Mechanism-based enhancement of scope and enantioselectivity for reactions involving a copper-substituted stereogenic carbon centre

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SUPPLEMENTARY INFORMATION

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1. Bibliography: Enantioselective Formation of Metal-substituted Stereogenic Carbon Centres

(a)Wang, Y-M., Bruno, N. C., Placeres, Á. L., Zhu, S. & Buchwald, S. L. Enantioselective synthesis of carbo- and heterocycles through a CuH-catalyzed hydroalkylation approach. *J. Am. Chem. Soc.* **137**, 10524–10527 (2015).

(b) Ascic, E. & Buchwald, S. L. Highly diastereo- and enantioselective CuH-catalyzed synthesis of 2,3-disubstituted indolines. *J. Am. Chem. Soc.* **137**, 4666–4669 (2015).

(c) Shi, S-l., Wong, Z. I. & Buchwald, S. L. Copper-catalysed enantioselective stereodivergent synthesis of amino alcohols. *Nature* **532**, 353–356 (2016).

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More Examples without *Highly Electron Deficient* Aryl Olefins

(j) Ascic, E. & Buchwald, S. L. Highly diastereo- and enantioselective CuH-catalyzed synthesis of 2,3-disubstituted indolines. *J. Am. Chem. Soc.* **137,** 4666–4669 (2015).

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More Example with *Highly Electron Deficient* Aryl Olefins but *Lower Selectivity*.

(l) Zhong, C., Kunii, S., Kosaka, Y., Sawamura, M. & Ito, H. Enantioselective synthesis of *trans*-aryl- and -heteroaryl-substituted cyclopropylboronates by copper(I)-catalyzed reactions of allylic phosphates with a diboron derivative. *J. Am. Chem. Soc.* **132**, 11440–11442 (2010).

More Example with *Less Reactive (electron rich) Electrophile* but *Low Selectivity*.

(m) Choi, B., Saxena, A., Smith, J. J., Churchill, G. H. & Lam, W. L. Enantioselective copper-catalyzed reductive coupling of vinylazaarenes with N-Boc aldimines. *Synlett.* **26,** 350–354 (2015).

More Examples with *Highly Electron Deficient* Aryl Olefins and *High Selectivity* (*1.2 to 5.0*

***equivalent* of electrophiles were used).**

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(o) Niu, D. & Buchwald, S. L. Design of modified amine transfer reagents allows the synthesis of α-chiral secondary amines via CuH-catalyzed hydroamination. *J. Am. Chem. Soc.* **137,** 9716–9721 (2015).

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(q) For non-enantioselective example, see: Smith, K. B., Logan, K. M., You, W. & Brown, K. M. Alkene carboboration enabled by synergistic catalysis. *Chem. Eur. J.* **20**, 12032–12036 (2014); Semba, K. & Nakao, Y. Arylboration of alkenes by cooperative palladium/copper catalysis. *J. Am. Chem. Soc.* **136,** 7567–7570 (2014); Logan, K. M. & Brown, M. K. Copper/palladium synergistic catalysis for the *syn*- and *anti*-selective carboboration of alkenes. *Angew. Chem. Int. Ed.* **54,** 5228–5231 (2015); Kato, K., Hirano, K. & Miura, M. Synthesis of β-boryl-α-aminosilanes by copper-catalyzed aminoboration of vinylsilanes. *Angew. Chem. Int. Ed.* **55,** 14400–14404 (2016).

2. General

Infrared (IR) spectra were recorded on a Bruker FT-IR Alpha (ATR mode) spectrophotometer, ν_{max} in cm^{-1}. Bands are characterized as broad (br), strong (s), medium (m), and weak (w). ^{1}H NMR spectra were recorded on Varian Unity INOVA 400 (400 MHz), 500 (500 MHz), or 600 (600 MHz) spectrometers. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 7.26 ppm). Data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, pent = pentet, m = multiplet, br = broad, app = apparent), and coupling constants (Hz). ^{13}C NMR spectra were recorded on Varian Unity INOVA 400 (100 MHz), 500 (125 MHz), or 600 (150 MHz) spectrometers with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 77.16 ppm). High-resolution mass spectrometry was performed on a JEOL AccuTOF DART (positive mode) at the Mass Spectrometry Facility, Boston College. Enantiomeric ratios were determined by HPLC analysis (high-performance liquid chromatography) with a Shimadzu chromatograph [Chiral Technologies Chiralcel AZ-H (4.6 x 250 mm), Chiral Technologies Chiralcel OC-H (4.6 x 250 mm), Chiral Technologies Chiralcel OD-H (4.6 x 250 mm), Chiral Technologies Chiralcel OJ-H (4.6 x 250 mm), Chiral Technologies Chiralcel OZ-H (4.6 x 250 mm), or Chiral Technologies Chiralpak AD-H (4.6 x 250 mm)] in comparison with authentic racemic materials. Specific rotations were measured on a Rudolph Research Analytical Autopol IV Polarimeter. Melting points were measured on a Thomas Hoover capillary melting point apparatus and are uncorrected. X-ray structures were obtained, as described in the cif file, with a Microfocus sealed Cu tube from Incote. It is well established that that aforementioned detector allows for the determination of absolute configuration of molecules that do not have a heavy atom.

Unless otherwise noted, reactions were carried out with distilled and degassed solvents under an atmosphere of dry N_2 in oven- (135 ºC) or flame-dried glassware with standard dry box or vacuum-line techniques. Hexanes was purified under a positive pressure of dry argon by a modified Innovative Technologies purification system through a copper oxide and alumina column. Tetrahydrofuran (thf; Aldrich Chemical Co.) was purified by distillation from sodium benzophenone ketyl immediately prior to use. All work-up and purification procedures were carried out with reagent grade solvents (purchased from Fisher Scientific) under air.

3. Reagents

Allyl phenyl carbonate (1e): purchased from Aldrich and used as received.

Allyl *tert*-butyl carbonate (1f): prepared according to a previously reported procedure.[1]

Bis(pinacolato)diboron [$B_2(pin)_2$]: purchased from Frontier Scientific, Inc., recrystallized from pentane and dried under vacuum prior to use.

***n*-Butyllithium (1.6 M in hexanes):** purchased from Aldrich and used as received.

Chlorotrimethylsilane: purchased from Acros and used as received.

Copper(I) chloride: purchased from Strem and used as received.

Deuterium oxide (D_2O): purchased from Cambridge Isotope Laboratories and used as received.

Diethyl allyl phosphate (1a): purchased from Aldrich and used as received.

Diisobutylaluminum hydride (dibal-H): purchased neat from Aldrich and used as received.

Di-*tert*-butyl-dicarbonate (Boc_2O): purchased from Advanced ChemTech and used as received.

Hoveyda-Grubbs catalyst 2nd generation: purchased from Aldrich and used as received.

Hydrogen peroxide (30 wt % in H_2O): purchased from Aldrich and used as received.

Imidazolinium salt NHC-1, 2, 3, 4, and 5: prepared according to a previously reported procedure.[2]

Imidazolinium salt NHC-6: prepared according to a previously reported procedure.[3]

Imidazolinium salt NHC-7: prepared according to a previously reported procedure.[4]

2-Isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane [*i*-PrOB(pin)]: purchased from Aldrich and used as received.

Oxone®, monopersulfate compound: purchased from Aldrich and used as received.

Phosphine L1: prepared according to a previously reported procedure.[5]

Phosphine ligands (L2, 3a–c, 4, 5, and 6): purchased from Strem and used as received.

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Pyridinium dichromate (PDC): purchased from Aldrich and used as received.

Sodium *tert*-butoxide: purchased from Strem and used as received.

Sodium hydroxide (2 M): prepared from NaOH purchased from Fisher (used as received) and deionized water.

Sulfuric acid: purchased from Fisher and used as received.

Tetrabutylammonium fluoride (tbaf, 1.0 M in thf): purchased from Oakwood and used as received.

Preparation of aryl or heteroaryl olefins: unless otherwise noted, olefins were purchased from Acros, Aldrich, Alfa Aesar, Combi-Blocks, Matrix Scientific, or TCI, and distilled over CaH_2 under reduced pressure prior to use.

The following olefins were synthesized from the corresponding aldehydes by Wittig olefination.[6]

1,4-Dimethoxy-2-methyl-5-vinylbenzene (9): Melting point: 41–42°C. IR (neat): 2995 (w), 2935 (w), 2830 (w), 1623 (w), 1501 (s), 1464 (m), 1416 (m), 1399 (m), 1207 (s), 1182 (m), 1042 (s), 996 (m), 902 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.02 (1H, dd, *J* = 18.0, 11.2 Hz), 6.95 (1H, s), 6.70 (1H, s), 5.68 (1H, dd, *J* = 17.8, 1.4 Hz), 5.22 (1H, dd, *J* = 11.2, 1.2 Hz), 3.82 (3H, s), 3.80 (3H, s), 2.23 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.0, 150.8, 131.7, 127.5, 124.5, 114.7, 113.3, 108.2, 56.4, 55.9, 16.4; HRMS (DART): Calcd for $C_{11}H_{15}O_2$ $[M+H]^+$: 179.1072, Found: 179.1069.

1-(Allyloxy)-3-vinylbenzene (substrate for 2aj and 2ak): The spectroscopic data match those reported previously.[7] ^1H NMR (400 MHz, $CDCl_3$): δ 7.24 (1H, t, *J* = 8.0 Hz), 7.03–6.96 (2H, m), 6.83 (1H, ddd, *J* = 8.2, 2.6, 0.9 Hz), 6.68 (1H, dd, *J* = 17.6, 10.8 Hz), 6.07 (1H, ddt, *J* = 17.3, 10.6, 5.3 Hz), 5.73 (1H, dd, *J* = 17.6, 0.9 Hz), 5.43 (1H, dq, *J* = 17.3, 1.6 Hz), 5.29 (1H, dq, *J* = 10.5, 1.4 Hz), 5.25 (1H, dd, *J* = 10.9, 0.9 Hz), 4.56 (2H, dt, *J* = 5.3, 1.5 Hz).

2-Vinylbenzofuran (substrate for 2ag): The spectroscopic data match those reported previously.[8] ^1H NMR (400 MHz, $CDCl_3$): δ 7.52 (1H, ddd, *J* = 7.6, 1.4, 0.7 Hz), 7.45 (1H, dq, *J* =8.2, 0.9 Hz), 7.30–7.24 (2H, m), 6.64 (1H, dd, *J* = 17.5, 11.2 Hz), 6.60 (1H, s), 5.96 (1H, ddd, *J* = 17.4, 1.3, 0.6 Hz), 5.41 (1H, dd, *J* = 11.2, 1.2 Hz).

***tert*-Butyl 5-vinyl-1*H*-indole-1-carboxylate (substrate for 2m)**: The spectroscopic data match those reported previously.[9] ^1H NMR (400 MHz, $CDCl_3$): δ 8.08 (1H, d, *J*= 8.0 Hz), 7.58–7.57 (2H, m), 7.41 (1H, dd, *J* = 8.4, 1.2 Hz), 6.81 (1H, dd, *J* = 17.6, 10.8 Hz), 6.55–6.54 (1H, m), 5.75 (1H, dd, *J* = 17.2, 1.2 Hz), 5.21 (1H, dd, *J* = 10.4, 0.8 Hz), 1.68 (9H, s).

The following olefins were synthesized from the corresponding aryl bromides by a two-step lithium halogen exchange/addition to TMSCl or *i*-PrOB(pin). To a flame-dried round bottom flask equipped

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with a stir bar was added 4-bromostyrene (0.71 mL, 5.5 mmol) and thf (30 mL) under N_2. The resulting solution was allowed to cool to –78 ºC (dry ice/acetone) and *n*-butyllithium (1.6 M in hexanes, 3.8 mL, 6.0 mmol) was added dropwise into the solution through syringe. The resulting light yellow solution was allowed to stir for 1 h at –78 ºC and then TMSCl (0.84 mL, 6.6 mmol) was added dropwise by syringe. The mixture was allowed to slowly warm up to 22 ºC. After 16 h, the reaction was quenched by the addition of H_2O (10 mL) and a saturated solution of aqueous NH_4Cl (10 mL). The layers were separated and the aqueous layer was washed with Et_2O (3 x 20 mL). The combined organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The resulting yellow oil was purified by silica gel chromatography (100% hexanes) to afford **trimethyl(4-vinylphenyl)silane** (substrate for **2ad**) as colorless oil (876 mg, 5.0 mmol, 91%): IR (neat): 3063 (w), 3008 (w), 2956 (m), 1629 (w), 1389 (m), 1248 (m), 1105 (m), 989 (m), 906 (m), 826 (s), 761 (m), 730 (m), 692 (m), 642 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.51 (2H, d, *J* = 7.6 Hz), 7.43 (2H, d, *J* = 8.0 Hz), 6.74 (1H, dd, *J* = 17.6, 10.9, Hz), 5.80 (1H, d, *J* = 17.6 Hz), 5.27 (1H, d, *J* = 10.9 Hz), 0.29 (9H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 140.3, 138.1, 137.0, 133.7, 125.7, 114.2, –1.0; HRMS (DART): Calcd for $C_{11}H_{17}Si$ $[M+H]^+$: 177.1100, Found: 177.1101.

4,4,5,5-Tetramethyl-2-(4-vinylphenyl)-1,3,2-dioxaborolane (substrate for 2j): Following the above procedure except *i*-PrOB(pin) was used instead of TMSCl, the product was obtained as colorless oil [purified by silica gel chromatography (hexanes:Et_2O = 25:1)] (1.0 g, 4.5 mmol, 82%). IR (neat): 2978 (m), 2930 (w), 1629 (m), 1552 (w), 1397 (m), 1356 (s), 1322 (s), 1269 (m), 1213 (w), 1142 (s), 1088 (s), 1018 (m), 990 (m), 962 (m), 830 (m), 758 (w), 682 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.82 (2H, d, *J* = 8.0 Hz), 7.44 (2H, d, *J* = 8.0 Hz), 6.76 (1H, dd, *J* = 17.6, 10.8 Hz), 5.84 (1H, dd, *J* = 17.6, 1.2 Hz), 5.32 (1H, dd, *J* = 10.8, 0.8 Hz), 1.38 (12H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 140.3, 137.0, 135.1, 125.6, 114.9, 83.8, 25.0, 24.9; HRMS (DART): Calcd for $C_{14}H_{20}BO_2$ $[M+H]^+$: 231.1556; Found: 231.1563.

4,4,5,5-Tetramethyl-2-(3-vinylphenyl)-1,3,2-dioxaborolane (substrate for 2f): Following the above except 3-bromostyrene and *i*-PrOB(pin) were used instead of 4-bromostyrene and TMSCl, respectively, the product was obtained as colorless oil [purified by silica gel chromatography (hexanes:Et_2O = 25:1)] (1.1 g, 4.7 mmol, 85%). IR (neat): 2978 (w), 2929 (m), 1380 (m), 1353 (s), 1319 (s), 1141 (s), 1079 (s), 990 (m), 963 (m), 908 (m), 831 (m), 710 (w), 699 (s), 681 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.87 (1H, s), 7.73 (1H, d, *J* = 7.3 Hz), 7.53 (1H, dt, *J* = 7.8, 1.6 Hz), 7.35 (1H, t, *J* = 7.5 Hz), 6.75 (1H, dd, 17.6, 10.9 Hz), 5.81 (1H, dd, *J* = 17.6, 0.9 Hz), 5.26 (1H, dd, *J* = 10.9, 0.9 Hz), 1.37 (12H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.0, 136.9, 134.3, 132.9, 129.0, 128.0, 114.0, 83.9, 25.0, 24.9; HRMS (DART): Calcd for $C_{14}H_{20}BO_2$ $[M+H]^+$: 231.1556, Found: 231.1567.

***tert*-Butyl 3-vinylbenzoate (substrate for 2g)**: Prepared according to the reported procedure.[10] IR (neat): 2978 (w), 2932 (w), 1711 (s), 1367 (m), 1294 (s), 1271 (m), 1256 (m), 1158 (s), 1113 (m), 1086 (m), 909 (m), 763 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.03 (1H, dd, *J* = 2.2, 1.0 Hz), 7.88 (1H, dt,

(10) Miller, W. H., Seefeld, M. A., Newlander, K. A., Uzinskas, I. N., Burgess, W. J., Heerding, D. A., Yuan, C. C. K., Head, M. S., Payne, D. J., Rittenhouse, S. F., Moore, T. D., Pearson, S. C., Berry, V., DeWolf, Jr., W. E., Keller, P. M., Polizzi, B. J., Qiu, X., Janson, C. A. & Huffman, W. F. *J. Med. Chem.* **45**, 3246–3256 (2000).

J = 7.6, 1.2 Hz), 7.57–7.55 (1H, m), 7.37 (1H, t, *J* = 7.8 Hz), 6.75 (1H, dd, *J* = 17.6, 10.8 Hz), 5.82 (1H, dd, *J* = 17.6, 0.4 Hz), 5.31 (1H, dd, *J* = 11.0, 0.6 Hz), 1.61 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.8, 137.8, 136.2, 132.4, 130.1, 128.8, 128.5, 127.3, 115.0, 81.2, 28.3, ; HRMS (DART): Calcd for $C_{13}H_{17}O_2$ $[M+H]^+$: 205.1229, Found: 205.1235.

***tert*-Butyl 4-vinylbenzoate (substrate for 2k)**: Prepared according to the reported procedure.[10] The spectroscopic data match those reported previously.[11] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (2H, d, *J*= 8.0 Hz), 7.44 (2H, d, *J* = 8.0 Hz), 6.75 (1H, dd, *J* = 17.6, 10.8 Hz), 5.84 (1H, dd, *J* = 17.6, 1.2 Hz), 5.36 (1H, dd, *J* = 11.0, 0.2 Hz), 1.60 (9H, s).

Preparation of allylic phosphates (substrates for 2n, 2p, and 2ak): Allylic alcohols were synthesized from the corresponding alkenyl bromides (purchased from Aldrich and used as received) by a two-step lithium halogen exchange/addition to formaldehyde sequence.[12] Subsequently, allylic alcohols were converted to the corresponding allylic phosphates based on an established method.[13]

Diethyl (2-phenylallyl) phosphate (substrates for 2n): IR (neat): 2983 (w), 2908 (w), 1444 (w), 1262 (m), 1165 (w), 1016 (s), 975 (s), 778 (m), 707 (m) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43–7.46 (2H, m), 7.28–7.37 (3H, m), 5.57 (1H, s), 5.44 (1H, s), 4.93 (2H, d, *J* = 7.2 Hz), 4.11–4.03 (4H, m), 1.31–1.28 (6H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.9 (d, *J* = 7.5 Hz), 137.7, 128.6, 128.2, 126.2, 115.4, 68.7 (d, *J* = 5.3 Hz), 63.9 (d, *J* = 5.3 Hz), 16.2 (d, *J* = 6.8 Hz); HRMS (DART): Calcd for $C_{13}H_{20}O_4P_1$ $[M+H]^+$: 271.1099, Found: 271.1087.

Diethyl (2-(trimethylsilyl)allyl) phosphate (substrate for 2p and 2ak): IR (neat): 2982 (w), 2957 (w), 2908 (m), 1394 (w), 1250 (m), 1167 (w), 1024 (s), 976 (m), 840 (s) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.85 (1H, s), 5.45 (1H, s), 4.65 (2H, d, *J* = 6.0 Hz), 4.15–4.08 (4H, m), 1.33 (6H, t, *J* = 7.0 Hz), 0.13 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.8 (d, *J* = 7.6 Hz), 125.1, 70.7 (d, *J* = 6.0 Hz), 63.9 (d, *J* = 6.1 Hz), 16.3 (d, *J* = 6.9 Hz), –1.5; HRMS (DART): Calcd for $C_{10}H_{24}O_4P_1Si_1$ $[M+H]^+$: 267.1182, Found: 267.1177.

Preparation of an allylic phosphate for 2o: 2-Methyl-2-propen-1-ol (purchased from Aldrich and used as received) was converted to the corresponding allylic phosphate based on a previously disclosed method.[13]

Diethyl (2-methylallyl) phosphate (substrate for 2o): IR (neat): 2983 (w), 2911 (w), 1447 (w), 1264 (m), 1166 (w), 1008 (s), 973 (s) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.94 (1H, s), 4.83 (1H, s), 4.32 (2H, d, *J* = 7.2 Hz), 4.05–3.98 (4H, m), 1.67 (3H, s), 1.26–1.21 (6H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.0 (d, *J* = 6.8 Hz), 113.0, 70.5 (d, *J* = 6.1 Hz), 63.7 (d, *J* = 6.1 Hz), 18.9, 16.0 (d, *J* = 6.8 Hz); HRMS (DART): Calcd for $C_8H_{18}O_4P_1$ $[M+H]^+$: 209.0943, Found: 209.0944.

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(12) Amat, M., Arioli, F., Pérez, M., Molins, E. & Bosch, J. *Org. Lett.* **15**, 2470–2473 (2013).

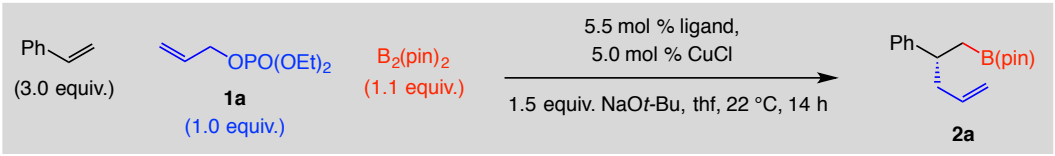
(13) Kacprzynski, M. A., May, T. L., Kazane, S. A. & Hoveyda, A. H. *Angew. Chem. Int. Ed.* **46**, 4554–4558 (2007).

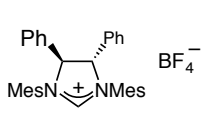
Preparation of allyl-1,1-d_2-diethyl phosphate (1a-d_2): Allylic alcohol was synthesized from the reported procedure.[14] Subsequently, allylic alcohol was converted to the corresponding allylic phosphates based on an established method.[13] IR (neat): 2984 (w), 2934 (w), 1265 (m), 1017(s), 976 (s), 801 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 5.91 (1H, dd, *J* = 17.2, 10.4 Hz), 5.33 (1H, dt, *J* = 17.2, 1.5 Hz), 5.21 (1H, dt, *J* = 10.0, 1.4 Hz), 4.12–4.04 (4H, m), 1.32–1.28 (6H, m); ^{13}C NMR (100 MHz, CDCl3): δ 135.6 (d, *J* = 6.8 Hz), 118.3, 63.8 (d, *J* = 6.1 Hz), 16.2 (d, *J* = 6.8 Hz); HRMS (DART): Calcd for $C_7H_{14}D_2O_4P_1$ [M+H]+: 197.0912, Found: 197.0920.

(14) Schuetz, R. D. & Millard, F. W. *J. Org. Chem.* **24**, 297–300 (1959).

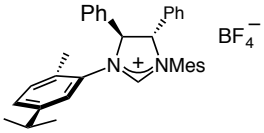
4. Examination of Different Types of Chiral Cu Complexes

Table 1 | Examination of different types of Cu complexes

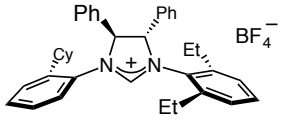




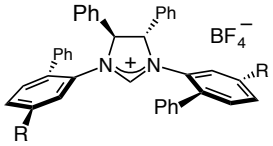
NHC-1



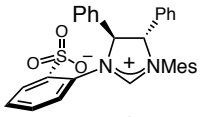
NHC-2



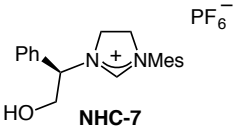
NHC-3



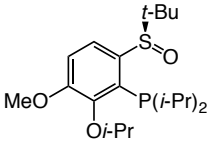
NHC-4 R = H, **NHC-5** R = *t*-Bu



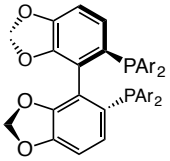
NHC-6



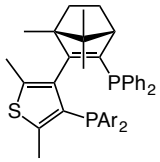
NHC-7



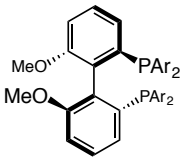
L1



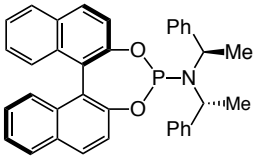
L2
Ar = 4-OMe-3,5-*t*-BuC_6H_2



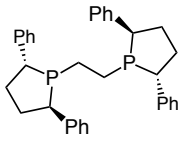
L3c
Ar = 3,5-$(Me)_2C_6H_3$



L4
Ar = 3,5-*t*-BuC_6H_3



L5



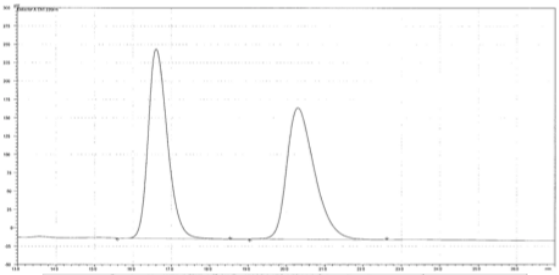
L6

Entry	Ligand	Conv. (%)§	Yield (%)§§	e.r.†
1	**NHC-1**	94	41	56:44
2	**NHC-2**	40	25	58:42
3	**NHC-3**	>98	78	56:44
4	**NHC-4**	80	71	61:39
5	**NHC-5**	35	25	17:83
6	**NHC-6**	44	<2 [only allyl–B(pin)]	NA
7	**NHC-7**	>98	<2 [only allyl–B(pin)]	NA
8	**L1**	15	6	9:91
9	**L2**	66	<2 [only allyl–B(pin)]	NA
8	**L3c**	>98	62	20:80
9	**L4**	86	11	51:49
10	**L5**	39	11	55:45
11	**L6**	>98	22	55:45

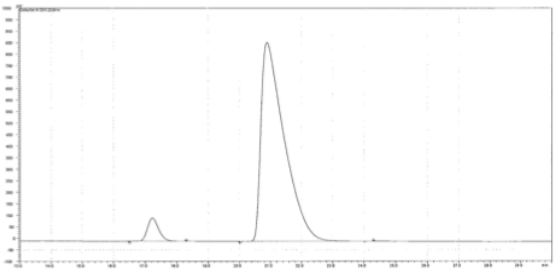
Reactions were carried out under N_2 atm.; see the Supplementary Information for details.
§ Conversion (conv.) was based on the disappearance of the limiting reagent (**1a**) and determined by analysis of the ^{1}H NMR spectra of the unpurified mixtures; the variance of values is estimated to be <±2%.
§§ Yield of isolated and purified product; the variance of values is estimated to be <±5%.
†Enantiomeric ratios were determined by HPLC analysis; the variance of values is estimated to be <±1%. See the Supplementary Information for details.
Abbreviation: NA, not applicable.

5. Representative Procedure for the Catalytic Enantioselective Boron-Allyl Addition to Aryl Alkenes

In an N_2-filled glove box, an oven-dried 1 dram vial equipped with a stir bar was charged with bisphosphine **L3a** (3.4 mg, 0.0055 mmol), NaO*t*-Bu (14 mg, 0.15 mmol), and CuCl (0.50 mg, 0.0050 mmol), and thf (1.0 mL). The mixture was allowed to stir for 1 h under N_2 at 22 °C; during this time the solution turned light yellow. Bis(pinacolato)diboron (28 mg, 0.11 mmol) was added to the mixture, causing the solution to turn dark brown immediately. Styrene (31 mg, 0.30 mmol), allylphosphate (**1a**) (19 mg, 0.10 mmol), and thf (0.50 mL) were added. The vial was sealed with a cap and electrical tape before removal from the glove box. The resulting mixture was allowed to stir at 22 °C for 14 h. The mixture was then passed through a short plug of silica gel (4 x 1 cm) and eluted with Et_2O. The organic layer was concentrated under reduced pressure, affording yellow oil, which was purified by silica gel chromatography (100% hexanes→hexanes:Et_2O = 10:1) to afford **2a** as colorless oil (18 mg, 0.067 mmol, 67% yield). **(*R*)-4,4,5,5-Tetramethyl-2-(2-phenylpent-4-en-1-yl)-1,3,2-dioxaborolane (2a):** 44% yield was obtained with 3:1 alkene:carbonate (**1e**). IR (neat): 3027 (w), 2977 (m), 2925 (w), 1452 (m), 1367 (s), 1319 (s), 1270 (w), 12134(w), 1164 (m), 1143 (s), 968 (m), 911 (m), 847 (m), 756 (m), 699 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.25–7.09 (5H, m), 5.68 (1H, ddt, *J* =17.2, 10.0, 7.2 Hz), 4.96–4.88 (2H, m), 2.96–2.88 (1H, m), 2.40–2.27 (2H, m), 1.23 (1H, dd, *J* =15.4, 6.6 Hz), 1.14–1.08 (1H, m), 1.10 (6H, s), 1.09 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 146.9, 137.3, 128.2, 127.6, 126.0, 116.1, 83.1, 43.9, 41.5, 24.83, 24.78; HRMS (DART): Calcd for $C_{17}H_{26}B_1O_2[M+H]^+$: 273.2026, Found: 273.2015. Specific rotation: $[\alpha]_D^{20}$ +6.7 (*c* 0.30, $CHCl_3$) for an enantiomerically enriched sample of 95:5 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OD–H column, 100% hexanes, 0.3 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area %
1	16.604	8995664	258220	50.067
2	20.296	8971612	179187	49.933
Total		17967275	437407	100.000

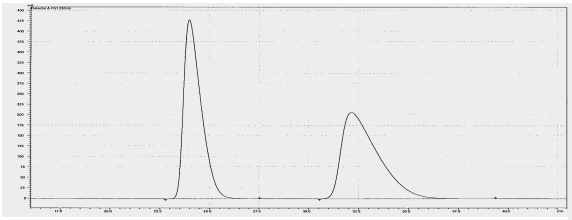


Peak#	Ret. Time	Area	Height	Area %
1	17.223	2468299	100781	5.239
2	20.890	44643911	865166	94.761
Total		47112211	965948	100.000

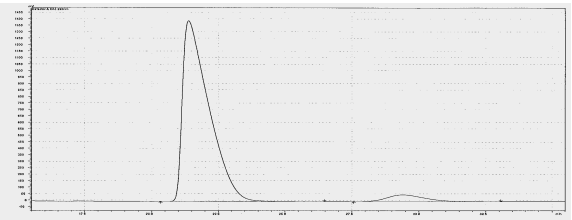
Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	16.604	50.067	1	17.223	5.239
2	20.296	49.933	2	20.890	94.761

(*R*)-2-(2-(2-Methoxyphenyl)pent-4-enyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2b): IR (neat): 2976 (w), 2929 (w), 2836 (w), 1599 (w), 1585 (w), 1491 (m), 1464 (w), 1438 (w), 1368 (s), 1318 (s), 1215 (s), 1143 (s), 1101 (s), 1031 (m), 968 (m), 909 (m), 885 (w), 749 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.17–7.10 (2H, m), 6.88 (1H, t, *J* = 7.4 Hz), 6.81 (1H, d, *J* = 8.4 Hz), 5.75–5.65 (1H, m), 4.96–4.88 (2H, m), 3.81 (3H, s), 3.42 (1H, app pent, *J* = 7.5 Hz), 2.44–2.26 (2H, m), 1.26–1.19 (1H,

m), 1.16–1.08 (1H, m), 1.11 (6H, s), 1.08 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.2, 137.8, 135.1, 127.8, 126.7, 120.4, 115.7, 110.6, 82.9, 55.5, 42.3, 33.9, 24.80, 24.77; HRMS (DART): Calcd for $C_{18}H_{28}B_1O_3$ $[M+H]^+$: 303.2132, Found: 303.2128; Specific Rotation: $[\alpha]_D^{20}$ +13.9 (*c* 1.61, $CHCl_3$) for an enantiomerically enriched sample of 95:5 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OZ–H column, 100% hexanes, 0.3 mL/min, 220 nm).



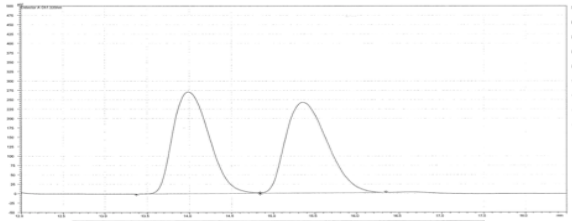
Peak#	Ret. Time	Area	Height	Area %
1	23.978	26303630	429169	50.115
2	32.136	26182411	207068	49.885
Total		52486041	636237	100.000



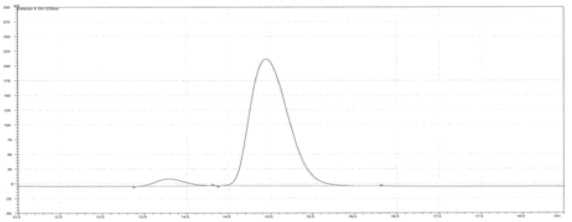
Peak#	Ret. Time	Area	Height	Area %
1	21.378	95311996	1394885	95.065
2	29.394	4947535	51312	4.935
Total		100259531	1446197	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	23.978	50.115	1	21.378	95.065
2	32.136	49.885	2	29.394	4.935

(*R*)-2-(2-(2-Fluorophenyl)pent-4-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2c): Following the representative procedure except **1e** was used. IR (neat): 2978 (w), 2931 (w), 1765 (s), 1490 (m), 1401 (s), 1369 (s), 1223 (m), 1144 (s), 968 (m), 913 (m), 846 (m), 754 (s) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.21 (1H, td, *J* = 7.6, 1.6 Hz), 7.13–7.10 (1H, m), 7.09–7.02 (1H, m), 6.98–6.94 (1H, m), 5.68 (1H, ddt, *J* = 16.8, 10.4, 6.8 Hz), 4.97–4.90 (2H, m), 3.35–3.27 (1H, m), 2.43–2.32 (2H, m), 1.28–1.22 (1H, m), 1.19–1.08 (1H, m), 1.11 (6H, s), 1.08 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.9 (d, *J* = 243.7 Hz), 136.9, 133.5 (d, *J* = 14.4 Hz), 128.8 (d, *J* = 5.3 Hz), 127.3 (d, *J* = 8.4 Hz), 123.9 (d, *J* = 3.8 Hz), 116.4, 115.3 (d, *J* = 22.8 Hz), 83.1, 42.5, 34.3, 24.8, 24.7; HRMS (DART): Calcd for $C_{17}H_{25}B_1F_1O_2$ $[M+H]^+$: 291.1932, Found: 291.1937; Specific Rotation: $[\alpha]_D^{20}$ +14.2 (*c* 0.87, $CHCl_3$) for an enantiomerically enriched sample of 96:4 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OD–H column, 100% hexanes, 0.3 mL/min, 220 nm).



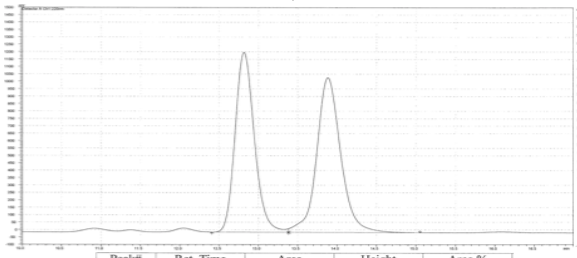
Peak#	Ret. Time	Area	Height	Area %
1	13.984	8054086	270865	48.955
2	15.351	8397818	241482	51.045
Total		16451904	512347	100.000



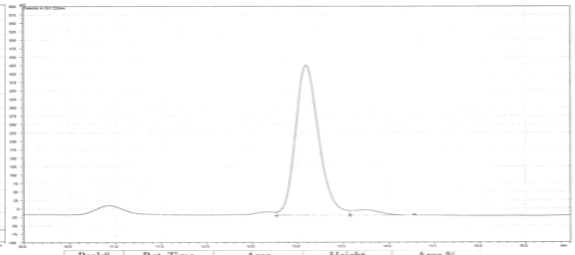
Peak#	Ret. Time	Area	Height	Area %
1	13.782	289017	12096	4.082
2	14.947	6790935	215149	95.918
Total		7079952	227246	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	13.984	48.955	1	13.782	4.082
2	15.351	51.045	2	14.947	95.918

(*R*)-4,4,5,5-Tetramethyl-2-(2-(2-(trifluoromethyl)phenyl)pent-4-en-1-yl)-1,3,2-dioxaborolane (2d): Following the representative procedure except except for 1:3 (0.1 mmol: 0.3 mmol) alkene:carbonate (**1e**) used. IR (neat): 2979 (w), 2928 (w), 1363 (m), 1312 (s), 1145 (s), 1124 (s), 1036 (m), 768 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.58 (1H, d, *J* = 8.0 Hz), 7.50–7.43 (2H, m), 7.26–7.22 (1H, m), 5.70 (1H, ddt, *J* = 18.0, 10.0, 7.2 Hz), 4.99–4.92 (2H, m), 3.42 (1H, app pent, *J* = 7.4 Hz), 2.45–2.25 (2H, m), 1.26 (1H, dd, *J* = 15.4, 7.0 Hz), 1.14 (1H, dd, *J* = 15.6, 8.4 Hz), 1.08 (6H, s), 1.05 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.5, 136.7, 131.8, 128.2 (q, *J* = 29.0 Hz), 128.18, 125.7, 125.6, 124.7 (q, *J* = 272.5 Hz), 116.6, 83.1, 43.9, 36.0, 24.7, 18.6 (br, C–B); HRMS (DART): Calcd for $C_{18}H_{25}B_1F_3O_2$ $[M+H]^+$: 341.1900, Found: 341.1903; Specific Rotation: $[\alpha]_D^{20}$ +11.9 (*c* 1.20, $CHCl_3$) for an enantiomerically enriched sample of 88:12 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OZ–H column, 100% hexanes, 0.3 mL/min, 220 nm).



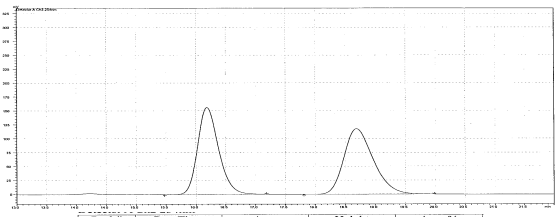
Peak#	Ret. Time	Area	Height	Area %
1	12.811	20832986	1213915	48.449
2	13.878	22166706	1044726	51.551
Total		42999693	2258641	100.000



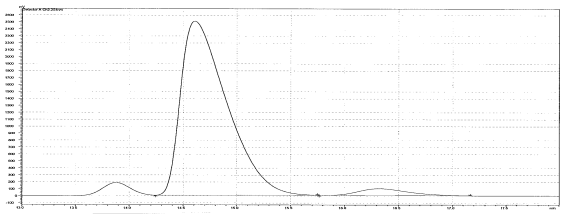
Peak#	Ret. Time	Area	Height	Area %
1	13.090	7952410	444664	96.273
2	13.739	307821	15826	3.727
Total		8260231	460490	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	12.811	48.449	1	13.090	96.273
2	13.878	51.551	2	13.739	3.727

(*R*)-4,4,5,5-Tetramethyl-2-(2-(naphthalen-2-yl)pent-4-en-1-yl)-1,3,2-dioxaborolane (2e): Following the representative procedure except for 1:3 (0.1 mmol: 0.3 mmol) alkene:phosphate used. IR (neat): 2976 (w), 2923 (s), 2853 (m), 1639 (w), 1362 (s), 1315 (s), 1143 (s), 968 (m), 911 (m), 847 (s), 814 (s), 744 (s), 476 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.81–7.73 (3H, m), 7.65–7.62 (1H, m), 7.46–7.35 (3H, m), 5.76–5.64 (1H, m), 5.01–4.89 (2H, m), 3.19–3.08 (1H, m), 2.55–2.37 (2H, m), 1.28–1.17(2H, m), 1.06 (6H, s), 1.07 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.5, 137.2, 133.6, 132.3, 127.82, 127.78, 127.74, 127.68, 126.3, 125.81, 125.79, 125.1, 116.3, 83.1, 43.6, 41.6, 24.85, 24.77; HRMS (DART): Calcd for $C_{21}H_{28}B_1O_2$ $[M+H]^+$: 323.2182, Found: 323.2194; Specific Rotation: $[\alpha]_D^{20}$ +16.4 (*c* 0.72, $CHCl_3$) for an enantiomerically enriched sample of 96:4 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OZ–H column, 100% hexanes, 0.3 mL/min, 254 nm).



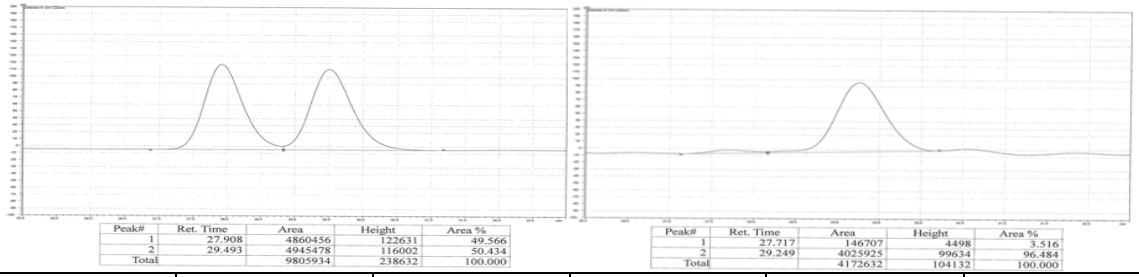
Peak#	Ret. Time	Area	Height	Area %
1	16.181	3853441	156647	48.876
2	18.684	4030671	117933	51.124
Total		7884112	274580	100.000



Peak#	Ret. Time	Area	Height	Area %
1	14.602	74811271	2504237	96.000
2	16.317	3116821	98231	4.000
Total		77928092	2602467	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	16.181	48.876	1	14.602	96.000
2	18.684	51.124	2	16.317	4.000

(*R*)-4,4,5,5-Tetramethyl-2-(3-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl)phenyl)-1,3,2-dioxaborolane (2f): Following the representative procedure except for 1:3 (0.1 mmol: 0.3 mmol) alkene:phosphate used. IR (neat): 2977 (m), 2926 (w), 2035 (w), 1611 (w), 1457 (w), 1399 (m), 1360 (s), 1320 (m), 1271 (w), 1214 (w), 1144 (s), 1090 (m), 964 (w), 860 (w), 829 (w), 659 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.66 (1H, s), 7.60 (1H, d, *J* = 7.1 Hz), 7.34–7.23 (2H, m), 5.68 (1H, ddt, *J* = 17.1, 10.1, 7.0 Hz), 4.97 (1H, dd, *J* = 17.2, 1.9 Hz), 4.94–4.89 (1H, m), 3.03–2.91 (1H, m), 2.49–2.29 (2H, m), 1.34 (6H, s), 1.33 (6H, s), 1.27–1.17 (2H, m), 1.10 (12H, s);^{13}C NMR ($CDCl_3$, 100 MHz): δ 146.2, 137.5, 134.2, 132.5, 130.3, 127.6, 116.0, 83.7, 83.0, 43.3, 41.4, 25.0, 24.9, 24.8; HRMS (DART): Calcd for $C_{23}H_{37}B_2O_4$ $[M+H]^+$: 399.2878, Found: 399.2887; Specific rotation: $[\alpha]_D^{20}$ +5.8 (*c* 0.43, $CHCl_3$) for an enantiomerically enriched sample of 96.5:3.5 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (96.5:3.5 e.r. shown; Chiralcel OD–H column, 98% hexanes, 2% *i*-PrOH, 0.3 mL/min, 220 nm).

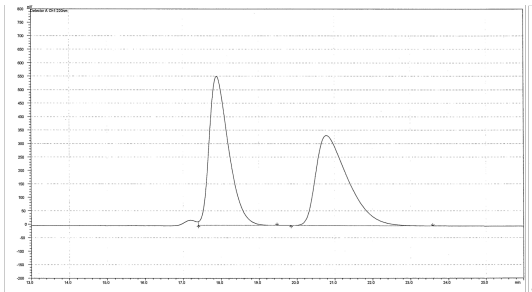


Peak#	Ret. Time	Area	Height	Area %
1	27.908	4860456	122631	49.566
2	29.493	4945478	116002	50.434
Total		9805934	238632	100.000

Peak#	Ret. Time	Area	Height	Area %
1	27.717	146707	4498	3.516
2	29.249	4025925	99634	96.484
Total		4172632	104132	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	27.908	49.566	1	27.717	3.516
2	29.493	50.434	2	29.249	96.484

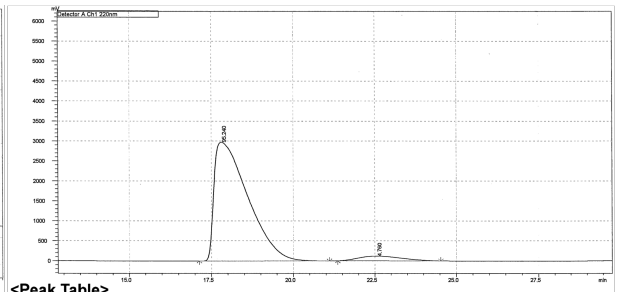
***tert*-Butyl (*R*)-3-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl)benzoate (2g):** Following the representative procedure except for 1:3 (0.1 mmol: 0.3 mmol) alkene:phosphate used. IR (neat): 2977 (w), 2929 (w), 1713 (s), 1440 (w), 1390 (w), 1367 (s), 1320 (m), 1294 (s), 1161 (s), 1144 (s), 1110 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.83 (1H, dd, *J* = 1.6, 1.2 Hz), 7.78 (1H, ddd, *J* = 7.7, 2.3, 1.1 Hz), 7.37 (1H, dd, *J* = 7.6, 1.6 Hz), 7.30 (1H, t, *J* = 7.4 Hz), 5.66 (1H, ddt, *J* = 17.2, 10.0, 7.2 Hz), 4.98–4.91 (2H, m), 3.04–2.96 (1H, m), 2.44–2.32 (2H, m), 1.59 (9H, s), 1.25 (1H, dd, *J* = 15.8, 7.0 Hz), 1.20–1.06 (13H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.2, 147.1, 137.0, 131.9, 131.6, 128.8, 128.1, 127.2, 116.5, 83.2, 80.9, 43.4, 41.4, 28.4, 24.9, 24.8; HRMS (DART): Calcd for $C_{22}H_{34}B_1O_4$ $[M+H]^+$: 373.2550, Found: 373.2565; Specific Rotation: $[\alpha]_D^{20}$ +4.9 (*c* 1.05, $CHCl_3$) for an enantiomerically enriched sample of 95:5 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OZ–H column, 100% hexanes, 0.3 mL/min, 220 nm).



PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.885	19631455	553324	50.079	62.322
2	20.783	19569298	334519	49.921	37.678
Total		39200753	887842	100.000	100.000



<Peak Table>

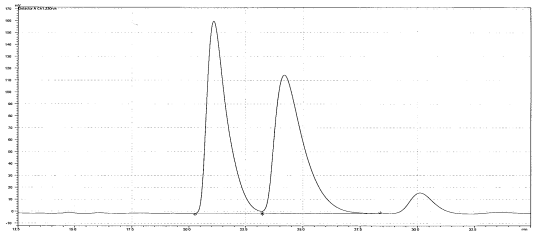
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	17.799	211784035	2977196	95.240	95.240
2	22.547	10584480	116111	4.760	4.760
Total		222368516	3093307		100.000

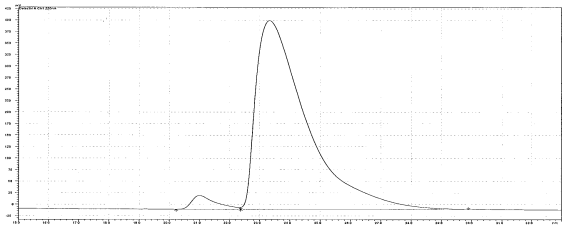
Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	17.885	50.079	1	17.799	95.240
2	20.783	49.921	2	22.547	4.760

***tert*-Butyl (*R*)-3-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl-5,5-d$_2$)benzoate [2g-*d*$_2$ (S_N2')]:** Following the representative procedure except **1b-*d*$_2$** and **L3b** was used. IR (neat): 2977 (w), 2929 (w), 1713 (s), 1367 (s), 1320 (m), 1295 (s), 1162 (s), 1145 (s), 1111 (m), 968 (m), 848 (m) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (1H, t, *J* = 1.6 Hz), 7.78 (1H, dt, *J* = 7.6, 1.6 Hz), 7.37 (1H, dt, *J* = 7.2, 1.6 Hz), 7.30 (1H, t, *J* = 7.8 Hz), 5.65 (1H, t, *J* = 7.0 Hz, 3.04–2.96 (1H, m), 2.44–2.32 (2H, m), 1.59 (9H, s), 1.25 (1H, dd, *J* = 15.2, 6.0 Hz) 1.11 (6H, s), 1.10 (6H, s), 1.12–1.06 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.2, 147.1, 136.8, 131.9, 131.6, 128.8, 128.1, 127.2, 83.2, 80.9, 43.3, 41.4, 28.4, 24.9, 24.8; HRMS (DART): Calcd for $C_{22}H_{35}D_2B_1N_1O_4$ [M+NH_4]$^+$: 392.2941, Found: 392.2954.

(*R*)-2-(2-(4-Methoxyphenyl)pent-4-enyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2h): 40% yield was obtained with 6:1 (0.6 mmol: 0.1 mmol) alkene:phosphate. IR (neat): 2976 (w), 2926 (w), 2834 (w), 1610 (w), 1511 (s), 1366 (s), 1319 (m), 1244 (s), 1214 (w), 1177 (m), 1165 (s), 1143 (w), 1104 (m), 1037 (m), 967 (m), 910 (w), 885 (w), 846 (m), 828 (m), 806 (w) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.12 (2H, dd, *J* = 6.4, 2.0 Hz), 6.80 (2H, dd, *J* = 6.4, 2.0 Hz), 5.67 (1H, ddt, *J* = 17.2, 9.6, 7.2 Hz), 4.97–4.90 (2H, m) 3.77 (3H, s), 2.94–2.86 (1H, m), 2.38–2.26 (2H, m), 1.25–1.18 (1H, m), 1.11–1.04 (13H, m). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.9, 139.1, 137.4, 128.4, 116.0, 113.6, 83.1, 55.4, 44.1, 40.7, 24.9, 24.8; HRMS (DART): Calcd for $C_{18}H_{28}BO_3$ [M+H]$^+$: 303.2132, Found: 303.2126; Specific Rotation: $[\alpha]_D^{20}$ +9.8 (*c* 0.76, $CHCl_3$) for an enantiomerically enriched sample of 97:3 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (97:3 e.r. shown; Chiralcel OD–H column, 100% hexanes, 0.3 mL/min, 220 nm).



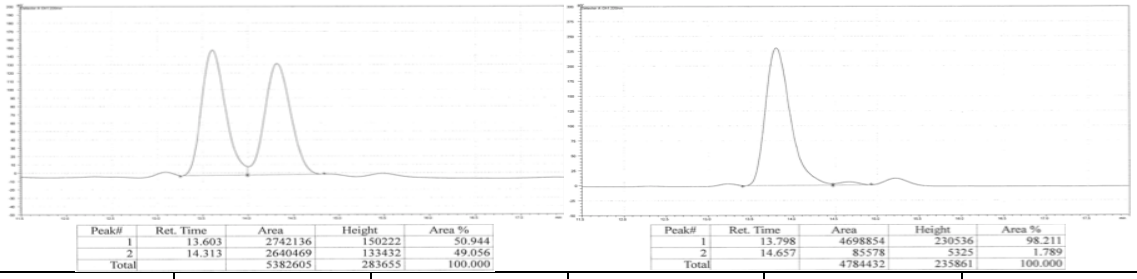
Peak#	Ret. Time	Area	Height	Area %
1	21.084	10063076	161641	49.788
2	24.175	10148737	116341	50.212
Total		20211813	277981	100.000



Peak#	Ret. Time	Area	Height	Area %
1	20.993	1662337	30072	3.369
2	23.315	47674508	409729	96.631
Total		49336845	439801	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	21.084	49.788	1	20.993	3.369
2	24.175	50.212	2	23.315	96.631

***(R)*-2-(2-(4-Fluorophenyl)pent-4-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2i):** Following the representative procedure except **1e** was used. IR (neat): 2978 (w), 2925 (w), 2855 (w), 1604 (w), 1509 (s), 1369 (s), 1322 (m), 1223 (m), 1144 (s), 968 (w), 912 (w), 832 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.17–7.13 (2H, m), 6.98–6.91 (2H, m), 5.65 (1H, ddt, *J* = 17.2, 10.0, 7.2 Hz), 4.96–4.91 (2H, m), 2.97–2.89 (1H, m), 2.36–2.27 (2H, m), 1.26–1.16 (1H, m), 1.09–1.04 (13H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.4 (d, *J* = 241.3 Hz), 142.5 (d, *J* = 3.0 Hz), 137.0, 128.9 (d, *J* = 7.6 Hz), 116.4, 114.9 (d, *J* = 20.5 Hz), 83.2, 44.0, 40.8, 24.8, 24.7; HRMS (DART): Calcd for $C_{17}H_{25}B_1F_1O_2$ $[M+H]^+$: 291.1932, Found: 291.1939; Specific Rotation: $[\alpha]_D^{20}$ +14.9 (*c* 1.20, $CHCl_3$) for an enantiomerically enriched sample of 92:8 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (98:2 e.r. shown; Chiralcel OZ–H column, 100% hexanes, 0.3 mL/min, 220 nm).

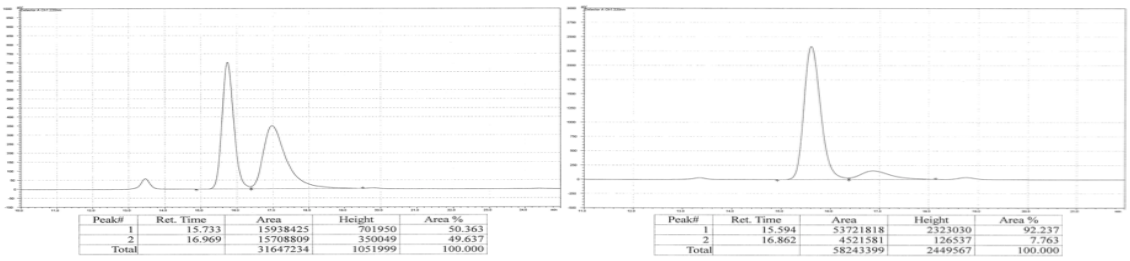


Peak#	Ret. Time	Area	Height	Area %
1	13.603	2742136	150222	50.944
2	14.313	2640469	133432	49.056
Total		5382605	283655	100.000

Peak#	Ret. Time	Area	Height	Area %
1	13.798	4698854	230536	98.211
2	14.657	85578	5325	1.789
Total		4784432	235861	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	13.603	50.944	1	13.798	98.211
2	14.313	49.056	2	14.657	1.789

(*R*)-4,4,5,5-Tetramethyl-2-(4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl)phenyl)-1,3,2-dioxaborolane (2j): Following the representative procedure except for 1:3 (0.1 mmol: 0.3 mmol) alkene:phosphate used. IR (neat): 2977 (m), 2925 (m), 2041 (w), 2034 (w), 2024 (w), 1611 (m), 1399 (m), 1360 (s), 1319 (m), 1271 (w), 1144 (m), 1090 (s), 964 (w), 860 (w), 830 (w), 660 (m)cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.70 (2H, d, *J*= 8.0 Hz), 7.21 (2H, d, *J* = 8.0 Hz), 5.73–5.57 (1H, m), 4.97–4.88 (2H, m), 3.01–2.90 (1H, m), 2.43–2.28 (2H, m), 1.33 (12H, s), 1.28–1.16 (2H, m), 1.12 (6H, s), 1.11 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 150.4, 137.2, 134.8, 127.0, 116.2, 83.6, 83.1, 43.5, 41.6, 25.0, 24.8; HRMS (DART): Calcd for $C_{23}H_{40}B_2N_1O_4$ $[M+NH_4]^+$: 416.3143, Found: 416.3158; Specific Rotation: $[\alpha]_D^{20}$ +9.1 (*c* 1.02, $CHCl_3$) for an enantiomerically enriched sample of 92:8 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (92:8 e.r. shown; Chiralcel AZ–H column, 99% hexanes, 1% *i*-PrOH, 0.3 mL/min, 220 nm).

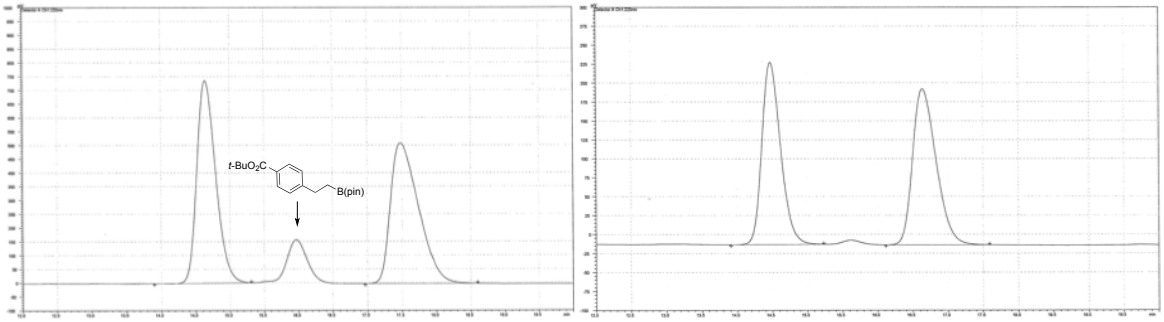


Peak#	Ret. Time	Area	Height	Area %
1	15.733	15938425	701950	50.363
2	16.969	15708809	350049	49.637
Total		31647234	1051999	100.000

Peak#	Ret. Time	Area	Height	Area %
1	15.594	53721818	2323030	92.237
2	16.862	4521581	126537	7.763
Total		58243399	2449567	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	15.733	50.363	1	15.594	92.237
2	16.969	49.637	2	16.862	7.763

***tert*-Butyl (*R*)-4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl)benzoate (2k):** IR (neat): 2978 (m), 2930 (w), 1712 (s), 1609 (w), 1367 (s), 1312 (m), 1290 (s), 1166 (s), 1145 (s), 1116 (s), 848 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.88 (2H, d, *J* = 8.0 Hz), 7.24 (2H, d, *J* = 8.0 Hz), 5.68–5.58 (1H, m), 4.96–4.90 (2H, m), 3.00 (1H, app pent, *J* = 7.5 Hz), 2.35 (2H, t, *J* = 7.2 Hz), 1.58 (9H, s), 1.27–1.21 (1H, m), 1.14–1.08, (1H, m) 1.12 (6H, s), 1.11 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.1, 152.0, 136.8, 129.9, 129.5, 127.4, 116.5, 83.2, 80.8, 43.5, 41.5, 28.4, 24.9, 24.8; HRMS (DART): Calcd for $C_{22}H_{34}B_1O_4$ $[M+H]^+$: 373.2550, Found: 373.2534; Specific Rotation: $[\alpha]_D^{20}$ –3.0 (*c* 1.00, $CHCl_3$) for an enantiomerically enriched sample of 67:33 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (52:48 e.r. shown; Chiralcel OD–H column, 100% hexanes, 0.3 mL/min, 220 nm).



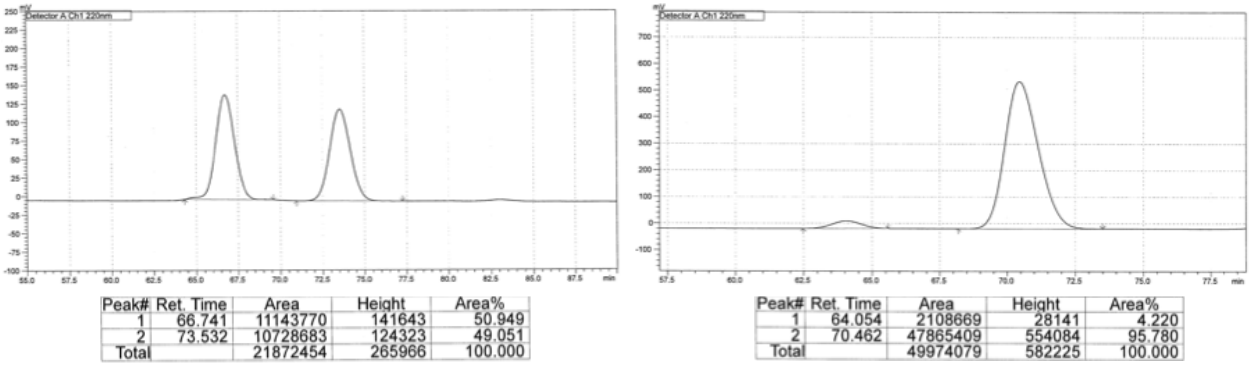
Peak#	Ret. Time	Area	Height	Area %
1	14.638	14061810	735507	49.374
2	17.479	14418511	510741	50.626
Total		28480320	1246248	100.000

Peak#	Ret. Time	Area	Height	Area %
1	14.474	4480291	240810	48.271
2	16.639	4801309	206218	51.729
Total		9281600	447028	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	14.638	49.374	1	14.474	48.271
2	17.479	50.626	2	16.639	51.729

(*R*)-4,4,5,5-Tetramethyl-2-(2-(4-(trifluoromethyl)phenyl)pent-4-en-1-yl)-1,3,2-dioxaborolane (2l): Following the representative procedure except for 1:3 (0.1 mmol: 0.3 mmol) alkene:carbonate (**1e**) used. The spectroscopic data match those reported previously.[5] ^1H NMR (400 MHz, $CDCl_3$): δ 7.58 (1H, d, *J* = 8.0 Hz), 7.50–7.43 (2H, m), 7.26–7.22 (1H, m), 5.70 (1H, ddt, *J* = 18.0, 10.0, 7.2 Hz), 4.99–4.92 (2H, m), 3.42 (1H, app pent, *J* = 7.4 Hz), 2.45–2.25 (2H, m), 1.26 (1H, dd, *J* = 15.4, 7.0 Hz), 1.14 (1H, dd, *J* = 15.6, 8.4 Hz), 1.08 (6H, s), 1.05 (6H, s). Specific Rotation: $[\alpha]_D^{20}$ +6.1 (*c* 0.45, $CHCl_3$) for an enantiomerically enriched sample of 96:4 e.r. Enantiomeric purity was determined by HPLC

analysis of the alcohol product after oxidation in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OZ–H column, 99% hexanes, 0.3 mL/min, 220 nm).

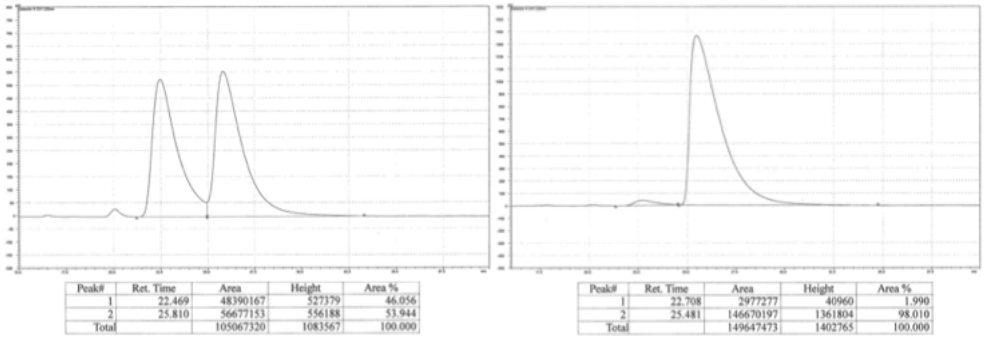


Peak#	Ret. Time	Area	Height	Area%
1	66.741	11143770	141643	50.949
2	73.532	10728683	124323	49.051
Total		21872454	265966	100.000

Peak#	Ret. Time	Area	Height	Area%
1	64.054	2108669	28141	4.220
2	70.462	47865409	554084	95.780
Total		49974079	582225	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	66.741	50.949	1	64.054	4.220
2	73.532	49.051	2	70.462	95.780

***tert*-Butyl (*R*)-5-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl)-1*H*-indole-1-carboxylate (2m)**: Following the representative procedure except for 6:1 (0.6 mmol: 0.1 mmol) alkene:phosphate used. IR (neat): 2977 (m), 2927 (w), 1731 (s), 1469 (m), 1441 (w), 1352 (s), 1318 (s), 1253 (m), 1162 (s), 1141 (s), 1081 (m), 1022 (m), 968 (w), 846 (w), 766 (m), 725 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.00 (1H, d, *J* = 8 Hz), 7.54 (1H, d, *J* = 3.6 Hz), 7.38 (1H, d, *J* = 1.6 Hz), 7.17 (1H, dd, *J* = 8.8, 2.0 Hz), 6.50 (1H, d, *J* = 3.6 Hz), 5.68 (1H, ddt, *J* = 17, 10.4, 6.4 Hz), 4.98–4.88 (2H, m), 3.04 (1H, app pent, *J* = 7.0 Hz), 2.46–2.34 (2H, m), 1.66 (9H, s), 1.30–1.25 (1H, m), 1.19–1.13 (1H, m), 1.09 (6H, s), 1.08 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.1, 141.4, 137.5, 133.8, 130.7, 125.9, 124.1, 119.5, 116.0, 114.8, 107.5, 83.5, 83.1, 44.2, 41.4, 28.4, 24.9, 24.8; HRMS (DART): Calcd for $C_{24}H_{35}B_1N_1O_4$ $[M+H]^+$: 412.2659, Found: 412.2653; Specific Rotation: $[\alpha]_D^{20}$ +17.1 (*c* 0.43, $CHCl_3$) for an enantiomerically enriched sample of 98:2 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (98:2 e.r. shown; Chiralcel AD–H column, 100% hexanes, 0.3 mL/min, 220 nm).

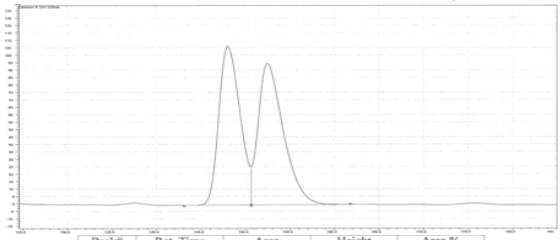


Peak#	Ret. Time	Area	Height	Area %
1	22.469	48390167	527379	46.056
2	25.810	56677153	556188	53.944
Total		105067320	1083567	100.000

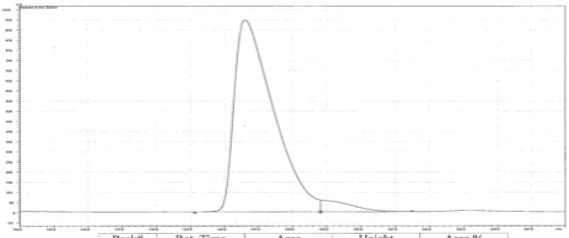
Peak#	Ret. Time	Area	Height	Area %
1	22.708	2977277	40960	1.990
2	25.481	146670197	1361804	98.010
Total		149647473	1402765	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	22.469	46.056	1	22.708	1.990
2	25.810	53.944	2	25.481	98.010

(*R*)-2-(2,4-Diphenylpent-4-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2n): Following the representative procedure except for 1:3 (0.1 mmol: 0.3 mmol) alkene:phosphate used. IR (neat): 3027 (w), 2977 (w), 2929 (w), 1494 (m), 1452 (w), 1369 (s), 1320 (s), 1145 (s), 699 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.39–7.36 (2H, m), 7.33–7.19 (5H, m), 7.14–7.09 (3H, m), 5.15 (1H, d, *J* = 2.0 Hz), 4.83 (1H, d, *J* = 1.2 Hz), 2.96 (1H, app pent, *J* = 7.7 Hz), 2.87 (1H, dd, *J* = 13.8, 7.0 Hz), 2.73 (1H, dd, *J* = 13.6, 8.0 Hz), 1.26 (1H, dd, *J* = 15.6, 6.8 Hz), 1.13 (1H, dd, *J* = 15.6, 9.2 Hz), 1.07 (6H, s), 1.05 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.9, 146.8, 141.2, 128.4, 128.1, 127.6, 127.4, 126.6, 125.9, 114.5, 83.1, 45.7, 39.9, 24.8, 24.7; HRMS (DART): Calcd for $C_{23}H_{30}B_1O_2$ $[M+H]^+$: 349.2339, Found: 349.2347; Specific Rotation: $[\alpha]_{20}^{D}$ –11.9 (c 0.50, $CHCl_3$) for an enantiomerically enriched sample of 88:12 e.r. Enantiomeric purity was determined by HPLC analysis of the alcohol product after oxidation in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OD–H column, 99% hexanes, 1% *i*-PrOH, 0.3 mL/min, 220 nm).



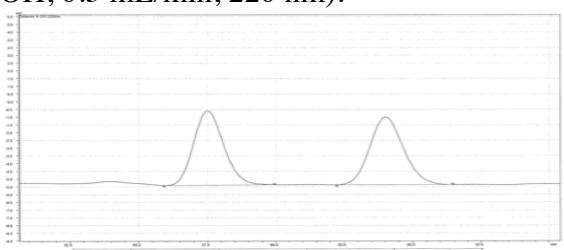
Peak#	Ret. Time	Area	Height	Area %
1	148.008	17684600	107007	48.370
2	152.465	18876400	95038	51.630
Total		36561001	202046	100.000



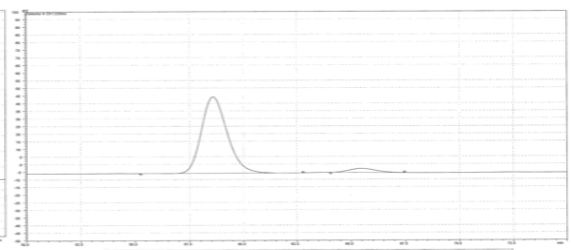
Peak#	Ret. Time	Area	Height	Area %
1	146.542	190523901	945369	95.605
2	152.058	8759003	57348	4.395
Total		199282904	1002718	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	148.008	48.370	1	146.542	95.605
2	152.465	51.630	2	152.058	4.395

(*R*)-4,4,5,5-Tetramethyl-2-(4-methyl-2-phenylpent-4-en-1-yl)-1,3,2-dioxaborolane (2o): Following the representative procedure except for 1:6 (0.1 mmol: 0.6 mmol) alkene:phosphate used. IR (neat): 3028 (w), 2978 (m), 2929 (m), 1453 (w), 1369 (s), 1320 (m), 1145 (s), 968 (w), 888 (w), 699 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.24–7.18 (4H, m), 7.13–7.10 (1H, m), 4.64 (1H, s), 4.56 (1H, s), 3.03 (1H, app pent, *J* = 7.7 Hz), 2.29 (2H, d, *J* = 7.6 Hz), 1.65 (3H, s), 1.24–1.16 (1H, m), 1.09–1.03 (13H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.2, 144.3, 128.1, 127.5, 125.9, 112.4, 83.0, 48.3, 39.8, 24.83, 24.75, 22.5; HRMS (DART): Calcd for $C_{18}H_{28}B_1O_2$ $[M+H]^+$: 287.2182, Found: 287.2189; Specific Rotation: $[\alpha]_D^{20}$ +5.7 (*c* 0.33, $CHCl_3$) for an enantiomerically enriched sample of 90:10 e.r. Enantiomeric purity was determined by HPLC analysis of the alcohol product after oxidation in comparison with authentic racemic material (95:5 e.r. shown; Chiralpak AD–H column, 99% hexanes, 1% *i*-PrOH, 0.3 mL/min, 220 nm).



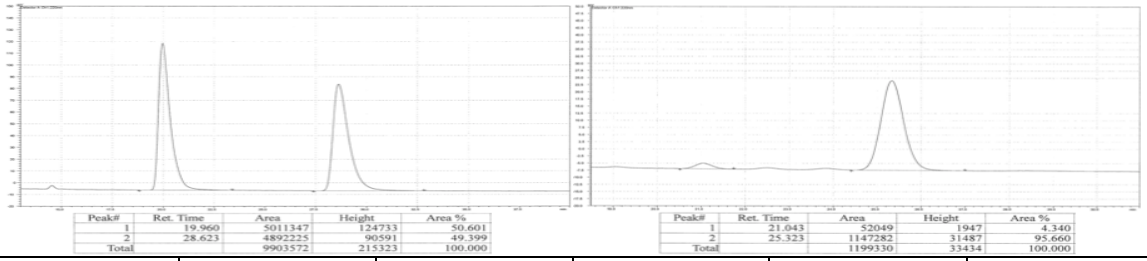
Peak#	Ret. Time	Area	Height	Area %
1	57.500	366961	4812	49.676
2	64.003	371750	4379	50.324
Total		738711	9191	100.000



Peak#	Ret. Time	Area	Height	Area %
1	58.582	4158680	50182	94.890
2	65.442	223953	2661	5.110
Total		4382633	52843	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	57.500	49.676	1	58.582	94.890
2	64.003	50.324	2	65.442	5.110

(*R*)-Trimethyl(4-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-1-en-2-yl)silane (2p): IR (neat): 2978 (w), 2955 (w), 1368 (s), 1319 (m), 1247 (m), 1145 (s), 968 (w), 836 (s), 757 (m), 699 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.25–7.18 (4H, m), 7.15–7.10 (1H, m), 5.45–5.44 (1H, m), 5.31 (1H, d, *J* = 3.2 Hz), 3.06–2.98 (1H, m), 2.49–2.35 (1H, m), 1.26–1.20 (1H, m), 1.09–1.01 (13H, m), 0.07 (9H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.3, 147.4, 128.1, 127.7, 126.5, 125.8, 83.0, 45.9, 40.7, 24.9, 24.8, –1.2; HRMS (DART): Calcd for $C_{20}H_{34}B_1O_2Si_1$ $[M+H]^+$: 345.2421, Found: 345.2424. Specific Rotation: $[\alpha]_D^{20}$ +7.9 (*c* 0.33, $CHCl_3$) for an enantiomerically enriched sample of 95:5 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OD–H column, 100% hexanes, 0.3 mL/min, 220 nm).

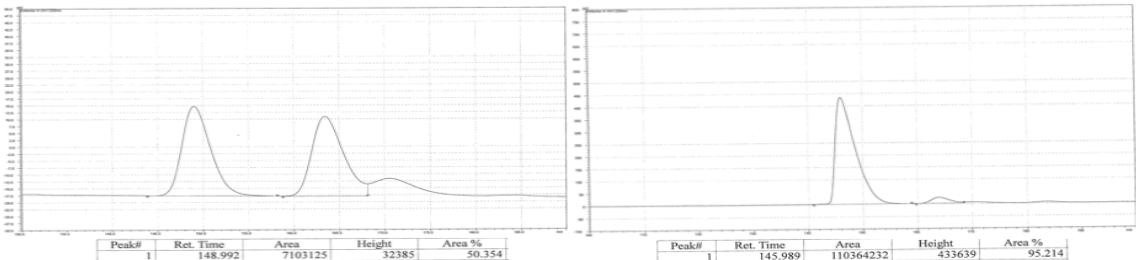


Peak#	Ret. Time	Area	Height	Area %
1	19.960	5011347	124733	50.601
2	28.623	4892225	90591	49.399
Total		9903572	215323	100.000

Peak#	Ret. Time	Area	Height	Area %
1	21.043	52049	1947	4.340
2	25.323	1147282	31487	95.660
Total		1199330	33434	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	19.960	50.601	1	21.043	4.340
2	28.623	49.399	2	25.323	95.660

(*R*)-6-Methyl-2-(4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl)phenyl)-1,3,6,2-dioxazaborocane-4,8-dione (2q): IR (neat): 2977 (w), 2927 (w), 1765 (s), 1457 (w), 1370 (m), 1334 (m), 1293 (m), 1235 (m), 1145 (m), 1040 (m), 993 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.40 (2H, d, *J* = 7.6 Hz), 7.23 (2H, d, *J* = 8.0 Hz), 5.69–5.59 (1H, m), 4.96–4.88 (2H, m), 3.93 (2H, d, *J* = 16.4 Hz), 3.75 (2H, d, *J* = 16.0 Hz), 2.95 (1H, app pent, *J* = 7.5 Hz), 2.51 (3H, s), 2.38–2.32 (2H, m), 1.23 (1H, dd, *J* = 15.2, 7.2 Hz), 1.12–1.06 (13H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.5, 149.0, 137.1, 132.2, 127.7, 116.3, 83.1, 61.8, 47.5, 43.6, 41.4, 24.9, 24.8; HRMS (DART): Calcd for $C_{22}H_{35}B_2N_2O_6$ $[M+NH_4]^+$: 445.2681, Found: 445.2689. Specific Rotation: $[\alpha]_D^{20}$ +6.4 (*c* 0.87, $CHCl_3$) for an enantiomerically enriched sample of 95:5 e.r. Enantiomeric purity was determined by HPLC analysis of the product from oxidation/acetylation in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OC–H column, 98% hexanes, 2% *i*-PrOH, 0.3 mL/min, 220 nm).



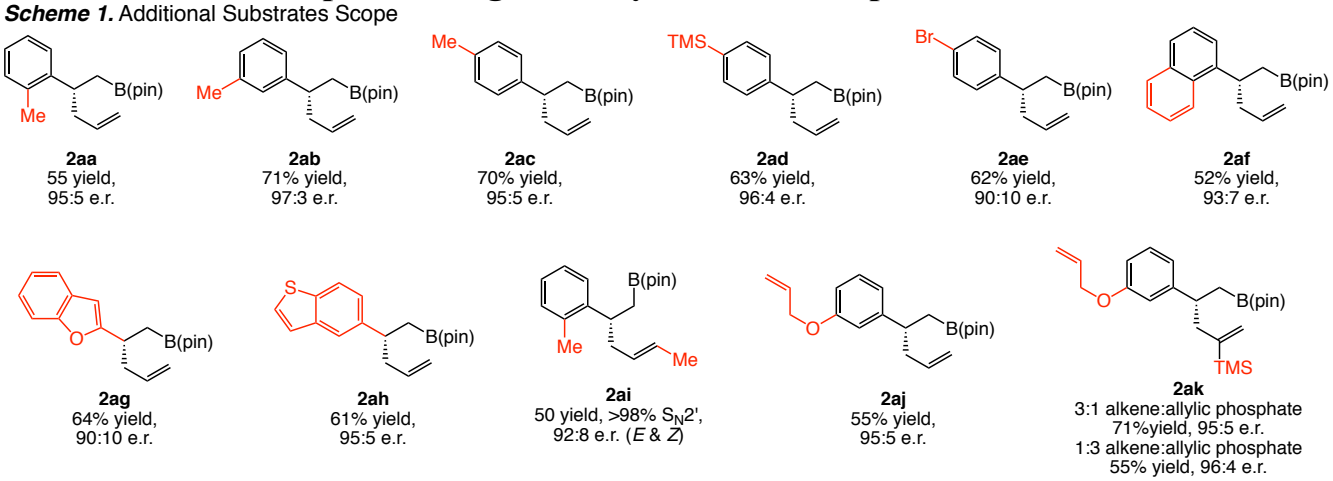
Peak#	Ret. Time	Area	Height	Area %
1	148.992	7103125	32385	50.354
2	163.447	7003134	28830	49.646
Total		14106259	61216	100.000

Peak#	Ret. Time	Area	Height	Area %
1	145.989	110364232	433639	95.214
2	163.902	5546930	24090	4.786
Total		115911162	457729	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	148.992	50.354	1	145.989	95.214
2	163.447	49.646	2	163.902	4.786

6. Additional Examples of Single-Catalyzed Multicomponent Reaction

Scheme 1. Additional Substrates Scope



2aa
55 yield,
95:5 e.r.

2ab
71% yield,
97:3 e.r.

2ac
70% yield,
95:5 e.r.

2ad
63% yield,
96:4 e.r.

2ae
62% yield,
90:10 e.r.

2af
52% yield,
93:7 e.r.

2ag
64% yield,
90:10 e.r.

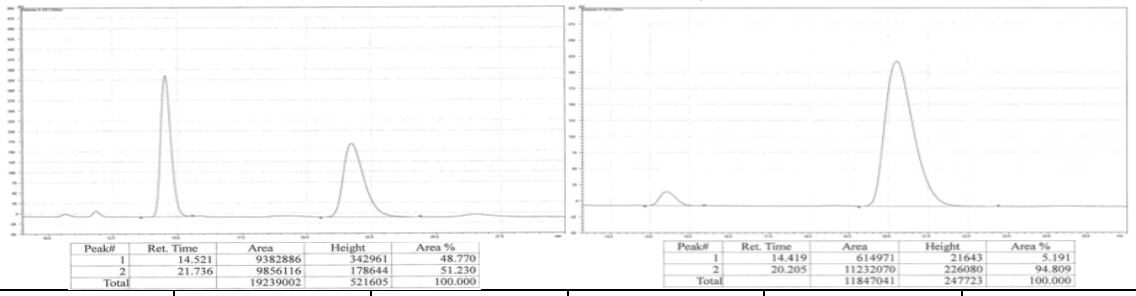
2ah
61% yield,
95:5 e.r.

2ai
50 yield, >98% S_N2',
92:8 e.r. (*E* & *Z*)

2aj
55% yield,
95:5 e.r.

2ak
3:1 alkene:allylic phosphate
71%yield, 95:5 e.r.
1:3 alkene:allylic phosphate
55% yield, 96:4 e.r.

(*R*)-4,4,5,5-Tetramethyl-2-(2-(*o*-tolyl)pent-4-en-1-yl)-1,3,2-dioxaborolane (2aa): IR (neat): 2977 (w), 2928 (w), 1365 (s), 1317 (s), 1144 (s), 968 (m), 911 (m), 846 (m), 758 (m), 726 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.20 (1H, d, *J* = 8.0 Hz), 7.14 (1H, t, *J* = 7.2 Hz), 7.09–7.01 (2H, m), 5.74–5.63 (1H, m), 4.99–4.91 (2H, m), 3.23 (1H, app pent, *J* = 7.3 Hz), 2.38–2.24 (2H, m), 2.36 (3H, s), 1.23 (1H, dd, *J* = 14.6, 7.8 Hz), 1.12 (1H, dd, *J* = 16.0, 8.0 Hz), 1.05 (s, 6H), 1.03 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 145.1, 137.3, 135.7, 130.0, 126.1, 125.6, 116.1, 83.0, 43.6, 36.0, 24.7, 20.0; HRMS (DART): Calcd for $C_{18}H_{28}B_1O_2$ $[M+H]^+$: 287.2182, Found: 287.2177; Specific Rotation: $[\alpha]_D^{20}$ +8.8 (*c* 1.32, $CHCl_3$) for an enantiomerically enriched sample of 95:5 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OD–H column, 100% hexanes, 0.3 mL/min, 220 nm).



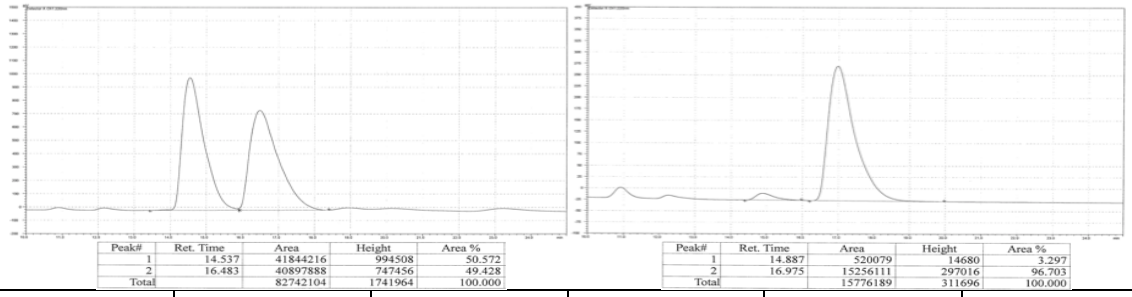
Peak#	Ret. Time	Area	Height	Area %
1	14.521	9382886	342961	48.770
2	21.736	9856116	178644	51.230
Total		19239002	521605	100.000

Peak#	Ret. Time	Area	Height	Area %
1	14.419	614971	21643	5.191
2	20.205	11232070	226080	94.809
Total		11847041	247723	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	14.521	48.770	1	14.419	5.191
2	21.736	51.230	2	20.205	94.809

(*R*)-4,4,5,5-Tetramethyl-2-(2-(*m*-tolyl)pent-4-en-1-yl)-1,3,2-dioxaborolane (2ab): IR (neat): 2977 (w), 2922 (w), 1366 (s), 1319 (s), 1144 (s), 968 (m), 847 (m), 704 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.15 (1H, dd, *J* = 9.0, 6.2 Hz), 7.00 (1H, s), 6.97–6.93 (2H, m), 5.72–5.62 (1H, m), 4.98–4.89 (2H, m), 2.89 (1H, app pent, *J* = 7.6 Hz), 2.40–2.26 (5H, m), 1.25–1.18 (1H, m), 1.11–1.03 (13H, m);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 146.9, 137.5, 137.46, 128.4, 128.1, 126.7, 124.5, 116.0, 83.1, 43.7, 41.4, 24.82, 24.79, 21.6; HRMS (DART): Calcd for $C_{18}H_{28}B_1O_2$ $[M+H]^+$: 287.2182, Found: 287.2188; Specific Rotation: $[\alpha]_D^{20}$ +16.9 (*c* 0.98, $CHCl_3$) for an enantiomerically enriched sample of 97:3 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (97:3 e.r. shown; Chiralcel OD–H column, 100% hexanes, 0.3 mL/min, 220 nm).

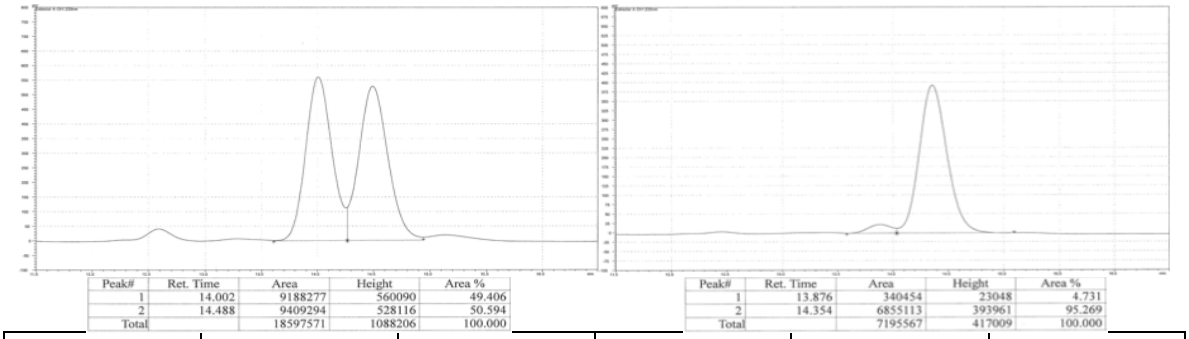


Peak#	Ret. Time	Area	Height	Area %
1	14.537	41844216	994508	50.572
2	16.483	40897888	747456	49.428
Total		82742104	1741964	100.000

Peak#	Ret. Time	Area	Height	Area %
1	14.887	520079	14680	3.297
2	16.975	15256111	297016	96.703
Total		15776189	311696	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	14.537	50.572	1	14.887	3.297
2	16.483	49.428	2	16.975	96.703

(*R*)-4,4,5,5-Tetramethyl-2-(2-(*p*-tolyl)pent-4-en-1-yl)-1,3,2-dioxaborolane (2ac): IR (neat): 2977 (m), 2924 (m), 1514 (w), 1368 (s), 1322 (s), 1145 (s), 968 (m), 911 (m), 846 (m), 813 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 7.09 (2H, d, *J* = 5.2 Hz), 7.06 (2H, d, *J* = 5.6 Hz), 5.71–5.64 (1H, m), 4.97–4.90 (2H, m), 2.91 (1H, app pent, *J* = 5.0 Hz), 2.39–2.30 (5H, m), 1.21 (1H, dd, *J* = 9.8, 4.2 Hz), 1.12–1.06 (13H, m); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 143.9, 137.5, 135.3, 128.9, 127.4, 116.0, 83.1, 43.8, 41.0, 24.84, 24.81, 21.1; HRMS (DART): Calcd for $C_{18}H_{28}B_1O_2$ $[M+H]^+$: 287.2182, Found: 287.2184; Specific Rotation: $[\alpha]_D^{20}$ +8.6 (*c* 1.00, $CHCl_3$) for an enantiomerically enriched sample of 95:5 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OD–H column, 100% hexanes, 0.3 mL/min, 220 nm).



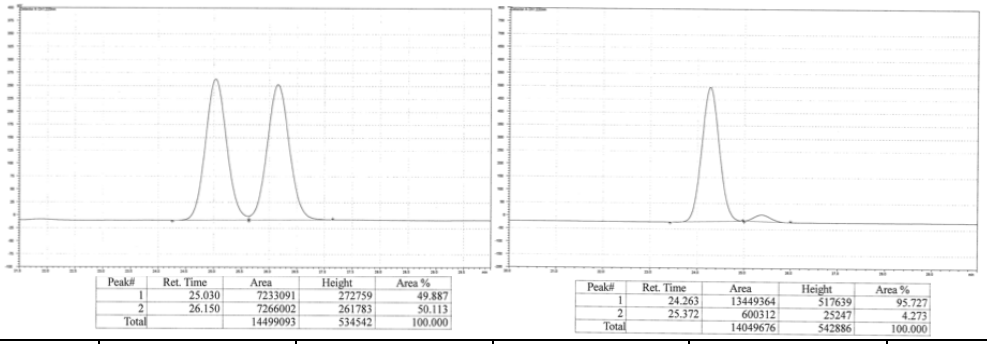
Peak#	Ret. Time	Area	Height	Area %
1	14.002	9188277	560090	49.406
2	14.488	9409294	528116	50.594
Total		18597571	1088206	100.000

Peak#	Ret. Time	Area	Height	Area %
1	13.876	340454	23048	4.731
2	14.354	6855113	393961	95.269
Total		7195567	417009	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	14.002	49.406	1	13.876	4.731
2	14.488	50.594	2	14.354	95.269

(*R*)-Trimethyl(4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl)phenyl)silane (2ad): IR (neat): 3068 (w), 2977 (m), 2955 (m), 2926 (w), 1640 (w), 1599 (w), 1365 (s), 1322 (s), 1164 (m), 1144 (s), 1110 (m), 997 (m), 968 (m), 911 (m), 837 (s), 757 (m), 725 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.41 (2H, d, *J* = 8.1 Hz), 7.23–7.17 (2H, m), 5.70 (1H, dddd, *J* = 16.8, 10.1, 7.6, 6.5 Hz),

4.98 (1H, ddt, *J* = 17.2, 2.5, 1.4 Hz), 4.93 (1H, ddt, *J* = 10.1, 2.1, 1.0 Hz), 2.99–2.88 (1H, m), 2.46–2.26 (2H, m), 1.29–1.20 (2H, m), 1.09 (6H, s), 1.08 (6H, s), 0.23 (9H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ147.6, 137.5, 137.3, 133.2, 127.0, 116.1, 83.0, 43.5, 41.4, 24.8, 24.7, –0.8, –0.9; HRMS (DART): Calcd for $C_{20}H_{34}BO_2Si$ $[M+H]^+$: 345.2421, Found: 345.2431; Specific Rotation: $[\alpha]_D^{20}$ +8.2 (*c* 0.85, $CHCl_3$) for an enantiomerically enriched sample of 96:4 e.r. Enantiomeric purity was determined by HPLC analysis of the alcohol product after oxidation in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel AZ–H column, 99% hexanes, 1% *i*-PrOH, 0.3 mL/min, 220 nm).

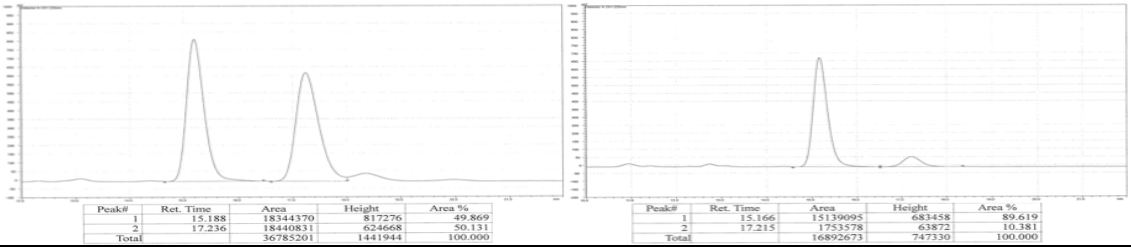


Peak#	Ret. Time	Area	Height	Area %
1	25.030	7233091	272759	49.887
2	26.150	7266002	261783	50.113
Total		14499093	534542	100.000

Peak#	Ret. Time	Area	Height	Area %
1	24.263	13449364	517639	95.727
2	25.372	600312	25247	4.273
Total		14049676	542886	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	25.030	49.887	1	24.263	95.727
2	26.150	50.113	2	25.372	4.273

(*R*)-2-(2-(4-Bromophenyl)pent-4-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2ae): Following the representative procedure except for 1:3 (0.1 mmol: 0.3 mmol) alkene:phosphate used. IR (neat): 2977 (w), 2926 (w), 1488 (w), 1368 (s), 1320 (s), 1143 (s), 1073 (m), 1010 (m), 968 (m), 913 (m), 846 (m), 820 (m) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 (2H, d, *J* = 6.4, Hz), 7.07 (2H, d, *J* = 7.6 Hz), 5.63 (1H, ddt, 17.2, 10.0, 7.2 Hz), 4.97–4.91 (2H, m), 2.94–2.87 (1H, m), 2.32 (2H, t, *J* = 7.0 Hz), 1.21 (1H, dd, *J* = 15.4, 6.6 Hz), 1.12 (6H, s), 1.10 (6H, s), 1.09–1.03 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.9, 136.8, 131.2, 129.4, 119.6, 116.5, 83.2, 43.6, 41.0, 24.9, 24.8; HRMS (DART): Calcd for $C_{17}H_{25}B_1Br_1O_2$ $[M+H]^+$: 351.1131, Found: 351.1141; Specific Rotation: $[\alpha]_D^{20}$ +4.1 (*c* 0.85, $CHCl_3$) for an enantiomerically enriched sample of 90:10 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (90:10 e.r. shown; Chiralcel OZ–H column, 100% hexanes, 0.3 mL/min, 220 nm).

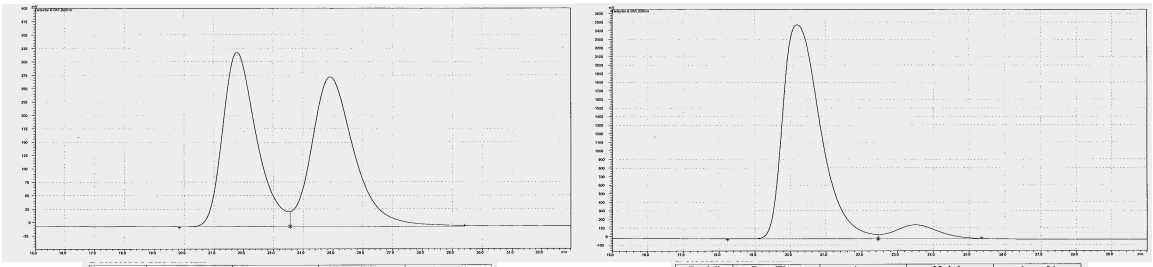


Peak#	Ret. Time	Area	Height	Area %
1	15.188	18344370	817276	49.869
2	17.236	18440831	624668	50.131
Total		36785201	1441944	100.000

Peak#	Ret. Time	Area	Height	Area %
1	15.166	15139095	683458	89.619
2	17.215	1753578	63872	10.381
Total		16892673	747330	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	15.188	49.869	1	15.166	89.619
2	17.236	50.131	2	17.215	10.381

(*R*)-4,4,5,5-Tetramethyl-2-(2-(naphthalen-1-yl)pent-4-enyl)-1,3,2-dioxaborolane (2af): IR (neat): 2976 (w), 2975 (w), 1367 (s), 1312 (s), 1251 (w), 1142 (s), 967 (m), 846 (m), 792 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.22 (1H, d, *J* = 8.1 Hz), 7.83 (1H, dd, *J* = 7.9, 1.6 Hz), 7.68 (1H, dd, *J* = 6.9, 2.5 Hz), 7.56–7.37 (4H, m), 5.75 (1H, ddt, *J* =17.2, 10.1, 7.0 Hz), 5.06–4.91 (2H, m), 3.90 (1H, app pent, *J* = 7.3 Hz), 2.66–2.53 (1H, m), 2.50–2.38 (1H, m), 1.47–1.35 (1H, m), 1.35–1.23 (1H, m), 1.04 (6H, s), 0.96 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 143.2, 137.2, 134.0, 131.8, 128.8, 126.4, 125.6, 125.6, 125.3, 123.9, 123.4, 116.4, 83.1, 43.3, 35.0, 24.7; HRMS (DART): Calcd for $C_{21}H_{28}B_1O_2$ $[M+H]^+$: 323.2182, Found: 323.2185; Specific Rotation: $[\alpha]_D^{20}$ +5.6 (*c* 1.08, $CHCl_3$) for an enantiomerically enriched sample of 93:7 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (93:7 e.r. shown; Chiralcel OJ–H column, 100% hexanes, 0.3 mL/min, 220 nm).

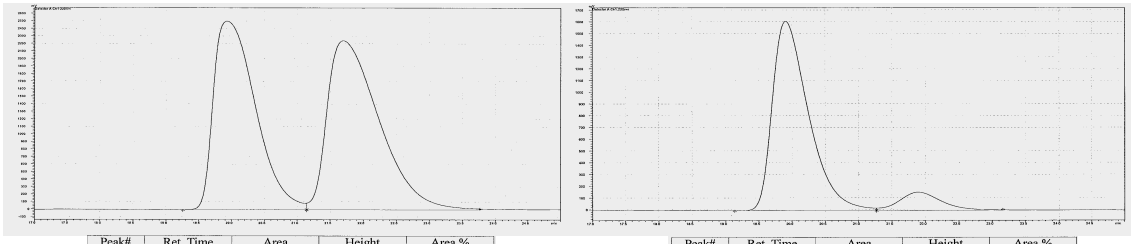


Peak#	Ret. Time	Area	Height	Area %
1	21.777	25778878	325680	48.483
2	24.906	27392466	279410	51.517
Total		53171343	605090	100.000

Peak#	Ret. Time	Area	Height	Area %
1	20.183	183585831	2496092	93.067
2	23.495	13676947	162887	6.933
Total		197262778	2658979	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	21.777	48.483	1	20.183	93.067
2	24.906	51.517	2	23.495	6.933

(*R*)-2-(2-(Benzofuran-2-yl)pent-4-enyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2ag) : IR (neat): 2977 (w), 2928 (w), 1584 (w), 1455 (m), 1370 (s), 1321 (s), 1253(w), 1142 (s), 1006 (m), 912 (m), 846 (m), 796 (m), 749 (s), 738 (s), 671 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.49–7.44 (1H, m), 7.42–7.38 (1H, m), 7.22–7.13 (2H, m), 6.38 (1H, s), 5.76 (1H, ddt, *J* = 17.2, 10.1, 7.1 Hz), 5.08–4.96 (2H, m), 3.26–3.16 (1H, m), 2.63–2.53 (1H, m), 2.49–2.38 (1H, m), 1.23 (2H, d, *J* = 7.7 Hz), 1.20 (6H, s), 1.18 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.3, 154.7, 136.3, 129.0, 123.1, 122.4, 120.4, 117.0, 110.9, 101.4, 83.3, 40.3, 35.0, 24.94, 24.88; HRMS (DART): Calcd for $C_{19}H_{26}BO_3$ $[M+H]^+$: 313.1975, Found: 313.1987; Specific Rotation: $[\alpha]_D^{20}$ +17.2 (*c* 1.67, $CHCl_3$) for an enantiomerically enriched sample of 90:10 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (90:10 e.r. shown; Chiralcel OZ–H column, 100% hexanes, 0.3 mL/min, 220 nm).

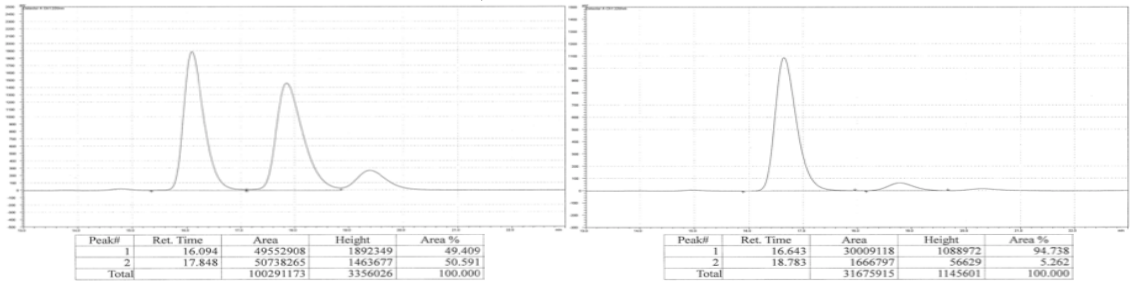


Peak#	Ret. Time	Area	Height	Area %
1	19.923	111510728	2504369	47.625
2	21.690	122634341	2245527	52.375
Total		234145069	4749896	100.000

Peak#	Ret. Time	Area	Height	Area %
1	19.900	61004630	1610521	90.179
2	21.888	6644064	153966	9.821
Total		67648694	1764486	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	19.923	47.625	1	19.900	90.179
2	21.690	52.375	2	21.888	9.821

(*R*)-2-(2-(Benzo[b]thiophen-5-yl)pent-4-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2ah): Following the representative procedure except for 1:3 (0.1 mmol: 0.3 mmol) alkene:phosphate used. IR (neat): 3073 (w), 2976 (w), 2924 (w), 1365 (s), 1319 (s), 11142 (s), 846 (m), 820 (m), 699 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.76 (1H, d, *J* = 8.4 Hz), 7.65 (1H, s), 7.38 (1H, dd, *J* = 5.4, 0.6 Hz), 7.27 (1H, d, *J* = 5.2 Hz), 7.22 (1H, d, *J* = 8.4 Hz), 5.74–5.64 (1H, m), 4.97 (1H, d, *J* = 17.2 Hz), 4.92 (1H, dd *J* = 10.4, 0.8 Hz), 3.08 (1H, app pent, *J* = 7.5 Hz), 2.48–2.36 (2H, m), 1.30 (1H, dd, *J* = 15.8, 7.0 Hz), 1.17 (1H, dd, *J* = 15.4, 9.0 Hz), 1.07 (12H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 152.3, 140.0, 139.2, 136.4, 124.0, 123.4, 122.9, 122.3, 119.8, 116.9, 83.4, 43.8, 37.6, 24.9, 24.8; HRMS (DART): Calcd for $C_{19}H_{26}B_1O_2S_1$ $[M+H]^+$: 329.1747, Found: 329.1744; Specific Rotation: $[\alpha]_D^{20}$ +18.0 (*c* 1.23, $CHCl_3$) for an enantiomerically enriched sample of 95:5 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OZ–H column, 100% hexanes, 0.3 mL/min, 220 nm).



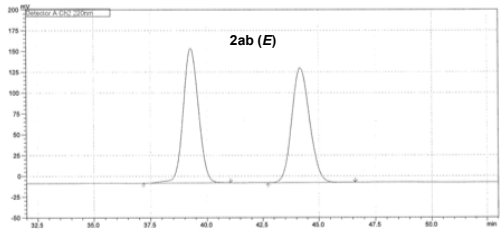
Peak#	Ret. Time	Area	Height	Area %
1	16.094	49552908	1892349	49.409
2	17.848	50738265	1463677	50.591
Total		100291173	3356026	100.000

Peak#	Ret. Time	Area	Height	Area %
1	16.643	30009118	1088972	94.738
2	18.783	1666797	56629	5.262
Total		31675915	1145601	100.000

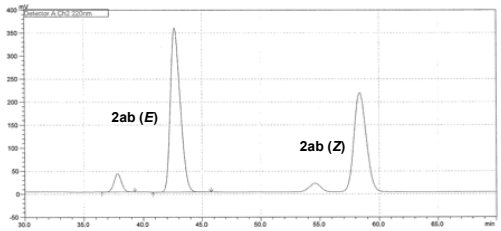
Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	16.094	49.409	1	16.643	94.738
2	17.848	50.591	2	18.783	5.262

(*R*)-4,4,5,5-Tetramethyl-2-(2-(*o*-tolyl)hex-4-en-1-yl)-1,3,2-dioxaborolane (2ai): Following the representative procedure except **L3b** was used. The spectroscopic data match those reported previously.[5] ^1H NMR (400 MHz, $CDCl_3$): δ 7.26–7.01 (8H, m, *E*/*Z*), 5.46–5.28 (4H, m, *E*/*Z*), 3.24–3.13 (2H, m, *E*/*Z*), 2.36 (3H, s, *E*) 2.35 (3H, s, *Z*), 2.32–2.13 (4H, m, *E*/*Z*), 1.59 (3H, d, *J* = 5.6 Hz, *E*), 1.54 (3H, d, *J* = 6 Hz, *Z*), 1.23–1.10 (4H, m, *E*/*Z*), 1.053 (6H, s, *E*), 1.045 (6H, s, *E*), 1.03 (6H, s, *Z*), 1.02 (6H, s, *Z*) Specific Rotation: $[\alpha]_D^{20}$ +6.1 (*c* 0.45, $CHCl_3$) for an enantiomerically enriched sample of 92:8 e.r. Enantiomeric purity was determined by HPLC analysis of the alcohol product after oxidation

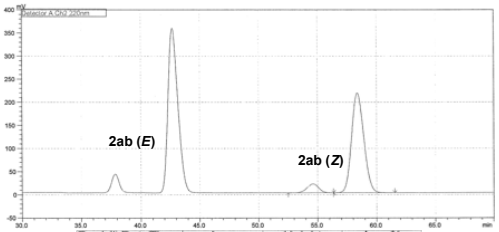
in comparison with authentic racemic material prepared according to the procedure reported previously obtaining ***rac-E*-2ab**.[5] (92:8 e.r. shown for *E* and *Z*; Chiralcel OJ–H column, 98% hexanes, 0.3 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area%
1	39.289	7684209	162000	50.239
2	44.190	7611006	137735	49.761
Total		15295214	299735	100.000



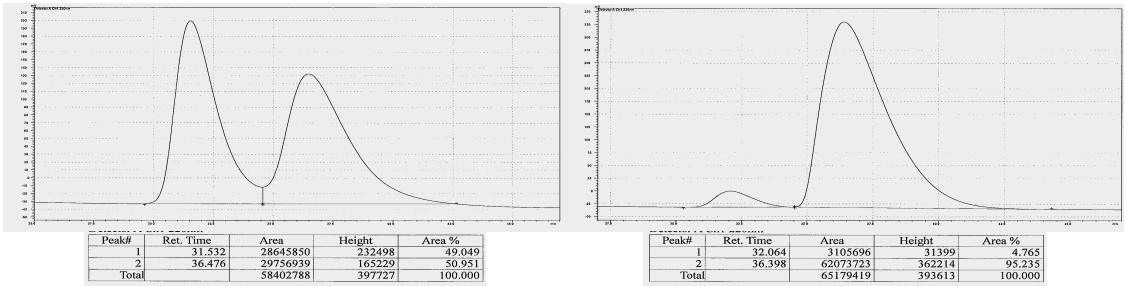
Peak#	Ret. Time	Area	Height	Area%
1	37.848	1739929	39964	7.697
2	42.673	20865572	356691	92.303
Total		22605501	396655	100.000



Peak#	Ret. Time	Area	Height	Area%
1	54.599	1289796	18912	7.644
2	58.361	15584373	215457	92.356
Total		16874169	234370	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1 (*rac*)	39.389	50.239	1 (*E*)	37.848	7.697
2 (*rac*)	44.190	49.761	2 (*E*)	42.673	92.303
			1 (*Z*)	54.599	7.644
			2 (*Z*)	58.361	92.356

(*R*)-2-(2-(3-(Allyloxy)phenyl)pent-4-enyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2aj): IR (neat): 3076 (w), 2977 (w), 2925 (w), 1600 (m), 1583 (m), 1422 (s), 1366 (s), 1265 (m), 1142 (s), 1034 (w), 913 (m), 846 (m), 776 (m), 699 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.16 (1H, t, *J* = 7.9 Hz), 6.84–6.76 (2H, m), 6.71 (1H, ddd, *J* = 8.2, 2.6, 0.9 Hz), 6.06 (1H, ddt *J* = 17.3, 10.6, 5.3 Hz), 5.67 (1H, dddd, *J* = 16.9, 10.1, 7.5, 6.6 Hz), 5.40 (1H, dd, *J* = 17.3, 1.6 Hz), 5.27 (1H, dd, *J* = 10.5, 1.5 Hz), 5.00–4.87 (2H, m), 4.52 (2H, dt, *J* = 5.3, 1.5 Hz), 3.04–2.82 (1H, m), 2.43–2.26 (2H, m), 1.29–1.16 (2H, m), 1.12 (6H, s), 1.11 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 158.6 148.7, 137.3, 133.7, 129.1, 120.2, 117.6, 116.2, 114.2, 112.2, 83.1, 68.8, 43.7, 41.5, 24.85, 24.82; HRMS (DART): Calcd for $C_{20}H_{30}B_1O_3$ $[M+H]^+$: 329.2288, Found: 329.2295; Specific Rotation: $[\alpha]_D^{20}$ +6.4 (*c* 1.17, $CHCl_3$) for an enantiomerically enriched sample of 95:5 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OD–H column, 100% hexanes, 0.3 mL/min, 220 nm).

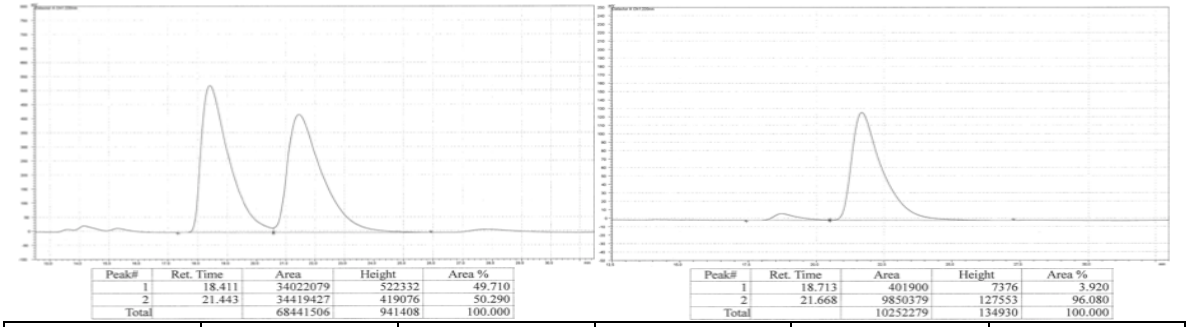


Peak#	Ret. Time	Area	Height	Area %
1	31.532	28645850	232498	49.049
2	36.476	29756939	165229	50.951
Total		58402788	397727	100.000

Peak#	Ret. Time	Area	Height	Area %
1	32.064	3105696	31399	4.765
2	36.398	62073723	362214	95.235
Total		65179419	393613	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	31.532	49.049	1	32.064	4.765
2	36.476	50.951	2	36.398	95.235

(*R*)-(4-(3-(Allyloxy)phenyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-1-en-2-yl)trimethylsilane (2ak): IR (neat): 2977 (w), 2954 (w), 1600 (w), 1584 (w), 1366 (m), 1317 (m), 1247 (m), 1144 (s), 924 (m), 836 (s) cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 7.14 (1H, t, *J* = 6.2 Hz), 6.80–6.77 (2H, m), 6.69 (1H, dd, *J* = 6.4, 2.0 Hz), 6.10–6.02 (1H, m), 5.45–5.38 (2H, m), 5.32–5.26 (2H, m), 4.52–4.51 (2H, m), 2.99 (1H, app pent, *J* = 6.1 Hz), 2.45 (1H, dd, *J* = 11.2, 6.0 Hz), 2.38 (1H, dd, *J* = 11.2, 6.0 Hz), 1.21 (1H, dd, *J* = 14.0, 3.6 Hz), 1.11 (6H, s), 1.09 (6H, s), 1.02 (1H, dd, *J* = 12.2, 7.0 Hz), 0.07 (9H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.5, 150.3, 149.3, 133.8, 129.0, 126.5, 120.4, 117.5, 114.3, 112.1, 83.0, 68.8, 45.7, 40.7, 24.9, 24.8, –1.2; HRMS (DART): Calcd for $C_{23}H_{38}B_1O_3Si_1$ $[M+H]^+$: 401.2683, Found: 401.2695; Specific Rotation: $[\alpha]_D^{20}$ +4.7 (*c* 0.88, $CHCl_3$) for an enantiomerically enriched sample of 95:5 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OD–H column, 100% hexanes, 0.3 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area %
1	18.411	34022079	522332	49.710
2	21.443	34419427	419076	50.290
Total		68441506	941408	100.000

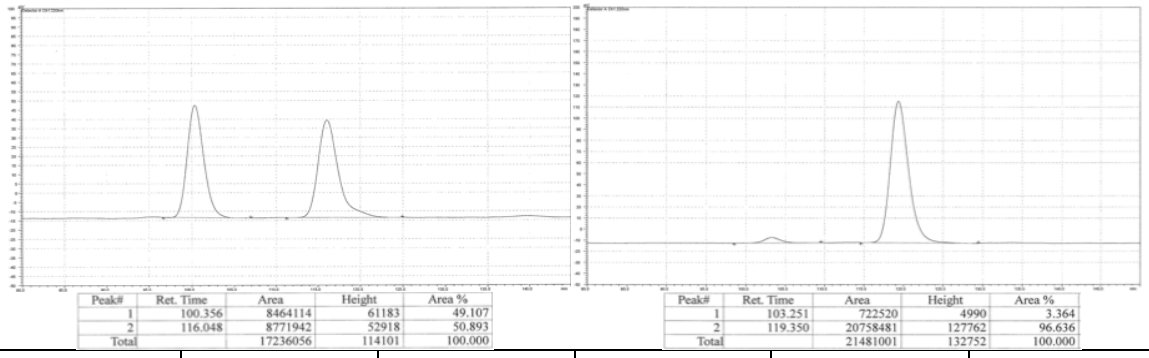
Peak#	Ret. Time	Area	Height	Area %
1	18.713	401900	7376	3.920
2	21.668	9850379	127553	96.080
Total		10252279	134930	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	18.411	49.710	1	18.713	3.920
2	21.443	50.290	2	21.668	96.080

7. Formal Synthesis of (+)-Heliespirone A and (–)-Heliespirone C

(*R*)-2-(2-(2,5-Dimethoxy-4-methylphenyl)pent-4-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2r): In a N_2-filled glove box, a flame-dried 100 mL round-bottom flask equipped with a stir bar was charged with bisphosphine **L3b** (188 mg, 0.28 mmol), NaO*t*-Bu (742 mg, 7.7 mmol), and CuCl (26 mg, 0.26 mmol). The flask was sealed with a septum and electrical tape before removal from the glove box. Tetrahydrofuran (20 mL) was added and the resulting yellow solution was allowed to stir for 1 h

under N_2 at 22 °C. A solution of $B_2(pin)_2$ (1.4 g, 5.7 mmol) in thf (15 mL) was added to the mixture at 0 °C, causing the solution to turn dark brown immediately. After 15 min, a solution of **9** (2.75 g, 15.5 mmol) in thf (5 mL) and allylphosphate (**1a**) [0.92 mL (1.0 g), 5.15 mmol] was added by syringe. The resulting mixture was allowed to stir at 22 °C for 18 h. Then, the mixture was passed through a short plug of silica gel (4x4 cm) and eluted with Et_2O. The organic layer was concentrated under reduced pressure, affording yellow oil, which was purified by silica gel chromatography (100% hexanes→hexanes:Et_2O = 10:1) to afford **2r** as colorless oil (1.1 g, 3.3 mmol, 64% yield) and recovered **9** (1.68 g, 9.4 mmol, 91%). IR (neat): 2976 (w), 2931 (w), 2830 (w), 1506 (m), 1465 (m), 1398 (m), 1369 (m), 1316 (m), 1207 (s), 1143 (s), 1046 (s), 968 (m), 846 (m), 802 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 6.68 (1H, s), 6.64 (1H, s), 5.71 (1H, ddt, *J* = 17.2, 9.8, 7.4 Hz), 4.98–4.89 (2H, m), 3.78 (3H, s), 3.76 (3H, s), 3.36 (1H, app pent, *J* = 7.5 Hz), 2.43–2.25 (2H, m), 2.18 (3H, s), 1.22 (1H, dd, *J* = 15.6, 7.6 Hz), 1.15–1.10 (1H, m), 1.13 (6H, s), 1.10 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.7, 151.0, 137.8, 133.2, 124.2, 115.7, 114.4, 110.9, 82.9, 56.5, 56.2, 42.3, 34.2, 24.84, 24.81, 16.2; HRMS (DART): Calcd for $C_{20}H_{32}B_1O_4$ $[M+H]^+$: 347.2394, Found: 347.2377; Specific Rotation: $[\alpha]_D^{20}$ +36.6 (*c* 0.56, $CHCl_3$) for an enantiomerically enriched sample of 97:3 e.r. Enantiomeric purity was determined by HPLC analysis of the alcohol product after oxidation in comparison with authentic racemic material (97:3 e.r. shown; Chiralpak AD–H column, 99% hexanes, 1% *i*-PrOH, 0.3 mL/min, 220 nm).



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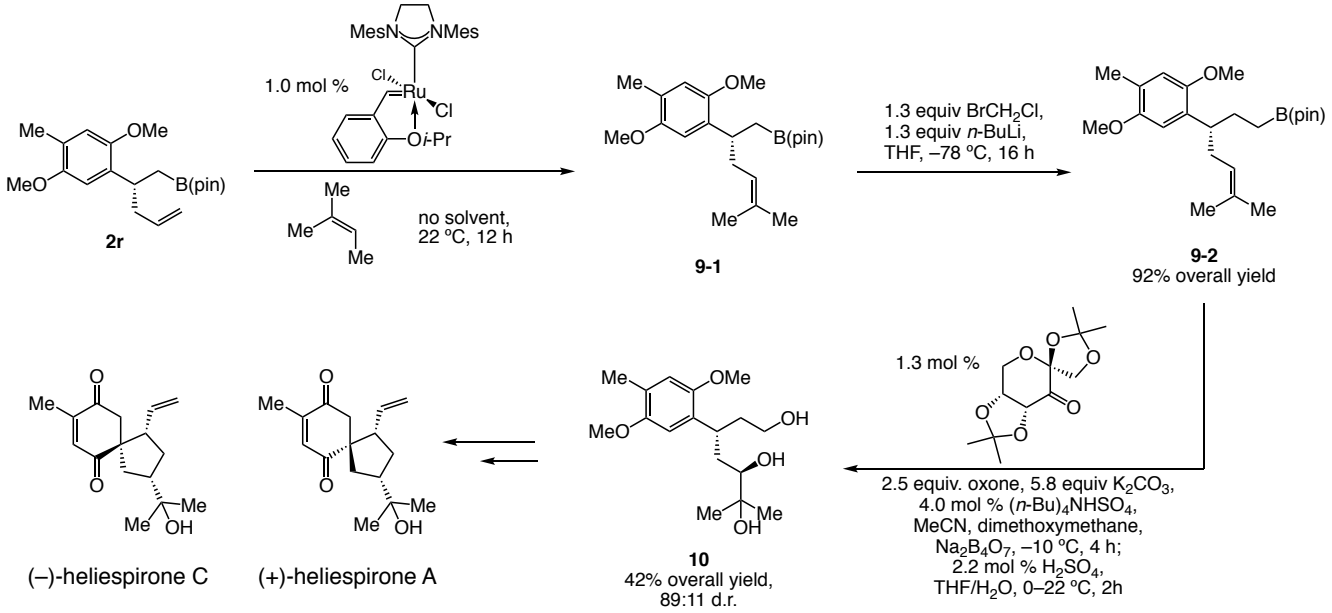
2	116.048	8771942	52918	50.893
Total		17236056	114101	100.000

Peak#	Ret. Time	Area	Height	Area %
1	103.251	722520	4990	3.364
2	119.350	20758481	127762	96.636
Total		21481001	132752	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	100.356	49.107	1	103.251	3.364
2	116.048	50.893	2	119.350	96.636

Scheme 2. Application to Enantioselective Synthesis of Heliespirone A and C



(*R*)-2-(3-(2,5-Dimethoxy-4-methylphenyl)-6-methylhept-5-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (9-2): Compound **2r** was converted to **9-2** by a two-step sequence olefin cross metathesis/homologation based on the reported procedures except Hoveyda-Grubbs catalyst 2nd generation was used in the cross metathesis.[15] IR (neat): 2977 (w), 2931 (w), 2854 (w), 1504 (m), 1466 (m), 1398 (m), 1372 (m), 1317 (m), 1208 (s), 1145 (m), 1049 (m), 968 (w) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.65 (1H, s), 6.62 (1H, s), 5.09–5.06 (1H, m), 3.77 (3H, s), 3.73 (3H, s), 3.02 (1H, app pent, J = 7.2 Hz), 2.35–2.19 (2H, m), 1.81 (3H, s), 1.80–1.70 (1H, m), 1.68–1.56 (4H, m), 1.54 (3H, s), 1.21 (12H, s), 0.74–0.60 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.9, 151.7, 132.1, 131.7, 124.2, 123.6, 114.5, 110.7, 82.9, 56.6, 56.2, 40.5, 33.8, 29.3, 25.9, 25.0, 24.9, 17.9, 16.2; HRMS (DART): Calcd for $C_{23}H_{38}B_1O_4$ $[M+H]^+$: 389.2863, Found: 389.2862; Specific Rotation: $[\alpha]_D^{20}$ +18.0 (*c* 0.50, $CHCl_3$).

(3*R*,5*R*)-3-(2,5-Dimethoxy-4-methylphenyl)-6-methylheptane-1,5,6-triol (10): Compound **9-2** was converted to **10** by a two step sequence enantioselective epoxidation/hydrolysis based on the reported procedures except the oxidation was performed with 2.5 equiv of oxone.[16] The spectroscopic data match those reported previously.[17] ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.72 (1H, s), 6.66 (1H, s), 3.80 (3H, s), 3.79 (3H, s), 3.58–3.53 (2H, m), 3.46–3.35 (2H, m), 2.20 (3H, s), 2.12–2.01 (1H, m), 1.88–1.84 (1H, m), 1.74–1.59 (2H, m), 1.21 (3H, s), 1.15 (3H, s); HRMS (DART): Calcd for $C_{17}H_{28}O_5$ $[M]^+$: 312.1937, Found: 312.1939. Specific Rotation: $[\alpha]_D^{20}$ +23.4 (*c* 0.23, $CHCl_3$). Literature precedence: $[\alpha]_D^{13}$ +29.2(*c* 0.10, CH_2Cl_2).[17]

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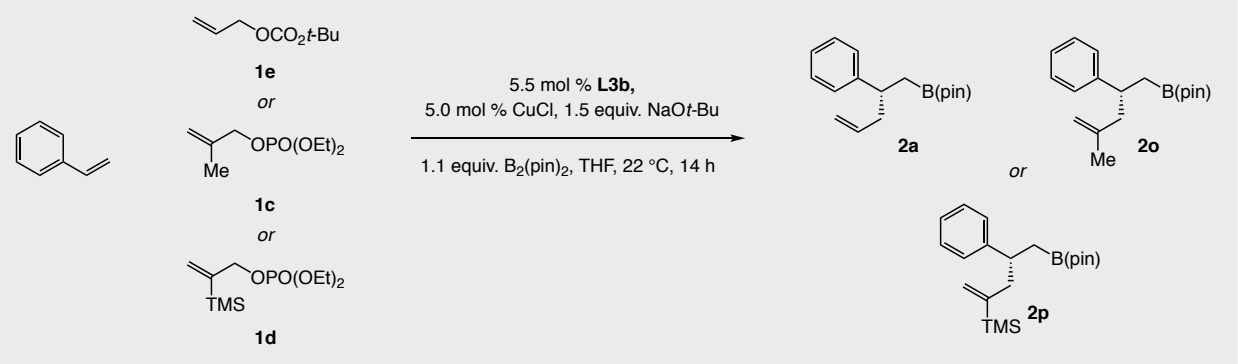
(15) For cross-metathesis, see: Chatterjee, A. K., Sanders, D. P. & Grubbs, R. H. *Org. Lett.* **4**, 1939–1942 (2002). For homologation, see: Kliman, L. T., Mlynarski, S. N. & Morken, J. P. *J. Am. Chem. Soc.* **131**, 13210–13211 (2009).

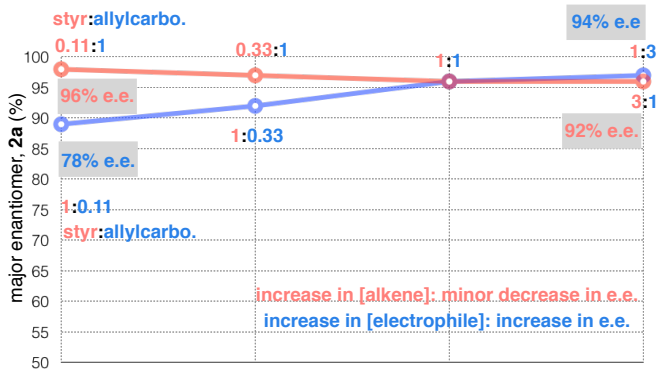
(16) Wang, Z.-X., Tu, Y., Frohn, M., Zhang, J.-R. & Shi, Y. *J. Am. Chem. Soc.* **119**, 11224–11235 (1997).

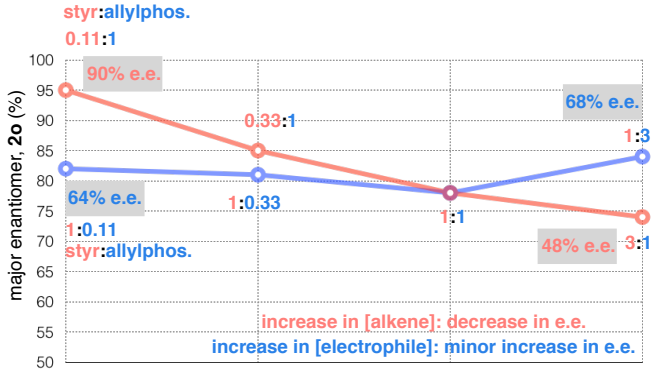
(17) Huang, C. & Liu, B. *Chem. Commun.* **46**, 5280–5282 (2010).

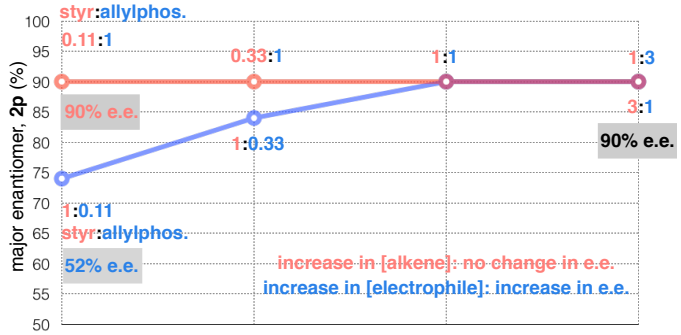
8. Additional Studies Regarding the Effect of Concentration Changes on Enantioselectivity

Scheme 3. Additional Studies Regarding the Effect of Aryl Olefin or Allyl Electrophile Concentration on Enantioselectivity



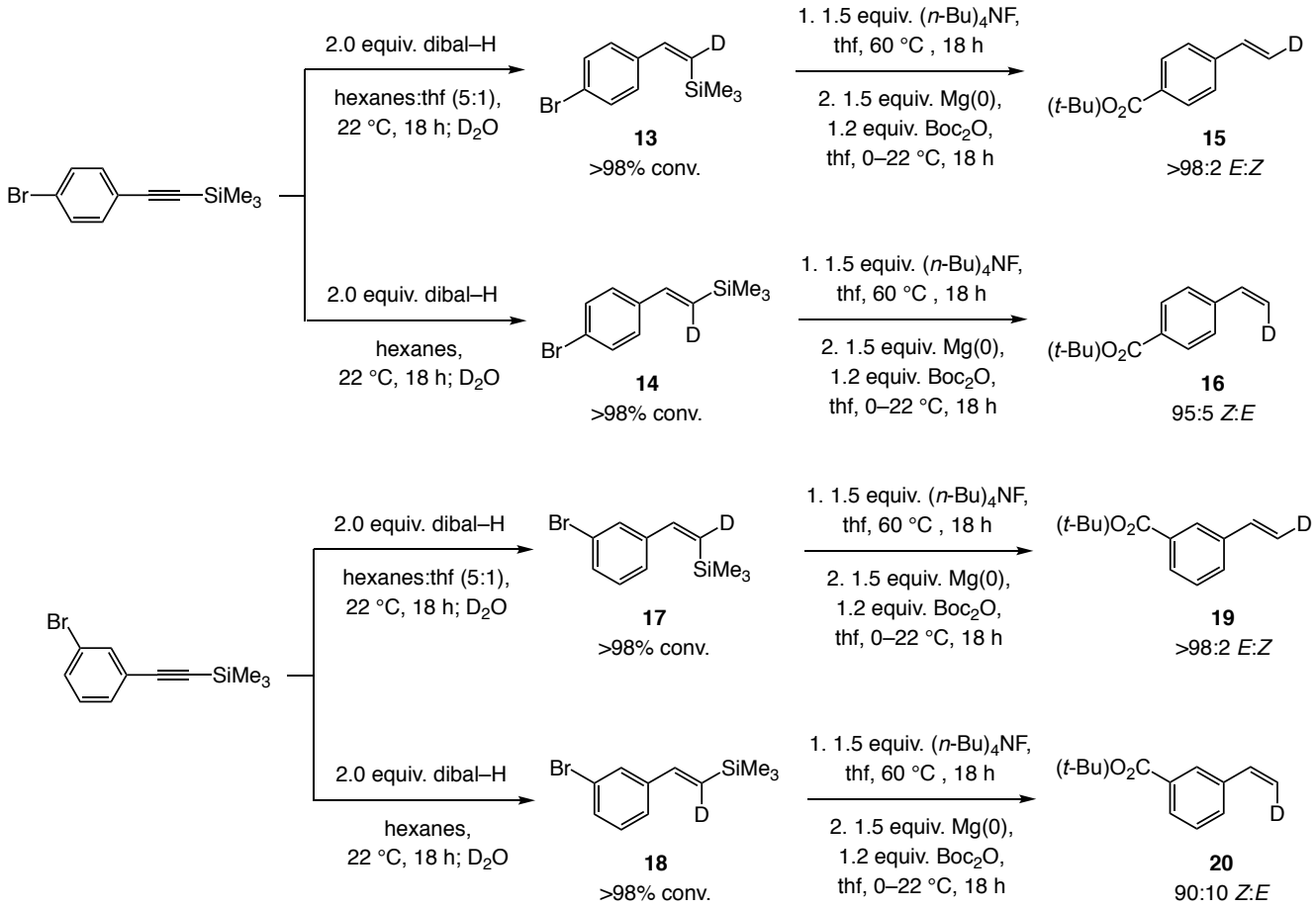






9. Study of the Possibility of Epimerization through Isotopic Labeling

Scheme 4. Synthesis of *E* and *Z* Deuterium-Labeled Aryl Olefins



(*Z*)-(2-(4-Bromophenyl)vinyl-1-*d*)trimethylsilane (13): To a flame-dried round bottom flask equipped with a stir bar was added hexanes (20 mL) under N_2, after which dibal–H (8.6 mL, 48 mmol, USE WITH CAUTION, PYROPHORIC) was added by a gas-tight syringe. The resulting mixture was allowed to cool to 0 °C, and a solution of trimethyl(4-bromophenylethynyl)silane (6.1 g, 24 mmol) in thf (4 mL) was added drop-wise by syringe. The mixture was allowed to stir for an additional 5 min at 0 °C and then warmed to 22 °C and allowed to stir for 23 h. The reaction was then quenched upon drop-wise addition of D_2O (1.2 mL, 72 mmol) at 0 °C and allowed to stir for 1 h at 22 °C. The mixture was transferred to a separatory funnel and Rochelle's salt (50 mL) and a saturated solution of aqueous ammonium chloride (40 mL) were added. The layers were separated, and the aqueous layer was washed with Et_2O (3 x 20 mL). The combined organic layers were dried over Na_2SO_4 and concentrated in vacuo. The resulting yellow oil was purified by silica gel chromatography (100% pentane) and Kugelrohr distillation to afford **13**.

(*E*)-(2-(4-Bromophenyl)vinyl-1-*d*)trimethylsilane (14): This compound was prepared similarly to **13**, except 100% hexanes (24 mL) was used instead of using 16.7% thf.

***tert*-Butyl-(*E*)-4-(vinyl-2-*d*)benzoate (15):** To a solution of **13** in thf (15 mL) was added $(n\text{Bu})_4\text{NF}$ (1.0 M in thf, 8.25 mL, 8.25 mmol) at 22 °C under N_2. The mixture was allowed to stir at 60 °C for 18

hours after which it was transferred to a separatory funnel; water (25 mL) was added and the layers separated. The aqueous layer was washed with Et_2O (3x20 mL). The combined organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The resulting yellow oil was purified by Kugelrohr distillation to afford **(*E*)-1-Bromo-4-(vinyl-2-*d*)benzene** which was converted to **15** following the previously reported procedure.[10] The resulting colorless oil was purified by silica gel chromatography and Kugelrohr distillation to afford **15** as colorless liquid (200 mg, >98% D, >98% *E)*. IR (neat): 2979 (w), 1709 (s), 1608 (w), 1393 (m), 1291 (s), 1162 (s), 1112 (s), 1066 (s), 1067 (m), 865 (s), 771 (s), 702 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.97–7.94 (2H, m), 7.43 (2H, d, *J* = 8.4 Hz), 6.74 (1H, d, *J* = 17.6 Hz), 5.82 (1H, d, *J* = 17.6 Hz), 1.60 (9H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.6, 141.5, 136.1, 131.3, 129.8, 127.2, 126.0, 121.4, 115.9 (t, *J* = 24.3 Hz), 81.0, 28.3; HRMS (DART): Calcd for $C_{13}H_{16}DO_2$ $[M+H]^+$: 206.1291; Found: 206.1300.

***tert*-Butyl-(*Z*)-4-(vinyl-2-*d*)benzoate (16):** To a solution of **14** in thf (15 mL) was added $(nBu)_4NF$ (1.0 M in thf, 8.25 mL, 8.25 mmol) at 22 °C under N_2. The mixture was allowed to stir at 60 °C for 18 h after which it was transferred to a separatory funnel, water (25 mL) was added and the layers separated. The aqueous layer was washed with Et_2O (3x20 mL). The combined organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The resulting yellow oil was purified by Kugelrohr distillation to afford **(*Z*)-1-Bromo-4-(vinyl-2-*d*)benzene** which was converted to **16** following the previously reported procedure.[10] The product was purified by silica gel chromatography and Kugelrohr distillation to afford **16** as colorless liquid (199.4 mg, >98%D, 95:5 *Z*:*E)*. IR (neat): 2977 (w), 1707 (s), 1607 (w), 1367 (m), 1287 (s), 1161 (s), 1104 (s), 1016 (m), 848 (s), 774 (s), 706 (s), 438 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.94 (2H, d, *J*= 8.4 Hz), 7.43 (2H, d, *J* = 8.4 Hz), 6.75–6.79 (1H, m), 5.35 (1H, *J* = 10.4 Hz), 1.60 (9H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.7, 141.5, 136.2, 131.3, 129.8, 126.1, 116.0 (t, *J* = 23.5 Hz), 81.0, 28.3 HRMS (DART): Calcd for $C_{13}H_{16}DO_2$ $[M+H]^+$: 206.1291; Found: 206.1293

tert*-Butyl-4-((1*S*,2*R*)-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl-1-*d*)benzoate (2k-*d from 15*):** Following the representative procedure except **L3b** and 1:3 alkene:phosphate used, **2k-*d was obtained as colorless oil (60:40 d.r., determined from ^1H NMR of the product after oxidation). IR (neat): 2977 (w), 2929 (w), 1711 (s), 1609 (w), 1391 (m), 1364 (s), 1312 (s), 1288 (s), 1255 (m), 1164 (s), 1143 (s), 1112 (s), 850 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.88 (2H, d, *J* = 8.0 Hz), 7.24 (2H, d, *J* = 8.0 Hz), 5.63 (1H, ddt, *J* = 17.2, 10.4, 6.8 Hz), 4.96–4.90 (2H, m), 2.99 (1H, app q, *J* = 7.2 Hz), 2.35 (2H, t, *J* = 7.0 Hz), 1.58 (9H, s), 1.22 (1H, br s), 1.12 (6H, s), 1.11 (2.46H, s, minor), 1.10 (3.54H, s, major); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 166.1, 151.95 (minor), 151.93 (major), 136.8, 129.8, 129.5, 127.4, 116.5, 83.2, 80.8, 43.51 (major), 43.48 (minor), 41.4, 28.4, 24.9, 24.80 (minor), 24.79 (major); HRMS (DART): Calcd for $C_{22}H_{33}D_1B_1O_4$ $[M+H]^+$: 374.2613; Found: 374.2620.

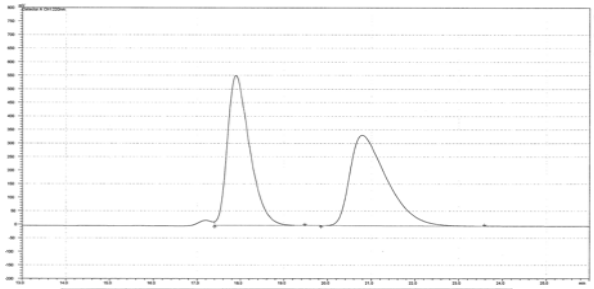
tert*-Butyl-4-((1*R*,2*R*)-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl-1-*d*)benzoate (2k-*d from 16*):** Following the representative procedure except **L3b** and 1:3 alkene:phosphate used, **2k-*d was obtained as colorless oil (35:65 d.r., determined from ^1H NMR of the product after oxidation). IR (neat): 2977 (w), 2929 (w), 1711 (s), 1609 (w), 1391 (m), 1364 (s), 1312 (s), 1288 (s), 1255 (m), 1164 (s), 1143 (s), 1112 (s), 850 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.88 (2H, d, *J* = 8.0 Hz), 7.24 (2H, d, *J* = 8.0 Hz), 5.63 (1H, ddt, *J* = 17.2, 10.4, 6.8 Hz), 4.96–4.90 (2H, m), 2.99 (1H,

app q, J = 7.5 Hz), 2.35 (2H, t, J = 7.0 Hz), 1.58 (9H, s), 1.22 (1H, br s), 1.12 (6H, s), 1.11 (3.76H, s, major), 1.10 (2.24H, s, minor); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 166.1, 151.95 (major), 151.93 (minor), 136.8, 129.8, 129.5, 127.4, 116.5, 83.2, 80.8, 43.51 (minor), 43.48 (major), 41.4, 28.4, 24.9, 24.80 (major), 24.79 (minor); HRMS (DART): Calcd for $C_{22}H_{33}D_1B_1O_4$ $[M+H]^+$: 374.2613; Found: 374.2620.

***tert*-Butyl-(*E*)-3-(vinyl-2-*d*)benzoate (19, substrate for synthesis of *anti*-2g-*d*):** Following the procedure for preparation of **15** except trimethyl(3-bromophenylethynyl)silane was used. The product was obtained as >98:2 *E*:*Z*. IR (neat): 2977 (w), 1710 (s), 1367 (m), 1297 (s), 1254 (m), 1157 (s), 1079 (m), 1036 (m), 999 (m), 883 (m), 785 (w), 753 (s), 408 (w) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (1H, s), 7.87 (1H, dt, J = 7.6, 1.2 Hz), 7.56–7.55 (1H, m), 7.35 (1H, t, J = 7.2 Hz), 6.75 (1H, d, J = 17.6 Hz), 5.80 (1H, d, J = 17.6 Hz), 1.60 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.7, 137.7, 136.1, 132.4, 130.1, 128.8, 128.5, 127.3, 114.7 (t, J = 24.3 Hz), 81.1, 28.3; HRMS (DART): Calcd for $C_{13}H_{16}D_1O_2$ $[M+H]^+$: 206.1291, Found: 206.1297.

***tert*-Butyl-(*Z*)-3-(vinyl-2-*d*)benzoate (20, substrate for synthesis of *syn*-2g-*d*):** Following the procedure for preparation of **16** except trimethyl(3-bromophenylethynyl)silane was used. The product was obtained as 90:10 *Z*:*E*. IR (neat): 2977 (w), 1711 (s), 1367 (m), 1291 (s), 1277 (s), 1156 (s), 1109 (m), 1082 (m), 848 (m), 818 (m), 755 (m), 697 (m), 406 (w) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (1H, t, J = 2 Hz), 7.88 (1H, dt, J = 7.6, 1.6 Hz), 7.57–7.55 (1H, m), 7.37 (1H, t, J = 7.6 Hz), 6.74 (1H, dt, J = 10.8, 2.4 Hz), 5.29 (1H, d, J = 10.8 Hz), 1.61 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.7, 137.7, 136.1, 132.4, 130.1, 128.7, 128.5, 127.3, 114.6 (t, J = 23.5 Hz), 81.1, 28.2; HRMS (DART): Calcd for $C_{13}H_{16}D_1O_2$ $[M+H]^+$: 206.1291, Found: 206.1302.

***tert*-Butyl-3-((1*S*,2*R*)-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl-1-*d*)benzoate (*anti*-2g-*d*):** IR (neat): 2977 (m), 2927 (w), 1713 (s), 1479 (w), 1366 (s), 1316 (s), 1295 (s), 1161 (s), 1145 (s), 1111 (m), 755 (m), 697 (w) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (1H, t, J = 1.8 Hz), 7.78 (1H, dt, J = 8.0, 1.2 Hz), 7.37 (1H, dt, J = 7.6, 1.2 Hz), 7.30 (1H, t, J = 7.6 Hz), 5.66 (1H, ddt, J = 17.0, 10.0, 7.2 Hz), 4.99–4.90 (2H, m), 2.99 (1H, q, J = 7.2 Hz), 2.44–2.32 (2H, m), 1.59 (9H, s), 1.22 (1H, d, J = 7.6 Hz), 1.11 (6H, s), 1.10 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.2, 147.1, 137.0, 131.9, 131.6, 128.8, 128.1, 127.2, 116.4, 83.2, 80.9, 43.4, 41.3, 28.4, 24.9, 24.8; HRMS (DART): Calcd for $C_{22}H_{33}D_1B_1O_4$ $[M+H]^+$: 374.2613, Found: 374.2614. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (87:13 e.r. shown; Chiralcel OZ–H column, 100% hexanes, 0.3 mL/min, 220 nm).



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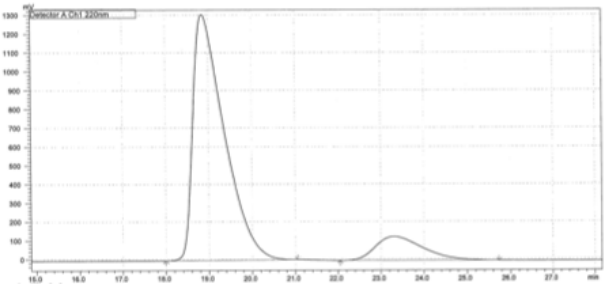

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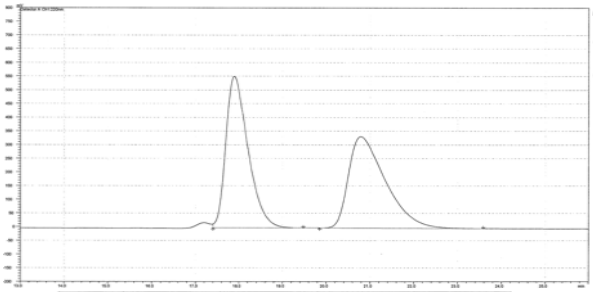
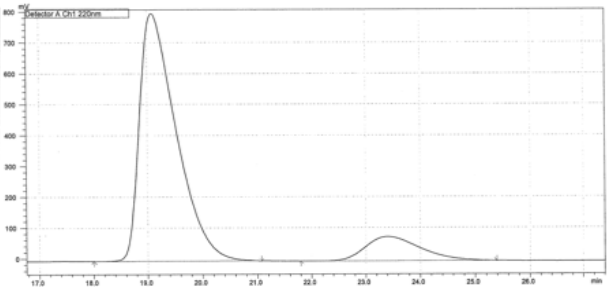
Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	17.885	50.079	1	18.855	87.254
2	20.783	49.921	2	23.306	12.746

***tert*-Butyl-3-((1*R*,2*R*)-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl-1-*d*)benzoate (*syn*-2g-*d*):** IR (neat): 2977 (m), 2927 (w), 1713 (s), 1479 (w), 1366 (s), 1316 (s), 1295 (s), 1161 (s), 1145 (s), 1111 (m), 755 (m), 697 (w) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.83 (1H, t, *J* = 1.6 Hz), 7.78 (1H, dt, *J* = 7.6, 1.2 Hz), 7.37 (1H, dt, *J* = 8, 1.6 Hz), 7.30 (1H, t, *J* = 7.6 Hz), 5.66 (1H, ddt, *J* = 17.0, 10.0, 7.2 Hz), 4.99–4.91 (2H, m), 2.99 (1H, q, *J* = 7.2 Hz), 2.44–2.32 (2H, m), 1.59 (9H, s), 1.11 (6H, s), 1.10 (6H, s), 1.07 (1H, d, *J* = 9.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.2, 147.1, 137.0, 131.9, 131.6, 128.8, 128.1, 127.2, 116.5, 83.2, 80.9, 43.4, 41.3, 28.4, 24.9, 24.8; HRMS (DART): Calcd for $C_{22}H_{33}D_1B_1O_4$ $[M+H]^+$: 374.2613, Found: 374.2614. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (87:13 e.r. shown; Chiralcel OZ–H column, 100% hexanes, 0.3 mL/min, 220 nm).



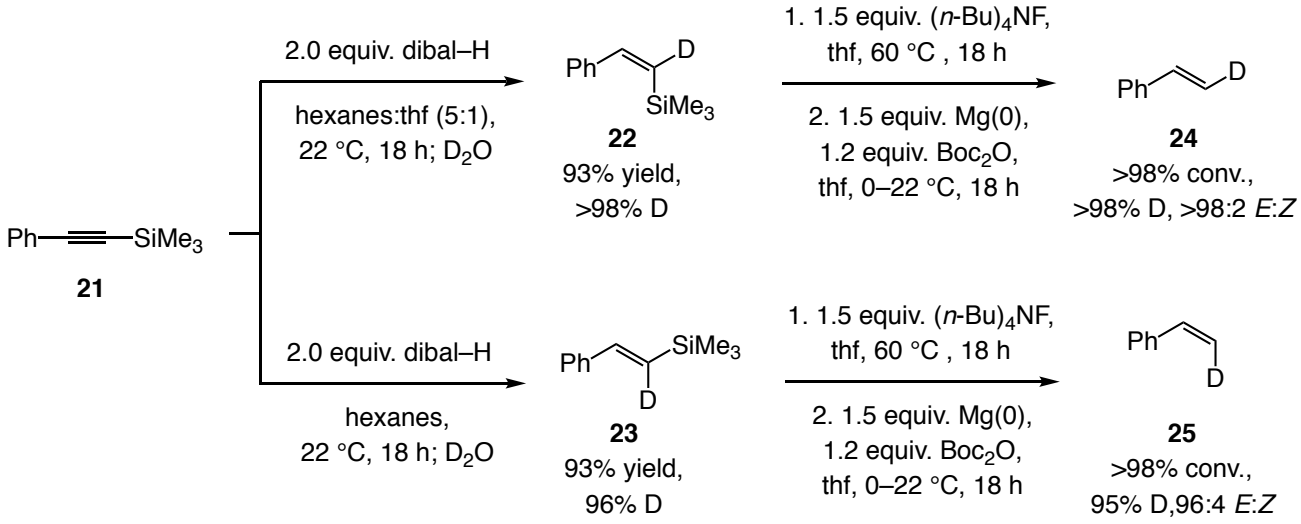
Peak#	Ret. Time	Area	Height	Area %
1	17.885	19631455	553324	50.079
2	20.783	19569298	334519	49.921
Total		39200753	887842	100.000



Peak#	Ret. Time	Area	Height	Conc.	Area%
1	19.082	37431307	801554	87.184	87.184
2	23.406	5502265	78389	12.816	12.816
Total		42933572	879943		100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	17.885	50.079	1	19.082	87.184
2	20.783	49.921	2	23.406	12.816

Scheme 5. Synthesis of *E* and *Z* Deuterium-Labeled Aryl Olefins



(*Z*)-Trimethyl(2-phenylvinyl-1-*d*)silane (22): To a flame-dried round bottom flask equipped with a stir bar was added hexanes (20 mL) and thf (4 mL) under N_2 after which dibal–H (8.6 mL, 48 mmol, USE CAUTION, PYROPHORIC) was added through a gas tight syringe. The mixture was allowed to cool to 0 °C (ice/water bath) and trimethyl(phenylethynyl)silane (4.8 mL, 24 mmol) was added by syringe drop-wise. The mixture was allowed to stir for an additional 5 min at 0 °C and then warm to 55 °C and stir for 23 h. The reaction was quenched upon drop-wise addition of D_2O (0.8 mL, 48 mmol) at 0 °C and stir for additional 1 h at 22 °C. The mixture was transferred to a separatory funnel after which Rochelle's salt (30 ml) and a saturated solution of aqueous ammonium chloride (30 ml) were added to separate the layers. The aqueous layer was washed with Et_2O (3 x 20 mL). The combined organic layers were dried over Na_2SO_4 and concentrated. The resulting yellow oil was purified by silica gel chromatography (100% pentane) and Kugelrohr distillation to afford **22** as colorless liquid (4.0 g, 93%, >98% D). IR (neat): 2954 (w), 2897 (w), 1590 (w), 1569 (w), 1491 (w), 1247 (m), 1073 (w), 833 (s), 755 (s), 695 (s), 619 (m), 486 (m), 458 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): 7.40–7.21 (6H, m), 0.06 (9H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 146.6, 128.4, 128.3, 128.0, 127.9, 127.5, 0.3; HRMS (DART): Calcd for $C_{11}H_{15}DSi$ $[M+H]^+$: 177.1084; Found: 177.1097.

(*E*)-Trimethyl(2-phenylvinyl-1-*d*)silane (23): Prepared similarly to **22**, 100% hexanes was used instead of using 16.7% thf to afford **S7** (4.0 g, 93%, 96% D) as a colorless liquid. IR (neat): 3025 (w), 2954 (w), 1594 (w), 1570 (w), 1494 (w), 1297 (s), 1082 (m), 922 (w), 834 (s), 754 (s), 692 (s), 485 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): 7.47–7.41 (2H, m), 7.36–7.13 (3H, m), 6.89–6.85 (1H, m), 0.16 (9H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 143.7, 128.7, 128.4, 128.1, 127.9, 126.5, 125.6, –1.1, –1.6; HRMS (DART): Calcd for $C_{11}H_{15}DSi$ $[M+H]^+$: 177.1084; Found: 177.1092.

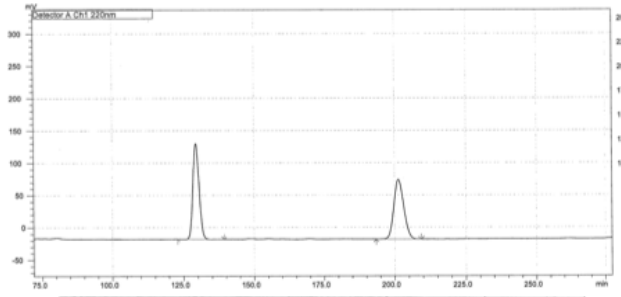
***trans*-Styrene-(β)-*d* (24):** To a solution of (*Z*)-trimethyl(2-phenylvinyl-1-*d*)silane (2.5 g, 14 mmol) in thf (15 mL) was added $(n\text{-Bu})_4NF$ (21 mL of 1M in thf) at 22 °C under N_2. The mixture was allowed to stir at 60 °C for 18 h, after which it was transferred to a separatory funnel. Water (25 mL) was added and the layers separated. The aqueous layer was washed with Et_2O (3 x 20 mL). The combined organic layers were dried over $MgSO_4$ and concentrated under house vacuum. The resulting yellow oil was purified by Kugelrohr distillation to afford the product (>98% *E*, >98% D) as colorless liquid. The spectroscopic data match those reported previously.[18] ^1H NMR ($CDCl_3$, 400 MHz): δ 7.45–7.23 (5H, m), 6.73 (1H, dt, *J* = 17.6, 1.6 Hz) 5.74 (1H, d, *J* = 17.6 Hz)

***cis*-Styrene-(β)-*d* (25):** This compound was prepared similarly to *trans*-Styrene-(β)-d, starting from (*E*)-trimethyl(2-phenylvinyl-1-*d*)silane (2.5 g, 14 mmol) and TBAF (56 mL of 1 M in thf) for 18 hours. The product was obtained as colorless liquid (96% *Z*, 95% D). The spectroscopic data match those reported previously.[21] ^1H NMR ($CDCl_3$, 400 MHz): δ 7.45–7.22 (5H, m), 6.72 (1H, dt, *J* = 10.9, 2.6 Hz), 5.23 (1H, d, *J* = 10.9 Hz)

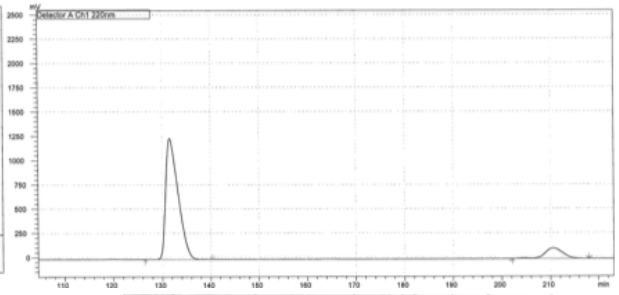
2-((1*R*,2*R*)-2,4-Diphenylpent-4-en-1-yl-1-*d*)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (*anti*-2n-*d*): Following the representative procedure except **L3b** and 6:1 alkene:phosphate used. IR (neat): 2923 (m), 2854 (w), 1453 (w), 1351 (m), 1314 (m), 1214 (w), 1143 (s), 969 (m), 896 (w), 777 (m), 734 (m), 698 (s), 547 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 600 MHz): δ 7.40–7.36 (2H, m), 7.33–7.29 (2H, m), 7.28–

(18) Kapeller, D., Barth, R., Mereiter, K. & Hammerschmidt, F. *J. Am. Chem. Soc.* **129**, 914–923 (2007).

7.19 (3H, m), 7.15–7.09 (3H, m), 5.15 (1H, d, *J* = 1.8 Hz), 4.83 (1H, *J* = 1.2 Hz), 2.95 (1H, q, *J* = 6.6 Hz), 2.87 (1H, dd, *J* = 13.2, 6 Hz), 2.73 (1H, dd, *J* = 12.6 7.8 Hz), 1.23 (1H, d, *J* = 6), 1.07 (6H, s), 1.05 (6H, s); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 146.9, 146.8, 141.2, 128.4, 128.1, 127.6, 127.4, 126.6, 125.9, 114.5, 83.0, 45.7, 39.9, 24.9, 24.7; HRMS (DART): Calcd for $C_{22}H_{27}DBO_2$ $[M+H]^+$: 336.2245; Found: 336.2241. Enantiomeric purity was determined by HPLC analysis of the alcohol product after oxidation in comparison with authentic racemic material (89:11 e.r. shown; Chiralcel OZ–H column, 99% hexanes, 1% *i*-PrOH, 0.3 mL/min, 220 nm).



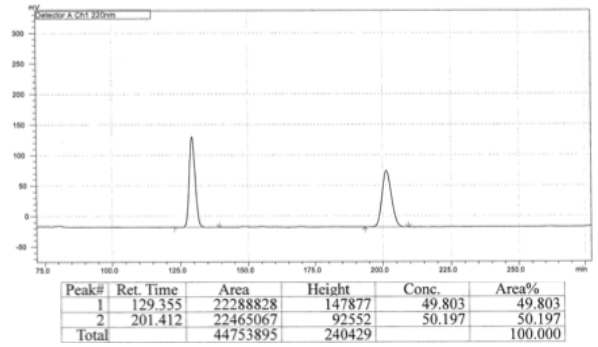
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	129.355	22288828	147877	49.803	49.803
2	201.412	22465067	92552	50.197	50.197
Total		44753895	240429		100.000



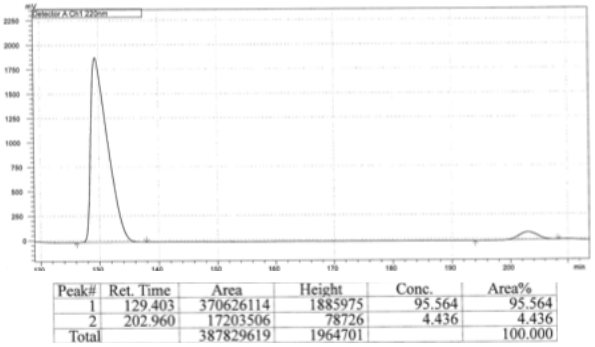
Peak#	Ret. Time	Area	Height	Conc.
1	131.578	221968013	1247086	88.668
2	210.567	28367150	110170	11.332
Total		250335164	1357256	

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	129.355	49.803	1	131.578	88.668
2	201.412	50.197	2	210.567	11.332

2-((1*S*,2*R*)-2,4-Diphenylpent-4-en-1-yl-1-*d*)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (*syn*-2n-*d*): Following the representative procedure except **L3b** and 6:1 alkene:phosphate used. IR (neat): 2977 (w), 2924 (m), 2854 (w), 1194 (w), 1389 (s), 1316 (s), 1142 (s), 1110 (w), 970 (m), 895 (m), 859 (m), 777 (m), 697 (s), 521 (w) cm^{-1}; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 7.42–7.35 (2H, m), 7.34–7.29 (2H, m), 7.28–7.19 (3H, m), 7.14–7.09 (3H, m), 5.15 (1H, d, *J* =1.2 Hz), 4.83 (1H, s), 2.96 (1H, q, *J* = 8.4 Hz), 2.87 (1H, dd, J = 13.8, 6 Hz), 2.73 (1H, dd, *J* = 13.2, 7.8 Hz), 1.11 (1H, d, *J* = 9 Hz), 1.08 (6H, s), 1.05 (6H, s); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 146.9, 146.8, 141.2, 128.4, 128.1, 127.6, 127.4, 126.7, 125.9, 114.5, 83.1, 45.6, 39.9, 24.9, 24.7; HRMS (DART): Calcd for $C_{22}H_{27}BO_2$ $[M+H]^+$: 336.2245; Found: 336.2245. Enantiomeric purity was determined by HPLC analysis of the alcohol product after oxidation in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OZ–H column, 99% hexanes, 1% *i*-PrOH, 0.3 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Conc.	Area%
1	129.355	22288828	147877	49.803	49.803
2	201.412	22465067	92552	50.197	50.197
Total		44753895	240429		100.000



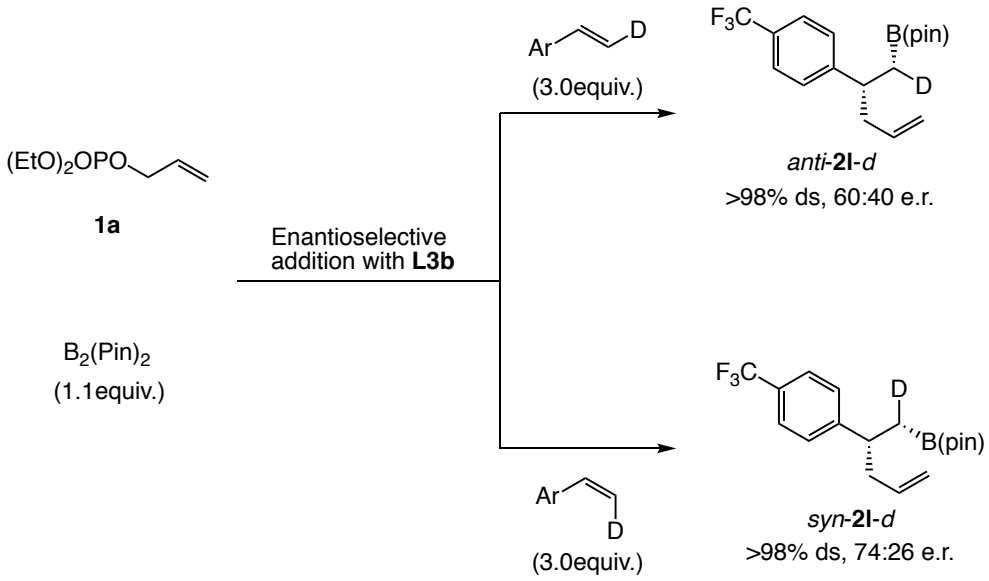
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	129.403	370626114	1885975	95.564	95.564
2	202.960	17203506	78726	4.436	4.436
Total		387829619	1964701		100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	129.355	49.803	1	129.403	95.564
2	201.412	50.197	2	202.960	4.436

(*E*)-1-(Trifluoromethyl)-4-(vinyl-2-*d*)benzene (substrate for synthesis of *anti*-2l-*d*): Following the procedure for preparation of **24** except 1-[(Trimethylsilyl)ethynyl]-4-(trifluoromethyl)benzene was used. The product was obtained in 91:9 *E*:*Z* selectivity. The spectroscopic data match those reported previously.[19] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (2H, d, *J* = 8.4 Hz), 7.50 (2H, d, *J* = 8.4 Hz), 6.75 (1H, d, *J* = 17.6 Hz), 5.83 (1H, d, *J* = 17.6 Hz).

(*Z*)-1-(Trifluoromethyl)-4-(vinyl-2-*d*)benzene (substrate for synthesis of *syn*-2l-*d*): Following the procedure for preparation of **25** except 1-[(Trimethylsilyl)ethynyl]-4-(trifluoromethyl)benzene was use. The product was obtained as a 90:10 ratio of *Z*:*E* isomers. IR (neat): 2954 (m), 2925 (m), 2854 (m), 1325 (s), 1168 (m), 1129 (m), 1068 (m) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (2H, d, *J* = 8.4 Hz), 7.48 (2H, d, *J* = 8.4 Hz), 6.72 (1H, dt, *J* = 11.2, 2.6 Hz), 5.36 (1H, d, *J* = 11.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.1, 135.7, 129.8 (q, *J* = 32.4 Hz), 126.5, 125.6, 124.3 (q, *J* = 270.2 Hz), 116.3 (t, *J* = 23.6 Hz); HRMS (EI): Calcd for $C_9H_7D_1F_3$ [M]$^+$: 173.0563, Found: 173.0560.

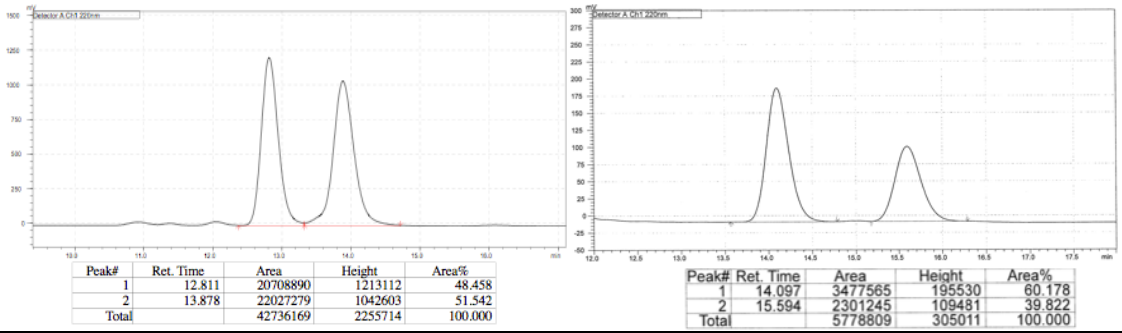
Scheme 6. Deuterated Alkenes Examination (for *p*-CF3 Styrene)



4,4,5,5-Tetramethyl-2-((1S,2R)-2-(4-(trifluoromethyl)phenyl)pent-4-en-1-yl-1-*d*)-1,3,2-dioxaborolane (*anti*-2l-*d*): Following the representative procedure except **L3b** used. IR (neat): 2979 (w), 2926 (w), 1359 (m), 1322 (s), 1162 (m), 1143 (m), 1120 (s), 1069 (m), 836 (m) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51 (2H, d, *J* = 8.0 Hz), 7.31 (2H, d, *J* = 8.4 Hz), 5.64 (1H, ddt, *J* = 17.0, 10.2, 7.0 Hz), 4.98–4.92 (2H, m), 3.00 (1H, q, *J* = 7.1 Hz), 2.36 (2H, t, *J* = 7.2 Hz), 1.22 (1H, d, *J* = 1.2 Hz), 1.10 (6H, s), 1.08 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.1, 136.5, 128.3 (q, *J* = 32.1 Hz), 127.9, 125.1 (q, *J* = 3.8 Hz), 124.5 (q, *J* = 270.4 Hz), 116.7, 83.3, 43.5, 41.4, 24.8, 24.7; HRMS (DART):

(19) Gao, F. & Hoveyda, A. H. *J. Am. Chem. Soc.* **132**, 10961–10963 (2010).

Calcd for $C_{18}H_{24}D_1B_1F_3O_2$ [M+H]$^+$: 342.1963, Found: 342.1961. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (60:40 e.r. shown; Chiralcel OZ–H column, 100% hexanes, 0.3 mL/min, 220 nm).

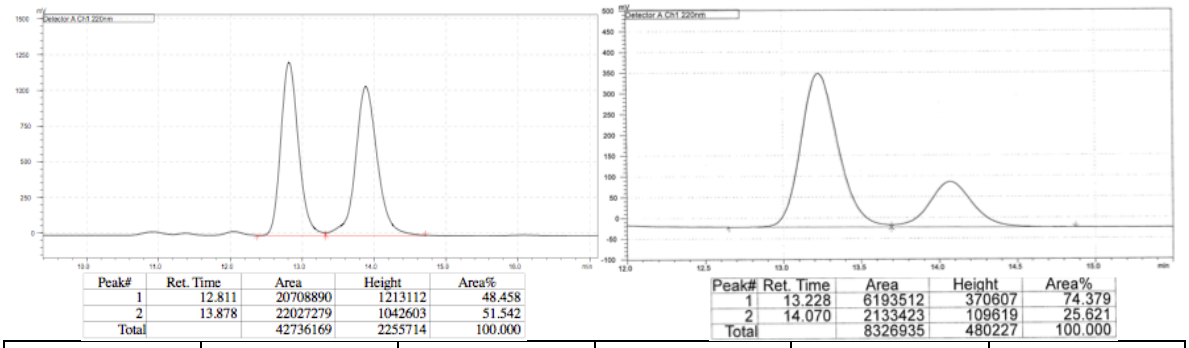


Peak#	Ret. Time	Area	Height	Area%
1	12.811	20708890	1213112	48.458
2	13.878	22027279	1042603	51.542
Total		42736169	2255714	100.000

Peak#	Ret. Time	Area	Height	Area%
1	14.097	3477565	195530	60.178
2	15.594	2301245	109481	39.822
Total		5778809	305011	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	12.811	48.458	1	14.097	60.178
2	13.878	51.542	2	15.594	39.822

4,4,5,5-Tetramethyl-2-((1R,2R)-2-(4-(trifluoromethyl)phenyl)pent-4-en-1-yl-1-d)-1,3,2-dioxaborolane (*syn*-2l-*d*): Following the representative procedure except **L3b** used. IR (neat): 2979 (w), 2926 (w), 1359 (m), 1322 (s), 1162 (m), 1143 (m), 1120 (s), 1069 (m), 836 (m) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51 (2H, d, *J* = 8.4 Hz), 7.31 (2H, d, *J* = 8.4 Hz), 5.64 (1H, ddt, *J* = 17.2, 10.4, 6.8 Hz), 4.98–4.91 (2H, m), 3.00 (1H, q, *J* = 7.9 Hz), 2.36 (2H, t, *J* = 7.2 Hz), 1.10 (6H, s), 1.09 (6H, s), 1.10–1.09 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.1, 136.5, 128.3 (q, *J* = 32.1 Hz), 127.9, 125.1 (q, *J* = 3.8 Hz), 124.5 (q, *J* = 270.2 Hz), 116.7, 83.3, 43.5, 41.4, 24.8, 24.7; HRMS (DART): Calcd for $C_{18}H_{24}D_1B_1F_3O_2$ [M+H]$^+$: 342.1963, Found: 342.1961. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (74:26 e.r. shown; Chiralcel OZ–H column, 100% hexanes, 0.3 mL/min, 220 nm).



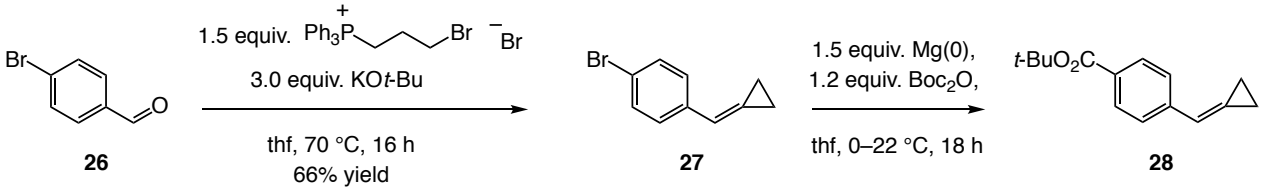
Peak#	Ret. Time	Area	Height	Area%
1	12.811	20708890	1213112	48.458
2	13.878	22027279	1042603	51.542
Total		42736169	2255714	100.000

Peak#	Ret. Time	Area	Height	Area%
1	13.228	6193512	370607	74.379
2	14.070	2133423	109619	25.621
Total		8326935	480227	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	12.811	48.458	1	13.228	74.379
2	13.878	51.542	2	14.070	25.621

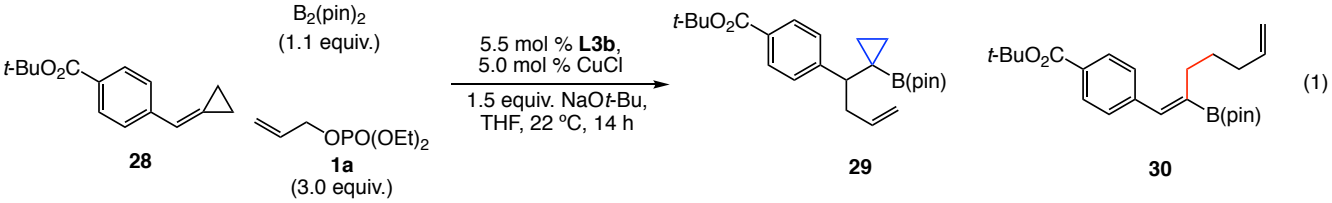
10. Study of the Possibility of Homolytic versus Heterolytic Cu–C Bond Cleavage

Scheme 7. Synthesis of Cyclopropane **28**



1-Bromo-4-(cyclopropylidenemethyl)benzene (27): Prepared from aldehyde **26** (purchased from Aldrich and used as received) by formerly reported procedure.[20] The spectroscopic data match those reported previously.[21] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46–7.42 (2H, m), 7.40–7.38 (2H, m), 6.70–6.68 (1H, m), 1.42–1.38 (2H, m), 1.20–1.16 (2H, m).

***tert*-Butyl-4-(cyclopropylidenemethyl)benzoate (28):** Prepared from **27** according to the reported procedure.[10] IR (neat): 2977 (w), 1706 (s), 1606 (m), 1367 (m), 1307 (s), 1292 (s), 1254 (m), 1161 (s), 1107 (s), 1015 (m), 863 (m), 849 (m), 757 (m) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (2H, d, J = 8.4 Hz), 7.55 (2H, d, J = 8.4 Hz), 6.79–6.78 (1H, m), 1.61 (9H, s), 1.48–1.42 (2H, m), 1.22–1.18 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.8, 142.3, 130.1, 129.7, 127.6, 126.3, 117.9, 80.8, 28.3, 4.5, 0.8; HRMS (DART): Calcd for $C_{15}H_{19}O_2$ [M+H]$^+$: 231.1391, Found: 231.1385.



>98% conv, 35% **29**; <2% **30**

***tert*-Butyl-(*S*)-4-(1-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cyclopropyl)but-3-en-1-yl)benzoate (29):** IR (neat): 2976 (w), 2932 (m), 1710 (s), 1640 (w), 1440 (m), 1409 (m), 1290 (s), 1164 (s), 1140 (s), 1113 (s), 851 (s), 708 (m), 685 (m), 420 (w) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (2H, d, J = 8), 7.38 (2H, d, J =8), 5.69 (1H, ddt, J = 17.2, 9.6, 7.2), 5.00–4.95 (1H, m), 4.89–4.85 (1H, m), 2.75–2.71 (2H, m), 1.20 (1H, t, J =7.8), 1.58 (9H, s), 1.20 (12H, s), 0.74 (1H, ddd, J = 9.2, 5.6, 3.2), 0.66 (1H, ddd, J = 8, 4.8, 2.8), 0.41 (1H, ddd, J =8.4, 5.2, 3.2), 0.35 (1H, ddd, J = 8.4, 5.2, 3.2); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.1, 150.3, 138.1, 129.8, 129.2, 128.5, 115.5, 83.1, 80.7, 53.4, 38.8, 28.4, 25.0, 24.5, 14.1, 10.2; HRMS (DART): Calcd for $C_{24}H_{36}BO_4$ [M+H]$^+$: 399.2707, Found: 399.2723. Enantiomeric purity was determined by HPLC analysis of the alcohol product after oxidation in comparison with authentic racemic material (54:46 e.r. shown; Chiralcel OZ–H column, 99% hexanes, 1% *i*-PrOH, 0.3 mL/min, 220 nm).

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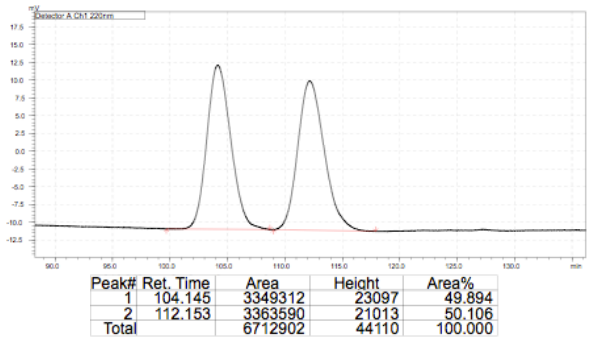
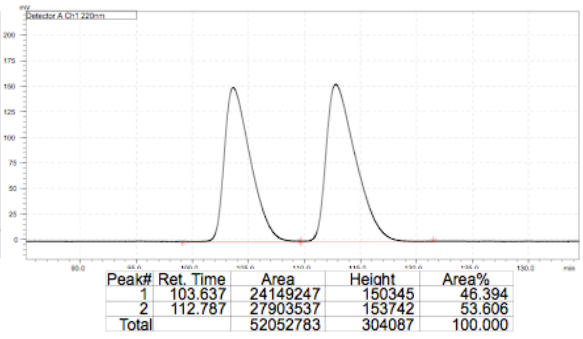
(20) Evans, P. A., Inglesby, P. A. & Kilbride, K. *Org. Lett.* **15**, 1798–1801 (2013).

(21) Katritzky, A. R., Du, W., Levell, J. R. & Li, J. *J. Org. Chem.* **63**, 6710–6711 (1998).



Peak#	Ret. Time	Area	Height	Area%
1	104.145	3349312	23097	49.894
2	112.153	3363590	21013	50.106
Total		6712902	44110	100.000

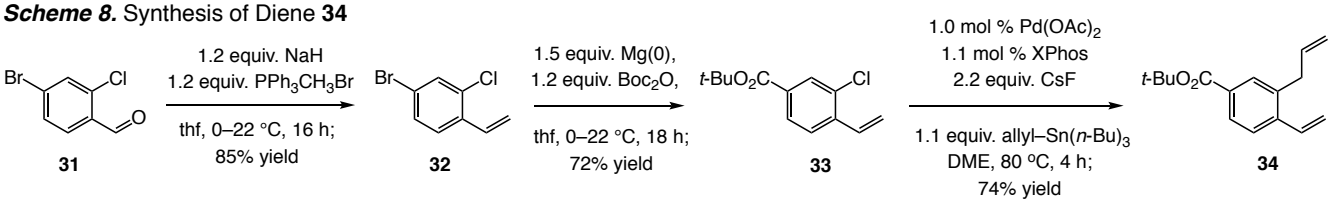


Peak#	Ret. Time	Area	Height	Area%
1	103.637	24149247	150345	46.394
2	112.787	27903537	153742	53.606
Total		52052783	304087	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	104.145	49.894	1	103.637	46.394
2	112.153	50.106	2	112.787	53.606

Additional support for cleavage/re-formation of the Cu–C bond is likely to be heterolytic in nature is that with diene **31** as the substrate, cyclopentenyl product **33** was not detected (Eq. 1).

Scheme 8. Synthesis of Diene **34**



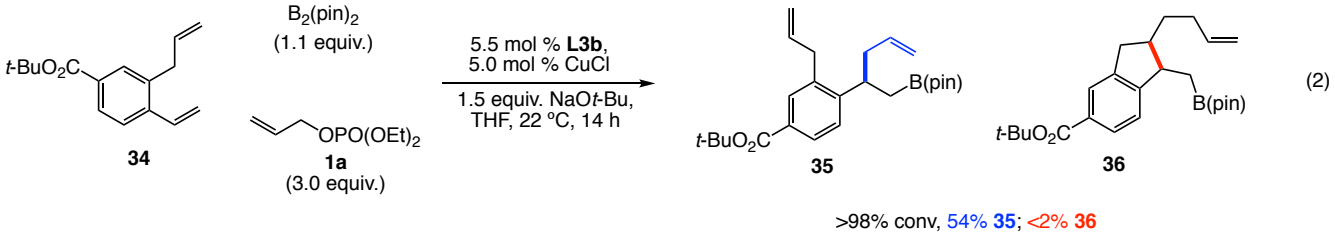
4-Bromo-2-chloro-1-vinylbenzene (32): Prepared from aldehyde **31** (purchased from Combi-Blocks and used as received) following the previously reported procedure.[6] IR (neat): 3089 (w), 3060 (w), 1579 (m), 1467 (s), 1371 (m), 1085 (m), 1049 (m), 985 (m), 917 (s), 867 (m), 812 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.53 (1H, s), 7.42 (1H, d, *J* = 8.4 Hz), 7.36 (1H, dd, *J* = 8.4, 1.6 Hz), 7.02 (1H, dd, *J* = 17.4, 11.0 Hz), 5.74 (1H, d, *J* = 17.2 Hz), 5.41 (1H, d, *J* = 10.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.9, 133.9, 132.4, 132.3, 130.2, 127.7, 121.7, 117.3; HRMS (DART): Calcd for $C_8H_7Br_1Cl_1$ $[M+H]^+$: 216.9420, Found: 216.9427.

***tert*-Butyl-3-chloro-4-vinylbenzoate (33):** Prepared from **32** according to the reported procedure.[10] IR (neat): 2978 (w), 2933 (w), 1716 (s), 1392 (m), 1368 (m), 1298 (s), 1258 (m), 1168 (s), 1118 (s), 773 (m), 849 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.95 (1H, d, *J* = 1.6 Hz), 7.83 (1H, dd, *J* = 8.5, 2.1 Hz), 7.59 (1H, d, *J* = 8.0 Hz), 7.11 (1H, dd, *J* = 17.6, 10.8 Hz), 5.82 (1H, dd, *J* = 17.4, 0.6 Hz), 5.48 (1H, dd, *J* = 11.0, 1.0 Hz), 1.59 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.5, 139.5, 133.1, 132.7, 132.5, 130.8, 127.8, 126.3, 118.6, 81.7, 28.3; HRMS (DART): Calcd for $C_{13}H_{16}Cl_1O_2$ $[M+H]^+$: 239.0839,

***tert*-Butyl-3-allyl-4-vinylbenzoate (34):** Prepared from **33** according to the reported procedure.[22] IR (neat): 2977 (w), 2931 (w), 1709 (s), 1367 (m), 1293 (s), 1253 (s), 1163 (s), 1118 (s), 989 (m), 914 (s), 849 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.82 (1H, dd, *J* = 7.8, 1.4 Hz), 7.78 (1H, d, *J* = 1.6 Hz), 7.53 (1H, d, *J* = 8.4 Hz), 6.97 (1H, dd, *J* = 17.2, 11.2 Hz), 6.01–5.91 (1H, m), 5.73 (1H, dd, *J* = 17.4, 1.4 Hz), 5.39 (1H, dd, *J* = 11.2, 1.2 Hz), 5.10–5.06 (1H, m), 5.00–4.94 (1H, m), 3.48 (2H, dt, J = 6.4, 1.6 Hz), 1.59 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.8, 140.9, 137.1, 136.4, 134.1, 131.4, 131.0,

(22) Naber, J. R. & Buchwald, S. L. *Adv. Synth. Catal.* **350**, 957–961 (2008).

127.8, 125.7, 117.5, 116.4, 81.0, 37.5, 28.3; HRMS (DART): Calcd for $C_{16}H_{21}O_2$ [M+H]$^+$: 244.1463, Found: 244.1471.

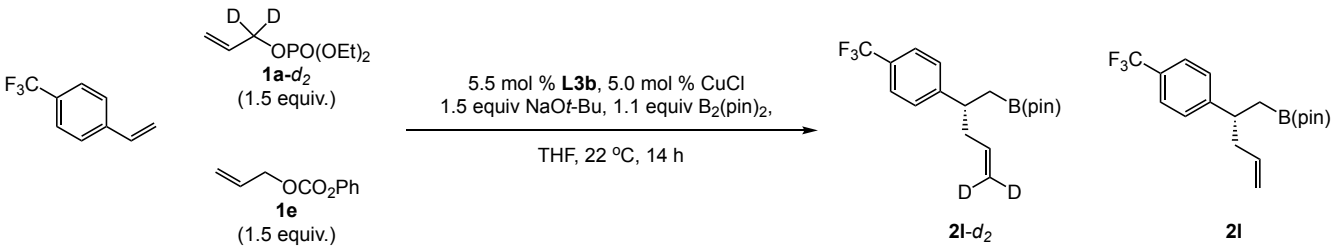


>98% conv, 54% **35**; <2% **36**

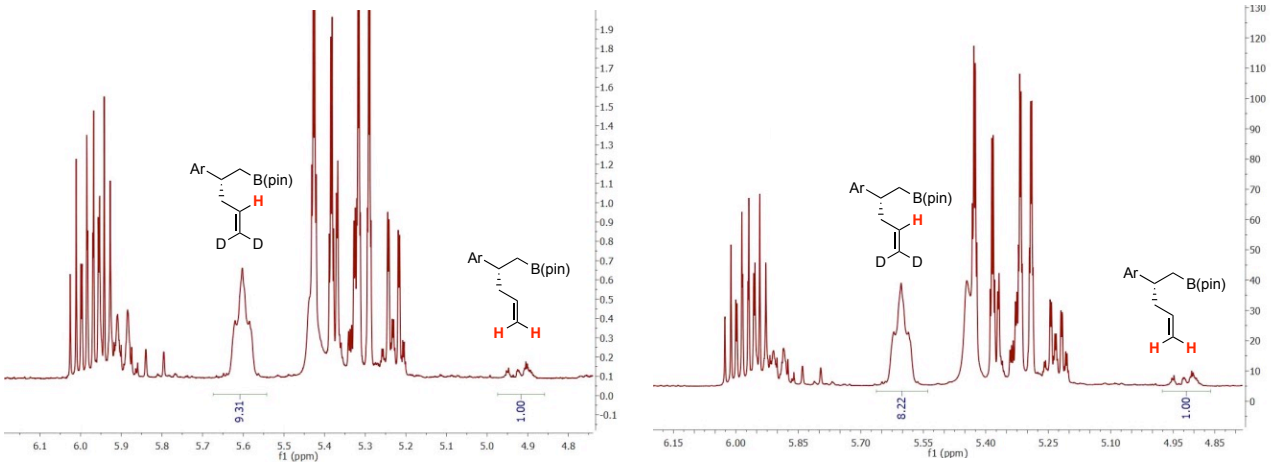
***tert*-Butyl-(*R*)-3-allyl-4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl)benzoate (35):** IR (neat): 2977 (w), 2930 (w), 1711 (s), 1367 (s), 1298 (s), 1253 (m), 1166 (s), 1143 (s), 1121 (m), 912 (m), 849 (m) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (1H, dd, *J* = 8.0, 2.0 Hz), 7.75 (1H, d, *J* = 2.0 Hz), 7.27 (1H, d, *J* = 7.6 Hz), 6.00 (1H, ddt, *J* = 17.0, 10.2, 6.2 Hz), 5.70–5.60 (1H, m), 5.09–5.02 (2H, m),), 4.99–4.91 (2H, m), 3.59–3.45 (2H, m), 3.32–3.24 (1H, m), 2.36–2.23 (2H, m), 1.58 (9H, s), 1.26–1.21 (1H, m), 1.08 (6H, s), 1.05 (6H, s), 1.12–1.05 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.2, 150.3, 137.6, 137.3, 136.8, 130.6, 129.5, 127.6, 126.4, 116.6, 116.1, 83.2, 80.7, 43.5, 37.4, 35.6, 28.4, 24.8, 24.77; HRMS (DART): Calcd for $C_{25}H_{38}B_1O_4$ [M+H]$^+$: 413.2863, Found: 413.2858.

11. Relative Reactivity of Allylphosphate and Allylphenyl Carbonate

In an N_2-filled glove box, an oven-dried 1-dram vial equipped with a stir bar was charged with bisphosphine **L3b** (3.7 mg, 0.0055 mmol), NaO*t*-Bu (14 mg, 0.15 mmol), and CuCl (0.50 mg, 0.0050 mmol), and THF was added (1.0 mL). The resulting solution was allowed to stir for one h under N_2 at 22 °C, during which the solution turned light yellow. Bis(pinacolato)diboron (28 mg, 0.11 mmol) was added to the mixture, which immediately caused the solution to turn dark brown. At this time the mixture was charged with *para*-trifluoromethyl styrene (14.8 μL, 0.10 mmol) followed by a solution containing labeled allylphosphate (**1a**-d_2; 29.4 mg, 0.15 mmol), allylphenyl carbonate (**1e**; 26.7 mg, 0.15 mmol), and THF (0.50 mL). The vial was sealed with a cap and electrical tape before removal from the glove box, and the mixture was allowed to stir at 22 °C for 14 h, after which it was passed through a plug of silica gel (4 x 1 cm) and eluted with Et_2O. The volatiles were removed *in vacuo* to afford yellow oil, which was dissolved in $CDCl_3$ for NMR analysis. Integration of the NMR signals provided the ratio of **2l** and **2l**-d_2, which was calculated as an average of two runs.

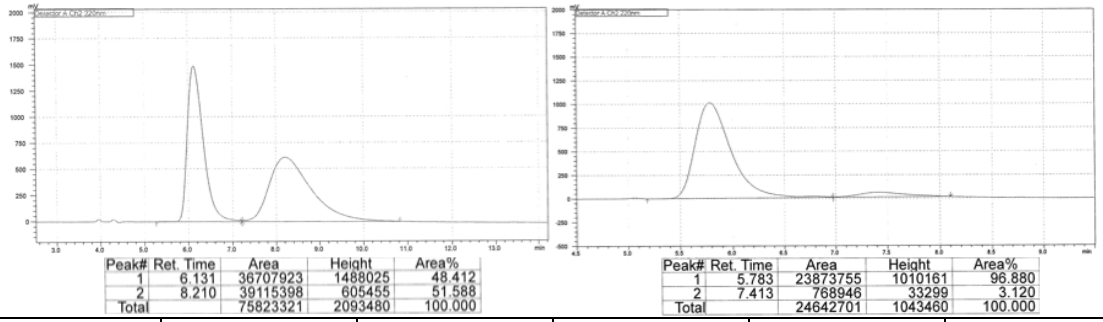


Conclusion: Allylphosphate is a considerably more effective electrophile compared to allylphenyl carbonate.



12. Relevance to Catalytic Processes that Involve Cu–H Additions

(*S*)-*N*,*N*-dibenzyl-1,2,3,4-tetrahydronaphthalen-1-amine (11): Following the previously reported procedure except 1:3 alkene:hydroxylamine was used. The spectroscopic data are consistent with those reported formerly.[23] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07 (1H, dt, *J* = 7.8, 1.2 Hz), 7.53 (4H, d, *J* = 7.3 Hz), 7.38 (4H, dd, *J* = 8.2, 6.9 Hz), 7.32–7.22 (3H, m), 7.17 (1H, tt, *J* = 7.3, 1.1 Hz), 7.09 (1H, d, *J* = 7.9 Hz), 4.00 (1H, dd, *J* = 10.2, 5.7 Hz), 3.87 (2H, d, *J* = 13.6 Hz), 3.54 (2H, d, *J* = 13.6 Hz), 2.91–2.66 (2H, m), 2.32–2.14 (1H, m), 2.06 (1H, dtt, *J* = 13.7, 5.6, 3.1 Hz), 1.85 (1H, tdd, *J* = 12.5, 10.1, 2.8 Hz), 1.76–1.58 (1H, m); Specific Rotation: $[\alpha]_D^{20}$ –62.0 (*c* 1.00, $CHCl_3$) for an enantiomerically enriched sample of 97:3 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (97:3 e.r. shown; Chiralcel OJ–H column, 97% hexanes, 3% *i*-PrOH, 0.8 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area%
1	6.131	36707923	1488025	48.412
2	8.210	39115398	605455	51.588
Total		75823321	2093480	100.000

Peak#	Ret. Time	Area	Height	Area%
1	5.783	23873755	1010161	96.880
2	7.413	768946	33299	3.120
Total		24642701	1043460	100.000

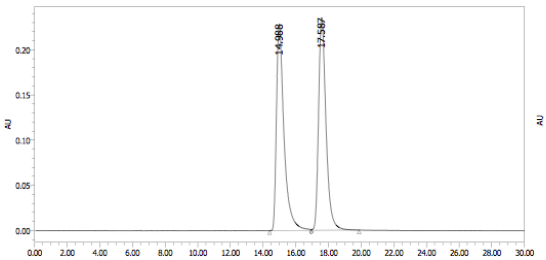
Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	6.131	48.412	1	5.783	96.880
2	8.210	51.588	2	7.413	3.120

***(R)*-2-(1-(3,4-Dihydroisoquinolin-2(1H)-yl)octyl)-2,3-dihydro-1H-naphtho[1,8-de][1,3,2]diazaborinine (12):** Following the previously reported procedure except 40 mol % of **8c** was used. The spectroscopic data match those reported previously.[24] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.10–7.01 (7H, m), 6.88 (1H, d, *J* = 6.8 Hz), 6.00 (2H, dd, 6.8, 1.6 Hz), 5.66 (2H, bs), 3.81 (1H, d, *J* = 14.8

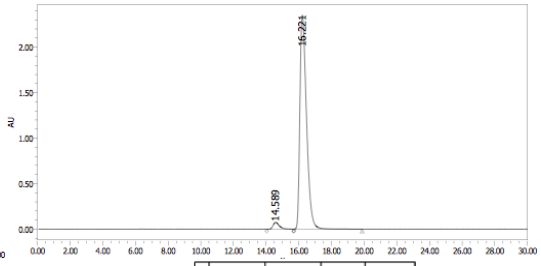
(23) Zhu, S., Niljianskul, N. & Buchwald, S. L. *J. Am. Chem. Soc.* **135**, 15746–15749 (2013).

(24) Nishikawa, D., Hirano, K. & Miura, M. *J. Am. Chem. Soc.* **137**, 15620–15623 (2015).

Hz), 3.55 (1H, d, *J* = 14.8 Hz), 2.86–2.79 (1H, m), 2.73–2.55 (3H, m), 1.78 (1H, dd, *J* = 9.2, 4.4 Hz), 1.71–1.64 (1H, m), 1.59–1.50 (1H, m), 1.46–1.37 (1H, m), 1.33–1.24 (9H, m), 0.89 (3H, t, *J* = 6.8 Hz); Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (97:3 e.r. shown; Chiralcel OD–H column, 95% hexanes, 5% *i*-PrOH, 0.5 mL/min, 330 nm).



	保持時間 (分)	面積 (μV秒)	%面積	高さ (μV)
1	14.988	7375266	49.72	228425
2	17.587	7458781	50.28	235465

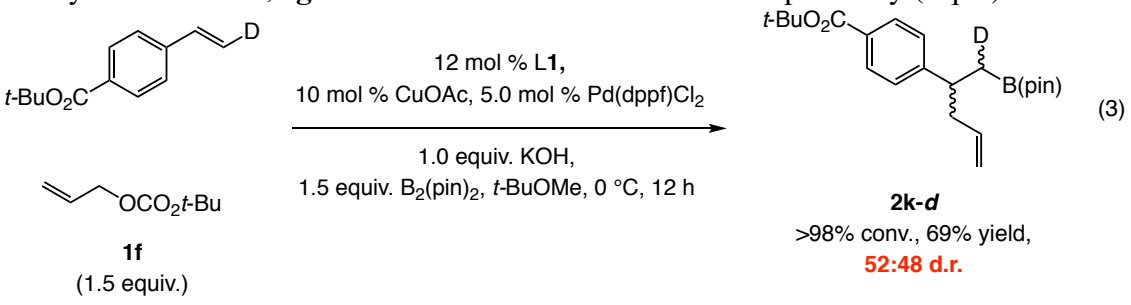


	保持時間 (分)	面積 (μV秒)	%面積	高さ (μV)
1	14.589	2038125	2.99	75250
2	16.221	66191474	97.01	2351533

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	14.988	49.72	1	14.589	2.99
2	17.587	50.28	2	16.221	97.01

13. Studies Regarding the Two-Catalyst (Cu/Pd) Approach

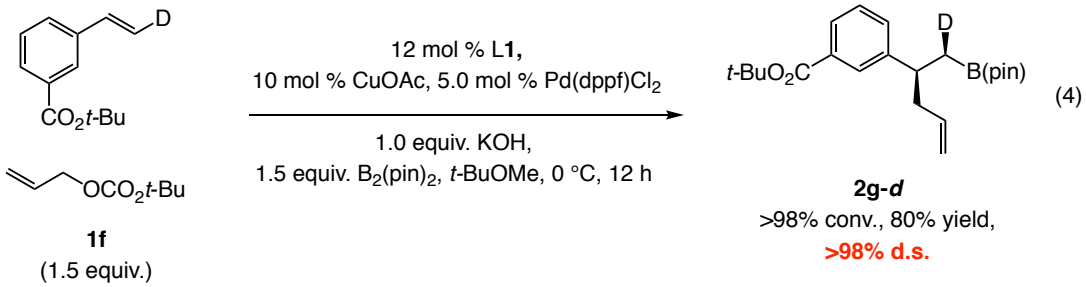
In the case of the two-catalyst (Pd/Cu) system, there is complete epimerization when the *para-tert*-butylester-substituted styrene is used as the substrate (Eq. 3). In contrast, when *meta-tert*-butylester-substituted styrene was used, **2g-d** was formed with >98% diastereospecificity (Eq. 4).



1f
(1.5 equiv.)

2k-*d*
>98% conv., 69% yield,
52:48 d.r.

(3)



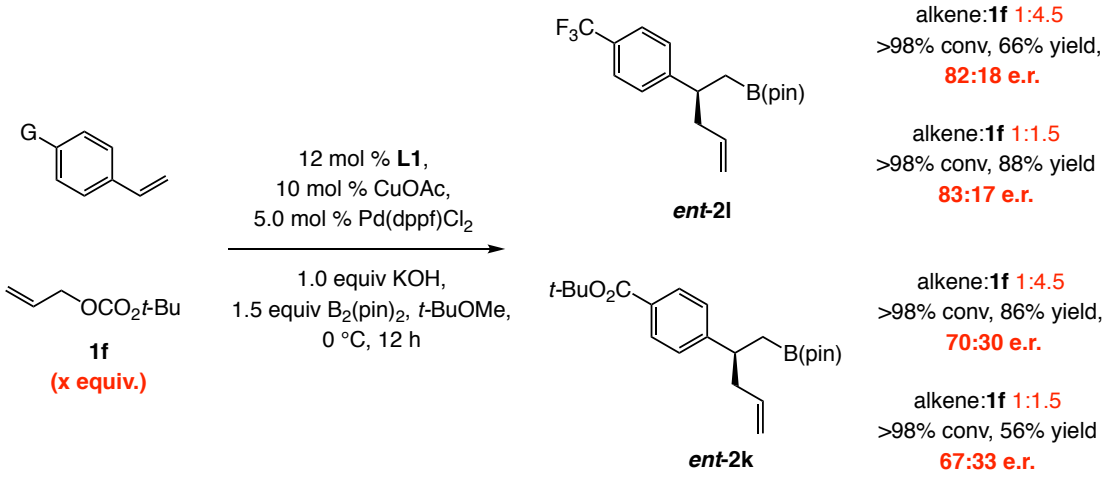
1f
(1.5 equiv.)

2g-*d*
>98% conv., 80% yield,
>98% d.s.

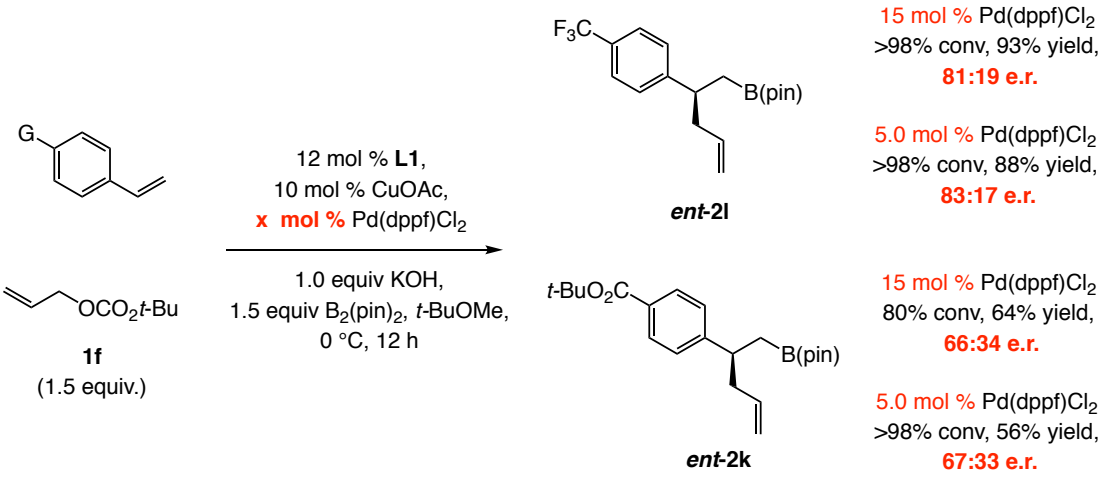
(4)

Moreover, increased amounts of allylcarbonate **1f** or Pd complex concentration (two-catalyst approach) does not improve e.r. (Scheme 9–10).

Scheme 9. Influence of Variations in Allylcarbonate Concentration on Enantioselectivity in the Two-Catalyst (Cu/Pd) System



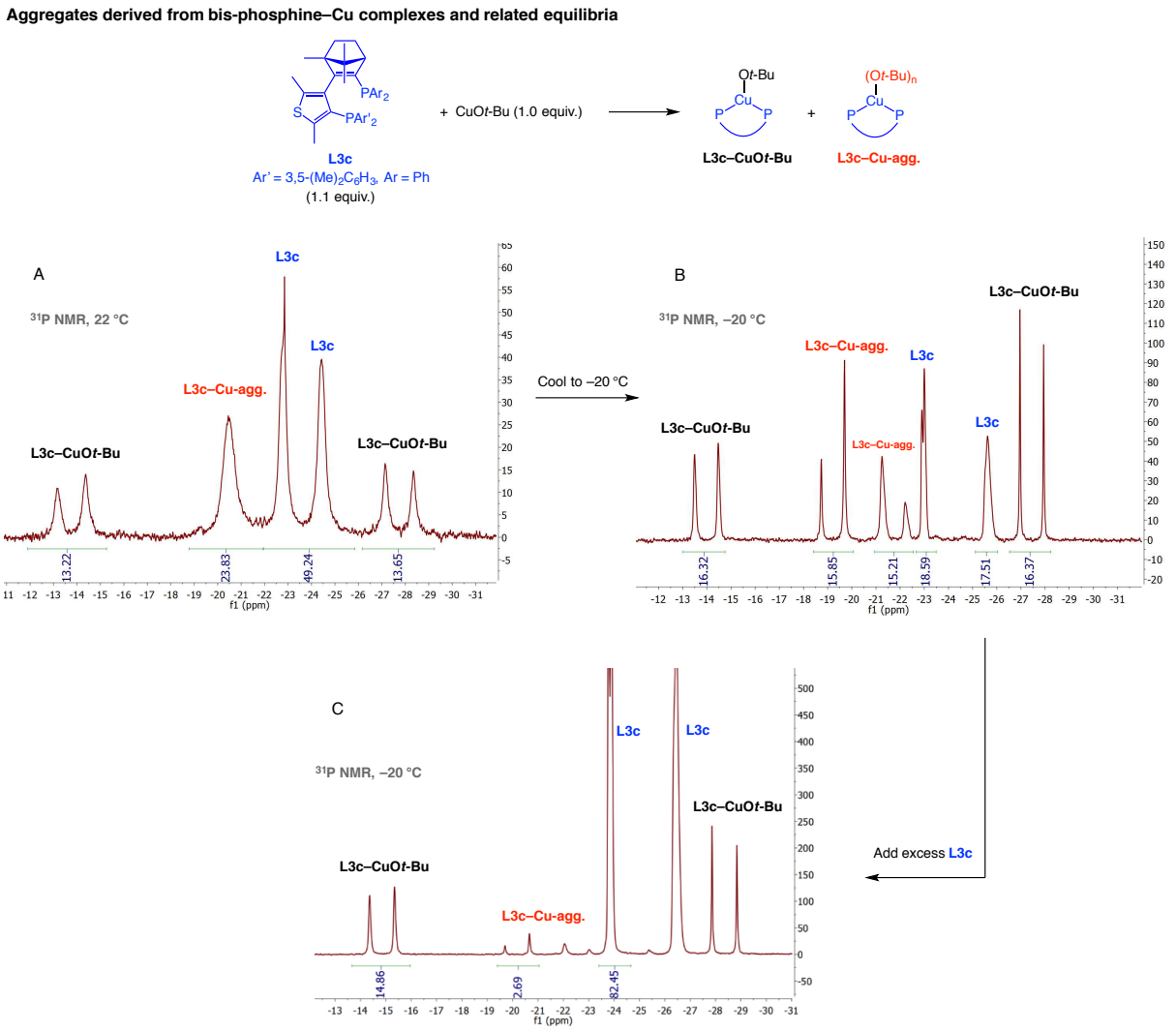
Scheme 10. Influence of Increased Loading of the Pd-based Co-Catalyst on Enantioselectivity in the Two-Catalyst (Cu/Pd) System



14. Spectroscopic Studies of Bis-Phosphine–Cu Complexes

Spectroscopic Detection of the Key Intermediates in the Catalytic Cycle

Detection of a chiral bis-phosphine–Cu complex and the corresponding aggregate structures. In an N_2-filled glove box, an oven-dried 2-dram vial was charged with CuO*t*-Bu (2.8 mg, 0.0203 mmol), bis-phosphine **L3c** (15 mg, 0.0224 mmol) and thf-d_8 (0.3 mL). The mixture was manually stirred leading to formation of a homogeneous light-green solution and was then transferred to an NMR tube after which the original vial was washed with 0.2 mL of thf-d_8. The tube was capped with a septum and sealed with paraffin before being removed from glove box.



The ^{31}P spectrum (A) was first acquired at 22 °C; there was ~30% un-coordinated bis-phosphine ligand. At –20 °C (spectrum B) peaks were generally sharper, suggesting that there is equilibrium among various complexes. Variations in temperature and concentration of **L3c** led to only slight changes in the chemical shift of the free ligand (as judged by the coupling constant values): whereas the $J_{P\text{-}P}$ **L3c** is 21.8 Hz, it is 110-190 Hz for the derived Cu complex the same coupling constant (depending on extent of complexation).

Conclusion: The increase in concentration of bis-phosphine–Cu complex (less unbound CuO*t*-Bu) due to excess **L3c** is consistent with the fact that there was considerable increase in e.r. when excess ligand was used even with unoptimal alkene:electrophile ratio (Fig. 4c, manuscript).

Addition of styrene, *para*-trifluoromethylstyrene or pentafluorostyrene (20 equiv.) did not result in a detectable change on the concentration of any of the organocopper species.

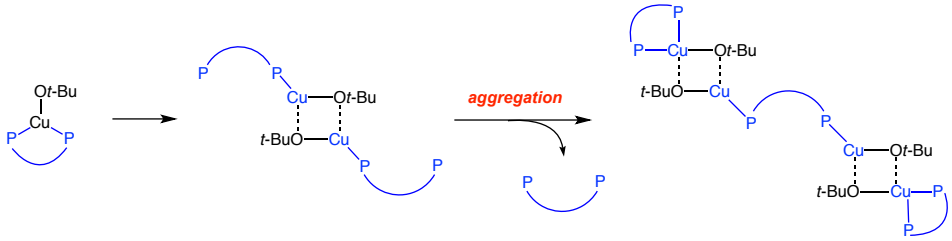
Conclusion: An alkene does not compete with the bis-phosphine ligand for copper coordination.

When excess **L3c** were added (60 mg, 0.112 mmol; spectrum C), the amount of bis-phosphine–Cu complex increased (i.e., from ~1:1 to ~5.5 **L3c-CuO*t*-Bu:L3c-Cu-agg.**).

Conclusion: L3c-Cu-agg. contains more than one Cu atom (dimer or larger aggregate) and may be converted to monomeric species by introducing more ligand. A similar observation has been reported involving $[CuO\textit{t}\text{-}Bu(PPh_3)]_2$.[25]

Bis-phosphine–CuOt-Bu complexes undergo ligand dissociation. Metal–oxygen bonds in alkoxide complexes are largely ionic. The polarity of the metal–oxygen bond is usually attenuated through π-donation by the oxygen atom into the metal d-orbitals in early transition metal systems. With late-transition metals, the ability of alkoxide ligands to serve as a σ- and π-donor systems is negligible. In the case of Cu(I) complexes (d^{10}), alkoxide and hydroxide ligands for the most part serve as σ-donors. Thus, the oxygen atoms retain considerable Lewis basicity, which can lead to the formation of oligomeric species by alkoxo bridging[25]. The large size of bis-phosphine ligand **L3c** and the *tert*-butoxide moiety translates into accelerated oligomer formation, a process that is driven by a decrease in steric pressure (Scheme 11).

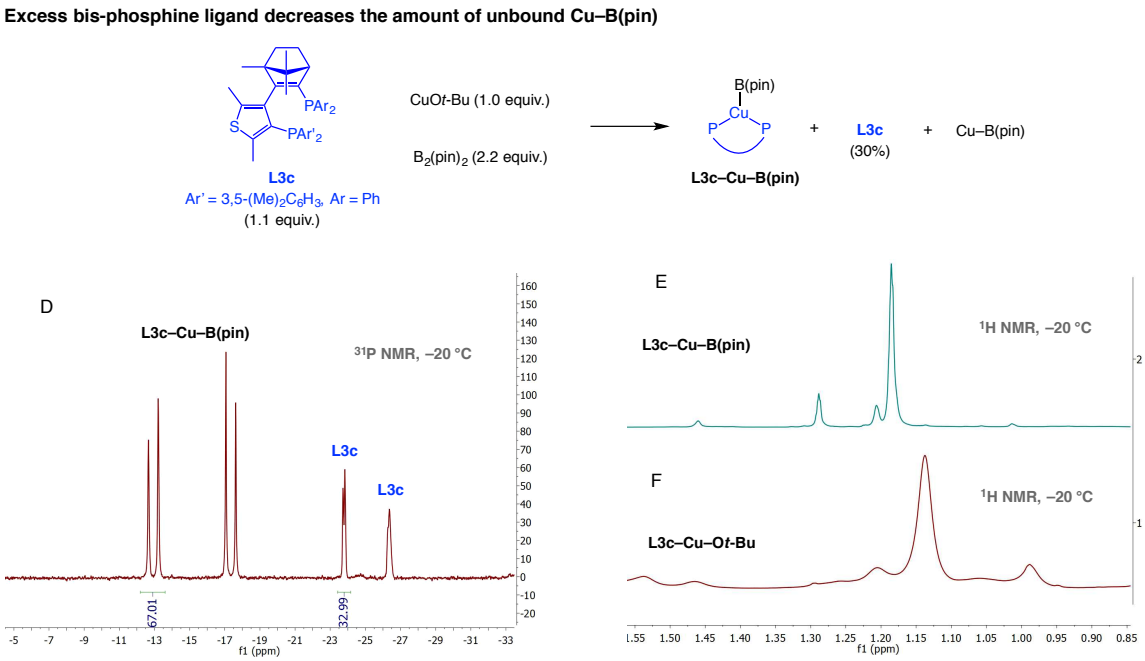
Scheme 11. Alkoxide Bridging Leads to Aggregation and Reduced Stereic Strain



Detection of bis-phosphine–Cu–B(pin) complex at –20 °C. In a N_2-filled glove box, a solution of $CuO\textit{t}\text{-}Bu$ (2.8 mg, 0.0203 mmol), **L3c** (15 mg, 0.0224 mmol), and $PhCH_2Ph$ (internal standard; 4.0 μL, 0.0233 mmol) in thf-d_8 (0.3 mL) was prepared in a two-dram vial. The mixture was manually stirred upon formation of a homogeneous light-green solution and then transferred to an NMR tube, after which the vial was washed with additional 0.2 mL of thf-d_8. The tube was capped with a septum and sealed with paraffin before being removed from glove box. The tube was then placed in a dry ice/acetone bath. A solution of bis(pinacolato)diboron (11.4 mg, 0.0449 mmol) was prepared in 0.2 mL of thf-d_8 in a separate vial and transferred by syringe to the solution in the NMR tube and stirred manually without removing the cooling bath to ensure minimal reaction occurring before being placed in the spectrometer. The spectrum was acquired at –20 ºC in a precooled spectrometer.

Resonances corresponding to bis-phosphine-Cu–Bpin and free **L3c** (30%) were detected by ^{31}P NMR spectroscopy (spectrum D). Complete disappearance of the initial signals assigned to L-$CuO\textit{t}\text{-}Bu$ was observed by ^{1}H NMR spectroscopy (spectrum E after the addition of B_2pin_2 solution, and spectrum F before the addition of B_2pin_2 solution).

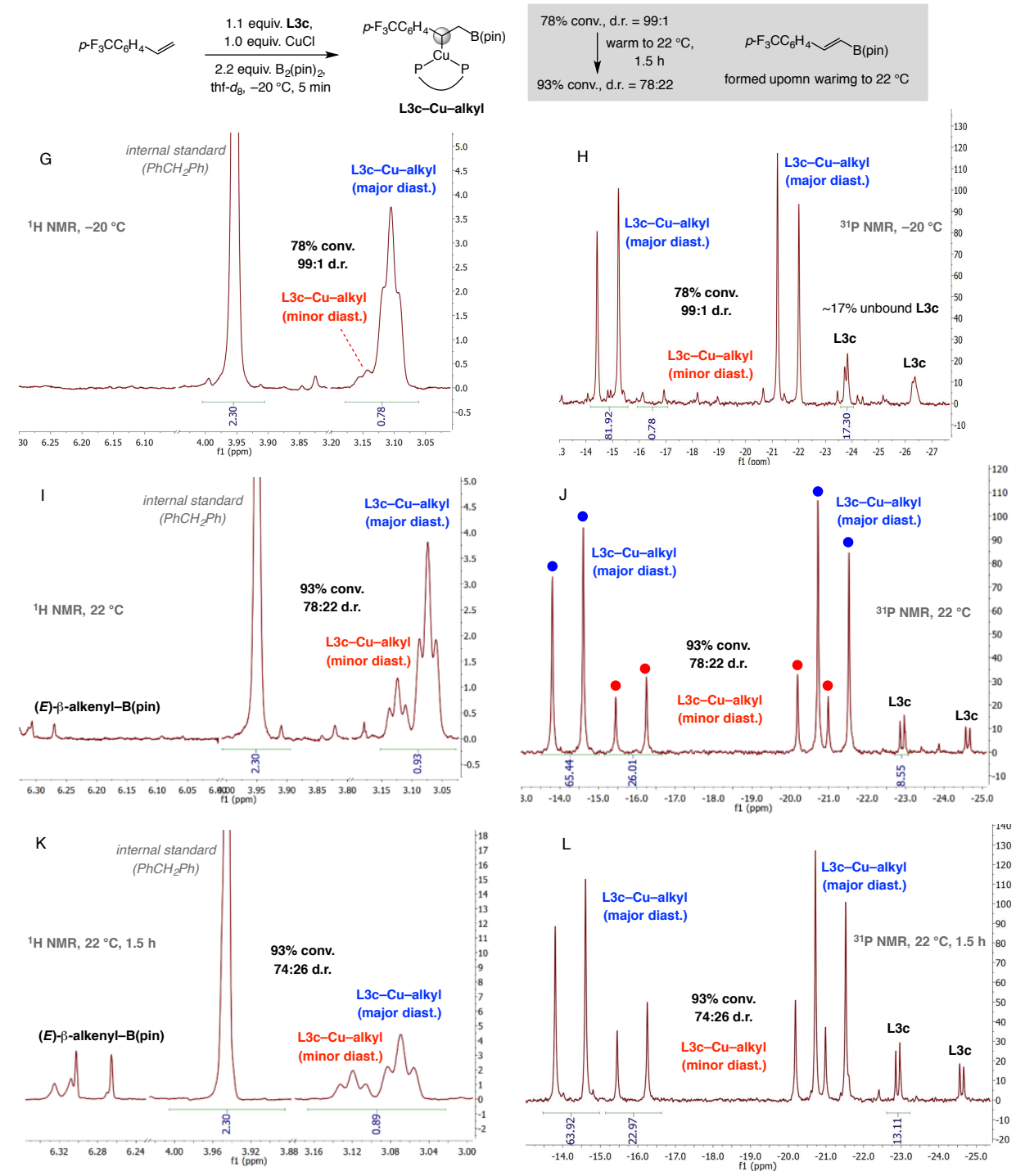
(25) Lemmen, T. H., Goeden, G. V., Huffman, J. C., Geerts, R. L. & Caulton, K. G. *Inorg. Chem.* **29**, 3680–3685 (1990).



Detection of alkyl–Cu diastereomers and evidence for Cu–H elimination. In an N_2-filled glove box, a solution of CuO*t*-Bu (2.8 mg, 0.0203 mmol), bis-phosphine **9c** (15 mg, 0.0224 mmol), *para*-trifluoromethylstyrene (5.0 μL, 0.0314 mmol) and $PhCH_2Ph$ (internal standard; 4.0 μL, 0.0233 mmol) in thf-d_8 (0.3 mL) were placed in a two-dram vial. The mixture was manually stirred upon formation of a homogeneous light-green solution and then transferred to an NMR tube, after which the vial was washed with additional 0.2 mL of thf-d_8. The tube was capped with a septum and sealed with paraffin before removal from glove box and placed into a dry ice/acetone bath. A solution of $B_2(pin)_2$ (11.4 mg, 0.0449 mmol) dissolved in 0.2 mL of thf-d_8 was at this time added and the resulting mixture was shaken/stirred manually without removing the cooling bath to minimize reaction occurring prior to positioning the tube in the spectrometer. The spectrum was then acquired at –20 °C.

As shown in spectra G and H below, the resonances corresponding to diastereomeric Cu-alkyl complexes (78% conv., 99:1 d.r.) were detected in the ^1H and ^{31}P NMR spectra; there was ~17% of uncoordinated bis-phosphine **L3c** also present. The sample was then allowed to warm to 22 °C (while in the spectrometer) and reaction progress monitored spectroscopically. There was further transformation to the Cu–alkyl complexes (93% conv.; spectra I and J) along with diminution of d.r. to 72:28. Additionally, the acquired spectra indicate the generation of the corresponding *E*-β-alkenyl–B(pin) byproduct formed through Cu–H elimination with significant amounts formed after 1.5 h at 22 °C (spectra K and L). The identity of the alkenyl–B(pin) compound was confirmed by spiking the tube with an authentic sample of the same material.

Kinetic enantioselectivity of Cu–B(pin) addition and reactivity of chiral vs. achiral Cu–B(pin) complexes



Conclusions. The above experiment show that the bis-phosphine–Cu–B(pin) complex adds to *para*-trifluoromethylstyrene readily and rapidly at –20 °C in a highly enantioselective manner. When the mixture was allowed to warm to 22 °C, the ratio between the two diastereomeric alkylcopper complexes decreased with time (from 99:1 to ~75:25) with more of the Cu–alkyl complex being formed (93% conv.). The decrease in d.r. may be attributed to lower reactivity of the un-coordinated

Cu–B(pin) complex, which can add to the alkene substrate only at a higher temperature, supporting the notion that such a species can engender diminution in enantioselectivity in cases where the olefin is more electrophilic/reactive. Once the aryl olefin is fully converted to the corresponding alkylcopper intermediate, there can be complete bis-phosphine–Cu coordination, leaving only the excess bis-phosphine unbound. It is also possible that some of the lowering in e.r. arises from preferential Cu–H elimination by the Cu–alkyl major diastereomer, accounting for the formation of the alkenyl–B(pin) byproduct at 22 °C.

Cu–H Addition to a β-Alkenyl–B(pin) Byproduct

Examination of bis-phosphine–Cu–H addition to an (E)-β-alkenyl–B(pin) compound. In an N_2-filled glove box, a solution of CuO*t*-Bu (2.8 mg, 0.0203 mmol), **L3c** (15 mg, 0.0224 mmol) and $PhCH_2Ph$ as the internal standard (5.0 μL, 0.03 mmol) was prepared in thf-d_8 (0.3 mL) in a two-dram vial. The mixture was manually stirred leading to the formation of a homogeneous light-green solution and was then transferred to an NMR tube. The vial was washed with an additional 0.2 mL of thf-d_8. The tube was capped with a septum and sealed with paraffin before removal from glove box and placed into a dry ice/acetone bath. A solution of polymethylhydrosiloxane (PMHS) (10 μL, 0.17 mmol) and (*E*)-2-[4-(trifluoromethyl)phenyl]vinylboronic acid pinacol ester (13.8 mg, 0.043 mmol) prepared in 0.2 mL of thf-d_8 was added by syringe and the resulting mixture was stirred manually (cooling bath retained to avoid any premature transformation). Reaction progress was monitored at 22 °C.

Resonances for **L3c-Cu–*iso*-alkyl-1** were detected in the ^{1}H NMR spectrum (M; ~80% conv.). The ^{31}P NMR spectrum (N) indicates 83:17 d.r. There were no detectable resonances for **L3c-Cu-alkyl-1**, but ~13% of 2-(4-trifluoromethylphenyl)ethyl-1-boronic acid pinacol ester (**β-alkyl–B(pin)-1**), probably formed due to reaction of organocopper with adventitious water, was detected. The same experiment was carried out with (*E*)-2-phenyl-vinylboronic acid pinacol ester (13.8 mg, 0.043 mmol). The resonances corresponding to **L3c-Cu–*iso*-alkyl-2** were detected by ^{1}H NMR (spectrum O; 73% conv.) along with 12% **β-alkyl–B(pin)-2**. As before, d.r. was determined by analysis of the ^{31}P NMR spectrum (P; 78:22).

Through the experiment shown in Eq. 5 we examined the issue of Cu–H addition to (*E*)-2-phenyl-vinylboronic acid pinacol ester followed by C–C bond formation. Only ***iso*-2a** was detected (11% conv.; <2% **2a**).

Conclusions. Due to reversal in alkene polarization due to the presence of the electron-withdrawing B(pin) group, Cu–H addition to (*E*)-*β*-alkenyl–B(pin) derivatives occurs with opposite site selectivity compared to Cu–B(pin) additions (i.e., homobenzylic Cu–C bond). Preferential formation of ***iso*-2a** is consistent with a study reported by Sadighi[26]. It is unlikely that Cu–H re-addition is responsible for the loss in enantioselectivity. We could not detect **L3c-Cu-alkyl-1** or **L3c-Cu-alkyl-2**.

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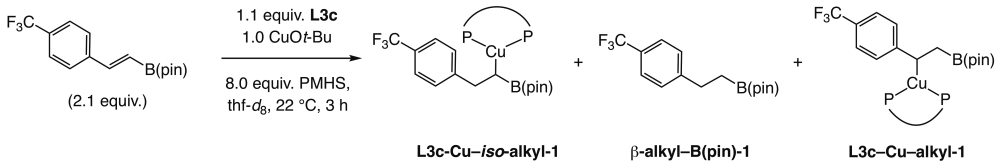
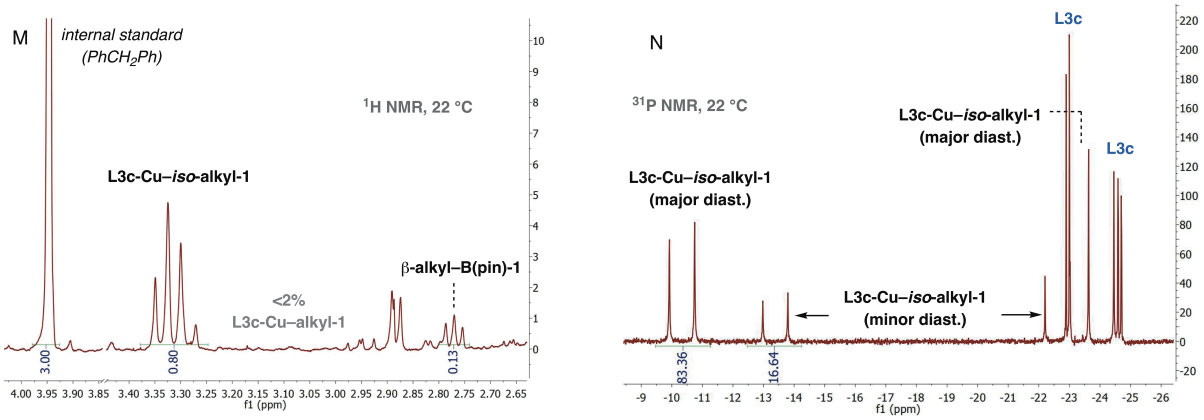
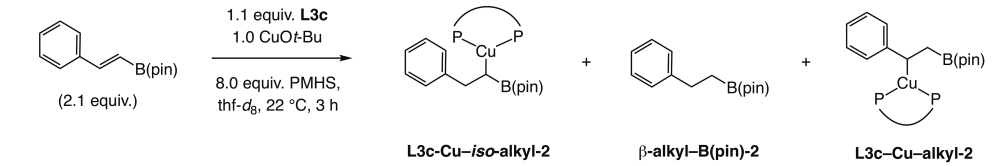
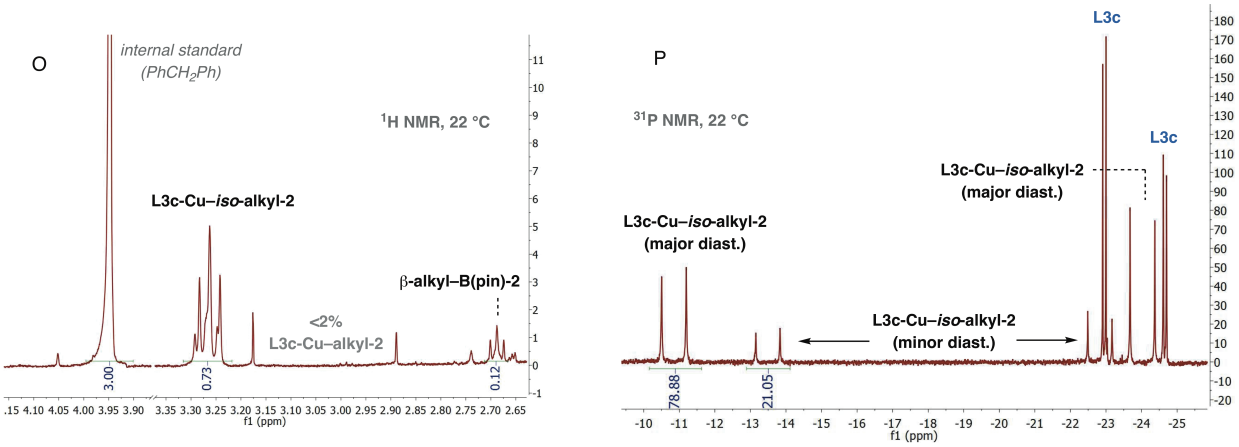
(26) Laita, D. S., Tsui, E. Y. & Sadighi, J. P. *Organometallics* **25**, 2405–2408 (2006).

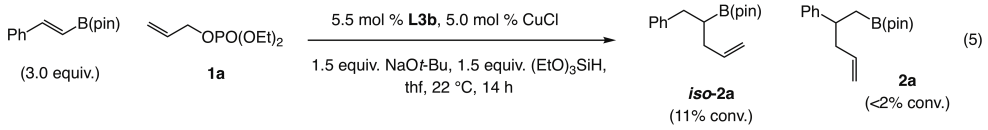
Regioselectivity of Cu–H addition to a β-alkenyl–B(pin) compound





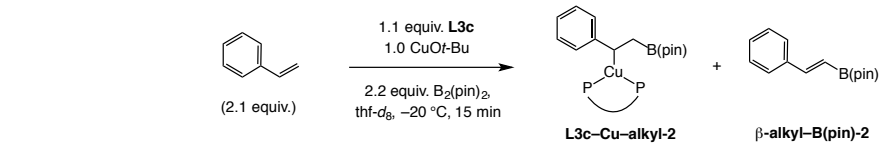


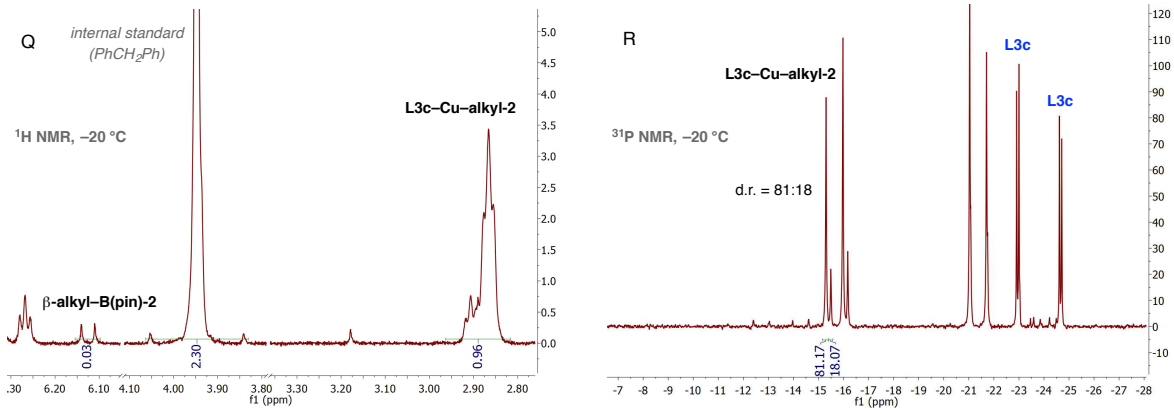


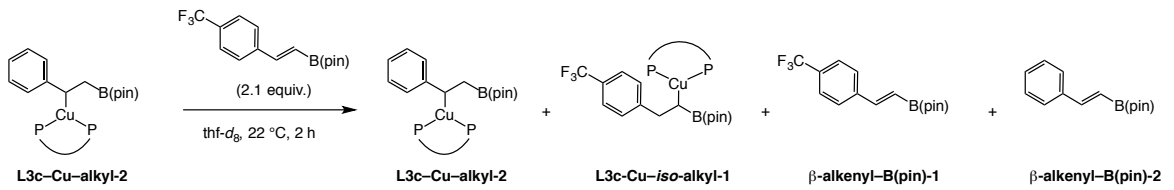


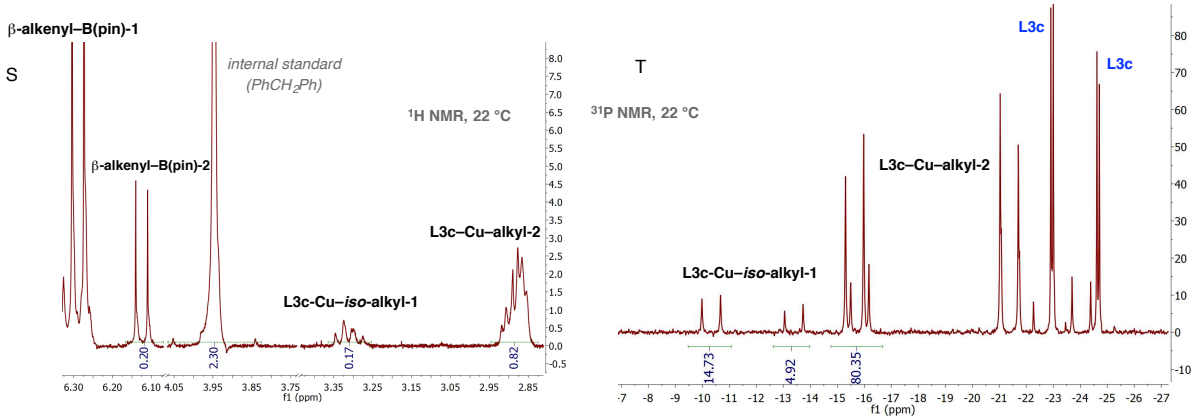
Probing the feasibility of Cu–H elimination/re-addition leading to loss of enantiomeric purity of a Cu–alkyl species; a cross-over experiment. In an N_2-filled glove box, a solution of CuO*t*-Bu (2.8 mg, 0.0203 mmol), **L3c** (15 mg, 0.0224 mmol), styrene (2.4 μL, 0.0203 mmol) and

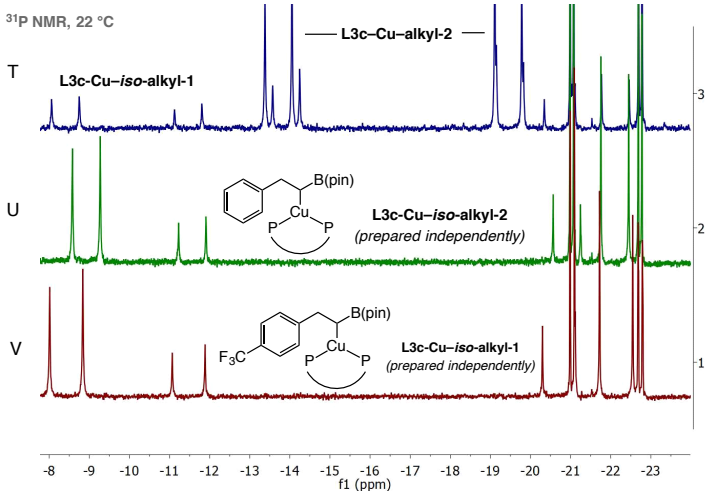
Evidence for Cu–H elimination; a cross-over experiment











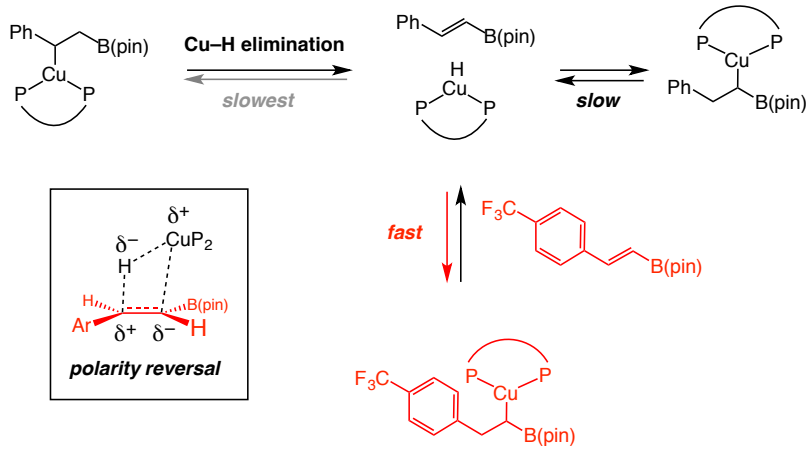
$PhCH_2Ph$ (internal standard; 4.0 μL, 0.0233 mmol) in thf-d_8 (0.3 mL) was prepared in a two-dram vial. The mixture was manually stirred leading to the formation of a homogeneous light-green solution and then transferred to an NMR tube, after which the vial was washed with additional 0.2 mL of thf-d_8. The tube was sealed with a septum and paraffin before removal from the glove box and introduced into a dry ice/acetone bath. A solution of bis(pinacolato)diboron (11.4 mg, 0.0449 mmol) in 0.2 mL thf-d_8 was then added by syringe and the mixture stirred manually without removing the cooling bath (to avoid premature transformation prior to the tube being placed in the spectrometer).

Resonances for diastereomers **L3c-Cu–alkyl-2** were detected by ^{1}H NMR (spectrum Q; 96% conv., 15 min, 22 °C); the corresponding alkenyl–B(pin) was detected in trace amounts (<5%). The ^{31}P NMR (spectrum R) indicates 81:19 d.r. for the formation of **L3c-Cu-alkyl-2**.

A solution of (*E*)-2-[4-(trifluoromethyl)phenyl]vinylboronic acid pinacol ester (13.8 mg, 0.043 mmol, 2.1 equiv.) in 0.2 mL thf-d_8 was added to the mixture transferred by syringe. After 2 h at 22 °C, spectroscopic analysis (spectra S and T) indicated depletion of **L3c-Cu-alkyl-2** concomitant with the appearance of resonances for **L3c-Cu-*iso*-alkyl-1** (17% conv.; 75:25 d.r. based on ^{31}P NMR spectrum T). Also shown for comparison are ^{31}P NMR spectra T, U and V, indicating the absence of any product from Cu–H addition to less electrophilic/reactive **β-alkenyl–B(pin)-2**.

Conclusions. A bis-phosphine–Cu–H complex can be generated from reaction of a Cu–alkyl complex generated from Cu–B(pin) addition to an alkene, and may subsequently be transferred by a Cu–H elimination/re-addition sequence to a different alkenyl–B(pin) compound but with the opposite regiochemistry (from benzylic to homobenzylic Cu–C bond); this is further illustrated in Scheme 12. It is therefore unlikely that Cu–H re-addition from the opposite face of the *same*

Scheme 12. Regiochemistry of Cu–H elimination/re-addition

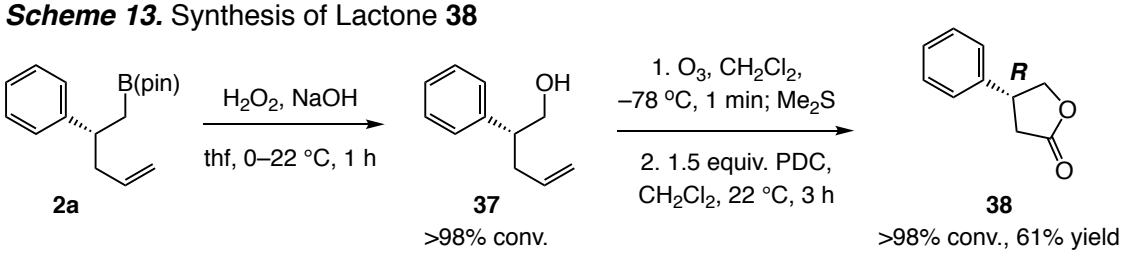


alkene can occur without dissociation from the original alkenyl–B(pin) by product. Furthermore, the observation that Cu–H can dissociate and then add to a different alkenyl–B(pin) compound points to a weak bis-phosphine–Cu–H⋯alkenyl–B(pin) coordination. The possibility of Cu–H re-addition to the same alkenyl–B(pin) is rendered especially unlikely considering the presence of substantially larger amounts of terminal alkene substrate under the catalytic condition (vs. any released alkenyl–B(pin)).

15. Determination of Absolute Stereochemistry

Other than comparison of specific rotation of **10** to the reported values suggesting a (*R*) configuration of the products, we synthesized **38** and obtained the X-ray crystal structure to ascertain the absolute stereochemical identity of the products.

Scheme 13. Synthesis of Lactone **38**



Compound **38** was synthesized from enantiomerically enriched **2a** (95:5 e.r.), as illustrated in Scheme 13. **(*R*)-4-Phenyldihydrofuran-2(3*H*)-one (38)**: The spectroscopic data match those reported previously.[27] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40–7.22 (5H, m), 4.67 (1H, dd, J = 8.8, 8.0 Hz), 4.28 (1H, dd, J = 9.0, 8.2 Hz), 3.79 (1H, app pent, J = 8.5 Hz), 2.93 (1H, dd, J = 17.6 and 8.8 Hz), 2.68 (1H, dd, J = 17.6, 8.8 Hz); Specific Rotation: $[\alpha]_D^{20}$ –40.8 (*c* 0.50, $CHCl_3$). The absolute configuration of **38** was established by X-ray analysis, which was assigned to be (*R*). Compound **2a** is thus assigned to possess the (*R*) configuration. The absolute stereochemistry for other enantiomerically enriched products has been assigned by inference.

16. Data for X-ray Crystallography of 38

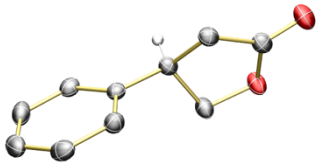


Table 2. **Crystal data and structure refinement for $C_{10}H_{10}O_2$**

Identification code	C10H10O2
Empirical formula	C10 H10 O2
Formula weight	162.18
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 6.1692(7) Å
	b = 7.7518(8) Å
	c = 8.6969(9) Å

(27) Malkov, A. V., Friscourt, F., Bell, M., Swarbrick, M. E. & Kočovský, P. *J. Org. Chem.* **73**, 3996–4003 (2008).

Volume	415.33(8) $Å^3$
Z	2
Density (calculated)	1.297 Mg/m^3
Absorption coefficient	0.729 mm^{-1}
F(000)	172
Crystal size	0.600 x 0.070 x 0.050 mm^3
Theta range for data collection	5.092 to 66.613°.
Index ranges	-7<=h<=7, -8<=k<=9, -10<=l<=10
Reflections collected	4434
Independent reflections	1435 [R(int) = 0.0455]
Completeness to theta = 67.679°	98.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7528 and 0.5867
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1435 / 1 / 109
Goodness-of-fit on F^2	1.091
Final R indices [I>2sigma(I)]	R1 = 0.0341, wR2 = 0.0848
R indices (all data)	R1 = 0.0346, wR2 = 0.0858
Absolute structure parameter	-0.05(11)
Extinction coefficient	na
Largest diff. peak and hole	0.145 and -0.213 e. $Å^{-3}$

Table 3. **Atomic coordinates (x10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $C_{10}H_{10}O_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor**

	x	y	z	U(eq)
O(1)	4872(2)	3283(2)	344(2)	29(1)
O(2)	8163(2)	4179(2)	-234(2)	34(1)
C(1)	6684(3)	4254(3)	609(2)	25(1)
C(2)	6464(3)	5329(3)	2029(2)	23(1)
C(3)	4017(3)	5331(3)	2238(2)	22(1)
C(4)	3365(3)	3581(3)	1546(2)	26(1)
C(5)	3258(3)	5568(2)	3851(2)	21(1)

C(6)	4294(3)	4761(3)	5124(2)	26(1)
C(7)	3475(4)	4930(3)	6572(2)	31(1)
C(8)	1594(4)	5872(3)	6774(2)	32(1)
C(9)	571(3)	6695(3)	5510(3)	31(1)
C(10)	1411(3)	6549(3)	4071(2)	24(1)

Table 4. **Bond lengths [Å] and angles [°] for $C_{10}H_{10}O_2$**

O(1)-C(1)	1.357(3)
O(1)-C(4)	1.453(2)
O(2)-C(1)	1.202(3)
C(1)-C(2)	1.502(3)
C(2)-C(3)	1.530(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(5)	1.513(3)
C(3)-C(4)	1.530(3)
C(3)-H(3)	1.0000
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(10)	1.392(3)
C(5)-C(6)	1.396(3)
C(6)-C(7)	1.388(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.390(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.393(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.384(3)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
C(1)-O(1)-C(4)	110.01(15)
O(2)-C(1)-O(1)	120.97(19)

O(2)-C(1)-C(2)	129.3(2)
O(1)-C(1)-C(2)	109.77(17)
C(1)-C(2)-C(3)	103.33(16)
C(1)-C(2)-H(2A)	111.1
C(3)-C(2)-H(2A)	111.1
C(1)-C(2)-H(2B)	111.1
C(3)-C(2)-H(2B)	111.1
H(2A)-C(2)-H(2B)	109.1
C(5)-C(3)-C(4)	112.65(16)
C(5)-C(3)-C(2)	117.74(15)
C(4)-C(3)-C(2)	101.13(16)
C(5)-C(3)-H(3)	108.3
C(4)-C(3)-H(3)	108.3
C(2)-C(3)-H(3)	108.3
O(1)-C(4)-C(3)	105.02(16)
O(1)-C(4)-H(4A)	110.7
C(3)-C(4)-H(4A)	110.7
O(1)-C(4)-H(4B)	110.7
C(3)-C(4)-H(4B)	110.7
H(4A)-C(4)-H(4B)	108.8
C(10)-C(5)-C(6)	118.66(18)
C(10)-C(5)-C(3)	119.28(17)
C(6)-C(5)-C(3)	121.98(18)
C(7)-C(6)-C(5)	120.31(19)
C(7)-C(6)-H(6)	119.8
C(5)-C(6)-H(6)	119.8
C(6)-C(7)-C(8)	120.6(2)
C(6)-C(7)-H(7)	119.7
C(8)-C(7)-H(7)	119.7
C(7)-C(8)-C(9)	119.20(18)
C(7)-C(8)-H(8)	120.4
C(9)-C(8)-H(8)	120.4
C(10)-C(9)-C(8)	120.0(2)
C(10)-C(9)-H(9)	120.0

C(8)-C(9)-H(9)	120.0
C(9)-C(10)-C(5)	121.13(19)
C(9)-C(10)-H(10)	119.4
C(5)-C(10)-H(10)	119.4

Symmetry transformations used to generate equivalent atoms:

Table 5. **Anisotropic displacement parameters ($Å^2x10^3$) for $C_{10}H_{10}O_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	25(1)	38(1)	24(1)	-7(1)	4(1)	-6(1)
O(2)	28(1)	46(1)	30(1)	-1(1)	8(1)	0(1)
C(1)	24(1)	28(1)	23(1)	3(1)	0(1)	1(1)
C(2)	20(1)	24(1)	25(1)	2(1)	0(1)	-1(1)
C(3)	21(1)	24(1)	22(1)	3(1)	0(1)	1(1)
C(4)	23(1)	34(1)	23(1)	-4(1)	3(1)	-3(1)
C(5)	21(1)	18(1)	24(1)	-2(1)	1(1)	-3(1)
C(6)	29(1)	23(1)	26(1)	1(1)	2(1)	2(1)
C(7)	42(1)	24(1)	25(1)	0(1)	-2(1)	-5(1)
C(8)	40(1)	31(1)	27(1)	-9(1)	9(1)	-10(1)
C(9)	25(1)	31(1)	37(1)	-11(1)	6(1)	0(1)
C(10)	21(1)	21(1)	30(1)	-2(1)	-2(1)	-2(1)

Table 6. **Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2 x10^3$) for $C_{10}H_{10}O_2$**

	x	y	z	U(eq)
H(2A)	7011	6515	1879	28
H(2B)	7263	4805	2930	28
H(3)	3343	6256	1569	27

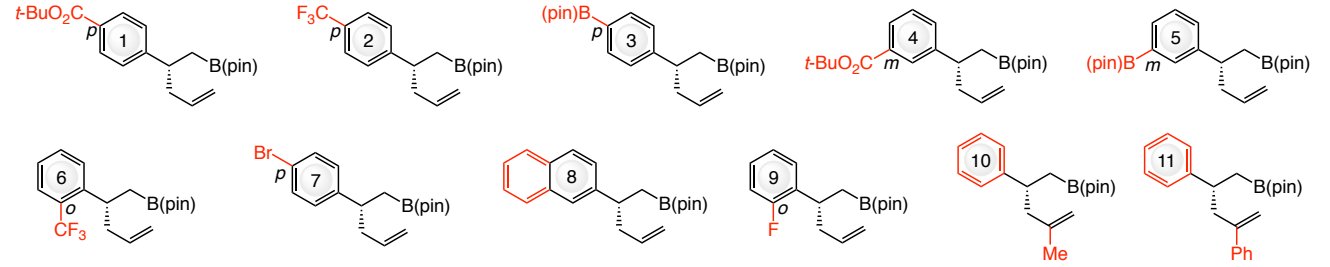
H(4A)	3494	2663	2336	31
H(4B)	1850	3610	1109	31
H(6)	5564	4094	4998	31
H(7)	4208	4395	7435	37
H(8)	1014	5954	7761	39
H(9)	-704	7357	5636	37
H(10)	715	7129	3218	29

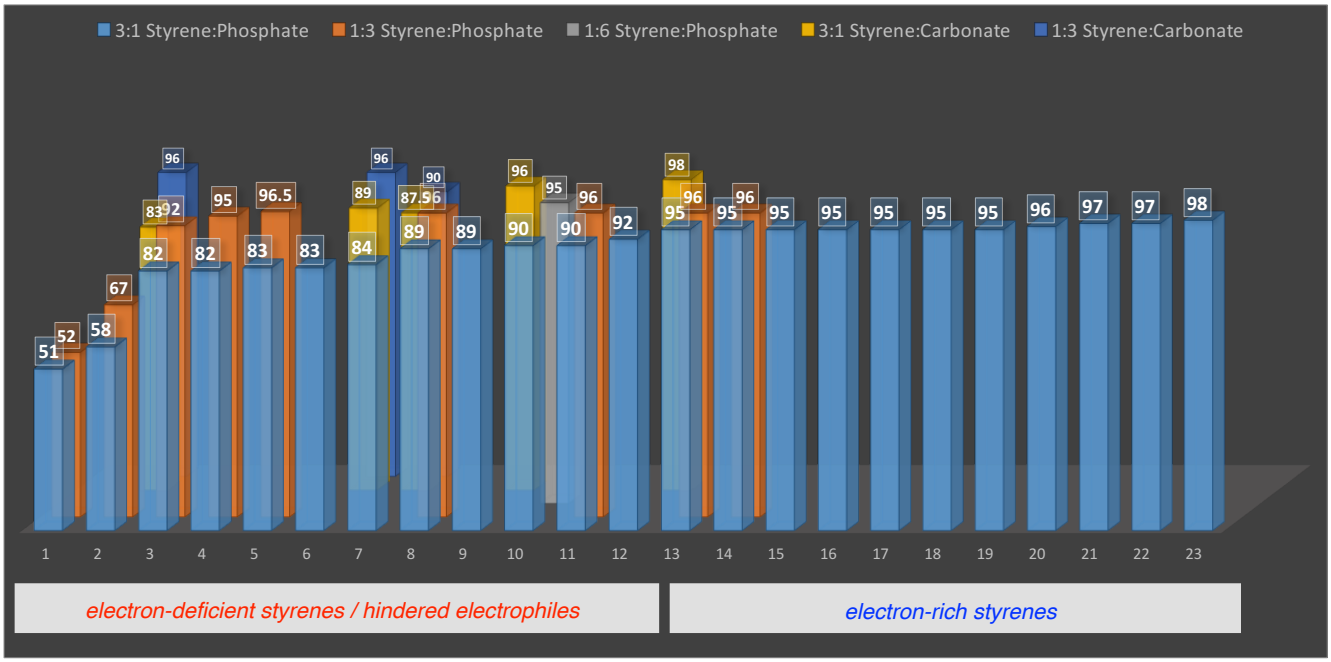
Table 7. **Torsion angles [°] for $C_{10}H_{10}O_2$**

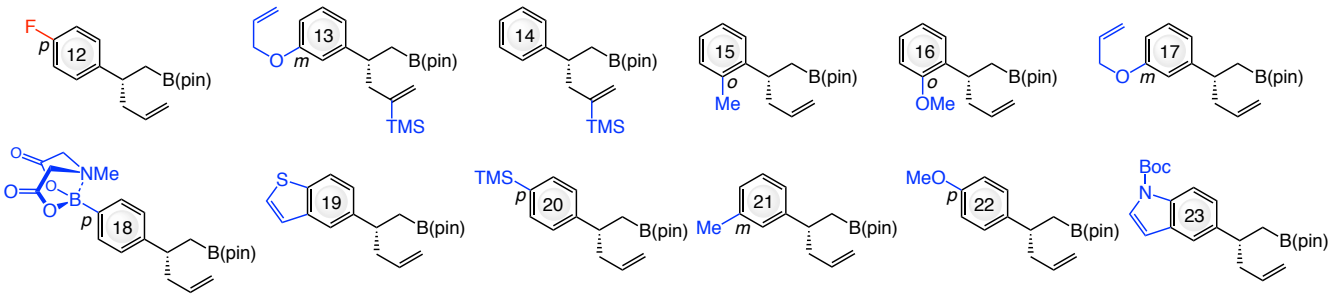
C(4)-O(1)-C(1)-O(2)	178.59(19)
C(4)-O(1)-C(1)-C(2)	-1.5(2)
O(2)-C(1)-C(2)-C(3)	161.0(2)
O(1)-C(1)-C(2)-C(3)	-18.9(2)
C(1)-C(2)-C(3)-C(5)	153.11(17)
C(1)-C(2)-C(3)-C(4)	29.95(18)
C(1)-O(1)-C(4)-C(3)	21.5(2)
C(5)-C(3)-C(4)-O(1)	-158.08(16)
C(2)-C(3)-C(4)-O(1)	-31.48(18)
C(4)-C(3)-C(5)-C(10)	-100.7(2)
C(2)-C(3)-C(5)-C(10)	142.14(19)
C(4)-C(3)-C(5)-C(6)	76.0(2)
C(2)-C(3)-C(5)-C(6)	-41.1(3)
C(10)-C(5)-C(6)-C(7)	0.5(3)
C(3)-C(5)-C(6)-C(7)	-176.25(19)
C(5)-C(6)-C(7)-C(8)	1.3(3)
C(6)-C(7)-C(8)-C(9)	-2.0(3)
C(7)-C(8)-C(9)-C(10)	0.9(3)
C(8)-C(9)-C(10)-C(5)	0.9(3)
C(6)-C(5)-C(10)-C(9)	-1.6(3)
C(3)-C(5)-C(10)-C(9)	175.24(19)

Symmetry transformations used to generate equivalent atoms:

17. Representative Products of Bis-Phosphine–Cu-Catalyzed Reactions







18. Density Functional Theory (DFT) Calculations

(**Please Note:** In the following section, the term Cu–rev is synonymous with the term Cu–*iso* used above.)

DFT computations[28] were performed with the Gaussian 09 suite of programs[29]. Geometries were optimized with density functional ωB97XD[30] and the Def2SVP basis set[31]. The effect of a polar reaction medium (tetrahydrofuran, THF) was approximated by means of the SMD solvation model[32]. Stationary points were probed through vibrational analysis and Gibbs free energy corrections were performed under standard conditions (298.15 K, 1.0 atm). Intrinsic reaction coordinate (IRC) calculations have been performed starting from selected transition states (**ts**) employing the L(ocal) Q(uadratic) A(approximation) method, followed by subsequent optimization to obtain structures and energies for educt (**ed**) and product (**prod**) on either side of the transition state[33]. We furthermore probed the performance of various density functionals through single point energy calculations at the geometries optimized at the levels described above by means of the SMD solvation model[32] with THF as solvent and the larger Def2TZVPP[31] basis set. Since the correct density functional is not known we tested several state of the art approaches that have been developed over the past decade[28,34]: ωB97XD[30],

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(31) Weigend, F. & Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297–3305.

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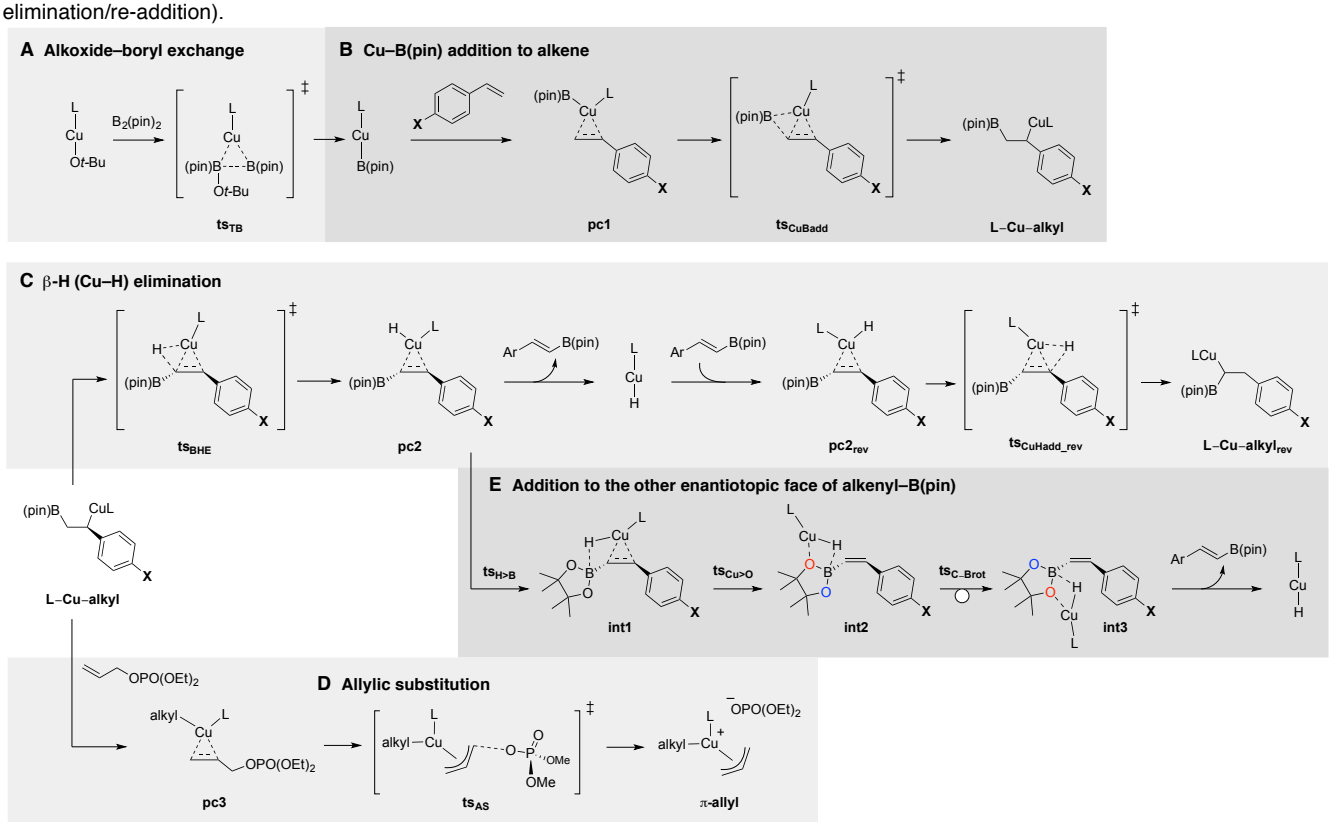
(34) For selected examples highlighting the importance of including treatment of dispersion interactions in modeling olefin metathesis reactions promoted by Ru carbene complexes, see: (a) Torker, S., Merki, D. & Chen. P. *J. Am. Chem. Soc.* **130**, 4808–4814 (2008). (b) Minenkov, Y., Occhipinti, G., Singstad, A. & Jensen, V. R. *Dalton Trans.* **41**, 5526–5541 (2012). (c) Minenkov, Y., Occhipinti, G. & Jensen, V. R. *Organometallics* **32**, 2099–2111 (2013). (d) Torker, S., Khan, R. K. M. & Hoveyda, A. H. *J. Am. Chem. Soc.* **136**, 3439–3455 (2014). (e) Khan, R. K. M., Torker, S. & Hoveyda, A. H. *J. Am. Chem. Soc.* **136**, 14337–14340 (2014). (f) Torker, S., Koh, M. J., Khan, R. K. M. & Hoveyda, A. H. *Organometallics* **35**, 543–562 (2016). (g) Mikus, M. S., Torker, S. & Hoveyda, A. H. *Angew. Chem. Int. Ed.* **55**, 4997–5002 (2016). For modeling allyl

M06[35], MN12SX[36], MN12L[36], M06L[35], BP86-D3BJ[28b,37] and PBE0-D3BJ[28b,38] (Figure 1–9). Electronic and Gibbs free energies for Figure 1–10 are provided in Section 19 and the entries used as the basis for Figures 6–7 are highlighted in red. A file for convenient viewing of computed geometries with the program Mercury 3.3 is appended as separate "coordinates.xyz" file in Section 20[39].

Scheme 14. General reaction sequence for Cu–B(pin) addition/allylic substitution including competitive side reactions (β-H or Cu–H elimination/re-addition).



Abbreviations: **TB**, transborylation [conversion of Cu–alkoxide to Cu–B(pin)]; **BHE**, β-hydride (or Cu–H) elimination; **pc**, π-complex; $\mathbf{ts_{H>B}}$, transition state for hydride migration to boron; $\mathbf{ts_{Cu>O}}$, transition state for Cu migration to oxygen on Bpin; $\mathbf{ts_{C\text{-}Brot}}$, transition state for C–B bond rotation; $\mathbf{ts_{CuHadd\_rev}}$, transition state Cu–H addition leading to Cu–alkyl$_{rev}$ species with opposite regiochemistry; **int**, intermediate; **Cu–H**, linear Cu-hydride species.

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addition to CF3-ketones, see: (h) Lee, K., Silverio, D. L., Torker, S., Robbins, D. W., Haeffner, F. & Hoveyda, A. H. *Nature Chem.* **8**, 768–777 (2016).

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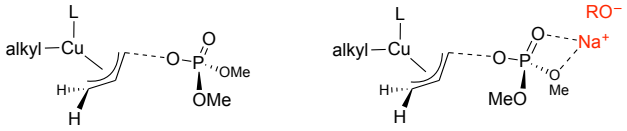
(39) Lichtenberger, D. L. & Gladysz, J. A. *Organometallics* **33**, 835–835 (2014). The "coordinates.xyz" file can be generated by copying all the coordinates in Section 20 into a text file without empty lines and changing the extension to ".xyz".

Background

Linear CuO*t*-Bu species that contain neutral ligands are labeled as **L–Cu–O*t*-Bu** [L = bis-phosphine **L3a**, a model NHC (**NHCMe$_2$**) and phosphine (**PMe$_3$**), tetrahydrofuran (thf) or an aryl olefin with *para* substituent X]. Formation of linear **L–Cu–B(pin)** complex is expected to occur by reaction with $B_2(pin)_2$ via transition state **ts$_{TB}$**. In Figures 1–10, **ed** and **prod** denote the minima on either side of **ts$_{TB}$**, which was obtained by IRC calculations and subsequent optimization. Complex **L–Cu–B(pin)** undergoes Cu–B(pin) addition through the following sequence: **pc1** → **ts$_{CuBadd}$** → **L–Cu–alkyl**. Complex **L–Cu–alkyl** can either participate in an allylic substitution reaction (**pc3** → **ts$_{AS}$** → **π-allyl**) or Cu–H elimination via transition state **ts$_{BHE}$** to generate π-complex **pc2**. Upon dissociation of the alkenyl–B(pin) species linear **L–Cu–H** is formed, which might then re-add with the opposite site selectivity [Cu at the carbon bearing the B(pin) unit] to form alkylcopper species **L–Cu–alkyl$_{rev}$** (**pc2$_{rev}$** → **ts$_{CuHadd_rev}$**).

Questions to be Addressed

Issues concerning the DFT calculations. The difficulty associated with modeling reactions that contain multiple ionic species notwithstanding, a number of DFT calculations were performed. Comparison of absolute free energies of transition states with different character (e.g., **ts$_{CuBadd}$** vs. **ts$_{AS}$**) is challenging and probably subject to somewhat large relative errors. This is particularly an issue with transtition state structures that may be envisioned for the allylic substitution (AS) step, such as those where the phosphate moiety is cleaved without the assistance of Na chelation and those where Na coordination is involved (but not necessarily intramolecular, see below).



ts$_{AS}$ without Na alkoxide **ts$_{AS}$** with Na alkoxide

Specific questions investigated. The major goal of these studies was to address the following questions:

(1) What is the most plausible stereochemical model for L–Cu–B(pin) addition to an aryl olefin with L being bis-phosphine ligand **L3a**?

(2) What are the most likely steps where the presence of an electron-deficient aryl olefin can lead to a lowering of enantioselectivity? Is it possible that electron-deficient alkene might be capable of activating Cu–O*t*-Bu clusters, breaking them into smaller, more reactive species, due to their ability to provide stronger back-bonding (lower energy π*)?

(3) Alternatively, does an electron-deficient aryl olefin allow for a more competitive Cu–B(pin) addition with an achiral complex?

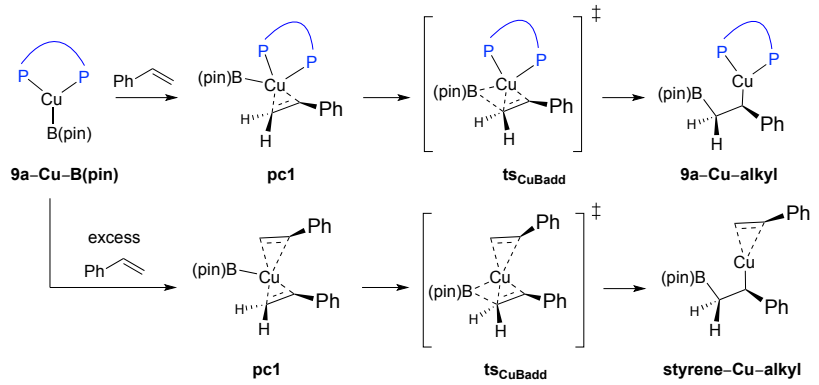
(4) Why does the allylic substitution step seem to be more difficult with bis-phosphine **L3a**, particularly with bulkier allyl elecrophiles? Does this allow for alternative reaction pathways to compete, leading to lower e.r. (enantiomeric ratio)?

(5) Is β–H (Cu–H) elimination within the alkylcopper intermediates critical to enantioselectivity fluctuations and, if so, is it followed by subsequent Cu–H re-addition from the opposite enantiotopic face?

(6) What is the basis for reactions, regardless of whether they contain an NHC or a phosphine ligand, being highly S_N2'-selective?

(7) Does displacement of the bis-phosphine ligand by an aryl olefin or a Lewis basic solvent molecule (i.e., thf) take place to a degree that influences the observed e.r. fluctuations? This might have several advantages: Although phosphines are better donors (compared to olefins) and should therefore bind more strongly to the metal center, the smaller size and π-accepting properties of styrenes could exert a positive influence on the rate of C–B bond formation. However, a competitive and non-selective Cu–B addition pathway starting form **L3a(9α)–Cu–B(pin)** would likely be second-order in the alkene (i.e., one styrene needed for displacement of **L3a** and another one is involved in Cu–B addition; Scheme 15). See the discussion associated with Figures 6–7 below.

Scheme 15. Enantioselective Cu–B(pin) addition and competitive bimolecular reaction.



Stereochemical Model for Addition of L3a–Cu–B(pin) to an Aryl Olefin (Figure 1.1–1.2)

The free energy surface for Cu–B(pin) addition with ligand **L3a** at the M06/Def2TZVPP$_{THF(SMD)}$//ωB97XD/ Def2SVP$_{THF(SMD)}$ level are shown in Figure 1.1. Reaction of **L3a–Cu–O*t*-Bu** generates **L3a–Cu–B(pin)** irreversibly (G_{rel} = 0.0 kcal/mol) via transition state **ts$_{TB}$** (G_{rel} = 36.3 kcal/mol). Two modes of addition were considered that might afford the major diastereomer of **L3a-Cu–alkyl** complex [**major01** with the phenyl group on styrene pointing to the front (G_{rel} = 16.9 kcal/mol) and **major02** with the phenyl ring facing to the rear (G_{rel} = 23.4 kcal/mol); Figure 1.1]. The same applies to the pathways leading to the minor diastereomer of **L3a–Cu–alkyl** [**minor01** (G_{rel} = 18.9 kcal/mol) and **minor02** (G_{rel} = 21.8 kcal/mol)]. The computed energies are in agreement with the experimental observations. Investigation with other density functionals (ωB97XD, MN12SX, MN12L, M06L, BP86-D3BJ and PBE0-D3BJ) revealed qualitatively similar trends albeit with some differences in the absolute energies (e.g., with BP86 including Grimme's D3 dispersion the reaction barriers relative to **L3a–Cu–B(pin)** are underestimated, likely due to overestimation of dispersion; 4.1 kcal/mol for **ts$_{CuBadd_major01}$**; Figure 1.2).

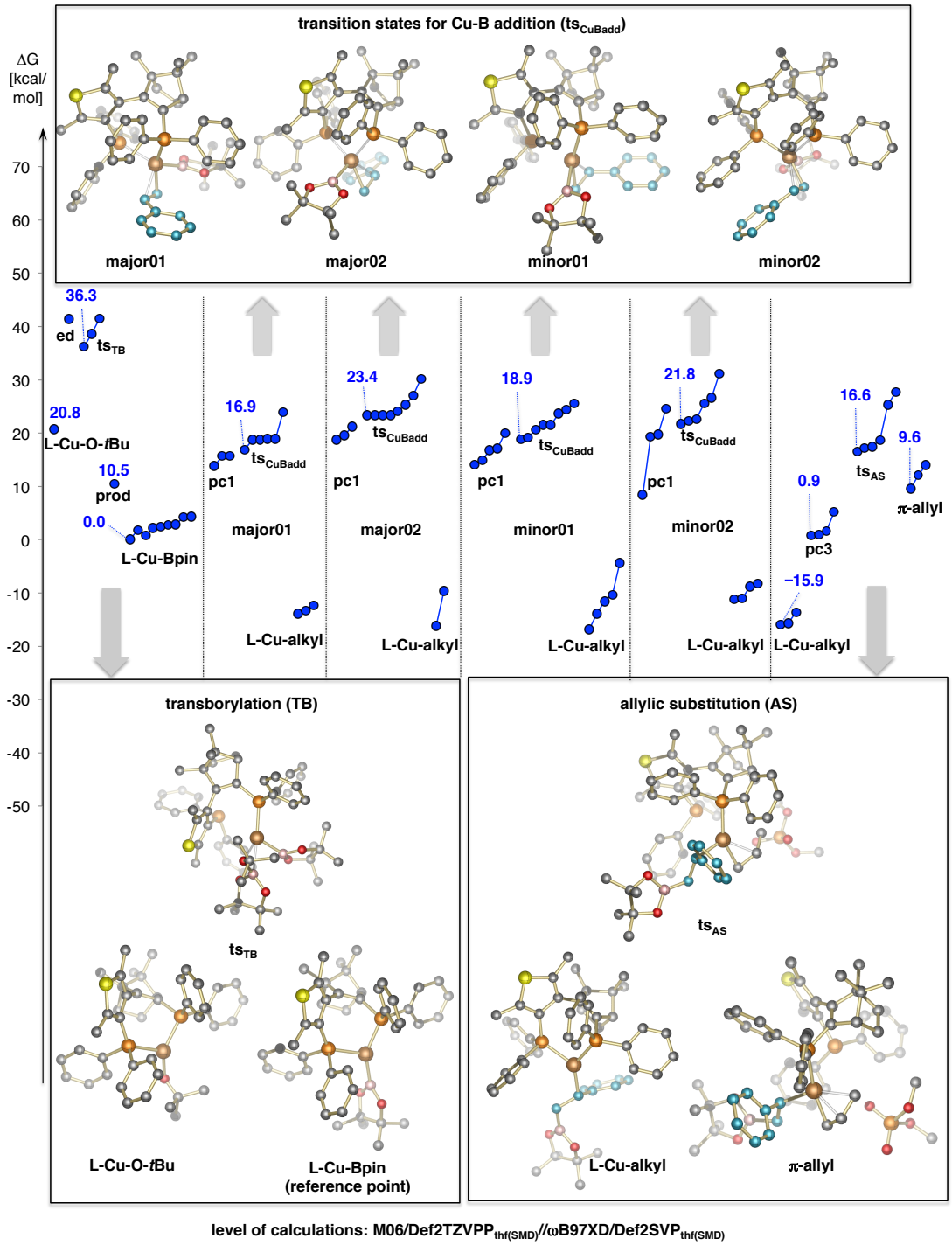


Figure 1.1. Free energy surfaces for the enantioselective Cu–B(pin) addition (CuBadd)/allylic substitution (AS) sequence with bis-phosphine **L3a** at the M06/DefTZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{thf(SMD)}$ level. Several conformers are shown for the two modes of addition leading to the major (**major01** and **major02**) and the minor enantiomer (**minor01** and **minor02**). The free energies have been referenced to the most stable **L3a–Cu–B(pin)** conformer. Only the AS transition states leading to the major enantiomer are shown. The computed structures of the lowest conformer for a given species are displayed. Abbreviations: **TB**, transborylation [conversion of Cu–alkoxide to Cu–B(pin)]; **pc**, π-complex.

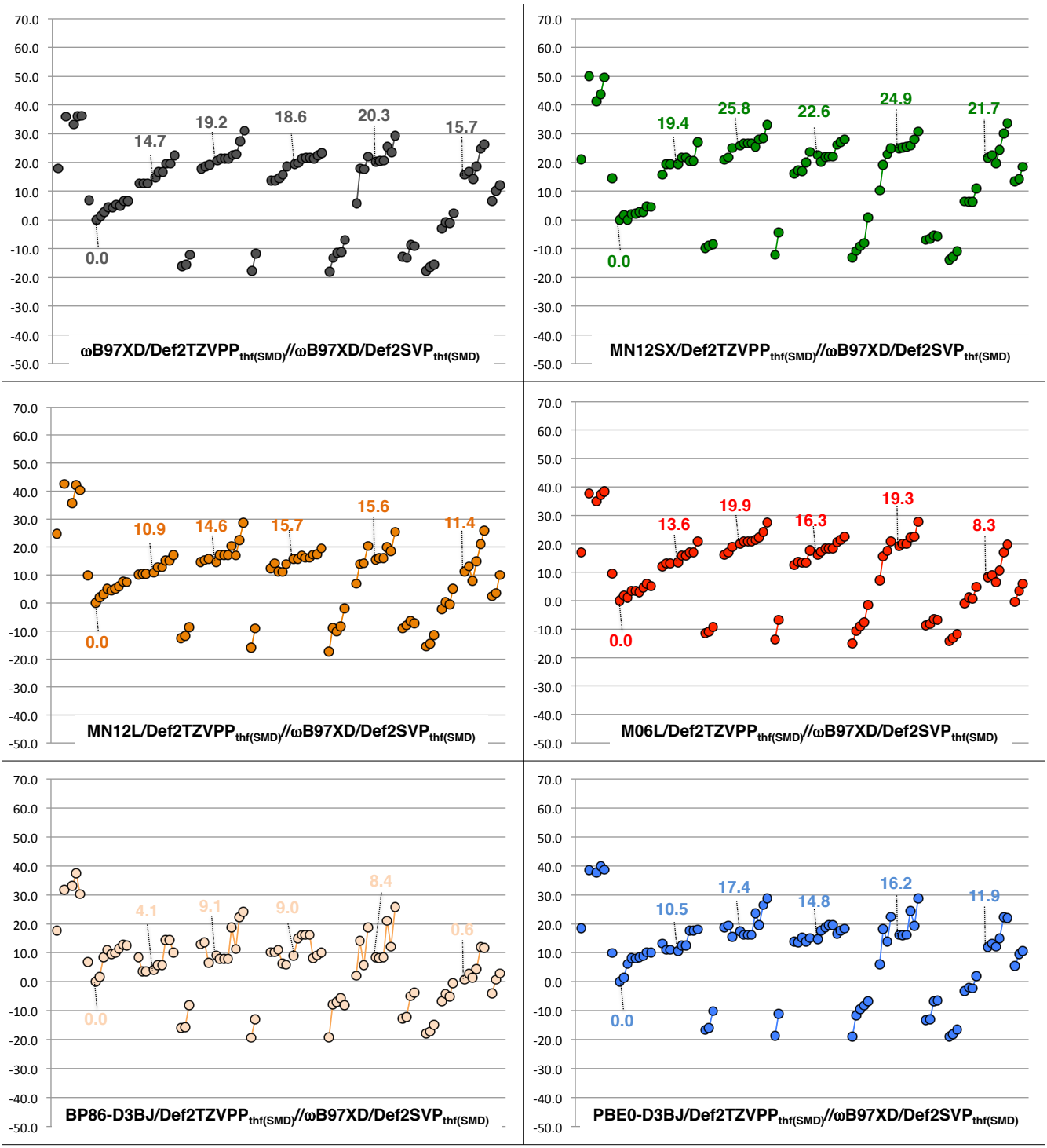


Figure 1.2. Free energy surfaces for the enantioselective Cu–B(pin) addition (CuBadd)/allylic substitution (AS) sequence with ligand **L3a** at the M06/DefTZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{thf(SMD)}$ level. Several conformers are shown for the two modes of addition that lead to the major (**major01** and **major02**) as well as the minor enantiomer (**minor01** and **minor02**). The free energies have been referenced to the most stable **L3a–Cu–B(pin)** conformer; only AS transition states leading to the major enantiomer are shown; the computed structures of the lowest conformer for a given species are displayed. Abbreviations: **TB** [conversion of Cu–alkoxide to Cu–B(pin)], transborylation; **pc**, π-complex.

Following Cu–B(pin) addition, the major alkylcopper diastereomer may undergo allylic substitution via $\mathbf{ts_{AS}}$ (G_{rel} = 16.6 kcal/mol for the most accessible conformer)[40,41,42,43]. Due to higher conformational complexity of $\mathbf{ts_{AS}}$ compared to $\mathbf{ts_{CuBadd}}$ we did not perform calculations for allylic substitution with the minor alkylcopper diastereomer; we judged that the energy difference relative to the major pathway would be masked by significant uncertainty.

Several structural features are worth highlighting, which explain why the major enantiomer is generated preferentially and shed light on coordination chemistry of the bis-phosphine ligands (Scheme 16). In the pathway leading to the major alkylcopper enantiomer there is, in addition to several edge-to-face aromatic interactions[44], a weak H-bonding association between one of the oxygen atoms of the B(pin) moiety and an *ortho*-hydrogen atom of an arylphosphine ring (Scheme 16a). Rather than consider this H-bonding interaction as purely attractive, this geometry may be viewed as the least repulsive; in other words, there is probably minimal electron density on that particular ortho proton on the phenyl ring, which favors propinquity with the B(pin) moiety.

The presence of the four *meta*-methyl groups of the diarylphosphine moieties in bis-phosphine **L3c** causes enantioselectivity reversal (20:80 e.r.); we propose this is because the aforementioned weak H-bonding interaction is sterically and electronically disrupted. It is also likely that the phosphine ligand adopts a more flexible coordination mode.

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(40) For mechanistic considerations regarding nucleophilic reaction promoted by Cu(I) species, see: Yoshikai, N. & Nakamura, E. *Chem. Rev.* **112**, 2339–2372 (2012). For a computational report regarding the nucleophilicity of d-orbitals in Cu-alkyl species, see: Mori, S., Hirai, A., Nakamura, M. & Nakamura, E. *Tetrahedron* **56**, 2805–2809 (2000).

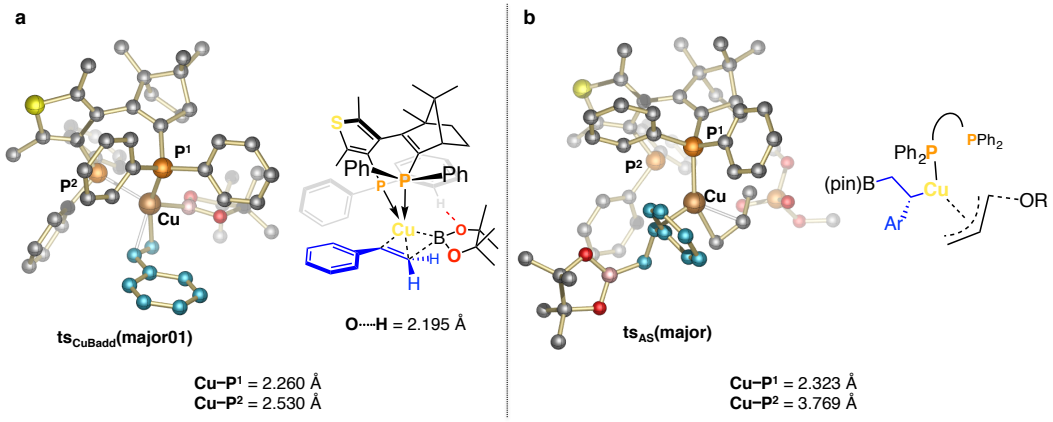
(41) For an early computational report regarding site selectivity in allylic substitution (AS) reactions involving anionic hetereocuprates, see: (a) Yoshikai, N., Zhang, S.-L. & Nakamura, E. *J. Am. Chem. Soc.* **130**, 12862–12863 (2008). For a report discussing regioselectivity during reductive elimination from Cu(III) π-allyl species, see: (b) Yamanaka, M., Kato, S. & Nakamura, E. *J. Am. Chem. Soc.* **126**, 6287–6293 (2004).

(42) For a dissusion of enantioselective allylic substitution promoted by Cu–R entities bearing NHC ligands with a pendant sulfonate group, see: (a) Shi, Y., Jung, B., Torker, S. & Hoveyda, A. H. *J. Am. Chem. Soc.* **137**, 8948–8964 (2015). (b) Lee, J., Torker, S. & Hoveyda, A. H. *Angew. Chem. Int. Ed.* **56**, 821–826 (2017).

(43) For additional stereochemical models regarding 1,4- or 1,6-additions to enoates or dienoates that also suggest the involvement of an intramolecular coordination of the substrate to a metal counterion, see: (a) Meng, F., Li, X., Torker, S., Shi, Y., Shen, X. & Hoveyda, A. H. *Nature* **537**, 387–393 (2016). (b) Li, X., Meng, F., Torker, S., Shi, Y. & Hoveyda, A. H. *Angew. Chem. Int. Ed.* **55**, 9997–10002 (2016).

(44) (a) Quan, R. W., Li Z. & Jacobsen, E. N. *J. Am. Chem. Soc.* **118**, 8156–8157 (1996). For a review on aromatic interactions, see: (b) Hunter, C. A., Lawson, K. R., Perkins, J. & Urch, C. J. *J. Chem. Soc., Perkin Trans. 2* 651–669 (2001).

Scheme 16. Key structural features in the transition states for Cu–B(pin) addition and allylic substitution with ligand **L3a**.



While bis-phosphine **L3a** probably coordinates to Cu in a bidentate manner during Cu–B(pin) addition (with a dissymmetric coordination of the two phosphine atoms; Cu–P^1 = 2.260 Å vs. Cu–P^2 = 2.530 Å; Scheme 16a), its coordination mode is monodentate during the allylic substitution process; this adjustment is required for accommodating the square planar geometry involving a π-allyl group (Scheme 16b). One of the phosphine atoms may therefore be displaced from Cu as reflected in a comparatively long Cu–P^2 distance (3.769 Å; Scheme 16b). The additional and undesired enthalpic penalty associated with cleavage of the Cu–P^2 bond implies that allylic substitution reactions, particularly those with sterically hindered electrophiles, are challenging and can allow side reactions to become more competitive.

Influence of Electronic Attributes of Aryl Olefins on the Barriers for Cu–B(pin) Addition, β-Hydride (Cu–H) Elimination and Allylic Substitution (Figures 2–3)

To gain insight vis-à-vis the impact of electronic alterations of aryl olefins, we probed the free energy surface for Cu–B(pin) addition with model NHC or phosphine ligands at the M06/Def2TZVPP$_{thf(SMD)}$//ωB97XD/ Def2SVP$_{thf(SMD)}$ level (Figure 2.1–2.2 for L = **$NHCMe_2$** and Figure 3.1–3.2 for L = **PMe_3**). We considered examining a model system to be more effective approach because the key electronic effects could be masked by large conformational complexity. We have referenced the energies relative to **L3a–Cu–B(pin)** and, as a result, the free energies in Figure 2.1 include that needed for displacement of the neutral bis-phosphine ligand [i.e., **L3a–Cu–B(pin)** + **Me_2NHC** → **Me_2NHC–Cu–B(pin)** + **L3a**].

Complex **Me_2NHC–Cu–O*t*-Bu** is likely monomeric (13.6 kcal/mol relative to **L3a–Cu–B(pin)** compared to 16.7 kcal/mol for the derived dimer; blue curve in Figure 2.1); it reacts with $B_2(pin)_2$ via transition state **ts_{TB}** (22.5 kcal/mol) to generate **Me_2NHC–Cu–B(pin)**, which is 2.8 kcal/mol more stable relative to **L3a–Cu–B(pin)**, suggesting that **$NHCMe_2$** coordinates more strongly to Cu than bis-phosphine **L3a**. **Me_2NHC–Cu–B(pin)** reacts irreversibly with styrene (11.6 kcal/mol for **ts_{CuBadd}**) to generate **Me_2NHC–Cu–alkyl** species (–19.9 kcal/mol for the conformer obtained by IRC calculation/optimization). Complex **Me_2NHC–Cu–alkyl** can either undergo Cu–H elimination via **ts_{BHE}** (5.1 kcal/mol) or allylic substitution (1.7 kcal/mol for **ts_{AS}**). Although these data suggest that reaction with the allyl phosphate (**ts_{AS}**) is more favorable than formation of the alkenyl–B(pin) (**ts_{BHE}**),

a more rigorous estimate of the relationship between $\mathbf{ts_{BHE}}$ and $\mathbf{ts_{AS}}$ would be difficult to establish. Firstly, unimolecular as opposed to bimolecular processes will show different dependencies on concentration. Secondly, as already mentioned, the precise idendity of $\mathbf{ts_{AS}}$ is probably unknown, although a structure resembling a π-allyl species should likely be entertained[40,41].

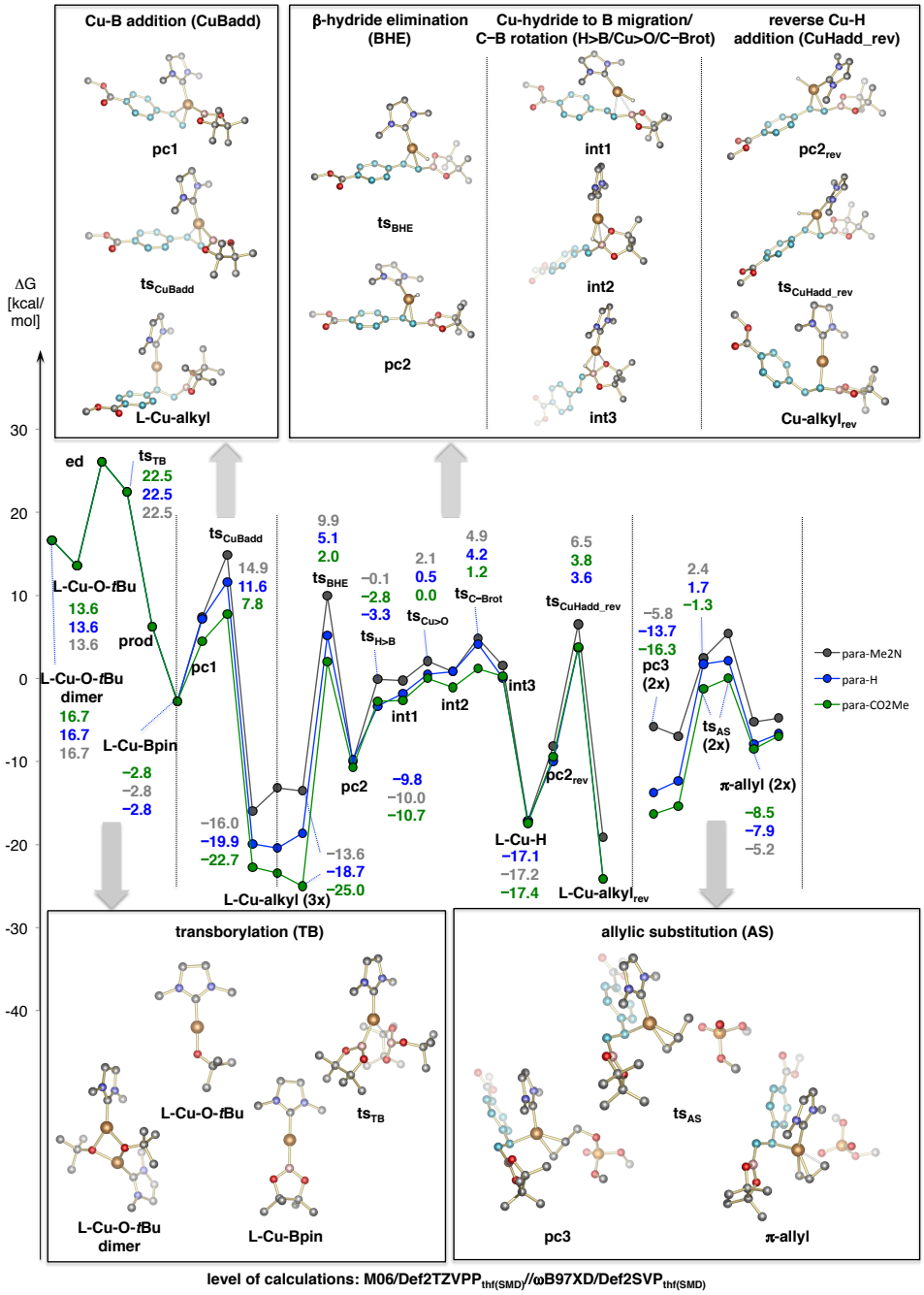


Figure 2.1. Free energy surfaces for the enantioselective Cu–B(pin) addition (CuBadd)/allylic substitution (AS) sequence with a model NHC ligand (**NHCMe$_2$**) for reaction with various aryl olefins (***p*-Me$_2$N**, grey; ***p*-H**, blue; ***p*-CO$_2$Me**, green) at the M06/DefTZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{thf(SMD)}$ level. Several conformers are shown for **ts$_{AS}$** and **L–Cu–alkyl**. The free energies have been referenced to the most stable **L3a–Cu–B(pin)** conformer, which takes into account the free energy for ligand displacement (cf. Figure 6.1); the computed structures for L = ***p*-CO$_2$Me-styrene** are displayed. Abbreviations: **TB**, transborylation [conversion of Cu–alkoxide to Cu–B(pin)]; **BHE**, β-hydride (or Cu–H) elimination; **pc**, π-complex; **ts$_{H>B}$**, transition state for hydride migration to boron; **ts$_{Cu>O}$**, transition state for Cu migration to oxygen on Bpin; **ts$_{C\text{-}Brot}$**, transition state for C–B bond rotation; **ts$_{CuHadd_rev}$**, transition state Cu–H addition leading to Cu–alkyl$_{rev}$ species with opposite regiochemistry; **int**, intermediate; **Cu–H**, linear Cu-hydride species.

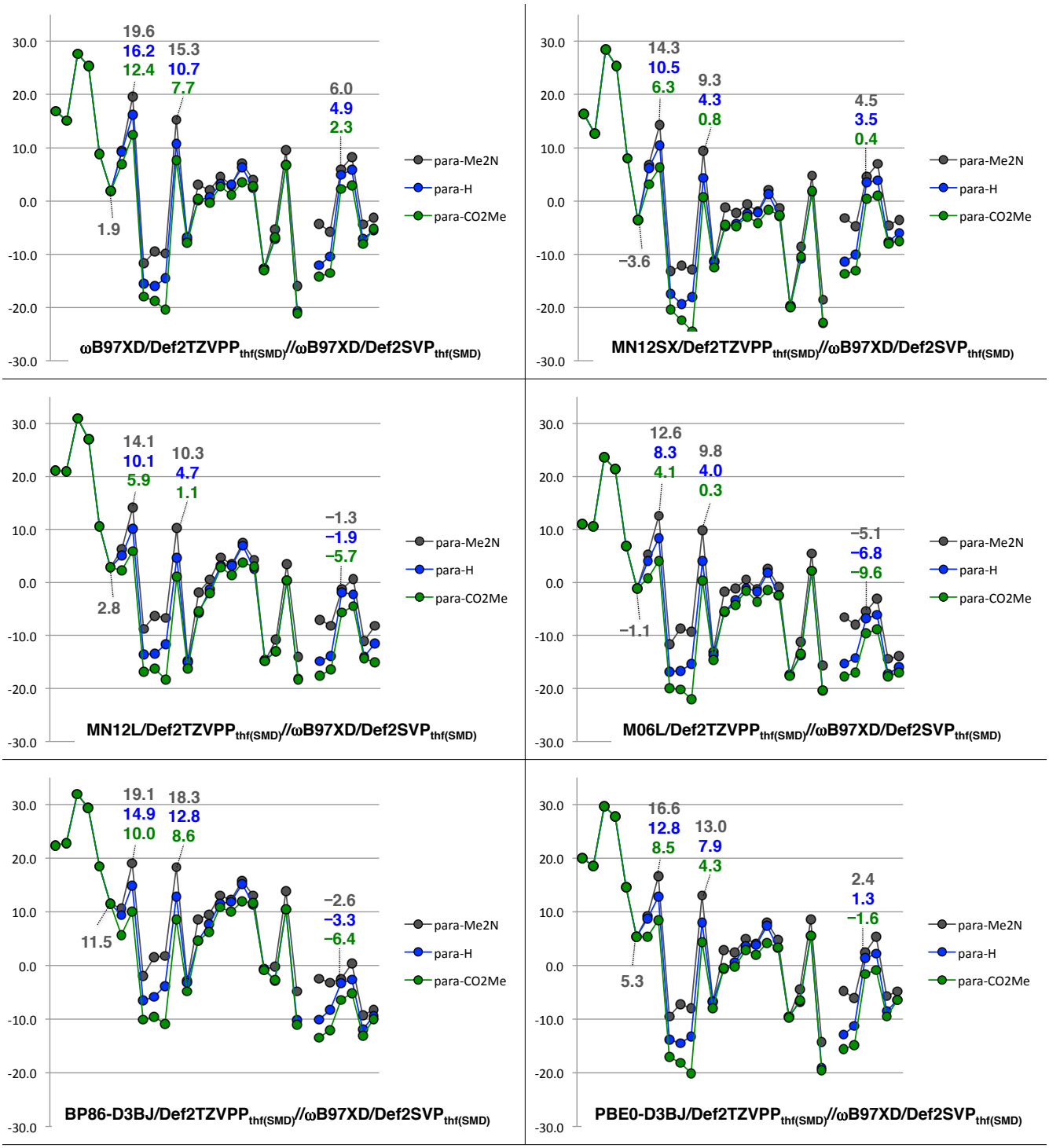


Figure 2.2. Free energy surfaces for the enantioselective Cu–B(pin) addition (CuBadd)/allylic substitution (AS) sequence with a model NHC ligand (**NHCMe$_2$**) for reaction with various styrene derivatives (***p*-Me$_2$N**, grey; ***p*-H (styrene)**, blue; ***p*-CO$_2$Me**, green) with various density functionals after optimization with ωB97XD/Def2SVP$_{thf(SMD)}$. For details, see Figure 2.1.

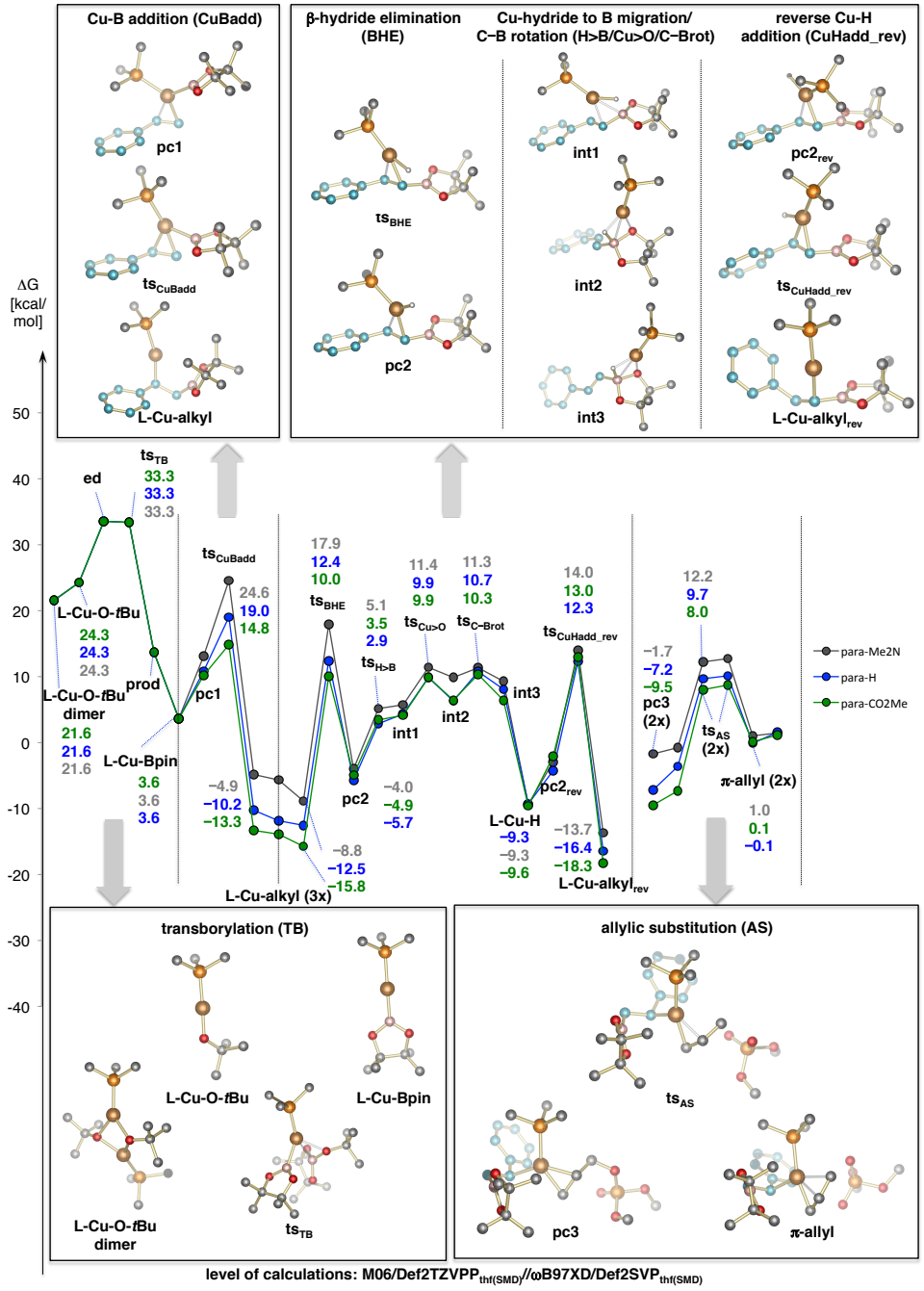


Figure 3.1. Free energy surfaces for the enantioselective Cu–B(pin) addition (CuBadd)/allylic substitution (AS) sequence with a model phosphine ligand (**PMe$_3$**) for reaction with various aryl olefins (***p*-Me$_2$N**, grey; ***p*-H (styrene)**, blue; ***p*-CO$_2$Me**, green) at the M06/DefTZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{thf(SMD)}$ level. Several conformers are shown for **ts$_{AS}$** and **L–Cu–alkyl**. The free energies have been referenced to the most stable **L3a**-Cu-Bpin conformer, which takes into account the free energy for ligand displacement (see Figure 6.1); the computed structures for L = ***p*-CO$_2$Me-styrene** are displayed. Abbreviations: **TB**, transborylation [conversion of Cu–alkoxide to Cu–B(pin)]; **BHE**, β-hydride (or Cu–H) elimination; **pc**, π-complex; **ts$_{H>B}$**, transition state for hydride migration to boron; **ts$_{Cu>O}$**, transition state for Cu migration to oxygen on Bpin; **ts$_{C\text{-}Brot}$**, transition state for C–B bond rotation; **ts$_{CuHadd_rev}$**, transition state Cu–H addition leading to Cu–alkyl$_{rev}$ species with reversal of regiochemistry; **int**, intermediate; **Cu–H**, linear Cu-hydride species.

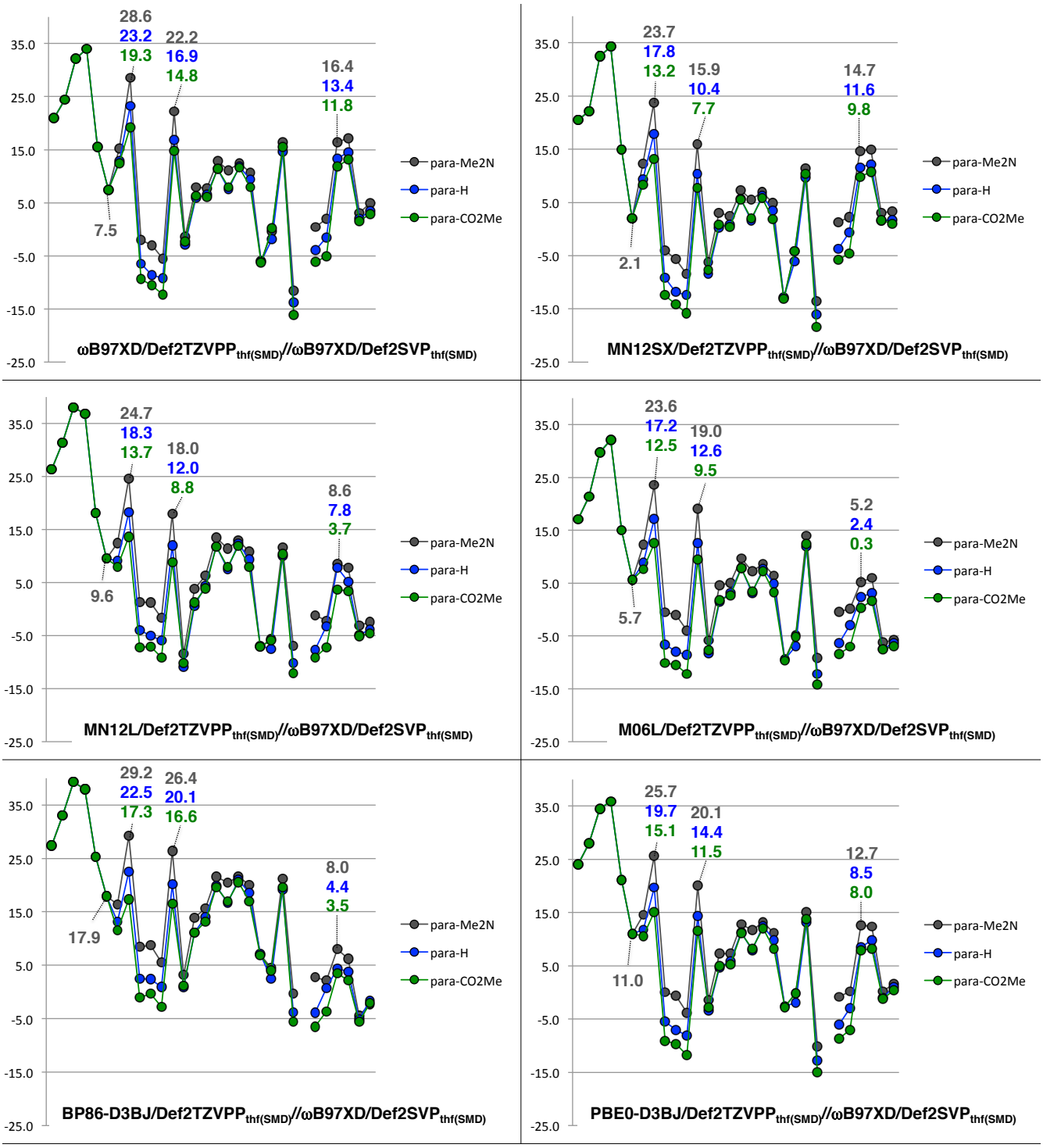
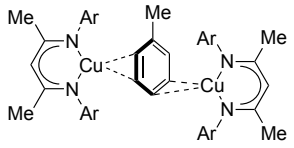


Figure 3.2. Free energy surfaces for the enantioselective Cu–B(pin) addition (CuBadd)/allylic substitution (AS) sequence with a model phosphine ligand (**PMe$_3$**) for reaction with various aryl olefins (***p*-Me$_2$N**, grey; ***p*-H (styrene)**, blue; ***p*-CO$_2$Me**, green) with various density functionals after optimization with ωB97XD/Def2SVP$_{thf(SMD)}$. For details, see Figure 3.1.

Feasibility of Cu–H re-addition as a possible reason for lowering of e.r. In search of a rationale regarding the diminution in enantioselectivity when allyl phosphate concentration is decreased, we first considered a Cu–H elimination/re-addition sequence. Nonetheless, Cu–H addition to the opposite enantiotopic face of the *same* alkenyl–B(pin) molecule seems unlikely, especially considering the substantial amounts of unreacted aryl olefin present.

Nevertheless, one feasible mechanism for Cu–H re-addition to the opposite face of the alkenyl–B(pin) without dissociation from that olefin might be as follows: migration of **L–Cu–H** from the double bond in **pc2** toward boron to generate borate[45] species **int2** (Figure 2.1), which would allow for rotation around the C–B bond ($\mathbf{ts_{Cu\text{-}Brot}}$, 3.6 kcal/mol) and addition to the opposite face of the olefin. Computational studies reveal that such a pathway would be energetically much less favored compared to formation of the separated entities [i.e., **L–Cu–H** + alkenyl–B(pin), –17.1 kcal/mol]. The absence of a stable adduct with the linear **L–Cu–H** species suggests that olefin exchange followed by Cu–H addition to a different olefin is preferred. What is more, we have been unable to locate a stable adduct between **L–Cu–H** and the aromatic ring moiety of the model alkenyl–B(pin) complex. Unlike bent β-diketiminate-Cu species (shown below), reported to form isolable adducts with toluene[45c], binding of a linear **L–Cu–H** species is unfavorable due to the energy required to distort the linear geometry (see Figure 10.1 for the **L–Cu–Me** species).



Site Selectivity of Cu–H addition to an aryl-substituted alkenyl–B(pin) compound. Cu–H addition to an alkenyl–B(pin) compound probably occurs with the opposite site selectivity compared to a monosubstituted aryl olefin (3.6 kcal/mol for $\mathbf{ts_{CuHadd\_rev}}$ vs. 5.1 kcal/mol for $\mathbf{ts_{BHE}}$), leading to linear $\mathbf{NHCMe_2–Cu–alkyl_{rev}}$ species with the Cu atom bound to homobenzylic carbon bearing the Bpin group (Figure 2.1). The latter scenario has been verified through spectroscopic investigations (see NMR experiments, Section 14) with ligand **L3c** (i.e., **L3c–Cu–H** generation from PHMS and **L3c–Cu–O*t*-Bu**, followed by addition to alkenyl–B(pin) substrates, synthesized independently, leads to generation of $\mathbf{L3c–Cu–alkyl_{rev}}$). The proposed site selectivity of Cu–H addition to an alkenyl–B(pin) is supported by the pioneering report of Sadighi[46].

Next, we investigated the significance of the electronic properties of aryl olefin substrates. Cu–B(pin) addition is significantly more favored with *p*-methylesterstyrene (7.8 kcal/mol for $\mathbf{ts_{CuBadd}}$) compared to *p*-dimethylaminostyrene (14.9 kcal/mol), which is also reflected in the greater reaction exothermicity

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(45) Copper–borohydride complexes are isolable compounds: (a) Lippard, S. J. & Melmed, K. M. *J. Am. Chem. Soc.* **89**, 3929–3930 (1967). (b) Lippard, S. J. & Ucko, D. A. *Inorg. Chem.* **7**, 1051–1056 (1968). (c) Nako, A. E., White, A. J. P. & Crimmin, M. R. *Dalton Trans.* **44**, 12530–12534 (2015). For a review on three-center/two-electron bonds in inorganic compounds, see: (d) Green, J. C., Green, M. L. H. & Parkin, G. *Chem. Commun.* **48**, 11481–11503 (2012).(

(46) Laitar, D. S., Tsui, E. Y. & Sadighi, J. P. *Organometallics* **25**, 2405–2408 (2006).

(–25.0 kcal/mol for the lowest **L–Cu–alkyl** conformer; green curve in Figure 2.1). The positive effect of an electron-withdrawing aryl substituent on reaction rate suggests that background reactivity starting from phosphine-free CuO*t*-Bu species might be significantly higher than association of bis-phosphine **L3a** with the phosphine-free Cu–Bpin intermediate (see Figure 4a in the manuscript).

The effect of an electron-withdrawing substituent on rate (transition state effect) appears to be considerably larger than the ability of an electron-withdrawing styrene to stabilize various $(CuO\textit{t}\text{-}Bu)_n$ species (ground state effect), ruling out styrene assisted deaggregation of oligomeric/polymeric $(CuO\textit{t}\text{-}Bu)_n$ species as reason for e.r. fluctuations (see also the discussion associated with Figures 8–9 below). Furthermore, the decreased nucleophilicity of the **Me_2NHC–Cu–alkyl** species derived from *p*-methylesterstyrene reduces the rate of allylic substitution (–1.3 kcal/mol for $\mathbf{ts_{AS}}$, which corresponds to a barrier of 26.3 kcal/mol relative to the most stable **Me_2NHC–Cu–alkyl** species; green curve, Figure 2.1). In the case of the substrate bearing a *p*-dimethylaminoaryl moiety the energy of $\mathbf{ts_{AS}}$ is 2.4 kcal/mol, corresponding to a barrier of only 18.4 kcal/mol (relative to the most stable **Me_2NHC–Cu–alkyl** species; grey curve, Figure 2.1). The lower reactivity of the **Me_2NHC–Cu–alkyl** species derived from *p*-methylesterstyrene towards allylic substitution (AS) renders the alternative Cu–H elimination pathway more competitive (2.0 kcal/mol for $\mathbf{ts_{BHE}}$, which is only 3.3 kcal/mol above $\mathbf{ts_{AS}}$). With *p*-dimethylaminoaryl system the energy difference between $\mathbf{ts_{BHE}}$ and $\mathbf{ts_{AS}}$ is larger (7.5 kcal/mol).

Similar trends are obtained when the calculations are performed in presence of a neutral **PMe_3** model ligand (Figure 3 compared to L = **$NHCMe_2$**, Figure 2). Notable distinctions are the greater propensity of the **Me_3P–Cu–O*t*-Bu** species to dimerize (21.6 kcal/mol for dimer vs. 24.3 kcal/mol for monomer; Figure 3.1), likely reflecting the lower nucleophilicity of the d orbitals on Cu in **Me_3P–Cu–O*t*-Bu**[40]. Further, **Me_3P–Cu–B(pin)** is 3.6 kcal/mol above **L3a–Cu–B(pin)**, whereas **Me_2NHC–Cu–B(pin)** is more stable than the reference point with ligand **L3a** (–2.8 kcal/mol; Figure 2.1). The lower binding affinity of phosphine as opposed to NHC ligands likely renders reactions promoted by phosphines more prone to undesired reactivity resulting from ligand loss.

Differences Between Density Functionals in Figures 2–3

Despite the similarity in trends between various density functionals there are notable distinctions. For example, **Me_2NHC–Cu–B(pin)** is more stable than **L3a–Cu–B(pin)** only with functionals M06, MN12SX and M06L (–2.8, –3.6 and –1.1 kcal/mol, respectively; Figure 2.2). PBE0-D3BJ and particularly BP86-D3BJ, which tend to overestimate dispersion when the large bis-phosphine **L3a** is involved, predict **Me_2NHC–Cu–B(pin)** to be 5.3 and 11.5 kcal/mol, respectively, less stable than **L3a–Cu–B(pin)** (Figure 2.2). Presumably, the energy for binding of the bis-phosphine ligand to Cu is overestimated. (Because spectroscopic experiments, as detailed in Section 14, indicate facile loss of the chiral ligand, the results with BP86-D3BJ are unlikely to be correct). Another instance where appropriate modeling of dispersion forces is central relates to the comparison of unimolecular (e.g., hydride Cu–H elimination) as opposed to bimolecular pathways (e.g., allylic substitution). For example, while there is a small energy gap between $\mathbf{ts_{BHE}}$ and $\mathbf{ts_{AS}}$ with functional M06 (5.1 vs. 1.7

kcal/mol; blue curve in Figure 2.1), with functional BP86-D3BJ $\mathbf{ts_{AS}}$ is favored significantly over $\mathbf{ts_{BHE}}$ (–3.3 vs. 12.8 kcal/mol; blue curve in Figure 2.2). Functional BP86-D3BJ probably provides an unsatisfactory representation of the mechanism, since the experimental results suggest competitiveness between Cu–H elimination and allylic substitution. The smallest energy gap between $\mathbf{ts_{BHE}}$ and $\mathbf{ts_{AS}}$ is predicted with functional MN12SX (4.3 vs. 3.5 kcal/mol; blue curve in Figure 2.2). Nearly identical trends to those described for L = $\mathbf{NHCMe_2}$ are observed with L = $\mathbf{PMe_3}$ as the model phosphine (Figure 3.2).

Regarding Displacement of a Bis-phosphine from a Cu Complex by an Aryl Olefin or a Solvent Molecule (Figures 4–7)

Comparison of free energy surfaces for Cu–B(pin) addition with various supporting ligands (L) at the M06/Def2TZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{thf(SMD)}$ level are shown in Figure 6.1. (For the individual free energy surfaces with L = styrene or thf, see Figures 4 and 5, respectively.) The graphs in Figure 6.1 offer insight regarding the ability of a select number of neutral ligands to stabilize intermediates and transition states along the catalytic cycle. For example, replacement of **L3a** from **L3a–Cu–B(pin)** (0.0 kcal/mol; grey curve in Figure 6.1) by $\mathbf{NHCMe_2}$ leads to an energy gain of 2.8 kcal/mol (red curve). Likewise, substitution of $\mathbf{PMe_3}$ affords a slightly less stable structure (3.6 kcal mol; brown curve).

Styrene and thf are relatively inferior Cu ligands (13.6 and 16.0 kcal/mol; blue and light blue curves). The high energies for transitions states $\mathbf{ts_{CuBadd}}$ and $\mathbf{ts_{BHE}}$ for L = thf (39.2 and 33.8 kcal/mol) rule out the feasibility of solvent-stabilized species as reactive intermediates. The situation is less straightforward with styrene. Changing the reference point from a common **L3a–Cu–B(pin)** intermediate to each individual **L–Cu–B(pin)** species (Figure 7) sheds some light on the impact of the electronic nature of L and the facility of each step. It appears that while π-donor ligands (thf) destabilize square planar transitions states $\mathbf{ts_{CuBadd}}$ and $\mathbf{ts_{BHE}}$ (23.2 and 17.8 kcal/mol; light blue curve in Figure 7), π-acceptor ligands exert a more positive impact in this regard (e.g., styrene; 9.3 and 4.8 kcal/mol; blue curve in Figure 7). Competitive π-back-donation from Cu to the styrene molecules may facilitate movement of the B(pin) nucleophile across the lobes of the transition metal's d_{xy} orbital. In other words, Cu–styrene coordination through σ-donation becomes more important, rendering the π*-orbital on styrene more electrophilic [more facile Cu–B(pin) addition]. These considerations suggest that, at sufficiently high styrene concentration, a Cu–B(pin) addition pathway that is bimolecular in styrene (cf. Scheme 15) might become competitive (23.0 and 16.9 kcal/mol for $\mathbf{ts_{CuBadd}}$ with L = styrene and L = **L3a**, respectively; Figures 6.1). Based on similar principles, β–H (or Cu–H) elimination might be favored with a π-accepting (electron-deficient) aryl olefin (4.8 and 17.8 kcal/mol for $\mathbf{ts_{BHE}}$ with L = styrene and L = thf; blue and light blue curves, Figure 7). It is therefore plausible that an aryl olefin might negatively impact enantioselectivity because competition between styrene and an allyl electrophile for **L3a–Cu–alkyl** could result in loss of the bis-phosphine ligand, followed by styrene-promoted Cu–H elimination via $\mathbf{ts_{BHE}}$ (L = styrene, 18.4 kcal/mol; blue curve, Figures 6.1); such a process is capable of being competitive with allylic substitution involving bis-phosphine–Cu–alkyl complex ($\mathbf{ts_{AS}}$ with L = **L3a** is 16.6 kcal/mol; grey curve, Figures 6.1). The findings illustrated in

Figure 7 further illustrate that allylic substitution processes involving **L3a–Cu–alkyl** might be particularly challenging due to steric hindrance. Whereas $\mathbf{ts_{CuBadd}}$ (15.4 kcal/mol) is significantly higher in energy compared to $\mathbf{ts_{AS}}$ (6.1 kcal/mol) with the smaller PMe_3 ligand, the two transition states have nearly identical energies with ligand **L3a** (16.9 and 16.6 kcal/mol, respectively; Figure 7).

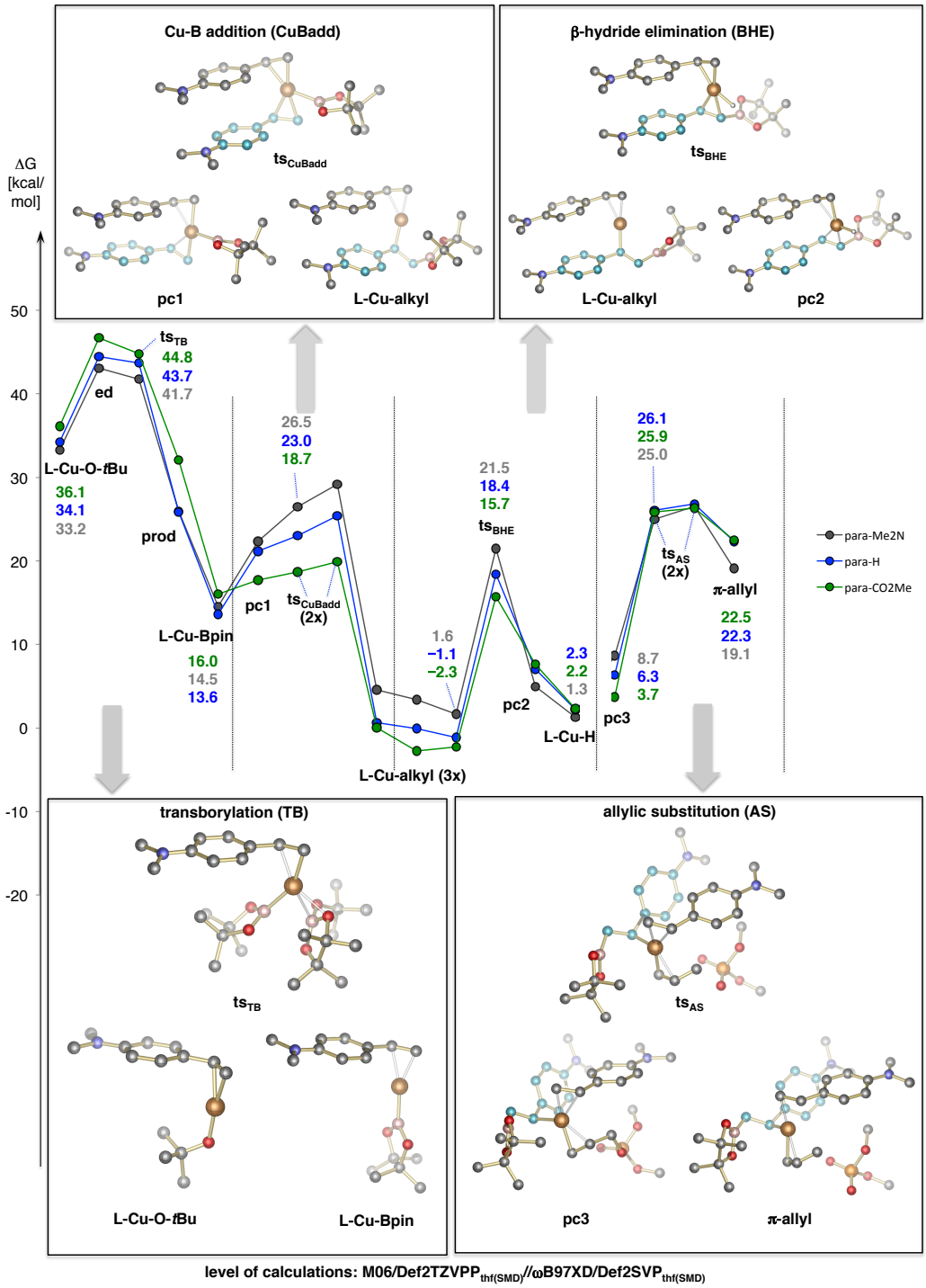

Figure 4.1. Free energy surfaces for the enantioselective Cu–B(pin) addition (CuBadd)/allylic substitution (AS) sequence with styrene derivatives as the supporting ligand (***p*-Me$_2$N**, grey; ***p*-H (styrene)**, blue; ***p*-CO$_2$Me**, green) at the M06/DefTZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{thf(SMD)}$ level. Several conformers are shown for **ts$_{CuBadd}$**, **ts$_{AS}$** and **L–Cu–alkyl**. The free energies have been referenced to the most stable **L3a–Cu–B(pin)** conformer, which takes into account the free energy for ligand displacement (see Figure 6.1); the computed structures for L = ***p*-Me$_2$N-styrene** are displayed. Abbreviations: **TB**, transborylation [conversion of Cu–alkoxide to Cu–B(pin)]; **BHE**, β-hydride (Cu–H) elimination; **pc**, π-complex.

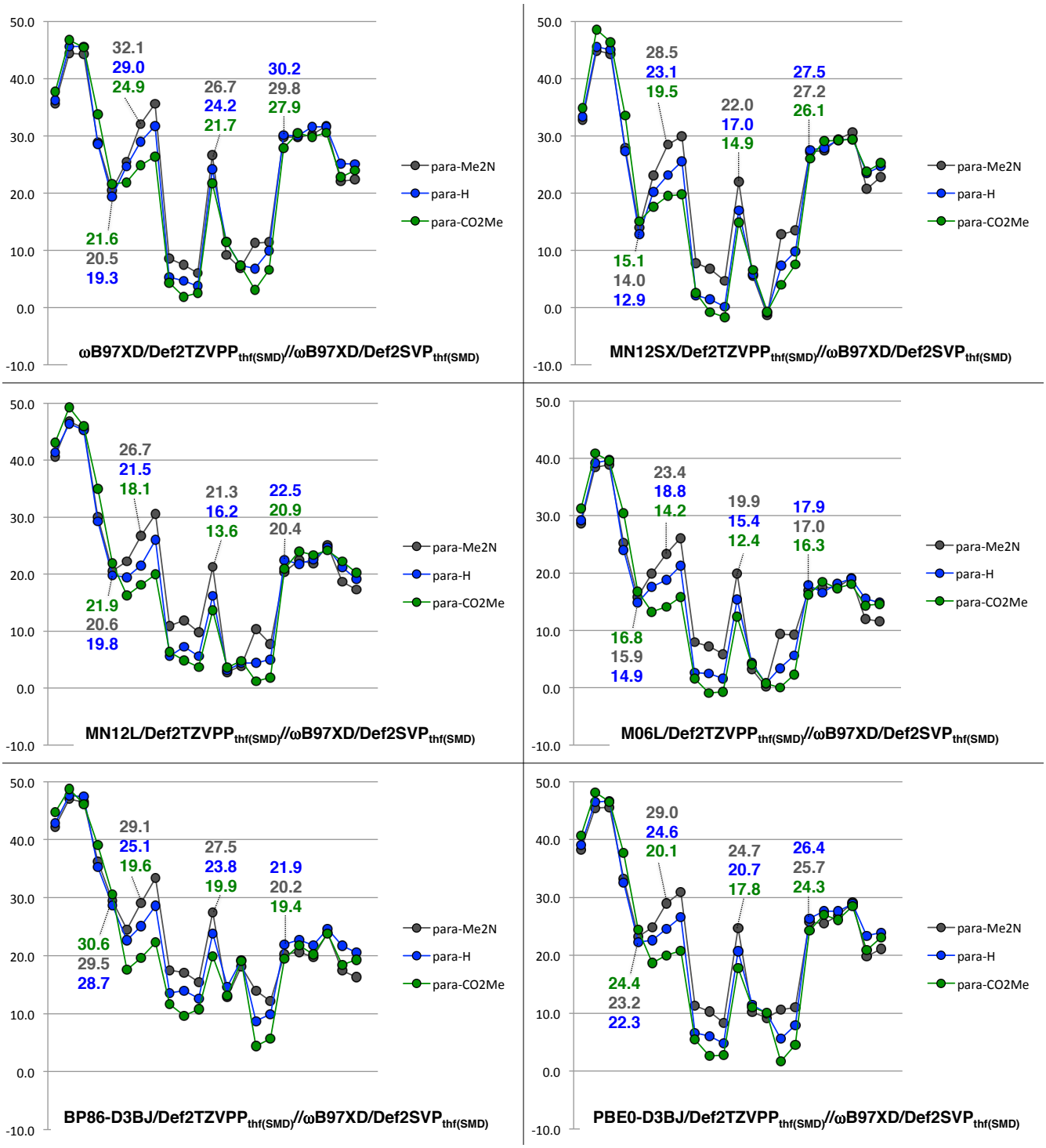

Figure 4.2. Free energy surfaces for the enantioselective Cu–B(pin) addition (CuBadd)/allylic substitution (AS) sequence with styrene derivatives as the supporting ligand (***p*-Me$_2$N**, grey; ***p*-H (styrene)**, blue; ***p*-CO$_2$Me**, green) with various density functionals after optimization with ωB97XD/Def2SVP$_{THF(SMD)}$. For more details, see Figure 4.1.

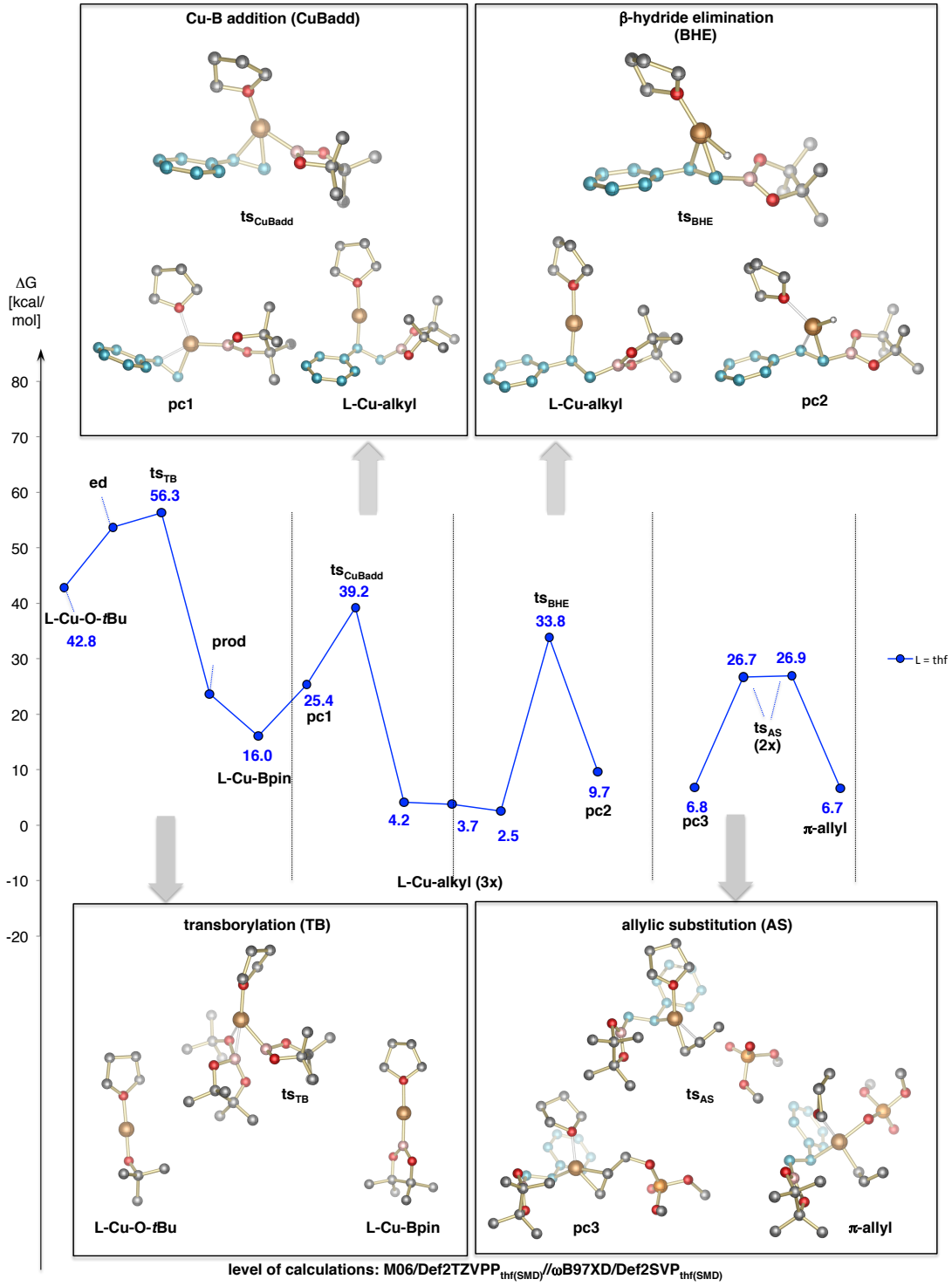

Figure 5.1. Free energy surfaces for the enantioselective Cu–B(pin) addition (CuBadd)/allylic substitution (AS) sequence with a thf molecule as the supporting ligand at the M06/DefTZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{thf(SMD)}$ level. Several conformers are shown for **ts$_{AS}$** and **L–Cu–alkyl**. The free energies have been referenced to the most stable **L3a–Cu–Bpin** conformer, which takes into account the free energy for ligand displacement (cf. Figure 6.1). Abbreviations: **TB**, transborylation [conversion of Cu–alkoxide to Cu–B(pin)]; **BHE**, β-hydride (Cu–H) elimination; **pc**, π-complex.

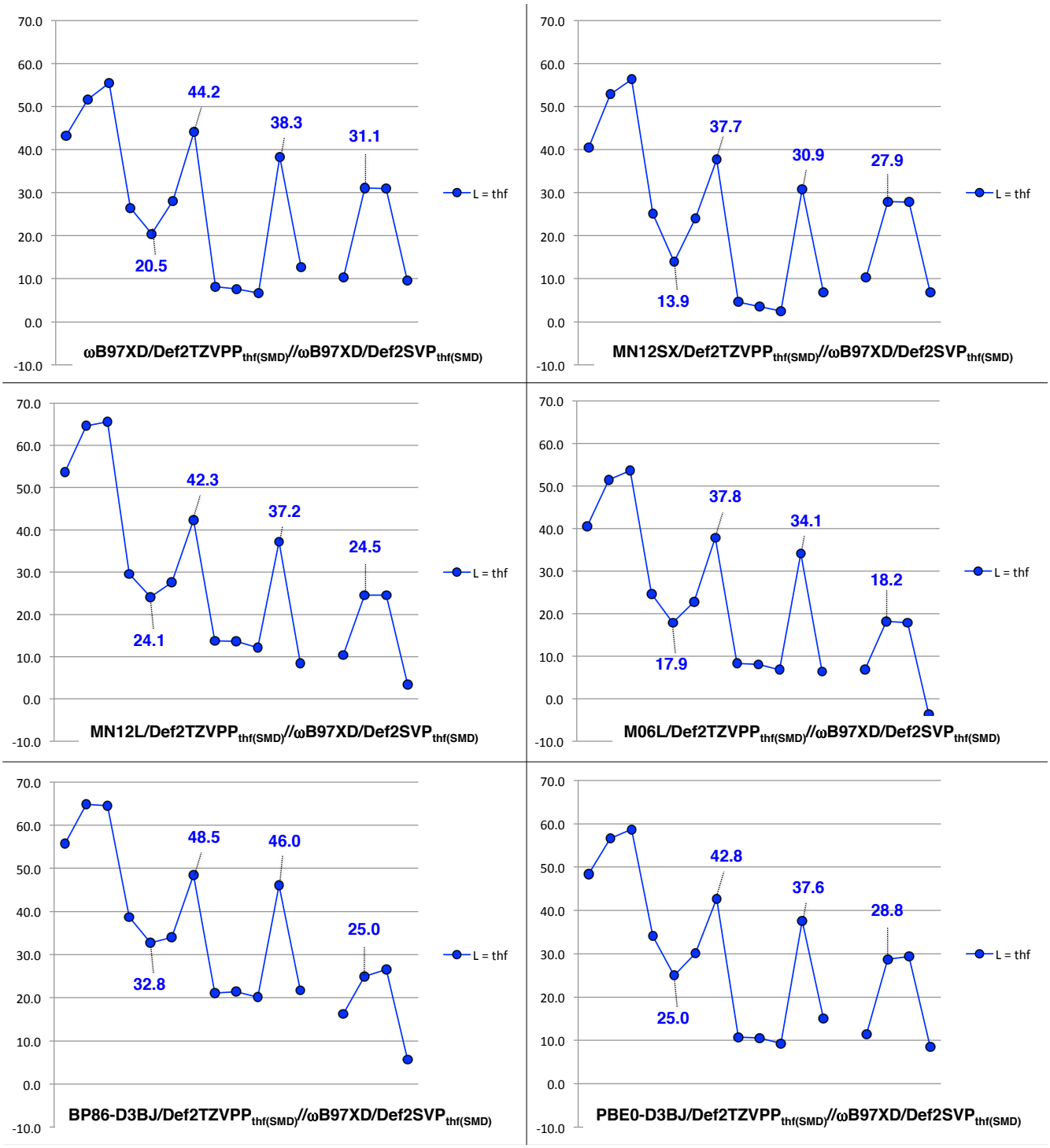

Figure 5.2. Free energy surfaces for the enantioselective Cu–B(pin) addition (CuBadd)/allylic substitution (AS) sequence with a thf molecule as the supporting ligand with different density functionals after optimization with ωB97XD/Def2SVP$_{THF(SMD)}$. For details, see Figure 5.1.

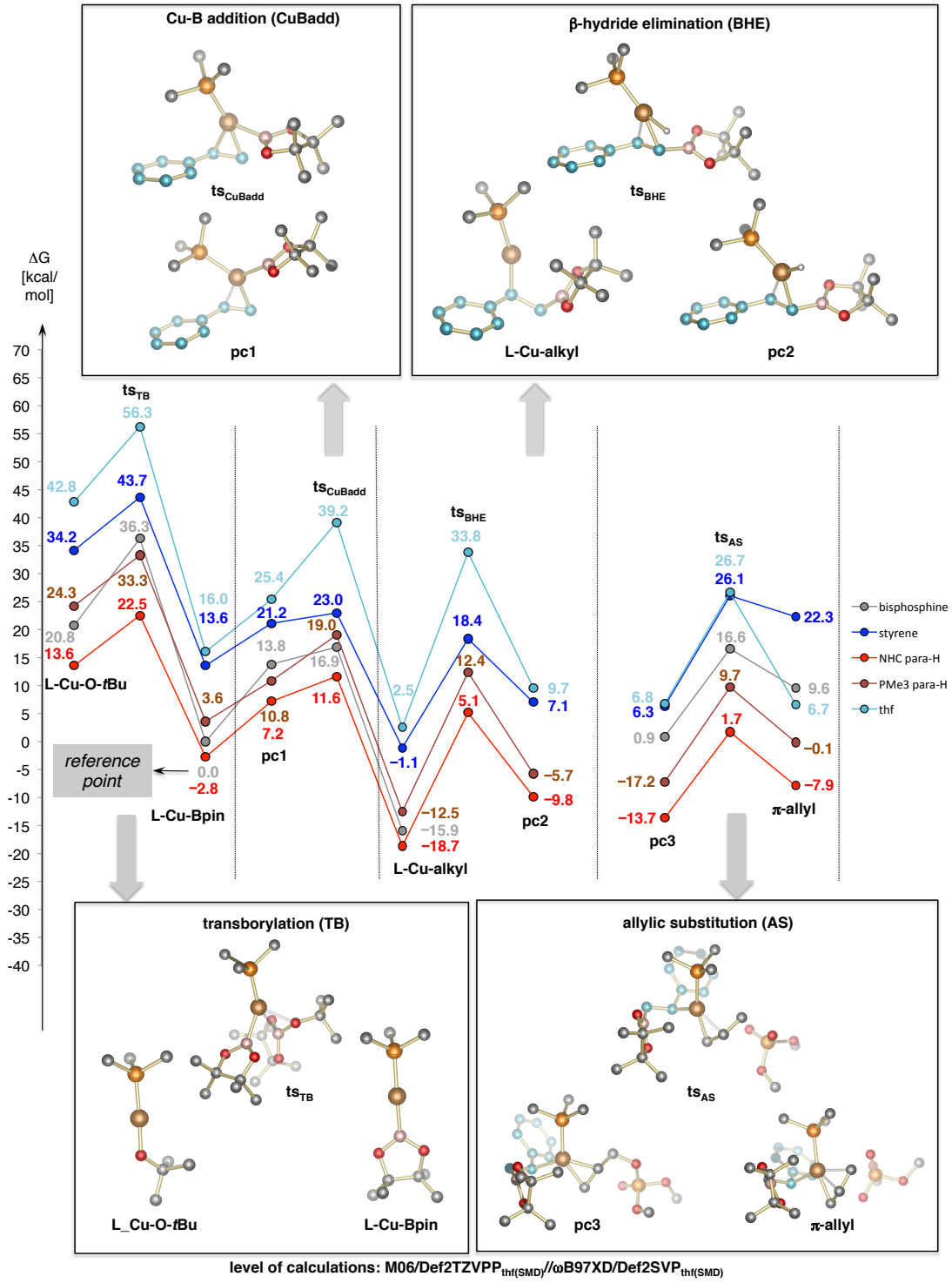

Figure 6.1. Free energy surfaces for the enantioselective Cu–B(pin) addition (CuBadd)/allylic substitution (AS) sequence in presence of various ligands L (**L3a**, grey; **styrene**, blue; model NHC ligand **NHCMe$_2$**, red; model phosphine ligand **PMe$_3$**, brown; **thf**, light blue) at the M06/DefTZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{thf(SMD)}$ level. All free energies have been referenced to the **L3a–Cu–B(pin)** species, which takes into account the free energy of ligand exchange; only computed structures for L = **PMe$_3$** are shown. Abbreviations: **TB**, transborylation [conversion of Cu–alkoxide to Cu–B(pin)]; **BHE**, β-hydride (Cu–H) elimination; **pc**, π-complex.

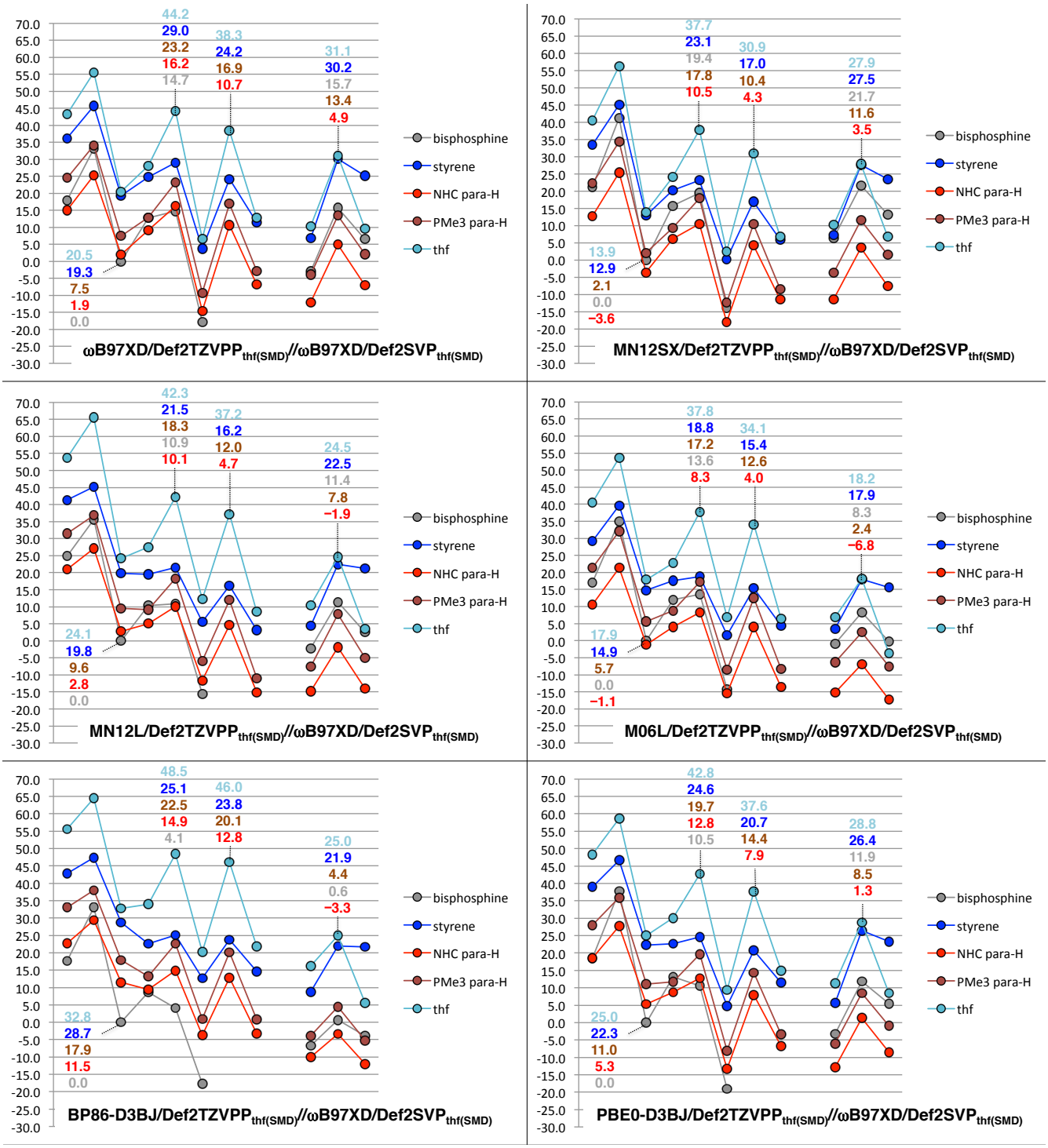

Figure 6.2. Free energy surfaces for the enantioselective Cu–B(pin) addition (CuBadd)/allylic substitution (AS) sequence in presence of various ligands L (**L3a**, grey; **styrene**, blue; model NHC ligand **NHCMe$_2$**, red; model phosphine ligand **PMe$_3$**, brown; **thf**, light blue) with various density functionals after optimization with ωB97XD/Def2SVP$_{thf(SMD)}$. For more details, see Figure 6.1.

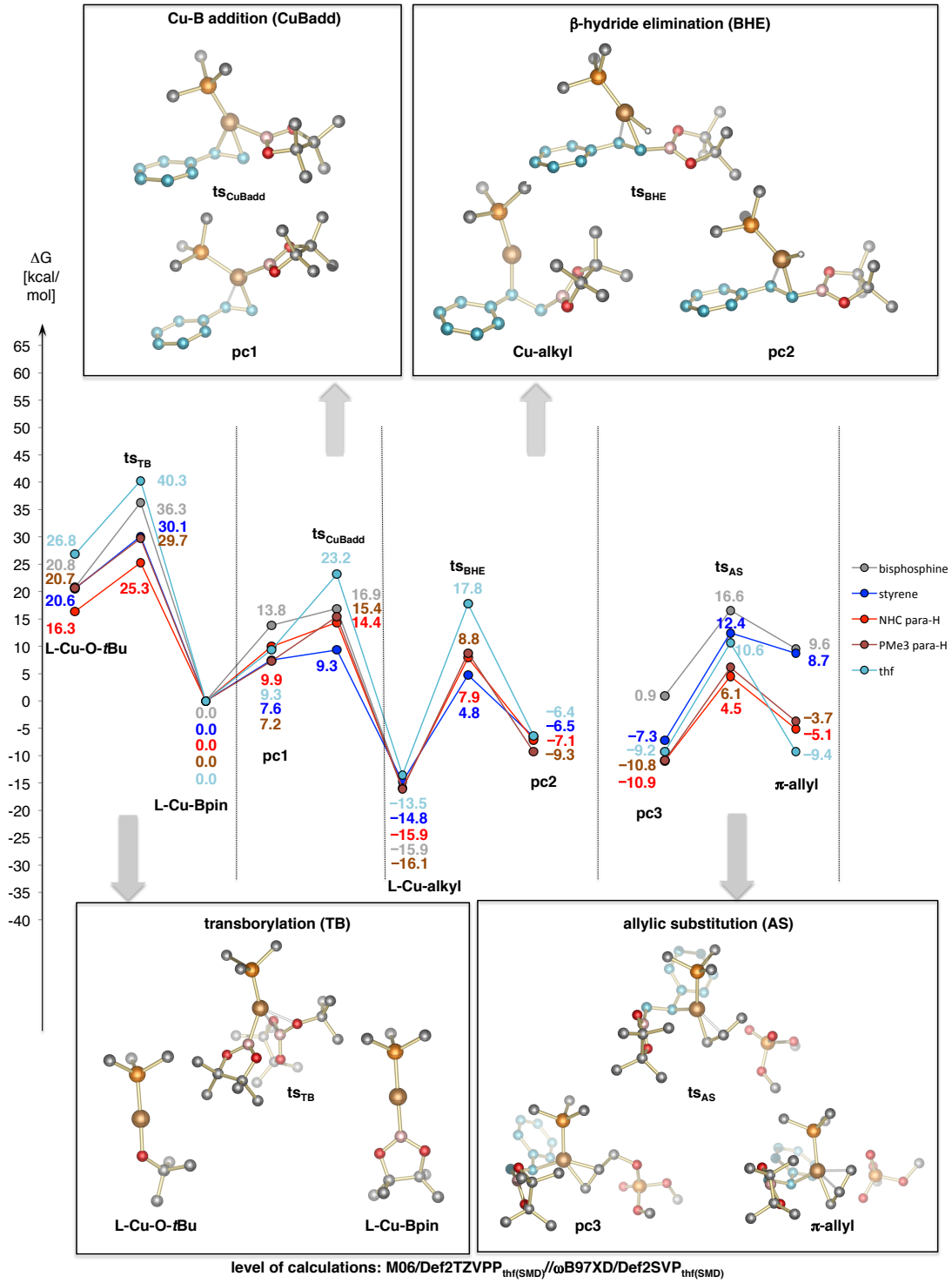

Figure 7. Free energy surfaces for the enantioselective Cu–Bpin addition (CuBadd)/allylic substitution (AS) sequence in presence of various ligands L (**L3a**, grey; **styrene**, blue; model NHC ligand **NHCMe$_2$**, red; model phosphine ligand **PMe$_3$**, brown; **thf**, light blue) at the M06/DefTZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{thf(SMD)}$ level. The free energies for a given ligand L have been referenced to the L–Cu–B(pin) species, which does not take into account the free energy of ligand exchange; only computed structures for L = **PMe$_3$** are shown. Abbreviations: **TB**, transborylation [conversion of Cu–alkoxide to Cu–B(pin)]; **BHE**, β-hydride (Cu–H) elimination; **pc**, π-complex.

Differences Between Density Functionals and the Negative Impact that an Aryl Olefins Might Have on Enantioselectivity (Figure 6.2)

There are noteworthy differences between various density functionals regarding the probability of competitive pathways, which would entail loss of bis-phosphine **L3a** and a pathway that is second-order in aryl olefin (see Scheme 15). For instance $\mathbf{ts_{CuBadd}}$ with L = **L3a** is less than 7 kcal/mol more stable than $\mathbf{ts_{CuBadd}}$ with L = styrene with M06 (6.1 kcal/mol; Figure 6.1), MN12SX (3.7 kcal/mol; Figure 6.2) and M06L (5.2 kcal/mol; Figure 6.2). (It should be noted that there is significant excess of styrene compared to bis-phosphine **L3a**.) With other density functionals a non-selective Cu–B(pin) addition mechanism that is second-order in styrene seems less likely. Similarly, styrene-induced β-hydride (Cu–H) elimination through the sequence entailing replacement of bis-phosphine **L3a**, followed by $\mathbf{ts_{BHE}}$ with L = styrene, could be responsible for lowering of enantioselectivty if predictions made with functionals M06 and particularly MN12SX were correct. That is, with MN12SX allylic substitution involving **L3a–Cu–alkyl** (21.7 kcal/mol; grey curve, Figure 6.2) is energetically more demanding than $\mathbf{ts_{BHE}}$ with L = styrene (17.0 kcal/mol; blue curve, Figure 6.2). In contrast, if the results with BP86-D3BJ, a functional, which tends to overestimate dispersion forces involving the bulky bisphosphine ligand, were correct (which is unlikely), a mechanism entailing styrene-promoted loss of ligand **L3a** could be entirely ruled out (i.e., the grey curve for L = **L3a** is significantly below the blue curve for L = styrene, Figure 6.2).

Coordinating Affinity of Aryl Olefins to CuO*t*-Bu, CuO*t*-Bu dimer, $Cu(O\textit{t}\text{-}Bu)_2^-$ and $Cu(O\textit{t}\text{-}Bu)_2^-Na^+$ (cf. Figures 8–9)

To examine the relationship between the electronic attributes of an aryl olefin and its ability to coordinate with various $(CuO\textit{t}\text{-}Bu)_n$ entities, we carried out the calculations illustrated in Figures 8–9 (M06/Def2TZVPP$_{thf(SMD)}$// ωB97XD/Def2SVP$_{thf(SMD)}$). These data show that replacement of bis-phosphine **L3a** from CuO*t*-Bu by styrene is significantly endergonic (13.4 kcal/mol, Figures 8.1) and that electron-rich aryl olefins stabilize linear alkene···Cu–O*t*-Bu structures more effectively (12.4 vs. 15.3 kcal/mol for *p*-dimethylaminostyrene vs. *p*-methylesterstyrene, respectively; Figure 8.1). The trend is reversed for the dimeric systems, where it appears that π-backbonding to the olefin becomes more of a factor (9.8, 9.6 and 8.8 kcal/mol for *p*-dimethylaminostyrene, styrene and *p*-methylesterstyrene, respectively; Figure 8.1). However, such ground states effects are unlikely to have a major impact on e.r. fluctuations because of the relatively small energy difference resulting from electronic attributes of an aryl olefin together with the relatively low binding affinity of olefins to CuO*t*-Bu species[47] comapred to a bis-phosphine.

Similar trends regarding the electronic nature of aryl olefins are observed vis-à-vis binding $Cu–(O\textit{t}\text{-}Bu)_2^-$ and $Cu–(O\textit{t}\text{-}Bu)_2^-Na^+$ (Figure 9.1). Association of *p*-methylesterstyrene is favored by 3.8

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(47) For a review on the chemistry of olefin–Cu(I) complexes, see: (a) Wang, X.-S., Zhao, H., Li, Y.-H., Xiong, R.-G. & You X.-Z. *Topics in Catalysis* **35**, 43–61 (2005). For the intramolecular chelation of olefins to Cu-O*t*Bu clusters, see: (b) Hakansson, M., Lopes, C. & Jagner, S. *Organometallics* **17**, 210–215 (1998). (c) Bellot, B. J. & Girolami, G. S. *Organometallics* **28**, 2046–2052 (2009). π-Backbonding is typically more pronounced in complexes with more nucleophilic anionic dinitrogen-containing ligands: (d) Oguadinma, P. O. & Schaper, F. *Organometallics* **28**, 6721–6731 (2009).

kcal/mol relative to *p*-NMe_2-styrene, although binding is overall highly endergonic (16.7 kcal/mol for *p*-CO_2Me-styrene; Figure 9.1); this might be attributed to the increase in repulsion between the alkoxide oxygen non-bonding electrons when they reside in a cis relationship[48]. In contrast, binding to the Cu(O*t*-Bu)$_2^-$Na$^+$ species is only slightly exergonic, with a slight preference for electron-deficient aryl olefins (0.5 and 1.1 kcal/mol relative stabilization for *p*-methylesterstyrene compared to *p*-NMe_2-styrene on the ΔG and ΔE surfaces, respectively; Figure 9.1). Here, repulsion caused by the alkoxide oxygen non-bonding electrons is countered by a Na ion[48], which can favor alkene–Cu association (G_{rel} = –0.7 kcal/mol for *p*-methylesterstyrene; Figure 9.1).

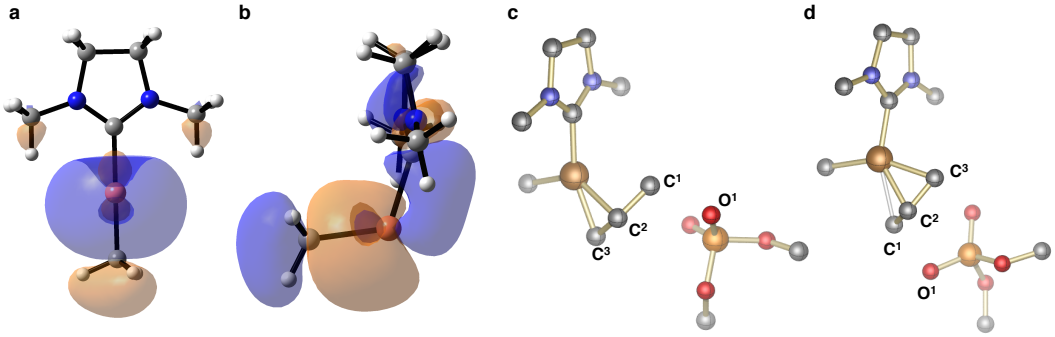
Factors that Impact S_N2' Selectivity (Figure 10)

The free energy transition states for the allylic substitution (AS) step was carried out with a system that contains a model phosphine (**PMe_3**) and NHC (**$NHCMe_2$**) ligand at the M06/Def2TZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{thf(SMD)}$ level (Figure 10.1). With L = **PMe_3** reaction of the linear nucleophilic L–Cu–Me species[40b] with allylphosphate in a S_N2'-type fashion (24.7 kcal/mol) is predicted to be 1.4 kcal/mol lower in free energy (compared to the S_N2-type transition state, 26.1 kcal/mol). A similar trend is observed with L = **$NHCMe_2$** (24.7 vs. 27.2 kcal/mol). Furthermore, it appears that the presence of an NHC ligand does not mean faster allylic substitution (compared to a phosphine); this can be attributed to the relatively high energy required to distort the L–Cu–Me species from its linear geometry into a bent form (18.0 kcal/mol required to reach a 115 ° angle vs. 14.5 kcal/mol for the corresponding PMe_3 species; Figure 10.1). It is likely that a potential positive influence of an NHC ligand may be attributed to diminished tendency for aggregate formation (as discussed above). As shown by Nakamura in connection to anionic cuprate complexes[40,41a], such "hetero-cuprate" Cu(I)–alkyl species in their bent form (Scheme 17a; stronger Me compared to weaker NHC/phosphine donor) display an increased orbital coefficient on the d_{xy} orbital lobe that is *cis* to the more nucleophilic alkyl group (HOMO at an angle of 115º; Scheme 17b); this favors addition of the allyl electrophile so that the larger coefficient on C3 is *trans* to less nucleophilc/neutral NHC/phoshpine ligand (Scheme 17c). In addition to these electronic effects, the involvement of a chelate interaction between a phosphate/carboxylate leaving group with either a cyanide ligand (as proposed by Nakamura)[41a] or a pendant sulfonate group[42] is probably not a necessary prerequisite for obtaining high S_N2'-selectivity, but it can assist in difficult cases such as those where a bulky allyl electrophile is involved. In other words, reactions promoted by alkyl–Cu–PR_3 species and a small/unsubstituted allyl electrophile are highly S_N2' selective (cf. Figure 4d in the manuscript). Our studies further show that allylic substitution transition state **$ts_{AS}(S_N2')$** is relatively early in character (i.e., it resembles the square-planar olefin π-complex generated from complexation to the C2=C3 double bond) with a relatively short Cu–C3 bond length of 1.978 Å and a comparatively extended Cu–C1 bond (2.468 Å). On the other hand, **$ts_{AS}(S_N2)$** is more "product-like" (that is, it more resembles the high-energy, square-planar π-allyl species), as indicated by the smaller difference between the Cu–C1

(48) A similar phenomenon has been described during polytopal rearrangements and olefin metathesis reactions of Ru carbene complexes. See: (a) Torker, S., Khan, R. K. M. & Hoveyda, A. H. *J. Am. Chem. Soc.* **136**, 3439–3455 (2014). (b) Khan, R. K. M., Torker, S. & Hoveyda, A. H. *J. Am. Chem. Soc.* **135**, 10258–10261 (2013).

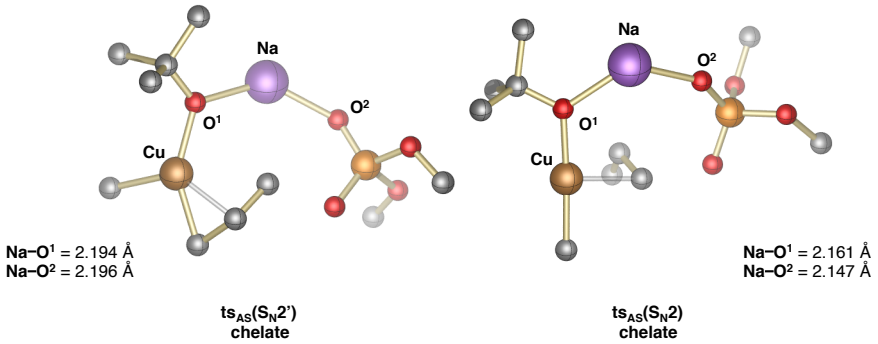
and Cu–C3 bond lengths (2.330 and 2.063 Å, respectively), which is in agreement with an earlier report[41a].

Scheme 17. S_N2' selectivity in allylic substitution (AS) promoted by "heterocuprate-like" **Me_2NHC–Cu–Me**; (a) HOMO of linear ground state; (b) HOMO of bent ground state (Me–Cu–C^{NHC} = 115 º); (c) transition state for S_N2'-type mode of addition; (d) transition state for S_N2-type mode of addition.



A similar trend, as described for Cu species bearing neutral NHC or phosphine ligands, is observed for the reaction catalyzed by **L–Cu–Me** (L = Na-O*t*Bu). The energies for **$ts_{AS}(S_N2')$** and **$ts_{AS}(S_N2)$** are 24.6 and 26.4 kcal/mol, respectively (left graph, Figure 10.1). (It should be noted that there is no intermolecular coordination between the phosphate leaving group and the Na counterion). In the alternative cases with intramolecular coordination of the phosphate leaving group to the Na cation bound to the alkoxide there is significant stabilization of both types of transition states (18.4 and 14.8 kcal/mol, respectively for **$ts_{AS}(S_N2')_{chelate}$** and **$ts_{AS}(S_N2)_{chelate}$**; cf. Figure 10.1), although this lowering in energy is likely overestimated and subject to significant uncertainties due to the presumably more complex coordination environment in solution (i.e., larger chelate structures with additional molecules of base, etc). Nonetheless, trends in energies and structural features might provide a hint for why background reactions [i.e., those catalyzed by **L–Cu–Me** (L = NaO*t*-Bu)] are less regioselective (Scheme 18). In case of the S_N2'-type transition state with a chelating interaction, the Na–O^1 and Na–O^2 bond lengths are 2.194 and 2.196 Å, respectively. This is significantly longer than when the Cu center displaces the phosphate with its d_{z^2} orbital through an S_N2-type mechanism (2.161 and 2.147 Å for Na–O^1 and Na–O^2, respectively; Scheme 18). These findings imply that **$ts_{AS}(S_N2')_{chelate}$** might be more strained, which is reflected in the larger entropy corrections to the free energy (ΔG_{corr} = 15.0 vs. 10.8 kcal/mol for **$ts_{AS}(S_N2')_{chelate}$** vs. **$ts_{AS}(S_N2)_{chelate}$**, respectively; Section 19).

Scheme 18. Geometries of transition states for allylic substitution (AS) for background reaction with a chelate bridge between *tert*-butoxide and phosphate through a Na counterion.



Intramolecular coordination of the phosphate leaving group to the Na cation bound to the alkoxide leads to significant stabilization of both types of transition states (18.4 and 14.8 kcal/mol, respectively for $\mathbf{ts_{AS}(S_N2')_{chelate}}$ and $\mathbf{ts_{AS}(S_N2)_{chelate}}$; cf. Figure 10.1), although this lowering in energy is likely overestimated and subject to significant uncertainties due to the presumably more complex coordination environment in solution (i.e., larger chelate structures with additional molecules of base, etc). Nonetheless, trends in energies and structural features might provide a hint for why background reactions are less regioselective (Scheme 18). In case of the S_N2'-type transition state with a chelating interaction, the Na–O^1 and Na–O^2 bond lengths are 2.194 and 2.196 Å, respectively. This is significantly longer than when the Cu center displaces the phosphate with its d_{z^2} orbital through an S_N2-type mechanism (2.161 and 2.147 Å for Na–O^1 and Na–O^2, respectively; Scheme 18). These findings imply that $\mathbf{ts_{AS}(S_N2')_{chelate}}$ might be more strained, which is reflected in the larger entropy corrections to the free energy (ΔG_{corr} = 15.0 vs. 10.8 kcal/mol for $\mathbf{ts_{AS}(S_N2')_{chelate}}$ vs. $\mathbf{ts_{AS}(S_N2)_{chelate}}$, respectively; Section 19).

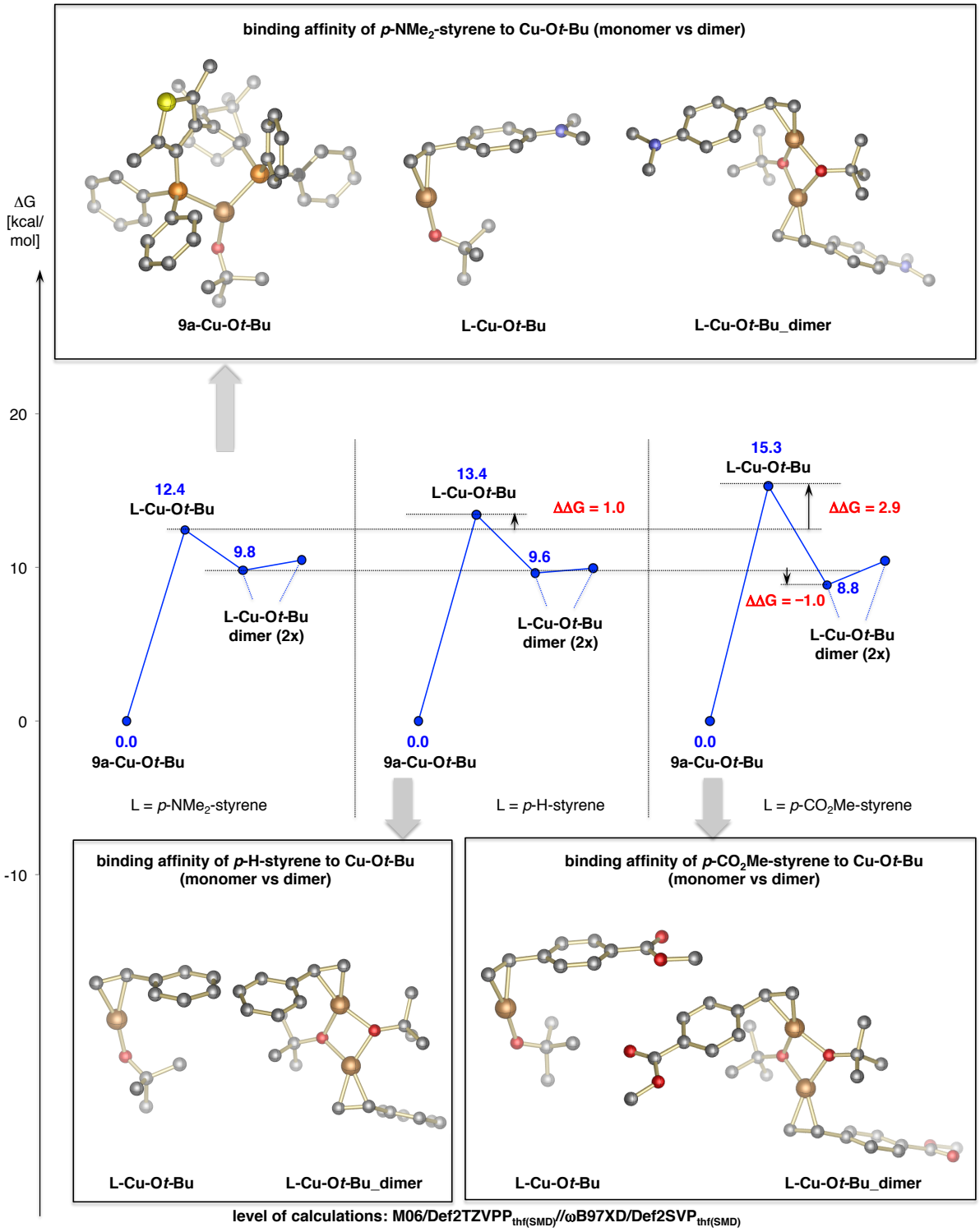


Figure 8.1. Free energy surfaces for binding affinity of various styrene derivatives (***p*-Me$_2$N**, left; ***p*-H (styrene)**, center; ***p*-CO$_2$Me**, right) to the **CuO*t*-Bu** monomer or dimer (**CuO*t*-Bu-dimer**) at the M06/DefTZVPP$_{thf(SMD)}$// ωB97XD/Def2SVP$_{thf(SMD)}$ level. Several conformers are shown for **L–CuO*t*-Bu-dimer**; the free energies have been referenced to **3La–Cu—O*t*-Bu**, which takes into account the free energy for ligand displacement (cf. Figure 6.1).

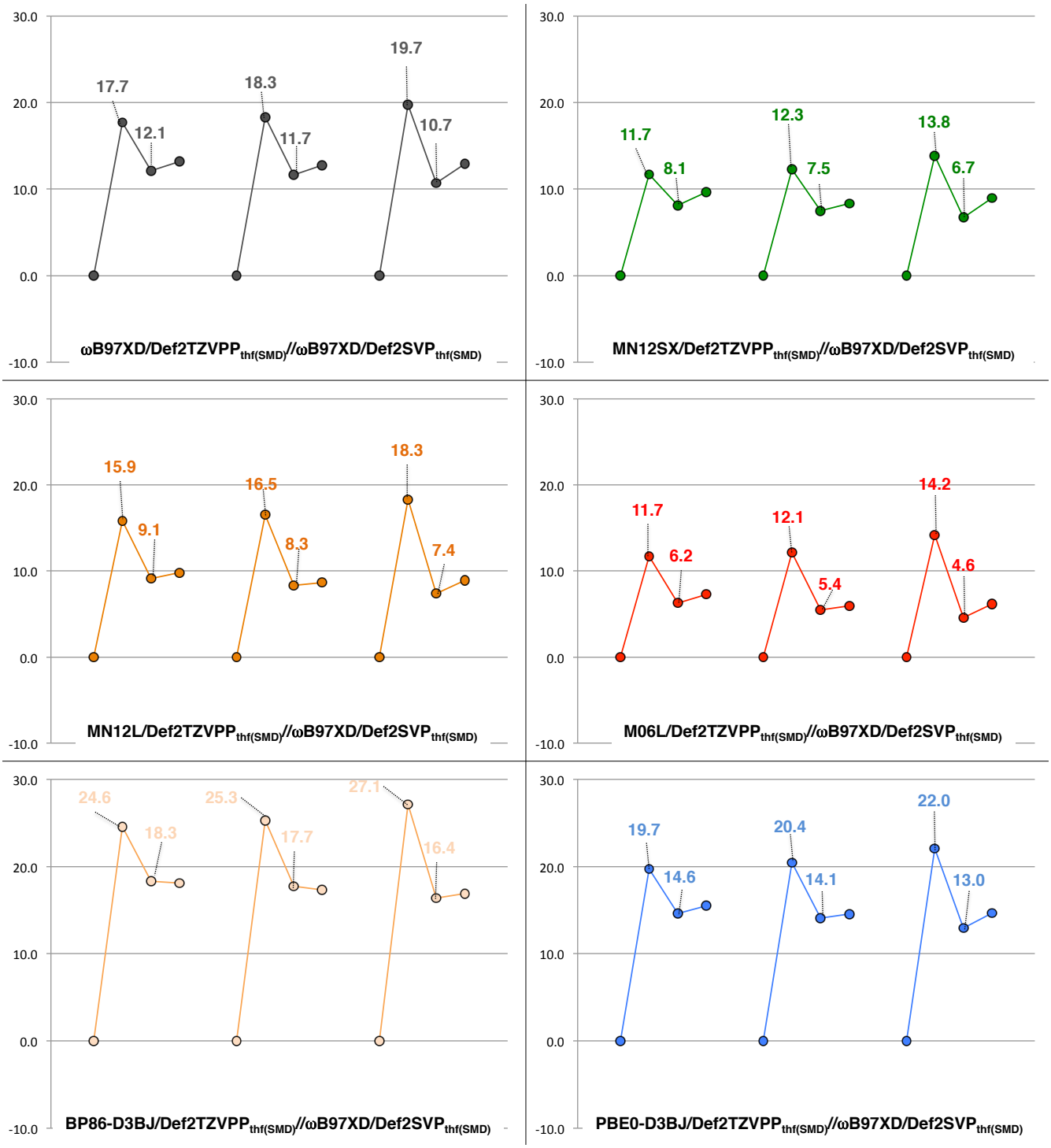


Figure 8.2. Free energy surfaces for binding affinity of various styrene derivatives (***p*-Me$_2$N**, left; ***p*-H (styrene)**, center; ***p*-CO$_2$Me**, right) to the **CuO*t*-Bu** monomer or dimer (**CuO*t*-Bu-dimer**) with various density functionals after optimization with ωB97XD/Def2SVP$_{thf(SMD)}$. For details, see Figure 8.1.

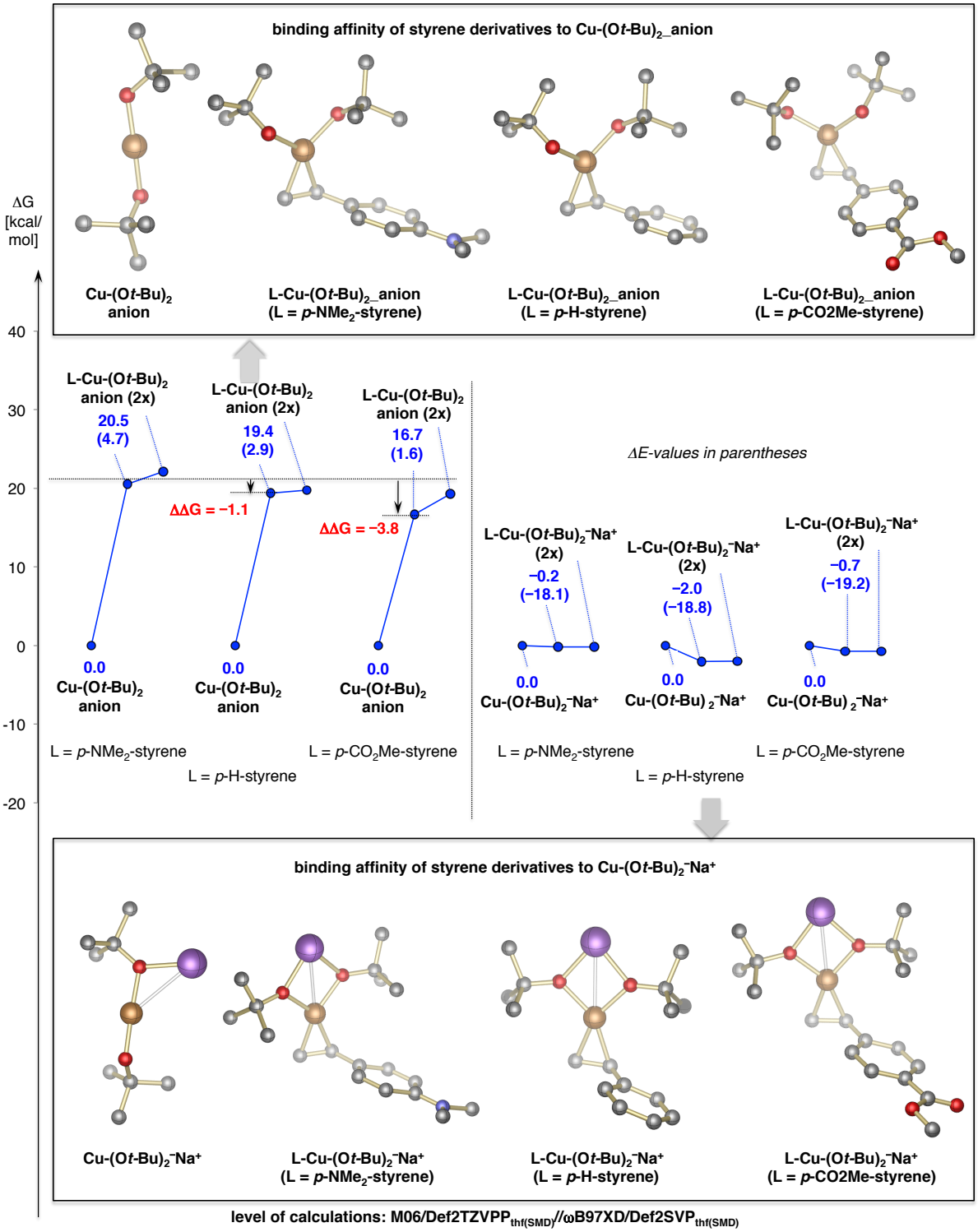


Figure 9.1. Free energy surfaces for binding affinity of various styrene derivatives (***p*-Me$_2$N**, ***p*-H** (styrene)and ***p*-CO$_2$Me**) to the **Cu–O*t*-Bu)$_2^-$** (left) and the species bound to Na (**Cu–O*t*-Bu)$_2^-$Na$^+$** (left) at the M06/DefTZVPP$_{thf(SMD)}$// ωB97XD/Def2SVP$_{thf(SMD)}$ level. Several conformers are shown. The free energies have been referenced to the linear structures for **Cu–O*t*-Bu)$_2^-$** and **Cu–O*t*-Bu)$_2^-$Na$^+$.**

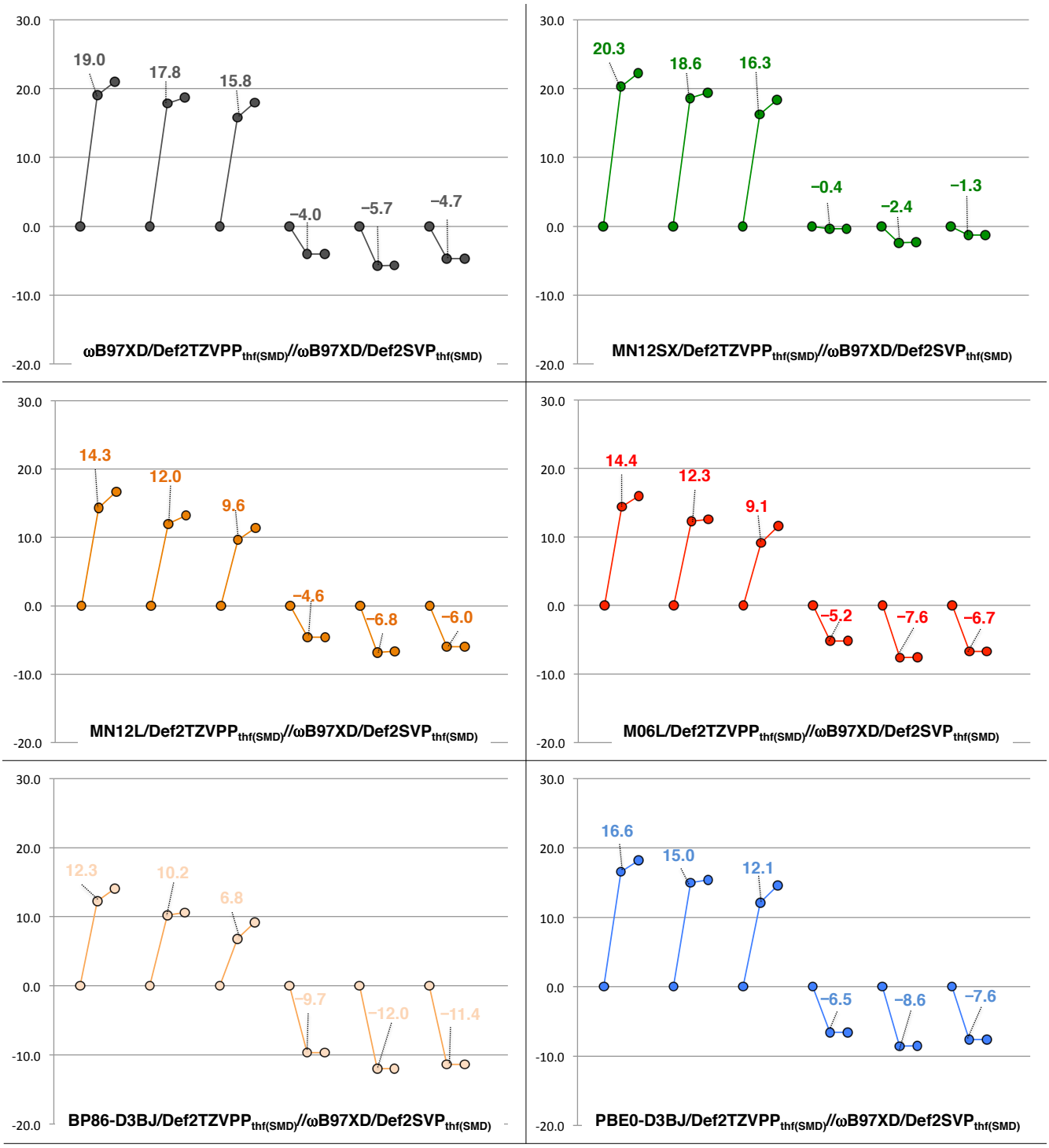


Figure 9.2. Free energy surfaces for binding affinity of various styrene derivatives (***p*-Me$_2$N**, ***p*-H** and ***p*-CO$_2$Me**) to the **Cu–O*t*-Bu)$_2^-$** (left) and the species bound to Na (**Cu–O*t*-Bu)$_2^-$Na$^+$** (left) with various density functionals after optimization with ωB97XD/Def2SVP$_{thf(SMD)}$. For details, see Figure 9.1.

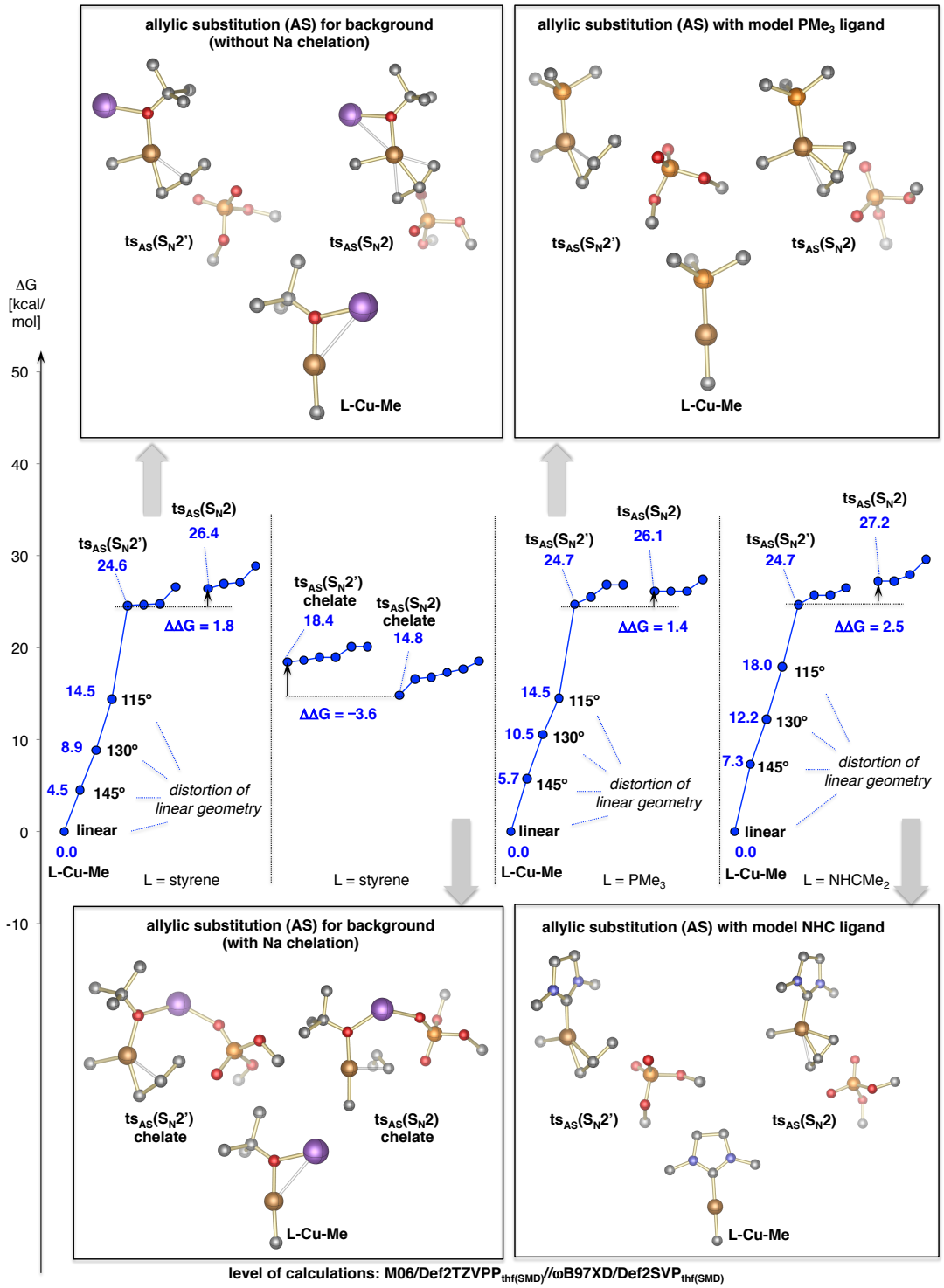


Figure 10.1. Free energy surfaces for S_N2'- and S_N2-type allylic substitution (AS) transition states with either a NaO*t*-Bu molecule, model phoshpine ligand (**PMe_3**) or model NHC ligand (**$NHCMe_2$**) as the supporting ligand at the M06/DefTZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{thf(SMD)}$ level. Several conformers are shown for **$ts_{AS}(S_N2')$** and **$ts_{AS}(S_N2)$**. The free energies have been referenced to linear Cu-alkyl species (**L–Cu–Me**); the alkyl group has been approximated by methyl (Me); only computed structures for the most stable conformers are displayed.

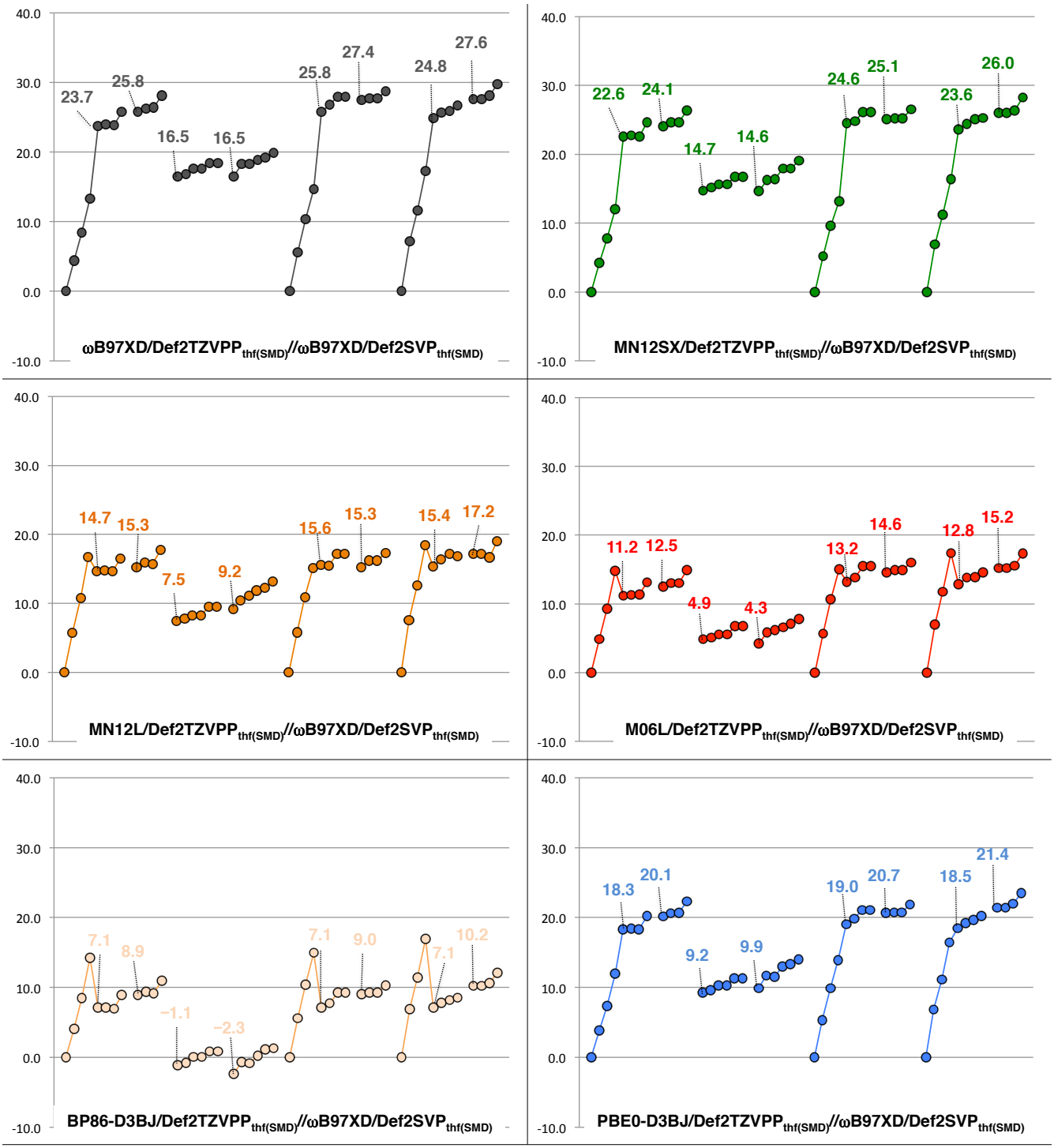


Figure 10.2. Free energy surfaces for S_N2'- and S_N2-type allylic substitution (AS) transition states with either a NaO*t*-Bu molecule, model phoshpine ligand (**PMe$_3$**) or model NHC ligand (**NHCMe$_2$**) as the supporting ligand with various density functionals after optimization with ωB97XD/Def2SVP$_{thf(SMD)}$. For details, see Figure 10.1.

19. Energies and Gibbs Free Energies

Optimization in Figures 1–10 with ωB97XD/Def2SVP in THF(SMD)

Structure	ωB97XD/Def2SVP in THF(SMD)							
	E [hartree]	E(sum) [hartree]	ΔE [kcal/mol]	G [hartree]	G(sum) [hartree]	ΔG [kcal/mol]	ΔG_{Corr} [kcal/mol]	Freq [cm^{-1}]
B2pin2	-821.73060091			-821.411205				32.2
tBuO-Bpin	-643.76963843			-643.500916				42.6
NaOtBu	-395.11737857			-395.027576				32.7
ligand L3a	-2627.35914104			-2626.737897				15.4
NHCMe2	-305.69353942			-305.575630				35.8
PMe3	-460.86841611			-460.785102				167.4
thf	-232.21317836			-232.123926				60.3
para-NMe2-styrene	-443.16696271			-442.996908				46.1
para-H-styrene	-309.32723533			-309.224950				23.5
para-CO2Me-styrene	-536.97246602			-536.832975				36.3
allylphosphate	-838.81191878			-838.683113				44.2
PMe3-Cu-H	-2101.82973385			-2101.744300				97.9
NHCMe2-Cu-H	-1946.68467112			-1946.562466				61.4
para-NMe2-styrene-Cu-H	-2084.11501069			-2083.940445				54.8
para-H-styrene-Cu-H	-1950.27347322			-1950.168006				32.1
para-CO2Me-styrene-Cu-H	-2177.91838845			-2177.775488				43.0
Figure 1								
Figure 1_L-Cu-OtBu	-4500.61984018	-2360.54889695	19.7	-4499.883173	-2360.280515	18.5	-1.2	-20.3
Figure 1_ed	-5322.37772681	-2360.57618267	2.6	-5321.284871	-2360.271008	24.5	21.9	19.1
Figure 1_ts(TB)_01	-5322.37787478	-2360.57633064	2.5	-5321.287061	-2360.273198	23.1	20.6	-98.5
Figure 1_ts(TB)_02	-5322.36659501	-2360.56505087	9.6	-5321.279707	-2360.265844	27.7	18.1	-95.3
Figure 1_ts(TB)_03	-5322.37581050	-2360.57426636	3.8	-5321.282963	-2360.269100	25.7	21.9	-111.0
Figure 1_prod	-5322.40355860	-2360.60201446	-13.6	-5321.318962	-2360.305099	3.1	16.7	15.2
Figure 1_L-Cu-Bpin_01	-4678.61224218	-2360.58033647	0.0	-4677.822972	-2360.310025	0.0	0.0	16.6
Figure 1_L-Cu-Bpin_02	-4678.61215750	-2360.58025179	0.1	-4677.820859	-2360.307912	1.3	1.3	15.2
Figure 1_L-Cu-Bpin_03	-4678.60409663	-2360.57219092	5.1	-4677.818156	-2360.305209	3.0	-2.1	12.8
Figure 1_L-Cu-Bpin_04	-4678.60278859	-2360.57088288	5.9	-4677.814737	-2360.301790	5.2	-0.8	10.3
Figure 1_L-Cu-Bpin_05	-4678.60699442	-2360.57508871	3.3	-4677.816027	-2360.303080	4.4	1.1	13.8
Figure 1_L-Cu-Bpin_06	-4678.60363299	-2360.57172728	5.4	-4677.813881	-2360.300934	5.7	0.3	17.3
Figure 1_L-Cu-Bpin_07	-4678.60209838	-2360.57019267	6.4	-4677.813830	-2360.300883	5.7	-0.6	15.7
Figure 1_L-Cu-Bpin_08	-4678.60272089	-2360.57081518	6.0	-4677.811593	-2360.298646	7.1	1.2	15.2
Figure 1_L-Cu-Bpin_09	-4678.60328369	-2360.57137798	5.6	-4677.811861	-2360.298914	7.0	1.4	16.3
Figure 1_pc1_major01_01	-4987.95820018	-2360.59905914	-11.7	-4987.035954	-2360.298057	7.5	19.3	20.3
Figure 1_pc1_major01_02	-4987.95729960	-2360.59815856	-11.2	-4987.036317	-2360.298420	7.3	18.5	12.2
Figure 1_pc1_major01_03	-4987.95729939	-2360.59815835	-11.2	-4987.036298	-2360.298401	7.3	18.5	12.4
Figure 1_ts(CuBadd)_major01_01	-4987.95489151	-2360.59575047	-9.7	-4987.034973	-2360.297076	8.1	17.8	-155.3
Figure 1_ts(CuBadd)_major01_02	-4987.95448195	-2360.59534091	-9.4	-4987.031999	-2360.294102	10.0	19.4	-142.5
Figure 1_ts(CuBadd)_major01_03	-4987.95448188	-2360.59534084	-9.4	-4987.031999	-2360.294102	10.0	19.4	-142.5
Figure 1_ts(CuBadd)_major01_04	-4987.94957683	-2360.59043579	-6.3	-4987.027592	-2360.289695	12.8	19.1	-183.2
Figure 1_ts(CuBadd)_major01_05	-4987.94957683	-2360.59043579	-6.3	-4987.027592	-2360.289695	12.8	19.1	-183.2
Figure 1_ts(CuBadd)_major01_06	-4987.94669284	-2360.58755180	-4.5	-4987.022574	-2360.284677	15.9	20.4	-34.6
Figure 1_L-Cu-alkyl_major01_01	-4988.00639632	-2360.64725528	-42.0	-4987.086183	-2360.348286	-24.0	18.0	6.0
Figure 1_L-Cu-alkyl_major01_02	-4988.00658408	-2360.64744304	-42.1	-4987.085455	-2360.347558	-23.6	18.6	16.0

Figure 1_L-Cu-alkyl_major01_03	-4988.00414970	-2360.64500866	-40.6	-4987.080469	-2360.342572	-20.4	20.2	20.4
Figure 1_pc1_major02_01	-4987.94730466	-2360.58816362	-4.9	-4987.028668	-2360.290771	12.1	17.0	7.2
Figure 1_pc1_major02_02	-4987.94730699	-2360.58816595	-4.9	-4987.027447	-2360.289550	12.8	17.8	9.8
Figure 1_pc1_major02_03	-4987.95173049	-2360.59258945	-7.7	-4987.026764	-2360.288867	13.3	21.0	15.2
Figure 1_ts(CuBadd)_major02_01	-4987.94649355	-2360.58735251	-4.4	-4987.024141	-2360.286244	14.9	19.3	-62.9
Figure 1_ts(CuBadd)_major02_02	-4987.94870159	-2360.58956055	-5.8	-4987.024476	-2360.286579	14.7	20.5	-97.7
Figure 1_ts(CuBadd)_major02_03	-4987.94870162	-2360.58956058	-5.8	-4987.024475	-2360.286578	14.7	20.5	-97.7
Figure 1_ts(CuBadd)_major02_04	-4987.94870153	-2360.58956049	-5.8	-4987.024475	-2360.286578	14.7	20.5	-97.7
Figure 1_ts(CuBadd)_major02_05	-4987.93948747	-2360.58034643	0.0	-4987.017450	-2360.279553	19.1	19.1	-189.6
Figure 1_ts(CuBadd)_major02_06	-4987.94647940	-2360.58733836	-4.4	-4987.020640	-2360.282743	17.1	21.5	-60.6
Figure 1_ts(CuBadd)_major02_07	-4987.93946936	-2360.58032832	0.0	-4987.015741	-2360.277844	20.2	20.2	-190.1
Figure 1_ts(CuBadd)_major02_08	-4987.93238186	-2360.57324082	4.5	-4987.009842	-2360.271945	23.9	19.4	-166.4
Figure 1_L-Cu-alkyl_major02_01	-4988.01015868	-2360.65101764	-44.4	-4987.088862	-2360.350965	-25.7	18.7	10.1
Figure 1_L-Cu-alkyl_major02_02	-4988.00339175	-2360.64425071	-40.1	-4987.079472	-2360.341575	-19.8	20.3	16.4
Figure 1_pc1_minor01_01	-4987.94988378	-2360.59074274	-6.5	-4987.032226	-2360.294329	9.8	16.4	16.6
Figure 1_pc1_minor01_02	-4987.95193410	-2360.59279306	-7.8	-4987.032908	-2360.295011	9.4	17.2	12.4
Figure 1_pc1_minor01_03	-4987.95470336	-2360.59556232	-9.6	-4987.031607	-2360.293710	10.2	19.8	27.1
Figure 1_pc1_minor01_04	-4987.95276732	-2360.59362628	-8.3	-4987.031341	-2360.293444	10.4	18.7	16.3
Figure 1_pc1_minor01_05	-4987.95012928	-2360.59098824	-6.7	-4987.027985	-2360.290088	12.5	19.2	21.5
Figure 1_ts(CuBadd)_minor01_01	-4987.94730051	-2360.58815947	-4.9	-4987.026703	-2360.288806	13.3	18.2	-107.9
Figure 1_ts(CuBadd)_minor01_02	-4987.94593447	-2360.58679343	-4.1	-4987.025448	-2360.287551	14.1	18.2	-131.7
Figure 1_ts(CuBadd)_minor01_03	-4987.94518213	-2360.58604109	-3.6	-4987.023435	-2360.285538	15.4	18.9	-182.9
Figure 1_ts(CuBadd)_minor01_04	-4987.94747424	-2360.58833320	-5.0	-4987.023545	-2360.285648	15.3	20.3	-174.4
Figure 1_ts(CuBadd)_minor01_05	-4987.94747424	-2360.58833320	-5.0	-4987.023545	-2360.285648	15.3	20.3	-174.4
Figure 1_ts(CuBadd)_minor01_06	-4987.94708758	-2360.58794654	-4.8	-4987.024219	-2360.286322	14.9	19.6	-81.7
Figure 1_ts(CuBadd)_minor01_07	-4987.94846380	-2360.58932276	-5.6	-4987.023375	-2360.285478	15.4	21.0	-106.3
Figure 1_ts(CuBadd)_minor01_08	-4987.94719470	-2360.58805366	-4.8	-4987.021546	-2360.283649	16.6	21.4	-103.8
Figure 1_L-Cu-alkyl_minor01_01	-4988.00887570	-2360.64973466	-43.5	-4987.089141	-2360.351244	-25.9	17.7	18.8
Figure 1_L-Cu-alkyl_minor01_02	-4987.99955082	-2360.64040978	-37.7	-4987.081186	-2360.343289	-20.9	16.8	14.4
Figure 1_L-Cu-alkyl_minor01_03	-4988.00110311	-2360.64196207	-38.7	-4987.079264	-2360.341367	-19.7	19.0	19.6
Figure 1_L-Cu-alkyl_minor01_04	-4987.99975913	-2360.64061809	-37.8	-4987.077693	-2360.339796	-18.7	19.1	21.3
Figure 1_L-Cu-alkyl_minor01_05	-4987.99842918	-2360.63928814	-37.0	-4987.072552	-2360.334655	-15.5	21.5	21.2
Figure 1_pc1_minor02_01	-4987.96129307	-2360.60215203	-13.7	-4987.044965	-2360.307068	1.9	15.5	14.5
Figure 1_pc1_minor02_02	-4987.94484714	-2360.58570610	-3.4	-4987.026370	-2360.288473	13.5	16.9	4.4
Figure 1_pc1_minor02_03	-4987.95227656	-2360.59313552	-8.0	-4987.030755	-2360.292858	10.8	18.8	8.2
Figure 1_pc1_minor02_04	-4987.93892719	-2360.57978615	0.3	-4987.019375	-2360.281478	17.9	17.6	7.9
Figure 1_ts(CuBadd)_minor02_01	-4987.94770508	-2360.58856404	-5.2	-4987.026330	-2360.288433	13.5	18.7	-69.3
Figure 1_ts(CuBadd)_minor02_02	-4987.95176996	-2360.59262892	-7.7	-4987.027283	-2360.289386	13.0	20.7	-106.0
Figure 1_ts(CuBadd)_minor02_03	-4987.95176079	-2360.59261975	-7.7	-4987.027164	-2360.289267	13.0	20.7	-108.5
Figure 1_ts(CuBadd)_minor02_04	-4987.94109714	-2360.58195610	-1.0	-4987.017140	-2360.279243	19.3	20.3	-155.1
Figure 1_ts(CuBadd)_minor02_05	-4987.94907131	-2360.58993027	-6.0	-4987.022458	-2360.284561	16.0	22.0	-186.3
Figure 1_ts(CuBadd)_minor02_06	-4987.93299261	-2360.57385157	4.1	-4987.009729	-2360.271832	24.0	19.9	-157.3
Figure 1_L-Cu-alkyl_minor02_01	-4988.00284447	-2360.64370343	-39.8	-4987.080286	-2360.342389	-20.3	19.5	18.5
Figure 1_L-Cu-alkyl_minor02_02	-4988.00460427	-2360.64546323	-40.9	-4987.080632	-2360.342735	-20.5	20.3	19.5
Figure 1_L-Cu-alkyl_minor02_03	-4987.99535033	-2360.63620929	-35.1	-4987.074610	-2360.336713	-16.7	18.3	13.4
Figure 1_L-Cu-alkyl_minor02_04	-4987.99700051	-2360.63785947	-36.1	-4987.075717	-2360.337820	-17.4	18.7	-32.4
Figure 1_L-Cu-alkyl_major_01	-4988.00213073	-2360.64298969	-39.3	-4987.085657	-2360.347760	-23.7	15.6	5.5
Figure 1_L-Cu-alkyl_major_02	-4988.00326436	-2360.64412332	-40.0	-4987.084106	-2360.346209	-22.7	17.3	12.4
Figure 1_L-Cu-alkyl_major_03	-4988.00032240	-2360.64118136	-38.2	-4987.082117	-2360.344220	-21.5	16.7	13.6
Figure 1_pc3_major_01	-5826.83109267	-2360.66003285	-50.0	-5825.753158	-2360.332148	-13.9	36.1	13.7
Figure 1_pc3_major_02	-5826.83024921	-2360.65918939	-49.5	-5825.751679	-2360.330669	-13.0	36.5	19.6
Figure 1_pc3_major_03	-5826.82859981	-2360.65753999	-48.4	-5825.751666	-2360.330656	-12.9	35.5	5.2
Figure 1_pc3_major_04	-5826.82790049	-2360.65684067	-48.0	-5825.746846	-2360.325836	-9.9	38.1	12.3
Figure 1_ts(AS)_major_01	-5826.79676454	-2360.62570472	-28.5	-5825.720386	-2360.299376	6.7	35.2	-342.4
Figure 1_ts(AS)_major_02	-5826.79516945	-2360.62410963	-27.5	-5825.718840	-2360.297830	7.7	35.1	-325.1
Figure 1_ts(AS)_major_03	-5826.79145442	-2360.62039460	-25.1	-5825.715540	-2360.294530	9.7	34.9	-196.6
Figure 1_ts(AS)_major_04	-5826.79527463	-2360.62421481	-27.5	-5825.716136	-2360.295126	9.3	36.9	-325.3
Figure 1_ts(AS)_major_05	-5826.77845892	-2360.60739910	-17.0	-5825.701647	-2360.280637	18.4	35.4	-202.7
Figure 1_ts(AS)_major_06	-5826.78081695	-2360.60975713	-18.5	-5825.702704	-2360.281694	17.8	36.2	-282.9

Figure 1_pi-allyl_major_01	-5826.81392270	-2360.64286288	-39.2	-5825.734019	-2360.313009	-1.9	37.4	20.4
Figure 1_pi-allyl_major_02	-5826.80177164	-2360.63071182	-31.6	-5825.726513	-2360.305503	2.8	34.4	15.5
Figure 1_pi-allyl_major_03	-5826.80299964	-2360.63193982	-32.4	-5825.724145	-2360.303135	4.3	36.7	13.0

Figure 2

Figure 2_L-Cu-OtBu_dimer	-4357.97211601	-2360.58071639	-0.2	-4357.482114	-2360.300666	5.9	6.1	-19.9
Figure 2_L-Cu-OtBu	-2178.96309100	-2360.55774939	14.2	-2178.731353	-2360.290962	12.0	-2.2	32.4
Figure 2_ed	-3000.72395415	-2360.58801163	-4.8	-3000.145542	-2360.293946	10.1	14.9	-18.4
Figure 2_ts(TB)	-3000.72314236	-2360.58719984	-4.3	-3000.146659	-2360.295063	9.4	13.7	-71.6
Figure 2_prod	-3000.74272641	-2360.60678389	-16.6	-3000.165591	-2360.313995	-2.5	14.1	20.4
Figure 2_L-Cu-Bpin	-2356.95154150	-2360.58523741	-3.1	-2356.666415	-2360.315735	-3.6	-0.5	22.1
Figure 2_para-NMe2_pc1	-2800.13914226	-2360.60587547	-16.0	-2799.660203	-2360.312615	-1.6	14.4	11.8
Figure 2_para-NMe2_ts(CuBadd)	-2800.12649875	-2360.59323196	-8.1	-2799.646765	-2360.299177	6.8	14.9	-191.7
Figure 2_para-NMe2_L-Cu-alkyl_01	-2800.18197688	-2360.64871009	-42.9	-2799.700849	-2360.353261	-27.1	15.8	12.1
Figure 2_para-NMe2_L-Cu-alkyl_02	-2800.17645420	-2360.64318741	-39.4	-2799.693286	-2360.345698	-22.4	17.1	21.4
Figure 2_para-NMe2_L-Cu-alkyl_03	-2800.17710480	-2360.64383801	-39.8	-2799.694336	-2360.346748	-23.0	16.8	-13.5
Figure 2_para-NMe2_ts(BHE)	-2800.13027722	-2360.59701043	-10.5	-2799.652836	-2360.305248	3.0	13.5	-940.8
Figure 2_para-NMe2_pc2	-2800.16816835	-2360.63490156	-34.2	-2799.690028	-2360.342440	-20.3	13.9	25.4
Figure 2_para-NMe2_ts(H>B)	-2800.15510862	-2360.62184183	-26.0	-2799.676241	-2360.328653	-11.7	14.4	-383.4
Figure 2_para-NMe2_int1	-2800.15704127	-2360.62377448	-27.3	-2799.677584	-2360.329996	-12.5	14.7	23.8
Figure 2_para-NMe2_ts(Cu>O)	-2800.15146860	-2360.61820181	-23.8	-2799.673509	-2360.325921	-10.0	13.8	-50.0
Figure 2_para-NMe2_int2	-2800.15550685	-2360.62224006	-26.3	-2799.678077	-2360.330489	-12.8	13.5	11.3
Figure 2_para-NMe2_ts(C-Brot)	-2800.15035858	-2360.61709179	-23.1	-2799.671196	-2360.323608	-8.5	14.5	-85.1
Figure 2_para-NMe2_int3	-2800.15493149	-2360.62166470	-25.9	-2799.676698	-2360.329110	-12.0	14.0	16.6
Figure 2_para-NMe2-alkenylBpin	-853.45693444	-2360.60833876	-17.6	-853.124922	-2360.339800	-18.7	-1.1	23.2
Figure 2_para-NMe2_pc2_rev	-2800.16441697	-2360.63115018	-31.9	-2799.685687	-2360.338099	-17.6	14.3	18.9
Figure 2_para-NMe2_ts(CuHadd_rev)	-2800.14106095	-2360.60779416	-17.2	-2799.662044	-2360.314456	-2.8	14.4	-810.5
Figure 2_para-NMe2_L-Cu-alkyl_rev	-2800.19059809	-2360.65733130	-48.3	-2799.706987	-2360.359399	-31.0	17.3	17.9
Figure 2_para-NMe2_pc3_01	-3639.01987332	-2360.67468775	-59.2	-3638.378684	-2360.347983	-23.8	35.4	17.3
Figure 2_para-NMe2_pc3_02	-3639.01951463	-2360.67432906	-59.0	-3638.381124	-2360.350423	-25.4	33.6	15.6
Figure 2_para-NMe2_ts(AS)_01	-3638.99054294	-2360.64535737	-40.8	-3638.356188	-2360.325487	-9.7	31.1	-333.2
Figure 2_para-NMe2_ts(AS)_02	-3638.99039008	-2360.64520451	-40.7	-3638.352747	-2360.322046	-7.5	33.2	-339.4
Figure 2_para-NMe2_pi-allyl_01	-3639.01658157	-2360.67139600	-57.1	-3638.374596	-2360.343895	-21.3	35.9	26.6
Figure 2_para-NMe2_pi-allyl_02	-3639.01320290	-2360.66801733	-55.0	-3638.373862	-2360.343161	-20.8	34.2	11.6

Figure 2_L-Cu-OtBu_dimer	-4357.97211601	-2360.58071639	-0.2	-4357.482114	-2360.300666	5.9	6.1	-19.9
Figure 2_L-Cu-OtBu	-2178.96309100	-2360.55774939	14.2	-2178.731353	-2360.290962	12.0	-2.2	32.4
Figure 2_ed	-3000.72395415	-2360.58801163	-4.8	-3000.145542	-2360.293946	10.1	14.9	-18.4
Figure 2_ts(TB)	-3000.72314236	-2360.58719984	-4.3	-3000.146659	-2360.295063	9.4	13.7	-71.6
Figure 2_prod	-3000.74272641	-2360.60678389	-16.6	-3000.165591	-2360.313995	-2.5	14.1	20.4
Figure 2_L-Cu-Bpin	-2356.95154150	-2360.58523741	-3.1	-2356.666415	-2360.315735	-3.6	-0.5	22.1
Figure 2_para-H_pc1	-2666.30230457	-2360.60876515	-17.8	-2665.888826	-2360.313196	-2.0	15.8	20.5
Figure 2_para-H_ts(CuBadd)	-2666.29368708	-2360.60014766	-12.4	-2665.880330	-2360.304700	3.3	15.8	-166.2
Figure 2_para-H_L-Cu-alkyl_01	-2666.34950794	-2360.65596852	-47.5	-2665.935157	-2360.359527	-31.1	16.4	22.1
Figure 2_para-H_L-Cu-alkyl_02	-2666.34283721	-2360.64929779	-43.3	-2665.931938	-2360.356308	-29.0	14.2	16.6
Figure 2_para-H_L-Cu-alkyl_03	-2666.34484998	-2360.65131056	-44.5	-2665.930477	-2360.354847	-28.1	16.4	19.0
Figure 2_para-H_ts(BHE)	-2666.29763823	-2360.60409881	-14.9	-2665.888544	-2360.312914	-1.8	13.1	-918.5
Figure 2_para-H_pc2	-2666.32935168	-2360.63581226	-34.8	-2665.917508	-2360.341878	-20.0	14.8	30.4
Figure 2_para-H_ts(H>B)	-2666.31628206	-2360.62274264	-26.6	-2665.908279	-2360.332649	-14.2	12.4	-410.7
Figure 2_para-H_int1	-2666.31795715	-2360.62441773	-27.7	-2665.907555	-2360.331925	-13.7	13.9	20.9
Figure 2_para-H_ts(Cu>O)	-2666.31305334	-2360.61951392	-24.6	-2665.903312	-2360.327682	-11.1	13.5	-46.5
Figure 2_para-H_int2	-2666.31784905	-2360.62430963	-27.6	-2665.906003	-2360.330373	-12.8	14.8	20.0
Figure 2_para-H_ts(C-Brot)	-2666.31236794	-2360.61882852	-24.2	-2665.900079	-2360.324449	-9.1	15.1	-119.6
Figure 2_para-H_int3	-2666.31707941	-2360.62353999	-27.1	-2665.907002	-2360.331372	-13.4	13.7	15.9
Figure 2_para-H-alkenylBpin	-719.61630693	-2360.60743863	-17.0	-719.353090	-2360.339926	-18.8	-1.8	11.9
Figure 2_para-H_pc2_rev	-2666.32621361	-2360.63267419	-32.8	-2665.916493	-2360.340863	-19.4	13.5	23.6
Figure 2_para-H_ts(CuHadd_rev)	-2666.30378750	-2360.61024808	-18.8	-2665.894788	-2360.319158	-5.7	13.0	-811.4
Figure 2_para-H_L-Cu-alkyl_rev	-2666.35607480	-2360.66253538	-51.6	-2665.941742	-2360.366112	-35.2	16.4	17.9

Figure 2_para-H_pc3_01	-3505.18603597	-2360.68057777	-62.9	-3504.619437	-2360.360694	-31.8	31.1	2.5
Figure 2_para-H_pc3_02	-3505.18914182	-2360.68368362	-64.9	-3504.618485	-2360.359742	-31.2	33.7	17.5
Figure 2_para-H_ts(AS)_01	-3505.15917847	-2360.65372027	-46.0	-3504.588265	-2360.329522	-12.2	33.8	-332.8
Figure 2_para-H_ts(AS)_02	-3505.15468151	-2360.64922331	-43.2	-3504.584192	-2360.325449	-9.7	33.5	-321.3
Figure 2_para-H_pi-allyl_01	-3505.17787296	-2360.67241476	-57.8	-3504.606590	-2360.347847	-23.7	34.0	22.6
Figure 2_para-H_pi-allyl_02	-3505.17326116	-2360.66780296	-54.9	-3504.601562	-2360.342819	-20.6	34.3	19.3
Figure 2_L-Cu-OtBu_dimer	-4357.97211601	-2360.58071639	-0.2	-4357.482114	-2360.300666	5.9	6.1	-19.9
Figure 2_L-Cu-OtBu	-2178.96309100	-2360.55774939	14.2	-2178.731353	-2360.290962	12.0	-2.2	32.4
Figure 2_ed	-3000.72395415	-2360.58801163	-4.8	-3000.145542	-2360.293946	10.1	14.9	-18.4
Figure 2_ts(TB)	-3000.72314236	-2360.58719984	-4.3	-3000.146659	-2360.295063	9.4	13.7	-71.6
Figure 2_prod	-3000.74272641	-2360.60678389	-16.6	-3000.165591	-2360.313995	-2.5	14.1	20.4
Figure 2_L-Cu-Bpin	-2356.95154150	-2360.58523741	-3.1	-2356.666415	-2360.315735	-3.6	-0.5	22.1
Figure 2_para-CO2Me_pc1	-2893.94952148	-2360.61075138	-19.1	-2893.500546	-2360.316891	-4.3	14.8	9.3
Figure 2_para-CO2Me_ts(CuBadd)	-2893.94492610	-2360.60615600	-16.2	-2893.494221	-2360.310566	-0.3	15.9	-121.7
Figure 2_para-CO2Me_L-Cu-alkyl_01	-2894.00090787	-2360.66213777	-51.3	-2893.547467	-2360.363812	-33.8	17.6	16.2
Figure 2_para-CO2Me_L-Cu-alkyl_02	-2893.99404152	-2360.65527142	-47.0	-2893.544487	-2360.360832	-31.9	15.1	8.6
Figure 2_para-CO2Me_L-Cu-alkyl_03	-2893.99568367	-2360.65691357	-48.1	-2893.547853	-2360.364198	-34.0	14.1	9.7
Figure 2_para-CO2Me_ts(BHE)	-2893.94910035	-2360.61033025	-18.8	-2893.501451	-2360.317796	-4.9	13.9	-771.3
Figure 2_para-CO2Me_pc2	-2893.97546090	-2360.63669080	-35.4	-2893.527042	-2360.343387	-20.9	14.4	25.5
Figure 2_para-CO2Me_ts(H>B)	-2893.96254522	-2360.62377512	-27.3	-2893.516557	-2360.332902	-14.4	12.9	-339.8
Figure 2_para-CO2Me_int1	-2893.96426596	-2360.62549586	-28.3	-2893.517383	-2360.333728	-14.9	13.5	12.2
Figure 2_para-CO2Me_ts(Cu>O)	-2893.95949767	-2360.62072757	-25.3	-2893.512055	-2360.328400	-11.5	13.8	-41.1
Figure 2_para-CO2Me_int2	-2893.96407343	-2360.62530333	-28.2	-2893.516917	-2360.333262	-14.6	13.6	14.8
Figure 2_para-CO2Me_ts(C-Brot)	-2893.95849867	-2360.61972857	-24.7	-2893.512981	-2360.329326	-12.1	12.6	-112.0
Figure 2_para-CO2Me_int3	-2893.96339570	-2360.62462560	-27.8	-2893.514582	-2360.330927	-13.1	14.7	19.1
Figure 2_para-CO2Me-alkenylBpin	-947.26105091	-2360.60695193	-16.7	-946.961606	-2360.340417	-19.1	-2.4	13.6
Figure 2_para-CO2Me_pc2_rev	-2893.97226879	-2360.63349869	-33.4	-2893.523913	-2360.340258	-19.0	14.4	18.4
Figure 2_para-CO2Me_ts(CuHadd_rev)	-2893.95003715	-2360.61126705	-19.4	-2893.502301	-2360.318646	-5.4	14.0	-793.4
Figure 2_para-CO2Me_L-Cu-alkyl_rev	-2894.00374351	-2360.66497341	-53.1	-2893.551213	-2360.367558	-36.1	17.0	15.9
Figure 2_para-CO2Me_pc3_01	-3732.83783511	-2360.68714623	-67.0	-3732.230981	-2360.364213	-34.0	33.0	8.9
Figure 2_para-CO2Me_pc3_02	-3732.83759747	-2360.68690859	-66.9	-3732.229842	-2360.363074	-33.3	33.6	15.3
Figure 2_para-CO2Me_ts(AS)_01	-3732.80314503	-2360.65245615	-45.3	-3732.197945	-2360.331177	-13.3	32.0	-348.4
Figure 2_para-CO2Me_ts(AS)_02	-3732.80085269	-2360.65016381	-43.8	-3732.196633	-2360.329865	-12.4	31.4	-311.2
Figure 2_para-CO2Me_pi-allyl_01	-3732.82691538	-2360.67622650	-60.2	-3732.216571	-2360.349803	-25.0	35.2	24.3
Figure 2_para-CO2Me_pi-allyl_02	-3732.82458329	-2360.67389441	-58.7	-3732.213792	-2360.347024	-23.2	35.5	17.3

Figure 3

Figure 3_L-Cu-OtBu_dimer	-4668.27269506	-2360.55612923	15.2	-4667.854184	-2360.277229	20.6	5.4	20.3
Figure 3_L-Cu-OtBu	-2334.10735270	-2360.52713440	33.4	-2333.909085	-2360.259222	31.9	-1.5	-39.1
Figure 3_ed	-3155.87460188	-2360.56378267	10.4	-3155.332660	-2360.271592	24.1	13.7	11.4
Figure 3_ts(TB)	-3155.86594930	-2360.55513009	15.8	-3155.324968	-2360.263900	28.9	13.1	-80.6
Figure 3_prod	-3155.88950452	-2360.57868531	1.0	-3155.347748	-2360.286680	14.6	13.6	21.6
Figure 3_L-Cu-Bpin	-2512.09747879	-2360.55629801	15.1	-2511.850121	-2360.289969	12.6	-2.5	23.7
Figure 3_para-NMe2_pc1	-2955.28953194	-2360.58138846	-0.7	-2954.844645	-2360.287585	14.1	14.7	19.2
Figure 3_para-NMe2_ts(CuBadd)	-2955.27152489	-2360.56338141	10.6	-2954.825911	-2360.268851	25.8	15.2	-202.8
Figure 3_para-NMe2_L-Cu-alkyl_01	-2955.32654850	-2360.61840502	-23.9	-2954.877605	-2360.320545	-6.6	17.3	24.9
Figure 3_para-NMe2_L-Cu-alkyl_02	-2955.32118714	-2360.61304366	-20.5	-2954.875276	-2360.318216	-5.1	15.4	17.2
Figure 3_para-NMe2_L-Cu-alkyl_03	-2955.32513805	-2360.61699457	-23.0	-2954.881276	-2360.324216	-8.9	14.1	19.5
Figure 3_para-NMe2_ts(BHE)	-2955.27529180	-2360.56714832	8.3	-2954.835480	-2360.278420	19.8	11.6	-965.5
Figure 3_para-NMe2_pc2	-2955.31547918	-2360.60733570	-16.9	-2954.873016	-2360.315956	-3.7	13.2	26.8
Figure 3_para-NMe2_ts(H>B)	-2955.30163554	-2360.59349206	-8.3	-2954.859784	-2360.302724	4.6	12.8	-466.1
Figure 3_para-NMe2_int1	-2955.30314274	-2360.59499926	-9.2	-2954.860784	-2360.303724	4.0	13.2	19.5
Figure 3_para-NMe2_ts(Cu>O)	-2955.29561577	-2360.58747229	-4.5	-2954.853892	-2360.296832	8.3	12.8	-37.8
Figure 3_para-NMe2_int2	-2955.30214865	-2360.59400517	-8.6	-2954.857692	-2360.300632	5.9	14.5	23.8
Figure 3_para-NMe2_ts(C-Brot)	-2955.29669845	-2360.58855497	-5.2	-2954.854769	-2360.297709	7.7	12.9	-78.5
Figure 3_para-NMe2_int3	-2955.30153963	-2360.59339615	-8.2	-2954.858468	-2360.301408	5.4	13.6	19.8
Figure 3_para-NMe2-alkenylBpin	-853.45693444	-2360.57852480	1.1	-853.124922	-2360.312162	-1.3	-2.5	23.2

Figure 3_para-NMe2_pc2_rev	-2955.31296303	-2360.60481955	-15.4	-2954.871281	-2360.314221	-2.6	12.7	21.3
Figure 3_para-NMe2_ts(CuHadd_rev)	-2955.28486892	-2360.57672544	2.3	-2954.843838	-2360.286778	14.6	12.3	-860.2
Figure 3_para-NMe2_L-Cu-alkyl_rev	-2955.33794627	-2360.62980279	-31.0	-2954.891338	-2360.334278	-15.2	15.8	26.0
Figure 3_para-NMe2_pc3_01	-3794.16568164	-2360.64561938	-41.0	-3793.565283	-2360.325110	-9.5	31.5	17.6
Figure 3_para-NMe2_pc3_02	-3794.16837386	-2360.64831160	-42.7	-3793.564335	-2360.324162	-8.9	33.8	22.6
Figure 3_para-NMe2_ts(AS)_01	-3794.13369549	-2360.61363323	-20.9	-3793.533619	-2360.293446	10.4	31.3	-333.2
Figure 3_para-NMe2_ts(AS)_02	-3794.13722913	-2360.61716687	-23.1	-3793.535109	-2360.294936	9.5	32.6	-346.5
Figure 3_para-NMe2_pi-allyl_01	-3794.16230939	-2360.64224713	-38.8	-3793.558684	-2360.318511	-5.3	33.5	19.9
Figure 3_para-NMe2_pi-allyl_02	-3794.15615510	-2360.63609284	-35.0	-3793.553802	-2360.313629	-2.3	32.7	16.2
Figure 3_L-Cu-OtBu_dimer	-4668.27269506	-2360.55612923	15.2	-4667.854184	-2360.277229	20.6	5.4	20.3
Figure 3_L-Cu-OtBu	-2334.10735270	-2360.52713440	33.4	-2333.909085	-2360.259222	31.9	-1.5	-39.1
Figure 3_ed	-3155.87460188	-2360.56378267	10.4	-3155.332660	-2360.271592	24.1	13.7	11.4
Figure 3_ts(TB)	-3155.86594930	-2360.55513009	15.8	-3155.324968	-2360.263900	28.9	13.1	-80.6
Figure 3_prod	-3155.88950452	-2360.57868531	1.0	-3155.347748	-2360.286680	14.6	13.6	21.6
Figure 3_L-Cu-Bpin	-2512.09747879	-2360.55629801	15.1	-2511.850121	-2360.289969	12.6	-2.5	23.7
Figure 3_para-H_pc1	-2821.45221106	-2360.58379495	-2.2	-2821.076429	-2360.291327	11.7	13.9	16.9
Figure 3_para-H_ts(CuBadd)	-2821.43913646	-2360.57072035	6.0	-2821.062850	-2360.277748	20.3	14.2	-187.7
Figure 3_para-H_L-Cu-alkyl_01	-2821.49278031	-2360.62436420	-27.6	-2821.113713	-2360.328611	-11.7	16.0	25.4
Figure 3_para-H_L-Cu-alkyl_02	-2821.48741938	-2360.61900327	-24.3	-2821.112237	-2360.327135	-10.7	13.5	16.3
Figure 3_para-H_L-Cu-alkyl_03	-2821.49162681	-2360.62321070	-26.9	-2821.115418	-2360.330316	-12.7	14.2	19.8
Figure 3_para-H_ts(BHE)	-2821.44270924	-2360.57429313	3.8	-2821.072157	-2360.287055	14.4	10.6	-1002.2
Figure 3_para-H_pc2	-2821.47614749	-2360.60773138	-17.2	-2821.103515	-2360.318413	-5.3	11.9	16.9
Figure 3_para-H_ts(H>B)	-2821.46264111	-2360.59422500	-8.7	-2821.091495	-2360.306393	2.3	11.0	-449.6
Figure 3_para-H_int1	-2821.46389768	-2360.59548157	-9.5	-2821.090845	-2360.305743	2.7	12.2	24.9
Figure 3_para-H_ts(Cu>O)	-2821.45732695	-2360.58891084	-5.4	-2821.083953	-2360.298851	7.0	12.4	-34.6
Figure 3_para-H_int2	-2821.46396376	-2360.59554765	-9.5	-2821.091500	-2360.306398	2.3	11.8	9.9
Figure 3_para-H_ts(C-Brot)	-2821.45857138	-2360.59015527	-6.2	-2821.083895	-2360.298793	7.0	13.2	-89.1
Figure 3_para-H_int3	-2821.46355865	-2360.59514254	-9.3	-2821.088477	-2360.303375	4.2	13.5	19.1
Figure 3_para-H-alkenylBpin	-719.61630693	-2360.57762467	1.7	-719.353090	-2360.312288	-1.4	-3.1	11.9
Figure 3_para-H_pc2_rev	-2821.47379868	-2360.60538257	-15.7	-2821.101733	-2360.316631	-4.1	11.6	7.9
Figure 3_para-H_ts(CuHadd_rev)	-2821.44750747	-2360.57909136	0.8	-2821.074354	-2360.289252	13.0	12.3	-855.6
Figure 3_para-H_L-Cu-alkyl_rev	-2821.50134039	-2360.63292428	-33.0	-2821.123765	-2360.338663	-18.0	15.0	25.2
Figure 3_para-H_pc3_01	-3660.33447417	-2360.65413928	-46.3	-3659.801282	-2360.333067	-14.5	31.9	14.6
Figure 3_para-H_pc3_02	-3660.33292348	-2360.65258859	-45.3	-3659.796342	-2360.328127	-11.4	34.0	26.5
Figure 3_para-H_ts(AS)_01	-3660.29889725	-2360.61856236	-24.0	-3659.767287	-2360.299072	6.9	30.9	-278.0
Figure 3_para-H_ts(AS)_02	-3660.30030627	-2360.61997138	-24.9	-3659.767032	-2360.298817	7.0	31.9	-282.4
Figure 3_para-H_pi-allyl_01	-3660.32333278	-2360.64299789	-39.3	-3659.787885	-2360.319670	-6.1	33.3	24.0
Figure 3_para-H_pi-allyl_02	-3660.31700817	-2360.63667328	-35.4	-3659.782777	-2360.314562	-2.8	32.5	17.2
Figure 3_L-Cu-OtBu_dimer	-4668.27269506	-2360.55612923	15.2	-4667.854184	-2360.277229	20.6	5.4	20.3
Figure 3_L-Cu-OtBu	-2334.10735270	-2360.52713440	33.4	-2333.909085	-2360.259222	31.9	-1.5	-39.1
Figure 3_ed	-3155.87460188	-2360.56378267	10.4	-3155.332660	-2360.271592	24.1	13.7	11.4
Figure 3_ts(TB)	-3155.86594930	-2360.55513009	15.8	-3155.324968	-2360.263900	28.9	13.1	-80.6
Figure 3_prod	-3155.88950452	-2360.57868531	1.0	-3155.347748	-2360.286680	14.6	13.6	21.6
Figure 3_L-Cu-Bpin	-2512.09747879	-2360.55629801	15.1	-2511.850121	-2360.289969	12.6	-2.5	23.7
Figure 3_para-CO2Me_pc1	-3049.09919044	-2360.58554365	-3.3	-3048.685324	-2360.292197	11.2	14.5	22.1
Figure 3_para-CO2Me_ts(CuBadd)	-3049.09101988	-2360.57737309	1.9	-3048.676983	-2360.283856	16.4	14.6	-166.5
Figure 3_para-CO2Me_L-Cu-alkyl_01	-3049.14412054	-2360.63047375	-31.5	-3048.726217	-2360.333090	-14.5	17.0	25.5
Figure 3_para-CO2Me_L-Cu-alkyl_02	-3049.13832151	-2360.62467472	-27.8	-3048.723644	-2360.330517	-12.9	15.0	19.4
Figure 3_para-CO2Me_L-Cu-alkyl_03	-3049.14208777	-2360.62844098	-30.2	-3048.728291	-2360.335164	-15.8	14.4	15.0
Figure 3_para-CO2Me_ts(BHE)	-3049.09404597	-2360.58039918	0.0	-3048.683758	-2360.290631	12.2	12.2	-926.9
Figure 3_para-CO2Me_pc2	-3049.12196245	-2360.60831566	-17.6	-3048.710639	-2360.317512	-4.7	12.9	28.4
Figure 3_para-CO2Me_ts(H>B)	-3049.10879459	-2360.59514780	-9.3	-3048.698614	-2360.305487	2.8	12.1	-424.7
Figure 3_para-CO2Me_int1	-3049.10990203	-2360.59625524	-10.0	-3048.699490	-2360.306363	2.3	12.3	12.4
Figure 3_para-CO2Me_ts(Cu>O)	-3049.10330689	-2360.58966010	-5.9	-3048.692181	-2360.299054	6.9	12.7	-56.5
Figure 3_para-CO2Me_int2	-3049.11054654	-2360.59689975	-10.4	-3048.698773	-2360.305646	2.7	13.1	19.4
Figure 3_para-CO2Me_ts(C-Brot)	-3049.10479731	-2360.59115052	-6.8	-3048.692246	-2360.299119	6.8	13.6	-95.6
Figure 3_para-CO2Me_int3	-3049.10988776	-2360.59624097	-10.0	-3048.698852	-2360.305725	2.7	12.7	14.5

Figure 3_para-CO2Me-alkenylBpin	-947.26105091	-2360.57713797	2.0	-946.961606	-2360.312779	-1.7	-3.7	13.6
Figure 3_para-CO2Me_pc2_rev	-3049.11948820	-2360.60584141	-16.0	-3048.706451	-2360.313324	-2.1	13.9	23.8
Figure 3_para-CO2Me_ts(CuHadd_rev)	-3049.09338527	-2360.57973848	0.4	-3048.681487	-2360.288360	13.6	13.2	-781.6
Figure 3_para-CO2Me_L-Cu-alkyl_rev	-3049.14832622	-2360.63467943	-34.1	-3048.734434	-2360.341307	-19.6	14.5	12.5
Figure 3_para-CO2Me_pc3_01	-3887.98535988	-2360.65979431	-49.9	-3887.412586	-2360.336346	-16.5	33.3	10.8
Figure 3_para-CO2Me_pc3_02	-3887.98357896	-2360.65801339	-48.7	-3887.410460	-2360.334220	-15.2	33.6	18.7
Figure 3_para-CO2Me_ts(AS)_01	-3887.94585044	-2360.62028487	-25.1	-3887.376034	-2360.299794	6.4	31.5	-275.1
Figure 3_para-CO2Me_ts(AS)_02	-3887.94832102	-2360.62275545	-26.6	-3887.377269	-2360.301029	5.6	32.3	-271.0
Figure 3_para-CO2Me_pi-allyl_01	-3887.97108875	-2360.64552318	-40.9	-3887.396707	-2360.320467	-6.6	34.4	20.9
Figure 3_para-CO2Me_pi-allyl_02	-3887.96383511	-2360.63826954	-36.4	-3887.391898	-2360.315658	-3.5	32.8	21.1

Figure 4

Figure 4_para-NMe2_L-Cu-OtBu	-2316.39314463	-2360.51437973	41.4	-2316.108013	-2360.246344	40.0	-1.4	15.1
Figure 4_para-NMe2_ed	-3138.15747466	-2360.54810886	20.2	-3137.527119	-2360.254245	35.0	14.8	11.3
Figure 4_para-NMe2_ts(TB)	-3138.15700613	-2360.54764033	20.5	-3137.525221	-2360.252347	36.2	15.7	-44.5
Figure 4_para-NMe2_prod	-3138.17640839	-2360.56704259	8.3	-3137.545471	-2360.272597	23.5	15.1	16.2
Figure 4_para-NMe2_L-Cu-Bpin	-2494.38389228	-2360.54416491	22.7	-2494.045272	-2360.273314	23.0	0.3	19.8
Figure 4_para-NMe2_pc1	-2937.58317342	-2360.57648334	2.4	-2937.044864	-2360.275998	21.4	18.9	-6.6
Figure 4_para-NMe2_ts(CuBadd)_01	-2937.57583746	-2360.56914738	7.0	-2937.037839	-2360.268973	25.8	18.7	-173.0
Figure 4_para-NMe2_ts(CuBadd)_02	-2937.56458202	-2360.55789194	14.1	-2937.030364	-2360.261498	30.5	16.4	-194.2
Figure 4_para-NMe2_L-Cu-alkyl_01	-2937.61855973	-2360.61186965	-19.8	-2937.078205	-2360.309339	0.4	20.2	28.2
Figure 4_para-NMe2_L-Cu-alkyl_02	-2937.61545910	-2360.60876902	-17.8	-2937.076244	-2360.307378	1.7	19.5	21.9
Figure 4_para-NMe2_L-Cu-alkyl_03	-2937.61764213	-2360.61095205	-19.2	-2937.080012	-2360.311146	-0.7	18.5	21.1
Figure 4_para-NMe2_ts(BHE)	-2937.57872574	-2360.57203566	5.2	-2937.045448	-2360.276582	21.0	15.8	-844.1
Figure 4_para-NMe2_pc2	-2937.60609935	-2360.59940927	-12.0	-2937.072623	-2360.303757	3.9	15.9	21.6
Figure 4_para-NMe2-alkenylBpin	-853.45693444	-2360.56525505	9.5	-853.124922	-2360.296501	8.5	-1.0	23.2
Figure 4_para-NMe2_pc3_01	-3776.45374198	-2360.63513312	-34.4	-3775.761820	-2360.309841	0.1	34.5	10.4
Figure 4_para-NMe2_pc3_02	-3776.46237503	-2360.64376617	-39.8	-3775.765792	-2360.313813	-2.4	37.4	23.4
Figure 4_para-NMe2_ts(AS)_01	-3776.41596452	-2360.59735566	-10.7	-3775.727752	-2360.275773	21.5	32.2	-320.2
Figure 4_para-NMe2_ts(AS)_02	-3776.41562681	-2360.59701795	-10.5	-3775.727284	-2360.275305	21.8	32.3	-278.6
Figure 4_para-NMe2_ts(AS)_03	-3776.42214536	-2360.60353650	-14.6	-3775.728174	-2360.276195	21.2	35.8	-265.5
Figure 4_para-NMe2_ts(AS)_04	-3776.41714465	-2360.59853579	-11.4	-3775.722917	-2360.270938	24.5	35.9	-193.5
Figure 4_para-NMe2_pi-allyl_01	-3776.42561792	-2360.60700906	-16.7	-3775.736771	-2360.284792	15.8	32.6	19.6
Figure 4_para-NMe2_pi-allyl_02	-3776.43298427	-2360.61437541	-21.4	-3775.737550	-2360.285571	15.3	36.7	24.8
Figure 4_para-H_L-Cu-OtBu	-2182.55158904	-2360.51255152	42.5	-2182.335076	-2360.245365	40.6	-2.0	27.4
Figure 4_para-H_ed	-3004.31675967	-2360.54712124	20.8	-3003.752996	-2360.252080	36.4	15.5	18.6
Figure 4_para-H_ts(TB)	-3004.31639795	-2360.54675952	21.1	-3003.751569	-2360.250653	37.3	16.2	-60.2
Figure 4_para-H_prod	-3004.33626287	-2360.56662444	8.6	-3003.774122	-2360.273206	23.1	14.5	26.4
Figure 4_para-H_L-Cu-Bpin	-2360.54260251	-2360.54260251	23.7	-2360.275158	-2360.275158	21.9	-1.8	16.9
Figure 4_para-H_pc1	-2669.90144009	-2360.57420476	3.8	-2669.501189	-2360.276239	21.2	17.4	-6.9
Figure 4_para-H_ts(CuBadd)_01	-2669.89657616	-2360.56934083	6.9	-2669.497256	-2360.272306	23.7	16.8	-163.1
Figure 4_para-H_ts(CuBadd)_02	-2669.89201608	-2360.56478075	9.8	-2669.492429	-2360.267479	26.7	16.9	-175.6
Figure 4_para-H_L-Cu-alkyl_01	-2669.93751624	-2360.61028091	-18.8	-2669.538752	-2360.313802	-2.4	16.4	16.8
Figure 4_para-H_L-Cu-alkyl_02	-2669.93402914	-2360.60679381	-16.6	-2669.536027	-2360.311077	-0.7	15.9	18.8
Figure 4_para-H_L-Cu-alkyl_03	-2669.93662784	-2360.60939251	-18.2	-2669.538961	-2360.314011	-2.5	15.7	14.2
Figure 4_para-H_ts(BHE)	-2669.89885582	-2360.57162049	5.5	-2669.504584	-2360.279634	19.1	13.6	-839.8
Figure 4_para-H_pc2	-2669.92145947	-2360.59422414	-8.7	-2669.524369	-2360.299419	6.7	15.4	-9.2
Figure 4_para-H-alkenylBpin	-719.61630693	-2360.56254481	11.2	-719.353090	-2360.296146	8.7	-2.5	11.9
Figure 4_para-H_pc3_01	-3508.77967897	-2360.64052486	-37.8	-3508.224920	-2360.316857	-4.3	33.5	-6.2
Figure 4_para-H_pc3_02	-3508.78340558	-2360.64425147	-40.1	-3508.223800	-2360.315737	-3.6	36.5	29.8
Figure 4_para-H_ts(AS)_01	-3508.73604808	-2360.59689397	-10.4	-3508.181939	-2360.273876	22.7	33.1	-180.6
Figure 4_para-H_ts(AS)_02	-3508.73603238	-2360.59687827	-10.4	-3508.181416	-2360.273353	23.0	33.4	-178.4
Figure 4_para-H_ts(AS)_03	-3508.73783576	-2360.59868165	-11.5	-3508.180685	-2360.272622	23.5	35.0	-216.1
Figure 4_para-H_ts(AS)_04	-3508.73372533	-2360.59457122	-8.9	-3508.178491	-2360.270428	24.8	33.8	-167.7
Figure 4_para-H_pi-allyl_01	-3508.74217018	-2360.60301607	-14.2	-3508.187544	-2360.279481	19.2	33.4	25.8
Figure 4_para-H_pi-allyl_02	-3508.74606185	-2360.60690774	-16.7	-3508.189032	-2360.280969	18.2	34.9	24.7

Figure 4_para-CO2Me_L-Cu-OtBu	-2410.19525632	-2360.51098811	43.5	-2409.941084	-2360.243348	41.8	-1.7	22.9
Figure 4_para-CO2Me_ed	-3231.96398916	-2360.54912005	19.6	-3231.360114	-2360.251173	36.9	17.3	15.2
Figure 4_para-CO2Me_ts(TB)	-3231.96311685	-2360.54824774	20.1	-3231.360676	-2360.251735	36.6	16.4	-92.4
Figure 4_para-CO2Me_prod	-3231.97269053	-2360.55782142	14.1	-3231.373692	-2360.264751	28.4	14.3	15.9
Figure 4_para-CO2Me_L-Cu-Bpin	-2588.18751234	-2360.54228166	23.9	-2587.879722	-2360.271697	24.1	0.2	14.5
Figure 4_para-CO2Me_pc1	-3125.20059961	-2360.58290291	-1.6	-3124.724852	-2360.283852	16.4	18.0	10.2
Figure 4_para-CO2Me_ts(CuBadd)_01	-3125.19811105	-2360.58041435	0.0	-3124.722317	-2360.281317	18.0	18.1	-136.2
Figure 4_para-CO2Me_ts(CuBadd)_02	-3125.18742203	-2360.56972533	6.7	-3124.716947	-2360.275947	21.4	14.7	-164.3
Figure 4_para-CO2Me_L-Cu-alkyl_01	-3125.23833982	-2360.62064312	-25.3	-3124.759063	-2360.318063	-5.0	20.2	21.0
Figure 4_para-CO2Me_L-Cu-alkyl_02	-3125.23509021	-2360.61739351	-23.3	-3124.760138	-2360.319138	-5.7	17.5	10.9
Figure 4_para-CO2Me_L-Cu-alkyl_03	-3125.23447326	-2360.61677656	-22.9	-3124.759140	-2360.318140	-5.1	17.8	15.8
Figure 4_para-CO2Me_ts(BHE)	-3125.19981935	-2360.58212265	-1.1	-3124.727569	-2360.286569	14.7	15.8	-841.5
Figure 4_para-CO2Me_pc2	-3125.21803273	-2360.60033603	-12.5	-3124.742909	-2360.301909	5.1	17.6	26.8
Figure 4_para-CO2Me-alkenylBpin	-947.26105091	-2360.56174266	11.7	-946.961606	-2360.296094	8.7	-2.9	13.6
Figure 4_para-CO2Me_pc3_01	-3964.07601958	-2360.64640410	-41.5	-3963.447610	-2360.323497	-8.5	33.0	7.3
Figure 4_para-CO2Me_pc3_02	-3964.08215085	-2360.65253537	-45.3	-3963.447118	-2360.323005	-8.1	37.2	18.9
Figure 4_para-CO2Me_ts(AS)_01	-3964.02907638	-2360.59946090	-12.0	-3963.402778	-2360.278665	19.7	31.7	-190.0
Figure 4_para-CO2Me_ts(AS)_02	-3964.02804325	-2360.59842777	-11.4	-3963.398459	-2360.274346	22.4	33.7	-184.6
Figure 4_para-CO2Me_ts(AS)_03	-3964.03280404	-2360.60318856	-14.3	-3963.401193	-2360.277080	20.7	35.0	-217.5
Figure 4_para-CO2Me_ts(AS)_04	-3964.02741833	-2360.59780285	-11.0	-3963.397368	-2360.273255	23.1	34.0	-157.6
Figure 4_para-CO2Me_pi-allyl_01	-3964.04377838	-2360.61416290	-21.2	-3963.412547	-2360.288434	13.5	34.8	17.7
Figure 4_para-CO2Me_pi-allyl_02	-3964.03936221	-2360.60974673	-18.5	-3963.408336	-2360.284223	16.2	34.6	10.5

Figure 5

Figure 5_L-Cu-OtBu	-2105.43166785	-2360.50668730	46.2	-2105.227438	-2360.238751	44.7	-1.5	-23.4
Figure 5_ed	-2927.19598297	-2360.54040151	25.1	-2926.648063	-2360.248171	38.8	13.8	14.3
Figure 5_ts(TB)	-2927.19056412	-2360.53498266	28.5	-2926.641767	-2360.241875	42.8	14.3	-26.2
Figure 5_prod	-2927.22806183	-2360.57248037	4.9	-2926.678851	-2360.278959	19.5	14.6	30.9
Figure 5_L-Cu-Bpin	-2283.43209458	-2360.54615155	21.5	-2283.176928	-2360.277952	20.1	-1.3	22.8
Figure 5_pc1	-2592.77992931	-2360.56675095	8.5	-2592.399223	-2360.275297	21.8	13.3	19.8
Figure 5_ts(CuBadd)	-2592.76023309	-2360.54705473	20.9	-2592.378720	-2360.254794	34.7	13.8	-243.4
Figure 5_L-Cu-alkyl_01	-2592.82066847	-2360.60749011	-17.0	-2592.436888	-2360.312962	-1.8	15.2	22.2
Figure 5_L-Cu-alkyl_02	-2592.81753394	-2360.60435558	-15.1	-2592.434281	-2360.310355	-0.2	14.9	23.4
Figure 5_L-Cu-alkyl_03	-2592.82107598	-2360.60789762	-17.3	-2592.437886	-2360.313960	-2.5	14.8	22.1
Figure 5_ts(BHE)	-2592.76459029	-2360.55141193	18.2	-2592.386396	-2360.262470	29.8	11.7	-958.2
Figure 5_pc2	-2592.80440429	-2360.59122593	-6.8	-2592.425209	-2360.301283	5.5	12.3	-3.3
Figure 5_pc3	-3431.66328451	-2360.63818737	-36.3	-3431.125429	-2360.318390	-5.2	31.1	14.4
Figure 5_ts(AS)_01	-3431.62747806	-2360.60238092	-13.8	-3431.087897	-2360.280858	18.3	32.1	-242.0
Figure 5_ts(AS)_02	-3431.62868825	-2360.60359111	-14.6	-3431.086959	-2360.279920	18.9	33.5	-257.5
Figure 5_pi-allyl	-3431.66797676	-2360.64287962	-39.2	-3431.127353	-2360.320314	-6.5	32.8	24.3

Figure 8

Figure 8_ L3a-Cu-OtBu	-4500.61984018	-1873.26069914	0.0	-4499.883173	-1873.145276	0.0	0.0	-20.3
Figure 8_para-NMe2-styrene-Cu-OtBu	-2316.39314463	-1873.22618192	21.7	-2316.108013	-1873.111105	21.4	-0.2	15.1
Figure 8_para-NMe2-styrene-Cu-OtBu_dimer_01	-4632.85611567	-1873.26109513	-0.2	-4632.257007	-1873.131596	8.6	8.8	17.1
Figure 8_para-NMe2-styrene-Cu-OtBu_dimer_02	-4632.85757242	-1873.26182350	-0.7	-4632.256999	-1873.131592	8.6	9.3	25.4
Figure 8_ L3a-Cu-OtBu	-4500.61984018	-1873.26069914	0.0	-4499.883173	-1873.145276	0.0	0.0	-20.3
Figure 8_para-H-styrene-Cu-OtBu	-2182.55158904	-1873.22435371	22.8	-2182.335076	-1873.110126	22.1	-0.8	27.4
Figure 8_para-H-styrene-Cu-OtBu_dimer_01	-4365.17726958	-1873.26139946	-0.4	-4364.713565	-1873.131833	8.4	8.9	25.6
Figure 8_para-H-styrene-Cu-OtBu_dimer_02	-4365.17671872	-1873.26112403	-0.3	-4364.713671	-1873.131886	8.4	8.7	25.6
Figure 8_ L3a-Cu-OtBu	-4500.61984018	-1873.26069914	0.0	-4499.883173	-1873.145276	0.0	0.0	-20.3
Figure 8_para-CO2Me-styrene-Cu-OtBu	-2410.19525632	-1873.22279030	23.8	-2409.941084	-1873.108109	23.3	-0.5	22.9
Figure 8_para-CO2Me-styrene-Cu-OtBu_dimer_01	-4820.46849056	-1873.26177926	-0.7	-4819.932581	-1873.133316	7.5	8.2	9.9
Figure 8_para-CO2Me-styrene-Cu-OtBu_dimer_02	-4820.47029487	-1873.26268142	-1.2	-4819.930546	-1873.132298	8.1	9.4	18.8

Figure 9

Figure 9_Cu-(OtBu)2_anion	-2106.15712863	-2106.15712863	0.0	-2105.951624	-2105.951624	0.0	0.0	16.1
Figure 9_para-NMe2-styrene-Cu-(OtBu)2_anion_01	-2549.33388221	-2106.16691950	-6.1	-2548.933046	-2105.936138	9.7	15.9	17.2
Figure 9_para-NMe2-styrene-Cu-(OtBu)2_anion_02	-2549.33285744	-2106.16589473	-5.5	-2548.930012	-2105.933104	11.6	17.1	28.2
Figure 9_Cu-(OtBu)2_anion	-2106.15712863	-2106.15712863	0.0	-2105.951624	-2105.951624	0.0	0.0	16.1
Figure 9_para-H-styrene-Cu-(OtBu)2_anion_01	-2415.49693836	-2106.16970303	-7.9	-2415.162831	-2105.937881	8.6	16.5	30.6
Figure 9_para-H-styrene-Cu-(OtBu)2_anion_02	-2415.49618477	-2106.16894944	-7.4	-2415.161886	-2105.936936	9.2	16.6	24.4
Figure 9_Cu-(OtBu)2_anion	-2106.15712863	-2106.15712863	0.0	-2105.951624	-2105.951624	0.0	0.0	16.1
Figure 9_para-CO2Me-styrene-Cu-(OtBu)2_anion_01	-2643.14335830	-2106.17089228	-8.6	-2642.774259	-2105.941284	6.5	15.1	9.0
Figure 9_para-CO2Me-styrene-Cu-(OtBu)2_anion_02	-2643.14401653	-2106.17155051	-9.0	-2642.770739	-2105.937764	8.7	17.7	-0.9
Figure 9_Cu-(OtBu)2_Na	-2268.34902130	-2268.34902130	0.0	-2268.144864	-2268.144864	0.0	0.0	24.5
Figure 9_para-NMe2-styrene-Cu-(OtBu)2_Na_01	-2711.56379480	-2268.39683209	-30.0	-2711.161060	-2268.164152	-12.1	17.9	26.0
Figure 9_para-NMe2-styrene-Cu-(OtBu)2_Na_02	-2711.56379480	-2268.39683209	-30.0	-2711.161060	-2268.164152	-12.1	17.9	26.0
Figure 9_Cu-(OtBu)2_Na	-2268.34902130	-2268.34902130	0.0	-2268.144864	-2268.144864	0.0	0.0	24.5
Figure 9_para-H-styrene-Cu-(OtBu)2_Na_01	-2577.72481829	-2268.39758296	-30.5	-2577.391693	-2268.166743	-13.7	16.7	26.2
Figure 9_para-H-styrene-Cu-(OtBu)2_Na_02	-2577.72480787	-2268.39757254	-30.5	-2577.391579	-2268.166629	-13.7	16.8	31.4
Figure 9_Cu-(OtBu)2_Na	-2268.34902130	-2268.34902130	0.0	-2268.144864	-2268.144864	0.0	0.0	24.5
Figure 9_para-CO2Me-styrene-Cu-(OtBu)2_Na_01	-2805.37090024	-2268.39843422	-31.0	-2804.997907	-2268.164932	-12.6	18.4	24.1
Figure 9_para-CO2Me-styrene-Cu-(OtBu)2_Na_02	-2805.37090023	-2268.39843421	-31.0	-2804.997906	-2268.164931	-12.6	18.4	24.1

Figure 10

Figure 10_NaOtBu-Cu-Me	-2075.35042459	-2914.16234337	0.0	-2075.229306	-2913.912419	0.0	0.0	-32.5
Figure 10_NaOtBu-Cu-Me_(145 deg)	-2075.34278322	-2914.15470200	4.8	-2075.222774	-2913.905887	4.1	-0.7	-11.4
Figure 10_NaOtBu-Cu-Me_(130 deg)	-2075.33621269	-2914.14813147	8.9	-2075.216580	-2913.899693	8.0	-0.9	39.9
Figure 10_NaOtBu-Cu-Me_(115 deg)	-2075.32884553	-2914.14076431	13.5	-2075.208226	-2913.891339	13.2	-0.3	-9.4
Figure 10_NaOtBu_ts(SN2')_01	-2914.15039392	-2914.15039392	7.5	-2913.876811	-2913.876811	22.3	14.8	-228.7
Figure 10_NaOtBu_ts(SN2')_02	-2914.15050466	-2914.15050466	7.4	-2913.876794	-2913.876794	22.4	14.9	-245.6
Figure 10_NaOtBu_ts(SN2')_03	-2914.14886171	-2914.14886171	8.5	-2913.876399	-2913.876399	22.6	14.1	-234.2
Figure 10_NaOtBu_ts(SN2')_04	-2914.14810523	-2914.14810523	8.9	-2913.874279	-2913.874279	23.9	15.0	-261.8
Figure 10_NaOtBu_ts(SN2)_01	-2914.14526307	-2914.14526307	10.7	-2913.873417	-2913.873417	24.5	13.8	-335.1
Figure 10_NaOtBu_ts(SN2)_02	-2914.14552014	-2914.14552014	10.6	-2913.872693	-2913.872693	24.9	14.4	-358.8
Figure 10_NaOtBu_ts(SN2)_03	-2914.14400540	-2914.14400540	11.5	-2913.872211	-2913.872211	25.2	13.7	-344.8
Figure 10_NaOtBu_ts(SN2)_04	-2914.14390216	-2914.14390216	11.6	-2913.869510	-2913.869510	26.9	15.4	-336.7
Figure 10_NaOtBu_ts(SN2')_chelate_01	-2914.16942813	-2914.16942813	-4.4	-2913.895677	-2913.895677	10.5	15.0	-377.0
Figure 10_NaOtBu_ts(SN2')_chelate_02	-2914.16958209	-2914.16958209	-4.5	-2913.895571	-2913.895571	10.6	15.1	-387.0
Figure 10_NaOtBu_ts(SN2')_chelate_03	-2914.17005408	-2914.17005408	-4.8	-2913.894634	-2913.894634	11.2	16.0	-394.1
Figure 10_NaOtBu_ts(SN2')_chelate_04	-2914.17005409	-2914.17005409	-4.8	-2913.894634	-2913.894634	11.2	16.0	-394.1
Figure 10_NaOtBu_ts(SN2')_chelate_05	-2914.16875021	-2914.16875021	-4.0	-2913.892367	-2913.892367	12.6	16.6	-369.0
Figure 10_NaOtBu_ts(SN2')_chelate_06	-2914.16875021	-2914.16875021	-4.0	-2913.892367	-2913.892367	12.6	16.6	-369.0
Figure 10_NaOtBu_ts(SN2)_chelate_01	-2914.16222070	-2914.16222070	0.1	-2913.895018	-2913.895018	10.9	10.8	-483.3
Figure 10_NaOtBu_ts(SN2)_chelate_02	-2914.16232564	-2914.16232564	0.0	-2913.892317	-2913.892317	12.6	12.6	-494.8
Figure 10_NaOtBu_ts(SN2)_chelate_03	-2914.16068298	-2914.16068298	1.0	-2913.891867	-2913.891867	12.9	11.9	-481.8
Figure 10_NaOtBu_ts(SN2)_chelate_04	-2914.16231279	-2914.16231279	0.0	-2913.891111	-2913.891111	13.4	13.4	-469.1
Figure 10_NaOtBu_ts(SN2)_chelate_05	-2914.16125846	-2914.16125846	0.7	-2913.890253	-2913.890253	13.9	13.2	-469.6
Figure 10_NaOtBu_ts(SN2)_chelate_06	-2914.16058712	-2914.16058712	1.1	-2913.889265	-2913.889265	14.5	13.4	-465.6
Figure 10_PMe3-Cu-Me	-2141.10632939	-2979.91824817	0.0	-2140.996008	-2979.679121	0.0	0.0	48.2
Figure 10_PMe3-Cu-Me_(145 deg)	-2141.09872349	-2979.91064227	4.8	-2140.986760	-2979.669873	5.8	1.0	70.7
Figure 10_PMe3-Cu-Me_(130 deg)	-2141.09184945	-2979.90376823	9.1	-2140.978995	-2979.662108	10.7	1.6	64.3

Figure 10_PMe3-Cu-Me_(115 deg)	-2141.08375606	-2979.89567484	14.2	-2140.971734	-2979.654847	15.2	1.1	53.8
Figure 10_PMe3_ts(SN2')_01	-2979.90366207	-2979.90366207	9.2	-2979.640377	-2979.640377	24.3	15.2	-311.5
Figure 10_PMe3_ts(SN2')_02	-2979.90320903	-2979.90320903	9.4	-2979.639845	-2979.639845	24.6	15.2	-287.9
Figure 10_PMe3_ts(SN2')_03	-2979.90323285	-2979.90323285	9.4	-2979.637616	-2979.637616	26.0	16.6	-289.3
Figure 10_PMe3_ts(SN2')_04	-2979.90323285	-2979.90323285	9.4	-2979.637616	-2979.637616	26.0	16.6	-289.3
Figure 10_PMe3_ts(SN2)_01	-2979.90175960	-2979.90175960	10.3	-2979.638284	-2979.638284	25.6	15.3	-328.9
Figure 10_PMe3_ts(SN2)_02	-2979.90254477	-2979.90254477	9.9	-2979.638179	-2979.638179	25.7	15.8	-358.4
Figure 10_PMe3_ts(SN2)_03	-2979.90254477	-2979.90254477	9.9	-2979.638178	-2979.638178	25.7	15.8	-358.4
Figure 10_PMe3_ts(SN2)_04	-2979.90029845	-2979.90029845	11.3	-2979.636977	-2979.636977	26.4	15.2	-334.5
Figure 10_NHCMe2-Cu-Me	-1985.96094373	-2824.77286251	0.0	-1985.814079	-2824.497192	0.0	0.0	47.1
Figure 10_NHCMe2-Cu-Me_(145 deg)	-1985.95101987	-2824.76293865	6.2	-1985.802010	-2824.485123	7.6	1.3	65.1
Figure 10_NHCMe2-Cu-Me_(130 deg)	-1985.94203020	-2824.75394898	11.9	-1985.794273	-2824.477386	12.4	0.6	66.0
Figure 10_NHCMe2-Cu-Me_(115 deg)	-1985.93143678	-2824.74335556	18.5	-1985.784721	-2824.467834	18.4	-0.1	49.3
Figure 10_NHCMe2_ts(SN2')_01	-2824.75801259	-2824.75801259	9.3	-2824.460014	-2824.460014	23.3	14.0	-332.6
Figure 10_NHCMe2_ts(SN2')_02	-2824.75692951	-2824.75692951	10.0	-2824.458601	-2824.458601	24.2	14.2	-329.6
Figure 10_NHCMe2_ts(SN2')_03	-2824.75750602	-2824.75750602	9.6	-2824.457526	-2824.457526	24.9	15.3	-318.4
Figure 10_NHCMe2_ts(SN2')_04	-2824.75669355	-2824.75669355	10.1	-2824.456634	-2824.456634	25.5	15.3	-334.2
Figure 10_NHCMe2_ts(SN2)_01	-2824.75588695	-2824.75588695	10.7	-2824.455687	-2824.455687	26.0	15.4	-385.6
Figure 10_NHCMe2_ts(SN2)_02	-2824.75588696	-2824.75588696	10.7	-2824.455684	-2824.455684	26.0	15.4	-385.6
Figure 10_NHCMe2_ts(SN2)_03	-2824.75502346	-2824.75502346	11.2	-2824.455686	-2824.455686	26.0	14.9	-384.8
Figure 10_NHCMe2_ts(SN2)_04	-2824.75341246	-2824.75341246	12.2	-2824.453336	-2824.453336	27.5	15.3	-372.6

E …….. electronic energy in hartree with ωB97XD/Def2SVP in THF(SMD)
E(sum).. sum of electronic energies in hartree with ωB97XD/Def2SVP in THF(SMD) after mass balance
ΔE …… relative electronic energy in kcal/mol with ωB97XD/Def2SVP in THF(SMD)
G …….. electronic and thermal free energy with ωB97XD/Def2SVP in THF(SMD)
G(sum).. sum of electronic and thermal free energies with ωB97XD/Def2SVP in THF(SMD) after mass balance
ΔG …… relative free energy in kcal/mol with ωB97XD/Def2SVP in THF(SMD)
ΔG_{corr} … thermal correction to free energy in kcal/mol obtained with ωB97XD/Def2SVP in THF(SMD) ($\Delta G = \Delta E + \Delta G_{corr}$)
Freq ..… lowest frequency

Single point energies in Figures 1–10 with ωB97XD, M06 and MN12SX

ωB97XD/Def2TZVPP thf(SMD)				M06/Def2TZVPP thf(SMD)				MN12SX/Def2TZVPP thf(SMD)			
E_{sp} [hartree]	E_{sp} (sum) [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	E_{sp} (sum) [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	E_{sp} (sum) [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-822.63742462				-822.34096278				-822.21045351			
-644.47941828				-644.23994397				-644.12896180			
-395.41732056				-395.32316214				-395.24870005			
-2629.35690509				-2628.58922077				-2628.46365510			
-306.03731489				-305.90630992				-305.86391504			
-461.12441594				-461.03901632				-460.98757969			
-232.47633068				-232.38382755				-232.34339344			
-443.63960534				-443.44045805				-443.40779969			
-309.65716057				-309.51465818				-309.50609487			
-537.56167268				-537.37175015				-537.31952508			
-839.55116847				-839.40607084				-839.28302153			
-2102.33511687				-2102.15846683				-2101.90776119			
-1947.26090385				-1947.04042106				-1946.79710435			
-2084.83222579				-2084.54535952				-2084.31184521			
-1950.84759171				-1950.61689125				-1950.40824573			
-2178.75183478				-2178.47354099				-2178.22118843			
	Figure 1										
-4503.11271283	-2361.57097464	19.2	18.0	-4502.15727169	-2361.18372791	22.0	20.8	-4501.78541783	-2360.90934931	22.3	21.1
-5325.75818708	-2361.57902427	14.1	36.0	-5324.50222760	-2361.18772105	19.5	41.4	-5323.98679573	-2360.90027370	28.0	49.9
-5325.76066125	-2361.58149844	12.6	33.2	-5324.50832965	-2361.19382310	15.7	36.3	-5323.99847408	-2360.91195205	20.7	41.3
-5325.75217508	-2361.57301227	17.9	36.0	-5324.50059201	-2361.18608546	20.5	38.7	-5323.99060089	-2360.90407886	25.6	43.7
-5325.75768104	-2361.57851823	14.4	36.3	-5324.50206025	-2361.18755370	19.6	41.5	-5323.98724846	-2360.90072643	27.7	49.6
-5325.79615264	-2361.61698983	-9.7	7.0	-5324.54316041	-2361.22865386	-6.2	10.5	-5324.03481486	-2360.94829283	-2.1	14.6
-4681.30126301	-2361.60151849	0.0	0.0	-4680.29335366	-2361.21879107	0.0	0.0	-4679.90245130	-2360.94489107	0.0	0.0
-4681.30106701	-2361.60132249	0.1	1.4	-4680.29243536	-2361.21787277	0.6	1.8	-4679.90171886	-2360.94415863	0.5	1.7
-4681.29350327	-2361.59375875	4.9	2.8	-4680.28875077	-2361.21418818	2.9	0.8	-4679.89907318	-2360.94151295	2.1	0.0
-4681.29312649	-2361.59338197	5.1	4.3	-4680.28852829	-2361.21396570	3.0	2.3	-4679.89810889	-2360.94054866	2.7	2.0
-4681.29621168	-2361.59646716	3.2	4.2	-4680.29108504	-2361.21652245	1.4	2.5	-4679.90071266	-2360.94315243	1.1	2.2
-4681.29322386	-2361.59347934	5.0	5.3	-4680.28940295	-2361.21484036	2.5	2.8	-4679.89864459	-2360.94108436	2.4	2.7
-4681.29226619	-2361.59252167	5.6	5.0	-4680.28775475	-2361.21319216	3.5	2.9	-4679.89684239	-2360.93928216	3.5	2.9
-4681.29266017	-2361.59291565	5.4	6.6	-4680.28838888	-2361.21382629	3.1	4.3	-4679.89691367	-2360.93935344	3.5	4.6
-4681.29290076	-2361.59315624	5.2	6.6	-4680.28860475	-2361.21404216	3.0	4.3	-4679.89736128	-2360.93980105	3.2	4.5
-4990.96873253	-2361.61182744	-6.5	12.8	-4989.81665075	-2361.22742998	-5.4	13.8	-4989.41412818	-2360.95047308	-3.5	15.8
-4990.96759415	-2361.61068906	-5.8	12.7	-4989.81249067	-2361.22326990	-2.8	15.7	-4989.40718567	-2360.94353057	0.9	19.3
-4990.96759442	-2361.61068933	-5.8	12.7	-4989.81249185	-2361.22327108	-2.8	15.7	-4989.40718643	-2360.94353133	0.9	19.3
-4990.96329565	-2361.60639056	-3.1	14.7	-4989.80947843	-2361.22025766	-0.9	16.9	-4989.40601438	-2360.94235928	1.6	19.4
-4990.96281341	-2361.60590832	-2.8	16.7	-4989.80897082	-2361.21975005	-0.6	18.8	-4989.40478921	-2360.94113411	2.4	21.8
-4990.96281305	-2361.60590796	-2.8	16.7	-4989.80897019	-2361.21974942	-0.6	18.8	-4989.40478830	-2360.94113320	2.4	21.8
-4990.95774691	-2361.60084182	0.4	19.5	-4989.80818047	-2361.21895970	-0.1	19.0	-4989.40643600	-2360.94278090	1.3	20.4
-4990.95774681	-2361.60084172	0.4	19.5	-4989.80818027	-2361.21895950	-0.1	19.0	-4989.40643587	-2360.94278077	1.3	20.4
-4990.95526170	-2361.59835661	2.0	22.4	-4989.80249014	-2361.21326937	3.5	23.9	-4989.39801364	-2360.93435854	6.6	27.0
-4991.01269673	-2361.65579164	-34.1	-16.1	-4989.85884735	-2361.26962658	-31.9	-13.9	-4989.45286250	-2360.98920740	-27.8	-9.8
-4991.01274487	-2361.65583978	-34.1	-15.5	-4989.85871857	-2361.26949780	-31.8	-13.3	-4989.45245036	-2360.98879526	-27.6	-9.0
-4991.00983046	-2361.65292537	-32.3	-12.1	-4989.85987246	-2361.27065169	-32.5	-12.4	-4989.45426081	-2360.99060571	-28.7	-8.5
-4990.95713259	-2361.60022750	0.8	17.8	-4989.80510101	-2361.21588024	1.8	18.8	-4989.40233862	-2360.93868352	3.9	20.9
-4990.95712444	-2361.60021935	0.8	18.6	-4989.80507078	-2361.21585001	1.8	19.6	-4989.40231806	-2360.93866296	3.9	21.7
-4990.96130800	-2361.60440291	-1.8	19.2	-4989.80761326	-2361.21839249	0.3	21.2	-4989.40192568	-2360.93827058	4.2	25.1

-4990.95645430	-2361.59954921	1.2	20.6	-4989.80158736	-2361.21236659	4.0	23.4	-4989.39827491	-2360.93461981	6.4	25.8
-4990.95690745	-2361.60000236	1.0	21.5	-4989.80342035	-2361.21419958	2.9	23.4	-4989.39890303	-2360.93524793	6.1	26.6
-4990.95690757	-2361.60000248	1.0	21.5	-4989.80342032	-2361.21419955	2.9	23.4	-4989.39890295	-2360.93524785	6.1	26.6
-4990.95690739	-2361.60000230	1.0	21.5	-4989.80342023	-2361.21419946	2.9	23.4	-4989.39890285	-2360.93524775	6.1	26.6
-4990.95307635	-2361.59617126	3.4	22.5	-4989.80012382	-2361.21090305	4.9	24.1	-4989.39840387	-2360.93474877	6.4	25.5
-4990.95639924	-2361.59949415	1.3	22.8	-4989.80191250	-2361.21269173	3.8	25.3	-4989.39822477	-2360.93456967	6.5	28.0
-4990.94701335	-2361.59010826	7.2	27.3	-4989.79713831	-2361.20791754	6.8	27.0	-4989.39545411	-2360.93179901	8.2	28.4
-4990.94003262	-2361.58312753	11.5	31.0	-4989.79087377	-2361.20165300	10.8	30.2	-4989.38673471	-2360.92307961	13.7	33.1
-4991.01663334	-2361.65972825	-36.5	-17.9	-4989.86363132	-2361.27441055	-34.9	-16.2	-4989.45775192	-2360.99409682	-30.9	-12.2
-4991.00934139	-2361.65243630	-32.0	-11.6	-4989.85567366	-2361.26645289	-29.9	-9.6	-4989.44797285	-2360.98431775	-24.7	-4.4
-4990.96262428	-2361.60571919	-2.6	13.7	-4989.81170293	-2361.22248216	-2.3	14.1	-4989.40869386	-2360.94503876	-0.1	16.3
-4990.96403496	-2361.60712987	-3.5	13.7	-4989.81176384	-2361.22254307	-2.4	14.9	-4989.40843601	-2360.94478091	0.1	17.3
-4990.96675951	-2361.60985442	-5.2	14.6	-4989.81273580	-2361.22351503	-3.0	16.8	-4989.41294327	-2360.94928817	-2.8	17.0
-4990.96308741	-2361.60618232	-2.9	15.8	-4989.81051818	-2361.22129741	-1.6	17.2	-4989.40643359	-2360.94277849	1.3	20.1
-4990.95943659	-2361.60253150	-0.6	18.6	-4989.80667493	-2361.21745416	0.8	20.0	-4989.40146307	-2360.93780797	4.4	23.6
-4990.95663692	-2361.59973183	1.1	19.3	-4989.80697068	-2361.21774991	0.7	18.9	-4989.40163073	-2360.93797563	4.3	22.6
-4990.95571174	-2361.59880665	1.7	19.9	-4989.80628489	-2361.21706412	1.1	19.2	-4989.40508369	-2360.94142859	2.2	20.3
-4990.95467292	-2361.59776783	2.4	21.3	-4989.80521477	-2361.21599400	1.8	20.7	-4989.40390830	-2360.94025320	2.9	21.9
-4990.95631690	-2361.59941181	1.3	21.6	-4989.80603730	-2361.21681653	1.2	21.6	-4989.40570346	-2360.94204836	1.8	22.1
-4990.95631681	-2361.59941172	1.3	21.6	-4989.80603723	-2361.21681646	1.2	21.6	-4989.40570341	-2360.94204831	1.8	22.1
-4990.95553530	-2361.59863021	1.8	21.5	-4989.80157073	-2361.21234996	4.0	23.7	-4989.39830544	-2360.93465034	6.4	26.1
-4990.95642322	-2361.59951813	1.3	22.3	-4989.80268673	-2361.21346596	3.3	24.4	-4989.39892003	-2360.93526493	6.0	27.1
-4990.95543240	-2361.59852731	1.9	23.3	-4989.80139646	-2361.21217569	4.2	25.5	-4989.39794838	-2360.93429328	6.7	28.0
-4991.01531444	-2361.65840935	-35.7	-18.0	-4989.86302095	-2361.27380018	-34.5	-16.8	-4989.45771896	-2360.99406386	-30.9	-13.2
-4991.00632345	-2361.64941836	-30.1	-13.2	-4989.85699350	-2361.26777273	-30.7	-13.9	-4989.45241716	-2360.98876206	-27.5	-10.7
-4991.00718221	-2361.65027712	-30.6	-11.6	-4989.85665126	-2361.26743049	-30.5	-11.5	-4989.45333196	-2360.98967686	-28.1	-9.1
-4991.00685767	-2361.64995258	-30.4	-11.2	-4989.85499978	-2361.26577901	-29.5	-10.3	-4989.45195091	-2360.98829581	-27.2	-8.1
-4991.00394535	-2361.64704026	-28.6	-7.0	-4989.84935186	-2361.26013109	-25.9	-4.4	-4989.44157757	-2360.97792247	-20.7	0.8
-4990.97404789	-2361.61714280	-9.8	5.7	-4989.81934440	-2361.23012363	-7.1	8.4	-4989.41692500	-2360.95326990	-5.3	10.3
-4990.95673406	-2361.59982897	1.1	18.0	-4989.80408925	-2361.21486848	2.5	19.4	-4989.40478299	-2360.94112789	2.4	19.3
-4990.96030903	-2361.60340394	-1.2	17.6	-4989.80646415	-2361.21724338	1.0	19.8	-4989.40202993	-2360.93837483	4.1	22.9
-4990.95135576	-2361.59445067	4.4	22.0	-4989.79688752	-2361.20766675	7.0	24.5	-4989.39693787	-2360.93328277	7.3	24.9
-4990.95594108	-2361.59903599	1.6	20.3	-4989.80315133	-2361.21393056	3.1	21.8	-4989.39874743	-2360.93509233	6.1	24.9
-4990.95866104	-2361.60175595	-0.1	20.5	-4989.80539739	-2361.21617662	1.6	22.3	-4989.40124308	-2360.93758798	4.6	25.2
-4990.95857682	-2361.60167173	-0.1	20.6	-4989.80505034	-2361.21582957	1.9	22.6	-4989.40113184	-2360.93747674	4.7	25.4
-4990.95015762	-2361.59325253	5.2	25.5	-4989.79967506	-2361.21045429	5.2	25.6	-4989.39972865	-2360.93607355	5.5	25.9
-4990.95618593	-2361.59928084	1.4	23.4	-4989.80069088	-2361.21147011	4.6	26.6	-4989.39903447	-2360.93537937	6.0	28.0
-4990.94340654	-2361.58650145	9.4	29.3	-4989.79005783	-2361.20083706	11.3	31.2	-4989.39124804	-2360.92759294	10.9	30.8
-4991.00988880	-2361.65298371	-32.3	-12.8	-4989.85679752	-2361.26757675	-30.6	-11.2	-4989.45063671	-2360.98698161	-26.4	-7.0
-4991.01185824	-2361.65495315	-33.5	-13.2	-4989.85788626	-2361.26866549	-31.3	-11.0	-4989.45126722	-2360.98761212	-26.8	-6.5
-4991.00145664	-2361.64455155	-27.0	-8.7	-4989.85114045	-2361.26191968	-27.1	-8.7	-4989.44637551	-2360.98272041	-23.7	-5.4
-4991.00277397	-2361.64586888	-27.8	-9.2	-4989.85076914	-2361.26154837	-26.8	-8.2	-4989.44744986	-2360.98379476	-24.4	-5.8
-4991.01180007	-2361.65489498	-33.5	-17.9	-4989.85830089	-2361.26908012	-31.6	-15.9	-4989.45549263	-2360.99183753	-29.5	-13.8
-4991.01214734	-2361.65524225	-33.7	-16.4	-4989.86071936	-2361.27149859	-33.1	-15.8	-4989.45663966	-2360.99298456	-30.2	-12.9
-4991.00984555	-2361.65294046	-32.3	-15.5	-4989.85637305	-2361.26715228	-30.3	-13.6	-4989.45246859	-2360.98881349	-27.6	-10.8
-5830.57189369	-2361.66382014	-39.1	-3.0	-5829.27024700	-2361.27495540	-35.2	0.9	-5828.73887762	-2360.99220099	-29.7	6.4
-5830.56914419	-2361.66107064	-37.4	-0.8	-5829.27079173	-2361.27550013	-35.6	0.9	-5828.73973496	-2360.99305833	-30.2	6.3
-5830.56799162	-2361.65991807	-36.6	-1.1	-5829.26812196	-2361.27283036	-33.9	1.6	-5828.73813491	-2360.99145828	-29.2	6.3
-5830.56651967	-2361.65844612	-35.7	2.4	-5829.26644529	-2361.27115369	-32.9	5.2	-5828.73478507	-2360.98810844	-27.1	11.0
-5830.54055918	-2361.63248563	-19.4	15.7	-5829.24369011	-2361.24839851	-18.6	16.6	-5828.71307869	-2360.96640206	-13.5	21.7
-5830.53878381	-2361.63071026	-18.3	16.8	-5829.24261449	-2361.24732289	-17.9	17.2	-5828.71160944	-2360.96493281	-12.6	22.5
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-5830.52537225	-2361.61729870	-9.9	26.3	-5829.22775442	-2361.23246282	-8.6	27.7	-5828.69587648	-2360.94919985	-2.7	33.5
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-5830.54836304	-2361.64028949	-24.3	10.1	-5829.24967736	-2361.25438576	-22.3	12.1	-5828.72388783	-2360.97721120	-20.3	14.2

-5830.54889015	-2361.64081660	-24.7	12.0	-5829.25024847	-2361.25495687	-22.7	14.0	-5828.72075678	-2360.97408015	-18.3	18.4

Figure 2

-4359.61300751	-2361.58435577	10.8	16.9	-4358.98519860	-2361.20196638	10.6	16.7	-4358.40966850	-2360.92850578	10.3	16.4
-2179.79614972	-2361.57400174	17.3	15.1	-2179.48426810	-2361.19363518	15.8	13.6	-2179.19743761	-2360.92110914	14.9	12.7
-3002.44083043	-2361.58125783	12.7	27.6	-3001.83253866	-2361.20094296	11.2	26.1	-3001.41017115	-2360.92338917	13.5	28.4
-3002.44252819	-2361.58295559	11.6	25.3	-3001.83632324	-2361.20472754	8.8	22.5	-3001.41319180	-2360.92640982	11.6	25.3
-3002.46950946	-2361.60993686	-5.3	8.8	-3001.86295691	-2361.23136121	-7.9	6.2	-3001.44135169	-2360.95456971	-6.1	8.0
-2357.97781700	-2361.59766268	2.4	1.9	-2357.61404083	-2361.22238910	-2.3	-2.8	-2357.30762783	-2360.94980766	-3.1	-3.6
-2801.62930346	-2361.60954380	-5.0	9.4	-2801.06201671	-2361.22990693	-7.0	7.4	-2800.72267142	-2360.95705156	-7.6	6.8
-2801.61371274	-2361.59395308	4.7	19.6	-2801.05085708	-2361.21874730	0.0	14.9	-2800.71150494	-2360.94588508	-0.6	14.3
-2801.66506261	-2361.64530295	-27.5	-11.7	-2801.10152093	-2361.26941115	-31.8	-16.0	-2800.75660686	-2360.99098700	-28.9	-13.2
-2801.66364796	-2361.64388830	-26.6	-9.5	-2801.09908506	-2361.26697528	-30.2	-13.2	-2800.75700934	-2360.99138948	-29.2	-12.1
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-2801.61841326	-2361.59865360	1.8	15.3	-2801.05652379	-2361.22441401	-3.5	9.9	-2800.71706387	-2360.95144401	-4.1	9.3
-2801.65497289	-2361.63521323	-21.1	-7.2	-2801.08897115	-2361.25686137	-23.9	-10.0	-2800.75054838	-2360.98492852	-25.1	-11.2
-2801.63923586	-2361.61947620	-11.3	3.1	-2801.07393617	-2361.24182639	-14.5	-0.1	-2800.73537827	-2360.96975841	-15.6	-1.2
-2801.64147925	-2361.62171959	-12.7	2.0	-2801.07473897	-2361.24262919	-15.0	-0.2	-2800.73753174	-2360.97191188	-17.0	-2.2
-2801.63591153	-2361.61615187	-9.2	4.6	-2801.06953973	-2361.23742995	-11.7	2.1	-2800.73347209	-2360.96785223	-14.4	-0.6
-2801.63796638	-2361.61820672	-10.5	3.0	-2801.07100210	-2361.23889232	-12.6	0.8	-2800.73511464	-2360.96949478	-15.4	-2.0
-2801.63318337	-2361.61342371	-7.5	7.1	-2801.06633154	-2361.23422176	-9.7	4.9	-2800.73030654	-2360.96468668	-12.4	2.1
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-3641.23661408	-2361.66568596	-40.3	-4.4	-3640.52250346	-2361.28432284	-41.1	-5.2	-3640.05799338	-2361.00935199	-40.4	-4.6
-3641.23196268	-2361.66103456	-37.3	-3.1	-3640.51918181	-2361.28100119	-39.0	-4.8	-3640.05366321	-2361.00502182	-37.7	-3.5

-4359.61300751	-2361.58435577	10.8	16.9	-4358.98519860	-2361.20196638	10.6	16.7	-4358.40966850	-2360.92850578	10.3	16.4
-2179.79614972	-2361.57400174	17.3	15.1	-2179.48426810	-2361.19363518	15.8	13.6	-2179.19743761	-2360.92110914	14.9	12.7
-3002.44083043	-2361.58125783	12.7	27.6	-3001.83253866	-2361.20094296	11.2	26.1	-3001.41017115	-2360.92338917	13.5	28.4
-3002.44252819	-2361.58295559	11.6	25.3	-3001.83632324	-2361.20472754	8.8	22.5	-3001.41319180	-2360.92640982	11.6	25.3
-3002.46950946	-2361.60993686	-5.3	8.8	-3001.86295691	-2361.23136121	-7.9	6.2	-3001.44135169	-2360.95456971	-6.1	8.0
-2357.97781700	-2361.59766268	2.4	1.9	-2357.61404083	-2361.22238910	-2.3	-2.8	-2357.30762783	-2360.94980766	-3.1	-3.6
-2667.64939867	-2361.61208379	-6.6	9.2	-2667.13892104	-2361.23261112	-8.7	7.2	-2666.82427884	-2360.96036380	-9.7	6.1
-2667.63813480	-2361.60081992	0.4	16.2	-2667.13171715	-2361.22540723	-4.2	11.6	-2666.81718486	-2360.95326982	-5.3	10.5
-2667.68966647	-2361.65235159	-31.9	-15.5	-2667.18295379	-2361.27664387	-36.3	-19.9	-2666.86274707	-2360.99883203	-33.8	-17.5
-2667.68701522	-2361.64970034	-30.2	-16.0	-2667.18034588	-2361.27403596	-34.7	-20.4	-2666.86222706	-2360.99831202	-33.5	-19.3
-2667.68819177	-2361.65087689	-31.0	-14.6	-2667.18099856	-2361.27468864	-35.1	-18.7	-2666.86365922	-2360.99974418	-34.4	-18.0
-2667.64266431	-2361.60534943	-2.4	10.7	-2667.13779876	-2361.23148884	-8.0	5.1	-2666.82281325	-2360.95889821	-8.8	4.3
-2667.67341838	-2361.63610350	-21.7	-6.9	-2667.16439493	-2361.25808501	-24.7	-9.8	-2666.85071508	-2360.98680004	-26.3	-11.5
-2667.65832772	-2361.62101284	-12.2	0.2	-2667.15018521	-2361.24387529	-15.7	-3.3	-2666.83620841	-2360.97229337	-17.2	-4.8
-2667.65999464	-2361.62267976	-13.3	0.6	-2667.15021920	-2361.24390928	-15.8	-1.8	-2666.83778618	-2360.97387114	-18.2	-4.3
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-2667.65289891	-2361.61558403	-8.8	6.3	-2667.14248990	-2361.23617998	-10.9	4.2	-2666.83080066	-2360.96688562	-13.8	1.3
-2667.65677882	-2361.61946394	-11.3	2.5	-2667.14685863	-2361.24054871	-13.7	0.1	-2666.83524081	-2360.97132577	-16.6	-2.9
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-2667.69786576	-2361.66055088	-37.0	-20.7	-2667.18965374	-2361.28334382	-40.5	-24.1	-2666.87157980	-2361.00766476	-39.4	-23.0

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-3507.23604058	-2361.64755723	-28.9	4.9	-3506.58233743	-2361.26995668	-32.1	1.7	-3506.14016701	-2360.99323044	-30.3	3.5
-3507.23407031	-2361.64558696	-27.7	5.9	-3506.58114889	-2361.26876814	-31.4	2.2	-3506.13909858	-2360.99216201	-29.7	3.9
-3507.25556325	-2361.66707990	-41.1	-7.1	-3506.59803888	-2361.28565813	-42.0	-7.9	-3506.15819863	-2361.01126206	-41.6	-7.6
-3507.25354805	-2361.66506470	-39.9	-5.6	-3506.59647729	-2361.28409654	-41.0	-6.7	-3506.15611107	-2361.00917450	-40.3	-6.0
-4359.61300751	-2361.58435577	10.8	16.9	-4358.98519860	-2361.20196638	10.6	16.7	-4358.40966850	-2360.92850578	10.3	16.4
-2179.79614972	-2361.57400174	17.3	15.1	-2179.48426810	-2361.19363518	15.8	13.6	-2179.19743761	-2360.92110914	14.9	12.7
-3002.44083043	-2361.58125783	12.7	27.6	-3001.83253866	-2361.20094296	11.2	26.1	-3001.41017115	-2360.92338917	13.5	28.4
-3002.44252819	-2361.58295559	11.6	25.3	-3001.83632324	-2361.20472754	8.8	22.5	-3001.41319180	-2360.92640982	11.6	25.3
-3002.46950946	-2361.60993686	-5.3	8.8	-3001.86295691	-2361.23136121	-7.9	6.2	-3001.44135169	-2360.95456971	-6.1	8.0
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-3735.13983544	-2361.64683998	-28.4	2.9	-3734.43828590	-2361.26881318	-31.4	0.0	-3733.95368094	-2360.99331416	-30.4	1.0
-3735.16340981	-2361.67041435	-43.2	-8.0	-3734.45789578	-2361.28842306	-43.7	-8.5	-3733.97408469	-2361.01371791	-43.2	-8.0
-3735.15945197	-2361.66645651	-40.7	-5.3	-3734.45588362	-2361.28641090	-42.4	-6.9	-3733.97381451	-2361.01344773	-43.0	-7.5

Figure 3

-4669.77209926	-2361.57680059	15.5	20.9	-4669.23265981	-2361.19299058	16.2	21.6	-4668.64174035	-2360.92087706	15.1	20.5
-2334.86939169	-2361.56014265	26.0	24.5	-2334.60107416	-2361.17773484	25.8	24.3	-2334.30714537	-2360.90715225	23.7	22.2
-3157.51884617	-2361.57217252	18.4	32.1	-3156.95144797	-2361.18714587	19.9	33.6	-3156.52541552	-2360.91496889	18.8	32.5
-3157.51487318	-2361.56819953	20.9	34.0	-3156.95088798	-2361.18658588	20.2	33.3	-3156.52159558	-2360.91114895	21.2	34.3
-3157.54523433	-2361.59856068	1.9	15.5	-3156.98294213	-2361.21864003	0.1	13.7	-3156.55323181	-2360.94278518	1.3	14.9
-2513.05289186	-2361.58563649	10.0	7.5	-2512.73342116	-2361.20906303	6.1	3.6	-2512.41904219	-2360.93755737	4.6	2.1
-2956.70764005	-2361.60077934	0.5	15.2	-2956.18614536	-2361.22132918	-1.6	13.1	-2955.83811276	-2360.94882825	-2.5	12.3
-2956.68706596	-2361.58020525	13.4	28.6	-2956.16864033	-2361.20382415	9.4	24.6	-2955.82060941	-2360.93132490	8.5	23.7
-2956.73908940	-2361.63222869	-19.3	-2.0	-2956.21888849	-2361.25407231	-22.1	-4.9	-2955.86811460	-2360.97883009	-21.3	-4.0
-2956.73763089	-2361.63077018	-18.4	-3.0	-2956.21709866	-2361.25228248	-21.0	-5.6	-2955.86767199	-2360.97838748	-21.0	-5.6
-2956.73971299	-2361.63285228	-19.7	-5.6	-2956.22013951	-2361.25532333	-22.9	-8.8	-2955.87001464	-2360.98073013	-22.5	-8.4
-2956.69143922	-2361.58457851	10.6	22.2	-2956.17352187	-2361.20870569	6.3	17.9	-2955.82717727	-2360.93789276	4.4	15.9
-2956.73174903	-2361.62488832	-14.7	-1.4	-2956.21106559	-2361.24624941	-17.2	-4.0	-2955.86513297	-2360.97584846	-19.4	-6.2
-2956.71608769	-2361.60922698	-4.8	8.0	-2956.19585738	-2361.23104120	-7.7	5.1	-2955.84967939	-2360.96039488	-9.7	3.1
-2956.71711609	-2361.61025538	-5.5	7.7	-2956.19538550	-2361.23056932	-7.4	5.8	-2955.85136120	-2360.96207669	-10.8	2.4
-2956.70822449	-2361.60136378	0.1	12.9	-2956.18580310	-2361.22098692	-1.4	11.4	-2955.84296400	-2360.95367949	-5.5	7.2
-2956.71368261	-2361.60682190	-3.3	11.1	-2956.19095667	-2361.22614049	-4.6	9.9	-2955.84842594	-2360.95914143	-8.9	5.5
-2956.70904112	-2361.60218041	-0.4	12.5	-2956.18608775	-2361.22127157	-1.6	11.3	-2955.84367500	-2360.95439049	-6.0	6.9

-2956.71300641	-2361.60614570	-2.9	10.7	-2956.19046893	-2361.22565275	-4.3	9.3	-2955.84813167	-2360.95884716	-8.8	4.8
-854.37878572	-2361.60704188	-3.5	-5.9	-854.03608245	-2361.22973310	-6.9	-9.3	-853.94312409	-2360.96160077	-10.5	-13.0
-2956.72928342	-2361.62242271	-13.1	-0.4	-2956.20859018	-2361.24377400	-15.7	-2.9	-2955.86106697	-2360.97178246	-16.9	-4.1
-2956.70180090	-2361.59494019	4.1	16.4	-2956.18096231	-2361.21614613	1.7	14.0	-2955.83554274	-2360.94625823	-0.9	11.5
-2956.75204295	-2361.64518224	-27.4	-11.6	-2956.23065120	-2361.26583502	-29.5	-13.7	-2955.88096400	-2360.99167949	-29.4	-13.5
-3796.30899013	-2361.65096096	-31.0	0.5	-3795.64262580	-2361.27173878	-33.2	-1.7	-3795.16525988	-2360.99295383	-30.2	1.3
-3796.31019724	-2361.65216807	-31.8	2.0	-3795.64474807	-2361.27386105	-34.6	-0.8	-3795.16740735	-2360.99510130	-31.5	2.3
-3796.28330188	-2361.62527271	-14.9	16.4	-3795.62005806	-2361.24917104	-19.1	12.2	-3795.14372434	-2360.97141829	-16.6	14.7
-3796.28401951	-2361.62599034	-15.4	17.2	-3795.62133099	-2361.25044397	-19.9	12.7	-3795.14528026	-2360.97297421	-17.6	15.0
-3796.30799724	-2361.64996807	-30.4	3.1	-3795.64152160	-2361.27063458	-32.5	1.0	-3795.16576035	-2360.99345430	-30.5	3.1
-3796.30372847	-2361.64569930	-27.7	5.0	-3795.63946213	-2361.26857511	-31.2	1.5	-3795.16398028	-2360.99167423	-29.4	3.4
-4669.77209926	-2361.57680059	15.5	20.9	-4669.23265981	-2361.19299058	16.2	21.6	-4668.64174035	-2360.92087706	15.1	20.5
-2334.86939169	-2361.56014265	26.0	24.5	-2334.60107416	-2361.17773484	25.8	24.3	-2334.30714537	-2360.90715225	23.7	22.2
-3157.51884617	-2361.57217252	18.4	32.1	-3156.95144797	-2361.18714587	19.9	33.6	-3156.52541552	-2360.91496889	18.8	32.5
-3157.51487318	-2361.56819953	20.9	34.0	-3156.95088798	-2361.18658588	20.2	33.3	-3156.52159558	-2360.91114895	21.2	34.3
-3157.54523433	-2361.59856068	1.9	15.5	-3156.98294213	-2361.21864003	0.1	13.7	-3156.55323181	-2360.94278518	1.3	14.9
-2513.05289186	-2361.58563649	10.0	7.5	-2512.73342116	-2361.20906303	6.1	3.6	-2512.41904219	-2360.93755737	4.6	2.1
-2822.72763759	-2361.60322165	-1.1	12.8	-2822.26269465	-2361.22367834	-3.1	10.8	-2821.93979615	-2360.95221646	-4.6	9.3
-2822.71160653	-2361.58719059	9.0	23.2	-2822.25014157	-2361.21112526	4.8	19.0	-2821.92677170	-2360.93919201	3.6	17.8
-2822.76168195	-2361.63726601	-22.4	-6.5	-2822.29953272	-2361.26051641	-26.2	-10.2	-2821.97239921	-2360.98481952	-25.1	-9.1
-2822.76113040	-2361.63671446	-22.1	-8.6	-2822.29828209	-2361.25926578	-25.4	-11.9	-2821.97289704	-2360.98531735	-25.4	-11.8
-2822.76317026	-2361.63875432	-23.4	-9.2	-2822.30037878	-2361.26136247	-26.7	-12.5	-2821.97481338	-2360.98723369	-26.6	-12.4
-2822.71595661	-2361.59154067	6.3	16.9	-2822.25497973	-2361.21596342	1.8	12.4	-2821.93283681	-2360.94525712	-0.2	10.4
-2822.74955277	-2361.62513683	-14.8	-2.9	-2822.28589290	-2361.24687659	-17.6	-5.7	-2821.96490323	-2360.97732354	-20.4	-8.4
-2822.73406328	-2361.60964734	-5.1	5.9	-2822.27074413	-2361.23172782	-8.1	2.9	-2821.94951866	-2360.96193897	-10.7	0.3
-2822.73495211	-2361.61053617	-5.7	6.5	-2822.27029385	-2361.23127754	-7.8	4.4	-2821.95055761	-2360.96297792	-11.3	0.8
-2822.72754078	-2361.60312484	-1.0	11.4	-2822.26185087	-2361.22283456	-2.5	9.9	-2821.94320765	-2360.95562796	-6.7	5.7
-2822.73274796	-2361.60833202	-4.3	7.5	-2822.26660776	-2361.22759145	-5.5	6.3	-2821.94863164	-2360.96105195	-10.1	1.7
-2822.72817612	-2361.60376018	-1.4	11.8	-2822.26173434	-2361.22271803	-2.5	10.7	-2821.94360625	-2360.95602656	-7.0	6.2
-2822.73236560	-2361.60794966	-4.0	9.4	-2822.26632440	-2361.22730809	-5.3	8.1	-2821.94826445	-2360.96068476	-9.9	3.6
-720.39540514	-2361.60610607	-2.9	-6.0	-720.10913981	-2361.22859032	-6.1	-9.3	-720.04021804	-2360.96039954	-9.7	-12.9
-2822.74736934	-2361.62295340	-13.5	-1.9	-2822.28304044	-2361.24402413	-15.8	-4.3	-2821.96050440	-2360.97292471	-17.6	-6.0
-2822.72211334	-2361.59769740	2.4	14.7	-2822.25778031	-2361.21876400	0.0	12.3	-2821.93650598	-2360.94892629	-2.5	9.7
-2822.77187935	-2361.64746341	-28.8	-13.8	-2822.30793957	-2361.26892326	-31.5	-16.4	-2821.98201867	-2360.99443898	-31.1	-16.1
-3662.33412928	-2361.65854488	-35.8	-3.9	-3661.72614189	-2361.28105474	-39.1	-7.2	-3661.27213145	-2361.00153022	-35.5	-3.7
-3662.33365747	-2361.65807307	-35.5	-1.5	-3661.72379560	-2361.27870845	-37.6	-3.6	-3661.27068848	-2361.00008725	-34.6	-0.7
-3662.30496845	-2361.62938405	-17.5	13.4	-3661.69758692	-2361.25249977	-21.2	9.7	-3661.24620526	-2360.97560403	-19.3	11.6
-3662.30471849	-2361.62913409	-17.3	14.6	-3661.69859631	-2361.25350916	-21.8	10.1	-3661.24683226	-2360.97623103	-19.7	12.2
-3662.32683470	-2361.65125030	-31.2	2.1	-3661.71709726	-2361.27201011	-33.4	-0.1	-3661.26608153	-2360.99548030	-31.7	1.5
-3662.32339383	-2361.64780943	-29.0	3.5	-3661.71317075	-2361.26808360	-30.9	1.6	-3661.26458741	-2360.99398618	-30.8	1.7
-4669.77209926	-2361.57680059	15.5	20.9	-4669.23265981	-2361.19299058	16.2	21.6	-4668.64174035	-2360.92087706	15.1	20.5
-2334.86939169	-2361.56014265	26.0	24.5	-2334.60107416	-2361.17773484	25.8	24.3	-2334.30714537	-2360.90715225	23.7	22.2
-3157.51884617	-2361.57217252	18.4	32.1	-3156.95144797	-2361.18714587	19.9	33.6	-3156.52541552	-2360.91496889	18.8	32.5
-3157.51487318	-2361.56819953	20.9	34.0	-3156.95088798	-2361.18658588	20.2	33.3	-3156.52159558	-2360.91114895	21.2	34.3
-3157.54523433	-2361.59856068	1.9	15.5	-3156.98294213	-2361.21864003	0.1	13.7	-3156.55323181	-2360.94278518	1.3	14.9
-2513.05289186	-2361.58563649	10.0	7.5	-2512.73342116	-2361.20906303	6.1	3.6	-2512.41904219	-2360.93755737	4.6	2.1
-3050.63364237	-2361.60471432	-2.0	12.4	-3050.12172158	-2361.22561330	-4.3	10.2	-3049.75571758	-2360.95470768	-6.2	8.3
-3050.62297347	-2361.59404542	4.7	19.3	-3050.11449614	-2361.21838786	0.3	14.8	-3049.74805579	-2360.94704589	-1.4	13.2
-3050.67246970	-2361.64354165	-26.4	-9.4	-3050.16312695	-2361.26701867	-30.3	-13.3	-3049.79280977	-2360.99179987	-29.4	-12.4
-3050.67105857	-2361.64213052	-25.5	-10.5	-3050.16085613	-2361.26474785	-28.8	-13.9	-3049.79217174	-2360.99116184	-29.0	-14.1
-3050.67290163	-2361.64397358	-26.6	-12.2	-3050.16296835	-2361.26686007	-30.2	-15.8	-3049.79410420	-2360.99309430	-30.2	-15.8
-3050.62633272	-2361.59740467	2.6	14.8	-3050.11837842	-2361.22227014	-2.2	10.0	-3049.75313112	-2360.95212122	-4.5	7.7
-3050.65459044	-2361.62566239	-15.2	-2.3	-3050.14315601	-2361.24704773	-17.7	-4.9	-3049.77859979	-2360.97758989	-20.5	-7.7
-3050.63974489	-2361.61081684	-5.8	6.3	-3050.12874143	-2361.23263315	-8.7	3.5	-3049.76383038	-2360.96282048	-11.3	0.9
-3050.64038005	-2361.61145200	-6.2	6.1	-3050.12789211	-2361.23178383	-8.2	4.1	-3049.76476264	-2360.96375274	-11.8	0.5

-3050.63259300	-2361.60366495	-1.3	11.4	-3050.11947396	-2361.22336568	-2.9	9.9	-3049.75736164	-2360.95635174	-7.2	5.5
-3050.63866956	-2361.60974151	-5.2	8.0	-3050.12556012	-2361.22945184	-6.7	6.5	-3049.76368083	-2360.96267093	-11.2	2.0
-3050.63362566	-2361.60469761	-2.0	11.6	-3050.12019470	-2361.22408642	-3.3	10.3	-3049.75832780	-2360.95731790	-7.8	5.8
-3050.63800178	-2361.60907373	-4.7	7.9	-3050.12484620	-2361.22873792	-6.2	6.4	-3049.76317571	-2360.96216581	-10.8	1.8
-948.29944412	-2361.60563294	-2.6	-6.3	-947.96574899	-2361.22810754	-5.8	-9.6	-947.85307460	-2360.95982589	-9.4	-13.1
-3050.65229183	-2361.62336378	-13.7	0.2	-3050.14045811	-2361.24434983	-16.0	-2.1	-3049.77473366	-2360.97372376	-18.1	-4.2
-3050.62672003	-2361.59779198	2.3	15.6	-3050.11529999	-2361.21919171	-0.3	13.0	-3049.75045712	-2360.94944722	-2.9	10.4
-3050.67911248	-2361.65018443	-30.5	-16.1	-3050.16709398	-2361.27098570	-32.8	-18.3	-3049.79822888	-2360.99721898	-32.8	-18.4
-3890.24452219	-2361.66442567	-39.5	-6.1	-3889.58924514	-2361.28706603	-42.8	-9.5	-3889.09123116	-2361.00719973	-39.1	-5.8
-3890.24319441	-2361.66309789	-38.6	-5.1	-3889.58614696	-2361.28396785	-40.9	-7.3	-3889.08969637	-2361.00566494	-38.1	-4.6
-3890.21301199	-2361.63291547	-19.7	11.8	-3889.55836828	-2361.25618917	-23.5	8.0	-3889.06351115	-2360.97947972	-21.7	9.8
-3890.21210397	-2361.63200745	-19.1	13.1	-3889.55843400	-2361.25625489	-23.5	8.8	-3889.06319921	-2360.97916778	-21.5	10.8
-3890.23380344	-2361.65370692	-32.7	1.6	-3889.57551902	-2361.27333991	-34.2	0.1	-3889.08107904	-2360.99704761	-32.7	1.6
-3890.22923599	-2361.64913947	-29.9	2.9	-3889.57141952	-2361.26924041	-31.7	1.2	-3889.07951502	-2360.99548359	-31.7	1.1

Figure 4

-2317.36690187	-2361.54246343	37.1	35.6	-2316.98833064	-2361.16354958	34.7	33.2	-2316.71057773	-2360.89036462	34.2	32.8
-3140.01613898	-2361.55427593	29.6	44.4	-3139.33941812	-2361.17367429	28.3	43.1	-3138.92759139	-2360.89692477	30.1	44.9
-3140.01783791	-2361.55597486	28.6	44.3	-3139.34301099	-2361.17726716	26.1	41.7	-3138.92982870	-2360.89916208	28.7	44.4
-3140.04156046	-2361.57969741	13.7	28.8	-3139.36727037	-2361.20152654	10.8	26.0	-3138.95512805	-2360.92446143	12.8	28.0
-2495.55181674	-2361.56937197	20.2	20.5	-2495.12197287	-2361.19617300	14.2	14.5	-2494.82487974	-2360.92317492	13.6	14.0
-2939.21318129	-2361.59113118	6.5	25.5	-2938.57959896	-2361.21334104	3.4	22.4	-2938.24772058	-2360.93821607	4.2	23.1
-2939.20235136	-2361.58030125	13.3	32.1	-2938.57271921	-2361.20646129	7.7	26.5	-2938.23886805	-2360.92936354	9.7	28.5
-2939.19289223	-2361.57084212	19.2	35.6	-2938.56460766	-2361.19834974	12.8	29.2	-2938.23286634	-2360.92336183	13.5	29.9
-2939.24216971	-2361.62011960	-11.7	8.5	-2938.60999256	-2361.24373464	-15.7	4.6	-2938.27418270	-2360.96467819	-12.4	7.8
-2939.24271839	-2361.62066828	-12.0	7.5	-2938.61074614	-2361.24448822	-16.1	3.4	-2938.27474081	-2360.96523630	-12.8	6.7
-2939.24343274	-2361.62138263	-12.5	6.0	-2938.61192871	-2361.24567079	-16.9	1.6	-2938.27634660	-2360.96684209	-13.8	4.7
-2939.20616414	-2361.58411403	10.9	26.7	-2938.57600096	-2361.20974304	5.7	21.5	-2938.24446582	-2360.93496131	6.2	22.0
-2939.23428499	-2361.61223488	-6.7	9.2	-2938.60248286	-2361.23622494	-10.9	5.0	-2938.27085032	-2360.96134581	-10.3	5.6
-854.37878572	-2361.58896140	7.9	6.9	-854.03608245	-2361.21518405	2.3	1.3	-853.94312409	-2360.94546479	-0.4	-1.3
-3778.81174713	-2361.63852856	-23.2	11.3	-3778.03301652	-2361.26068777	-26.3	8.2	-3777.57203416	-2360.97950812	-21.7	12.8
-3778.81618364	-2361.64296507	-26.0	11.4	-3778.03697097	-2361.26464222	-28.8	8.7	-3777.57559137	-2360.98306533	-24.0	13.5
-3778.77847783	-2361.60525926	-2.3	29.8	-3778.00496283	-2361.23263408	-8.7	23.5	-3777.54533791	-2360.95281187	-5.0	27.2
-3778.77868129	-2361.60546272	-2.5	29.8	-3778.00459802	-2361.23226927	-8.5	23.8	-3777.54509560	-2360.95256956	-4.8	27.4
-3778.78353270	-2361.61031413	-5.5	30.3	-3778.00829428	-2361.23596553	-10.8	25.0	-3777.54750553	-2360.95497949	-6.3	29.5
-3778.78147992	-2361.60826135	-4.2	31.7	-3778.00616179	-2361.23383304	-9.4	26.5	-3777.54587486	-2360.95334882	-5.3	30.6
-3778.79145876	-2361.61824019	-10.5	22.1	-3778.01367631	-2361.24134756	-14.2	18.4	-3777.55636077	-2360.96383473	-11.9	20.7
-3778.79752260	-2361.62430403	-14.3	22.4	-3778.01920581	-2361.24687706	-17.6	19.1	-3777.55944481	-2360.96691877	-13.8	22.9
-2183.38259128	-2361.54059762	38.2	36.3	-2183.06013021	-2361.16114902	36.2	34.2	-2182.80705398	-2360.88854569	35.4	33.4
-3006.03298668	-2361.55356840	30.1	45.6	-3005.41258963	-2361.17264566	29.0	44.5	-3005.02607325	-2360.89711145	30.0	45.5
-3006.03397482	-2361.55455654	29.5	45.7	-3005.41487162	-2361.17492765	27.5	43.7	-3005.02786110	-2360.89889930	28.9	45.0
-3006.05851995	-2361.57910167	14.1	28.6	-3005.44065211	-2361.20070814	11.3	25.8	-3005.05339229	-2360.92443049	12.8	27.3
-2361.56784893	-2361.56784893	21.1	19.3	-2361.19419447	-2361.19419447	15.4	13.6	-2360.92154454	-2360.92154454	14.7	12.9
-2671.24696206	-2361.58980150	7.4	24.7	-2670.72739719	-2361.21273901	3.8	21.2	-2670.44638441	-2360.94028954	2.9	20.2
-2671.23921738	-2361.58205682	12.2	29.0	-2670.72354577	-2361.20888759	6.2	23.0	-2670.44083345	-2360.93473858	6.4	23.1
-2671.23512250	-2361.57796194	14.8	31.7	-2670.71994186	-2361.20528368	8.5	25.4	-2670.43722988	-2360.93113501	8.6	25.6
-2671.27632493	-2361.61916437	-11.1	5.3	-2670.75857536	-2361.24391718	-15.8	0.7	-2670.47370663	-2360.96761176	-14.3	2.2
-2671.27658543	-2361.61942487	-11.2	4.7	-2670.75899634	-2361.24433816	-16.0	-0.1	-2670.47411469	-2360.96801982	-14.5	1.4
-2671.27781851	-2361.62065795	-12.0	3.7	-2670.76033476	-2361.24567658	-16.9	-1.1	-2670.47578918	-2360.96969431	-15.6	0.2
-2671.24176129	-2361.58460073	10.6	24.2	-2670.72579016	-2361.21113198	4.8	18.4	-2670.44562330	-2360.93952843	3.4	17.0
-2671.26486003	-2361.60769947	-3.9	11.5	-2670.74668546	-2361.23202728	-8.3	7.1	-2670.46613006	-2360.96003519	-9.5	5.9
-720.39540514	-2361.58583629	9.8	7.4	-720.10913981	-2361.21137288	4.7	2.2	-720.04021804	-2360.94236890	1.6	-0.9
-3510.85236808	-2361.64403905	-26.7	6.8	-3510.18739624	-2361.26666722	-30.0	3.4	-3509.77574835	-2360.98663195	-26.2	7.3
-3510.85224938	-2361.64392035	-26.6	9.9	-3510.18760913	-2361.26688011	-30.2	6.3	-3509.77645414	-2360.98733774	-26.6	9.9
-3510.81449615	-2361.60616712	-2.9	30.2	-3510.15317917	-2361.23245015	-8.6	24.5	-3509.74283925	-2360.95372285	-5.5	27.5

-3510.81531096	-2361.60698193	-3.4	30.0	-3510.15317279	-2361.23244377	-8.6	24.8	-3509.74267533	-2360.95355893	-5.4	28.0
-3510.81526236	-2361.60693333	-3.4	31.6	-3510.15373363	-2361.23300461	-8.9	26.1	-3509.74312742	-2360.95401102	-5.7	29.3
-3510.81335575	-2361.60502672	-2.2	31.6	-3510.15058128	-2361.22985226	-6.9	26.8	-3509.74091207	-2360.95179567	-4.3	29.4
-3510.82296746	-2361.61463843	-8.2	25.2	-3510.15795596	-2361.23722694	-11.6	21.8	-3509.74979321	-2360.96067681	-9.9	23.5
-3510.82556479	-2361.61723576	-9.9	25.0	-3510.15956490	-2361.23883588	-12.6	22.3	-3509.75033698	-2360.96122058	-10.2	24.7
-2411.28528688	-2361.53878110	39.4	37.7	-2410.91470078	-2361.15862762	37.8	36.1	-2410.61849826	-2360.88655976	36.6	34.9
-3233.93860735	-2361.55467696	29.4	46.7	-3233.26903936	-2361.17200343	29.4	46.7	-3232.83754085	-2360.89514884	31.2	48.6
-3233.93924854	-2361.55531815	29.0	45.4	-3233.27062309	-2361.17358716	28.4	44.8	-3232.83950248	-2360.89711047	30.0	46.4
-3233.95435973	-2361.57042934	19.5	33.8	-3233.28750521	-2361.19046928	17.8	32.1	-3232.85651679	-2360.91412478	19.3	33.6
-2589.47195083	-2361.56743872	21.4	21.6	-2589.05063594	-2361.19354398	15.8	16.0	-2588.73453207	-2360.92110186	14.9	15.1
-3127.06147307	-2361.59528828	3.9	21.9	-3126.44811408	-2361.21927197	-0.3	17.7	-3126.07846191	-2360.94550663	-0.4	17.6
-3127.05687110	-2361.59068631	6.8	24.9	-3126.44668525	-2361.21784314	0.6	18.7	-3126.07552275	-2360.94256747	1.5	19.5
-3127.04911246	-2361.58292767	11.7	26.4	-3126.43935392	-2361.21051181	5.2	19.9	-3126.06975990	-2360.93680462	5.1	19.8
-3127.09295277	-2361.62676798	-15.8	4.4	-3126.47985647	-2361.25101436	-20.2	0.0	-3126.10602698	-2360.97307170	-17.7	2.6
-3127.09258354	-2361.62639875	-15.6	1.9	-3126.47995870	-2361.25111659	-20.3	-2.7	-3126.10708874	-2360.97413346	-18.3	-0.8
-3127.09194220	-2361.62575741	-15.2	2.6	-3126.47958738	-2361.25074527	-20.1	-2.3	-3126.10881770	-2360.97586242	-19.4	-1.7
-3127.05835155	-2361.59216676	5.9	21.7	-3126.44783915	-2361.21899704	-0.1	15.7	-3126.07932879	-2360.94637351	-0.9	14.9
-3127.07756150	-2361.61137671	-6.2	11.5	-3126.46358182	-2361.23473971	-10.0	7.6	-3126.09549802	-2360.96254274	-11.1	6.6
-948.29944412	-2361.58509411	10.3	7.4	-947.96574899	-2361.21044786	5.2	2.3	-947.85307460	-2360.94130775	2.2	-0.7
-3966.66647880	-2361.64912554	-29.9	3.1	-3965.90647325	-2361.27156030	-33.1	-0.1	-3965.40716358	-2360.99118676	-29.1	4.0
-3966.66758202	-2361.65022876	-30.6	6.6	-3965.90700643	-2361.27209348	-33.4	3.7	-3965.40803835	-2360.99206153	-29.6	7.6
-3966.62492518	-2361.60757192	-3.8	27.9	-3965.86823577	-2361.23332282	-9.1	22.6	-3965.36983234	-2360.95385552	-5.6	26.1
-3966.62409267	-2361.60673941	-3.3	30.5	-3965.86729775	-2361.23238480	-8.5	25.2	-3965.36827568	-2360.95229886	-4.6	29.1
-3966.62708255	-2361.60972929	-5.2	29.9	-3965.86829715	-2361.23338420	-9.2	25.9	-3965.37011654	-2360.95413972	-5.8	29.2
-3966.62443236	-2361.60707910	-3.5	30.5	-3965.86597201	-2361.23105906	-7.7	26.3	-3965.36825106	-2360.95227424	-4.6	29.4
-3966.63793374	-2361.62058048	-12.0	22.8	-3965.87702651	-2361.24211356	-14.6	20.1	-3965.37829168	-2360.96231486	-10.9	23.8
-3966.63594647	-2361.61859321	-10.7	23.9	-3965.87309838	-2361.23818543	-12.2	22.5	-3965.37587090	-2360.95989408	-9.4	25.2

Figure 5

-2106.19134423	-2361.53018045	44.8	43.3	-2105.91630879	-2361.14815823	44.3	42.8	-2105.63389414	-2360.87808728	41.9	40.4
-2928.83966192	-2361.54107352	37.9	51.7	-2928.26426259	-2361.15514925	39.9	53.7	-2927.84891605	-2360.88265568	39.1	52.8
-2928.83444256	-2361.53585416	41.2	55.5	-2928.26096803	-2361.15185469	42.0	56.3	-2927.84424808	-2360.87798771	42.0	56.3
-2928.88110424	-2361.58251584	11.9	26.5	-2928.31336052	-2361.20424718	9.1	23.7	-2927.89436006	-2360.92809969	10.5	25.1
-2284.38590730	-2361.56673718	21.8	20.5	-2284.06027233	-2361.19110296	17.4	16.0	-2283.75795726	-2360.92065869	15.2	13.9
-2594.05413865	-2361.57780797	14.9	28.1	-2593.58333865	-2361.19951110	12.1	25.4	-2593.27110414	-2360.92771070	10.8	24.0
-2594.02935905	-2361.55302837	30.4	44.2	-2593.56204859	-2361.17822104	25.5	39.2	-2593.25018949	-2360.90679605	23.9	37.7
-2594.08902916	-2361.61269848	-7.0	8.2	-2593.62021606	-2361.23638851	-11.0	4.2	-2593.30514157	-2360.96174813	-10.6	4.6
-2594.08943424	-2361.61310356	-7.3	7.6	-2593.62034695	-2361.23651940	-11.1	3.7	-2593.30628945	-2360.96289601	-11.3	3.6
-2594.09087066	-2361.61453998	-8.2	6.7	-2593.62219447	-2361.23836692	-12.3	2.5	-2593.30791620	-2360.96452276	-12.3	2.5
-2594.03539479	-2361.55906411	26.6	38.3	-2593.56737344	-2361.18354589	22.1	33.8	-2593.25765499	-2360.91426155	19.2	30.9
-2594.07712437	-2361.60079369	0.5	12.8	-2593.60682566	-2361.22299811	-2.6	9.7	-2593.29713769	-2360.95374425	-5.6	6.8
-3433.66207959	-2361.63458044	-20.7	10.3	-3433.04729433	-2361.25739594	-24.2	6.8	-3432.60446649	-2360.97805152	-20.8	10.2
-3433.63068766	-2361.60318851	-1.0	31.1	-3433.01737988	-2361.22748149	-5.5	26.7	-3432.57805074	-2360.95163577	-4.2	27.9
-3433.63304132	-2361.60554217	-2.5	31.0	-3433.01919408	-2361.22929569	-6.6	26.9	-3432.58029238	-2360.95387741	-5.6	27.8
-3433.66609220	-2361.63859305	-23.3	9.5	-3433.05027607	-2361.26037768	-26.1	6.7	-3432.61279303	-2360.98637806	-26.0	6.8

Figure 8

-4503.11271283	-1873.75580774	0.0	0.0	-4502.15727169	-1873.56805092	0.0	0.0	-4501.78541783	-1873.32176273	0.0	0.0
-2317.36690187	-1873.72729653	17.9	17.7	-2316.98833064	-1873.54787259	12.7	12.4	-2316.71057773	-1873.30277804	11.9	11.7
-4634.78038567	-1873.75058750	3.3	12.1	-4634.01396968	-1873.56652679	1.0	9.8	-4633.46132974	-1873.32286518	-0.7	8.1
-4634.77839369	-1873.74959151	3.9	13.2	-4634.01323785	-1873.56616087	1.2	10.5	-4633.45793193	-1873.32116628	0.4	9.7
-4503.11271283	-1873.75580774	0.0	0.0	-4502.15727169	-1873.56805092	0.0	0.0	-4501.78541783	-1873.32176273	0.0	0.0
-2183.38259128	-1873.72543072	19.1	18.3	-2183.06013021	-1873.54547203	14.2	13.4	-2182.80705398	-1873.30095911	13.1	12.3

-4366.81705247	-1873.75136567	2.8	11.7	-4366.16304146	-1873.56686255	0.7	9.6	-4365.66015933	-1873.32398480	-1.4	7.5
-4366.81285308	-1873.74926598	4.1	12.8	-4366.16139649	-1873.56604006	1.3	9.9	-4365.65668412	-1873.32224719	-0.3	8.4
-4503.11271283	-1873.75580774	0.0	0.0	-4502.15727169	-1873.56805092	0.0	0.0	-4501.78541783	-1873.32176273	0.0	0.0
-2411.28528688	-1873.72361420	20.2	19.7	-2410.91470078	-1873.54295063	15.8	15.3	-2410.61849826	-1873.29897318	14.3	13.8
-4822.62694368	-1873.75179916	2.5	10.7	-4821.87752107	-1873.56701039	0.7	8.8	-4821.28731798	-1873.32413391	-1.5	6.7
-4822.62379779	-1873.75022622	3.5	12.9	-4821.87627623	-1873.56638797	1.0	10.4	-4821.28387705	-1873.32241345	-0.4	9.0

Figure 9

-2106.92922907	-2106.92922907	0.0	0.0	-2106.65682553	-2106.65682553	0.0	0.0	-2106.36543988	-2106.36543988	0.0	0.0
-2550.56380078	-2106.92419544	3.2	19.0	-2550.08981831	-2106.64936026	4.7	20.5	-2549.76618498	-2106.35838529	4.4	20.3
-2550.56271851	-2106.92311317	3.8	21.0	-2550.08932110	-2106.64886305	5.0	22.1	-2549.76507851	-2106.35727882	5.1	22.2
-2106.92922907	-2106.92922907	0.0	0.0	-2106.65682553	-2106.65682553	0.0	0.0	-2106.36543988	-2106.36543988	0.0	0.0
-2416.58432207	-2106.92716151	1.3	17.8	-2416.16693407	-2106.65227589	2.9	19.4	-2415.86821358	-2106.36211871	2.1	18.6
-2416.58310190	-2106.92594134	2.1	18.7	-2416.16652377	-2106.65186559	3.1	19.7	-2415.86709800	-2106.36100313	2.8	19.4
-2106.92922907	-2106.92922907	0.0	0.0	-2106.65682553	-2106.65682553	0.0	0.0	-2106.36543988	-2106.36543988	0.0	0.0
-2644.48985869	-2106.92818601	0.7	15.8	-2644.02606598	-2106.65431583	1.6	16.7	-2643.68316972	-2106.36364464	1.1	16.3
-2644.49059793	-2106.92892525	0.2	17.9	-2644.02613927	-2106.65438912	1.5	19.3	-2643.68400518	-2106.36448010	0.6	18.3
-2269.16839209	-2269.16839209	0.0	0.0	-2268.89240162	-2268.89240162	0.0	0.0	-2268.57328139	-2268.57328139	0.0	0.0
-2712.84291433	-2269.20330899	-21.9	-4.0	-2712.36166654	-2268.92120849	-18.1	-0.2	-2712.01018455	-2268.60238486	-18.3	-0.4
-2712.84291431	-2269.20330897	-21.9	-4.0	-2712.36166652	-2268.92120847	-18.1	-0.2	-2712.01018460	-2268.60238491	-18.3	-0.4
-2269.16839209	-2269.16839209	0.0	0.0	-2268.89240162	-2268.89240162	0.0	0.0	-2268.57328139	-2268.57328139	0.0	0.0
-2578.86139078	-2269.20423022	-22.5	-5.7	-2578.43696714	-2268.92230896	-18.8	-2.0	-2578.10988229	-2268.60378742	-19.1	-2.4
-2578.86137289	-2269.20421233	-22.5	-5.7	-2578.43703689	-2268.92237871	-18.8	-2.0	-2578.10985352	-2268.60375865	-19.1	-2.3
-2269.16839209	-2269.16839209	0.0	0.0	-2268.89240162	-2268.89240162	0.0	0.0	-2268.57328139	-2268.57328139	0.0	0.0
-2806.76683537	-2269.20516269	-23.1	-4.7	-2806.29467721	-2268.92292706	-19.2	-0.7	-2805.92419265	-2268.60466757	-19.7	-1.3
-2806.76683534	-2269.20516266	-23.1	-4.7	-2806.29467719	-2268.92292704	-19.2	-0.7	-2805.92419267	-2268.60466759	-19.7	-1.3

Figure 10

-2075.95535431	-2915.50652278	0.0	0.0	-2075.75288285	-2915.15895369	0.0	0.0	-2075.46966696	-2914.75268849	0.0	0.0
-2075.94725779	-2915.49842626	5.1	4.4	-2075.74456426	-2915.15063510	5.2	4.5	-2075.46184812	-2914.74486965	4.9	4.2
-2075.94045346	-2915.49162193	9.4	8.4	-2075.73726671	-2915.14333755	9.8	8.9	-2075.45576405	-2914.73878558	8.7	7.8
-2075.93358333	-2915.48475180	13.7	13.3	-2075.72935521	-2915.13542605	14.8	14.5	-2075.44990448	-2914.73292601	12.4	12.1
-2915.49236370	-2915.49236370	8.9	23.7	-2915.14340495	-2915.14340495	9.8	24.6	-2914.74039591	-2914.74039591	7.7	22.6
-2915.49221196	-2915.49221196	9.0	23.9	-2915.14340873	-2915.14340873	9.8	24.7	-2914.74025406	-2914.74025406	7.8	22.7
-2915.49107742	-2915.49107742	9.7	23.8	-2915.14199692	-2915.14199692	10.6	24.8	-2914.73923049	-2914.73923049	8.4	22.6
-2915.48939000	-2915.48939000	10.8	25.7	-2915.14043382	-2915.14043382	11.6	26.6	-2914.73724489	-2914.73724489	9.7	24.7
-2915.48740784	-2915.48740784	12.0	25.8	-2915.13877223	-2915.13877223	12.7	26.4	-2914.73619567	-2914.73619567	10.3	24.1
-2915.48764463	-2915.48764463	11.8	26.2	-2915.13897566	-2915.13897566	12.5	26.9	-2914.73632776	-2914.73632776	10.3	24.6
-2915.48627085	-2915.48627085	12.7	26.4	-2915.13762899	-2915.13762899	13.4	27.1	-2914.73525198	-2914.73525198	10.9	24.7
-2915.48621503	-2915.48621503	12.7	28.1	-2915.13739082	-2915.13739082	13.5	28.9	-2914.73506760	-2914.73506760	11.1	26.4
-2915.50404523	-2915.50404523	1.6	16.5	-2915.15339595	-2915.15339595	3.5	18.4	-2914.75309538	-2914.75309538	-0.3	14.7
-2915.50376321	-2915.50376321	1.7	16.8	-2915.15338024	-2915.15338024	3.5	18.6	-2914.75265712	-2914.75265712	0.0	15.1
-2915.50401979	-2915.50401979	1.6	17.6	-2915.15426424	-2915.15426424	2.9	18.9	-2914.75329538	-2914.75329538	-0.4	15.6
-2915.50401977	-2915.50401977	1.6	17.6	-2915.15426424	-2915.15426424	2.9	18.9	-2914.75329535	-2914.75329535	-0.4	15.6
-2915.50359141	-2915.50359141	1.8	18.4	-2915.15331094	-2915.15331094	3.5	20.1	-2914.75249895	-2914.75249895	0.1	16.7
-2915.50359134	-2915.50359134	1.8	18.4	-2915.15331089	-2915.15331089	3.5	20.1	-2914.75249890	-2914.75249890	0.1	16.7

-2915.49758377	-2915.49758377	5.6	16.5	-2915.15259834	-2915.15259834	4.0	14.8	-2914.74668142	-2914.74668142	3.8	14.6
-2915.49743197	-2915.49743197	5.7	18.3	-2915.15253173	-2915.15253173	4.0	16.6	-2914.74679282	-2914.74679282	3.7	16.3
-2915.49621977	-2915.49621977	6.5	18.3	-2915.15107993	-2915.15107993	4.9	16.8	-2914.74545156	-2914.74545156	4.5	16.4
-2915.49770861	-2915.49770861	5.5	18.9	-2915.15266414	-2915.15266414	3.9	17.3	-2914.74537387	-2914.74537387	4.6	17.9
-2915.49699588	-2915.49699588	6.0	19.2	-2915.15189705	-2915.15189705	4.4	17.7	-2914.74516804	-2914.74516804	4.7	17.9
-2915.49627893	-2915.49627893	6.4	19.9	-2915.15082137	-2915.15082137	5.1	18.5	-2914.74373759	-2914.74373759	5.6	19.0
-2141.65269802	-2981.20386649	0.0	0.0	-2141.45816208	-2980.86423292	0.0	0.0	-2141.19963466	-2980.48265619	0.0	0.0
-2141.64537736	-2981.19654583	4.6	5.6	-2141.45064242	-2980.85671326	4.7	5.7	-2141.19296088	-2980.47598241	4.2	5.2
-2141.63872531	-2981.18989378	8.8	10.4	-2141.44389024	-2980.84996108	9.0	10.5	-2141.18687164	-2980.46989317	8.0	9.6
-2141.63101767	-2981.18218614	13.6	14.7	-2141.43669753	-2980.84276837	13.5	14.5	-2141.18029773	-2980.46331926	12.1	13.2
-2981.18697803	-2981.18697803	10.6	25.8	-2980.84896107	-2980.84896107	9.6	24.7	-2980.46767442	-2980.46767442	9.4	24.6
-2981.18540881	-2981.18540881	11.6	26.8	-2980.84781710	-2980.84781710	10.3	25.5	-2980.46735368	-2980.46735368	9.6	24.8
-2981.18577873	-2981.18577873	11.4	28.0	-2980.84795420	-2980.84795420	10.2	26.8	-2980.46753052	-2980.46753052	9.5	26.1
-2981.18577867	-2981.18577867	11.4	28.0	-2980.84795413	-2980.84795413	10.2	26.8	-2980.46753046	-2980.46753046	9.5	26.1
-2981.18452758	-2981.18452758	12.1	27.4	-2980.84693685	-2980.84693685	10.9	26.1	-2980.46707835	-2980.46707835	9.8	25.1
-2981.18498651	-2981.18498651	11.8	27.7	-2980.84777627	-2980.84777627	10.3	26.2	-2980.46770767	-2980.46770767	9.4	25.2
-2981.18498655	-2981.18498655	11.8	27.7	-2980.84777627	-2980.84777627	10.3	26.2	-2980.46770771	-2980.46770771	9.4	25.2
-2981.18237254	-2981.18237254	13.5	28.7	-2980.84473125	-2980.84473125	12.2	27.4	-2980.46460061	-2980.46460061	11.3	26.5
-1986.57814044	-2826.12930891	0.0	0.0	-1986.33955582	-2825.74562666	0.0	0.0	-1986.08883022	-2825.37185175	0.0	0.0
-1986.56895352	-2826.12012199	5.8	7.1	-1986.33000606	-2825.73607690	6.0	7.3	-1986.07998002	-2825.36300155	5.6	6.9
-1986.56053382	-2826.11170229	11.0	11.6	-1986.32094249	-2825.72701333	11.7	12.2	-1986.07183061	-2825.35485214	10.7	11.2
-1986.55046689	-2826.10163536	17.4	17.3	-1986.31078417	-2825.71685501	18.1	18.0	-1986.06267282	-2825.34569435	16.4	16.3
-2826.11208469	-2826.11208469	10.8	24.8	-2825.72859180	-2825.72859180	10.7	24.7	-2825.35659278	-2825.35659278	9.6	23.6
-2826.11104038	-2826.11104038	11.5	25.7	-2825.72734835	-2825.72734835	11.5	25.7	-2825.35559374	-2825.35559374	10.2	24.4
-2826.11241313	-2826.11241313	10.6	25.9	-2825.72896742	-2825.72896742	10.5	25.7	-2825.35609097	-2825.35609097	9.9	25.1
-2826.11123022	-2826.11123022	11.3	26.6	-2825.72776919	-2825.72776919	11.2	26.5	-2825.35603124	-2825.35603124	9.9	25.2
-2826.10978056	-2826.10978056	12.3	27.6	-2825.72677023	-2825.72677023	11.8	27.2	-2825.35499642	-2825.35499642	10.6	26.0
-2826.10978071	-2826.10978071	12.3	27.6	-2825.72677046	-2825.72677046	11.8	27.2	-2825.35499658	-2825.35499658	10.6	26.0
-2826.10819802	-2826.10819802	13.2	28.1	-2825.72478699	-2825.72478699	13.1	27.9	-2825.35353093	-2825.35353093	11.5	26.3
-2826.10632792	-2826.10632792	14.4	29.7	-2825.72283806	-2825.72283806	14.3	29.6	-2825.35124742	-2825.35124742	12.9	28.2

E_{sp} …… single point electronic energy in thf (SMD) in hartree with Def2TZVPP
E_{sp} (sum) single point electronic energy in thf (SMD) in hartree with Def2TZVPP after mass balance
ΔE_{sp} … relative single point electronic energy in thf(SMD) in kcal/mol with Def2TZVPP
ΔG_{sp} … relative single point free energy in thf(SMD) in kcal/mol ($\Delta G_{sp} = \Delta E_{sp}$/Def2TZVPP + ΔG_{corr}[level of optimization])

Single point energies in Figures 1–10 with MN12L and M06L

MN12L/Def2TZVPP thf(SMD)				M06L/Def2TZVPP thf(SMD)			
E_{sp} [hartree]	E_{sp} (sum) [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	E_{sp} (sum) [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-822.04607631				-822.75545796			
-643.98578532				-644.57034955			
-395.19783002				-395.45310892			
-2628.23171756				-2629.63211447			
-305.79116114				-306.08269389			
-460.94909718				-461.13567381			
-232.28527940				-232.50842306			
-443.32250906				-443.72359397			
-309.45547799				-309.72019656			
-537.23585868				-537.66849954			
-839.18651749				-839.62646710			
-2101.65341983				-2102.24570645			
-1946.51000347				-1947.20767662			
-2084.01167846				-2084.82069541			
-1950.14284503				-1950.81515487			
-2177.92257168				-2178.76324286			
	Figure 1						
-4501.28636762	-2360.57041905	26.0	24.8	-4503.31808352	-2361.59127402	18.2	17.0
-5323.34098806	-2360.57896318	20.7	42.6	-5326.07741129	-2361.59514383	15.8	37.7
-5323.34996829	-2360.58794341	15.0	35.6	-5326.07953936	-2361.59727190	14.4	35.0
-5323.33569668	-2360.57367180	24.0	42.1	-5326.07193576	-2361.58966830	19.2	37.3
-5323.34444374	-2360.58241886	18.5	40.4	-5326.07616090	-2361.59389344	16.6	38.4
-5323.38475313	-2360.62272825	-6.8	9.9	-5326.11380739	-2361.63153993	-7.1	9.6
-4679.38816199	-2360.61192242	0.0	0.0	-4681.53220507	-2361.62028716	0.0	0.0
-4679.38689947	-2360.61065990	0.8	2.1	-4681.53133506	-2361.61941715	0.5	1.8
-4679.37981569	-2360.60357612	5.2	3.1	-4681.52699502	-2361.61507711	3.3	1.2
-4679.37890877	-2360.60266920	5.8	5.0	-4681.52543652	-2361.61351861	4.2	3.5
-4679.38299196	-2360.60675239	3.2	4.3	-4681.52821068	-2361.61629277	2.5	3.6
-4679.38051466	-2360.60427509	4.8	5.1	-4681.52777463	-2361.61585672	2.8	3.1
-4679.37765467	-2360.60141510	6.6	6.0	-4681.52379342	-2361.61187551	5.3	4.6
-4679.37791686	-2360.60167729	6.4	7.6	-4681.52474041	-2361.61282250	4.7	5.8
-4679.37839074	-2360.60215117	6.1	7.5	-4681.52613391	-2361.61421600	3.8	5.2
-4988.85796259	-2360.62624503	-9.0	10.3	-4991.26394184	-2361.63182737	-7.2	12.0
-4988.85640998	-2360.62469242	-8.0	10.5	-4991.26099070	-2361.62887623	-5.4	13.1
-4988.85640960	-2360.62469204	-8.0	10.5	-4991.26099193	-2361.62887746	-5.4	13.1
-4988.85465094	-2360.62293338	-6.9	10.9	-4991.25908183	-2361.62696736	-4.2	13.6
-4988.85421704	-2360.62249948	-6.6	12.8	-4991.25817285	-2361.62605838	-3.6	15.8
-4988.85421650	-2360.62249894	-6.6	12.8	-4991.25817216	-2361.62605769	-3.6	15.8
-4988.84972826	-2360.61801070	-3.8	15.3	-4991.25601019	-2361.62389572	-2.3	16.8
-4988.84972815	-2360.61801059	-3.8	15.3	-4991.25601013	-2361.62389566	-2.3	16.8
-4988.84884346	-2360.61712590	-3.3	17.2	-4991.25158736	-2361.61947289	0.5	20.9
-4988.89252289	-2360.66080533	-30.7	-12.7	-4991.29942301	-2361.66730854	-29.5	-11.5
-4988.89204016	-2360.66032260	-30.4	-11.8	-4991.29931015	-2361.66719568	-29.4	-10.9
-4988.88948445	-2360.65776689	-28.8	-8.6	-4991.29924045	-2361.66712598	-29.4	-9.2
-4988.84745639	-2360.61573883	-2.4	14.6	-4991.25358081	-2361.62146634	-0.7	16.3
-4988.84744680	-2360.61572924	-2.4	15.4	-4991.25355576	-2361.62144129	-0.7	17.0
-4988.85201242	-2360.62029486	-5.3	15.7	-4991.25581983	-2361.62370536	-2.1	18.8

-4988.85122013	-2360.61950257	-4.8	14.6	-4991.25140935	-2361.61929488	0.6	19.9
-4988.84893142	-2360.61721386	-3.3	17.2	-4991.25181670	-2361.61970223	0.4	20.9
-4988.84893120	-2360.61721364	-3.3	17.2	-4991.25181662	-2361.61970215	0.4	20.9
-4988.84893115	-2360.61721359	-3.3	17.2	-4991.25181661	-2361.61970214	0.4	20.9
-4988.84171584	-2360.60999828	1.2	20.3	-4991.24893907	-2361.61682460	2.2	21.3
-4988.85078797	-2360.61907041	-4.5	17.0	-4991.25136200	-2361.61924753	0.7	22.2
-4988.83995646	-2360.60823890	2.3	22.5	-4991.24602377	-2361.61390930	4.0	24.2
-4988.82888840	-2360.59717084	9.3	28.7	-4991.23932875	-2361.60721428	8.2	27.6
-4988.89883787	-2360.66712031	-34.6	-16.0	-4991.30403699	-2361.67192252	-32.4	-13.7
-4988.89053079	-2360.65881323	-29.4	-9.1	-4991.29577067	-2361.66365620	-27.2	-6.9
-4988.84988219	-2360.61816463	-3.9	12.5	-4991.25851367	-2361.62639920	-3.8	12.5
-4988.84839884	-2360.61668128	-3.0	14.3	-4991.25794845	-2361.62583398	-3.5	13.8
-4988.85710959	-2360.62539203	-8.5	11.3	-4991.26246346	-2361.63034899	-6.3	13.5
-4988.85565429	-2360.62393673	-7.5	11.2	-4991.26088577	-2361.62877130	-5.3	13.4
-4988.85194662	-2360.62022906	-5.2	14.0	-4991.25472840	-2361.62261393	-1.5	17.7
-4988.84765355	-2360.61593599	-2.5	15.7	-4991.25552841	-2361.62341394	-2.0	16.3
-4988.84756235	-2360.61584479	-2.5	15.7	-4991.25397400	-2361.62185953	-1.0	17.2
-4988.84672813	-2360.61501057	-1.9	17.0	-4991.25304728	-2361.62093281	-0.4	18.5
-4988.85031611	-2360.61859855	-4.2	16.1	-4991.25538090	-2361.62326643	-1.9	18.4
-4988.85031606	-2360.61859850	-4.2	16.1	-4991.25538084	-2361.62326637	-1.9	18.4
-4988.84730053	-2360.61558297	-2.3	17.4	-4991.25088060	-2361.61876613	1.0	20.6
-4988.84931666	-2360.61759910	-3.6	17.5	-4991.25151932	-2361.61940485	0.6	21.6
-4988.84650189	-2360.61478433	-1.8	19.6	-4991.25057160	-2361.61845713	1.1	22.5
-4988.89941353	-2360.66769597	-35.0	-17.3	-4991.30473639	-2361.67262192	-32.8	-15.2
-4988.88473808	-2360.65302052	-25.8	-9.0	-4991.29619501	-2361.66408054	-27.5	-10.7
-4988.89024863	-2360.65853107	-29.2	-10.2	-4991.29721136	-2361.66509689	-28.1	-9.1
-4988.88750185	-2360.65578429	-27.5	-8.4	-4991.29514275	-2361.66302828	-26.8	-7.7
-4988.88096605	-2360.64924849	-23.4	-1.9	-4991.28929904	-2361.65718457	-23.2	-1.6
-4988.85724806	-2360.62553050	-8.5	7.0	-4991.26579956	-2361.63368509	-8.4	7.1
-4988.84849552	-2360.61677796	-3.0	13.8	-4991.25431121	-2361.62219674	-1.2	15.7
-4988.85092131	-2360.61920375	-4.6	14.2	-4991.25450762	-2361.62239315	-1.3	17.5
-4988.83922038	-2360.60750282	2.8	20.3	-4991.24722592	-2361.61511145	3.2	20.8
-4988.84861621	-2360.61689865	-3.1	15.6	-4991.25142667	-2361.61931220	0.6	19.3
-4988.85095232	-2360.61923476	-4.6	16.1	-4991.25362567	-2361.62151120	-0.8	19.9
-4988.85117418	-2360.61945662	-4.7	16.0	-4991.25350469	-2361.62139022	-0.7	20.0
-4988.84429569	-2360.61257813	-0.4	19.9	-4991.24913990	-2361.61702543	2.0	22.4
-4988.84898617	-2360.61726861	-3.4	18.6	-4991.25163100	-2361.61951653	0.5	22.5
-4988.83475407	-2360.60303651	5.6	25.5	-4991.23997512	-2361.60786065	7.8	27.7
-4988.88907097	-2360.65735341	-28.5	-9.1	-4991.29712588	-2361.66501141	-28.1	-8.6
-4988.88873731	-2360.65701975	-28.3	-8.0	-4991.29782361	-2361.66570914	-28.5	-8.2
-4988.88302940	-2360.65131184	-24.7	-6.4	-4991.29192643	-2361.65981196	-24.8	-6.5
-4988.88488031	-2360.65316275	-25.9	-7.2	-4991.29273887	-2361.66062440	-25.3	-6.7
-4988.89343366	-2360.66171610	-31.2	-15.6	-4991.30003169	-2361.66791722	-29.9	-14.3
-4988.89457434	-2360.66285678	-32.0	-14.6	-4991.30099393	-2361.66887946	-30.5	-13.2
-4988.88863184	-2360.65691428	-28.2	-11.5	-4991.29750798	-2361.66539351	-28.3	-11.6
-5828.09124695	-2360.67301190	-38.3	-2.2	-5830.93795352	-2361.67937195	-37.1	-0.9
-5828.08774704	-2360.66951199	-36.1	0.4	-5830.93524803	-2361.67666646	-35.4	1.1
-5828.08753594	-2360.66930089	-36.0	-0.5	-5830.93404836	-2361.67546679	-34.6	0.9
-5828.08287841	-2360.66464336	-33.1	5.0	-5830.93194926	-2361.67336769	-33.3	4.8
-5828.06800600	-2360.64977095	-23.8	11.4	-5830.92172687	-2361.66314530	-26.9	8.3
-5828.06513123	-2360.64689618	-21.9	13.2	-5830.92029553	-2361.66171396	-26.0	9.1
-5828.07308655	-2360.65485150	-26.9	7.9	-5830.92432287	-2361.66574130	-28.5	6.3
-5828.06526714	-2360.64703209	-22.0	14.9	-5830.92049597	-2361.66191440	-26.1	10.8
-5828.05303669	-2360.63480164	-14.4	21.1	-5830.90838941	-2361.64980784	-18.5	16.9
-5828.04656461	-2360.62832956	-10.3	25.9	-5830.90508102	-2361.64649945	-16.4	19.8
-5828.08581243	-2360.66757738	-34.9	2.4	-5830.93879609	-2361.68021452	-37.6	-0.2
-5828.07946615	-2360.66123110	-30.9	3.5	-5830.92803846	-2361.66945689	-30.9	3.6

-5828.07273533	-2360.65450028	-26.7	10.0	-5830.92763250	-2361.66905093	-30.6	6.1

Figure 2

-4357.72683468	-2360.58802518	15.0	21.1	-4359.57953482	-2361.61237849	5.0	11.1
-2178.85030206	-2360.57490990	23.2	21.0	-2179.77731897	-2361.59993005	12.8	10.6
-3000.90779644	-2360.58632797	16.1	31.0	-3002.53929522	-2361.60644834	8.7	23.6
-3000.91212273	-2360.59065426	13.3	27.0	-3002.54097568	-2361.60812880	7.6	21.3
-3000.93893076	-2360.61746229	-3.5	10.6	-3002.56473570	-2361.63188882	-7.3	6.8
-2356.94231187	-2360.60662872	3.3	2.8	-2357.98375042	-2361.62125308	-0.6	-1.1
-2800.28316903	-2360.62497682	-8.2	6.2	-2801.72091381	-2361.63482251	-9.1	5.3
-2800.27137083	-2360.61317862	-0.8	14.1	-2801.71011758	-2361.62402628	-2.3	12.6
-2800.30916518	-2360.65097297	-24.5	-8.7	-2801.75010359	-2361.66401229	-27.4	-11.7
-2800.30729069	-2360.64909848	-23.3	-6.3	-2801.74744348	-2361.66135218	-25.8	-8.7
-2800.30756708	-2360.64937487	-23.5	-6.7	-2801.74790700	-2361.66181570	-26.1	-9.3
-2800.27517436	-2360.61698215	-3.2	10.3	-2801.71214598	-2361.62605468	-3.6	9.8
-2800.31578308	-2360.65759087	-28.7	-14.8	-2801.74926939	-2361.66317809	-26.9	-13.0
-2800.29604255	-2360.63785034	-16.3	-1.9	-2801.73195409	-2361.64586279	-16.0	-1.7
-2800.29262713	-2360.63443492	-14.1	0.6	-2801.73167493	-2361.64558363	-15.9	-1.1
-2800.28452615	-2360.62633394	-9.0	4.7	-2801.72741804	-2361.64132674	-13.2	0.6
-2800.28616449	-2360.62797228	-10.1	3.4	-2801.72982465	-2361.64373335	-14.7	-1.3
-2800.28137484	-2360.62318263	-7.1	7.5	-2801.72551993	-2361.63942863	-12.0	2.5
-2800.28553544	-2360.62734323	-9.7	4.3	-2801.72995096	-2361.64385966	-14.8	-0.8
-853.78202880	-2360.63384006	-13.8	-14.9	-854.52473821	-2361.64632353	-16.3	-17.5
-2800.31005102	-2360.65185881	-25.1	-10.8	-2801.74694127	-2361.66084997	-25.5	-11.2
-2800.28764106	-2360.62944885	-11.0	3.5	-2801.72064153	-2361.63455023	-9.0	5.5
-2800.32002571	-2360.66183350	-31.3	-14.0	-2801.75891341	-2361.67282211	-33.0	-15.6
-3639.52420143	-2360.67949173	-42.4	-7.0	-3641.39967563	-2361.68711723	-41.9	-6.5
-3639.52323183	-2360.67852213	-41.8	-8.2	-3641.39911247	-2361.68655407	-41.6	-8.0
-3639.50825065	-2360.66354095	-32.4	-1.3	-3641.39098795	-2361.67842955	-36.5	-5.4
-3639.50840858	-2360.66369888	-32.5	0.7	-3641.39055237	-2361.67799397	-36.2	-3.0
-3639.53146649	-2360.68675679	-47.0	-11.1	-3641.41306684	-2361.70050844	-50.3	-14.5
-3639.52425098	-2360.67954128	-42.4	-8.2	-3641.40953288	-2361.69697448	-48.1	-13.9

-4357.72683468	-2360.58802518	15.0	21.1	-4359.57953482	-2361.61237849	5.0	11.1
-2178.85030206	-2360.57490990	23.2	21.0	-2179.77731897	-2361.59993005	12.8	10.6
-3000.90779644	-2360.58632797	16.1	31.0	-3002.53929522	-2361.60644834	8.7	23.6
-3000.91212273	-2360.59065426	13.3	27.0	-3002.54097568	-2361.60812880	7.6	21.3
-3000.93893076	-2360.61746229	-3.5	10.6	-3002.56473570	-2361.63188882	-7.3	6.8
-2356.94231187	-2360.60662872	3.3	2.8	-2357.98375042	-2361.62125308	-0.6	-1.1
-2666.42032407	-2360.62916293	-10.8	5.0	-2667.72182456	-2361.63913067	-11.8	4.0
-2666.41214083	-2360.62097969	-5.7	10.1	-2667.71490453	-2361.63221064	-7.5	8.3
-2666.45084526	-2360.65968412	-30.0	-13.6	-2667.75589650	-2361.67320261	-33.2	-16.8
-2666.44729515	-2360.65613401	-27.7	-13.5	-2667.75214943	-2361.66945554	-30.9	-16.6
-2666.44780530	-2360.65664416	-28.1	-11.7	-2667.75363075	-2361.67093686	-31.8	-15.4
-2666.41653719	-2360.62537605	-8.4	4.7	-2667.71751210	-2361.63481821	-9.1	4.0
-2666.45076636	-2360.65960522	-29.9	-15.1	-2667.74833181	-2361.66563792	-28.5	-13.6
-2666.43203350	-2360.64087236	-18.2	-5.8	-2667.73173197	-2361.64903808	-18.0	-5.6
-2666.42739608	-2360.63623494	-15.3	-1.3	-2667.73053441	-2361.64784052	-17.3	-3.4
-2666.41941305	-2360.62825191	-10.2	3.3	-2667.72612157	-2361.64342768	-14.5	-1.0
-2666.42163297	-2360.63047183	-11.6	3.2	-2667.72942134	-2361.64672745	-16.6	-1.8
-2666.41606704	-2360.62490590	-8.1	7.0	-2667.72409388	-2361.64139999	-13.2	1.9
-2666.42091230	-2360.62975116	-11.2	2.5	-2667.72880142	-2361.64610753	-16.2	-2.5
-719.91359626	-2360.63243859	-12.9	-14.6	-720.52025101	-2361.64523374	-15.7	-17.4
-2666.44530626	-2360.65414512	-26.5	-13.0	-2667.74637394	-2361.66368005	-27.2	-13.7
-2666.42337203	-2360.63221089	-12.7	0.3	-2667.72028171	-2361.63758782	-10.9	2.2
-2666.45822105	-2360.66705991	-34.6	-18.2	-2667.76169530	-2361.67900141	-36.8	-20.5

-3505.66278446	-2360.68510582	-45.9	-14.8	-3507.40333005	-2361.69416906	-46.4	-15.3
-3505.66537332	-2360.68769468	-47.5	-13.9	-3507.40580883	-2361.69664784	-47.9	-14.3
-3505.64652209	-2360.66884345	-35.7	-1.9	-3507.39421409	-2361.68505310	-40.6	-6.8
-3505.64661905	-2360.66894041	-35.8	-2.2	-3507.39264679	-2361.68348580	-39.7	-6.1
-3505.66615823	-2360.68847959	-48.0	-14.0	-3507.41119479	-2361.70203380	-51.3	-17.3
-3505.66267111	-2360.68499247	-45.9	-11.5	-3507.40952149	-2361.70036050	-50.2	-15.9
-4357.72683468	-2360.58802518	15.0	21.1	-4359.57953482	-2361.61237849	5.0	11.1
-2178.85030206	-2360.57490990	23.2	21.0	-2179.77731897	-2361.59993005	12.8	10.6
-3000.90779644	-2360.58632797	16.1	31.0	-3002.53929522	-2361.60644834	8.7	23.6
-3000.91212273	-2360.59065426	13.3	27.0	-3002.54097568	-2361.60812880	7.6	21.3
-3000.93893076	-2360.61746229	-3.5	10.6	-3002.56473570	-2361.63188882	-7.3	6.8
-2356.94231187	-2360.60662872	3.3	2.8	-2357.98375042	-2361.62125308	-0.6	-1.1
-2894.20341177	-2360.63186994	-12.5	2.3	-2895.67357946	-2361.64258258	-14.0	0.8
-2894.19930669	-2360.62776486	-9.9	5.9	-2895.67008865	-2361.63909177	-11.8	4.1
-2894.23824948	-2360.66670765	-34.4	-16.8	-2895.71115078	-2361.68015390	-37.6	-20.0
-2894.23349154	-2360.66194971	-31.4	-16.3	-2895.70751386	-2361.67651698	-35.3	-20.1
-2894.23509360	-2360.66355177	-32.4	-18.3	-2895.70884186	-2361.67784498	-36.1	-22.1
-2894.20395121	-2360.63240938	-12.9	1.1	-2895.67302072	-2361.64202384	-13.6	0.3
-2894.23231395	-2360.66077212	-30.7	-16.2	-2895.69760040	-2361.66660352	-29.1	-14.6
-2894.21271538	-2360.64117355	-18.4	-5.5	-2895.68042295	-2361.64942607	-18.3	-5.4
-2894.20811608	-2360.63657425	-15.5	-2.0	-2895.67946156	-2361.64846468	-17.7	-4.2
-2894.20100942	-2360.62946759	-11.0	2.8	-2895.67571927	-2361.64472239	-15.3	-1.5
-2894.20309388	-2360.63155205	-12.3	1.3	-2895.67874496	-2361.64774808	-17.2	-3.6
-2894.19755718	-2360.62601535	-8.8	3.8	-2895.67370760	-2361.64271072	-14.1	-1.5
-2894.20204965	-2360.63050782	-11.7	3.0	-2895.67850972	-2361.64751284	-17.1	-2.4
-947.69330999	-2360.63177163	-12.5	-14.8	-948.46798210	-2361.64466184	-15.3	-17.7
-2894.22700355	-2360.65546172	-27.3	-12.9	-2895.69570033	-2361.66470345	-27.9	-13.5
-2894.20506833	-2360.63352650	-13.6	0.4	-2895.67007487	-2361.63907799	-11.8	2.2
-2894.23970774	-2360.66816591	-35.3	-18.3	-2895.71085309	-2361.67985621	-37.4	-20.4
-3733.45069252	-2360.69263320	-50.6	-17.6	-3735.35869266	-2361.70122868	-50.8	-17.8
-3733.44957375	-2360.69151443	-49.9	-16.4	-3735.35831840	-2361.70085442	-50.6	-17.0
-3733.43000564	-2360.67194632	-37.7	-5.7	-3735.34406823	-2361.68660425	-41.6	-9.6
-3733.42707697	-2360.66901765	-35.8	-4.5	-3735.34179114	-2361.68432716	-40.2	-8.8
-3733.44893775	-2360.69087843	-49.5	-14.3	-3735.36222004	-2361.70475606	-53.0	-17.8
-3733.45066894	-2360.69260962	-50.6	-15.1	-3735.36145478	-2361.70399080	-52.5	-17.0

Figure 3

-4668.02366684	-2360.57850523	21.0	26.4	-4669.66412365	-2361.60169299	11.7	17.1
-2333.99270111	-2360.55937292	33.0	31.5	-2334.81423481	-2361.58386597	22.9	21.3
-3156.05264696	-2360.57324246	24.3	38.0	-3157.58061615	-2361.59478935	16.0	29.7
-3156.05347454	-2360.57407004	23.8	36.9	-3157.57594475	-2361.59011795	18.9	32.1
-3156.08416012	-2360.60475562	4.5	18.1	-3157.60387047	-2361.61804367	1.4	15.0
-2512.08633547	-2360.59271629	12.1	9.6	-2513.02274452	-2361.60726727	8.2	5.7
-2955.43174365	-2360.61561541	-2.3	12.4	-2956.76332928	-2361.62425806	-2.5	12.2
-2955.41295284	-2360.59682460	9.5	24.7	-2956.74591946	-2361.60684824	8.4	23.6
-2955.45351047	-2360.63738223	-16.0	1.3	-2956.78771712	-2361.64864590	-17.8	-0.5
-2955.45062982	-2360.63450158	-14.2	1.2	-2956.78550648	-2361.64643526	-16.4	-1.0
-2955.45319327	-2360.63706503	-15.8	-1.7	-2956.78808178	-2361.64901056	-18.0	-3.9
-2955.41783673	-2360.60170849	6.4	18.0	-2956.74747497	-2361.60840375	7.5	19.0
-2955.46246899	-2360.64634075	-21.6	-8.4	-2956.78972398	-2361.65065276	-19.1	-5.8
-2955.44245333	-2360.62632509	-9.0	3.8	-2956.77255799	-2361.63348677	-8.3	4.6
-2955.43900075	-2360.62287251	-6.9	6.3	-2956.77229827	-2361.63322705	-8.1	5.0
-2955.42687915	-2360.61075091	0.7	13.5	-2956.76419560	-2361.62512438	-3.0	9.7
-2955.43290666	-2360.61677842	-3.0	11.4	-2956.77094386	-2361.63187264	-7.3	7.2
-2955.42788655	-2360.61175831	0.1	13.0	-2956.76612071	-2361.62704949	-4.2	8.6

-2955.43252825	-2360.61640001	-2.8	10.8	-2956.77076389	-2361.63169267	-7.2	6.4
-853.78202880	-2360.61932039	-4.6	-7.1	-854.52473821	-2361.63137344	-7.0	-9.4
-2955.45734947	-2360.64122123	-18.4	-5.7	-2956.78741134	-2361.64834012	-17.6	-4.9
-2955.42907548	-2360.61294724	-0.6	11.7	-2956.75666048	-2361.61758926	1.7	14.0
-2955.46431481	-2360.64818657	-22.8	-6.9	-2956.79914108	-2361.66006986	-25.0	-9.1
-3794.66657155	-2360.66392582	-32.6	-1.1	-3796.43671483	-2361.67117651	-31.9	-0.4
-3794.67188479	-2360.66923906	-36.0	-2.2	-3796.43932285	-2361.67378453	-33.6	0.2
-3794.65068312	-2360.64803739	-22.7	8.6	-3796.42739291	-2361.66185459	-26.1	5.2
-3794.65398544	-2360.65133971	-24.7	7.8	-3796.42811214	-2361.66257382	-26.5	6.0
-3794.67289222	-2360.67024649	-36.6	-3.1	-3796.44918054	-2361.68364222	-39.8	-6.2
-3794.67056357	-2360.66791784	-35.1	-2.4	-3796.44716339	-2361.68162507	-38.5	-5.8
-4668.02366684	-2360.57850523	21.0	26.4	-4669.66412365	-2361.60169299	11.7	17.1
-2333.99270111	-2360.55937292	33.0	31.5	-2334.81423481	-2361.58386597	22.9	21.3
-3156.05264696	-2360.57324246	24.3	38.0	-3157.58061615	-2361.59478935	16.0	29.7
-3156.05347454	-2360.57407004	23.8	36.9	-3157.57594475	-2361.59011795	18.9	32.1
-3156.08416012	-2360.60475562	4.5	18.1	-3157.60387047	-2361.61804367	1.4	15.0
-2512.08633547	-2360.59271629	12.1	9.6	-2513.02274452	-2361.60726727	8.2	5.7
-2821.56867261	-2360.61957544	-4.8	9.1	-2822.76396379	-2361.62828998	-5.0	8.9
-2821.55458628	-2360.60548911	4.0	18.3	-2822.75127377	-2361.61559996	2.9	17.2
-2821.59276964	-2360.64367247	-19.9	-4.0	-2822.79193165	-2361.65625784	-22.6	-6.6
-2821.59050576	-2360.64140859	-18.5	-5.0	-2822.79024703	-2361.65457322	-21.5	-8.0
-2821.59302499	-2360.64392782	-20.1	-5.9	-2822.79214528	-2361.65647147	-22.7	-8.5
-2821.55885343	-2360.60975626	1.4	12.0	-2822.75280606	-2361.61713225	2.0	12.6
-2821.59739772	-2360.64830055	-22.8	-10.9	-2822.78820671	-2361.65253290	-20.2	-8.3
-2821.57756198	-2360.62846481	-10.4	0.6	-2822.77110010	-2361.63542629	-9.5	1.5
-2821.57345899	-2360.62436182	-7.8	4.4	-2822.77035356	-2361.63467975	-9.0	3.2
-2821.56187133	-2360.61277416	-0.5	11.9	-2822.76308106	-2361.62740725	-4.5	7.9
-2821.56785385	-2360.61875668	-4.3	7.5	-2822.76984926	-2361.63417545	-8.7	3.1
-2821.56236839	-2360.61327122	-0.8	12.4	-2822.76469219	-2361.62901838	-5.5	7.7
-2821.56756206	-2360.61846489	-4.1	9.4	-2822.76961279	-2361.63393898	-8.6	4.9
-719.91359626	-2360.61791892	-3.8	-6.9	-720.52025101	-2361.63028365	-6.3	-9.4
-2821.59155404	-2360.64245687	-19.2	-7.6	-2822.78547624	-2361.64980243	-18.5	-6.9
-2821.56465884	-2360.61556167	-2.3	10.0	-2822.75651358	-2361.62083977	-0.3	11.9
-2821.60123556	-2360.65213839	-25.2	-10.2	-2822.79934760	-2361.66367379	-27.2	-12.2
-3660.81041560	-2360.67480093	-39.5	-7.6	-3662.44327896	-2361.68113805	-38.2	-6.3
-3660.80672447	-2360.67110980	-37.1	-3.2	-3662.44127263	-2361.67913172	-36.9	-2.9
-3660.78424951	-2360.64863484	-23.0	7.8	-3662.42777971	-2361.66563880	-28.5	2.4
-3660.79016001	-2360.65454534	-26.7	5.2	-3662.42831798	-2361.66617707	-28.8	3.1
-3660.80837623	-2360.67276156	-38.2	-4.9	-3662.44735085	-2361.68520994	-40.7	-7.5
-3660.80540300	-2360.66978833	-36.3	-3.8	-3662.44430160	-2361.68216069	-38.8	-6.3
-4668.02366684	-2360.57850523	21.0	26.4	-4669.66412365	-2361.60169299	11.7	17.1
-2333.99270111	-2360.55937292	33.0	31.5	-2334.81423481	-2361.58386597	22.9	21.3
-3156.05264696	-2360.57324246	24.3	38.0	-3157.58061615	-2361.59478935	16.0	29.7
-3156.05347454	-2360.57407004	23.8	36.9	-3157.57594475	-2361.59011795	18.9	32.1
-3156.08416012	-2360.60475562	4.5	18.1	-3157.60387047	-2361.61804367	1.4	15.0
-2512.08633547	-2360.59271629	12.1	9.6	-2513.02274452	-2361.60726727	8.2	5.7
-3049.35173339	-2360.62225553	-6.5	8.0	-3050.71518151	-2361.63120471	-6.9	7.6
-3049.34279685	-2360.61331899	-0.9	13.7	-3050.70748183	-2361.62350503	-2.0	12.5
-3049.37999853	-2360.65052067	-24.2	-7.2	-3050.74744602	-2361.66346922	-27.1	-10.1
-3049.37647830	-2360.64700044	-22.0	-7.0	-3050.74481330	-2361.66083650	-25.4	-10.5
-3049.37884777	-2360.64936991	-23.5	-9.1	-3050.74662773	-2361.66265093	-26.6	-12.2
-3049.34680829	-2360.61733043	-3.4	8.8	-3050.70851787	-2361.62454107	-2.7	9.5
-3049.37796617	-2360.64848831	-22.9	-10.1	-3050.73687675	-2361.65289995	-20.5	-7.6
-3049.35882410	-2360.62934624	-10.9	1.2	-3050.72079536	-2361.63681856	-10.4	1.8
-3049.35471656	-2360.62523870	-8.4	3.9	-3050.71961650	-2361.63563970	-9.6	2.7

-3049.34282657	-2360.61334871	-0.9	11.8	-3050.71209175	-2361.62811495	-4.9	7.8
-3049.34978523	-2360.62030737	-5.3	7.9	-3050.71972442	-2361.63574762	-9.7	3.4
-3049.34404412	-2360.61456626	-1.7	12.0	-3050.71435123	-2361.63037443	-6.3	7.3
-3049.34902889	-2360.61955103	-4.8	7.9	-3050.71925529	-2361.63527849	-9.4	3.3
-947.69330999	-2360.61725196	-3.3	-7.1	-948.46798210	-2361.62971175	-5.9	-9.6
-3049.37305057	-2360.64357271	-19.9	-5.9	-3050.73462261	-2361.65064581	-19.1	-5.1
-3049.34583522	-2360.61635736	-2.8	10.4	-3050.70546576	-2361.62148896	-0.8	12.5
-3049.38372100	-2360.65424314	-26.6	-12.1	-3050.74998920	-2361.66601240	-28.7	-14.2
-3888.59557000	-2360.67957465	-42.5	-9.1	-3890.39731555	-2361.68687165	-41.8	-8.4
-3888.59293034	-2360.67693499	-40.8	-7.2	-3890.39533822	-2361.68489432	-40.5	-7.0
-3888.57215316	-2360.65615781	-27.8	3.7	-3890.38038994	-2361.66994604	-31.2	0.3
-3888.57389039	-2360.65789504	-28.8	3.4	-3890.37958558	-2361.66914168	-30.7	1.6
-3888.59070815	-2360.67471280	-39.4	-5.0	-3890.39754616	-2361.68710226	-41.9	-7.6
-3888.58747342	-2360.67147807	-37.4	-4.6	-3890.39404561	-2361.68360171	-39.7	-6.9

Figure 4

-2316.35155405	-2360.54481398	42.1	40.7	-2317.39059075	-2361.57230175	30.1	28.7
-3138.41370631	-2360.56088993	32.0	46.8	-3140.15633505	-2361.58258810	23.7	38.4
-3138.41704256	-2360.56422618	29.9	45.6	-3140.15708512	-2361.58333817	23.2	38.9
-3138.44111550	-2360.58829912	14.8	30.0	-3140.17805588	-2361.60430893	10.0	25.2
-2494.44667915	-2360.57964809	20.3	20.6	-2495.59893082	-2361.59553341	15.5	15.9
-2937.79614532	-2360.60660520	3.3	22.3	-2939.34569103	-2361.61869966	1.0	19.9
-2937.78880607	-2360.59926595	7.9	26.7	-2939.33983165	-2361.61284028	4.7	23.4
-2937.77886975	-2360.58932963	14.2	30.5	-2939.33187354	-2361.60488217	9.7	26.0
-2937.81630486	-2360.62676474	-9.3	10.9	-2939.36688970	-2361.63989833	-12.3	7.9
-2937.81355803	-2360.62401791	-7.6	11.9	-2939.36681224	-2361.63982087	-12.3	7.2
-2937.81534669	-2360.62580657	-8.7	9.8	-2939.36741443	-2361.64042306	-12.6	5.9
-2937.79265217	-2360.60311205	5.5	21.3	-2939.34076928	-2361.61377791	4.1	19.9
-2937.82231063	-2360.63277051	-13.1	2.8	-2939.36745170	-2361.64046033	-12.7	3.2
-853.78202880	-2360.60416714	4.9	3.9	-854.52473821	-2361.61844224	1.2	0.2
-3777.02648401	-2360.65042640	-24.2	10.3	-3779.01385830	-2361.66039983	-25.2	9.3
-3777.03525859	-2360.65920098	-29.7	7.8	-3779.01870981	-2361.66525134	-28.2	9.2
-3777.00677230	-2360.63071469	-11.8	20.4	-3778.99796003	-2361.64450156	-15.2	17.0
-3777.00363213	-2360.62757452	-9.8	22.4	-3778.99719929	-2361.64374082	-14.7	17.5
-3777.01019105	-2360.63413344	-13.9	21.8	-3779.00303997	-2361.64958150	-18.4	17.4
-3777.00534283	-2360.62928522	-10.9	25.1	-3779.00063716	-2361.64717869	-16.9	19.1
-3777.01015070	-2360.63409309	-13.9	18.7	-3779.00650925	-2361.65305078	-20.6	12.0
-3777.01892753	-2360.64286992	-19.4	17.3	-3779.01379530	-2361.66033683	-25.1	11.6
-2182.48260214	-2360.54289313	43.3	41.4	-2183.38563437	-2361.57074278	31.1	29.1
-3004.54846505	-2360.56267973	30.9	46.4	-3006.15291285	-2361.58256331	23.7	39.2
-3004.55139767	-2360.56561235	29.1	45.2	-3006.15320929	-2361.58285975	23.5	39.7
-3004.57418159	-2360.58839627	14.8	29.3	-3006.17543459	-2361.60508505	9.5	24.0
-2360.57748535	-2360.57748535	21.6	19.8	-2361.59374933	-2361.59374933	16.7	14.9
-2670.06403240	-2360.60855441	2.1	19.5	-2671.34014222	-2361.61994567	0.2	17.6
-2670.05980181	-2360.60432382	4.8	21.5	-2671.33724905	-2361.61705250	2.0	18.8
-2670.05301436	-2360.59753637	9.0	26.0	-2671.33358714	-2361.61339059	4.3	21.3
-2670.08466310	-2360.62918511	-10.8	5.6	-2671.36250075	-2361.64230420	-13.8	2.6
-2670.08127030	-2360.62579231	-8.7	7.2	-2671.36192322	-2361.64172667	-13.5	2.5
-2670.08354222	-2360.62806423	-10.1	5.6	-2671.36297950	-2361.64278295	-14.1	1.6
-2670.06330442	-2360.60782643	2.6	16.2	-2671.33762513	-2361.61742858	1.8	15.4
-2670.08687673	-2360.63139874	-12.2	3.1	-2671.35796999	-2361.63777344	-11.0	4.4
-719.91359626	-2360.60096330	6.9	4.4	-720.52025101	-2361.61520932	3.2	0.7
-3509.30027501	-2360.65827952	-29.1	4.4	-3511.01482605	-2361.66816240	-30.0	3.4
-3509.30407582	-2360.66208033	-31.5	5.0	-3511.01617062	-2361.66950697	-30.9	5.6
-3509.27081329	-2360.62881780	-10.6	22.5	-3510.99105736	-2361.64439371	-15.1	17.9

-3509.27246028	-2360.63046479	-11.6	21.8	-3510.99373044	-2361.64706679	-16.8	16.6
-3509.27371772	-2360.63172223	-12.4	22.6	-3510.99375582	-2361.64709217	-16.8	18.2
-3509.26852553	-2360.62653004	-9.2	24.6	-3510.99051693	-2361.64385328	-14.8	19.0
-3509.27335061	-2360.63135512	-12.2	21.2	-3510.99538739	-2361.64872374	-17.8	15.6
-3509.27906286	-2360.63706737	-15.8	19.1	-3510.99894487	-2361.65228122	-20.1	14.8
-2410.26062260	-2360.54053291	44.8	43.1	-2411.33108586	-2361.56789128	32.9	31.2
-3232.32726546	-2360.56109946	31.9	49.2	-3234.10143029	-2361.58277776	23.5	40.9
-3232.33095360	-2360.56478760	29.6	46.0	-3234.10198795	-2361.58333542	23.2	39.6
-3232.34503302	-2360.57886702	20.7	35.0	-3234.11325730	-2361.59460477	16.1	30.4
-2588.35763461	-2360.57725393	21.8	21.9	-2589.54203182	-2361.59372883	16.7	16.8
-3125.63102428	-2360.61478492	-1.8	16.2	-3127.24468537	-2361.62788284	-4.8	13.3
-3125.62814292	-2360.61190356	0.0	18.1	-3127.24332190	-2361.62651937	-3.9	14.2
-3125.61986331	-2360.60362395	5.2	19.9	-3127.23538629	-2361.61858376	1.1	15.8
-3125.65040280	-2360.63416344	-14.0	6.3	-3127.26678192	-2361.64997939	-18.6	1.6
-3125.64833486	-2360.63209550	-12.7	4.9	-3127.26656262	-2361.64976009	-18.5	-1.0
-3125.65059922	-2360.63435986	-14.1	3.7	-3127.26647745	-2361.64967492	-18.4	-0.7
-3125.63166393	-2360.61542457	-2.2	13.6	-3127.24261450	-2361.62581197	-3.5	12.4
-3125.65053661	-2360.63429725	-14.0	3.6	-3127.25878147	-2361.64197894	-13.6	4.0
-947.69330999	-2360.59964231	7.7	4.8	-948.46798210	-2361.61442242	3.7	0.8
-3964.86537215	-2360.66261530	-31.8	1.2	-3966.91617691	-2361.67290728	-33.0	0.0
-3964.87099805	-2360.66824120	-35.3	1.8	-3966.91911991	-2361.67585028	-34.9	2.3
-3964.83192362	-2360.62916677	-10.8	20.9	-3966.88808964	-2361.64482001	-15.4	16.3
-3964.83025407	-2360.62749722	-9.8	24.0	-3966.88787055	-2361.64460092	-15.3	18.5
-3964.83329981	-2360.63054296	-11.7	23.3	-3966.89168136	-2361.64841173	-17.6	17.4
-3964.83046656	-2360.62770971	-9.9	24.1	-3966.88896723	-2361.64569760	-15.9	18.1
-3964.83467890	-2360.63192205	-12.5	22.2	-3966.89610917	-2361.65283954	-20.4	14.3
-3964.83758434	-2360.63482749	-14.4	20.3	-3966.89550631	-2361.65223668	-20.0	14.6

Figure 5

-2105.29353601	-2360.52402560	55.2	53.7	-2106.15647146	-2361.55335336	42.0	40.5
-2927.34643927	-2360.53085255	50.9	64.6	-2928.91884570	-2361.56026965	37.7	51.4
-2927.34582967	-2360.53024295	51.3	65.6	-2928.91629015	-2361.55771410	39.3	53.6
-2927.40351854	-2360.58793182	15.1	29.6	-2928.96282305	-2361.60424700	10.1	24.6
-2283.40117354	-2360.57137213	25.4	24.1	-2284.37791805	-2361.58969154	19.2	17.9
-2592.87444071	-2360.58916131	14.3	27.5	-2594.11352308	-2361.60510002	9.5	22.8
-2592.85171386	-2360.56643446	28.5	42.3	-2594.09041397	-2361.58199091	24.0	37.8
-2592.89952742	-2360.61424802	-1.5	13.7	-2594.13969762	-2361.63127456	-6.9	8.3
-2592.89923466	-2360.61395526	-1.3	13.6	-2594.13957453	-2361.63115147	-6.8	8.0
-2592.90142514	-2360.61614574	-2.7	12.2	-2594.14144431	-2361.63302125	-8.0	6.8
-2592.85649333	-2360.57121393	25.5	37.2	-2594.09304137	-2361.58461831	22.4	34.1
-2592.90325737	-2360.61797797	-3.8	8.5	-2594.13815374	-2361.62973068	-5.9	6.4
-3432.11661049	-2360.64481360	-20.6	10.4	-3433.79359523	-2361.65870507	-24.1	6.9
-3432.09583327	-2360.62403638	-7.6	24.5	-3433.77743644	-2361.64254628	-14.0	18.2
-3432.09787875	-2360.62608186	-8.9	24.6	-3433.78006244	-2361.64517228	-15.6	17.9
-3432.13037187	-2360.65857498	-29.3	3.5	-3433.81336741	-2361.67847725	-36.5	-3.7

Figure 8

-4501.28636762	-1873.05465006	0.0	0.0	-4503.31808352	-1873.68596905	0.0	0.0
-2316.35155405	-1873.02904499	16.1	15.9	-2317.39059075	-1873.66699679	11.9	11.7
-4632.75334354	-1873.05416271	0.3	9.1	-4634.82738877	-1873.69010042	-2.6	6.2
-4632.75266233	-1873.05382211	0.5	9.8	-4634.82566708	-1873.68923958	-2.1	7.2
-4501.28636762	-1873.05465006	0.0	0.0	-4503.31808352	-1873.68596905	0.0	0.0
-2182.48260214	-1873.02712415	17.3	16.5	-2183.38563437	-1873.66543782	12.9	12.1

-4365.02200811	-1873.05552606	-0.5	8.3	-4366.82325217	-1873.69142953	-3.4	5.4
-4365.02027833	-1873.05466117	0.0	8.7	-4366.82105432	-1873.69033061	-2.7	5.9
-4501.28636762	-1873.05465006	0.0	0.0	-4503.31808352	-1873.68596905	0.0	0.0
-2410.26062260	-1873.02476392	18.8	18.3	-2411.33108586	-1873.66258632	14.7	14.2
-4820.58353572	-1873.05590918	-0.8	7.4	-4822.72041747	-1873.69170919	-3.6	4.6
-4820.58254522	-1873.05541393	-0.5	8.9	-4822.71930640	-1873.69115366	-3.3	6.1

Figure 9

-2106.01986092	-2106.01986092	0.0	0.0	-2106.89488626	-2106.89488626	0.0	0.0
-2549.34485975	-2106.02235069	-1.6	14.3	-2550.62074583	-2106.89715187	-1.4	14.4
-2549.34303493	-2106.02052587	-0.4	16.7	-2550.62024326	-2106.89664930	-1.1	16.0
-2106.01986092	-2106.01986092	0.0	0.0	-2106.89488626	-2106.89488626	0.0	0.0
-2415.48251933	-2106.02704134	-4.5	12.0	-2416.62184512	-2106.90164857	-4.2	12.3
-2415.48084182	-2106.02536383	-3.5	13.2	-2416.62154008	-2106.90134353	-4.1	12.6
-2106.01986092	-2106.01986092	0.0	0.0	-2106.89488626	-2106.89488626	0.0	0.0
-2643.26446591	-2106.02860723	-5.5	9.6	-2644.57292623	-2106.90442669	-6.0	9.1
-2643.26586213	-2106.03000345	-6.4	11.4	-2644.57318368	-2106.90468414	-6.1	11.6
-2268.24693747	-2268.24693747	0.0	0.0	-2269.13807551	-2269.13807551	0.0	0.0
-2711.60533739	-2268.28282833	-22.5	-4.6	-2712.89841293	-2269.17481897	-23.1	-5.2
-2711.60533760	-2268.28282854	-22.5	-4.6	-2712.89841299	-2269.17481903	-23.1	-5.2
-2268.24693747	-2268.24693747	0.0	0.0	-2269.13807551	-2269.13807551	0.0	0.0
-2577.73996610	-2268.28448811	-23.6	-6.8	-2578.89705234	-2269.17685579	-24.3	-7.6
-2577.73979530	-2268.28431731	-23.5	-6.6	-2578.89706616	-2269.17686961	-24.3	-7.5
-2268.24693747	-2268.24693747	0.0	0.0	-2269.13807551	-2269.13807551	0.0	0.0
-2805.52168423	-2268.28582555	-24.4	-6.0	-2806.84660944	-2269.17810990	-25.1	-6.7
-2805.52168431	-2268.28582563	-24.4	-6.0	-2806.84660942	-2269.17810988	-25.1	-6.7

Fig. S10

-2075.19265695	-2914.37917444	0.0	0.0	-2075.89824977	-2915.52471687	0.0	0.0
-2075.18240589	-2914.36892338	6.4	5.7	-2075.88936094	-2915.51582804	5.6	4.9
-2075.17405895	-2914.36057644	11.7	10.7	-2075.88191308	-2915.50838018	10.3	9.3
-2075.16548971	-2914.35200720	17.0	16.7	-2075.87419945	-2915.50066655	15.1	14.8
-2914.37946319	-2914.37946319	-0.2	14.7	-2915.53060384	-2915.53060384	-3.7	11.2
-2914.37945489	-2914.37945489	-0.2	14.8	-2915.53051616	-2915.53051616	-3.6	11.3
-2914.37832153	-2914.37832153	0.5	14.7	-2915.52915693	-2915.52915693	-2.8	11.4
-2914.37681722	-2914.37681722	1.5	16.5	-2915.52760834	-2915.52760834	-1.8	13.2
-2914.37668368	-2914.37668368	1.6	15.3	-2915.52672711	-2915.52672711	-1.3	12.5
-2914.37674569	-2914.37674569	1.5	15.9	-2915.52685906	-2915.52685906	-1.3	13.0
-2914.37596634	-2914.37596634	2.0	15.7	-2915.52586131	-2915.52586131	-0.7	13.0
-2914.37544645	-2914.37544645	2.3	17.7	-2915.52533653	-2915.52533653	-0.4	15.0
-2914.39108658	-2914.39108658	-7.5	7.5	-2915.54071711	-2915.54071711	-10.0	4.9
-2914.39074163	-2914.39074163	-7.3	7.9	-2915.54069969	-2915.54069969	-10.0	5.1
-2914.39148707	-2914.39148707	-7.7	8.3	-2915.54131709	-2915.54131709	-10.4	5.6
-2914.39148705	-2914.39148705	-7.7	8.3	-2915.54131711	-2915.54131711	-10.4	5.6
-2914.39047688	-2914.39047688	-7.1	9.5	-2915.54045518	-2915.54045518	-9.9	6.7
-2914.39047684	-2914.39047684	-7.1	9.5	-2915.54045517	-2915.54045517	-9.9	6.7

-2914.38178913	-2914.38178913	-1.6	9.2	-2915.53520027	-2915.53520027	-6.6	4.3
-2914.38260788	-2914.38260788	-2.2	10.4	-2915.53540450	-2915.53540450	-6.7	5.9
-2914.38039449	-2914.38039449	-0.8	11.1	-2915.53369427	-2915.53369427	-5.6	6.2
-2914.38152590	-2914.38152590	-1.5	11.9	-2915.53549564	-2915.53549564	-6.8	6.6
-2914.38073918	-2914.38073918	-1.0	12.2	-2915.53441854	-2915.53441854	-6.1	7.1
-2914.37955350	-2914.37955350	-0.2	13.2	-2915.53363176	-2915.53363176	-5.6	7.8
-2140.93383702	-2980.12035451	0.0	0.0	-2141.57039794	-2981.19686504	0.0	0.0
-2140.92618067	-2980.11269816	4.8	5.8	-2141.56294282	-2981.18940992	4.7	5.7
-2140.91898069	-2980.10549818	9.3	10.9	-2141.55598597	-2981.18245307	9.0	10.6
-2140.91137789	-2980.09789538	14.1	15.2	-2141.54815693	-2981.17462403	14.0	15.0
-2980.11965190	-2980.11965190	0.4	15.6	-2981.19993262	-2981.19993262	-1.9	13.2
-2980.11994435	-2980.11994435	0.3	15.5	-2981.19903574	-2981.19903574	-1.4	13.8
-2980.11947742	-2980.11947742	0.6	17.2	-2981.19873048	-2981.19873048	-1.2	15.5
-2980.11947737	-2980.11947737	0.6	17.2	-2981.19873041	-2981.19873041	-1.2	15.5
-2980.12030703	-2980.12030703	0.0	15.3	-2981.19793706	-2981.19793706	-0.7	14.6
-2980.11981392	-2980.11981392	0.3	16.2	-2981.19830483	-2981.19830483	-0.9	14.9
-2980.11981396	-2980.11981396	0.3	16.2	-2981.19830487	-2981.19830487	-0.9	14.9
-2980.11705353	-2980.11705353	2.1	17.3	-2981.19559112	-2981.19559112	0.8	16.0
-1985.79035676	-2824.97687425	0.0	0.0	-1986.53187940	-2826.15834650	0.0	0.0
-1985.78046851	-2824.96698600	6.2	7.6	-1986.52281850	-2826.14928560	5.7	7.0
-1985.77120101	-2824.95771850	12.0	12.6	-1986.51406654	-2826.14053364	11.2	11.7
-1985.76082970	-2824.94734719	18.5	18.4	-1986.50407463	-2826.13054173	17.4	17.4
-2824.97470147	-2824.97470147	1.4	15.4	-2826.16021083	-2826.16021083	-1.2	12.8
-2824.97351672	-2824.97351672	2.1	16.3	-2826.15894139	-2826.15894139	-0.4	13.8
-2824.97383096	-2824.97383096	1.9	17.2	-2826.16050741	-2826.16050741	-1.4	13.9
-2824.97438576	-2824.97438576	1.6	16.9	-2826.15952749	-2826.15952749	-0.7	14.6
-2824.97398663	-2824.97398663	1.8	17.2	-2826.15864400	-2826.15864400	-0.2	15.2
-2824.97398670	-2824.97398670	1.8	17.2	-2826.15864426	-2826.15864426	-0.2	15.2
-2824.97394208	-2824.97394208	1.8	16.7	-2826.15728740	-2826.15728740	0.7	15.5
-2824.97094555	-2824.97094555	3.7	19.0	-2826.15515051	-2826.15515051	2.0	17.3

E_{sp} …… single point electronic energy in thf (SMD) in hartree with Def2TZVPP
E_{sp} (sum) single point electronic energy in thf (SMD) in hartree with Def2TZVPP after mass balance
ΔE_{sp} … relative single point electronic energy in thf(SMD) in kcal/mol with Def2TZVPP
ΔG_{sp} … relative single point free energy in thf(SMD) in kcal/mol ($\Delta G_{sp} = \Delta E_{sp}$/Def2TZVPP + ΔG_{corr}[level of optimization])

Single point energies in Figures 1–10 with BP86-D3BJ and PBE0-D3BJ

BP86-D3BJ/Def2TZVPP thf(SMD)				PBE0-D3BJ/Def2TZVPP thf(SMD)			
E_{sp} [hartree]	E_{sp} (sum) [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	E_{sp} (sum) [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-822.91432061				-821.94869064			
-644.69434069				-643.93532528			
-395.51182271				-395.11999426			
-2630.16132995				-2627.72774896			
-306.15260557				-305.77960062			
-461.20902678				-460.88581488			
-232.55698528				-232.28199333			
-443.82238654				-443.27274318			
-309.78612087				-309.40128801			
-537.77787666				-537.13780135			
-839.77094997				-839.03710930			
-2102.64636097				-2101.80357820			
-1947.60447108				-1946.71054354			
-2085.24428915				-2084.17399646			
-1951.20535915				-1950.30012369			
-2179.19720728				-2178.03642956			
	Figure 1						
-4504.24272347	-2362.08749432	18.8	17.6	-4501.00064360	-2360.68754801	19.8	18.6
-5327.17133101	-2362.10178125	9.9	31.7	-5322.95431599	-2360.69252976	16.6	38.5
-5327.16724659	-2362.09769683	12.4	33.0	-5322.95351526	-2360.69172903	17.1	37.7
-5327.15615544	-2362.08660568	19.4	37.5	-5322.94599781	-2360.68421158	21.9	40.0
-5327.17369281	-2362.10414305	8.4	30.2	-5322.95410216	-2360.69231593	16.8	38.7
-5327.20291007	-2362.13336031	-10.0	6.7	-5322.99174808	-2360.72996185	-6.8	9.9
-4682.49270204	-2362.11749296	0.0	0.0	-4679.04551613	-2360.71905518	0.0	0.0
-4682.49220628	-2362.11699720	0.3	1.6	-4679.04510348	-2360.71864253	0.3	1.5
-4682.47604050	-2362.10083142	10.5	8.4	-4679.03240069	-2360.70593974	8.2	6.1
-4682.47396352	-2362.09875444	11.8	11.0	-4679.03127559	-2360.70481464	8.9	8.2
-4682.47943375	-2362.10422467	8.3	9.4	-4679.03431305	-2360.70785210	7.0	8.1
-4682.47730342	-2362.10209434	9.7	10.0	-4679.03238462	-2360.70592367	8.2	8.5
-4682.47336530	-2362.09815622	12.1	11.5	-4679.03037064	-2360.70390969	9.5	8.9
-4682.47432383	-2362.09911475	11.5	12.7	-4679.03107269	-2360.70461174	9.1	10.2
-4682.47507980	-2362.09987072	11.1	12.4	-4679.03163754	-2360.70517659	8.7	10.1
-4992.29584886	-2362.13451891	-10.7	8.6	-4988.45656909	-2360.72882013	-6.1	13.1
-4992.30266822	-2362.14133827	-15.0	3.5	-4988.45858943	-2360.73084047	-7.4	11.1
-4992.30266775	-2362.14133780	-15.0	3.5	-4988.45858953	-2360.73084057	-7.4	11.1
-4992.30063693	-2362.13930698	-13.7	4.1	-4988.45844205	-2360.73069309	-7.3	10.5
-4992.30055643	-2362.13922648	-13.6	5.8	-4988.45774391	-2360.72999495	-6.9	12.5
-4992.30055659	-2362.13922664	-13.6	5.8	-4988.45774363	-2360.72999467	-6.9	12.5
-4992.28610058	-2362.12477063	-4.6	14.5	-4988.44892493	-2360.72117597	-1.3	17.8
-4992.28610050	-2362.12477055	-4.6	14.5	-4988.44892492	-2360.72117596	-1.3	17.8
-4992.29524444	-2362.13391449	-10.3	10.1	-4988.45051381	-2360.72276485	-2.3	18.1
-4992.33307614	-2362.17174619	-34.0	-16.1	-4988.50191476	-2360.77416580	-34.6	-16.6
-4992.33341996	-2362.17209001	-34.3	-15.7	-4988.50192258	-2360.77417362	-34.6	-16.0
-4992.32382908	-2362.16249913	-28.2	-8.1	-4988.49491398	-2360.76716502	-30.2	-10.0
-4992.28547747	-2362.12414752	-4.2	12.8	-4988.44413553	-2360.71638657	1.7	18.7
-4992.28547095	-2362.12414100	-4.2	13.6	-4988.44411767	-2360.71636871	1.7	19.4
-4992.30177785	-2362.14044790	-14.4	6.6	-4988.45555405	-2360.72780509	-5.5	15.5

-4992.29504212	-2362.13371217	-10.2	9.1	-4988.44990015	-2360.72215119	-1.9	17.4
-4992.29902117	-2362.13769122	-12.7	7.8	-4988.45375328	-2360.72600432	-4.4	16.1
-4992.29902127	-2362.13769132	-12.7	7.8	-4988.45375338	-2360.72600442	-4.4	16.1
-4992.29902122	-2362.13769127	-12.7	7.8	-4988.45375326	-2360.72600430	-4.4	16.1
-4992.27920335	-2362.11787340	-0.2	18.9	-4988.43958747	-2360.71183851	4.5	23.7
-4992.29511033	-2362.13378038	-10.2	11.3	-4988.44994906	-2360.72220010	-2.0	19.5
-4992.27554793	-2362.11421798	2.1	22.2	-4988.43682845	-2360.70907949	6.3	26.4
-4992.27128282	-2362.10995287	4.7	24.2	-4988.43190028	-2360.70415132	9.4	28.8
-4992.33924927	-2362.17791932	-37.9	-19.3	-4988.50629584	-2360.77854688	-37.3	-18.7
-4992.33176795	-2362.17043800	-33.2	-12.9	-4988.49665871	-2360.76890975	-31.3	-11.0
-4992.28872524	-2362.12739529	-6.2	10.2	-4988.45099450	-2360.72324554	-2.6	13.7
-4992.29003748	-2362.12870753	-7.0	10.2	-4988.45254696	-2360.72479800	-3.6	13.6
-4992.29285904	-2362.13152909	-8.8	11.0	-4988.45419026	-2360.72644130	-4.6	15.2
-4992.29868181	-2362.13735186	-12.5	6.3	-4988.45476242	-2360.72701346	-5.0	13.8
-4992.29999437	-2362.13866442	-13.3	5.9	-4988.45338778	-2360.72563882	-4.1	15.1
-4992.29357754	-2362.13224759	-9.3	9.0	-4988.45222110	-2360.72447214	-3.4	14.8
-4992.28407140	-2362.12274145	-3.3	14.9	-4988.44742441	-2360.71967545	-0.4	17.8
-4992.28318208	-2362.12185213	-2.7	16.2	-4988.44702418	-2360.71927522	-0.1	18.8
-4992.28544888	-2362.12411893	-4.2	16.2	-4988.44804601	-2360.72029705	-0.8	19.5
-4992.28544875	-2362.12411880	-4.2	16.2	-4988.44804595	-2360.72029699	-0.8	19.5
-4992.29708987	-2362.13575992	-11.5	8.2	-4988.45176370	-2360.72401474	-3.1	16.5
-4992.29788417	-2362.13655422	-12.0	9.1	-4988.45208615	-2360.72433719	-3.3	17.7
-4992.29676812	-2362.13543817	-11.3	10.1	-4988.45175505	-2360.72400609	-3.1	18.3
-4992.33743508	-2362.17610513	-36.8	-19.1	-4988.50503421	-2360.77728525	-36.5	-18.9
-4992.31827702	-2362.15694707	-24.8	-7.9	-4988.49226555	-2360.76451659	-28.5	-11.7
-4992.32008420	-2362.15875425	-25.9	-6.9	-4988.49223747	-2360.76448851	-28.5	-9.5
-4992.31813818	-2362.15680823	-24.7	-5.5	-4988.49049779	-2360.76274883	-27.4	-8.3
-4992.32601546	-2362.16468551	-29.6	-8.1	-4988.49185016	-2360.76410120	-28.3	-6.7
-4992.30013663	-2362.13880668	-13.4	2.2	-4988.46205321	-2360.73430425	-9.6	6.0
-4992.28326853	-2362.12193858	-2.8	14.1	-4988.44461235	-2360.71686339	1.4	18.3
-4992.29976449	-2362.13843454	-13.1	5.7	-4988.45471671	-2360.72696775	-5.0	13.8
-4992.27709722	-2362.11576727	1.1	18.7	-4988.43903019	-2360.71128123	4.9	22.4
-4992.29518701	-2362.13385706	-10.3	8.4	-4988.45075016	-2360.72300120	-2.5	16.2
-4992.29878614	-2362.13745619	-12.5	8.1	-4988.45422058	-2360.72647162	-4.7	16.0
-4992.29864407	-2362.13731412	-12.4	8.3	-4988.45404615	-2360.72629719	-4.5	16.2
-4992.27775258	-2362.11642263	0.7	21.0	-4988.44034497	-2360.71259601	4.1	24.4
-4992.29448468	-2362.13315473	-9.8	12.2	-4988.45121626	-2360.72346730	-2.8	19.2
-4992.26967090	-2362.10834095	5.7	25.6	-4988.43272178	-2360.70497282	8.8	28.7
-4992.33015563	-2362.16882568	-32.2	-12.8	-4988.49893339	-2360.77118443	-32.7	-13.3
-4992.33049576	-2362.16916581	-32.4	-12.1	-4988.49987406	-2360.77212510	-33.3	-13.0
-4992.31586160	-2362.15453165	-23.2	-4.9	-4988.48687826	-2360.75912930	-25.1	-6.8
-4992.31479007	-2362.15346012	-22.6	-3.9	-4988.48676831	-2360.75901935	-25.1	-6.4
-4992.33192533	-2362.17059538	-33.3	-17.7	-4988.50207232	-2360.77432336	-34.7	-19.0
-4992.33377868	-2362.17244873	-34.5	-17.2	-4988.50311926	-2360.77537030	-35.3	-18.0
-4992.32934295	-2362.16801300	-31.7	-15.0	-4988.49983752	-2360.77208856	-33.3	-16.6
-5832.11806960	-2362.18578968	-42.9	-6.7	-5827.54669293	-2360.78183467	-39.4	-3.3
-5832.11462784	-2362.18234792	-40.7	-4.2	-5827.54534837	-2360.78049011	-38.6	-2.0
-5832.11447861	-2362.18219869	-40.6	-5.1	-5827.54410304	-2360.77924478	-37.8	-2.3
-5832.11144880	-2362.17916888	-38.7	-0.6	-5827.54161102	-2360.77675276	-36.2	1.9
-5832.10477013	-2362.17249021	-34.5	0.6	-5827.52096736	-2360.75610910	-23.3	11.9
-5832.10143625	-2362.16915633	-32.4	2.7	-5827.51889605	-2360.75403779	-22.0	13.2
-5832.10333487	-2362.17105495	-33.6	1.2	-5827.52020318	-2360.75534492	-22.8	12.1
-5832.10157794	-2362.16929802	-32.5	4.4	-5827.51895341	-2360.75409515	-22.0	14.9
-5832.08712196	-2362.15484204	-23.4	12.0	-5827.50476178	-2360.73990352	-13.1	22.3
-5832.08894247	-2362.15666255	-24.6	11.7	-5827.50656449	-2360.74170623	-14.2	22.0
-5832.11559801	-2362.18331809	-41.3	-3.9	-5827.53479288	-2360.76993462	-31.9	5.4
-5832.10346598	-2362.17118606	-33.7	0.8	-5827.52375299	-2360.75889473	-25.0	9.4

-5832.10359822	-2362.17131830	-33.8	2.9	-5827.52549046	-2360.76063220	-26.1	10.6

Figure 2

-4360.47632744	-2362.09165895	16.2	22.3	-4358.12370978	-2360.69690764	13.9	20.0
-2180.22422384	-2362.07771907	25.0	22.7	-2179.05096916	-2360.68602191	20.7	18.5
-3003.15119932	-2362.09037394	17.0	31.9	-3001.00926782	-2360.69562993	14.7	29.6
-3003.15333331	-2362.09250793	15.7	29.4	-3001.01023197	-2360.69659408	14.1	27.8
-3003.17139069	-2362.11056531	4.3	18.5	-3001.03192144	-2360.71828355	0.5	14.6
-2358.46477953	-2362.09829484	12.0	11.5	-2357.08807640	-2360.70976379	5.8	5.3
-2802.31250457	-2362.12363334	-3.9	10.5	-2800.37828378	-2360.72722799	-5.1	9.3
-2802.29968020	-2362.11080897	4.2	19.1	-2800.36739959	-2360.71634380	1.7	16.6
-2802.33460888	-2362.14573765	-17.7	-1.9	-2800.41039155	-2360.75933576	-25.3	-9.5
-2802.33109962	-2362.14222839	-15.5	1.5	-2800.40878043	-2360.75772464	-24.3	-7.2
-2802.33036803	-2362.14149680	-15.1	1.7	-2800.40952158	-2360.75846579	-24.7	-7.9
-2802.29865247	-2362.10978124	4.8	18.3	-2800.37083910	-2360.71978331	-0.5	13.0
-2802.33309542	-2362.14422419	-16.8	-2.9	-2800.40293277	-2360.75187698	-20.6	-6.7
-2802.31567483	-2362.12680360	-5.8	8.5	-2800.38836940	-2360.73731361	-11.5	2.9
-2802.31478250	-2362.12591127	-5.3	9.4	-2800.38970037	-2360.73864458	-12.3	2.4
-2802.30758077	-2362.11870954	-0.8	13.0	-2800.38408841	-2360.73303262	-8.8	5.0
-2802.30834457	-2362.11947334	-1.2	12.2	-2800.38509692	-2360.73404113	-9.4	4.0
-2802.30444251	-2362.11557128	1.2	15.7	-2800.38049305	-2360.72943726	-6.5	8.0
-2802.30780607	-2362.11893484	-0.9	13.1	-2800.38474254	-2360.73368675	-9.2	4.8
-854.70137435	-2362.11697420	0.3	-0.8	-853.67310338	-2360.73259113	-8.5	-9.6
-2802.32938681	-2362.14051558	-14.4	-0.2	-2800.40006752	-2360.74901173	-18.8	-4.5
-2802.30738774	-2362.11851651	-0.6	13.8	-2800.37945364	-2360.72839785	-5.9	8.6
-2802.34167989	-2362.15280866	-22.2	-4.8	-2800.42042163	-2360.76936584	-31.6	-14.2
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-3642.13605384	-2362.17623263	-36.9	-3.2	-3639.47053199	-2360.78236689	-39.7	-6.1
-3642.13096741	-2362.17114620	-33.7	-2.6	-3639.45287975	-2360.76471465	-28.7	2.4
-3642.12964829	-2362.16982708	-32.8	0.3	-3639.45153742	-2360.76337232	-27.8	5.4
-3642.14941236	-2362.18959115	-45.2	-9.4	-3639.47338682	-2360.78522172	-41.5	-5.6
-3642.14489779	-2362.18507658	-42.4	-8.2	-3639.46947171	-2360.78130661	-39.1	-4.8

-4360.47632744	-2362.09165895	16.2	22.3	-4358.12370978	-2360.69690764	13.9	20.0
-2180.22422384	-2362.07771907	25.0	22.7	-2179.05096916	-2360.68602191	20.7	18.5
-3003.15119932	-2362.09037394	17.0	31.9	-3001.00926782	-2360.69562993	14.7	29.6
-3003.15333331	-2362.09250793	15.7	29.4	-3001.01023197	-2360.69659408	14.1	27.8
-3003.17139069	-2362.11056531	4.3	18.5	-3001.03192144	-2360.71828355	0.5	14.6
-2358.46477953	-2362.09829484	12.0	11.5	-2357.08807640	-2360.70976379	5.8	5.3
-2668.28041145	-2362.12780588	-6.5	9.4	-2666.51005975	-2360.73045913	-7.2	8.7
-2668.27150585	-2362.11890028	-0.9	14.9	-2666.50335902	-2360.72375840	-3.0	12.8
-2668.30668156	-2362.15407599	-23.0	-6.6	-2666.54680865	-2360.76720803	-30.2	-13.8
-2668.30209438	-2362.14948881	-20.1	-5.8	-2666.54442894	-2360.76482832	-28.7	-14.5
-2668.30229726	-2362.14969169	-20.2	-3.8	-2666.54591207	-2360.76631145	-29.7	-13.2
-2668.27063968	-2362.11803411	-0.3	12.8	-2666.50688012	-2360.72727950	-5.2	7.9
-2668.29880893	-2362.14620336	-18.0	-3.2	-2666.53303311	-2360.75343249	-21.6	-6.7
-2668.28244941	-2362.12984384	-7.8	4.7	-2666.51940988	-2360.73980926	-13.0	-0.6
-2668.27995858	-2362.12735301	-6.2	7.7	-2666.51990862	-2360.74030800	-13.3	0.6
-2668.27331006	-2362.12070449	-2.0	11.5	-2666.51454815	-2360.73494753	-10.0	3.5
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-2668.27000979	-2362.11740422	0.1	15.2	-2666.51101507	-2360.73141445	-7.8	7.3
-2668.27390089	-2362.12129532	-2.4	11.3	-2666.51544353	-2360.73584291	-10.5	3.2
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-2668.29611377	-2362.14350820	-16.3	-2.8	-2666.53097202	-2360.75137140	-20.3	-6.8
-2668.27422873	-2362.12162316	-2.6	10.4	-2666.51059750	-2360.73099688	-7.5	5.5
-2668.31245107	-2362.15984550	-26.6	-10.2	-2666.55528575	-2360.77568513	-35.5	-19.2

-3508.10662325	-2362.18306771	-41.1	-10.0	-3505.60590644	-2360.78919652	-44.0	-12.9
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-3508.09870330	-2362.17514776	-36.2	-2.6	-3505.58577727	-2360.76906735	-31.4	2.2
-3508.11434739	-2362.19079185	-46.0	-11.9	-3505.60356916	-2360.78685924	-42.5	-8.5
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-4360.47632744	-2362.09165895	16.2	22.3	-4358.12370978	-2360.69690764	13.9	20.0
-2180.22422384	-2362.07771907	25.0	22.7	-2179.05096916	-2360.68602191	20.7	18.5
-3003.15119932	-2362.09037394	17.0	31.9	-3001.00926782	-2360.69562993	14.7	29.6
-3003.15333331	-2362.09250793	15.7	29.4	-3001.01023197	-2360.69659408	14.1	27.8
-3003.17139069	-2362.11056531	4.3	18.5	-3001.03192144	-2360.71828355	0.5	14.6
-2358.46477953	-2362.09829484	12.0	11.5	-2357.08807640	-2360.70976379	5.8	5.3
-2896.27637605	-2362.13201470	-9.1	5.7	-2894.25025225	-2360.73413829	-9.5	5.3
-2896.27116845	-2362.12680710	-5.8	10.0	-2894.24689297	-2360.73077901	-7.4	8.5
-2896.30590006	-2362.16153871	-27.6	-10.1	-2894.29036869	-2360.77425473	-34.6	-17.1
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-2896.30152330	-2362.15716195	-24.9	-10.8	-2894.28949316	-2360.77337920	-34.1	-20.0
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-2896.27515251	-2362.13079116	-8.3	4.6	-2894.25658153	-2360.74046757	-13.4	-0.5
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-2896.26287815	-2362.11851680	-0.6	12.0	-2894.24846473	-2360.73235077	-8.3	4.3
-2896.26679722	-2362.12243587	-3.1	11.6	-2894.25317564	-2360.73706168	-11.3	3.4
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-2896.30651376	-2362.16215241	-28.0	-11.0	-2894.29342692	-2360.77731296	-36.6	-19.5
-3736.10684488	-2362.19153355	-46.5	-13.4	-3733.34977682	-2360.79655356	-48.6	-15.6
-3736.10555637	-2362.19024504	-45.7	-12.1	-3733.34947793	-2360.79625467	-48.4	-14.9
-3736.09402901	-2362.17871768	-38.4	-6.4	-3733.32575966	-2360.77253640	-33.6	-1.6
-3736.09103472	-2362.17572339	-36.5	-5.2	-3733.32367873	-2360.77045547	-32.3	-0.9
-3736.10963726	-2362.19432593	-48.2	-13.0	-3733.34346873	-2360.79024547	-44.7	-9.5
-3736.10527829	-2362.18996696	-45.5	-10.0	-3733.33912217	-2360.78589891	-41.9	-6.5

Figure 3

-4670.57063203	-2362.08239004	22.0	27.4	-4668.32094893	-2360.68931295	18.7	24.1
-2335.26533567	-2362.06240969	34.6	33.1	-2334.14321579	-2360.67205428	29.5	28.0
-3158.19402668	-2362.07678009	25.5	39.3	-3156.10574755	-2360.68589540	20.8	34.5
-3158.19516744	-2362.07792085	24.8	38.0	-3156.10260300	-2360.68275085	22.8	35.9
-3158.21604175	-2362.09879516	11.7	25.3	-3156.12682880	-2360.70697665	7.6	21.2
-2513.50791312	-2362.08500722	20.4	17.9	-2512.18201965	-2360.69749278	13.5	11.0
-2957.36020975	-2362.11491731	1.6	16.4	-2955.47656294	-2360.71929289	-0.1	14.6
-2957.34052133	-2362.09522889	14.0	29.2	-2955.45962540	-2360.70235535	10.5	25.7
-2957.37693803	-2362.13164559	-8.9	8.4	-2955.50376269	-2360.74649264	-17.2	0.1
-2957.37338588	-2362.12809344	-6.7	8.7	-2955.50186761	-2360.74459756	-16.0	-0.6
-2957.37643921	-2362.13114677	-8.6	5.5	-2955.50479459	-2360.74752454	-17.9	-3.8
-2957.33915972	-2362.09386728	14.8	26.4	-2955.46277502	-2360.70550497	8.5	20.1
-2957.37874277	-2362.13345033	-10.0	3.2	-2955.49959647	-2360.74232642	-14.6	-1.4
-2957.36103444	-2362.11574200	1.1	13.9	-2955.48510984	-2360.72783979	-5.5	7.3
-2957.35884269	-2362.11355025	2.5	15.6	-2955.48566499	-2360.72839494	-5.9	7.3
-2957.34872400	-2362.10343156	8.8	21.6	-2955.47618990	-2360.71891985	0.1	12.8
-2957.35319728	-2362.10790484	6.0	20.5	-2955.48068042	-2360.72341037	-2.7	11.7
-2957.34888001	-2362.10358757	8.7	21.6	-2955.47594816	-2360.71867811	0.2	13.1

-2957.35246723	-2362.10717479	6.5	20.1	-2955.48010840	-2360.72283835	-2.4	11.2
-854.70137435	-2362.10244288	9.4	7.0	-853.67310338	-2360.71941153	-0.2	-2.7
-2957.37583509	-2362.13054265	-8.2	4.5	-2955.49680028	-2360.73953023	-12.8	-0.1
-2957.34868388	-2362.10339144	8.8	21.2	-2955.47188254	-2360.71461249	2.8	15.1
-2957.38848904	-2362.14319660	-16.1	-0.3	-2955.51753094	-2360.76026089	-25.9	-10.0
-3797.17954175	-2362.16329934	-28.7	2.8	-3794.56493617	-2360.77055682	-32.3	-0.8
-3797.18421057	-2362.16796816	-31.7	2.1	-3794.56688922	-2360.77250987	-33.5	0.2
-3797.17091601	-2362.15467360	-23.3	8.0	-3794.54309459	-2360.74871524	-18.6	12.7
-3797.17574877	-2362.15950636	-26.4	6.2	-3794.54563290	-2360.75125355	-20.2	12.4
-3797.19424206	-2362.17799965	-38.0	-4.4	-3794.56646953	-2360.77209018	-33.3	0.2
-3797.18948531	-2362.17324290	-35.0	-2.3	-3794.56301189	-2360.76863254	-31.1	1.6
-4670.57063203	-2362.08239004	22.0	27.4	-4668.32094893	-2360.68931295	18.7	24.1
-2335.26533567	-2362.06240969	34.6	33.1	-2334.14321579	-2360.67205428	29.5	28.0
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-3158.19516744	-2362.07792085	24.8	38.0	-3156.10260300	-2360.68275085	22.8	35.9
-3158.21604175	-2362.09879516	11.7	25.3	-3156.12682880	-2360.70697665	7.6	21.2
-2513.50791312	-2362.08500722	20.4	17.9	-2512.18201965	-2360.69749278	13.5	11.0
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-2823.31325039	-2362.10422362	8.3	22.5	-2821.59612136	-2360.71030648	5.5	19.7
-2823.34795525	-2362.13892848	-13.5	2.5	-2821.63907662	-2360.75326174	-21.5	-5.5
-2823.34426446	-2362.13523769	-11.1	2.4	-2821.63758963	-2360.75177475	-20.5	-7.0
-2823.34753047	-2362.13850370	-13.2	1.0	-2821.64035280	-2360.75453792	-22.3	-8.1
-2823.31142514	-2362.10239837	9.5	20.1	-2821.59890418	-2360.71308930	3.7	14.4
-2823.34415674	-2362.13512997	-11.1	0.9	-2821.62924844	-2360.74343356	-15.3	-3.4
-2823.32628260	-2362.11725583	0.1	11.1	-2821.61489069	-2360.72907581	-6.3	4.7
-2823.32355924	-2362.11453247	1.9	14.0	-2821.61497660	-2360.72916172	-6.3	5.8
-2823.31453913	-2362.10551236	7.5	19.9	-2821.60665638	-2360.72084150	-1.1	11.3
-2823.31879975	-2362.10977298	4.8	16.7	-2821.61096434	-2360.72514946	-3.8	8.0
-2823.31407406	-2362.10504729	7.8	21.0	-2821.60596612	-2360.72015124	-0.7	12.5
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-720.66376017	-2362.10109437	10.3	7.2	-719.80039546	-2360.71815878	0.6	-2.6
-2823.34101367	-2362.13198690	-9.1	2.5	-2821.62637719	-2360.74056231	-13.5	-1.9
-2823.31547557	-2362.10644880	6.9	19.2	-2821.60333376	-2360.71751888	1.0	13.2
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-3663.15048717	-2362.17051042	-33.3	0.7	-3660.70079317	-2360.77786899	-36.9	-2.9
-3663.13961990	-2362.15964315	-26.4	4.4	-3660.67767942	-2360.75475524	-22.4	8.5
-3663.14226293	-2362.16228618	-28.1	3.8	-3660.67710061	-2360.75417643	-22.0	9.9
-3663.15870065	-2362.17872390	-38.4	-5.2	-3660.69651658	-2360.77359240	-34.2	-1.0
-3663.15173689	-2362.17176014	-34.1	-1.5	-3660.69226675	-2360.76934257	-31.6	0.9
-4670.57063203	-2362.08239004	22.0	27.4	-4668.32094893	-2360.68931295	18.7	24.1
-2335.26533567	-2362.06240969	34.6	33.1	-2334.14321579	-2360.67205428	29.5	28.0
-3158.19402668	-2362.07678009	25.5	39.3	-3156.10574755	-2360.68589540	20.8	34.5
-3158.19516744	-2362.07792085	24.8	38.0	-3156.10260300	-2360.68275085	22.8	35.9
-3158.21604175	-2362.09879516	11.7	25.3	-3156.12682880	-2360.70697665	7.6	21.2
-2513.50791312	-2362.08500722	20.4	17.9	-2512.18201965	-2360.69749278	13.5	11.0
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-3051.31389720	-2362.11311464	2.7	17.3	-3049.34048350	-2360.71815528	0.6	15.1
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-3051.34560278	-2362.14482022	-17.1	-2.7	-3049.38311052	-2360.76078230	-26.2	-11.8
-3051.31131502	-2362.11053246	4.4	16.6	-3049.34247635	-2360.72014813	-0.7	11.5
-3051.33694970	-2362.13616714	-11.7	1.1	-3049.36644434	-2360.74411612	-15.7	-2.9
-3051.32001556	-2362.11923300	-1.1	11.0	-3049.35282087	-2360.73049265	-7.2	5.0
-3051.31680607	-2362.11602351	0.9	13.2	-3049.35250206	-2360.73017384	-7.0	5.3

-3051.30726807	-2362.10648551	6.9	19.6	-3049.34398378	-2360.72165556	-1.6	11.1
-3051.31228524	-2362.11150268	3.8	16.9	-3049.34915261	-2360.72682439	-4.9	8.3
-3051.30727917	-2362.10649661	6.9	20.5	-3049.34385068	-2360.72152246	-1.5	12.1
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-948.65494511	-2362.10052352	10.6	6.9	-947.53631151	-2360.71756149	0.9	-2.8
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-3051.30808910	-2362.10730654	6.4	19.6	-3049.34032878	-2360.71800056	0.7	13.9
-3051.35014839	-2362.14936583	-20.0	-5.5	-3049.38825641	-2360.76592819	-29.4	-14.9
-3891.15266145	-2362.18092892	-39.8	-6.5	-3888.44531453	-2360.78587701	-41.9	-8.6
-3891.14841598	-2362.17668345	-37.1	-3.6	-3888.44312299	-2360.78368547	-40.6	-7.0
-3891.13384232	-2362.16210979	-28.0	3.5	-3888.41598775	-2360.75655023	-23.5	8.0
-3891.13718580	-2362.16545327	-30.1	2.2	-3888.41676487	-2360.75732735	-24.0	8.2
-3891.15284365	-2362.18111112	-39.9	-5.6	-3888.43520983	-2360.77577231	-35.6	-1.2
-3891.14480071	-2362.17306818	-34.9	-2.1	-3888.43012379	-2360.77068627	-32.4	0.4

Figure 4

-2317.86425799	-2362.04797225	43.6	42.2	-2316.51382701	-2360.65573719	39.7	38.3
-3140.79680578	-2362.06619943	32.2	47.0	-3138.47699289	-2360.67021244	30.6	45.4
-3140.79902799	-2362.06842164	30.8	46.5	-3138.47811300	-2360.67133255	29.9	45.6
-3140.81445072	-2362.08384437	21.1	36.3	-3138.49695665	-2360.69017620	18.1	33.3
-2496.10730110	-2362.07103544	29.2	29.5	-2494.55400936	-2360.68255419	22.9	23.2
-2939.96726730	-2362.10861510	5.6	24.5	-2937.85385387	-2360.70965552	5.9	24.8
-2939.95966468	-2362.10101248	10.3	29.1	-2937.84695018	-2360.70275183	10.2	29.0
-2939.94900482	-2362.09035262	17.0	33.4	-2937.84010006	-2360.69590171	14.5	30.9
-2939.98049523	-2362.12184303	-2.7	17.5	-2937.87742763	-2360.73322928	-8.9	11.3
-2939.97994238	-2362.12129018	-2.4	17.1	-2937.87788576	-2360.73368741	-9.2	10.3
-2939.98107215	-2362.12241995	-3.1	15.4	-2937.87946080	-2360.73526245	-10.2	8.3
-2939.95748522	-2362.09883302	11.7	27.5	-2937.84898712	-2360.70478877	9.0	24.7
-2939.98094644	-2362.12229424	-3.0	12.9	-2937.87238035	-2360.72818200	-5.7	10.2
-854.70137435	-2362.08701130	19.1	18.2	-853.67310338	-2360.70290149	10.1	9.2
-3779.77981729	-2362.15021511	-20.5	14.0	-3776.93843114	-2360.75712348	-23.9	10.6
-3779.78739730	-2362.15779512	-25.3	12.1	-3776.94249159	-2360.76118393	-26.4	11.0
-3779.76616804	-2362.13656586	-12.0	20.2	-3776.91061422	-2360.72930656	-6.4	25.7
-3779.76561310	-2362.13601092	-11.6	20.6	-3776.91106822	-2360.72976056	-6.7	25.5
-3779.77265969	-2362.14305751	-16.0	19.7	-3776.91467739	-2360.73336973	-9.0	26.8
-3779.76627667	-2362.13667449	-12.0	23.9	-3776.91130205	-2360.72999439	-6.9	29.1
-3779.77126668	-2362.14166450	-15.2	17.4	-3776.92080997	-2360.73950231	-12.8	19.7
-3779.77952728	-2362.14992510	-20.4	16.4	-3776.92526825	-2360.74396059	-15.6	21.1
-2183.82604476	-2362.04602468	44.8	42.9	-2182.64042804	-2360.65379340	41.0	39.0
-3006.76059970	-2362.06625901	32.1	47.7	-3004.60508706	-2360.66976178	30.9	46.5
-3006.76207419	-2362.06773350	31.2	47.4	-3004.60577282	-2360.67044754	30.5	46.7
-3006.77879693	-2362.08445624	20.7	35.2	-3004.62564132	-2360.69031604	18.0	32.5
-2362.06892991	-2362.06892991	30.5	28.7	-2360.68065789	-2360.68065789	24.1	22.3
-2671.89519110	-2362.10907023	5.3	22.6	-2670.11193861	-2360.71065060	5.3	22.6
-2671.89041125	-2362.10429038	8.3	25.1	-2670.10787206	-2360.70658405	7.8	24.6
-2671.88504031	-2362.09891944	11.7	28.6	-2670.10495203	-2360.70366402	9.7	26.6
-2671.90819225	-2362.12207138	-2.9	13.5	-2670.13593661	-2360.73464860	-9.8	6.6
-2671.90681835	-2362.12069748	-2.0	13.9	-2670.13613432	-2360.73484631	-9.9	6.0
-2671.90851295	-2362.12239208	-3.1	12.7	-2670.13779126	-2360.73650325	-10.9	4.8
-2671.88736165	-2362.10124078	10.2	23.8	-2670.10897233	-2360.70768432	7.1	20.7
-2671.90471497	-2362.11859410	-0.7	14.7	-2670.12656454	-2360.72527653	-3.9	11.5
-720.66376017	-2362.08299845	21.6	19.2	-719.80039546	-2360.69923113	12.4	10.0
-3511.71396340	-2362.15689255	-24.7	8.8	-3509.20191096	-2360.76351364	-27.9	5.6
-3511.71694476	-2362.15987391	-26.6	9.9	-3509.20295397	-2360.76455665	-28.6	8.0
-3511.69234467	-2362.13527382	-11.2	21.9	-3509.16810666	-2360.72970934	-6.7	26.4

-3511.69155879	-2362.13448794	-10.7	22.7	-3509.16667900	-2360.72828168	-5.8	27.6
-3511.69553510	-2362.13846425	-13.2	21.8	-3509.16919391	-2360.73079659	-7.4	27.6
-3511.68920320	-2362.13213235	-9.2	24.6	-3509.16528831	-2360.72689099	-4.9	28.9
-3511.69316069	-2362.13608984	-11.7	21.7	-3509.17341982	-2360.73502250	-10.0	23.4
-3511.69747061	-2362.14039976	-14.4	20.5	-3509.17488747	-2360.73649015	-10.9	24.0
-2411.81534783	-2362.04357197	46.4	44.7	-2410.37482365	-2360.65167567	42.3	40.6
-3234.75354776	-2362.06745129	31.4	48.7	-3232.34181043	-2360.66997181	30.8	48.1
-3234.75626346	-2362.07016699	29.7	46.1	-3232.34296949	-2360.67113087	30.1	46.5
-3234.76414882	-2362.07805235	24.7	39.0	-3232.35365484	-2360.68181622	23.4	37.6
-2590.06082504	-2362.06906926	30.4	30.6	-2588.41694708	-2360.68043374	24.2	24.4
-3127.88785672	-2362.11822428	-0.5	17.6	-3125.59228059	-2360.71796590	0.7	18.7
-3127.88463210	-2362.11499966	1.6	19.6	-3125.59020366	-2360.71588897	2.0	20.1
-3127.87516281	-2362.10553037	7.5	22.2	-3125.58366942	-2360.70935473	6.1	20.8
-3127.90086739	-2362.13123495	-8.6	11.6	-3125.61695965	-2360.74264496	-14.8	5.4
-3127.89971028	-2362.13007784	-7.9	9.6	-3125.61716309	-2360.74284840	-14.9	2.6
-3127.89835685	-2362.12872441	-7.0	10.7	-3125.61725887	-2360.74294418	-15.0	2.8
-3127.88063840	-2362.11100596	4.1	19.9	-3125.59016947	-2360.71585478	2.0	17.8
-3127.89439788	-2362.12476544	-4.6	13.1	-3125.60388559	-2360.72957090	-6.6	11.0
-948.65494511	-2362.08251995	21.9	19.0	-947.53631151	-2360.69842637	12.9	10.0
-3967.70364194	-2362.16305953	-28.6	4.4	-3964.68048915	-2360.76906515	-31.4	1.6
-3967.70820957	-2362.16762716	-31.5	5.7	-3964.68238315	-2360.77095915	-32.6	4.6
-3967.67759485	-2362.13701244	-12.2	19.4	-3964.64230992	-2360.73088592	-7.4	24.3
-3967.67709745	-2362.13651504	-11.9	21.8	-3964.64126905	-2360.72984505	-6.8	27.0
-3967.68169211	-2362.14110970	-14.8	20.2	-3964.64463257	-2360.73320857	-8.9	26.1
-3967.67436652	-2362.13378411	-10.2	23.8	-3964.63937302	-2360.72794902	-5.6	28.5
-3967.68414030	-2362.14355789	-16.4	18.4	-3964.65257835	-2360.74115435	-13.9	20.9
-3967.68260189	-2362.14201948	-15.4	19.3	-3964.64895594	-2360.73753194	-11.6	23.1

Figure 5

-2106.57730947	-2362.02642498	57.1	55.7	-2105.50691500	-2360.63957504	49.9	48.4
-2929.50135186	-2362.03614676	51.0	64.8	-2927.46687234	-2360.65084175	42.8	56.6
-2929.50263869	-2362.03743359	50.2	64.5	-2927.46437544	-2360.64834485	44.4	58.7
-2929.54423314	-2362.07902804	24.1	38.7	-2927.50398092	-2360.68795033	19.5	34.1
-2284.83402203	-2362.06315762	34.1	32.8	-2283.55777781	-2360.67707250	26.3	25.0
-2594.64152253	-2362.08453725	20.7	33.9	-2592.97416006	-2360.69216673	16.9	30.1
-2594.61915451	-2362.06216923	34.7	48.5	-2592.95483229	-2360.67283896	29.0	42.8
-2594.66515284	-2362.10816756	5.9	21.0	-2593.00804461	-2360.72605128	-4.4	10.8
-2594.66403664	-2362.10705136	6.6	21.4	-2593.00786385	-2360.72587052	-4.3	10.6
-2594.66592945	-2362.10894417	5.4	20.2	-2593.00978957	-2360.72779624	-5.5	9.3
-2594.61972596	-2362.06274068	34.4	46.0	-2592.95977277	-2360.67777944	25.9	37.6
-2594.65942893	-2362.10244365	9.4	21.8	-2592.99675033	-2360.71475700	2.7	15.0
-3434.46899737	-2362.14106211	-14.8	16.3	-3432.06952210	-2360.75041947	-19.7	11.4
-3434.45679998	-2362.12886472	-7.1	25.0	-3432.04352414	-2360.72442151	-3.4	28.8
-3434.45653368	-2362.12859842	-7.0	26.5	-3432.04470461	-2360.72560198	-4.1	29.4
-3434.48864004	-2362.16070478	-27.1	5.7	-3432.07690280	-2360.75780017	-24.3	8.5

Figure 8

-4504.24272347	-1874.08139352	0.0	0.0	-4501.00064360	-1873.27289464	0.0	0.0
-2317.86425799	-1874.04187145	24.8	24.6	-2316.51382701	-1873.24108383	20.0	19.7
-4635.77729512	-1874.06626102	9.5	18.3	-4633.07287230	-1873.26369297	5.8	14.6
-4635.77947613	-1874.06735153	8.8	18.1	-4633.07158142	-1873.26304753	6.2	15.5
-4504.24272347	-1874.08139352	0.0	0.0	-4501.00064360	-1873.27289464	0.0	0.0
-2183.82604476	-1874.03992389	26.0	25.3	-2182.64042804	-1873.23914003	21.2	20.4

-4367.70685388	-1874.06730607	8.8	17.7	-4365.33180070	-1873.26461234	5.2	14.1
-4367.70750636	-1874.06763231	8.6	17.3	-4365.32964724	-1873.26353561	5.9	14.5
-4504.24272347	-1874.08139352	0.0	0.0	-4501.00064360	-1873.27289464	0.0	0.0
-2411.81534783	-1874.03747117	27.6	27.1	-2410.37482365	-1873.23702230	22.5	22.0
-4823.69240369	-1874.06832519	8.2	16.4	-4820.80616522	-1873.26528126	4.8	13.0
-4823.69463838	-1874.06944253	7.5	16.9	-4820.80454925	-1873.26447327	5.3	14.7

Figure 9

-2107.32249855	-2107.32249855	0.0	0.0	-2106.23819998	-2106.23819998	0.0	0.0
-2551.15059130	-2107.32820476	-3.6	12.3	-2549.50982555	-2106.23708237	0.7	16.6
-2551.14967990	-2107.32729336	-3.0	14.1	-2549.50919594	-2106.23645276	1.1	18.2
-2107.32249855	-2107.32249855	0.0	0.0	-2106.23819998	-2106.23819998	0.0	0.0
-2417.11868149	-2107.33256062	-6.3	10.2	-2415.64188390	-2106.24059589	-1.5	15.0
-2417.11819512	-2107.33207425	-6.0	10.6	-2415.64149686	-2106.24020885	-1.3	15.4
-2107.32249855	-2107.32249855	0.0	0.0	-2106.23819998	-2106.23819998	0.0	0.0
-2645.11357152	-2107.33569486	-8.3	6.8	-2643.38079020	-2106.24298885	-3.0	12.1
-2645.11408878	-2107.33621212	-8.6	9.1	-2643.38101249	-2106.24321114	-3.1	14.6
-2269.56973253	-2269.56973253	0.0	0.0	-2268.37991415	-2268.37991415	0.0	0.0
-2713.43607990	-2269.61369336	-27.6	-9.7	-2711.69159394	-2268.41885076	-24.4	-6.5
-2713.43607997	-2269.61369343	-27.6	-9.7	-2711.69159394	-2268.41885076	-24.4	-6.5
-2269.56973253	-2269.56973253	0.0	0.0	-2268.37991415	-2268.37991415	0.0	0.0
-2579.40166003	-2269.61553916	-28.7	-12.0	-2577.82151905	-2268.42023104	-25.3	-8.6
-2579.40168939	-2269.61556852	-28.8	-12.0	-2577.82155579	-2268.42026778	-25.3	-8.5
-2269.56973253	-2269.56973253	0.0	0.0	-2268.37991415	-2268.37991415	0.0	0.0
-2807.39508278	-2269.61720612	-29.8	-11.4	-2805.55919117	-2268.42138982	-26.0	-7.6
-2807.39508278	-2269.61720612	-29.8	-11.4	-2805.55919115	-2268.42138980	-26.0	-7.6

Figure 10

-2076.29051321	-2916.06146318	0.0	0.0	-2075.32688262	-2914.36399192	0.0	0.0
-2076.28285776	-2916.05380773	4.8	4.1	-2075.31964647	-2914.35675577	4.5	3.8
-2076.27556408	-2916.04651405	9.4	8.4	-2075.31366831	-2914.35077761	8.3	7.4
-2076.26727150	-2916.03822147	14.6	14.3	-2075.30732176	-2914.34443106	12.3	12.0
-2916.07385107	-2916.07385107	-7.8	7.1	-2914.35852097	-2914.35852097	3.4	18.3
-2916.07390160	-2916.07390160	-7.8	7.1	-2914.35849217	-2914.35849217	3.5	18.4
-2916.07286877	-2916.07286877	-7.2	7.0	-2914.35740160	-2914.35740160	4.1	18.3
-2916.07118284	-2916.07118284	-6.1	8.9	-2914.35564557	-2914.35564557	5.2	20.2
-2916.06922963	-2916.06922963	-4.9	8.9	-2914.35384506	-2914.35384506	6.4	20.1
-2916.06943639	-2916.06943639	-5.0	9.4	-2914.35407459	-2914.35407459	6.2	20.6
-2916.06868455	-2916.06868455	-4.5	9.2	-2914.35286293	-2914.35286293	7.0	20.7
-2916.06846090	-2916.06846090	-4.4	11.0	-2914.35291412	-2914.35291412	7.0	22.3
-2916.08703769	-2916.08703769	-16.0	-1.1	-2914.37310824	-2914.37310824	-5.7	9.2
-2916.08677205	-2916.08677205	-15.9	-0.8	-2914.37272743	-2914.37272743	-5.5	9.6
-2916.08687663	-2916.08687663	-15.9	0.1	-2914.37313173	-2914.37313173	-5.7	10.3
-2916.08687665	-2916.08687665	-15.9	0.1	-2914.37313171	-2914.37313171	-5.7	10.3
-2916.08653577	-2916.08653577	-15.7	0.9	-2914.37241847	-2914.37241847	-5.3	11.3
-2916.08653583	-2916.08653583	-15.7	0.9	-2914.37241842	-2914.37241842	-5.3	11.3

-2916.08243503	-2916.08243503	-13.2	-2.3	-2914.36549210	-2914.36549210	-0.9	9.9
-2916.08255224	-2916.08255224	-13.2	-0.6	-2914.36546478	-2914.36546478	-0.9	11.7
-2916.08172513	-2916.08172513	-12.7	-0.9	-2914.36451660	-2914.36451660	-0.3	11.5
-2916.08227242	-2916.08227242	-13.1	0.3	-2914.36452214	-2914.36452214	-0.3	13.0
-2916.08074477	-2916.08074477	-12.1	1.1	-2914.36378329	-2914.36378329	0.1	13.4
-2916.08078650	-2916.08078650	-12.1	1.3	-2914.36299532	-2914.36299532	0.6	14.1
-2141.98112815	-2981.75207812	0.0	0.0	-2141.08592854	-2980.12303784	0.0	0.0
-2141.97388588	-2981.74483585	4.5	5.6	-2141.07906502	-2980.11617432	4.3	5.3
-2141.96709559	-2981.73804556	8.8	10.4	-2141.07272240	-2980.10983170	8.3	9.9
-2141.95903906	-2981.72998903	13.9	14.9	-2141.06541525	-2980.10252455	12.9	13.9
-2981.76497869	-2981.76497869	-8.1	7.1	-2980.11684251	-2980.11684251	3.9	19.0
-2981.76399367	-2981.76399367	-7.5	7.7	-2980.11562670	-2980.11562670	4.7	19.9
-2981.76389605	-2981.76389605	-7.4	9.2	-2980.11591310	-2980.11591310	4.5	21.1
-2981.76389605	-2981.76389605	-7.4	9.2	-2980.11591304	-2980.11591304	4.5	21.1
-2981.76205927	-2981.76205927	-6.3	9.0	-2980.11443974	-2980.11443974	5.4	20.7
-2981.76254123	-2981.76254123	-6.6	9.3	-2980.11527428	-2980.11527428	4.9	20.7
-2981.76254126	-2981.76254126	-6.6	9.3	-2980.11527430	-2980.11527430	4.9	20.7
-2981.75989836	-2981.75989836	-4.9	10.3	-2980.11241687	-2980.11241687	6.7	21.8
-1986.93873275	-2826.70968272	0.0	0.0	-1985.99257465	-2825.02968395	0.0	0.0
-1986.92991494	-2826.70086491	5.5	6.9	-1985.98386763	-2825.02097693	5.5	6.8
-1986.92140791	-2826.69235788	10.9	11.4	-1985.97570303	-2825.01281233	10.6	11.1
-1986.91153355	-2826.68248352	17.1	17.0	-1985.96623953	-2825.00334883	16.5	16.4
-2826.72076203	-2826.72076203	-7.0	7.1	-2825.02260559	-2825.02260559	4.4	18.5
-2826.71991922	-2826.71991922	-6.4	7.8	-2825.02178040	-2825.02178040	5.0	19.2
-2826.72097467	-2826.72097467	-7.1	8.2	-2825.02275142	-2825.02275142	4.4	19.6
-2826.72047286	-2826.72047286	-6.8	8.5	-2825.02189370	-2825.02189370	4.9	20.2
-2826.71795387	-2826.71795387	-5.2	10.2	-2825.02010098	-2825.02010098	6.0	21.4
-2826.71795411	-2826.71795411	-5.2	10.2	-2825.02010115	-2825.02010115	6.0	21.4
-2826.71643793	-2826.71643793	-4.2	10.6	-2825.01834091	-2825.01834091	7.1	22.0
-2826.71480928	-2826.71480928	-3.2	12.1	-2825.01666444	-2825.01666444	8.2	23.5

E_{sp} …… single point electronic energy in thf (SMD) in hartree with Def2TZVPP
E_{sp} (sum) single point electronic energy in thf (SMD) in hartree with Def2TZVPP after mass balance
ΔE_{sp} … relative single point electronic energy in thf(SMD) in kcal/mol with Def2TZVPP
ΔG_{sp} … relative single point free energy in thf(SMD) in kcal/mol ($\Delta G_{sp} = \Delta E_{sp}$/Def2TZVPP + ΔG_{corr}[level of optimization])

20. Coordinates after optimization with ωB97XD/Def2SVP in THF(SMD)

```
42
B2pin2 / electronic energy: -821.730600906 a.u. / lowest freq: 32.24 cm-1
 H   -3.603963    0.156774    2.351574
 H   -2.641967    1.952160    1.305027
 H   -3.828098   -1.597532    2.177961
 C   -3.894435   -0.635133    1.649322
 O   -1.618685   -0.748124    0.855381
 H   -4.331140    1.951526    0.725984
 C   -3.279144    1.909655    0.409051
 H   -4.943860   -0.479100    1.357330
 B   -0.856260   -0.000012   -0.000003
 H   -3.067634    2.802414   -0.197554
 C   -2.993848   -0.661562    0.424433
 C   -2.993842    0.661563   -0.424434
 O   -1.618679    0.748109   -0.855386
 H   -3.067664   -2.802412    0.197554
 C   -3.279168   -1.909651   -0.409050
 H   -4.331167   -1.951511   -0.725977
 H   -2.641997   -1.952163   -1.305030
 H   -4.943860    0.479131   -1.357323
 C   -3.894433    0.635145   -1.649319
 H   -3.828081    1.597541   -2.177962
 H   -3.603977   -0.156769   -2.351570
 H    3.603967   -0.156765    2.351574
 H    4.331171   -1.951506    0.725981
 H    2.642000   -1.952165    1.305030
 C    3.279173   -1.909650    0.409052
 H    4.943854    0.479132    1.357331
 H    3.067673   -2.802411   -0.197553
 C    3.894426    0.635148    1.649323
 H    3.828073    1.597545    2.177963
 C    2.993840    0.661564    0.424434
 C    2.993851   -0.661562   -0.424432
 O    1.618675    0.748109    0.855382
 H    4.943863   -0.479097   -1.357326
 B    0.856259   -0.000013   -0.000003
 H    3.828102   -1.597529   -2.177960
 C    3.894438   -0.635131   -1.649320
 O    1.618688   -0.748128   -0.855382
 H    4.331140    1.951528   -0.725981
 C    3.279143    1.909656   -0.409051
 H    3.067630    2.802415    0.197554
 H    3.603966    0.156777   -2.351571
 H    2.641969    1.952159   -1.305028
35
tBuO-Bpin / electronic energy: -643.769638430 a.u. / lowest freq: 42.61 cm-1
 H    1.950589    2.581737    1.245788
 H    1.282998    2.573049   -1.114890
 C    2.274938    1.530707    1.221317
 H    3.366790    1.515587    1.085137
 H    2.035833    1.079159    2.192877
 H    2.819476    1.743064   -1.465409
 C    1.758323    1.587017   -1.223856
 O    0.173872    0.730324    0.345211
 C    1.586120    0.805598    0.077611
 H    1.279590    1.071739   -2.070267
 B   -0.273784   -0.458619   -0.181414
 C    1.969903   -0.713473   -0.066962
 H    4.016985   -0.475407   -0.740030
 H    1.470341   -1.171356    2.009916
 H    3.222625   -1.039223    1.696833
 H    2.836380   -0.670187   -2.066266
 C    2.264659   -1.378292    1.276902
 C    3.095618   -0.991696   -1.049127
 O    0.750347   -1.286304   -0.568902
 H    2.318018   -2.467244    1.132369
 H    3.304871   -2.071386   -1.079033
 H   -3.900376   -1.846746    0.185679
 H   -3.892534   -1.136209   -1.449810
 O   -1.561156   -0.836183   -0.327443
 C   -3.912419   -0.899975   -0.375151
 H   -4.853198   -0.375327   -0.151935
 C   -2.710277   -0.040251    0.003450
 H   -2.679818   -0.688402    2.074890
 H   -2.647087    1.023616   -1.890076
 C   -2.714720    0.252090    1.503790
 C   -2.700140    1.251496   -0.814221
 H   -1.848901    0.866578    1.788630
 H   -3.630700    0.791980    1.787079
 H   -1.839124    1.879940   -0.547103
 H   -3.620368    1.826118   -0.630742
15
NaOtBu / electronic energy: -395.117378571 a.u. / lowest freq: 32.67 cm-1
 O   -0.737133   -0.009141    0.003654
 C    0.624960   -0.000675   -0.000009
 C    1.181519   -1.414753   -0.289909
 H    2.284457   -1.455957   -0.304558
 H    0.819613   -2.118024    0.477986
 H    0.809650   -1.764308   -1.267141
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 C    1.175601    0.461725    1.370139
 H    2.278378    0.484748    1.411897
 H    0.800290    1.473434    1.596181
 H    0.814389   -0.215472    2.161532
 C    1.165629    0.961801   -1.084173
 H    0.789122    1.980374   -0.894033
 H    2.268079    1.001909   -1.121930
 H    0.797342    0.647083   -2.074606
Na   -2.786410   -0.000841    0.000833
83
ligand L3a / electronic energy: -2627.35914104 a.u. / lowest freq: 15.38 cm-1
 H    7.765869   -1.234940   -0.969707
 H    2.614901    5.052847   -0.752008
 H    7.149337    1.088242   -0.310777
 C    6.715261   -0.952941   -0.867998
 H   -7.112877   -0.977234    1.654310
 C    6.369636    0.346740   -0.501643
 H    5.966870   -2.912428   -1.395917
 H   -5.265454   -1.558219    3.222556
 H    2.903279    2.737044   -1.564531
 C    2.313544    4.216012   -0.117375
 C    5.708762   -1.890557   -1.107339
 C   -6.100531   -0.609625    1.470189
 H    1.574160    5.478806    1.474358
 C   -5.066468   -0.936710    2.346161
 C    2.484058    2.909962   -0.568535
 C    5.028276    0.708669   -0.365094
 C    1.731304    4.454358    1.128972
 H    4.780774    1.726385   -0.055503
 H   -6.646255    0.458071   -0.328731
 C    4.369947   -1.525297   -0.985196
 C   -5.839064    0.194532    0.359032
 C    4.012603   -0.224278   -0.598619
 C   -3.775072   -0.464140    2.107881
 H    3.591132   -2.269585   -1.178917
 H   -2.966581   -0.725490    2.796941
 H    4.493607   -1.293955    1.992683
 C    2.106968    1.818303    0.231087
 C    1.342001    3.378811    1.924388
 C   -4.547579    0.660227    0.119160
 C   -3.497637    0.330529    0.987952
 C    1.536697    2.068510    1.483788
 P    2.205901    0.144713   -0.519241
 H    0.876704    3.555529    2.896967
 C    3.643788   -0.774224    2.463501
 H   -4.356151    1.286646   -0.755499
 H    3.747533    0.296941    2.243292
 H    3.729671   -0.908098    3.551347
 H   -3.106470   -2.263388    0.096077
 P   -1.724032    0.756409    0.694172
 C    2.335583   -1.296228    1.956163
 H    1.217366    1.235945    2.113681
 C    1.644426   -0.992924    0.803661
 H   -4.288965   -2.482736   -1.198271
 C   -3.259621   -2.722053   -0.887608
 H   -3.200867   -3.816360   -0.771742
 H   -0.237492    1.941190   -1.568903
 C   -1.391341   -0.472707   -0.612127
 C    0.387984   -1.714027    0.697358
 C   -1.824954    2.375496   -0.167672
 S    1.475768   -2.469623    2.888151
 C   -0.575611   -1.529308   -0.413828
 C   -0.937790    2.694486   -1.202922
 H   -2.978476   -0.093072   -2.133891
 H   -3.366893    3.167242    1.136121
 H   -0.809102   -4.410811   -0.587033
 C   -2.676353    3.381544    0.315826
 C    0.168424   -2.559490    1.757471
 C   -2.073708   -0.689594   -1.955375
 C   -2.266585   -2.234677   -1.944777
 C   -0.919128    3.972639   -1.760844
 C   -0.750858   -2.481328   -1.605066
 H   -3.704457   -2.408394   -3.559139
 H   -0.218039    4.198036   -2.568064
 C   -0.285227   -3.909926   -1.414462
 C   -2.659143    4.658404   -0.242172
 H   -0.731090   -4.506375    2.032673
 C   -1.006737   -3.439775    2.043646
 C   -2.723700   -2.827449   -3.282374
 H   -1.788506   -3.283962    1.291361
 C   -1.782034    4.958641   -1.285462
 H   -2.850525   -3.917967   -3.192168
 H    0.794314   -3.948240   -1.198215
 H   -3.336218    5.424982    0.142828
 C   -0.967616   -0.519296   -3.035660
 H   -0.460407   -4.496213   -2.330185
 H   -0.433387    0.432286   -2.925281
 H   -1.769014    5.959433   -1.723508
 C   -0.056422   -1.740966   -2.788767
 H   -1.443886   -3.223325    3.030813
 H   -2.039072   -2.646314   -4.120245
 H   -1.406798   -0.529800   -4.043747
 H    0.970876   -1.456349   -2.523324
 H    0.003775   -2.401285   -3.667013
17
NHCMe2 / electronic energy: -305.693539420 a.u. / lowest freq: 35.85 cm-1
 C   -0.766605    1.222492   -0.000015
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 H   -1.194780    1.714234    0.889170
 C    0.766606    1.222492    0.000015
 H    1.194780    1.714234   -0.889170
 C    0.000000   -1.018377    0.000000
 N   -1.072810   -0.209587    0.000011
 N    1.072810   -0.209588   -0.000011
 H    1.194744    1.714191    0.889241
 H   -1.194744    1.714191   -0.889241
 C   -2.440866   -0.652458    0.000002
 H   -2.457478   -1.749081    0.000023
 H   -2.979571   -0.288634    0.892010
 H   -2.979552   -0.288668   -0.892032
 C    2.440866   -0.652458   -0.000002
 H    2.979551   -0.288668    0.892032
 H    2.457478   -1.749081   -0.000023
 H    2.979572   -0.288634   -0.892010
13
PMe3 / electronic energy: -460.868416109 a.u. / lowest freq: 167.39 cm-1
 P   -0.000338    0.000102   -0.594729
 C    0.584291   -1.525343    0.274538
 H    1.620053   -1.746096   -0.024732
 H    0.546134   -1.418301    1.370846
 H   -0.041774   -2.380912   -0.020763
 C    1.029583    1.268275    0.274512
 H    2.082777    1.155899   -0.024160
 H    0.701219    2.276321   -0.020713
 H    0.959458    1.178298    1.370763
 C   -1.613350    0.256983    0.274797
 H   -2.321224   -0.532226   -0.020573
 H   -1.500738    0.241234    1.371091
 H   -2.043983    1.224754   -0.023911
13
thf / electronic energy: -232.213178364 a.u. / lowest freq: 60.28 cm-1
 C   -0.729532    0.989834   -0.227142
 C    0.729533    0.989833    0.227142
 C   -1.158358   -0.431440    0.131766
 H   -0.791959    1.147286   -1.315596
 H   -1.344762    1.756834    0.263102
 C    1.158358   -0.431441   -0.131767
 H    0.791960    1.147284    1.315597
 H    1.344764    1.756833   -0.263101
 O    0.000000   -1.238426    0.000001
 H   -1.950010   -0.820430   -0.528067
 H   -1.532900   -0.480344    1.171812
 H    1.950011   -0.820432    0.528064
 H    1.532897   -0.480344   -1.171814
24
para-NMe2-styrene / electronic energy: -443.166962707 a.u. / lowest freq: 46.13 cm-1
 C   -1.001621    1.367094    0.000000
 C    0.384629    1.273883   -0.000002
 C   -1.829461    0.234869    0.000002
 C    1.028265    0.013666   -0.000005
 C   -1.188277   -1.015137    0.000005
 C    0.193460   -1.133042    0.000002
 C   -3.292425    0.400175    0.000003
 C   -4.224681   -0.561132   -0.000005
 H    0.630545   -2.131314    0.000007
 H   -1.783119   -1.932381    0.000013
 H    0.968381    2.194269   -0.000004
 H   -1.459369    2.360836   -0.000001
 H   -5.287906   -0.306563   -0.000004
 H   -3.975223   -1.626890   -0.000013
 H   -3.630810    1.443590    0.000010
 H    2.750606   -1.990268   -0.892343
 H    4.110298   -1.276169    0.000013
 C    3.020741   -1.397949    0.000000
 H    2.750584   -1.990260    0.892344
 N    2.395339   -0.095548   -0.000012
 H    3.033100    1.721348   -0.892262
 H    4.271950    0.812102   -0.000021
 C    3.212780    1.095778    0.000005
 H    3.033130    1.721307    0.892307
16
para-H-styrene / electronic energy: -309.327235333 a.u. / lowest freq: 23.45 cm-1
 C    0.512682   -0.226965   -0.000001
 C   -0.409996   -1.284277   -0.000001
 C    0.015494    1.087347    0.000000
 C   -1.354543    1.331056    0.000001
 C   -2.260833    0.267881    0.000000
 C   -1.783088   -1.041654   -0.000001
 H    0.707601    1.932393    0.000000
 H   -1.720740    2.360625    0.000002
 H   -3.335980    0.462131    0.000001
 H   -2.483584   -1.880208   -0.000001
 H   -0.041395   -2.313890   -0.000002
 C    1.957762   -0.536594   -0.000001
 C    2.966585    0.340887    0.000002
 H    2.197140   -1.606375   -0.000004
 H    2.808763    1.423612    0.000005
 H    4.003818   -0.004370    0.000001
22
para-CO2Me-styrene / electronic energy: -536.972466017 a.u. / lowest freq: 36.27 cm-1
 C   -2.177029   -0.273944   -0.000002
 C   -1.288457   -1.360405   -0.000006
 C   -1.638856    1.024705    0.000001
 C   -0.265795    1.223967    0.000001
 C    0.611262    0.131581   -0.000002
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 C    0.088912   -1.165460   -0.000005
 H   -2.301589    1.892476    0.000003
 H    0.147069    2.234463    0.000003
 C    2.078496    0.403327   -0.000003
 H    0.763300   -2.022664   -0.000007
 H   -1.688181   -2.377645   -0.000009
 C   -3.629628   -0.539756   -0.000003
 C   -4.608155    0.371151    0.000010
 H   -3.902499   -1.601050   -0.000014
 H   -4.416278    1.448163    0.000022
 H   -5.656147    0.060285    0.000008
 O    2.563111    1.509790   -0.000011
 O    2.807344   -0.712177    0.000008
 C    4.219407   -0.553732    0.000008
 H    4.642711   -1.564424    0.000021
 H    4.553514   -0.009542    0.895244
 H    4.553517   -0.009561   -0.895238
21
allylphosphate / electronic energy: -838.811918777 a.u. / lowest freq: 44.19 cm-1
 C   -4.228065   -0.213625   -0.450712
 C   -3.126548   -0.470342    0.252592
 C   -1.864256    0.322400    0.141664
 O   -0.783039   -0.563443   -0.176535
 P    0.707286   -0.141276    0.217233
 O    0.970662    0.121311    1.650298
 O    1.460311   -1.365735   -0.468955
 O    1.061740    1.104182   -0.737886
 C    2.879635   -1.448876   -0.389717
 C    1.322758    2.400172   -0.210050
 H   -5.142764   -0.796179   -0.309890
 H   -4.259343    0.593594   -1.190453
 H   -3.110287   -1.285179    0.985530
 H   -1.947579    1.092560   -0.642170
 H   -1.655843    0.823591    1.102977
 H    1.710475    3.008958   -1.036651
 H    2.070246    2.360904    0.595111
 H    0.403000    2.866284    0.175408
 H    3.173659   -2.389342   -0.871246
 H    3.217914   -1.455776    0.657446
 H    3.352692   -0.609183   -0.922604
15
PMe3-Cu-H / electronic energy: -2101.82973385 a.u. / lowest freq: 97.88 cm-1
 H   -1.104721    2.225261   -0.852565
 H   -1.093050    1.368789    1.951436
 C   -1.425922    1.209357   -1.126228
 C   -1.415982    0.373096    1.612246
 H   -2.524071    1.151181   -1.073457
 H   -1.103202    1.014093   -2.159812
 H   -2.514845    0.353775    1.545124
 H   -1.085574   -0.366086    2.356940
 P   -0.639847   -0.000027   -0.001647
 C   -1.420666   -1.584277   -0.479814
 H   -2.519328   -1.515999   -0.452390
 H   -1.101926   -1.859866   -1.496268
 H   -1.090664   -2.375237    0.209827
Cu    1.591472    0.000552   -0.001554
 H    3.157819   -0.000576    0.003704
19
NHCMe2-Cu-H / electronic energy: -1946.68467112 a.u. / lowest freq: 61.43 cm-1
Cu   -1.869884   -0.000005    0.000000
 H   -3.434689    0.000004    0.000023
 H    0.766219   -2.982321    0.893811
 H    2.777359   -1.194948    0.890330
 C    0.405973   -2.446840   -0.000004
 H   -0.692131   -2.453571   -0.000001
 H    2.777351    1.194965    0.890332
 N    0.862080   -1.081548   -0.000001
 C    2.289525   -0.767453    0.000002
 H    0.766213   -2.982315   -0.893826
 C    0.076079   -0.000001   -0.000001
 C    2.289519    0.767469    0.000004
 H    0.766207    2.982332    0.893799
 H    2.777362   -1.194946   -0.890324
 N    0.862071    1.081552    0.000004
 C    0.405953    2.446841   -0.000006
 H    2.777352    1.194968   -0.890323
 H   -0.692152    2.453561    0.000013
 H    0.766175    2.982311   -0.893837
26
para-NMe2-styrene-Cu-H / electronic energy: -2084.11501069 a.u. / lowest freq: 54.80 cm-1
Cu    2.999355   -0.200226   -0.784375
 H    3.390503   -0.553581   -2.255182
 H   -1.680785   -2.065887    0.489478
 C   -1.285578   -1.051929    0.438423
 H    0.669238   -1.726373    0.949773
 C    0.058923   -0.853889    0.703441
 C   -2.135974    0.033861    0.101829
 H    2.767965   -1.270333    1.561962
 C   -1.544589    1.320062    0.048408
 C    0.644926    0.422769    0.652207
 C    3.016212   -0.233340    1.313107
 H   -2.142215    2.194676   -0.206600
 C   -0.194256    1.495109    0.314010
 C    2.073169    0.671820    0.904129
 H    0.226432    2.503063    0.256107
 H    2.372759    1.725344    0.838707
 H    4.015062    0.111062    1.595736
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 H   -3.945377    1.450017   -1.465372
 H   -5.321099    0.620744   -0.704579
 C   -4.295008    0.967264   -0.535689
 H   -4.326805    1.737147    0.254466
 H   -3.576612   -2.154572   -0.875995
 N   -3.465134   -0.155951   -0.160897
 H   -5.105988   -1.429174   -0.331347
 C   -4.031155   -1.486017   -0.123291
 H   -3.908464   -1.958205    0.866568
18
para-H-styrene-Cu-H / electronic energy: -1950.27347322 a.u. / lowest freq: 32.14 cm-1
Cu    2.028179   -0.305190   -0.495135
 H    2.754416   -1.205888   -1.547483
 H   -2.465572   -2.384578    0.628580
 C   -2.229727   -1.348873    0.373629
 H   -0.187384   -1.522477    1.021800
 H   -4.213626   -0.913226   -0.365976
 C   -0.946915   -0.859504    0.599853
 C   -3.207963   -0.525491   -0.187817
 H    1.458986   -0.291086    2.040851
 C   -2.892328    0.789499   -0.527405
 C   -0.619222    0.465804    0.269134
 C    1.663136    0.554436    1.375717
 H   -3.650810    1.439378   -0.969886
 C   -1.605787    1.278422   -0.307310
 C    0.730962    1.029030    0.495676
 H   -1.361356    2.309237   -0.576875
 H    0.923428    1.989718    0.002777
 H    2.571781    1.129505    1.576274
24
para-CO2Me-styrene-Cu-H / electronic energy: -2177.91838845 a.u. / lowest freq: 43.01 cm-1
Cu    3.335163   -0.143092   -0.820022
 H    3.787606   -0.552242   -2.258376
 H   -1.275705   -2.172070    0.499056
 C   -0.885854   -1.153198    0.465705
 H    1.129434   -1.749438    0.880268
 C    0.461958   -0.908180    0.683380
 C   -1.765161   -0.097257    0.196181
 H    3.142717   -1.191536    1.549225
 C   -1.273412    1.210560    0.146107
 C    0.965853    0.403176    0.640182
 C    3.361484   -0.153917    1.278133
 H   -1.950576    2.038580   -0.066274
 C    0.078691    1.453563    0.364021
 C    2.395498    0.716998    0.856725
 H    0.457183    2.477650    0.319929
 H    2.654601    1.778940    0.771682
 H    4.355868    0.220045    1.537928
 H   -5.760531    1.446488   -0.690765
 C   -5.326819    0.455543   -0.514822
 H   -5.800336   -0.007852    0.362848
 H   -5.492971   -0.186544   -1.391846
 O   -3.938039    0.661363   -0.292397
 C   -3.205491   -0.419598   -0.032247
 O   -3.662896   -1.536174    0.013244
98
Figure 1_L-Cu-OtBu / electronic energy: -4500.61984018 a.u. / lowest freq: -20.29 cm-1
 P   -1.580542    0.896725    0.507317
 C   -2.908207    3.157185   -0.383641
 C   -4.006725    3.985801   -0.616704
 C   -3.065934    1.952882    0.310453
 C   -5.267815    3.615698   -0.152099
 C   -4.334988    1.587341    0.777167
 C   -5.430677    2.415956    0.544998
 C   -2.523549   -1.468960    3.766793
 C   -2.433956   -0.995007    2.458931
 C   -1.750721    0.195213    2.185586
 C   -1.940215   -0.754291    4.813269
 C   -1.270557    0.441252    4.550950
 C   -1.173132    0.911691    3.242472
 C   -2.488216   -0.166613   -2.032914
 C   -1.872393   -0.448550   -0.671022
 C   -1.299140   -1.669779   -0.734533
 C   -1.272709    0.069693   -2.972172
 C   -0.635837   -1.334154   -3.044849
 C   -1.568682   -2.215154   -2.148736
 C   -1.395589   -3.700880   -2.383493
 C   -2.968758   -1.580997   -2.446504
 C   -3.416732   -1.695439   -3.906676
 C   -4.117793   -2.103832   -1.580032
 C   -0.402948   -2.359373    0.224528
 C   -0.776860   -3.505808    0.883773
 C    0.975407   -1.984659    0.502411
 S    0.536953   -4.140203    1.811096
 C    1.617684   -2.882805    1.327412
 C   -2.109087   -4.184545    0.927504
 C    3.027464   -2.915300    1.833201
 P    1.678909   -0.407382   -0.087965
 C    3.102106    0.859929    3.522479
 C    2.302495    0.358977    2.498979
 C    4.452175    1.127830    3.286856
 C    2.843742    0.105397    1.231146
 C    4.993844    0.884481    2.025620
 C    4.195075    0.374971    1.000685
 C    3.810868    0.068843   -3.514968
 C    3.023741    0.281283   -2.383591
 C    4.288299   -1.209367   -3.809490
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 C    2.730665   -0.792862   -1.528752
 C    3.979451   -2.281011   -2.970507
 C    3.204103   -2.074442   -1.829949
 H   -1.915778    3.440512   -0.746059
 H   -3.873260    4.924573   -1.159108
 H   -6.129053    4.263617   -0.331942
 H   -4.472168    0.649243    1.321329
 H   -6.418530    2.124936    0.910059
 H   -3.052633   -2.403325    3.968939
 H   -2.893523   -1.557737    1.644298
 H   -2.009117   -1.130195    5.836777
 H   -0.813928    1.005846    5.367081
 H   -0.634680    1.841763    3.037295
 H   -3.246522    0.627518   -2.056758
 H   -0.589719    0.827995   -2.558260
 H   -1.599587    0.429651   -3.958197
 H    0.397965   -1.358219   -2.675070
 H   -0.612264   -1.725800   -4.072823
 H   -1.570304   -3.939191   -3.444195
 H   -2.092416   -4.304994   -1.785566
 H   -0.372211   -4.024525   -2.136174
 H   -4.283813   -1.039932   -4.086553
 H   -3.735264   -2.726536   -4.127997
 H   -2.643849   -1.427048   -4.637860
 H   -5.049987   -1.574746   -1.833824
 H   -3.945257   -1.962235   -0.505502
 H   -4.291685   -3.176350   -1.763069
 H   -2.830286   -3.652783    0.295310
 H   -2.511139   -4.201379    1.953149
 H   -2.051970   -5.227314    0.578596
 H    3.133815   -2.345375    2.769850
 H    3.720647   -2.481976    1.101170
 H    3.345945   -3.948938    2.031729
 H    2.665823    1.045999    4.506885
 H    1.245355    0.156678    2.688849
 H    5.080940    1.527152    4.086046
 H    6.049214    1.091790    1.833772
 H    4.633959    0.190791    0.017398
 H    4.040865    0.905396   -4.179302
 H    2.611508    1.276687   -2.160485
 H    4.894279   -1.374226   -4.703735
 H    4.343260   -3.284201   -3.205138
 H    2.955927   -2.917868   -1.180520
Cu    0.417430    1.531952   -0.315265
 H    1.533422    5.234717   -2.570756
 H    2.752520    5.897866   -1.444814
 H    3.117535    4.440494   -2.410028
 C    2.325100    4.966405   -1.852792
 H   -0.149226    5.110504   -0.667688
 C    1.752337    4.045194   -0.761300
 H    1.046191    5.717534    0.511698
 O    1.233972    2.914790   -1.363084
 C    0.662151    4.810177    0.015323
 H    3.662168    3.098170   -0.312532
 H    3.360480    4.550221    0.683303
 C    2.883951    3.670816    0.217078
 H    0.224040    4.154997    0.787863
 H    2.491679    3.029307    1.024769
140
Figure 1_ed / electronic energy: -5322.37772681 a.u. / lowest freq: 19.05 cm-1
 P   -1.547195    1.304450    1.048267
 C   -0.430925    3.863086    1.043101
 C   -0.447728    5.254931    1.170371
 C   -1.605414    3.127758    1.213465
 C   -1.638136    5.915613    1.458426
 C   -2.803828    3.800895    1.499630
 C   -2.820605    5.186125    1.619324
 C   -3.327289   -1.020465    3.954702
 C   -2.866831   -0.544656    2.728353
 C   -2.331137    0.744996    2.616052
 C   -3.248114   -0.220419    5.094159
 C   -2.704538    1.059339    4.995362
 C   -2.246958    1.538789    3.768678
 C   -2.930174    2.064722   -1.375651
 C   -2.704765    0.986821   -0.321920
 C   -3.153769   -0.174768   -0.845093
 C   -1.872684    1.752088   -2.460597
 C   -2.391709    0.428171   -3.057153
 C   -3.704160    0.152177   -2.250564
 C   -4.620533   -0.847906   -2.924612
 C   -4.248285    1.600403   -2.033048
 C   -4.601040    2.340702   -3.326353
 C   -5.454326    1.719931   -1.098426
 C   -3.065595   -1.592398   -0.417185
 C   -4.206747   -2.292385   -0.098851
 C   -1.886669   -2.445210   -0.475491
 S   -3.876353   -3.978551    0.046720
 C   -2.198597   -3.780239   -0.303250
 C   -5.581148   -1.779939    0.189394
 C   -1.354435   -5.015900   -0.388730
 P   -0.156384   -1.818798   -0.539295
 C    0.786081   -3.997748    2.788146
 C    0.224185   -3.100075    1.885184
 C    1.843183   -4.818463    2.391163
 C    0.692114   -3.022515    0.568671
 C    2.329895   -4.727784    1.088545
 C    1.761725   -3.831389    0.182943
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C	2.251664	-2.253905	-3.818461
C	1.764904	-1.947318	-2.548781
C	1.412257	-2.814807	-4.782712
C	0.432547	-2.241159	-2.221731
C	0.081201	-3.085013	-4.468056
C	-0.404769	-2.807779	-3.189824
H	0.505688	3.354401	0.801614
H	0.478902	5.818745	1.041500
H	-1.650640	7.003555	1.559186
H	-3.731113	3.235218	1.626678
H	-3.758070	5.702154	1.839069
H	-3.744796	-2.028268	4.016609
H	-2.919218	-1.196081	1.856834
H	-3.605017	-0.595048	6.056308
H	-2.629216	1.693641	5.881653
H	-1.808824	2.537227	3.721107
H	-2.915281	3.099843	-1.016079
H	-0.872090	1.647907	-2.021689
H	-1.832472	2.556856	-3.207990
H	-1.678260	-0.399080	-2.942625
H	-2.609442	0.514469	-4.132078
H	-4.856840	-0.508497	-3.945321
H	-5.571482	-0.976151	-2.388629
H	-4.144513	-1.836877	-3.010063
H	-4.752597	3.412167	-3.119371
H	-5.543999	1.952685	-3.743289
H	-3.839030	2.260843	-4.112041
H	-5.724791	2.780512	-0.974141
H	-5.265236	1.312766	-0.096885
H	-6.333802	1.207036	-1.519651
H	-5.660840	-0.719198	-0.072302
H	-5.810520	-1.870380	1.263919
H	-6.356415	-2.333312	-0.362050
H	-0.889560	-5.263941	0.577842
H	-0.551382	-4.893664	-1.126611
H	-1.966287	-5.876247	-0.697484
H	0.397982	-4.054218	3.807976
H	-0.601473	-2.460661	2.208461
H	2.285921	-5.525136	3.097118
H	3.159189	-5.363259	0.768616
H	2.151121	-3.785790	-0.835087
H	3.296709	-2.042638	-4.058898
H	2.416565	-1.480774	-1.802398
H	1.796485	-3.040175	-5.780635
H	-0.584895	-3.519837	-5.217116
H	-1.446131	-3.034108	-2.949453
H	0.670018	2.071794	2.804974
H	2.426314	2.368961	2.686458
O	1.929360	-0.152095	1.878567
C	1.646371	1.839205	3.251615
H	1.642346	2.217713	4.285739
C	1.900954	0.329626	3.221723
H	-0.171351	-0.315763	3.355895
H	4.035711	0.585794	3.568264
C	0.761772	-0.407283	3.924490
C	3.198095	0.007016	3.969096
H	0.999276	-1.475299	4.025996
H	0.592182	0.006383	4.930600
H	3.428380	-1.065543	3.882133
H	3.080786	0.239712	5.039683
Cu	0.396616	0.248269	0.480918
H	4.501374	3.509594	-2.264572
H	3.875068	2.057661	-4.250465
H	4.247900	1.268416	-2.700795
C	3.475891	1.397803	-3.466780
H	3.509620	4.444103	-3.416382
H	3.279512	0.413394	-3.914115
C	3.570788	4.079501	-2.379538
H	3.629261	4.955346	-1.715965
C	2.344141	3.249510	-2.026478
C	2.170370	1.943345	-2.886748
O	2.499468	2.733692	-0.694623
H	1.558092	2.729927	-4.806307
B	2.084067	1.415139	-0.633221
H	1.025361	1.061262	-4.484426
C	1.171259	2.052745	-4.029472
O	1.707269	1.000998	-1.907429
H	0.957349	4.619401	-3.015866
C	1.106256	4.143888	-2.035167
H	1.232112	4.939196	-1.286328
H	0.196373	2.425560	-3.708565
H	0.198683	3.581199	-1.776755
H	5.880284	-0.149264	2.751331
H	4.404211	-1.786359	2.188543
H	6.407634	1.480767	2.283518
C	6.206763	0.466673	1.904829
O	3.954429	1.060867	1.290203
H	5.986517	-2.215060	1.470182
C	4.926592	-2.013870	1.251054
H	7.155645	0.054007	1.526583
B	2.806496	0.342354	0.769922
H	4.481637	-2.932124	0.842471
C	5.163405	0.533333	0.788888
C	4.744587	-0.887302	0.229029
O	3.367225	-0.737028	-0.036971
H	5.827248	2.482376	0.163325
C	5.690538	1.487359	-0.286037

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 H     6.651682    1.162381   -0.711767
 H     4.960765    1.597588   -1.093068
 H     6.545622   -1.327315   -0.927257
 C     5.453794   -1.280566   -1.064987
 H     5.113536   -2.277053   -1.388253
 H     5.232620   -0.573918   -1.875807
140
Figure 1_ts(TB)_01 / electronic energy: -5322.37787478 a.u. / lowest freq: -98.49 cm-1
 P     0.567604    1.984871    0.215083
 C     0.435192    1.076768    2.845831
 C     0.533084    1.174687    4.232885
 C     0.608943    2.207356    2.040187
 C     0.778821    2.410890    4.828906
 C     0.855456    3.445804    2.644560
 C     0.933434    3.546988    4.032706
 C    -1.745129    5.281135   -0.474281
 C    -1.251737    4.066706   -0.005659
 C     0.031414    3.634756   -0.373198
 C    -0.969942    6.072925   -1.324363
 C     0.300893    5.643259   -1.701722
 C     0.801212    4.429185   -1.226817
 C     3.450211    2.721609    0.390540
 C     2.329997    1.861609   -0.177371
 C     2.907629    0.827083   -0.822291
 C     4.042097    1.885200    1.560290
 C     4.711477    0.708484    0.819769
 C     4.428185    1.000925   -0.689275
 C     5.292578    0.198577   -1.638783
 C     4.546577    2.565109   -0.704750
 C     5.919695    3.109422   -0.295648
 C     4.207040    3.210339   -2.048434
 C     2.234308   -0.312926   -1.491920
 C     1.981190   -0.300871   -2.843310
 C     1.786218   -1.533822   -0.847454
 S     1.178436   -1.749737   -3.321705
 C     1.191422   -2.410382   -1.731711
 C     2.294367    0.760062   -3.853094
 C     0.598031   -3.763424   -1.500443
 P     2.127293   -1.810926    0.928221
 C     0.132824   -5.079367    2.540473
 C     1.138694   -4.279031    1.998561
 C    -1.178722   -4.608725    2.615071
 C     0.845798   -2.996975    1.513865
 C    -1.477385   -3.333289    2.137595
 C    -0.474826   -2.536043    1.591249
 C     5.534292   -3.744516    2.131089
 C     4.351887   -3.008857    2.086933
 C     6.051019   -4.306626    0.962554
 C     3.654401   -2.842932    0.880377
 C     5.375185   -4.133853   -0.244544
 C     4.182638   -3.409320   -0.285457
 H     0.214525    0.112080    2.386871
 H     0.404154    0.280641    4.846841
 H     0.846527    2.492240    5.916339
 H     0.983203    4.341632    2.032142
 H     1.118866    4.518830    4.496035
 H    -2.747796    5.604444   -0.184381
 H    -1.879573    3.433771    0.628122
 H    -1.361202    7.022417   -1.697535
 H     0.912679    6.255269   -2.368677
 H     1.796117    4.102791   -1.530150
 H     3.171766    3.750735    0.657928
 H     3.257220    1.555157    2.253406
 H     4.764464    2.476176    2.141455
 H     4.304668   -0.264056    1.116814
 H     5.796990    0.665245    0.992135
 H     6.359281    0.400759   -1.455668
 H     5.079426    0.430771   -2.692740
 H     5.131680   -0.881072   -1.493351
 H     5.858584    4.200647   -0.155321
 H     6.656528    2.925890   -1.093477
 H     6.326754    2.682758    0.629205
 H     4.198755    4.307955   -1.953713
 H     3.236923    2.895259   -2.445299
 H     4.971395    2.955684   -2.799448
 H     3.378130    0.933573   -3.928317
 H     1.820323    1.714999   -3.585294
 H     1.934847    0.480317   -4.853216
 H    -0.372824   -3.657665   -0.995784
 H     1.252646   -4.384727   -0.874041
 H     0.435860   -4.290738   -2.451516
 H     0.378935   -6.079106    2.907195
 H     2.157493   -4.669173    1.945566
 H    -1.964151   -5.236188    3.043719
 H    -2.489373   -2.927519    2.182806
 H    -0.754852   -1.552703    1.202174
 H     6.060534   -3.870045    3.080333
 H     3.963277   -2.554443    3.003476
 H     6.984926   -4.872953    0.992903
 H     5.777255   -4.566314   -1.163974
 H     3.664160   -3.278984   -1.238105
 H    -1.294299    2.635864   -4.292559
 H    -3.384493    1.283643   -5.014995
 H    -0.435815    1.071131   -4.228817
 C    -1.043978    1.779170   -3.648949
 H    -3.446966    2.931406   -3.000928
 H    -2.460236   -0.232700   -4.853686
```

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 C   -3.084413    0.492945   -4.309961
 H   -0.441116    2.146468   -2.804475
 C   -2.305172    1.092625   -3.139672
 H   -3.987996   -0.015152   -3.948497
 C   -3.166580    2.082980   -2.357866
 H   -2.610601    2.473482   -1.495614
 H   -4.077610    1.602308   -1.979864
 H   -2.966397   -2.324673   -3.761776
 H   -5.254782   -2.081807   -3.555303
 O   -1.842330    0.026632   -2.294899
 H   -6.483714   -1.667950   -2.339369
 H   -3.656253   -3.964148   -3.594404
 C   -2.944805   -3.244928   -3.161673
 C   -5.617962   -2.315598   -2.545663
 O   -4.053880   -0.754412   -1.613169
 B   -2.660131   -0.766657   -1.437490
 H   -5.966400   -3.360126   -2.532963
Cu   -1.026678    0.464282   -0.354427
 C   -4.544610   -2.090379   -1.488862
 O   -2.227137   -2.087732   -1.195677
 C   -3.244118   -2.955137   -1.687830
 H   -5.925429   -1.488523    0.037636
 B   -2.703175    0.331249    0.831966
 C   -5.146123   -2.252966   -0.097997
 O   -3.377438    1.534487    1.015534
 C   -3.237277   -4.258945   -0.902687
 H   -4.082852   -4.897468   -1.202744
 H   -5.610783   -3.240744    0.038228
 H   -4.380493   -2.100784    0.673785
 H   -3.297324   -4.080625    0.177373
 O   -2.957981   -0.494183    1.914664
 C   -3.913422    1.630029    2.340679
 H   -5.316183    3.175776    1.808900
 H   -5.965398    1.538664    1.592388
 C   -5.338151    2.164046    2.240790
 H   -5.670200   -0.542146    1.996150
 C   -3.795816    0.146806    2.887966
 C   -5.129419   -0.593779    2.947267
 H   -4.947820   -1.654565    3.176483
 H   -5.812130    2.228457    3.231782
 C   -3.106952    0.022631    4.243119
 H   -3.021956   -1.041101    4.511898
 H   -5.776252   -0.181749    3.735777
 H   -3.682611    0.528349    5.032880
 H   -1.934133   -3.671833   -3.239881
 H   -2.309256   -4.816302   -1.100496
 H   -3.121756    3.619837    2.622647
 C   -3.055428    2.635704    3.110549
 H   -3.398548    2.752927    4.148882
 H   -1.998172    2.338012    3.123185
 H   -2.094743    0.444130    4.222265
140
Figure 1_ts(TB)_02 / electronic energy: -5322.36659501 a.u. / lowest freq: -95.28 cm-1
 P    0.265119   -1.141472    1.346455
 C   -1.418511    0.443284    2.852114
 C   -2.148263    0.844838    3.967495
 C   -0.515889   -0.622615    2.929029
 C   -1.974132    0.183491    5.183475
 C   -0.353508   -1.288355    4.148938
 C   -1.076881   -0.881367    5.270438
 C    3.649260   -2.655958    3.085660
 C    2.552010   -1.859938    2.769974
 C    1.594447   -2.300325    1.845434
 C    3.817631   -3.895628    2.466935
 C    2.883402   -4.329755    1.528664
 C    1.780102   -3.535022    1.215620
 C   -1.590692   -3.464309    1.255935
 C   -1.056396   -2.168162    0.659709
 C   -1.881238   -1.821989   -0.350270
 C   -2.915743   -3.079548    1.972755
 C   -3.851097   -2.740147    0.792356
 C   -2.943889   -2.929004   -0.463384
 C   -3.679124   -3.009832   -1.784419
 C   -2.108692   -4.185293   -0.020824
 C   -2.942680   -5.439445    0.263104
 C   -1.018717   -4.603969   -1.008546
 C   -1.828097   -0.628695   -1.234640
 C   -0.932095   -0.571361   -2.277243
 C   -2.718232    0.522732   -1.198499
 S   -1.173953    0.857055   -3.214717
 C   -2.479088    1.407300   -2.231098
 C    0.116816   -1.556938   -2.683413
 C   -3.144693    2.702665   -2.585829
 P   -3.967278    0.716929    0.129864
 C   -5.485755    4.576395    0.380156
 C   -5.375571    3.209973    0.119932
 C   -4.390692    5.294115    0.859302
 C   -4.165653    2.538518    0.334921
 C   -3.183072    4.632651    1.085501
 C   -3.076164    3.266543    0.834502
 C   -7.850503   -0.475854   -0.373693
 C   -6.623496   -0.079533    0.155871
 C   -8.011132   -0.584887   -1.755406
 C   -5.545473    0.230966   -0.686211
 C   -6.941626   -0.291831   -2.601337
 C   -5.717081    0.114797   -2.070686
 H   -1.575327    0.943527    1.895232
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 H   -2.857098    1.671990    3.882207
 H   -2.540993    0.494982    6.063991
 H    0.330824   -2.135269    4.230743
 H   -0.941832   -1.406771    6.218730
 H    4.384457   -2.300271    3.810976
 H    2.442921   -0.881296    3.244901
 H    4.681595   -4.517926    2.711539
 H    3.012537   -5.292830    1.029335
 H    1.068067   -3.882345    0.466270
 H   -0.886842   -4.026278    1.884524
 H   -2.767986   -2.229179    2.652064
 H   -3.293187   -3.917885    2.575827
 H   -4.243946   -1.720354    0.853989
 H   -4.716692   -3.416277    0.732628
 H   -4.370634   -3.866853   -1.793971
 H   -2.980766   -3.121992   -2.628378
 H   -4.275966   -2.103675   -1.962214
 H   -2.298868   -6.220487    0.698117
 H   -3.356312   -5.844878   -0.673832
 H   -3.780798   -5.285059    0.953346
 H   -0.423224   -5.430210   -0.588917
 H   -0.332678   -3.791583   -1.268213
 H   -1.468130   -4.973676   -1.943897
 H   -0.304817   -2.366597   -3.301169
 H    0.580103   -2.004891   -1.794310
 H    0.921846   -1.063449   -3.240397
 H   -2.776675    3.530424   -1.959707
 H   -4.231449    2.641671   -2.443722
 H   -2.953310    2.965440   -3.636137
 H   -6.436974    5.083462    0.201021
 H   -6.242073    2.670708   -0.268889
 H   -4.478660    6.364584    1.058684
 H   -2.317246    5.181049    1.464646
 H   -2.120813    2.769813    1.014459
 H   -8.680359   -0.712329    0.296456
 H   -6.499453   -0.011155    1.240903
 H   -8.968305   -0.906157   -2.172905
 H   -7.058951   -0.383418   -3.683701
 H   -4.884049    0.329665   -2.743898
 H   -0.586704    4.659723   -0.561602
 H   -0.015254    4.002658    1.841903
 H   -0.624272    2.916309   -0.954726
 C    0.021393    3.804563   -0.892861
 H    1.578038    5.632708    0.439176
 H    0.041645    2.271329    1.404636
 C    0.631477    3.197853    1.459704
 H    0.406627    4.014214   -1.902085
 C    1.172387    3.531743    0.070471
 H    1.451567    3.028673    2.169710
 C    2.121379    4.725785    0.131926
 H    2.580236    4.911053   -0.850423
 H    2.919291    4.544027    0.864906
 H    4.769064    3.852190    2.465075
 H    4.946253    4.485367    0.356533
 O    1.833638    2.385223   -0.474333
 H    5.992096    4.093910   -1.021113
 H    6.244451    2.902395    2.792015
 C    5.156214    2.839487    2.639479
 C    5.763799    3.833850    0.023470
 O    4.281692    2.164574   -0.807062
 B    3.105420    1.873018   -0.078955
 H    6.653940    4.051751    0.632299
Cu    1.508076    0.234996    0.026254
 C    5.380243    2.353502    0.083271
 O    3.406489    1.918790    1.300853
 C    4.813177    1.892329    1.493531
 H    6.934782    1.897437   -1.353101
 B    3.169156   -0.159690   -1.163006
 C    6.570108    1.522538   -0.384435
 O    2.979632   -0.122150   -2.540219
 C    5.217514    0.469887    1.888411
 H    6.298155    0.389972    2.078699
 H    7.401618    1.592315    0.333455
 H    6.288614    0.470256   -0.502420
 H    4.936203   -0.258451    1.116538
 O    4.231789   -1.012885   -0.876813
 C    4.056419   -0.803365   -3.197485
 H    4.560929    0.975801   -4.295744
 H    5.431465    0.820561   -2.759985
 C    5.064729    0.260106   -3.629198
 H    6.657679   -1.042398   -2.019164
 C    4.589095   -1.739896   -2.059747
 C    6.090990   -1.979886   -2.080228
 H    6.379668   -2.607813   -1.223612
 H    5.917022   -0.175705   -4.171429
 C    3.853208   -3.079794   -1.994442
 H    4.119274   -3.583762   -1.054041
 H    6.387955   -2.504729   -3.001371
 H    4.123174   -3.740680   -2.831462
 H    4.706188    2.465031    3.571451
 H    4.694288    0.207458    2.819507
 H    3.134280   -0.806703   -5.149624
 C    3.523805   -1.534941   -4.422066
 H    4.327677   -2.105256   -4.913254
 H    2.711580   -2.229463   -4.171420
 H    2.762793   -2.932699   -1.998677
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Figure 1_ts(TB)_03 / electronic energy: -5322.37581050 a.u. / lowest freq: -110.98 cm-1

P	-1.491735	1.190092	1.171624
C	-0.294720	3.700702	1.414231
C	-0.264164	5.072734	1.680008
C	-1.491329	2.990162	1.528115
C	-1.428037	5.740087	2.050084
C	-2.662466	3.669578	1.899142
C	-2.631858	5.036064	2.156057
C	-3.468256	-1.311322	3.796501
C	-2.971186	-0.731966	2.630081
C	-2.328522	0.511921	2.664885
C	-3.322468	-0.662281	5.021739
C	-2.678353	0.573361	5.068709
C	-2.183244	1.155339	3.902702
C	-2.807844	2.260281	-1.176845
C	-2.636910	1.068048	-0.241382
C	-3.136144	-0.010025	-0.884665
C	-1.763837	2.022707	-2.294947
C	-2.332448	0.787385	-3.020688
C	-3.660493	0.485986	-2.248951
C	-4.611337	-0.397767	-3.029875
C	-4.143175	1.925359	-1.879351
C	-4.462969	2.808819	-3.089254
C	-5.347627	1.996580	-0.936923
C	-3.111139	-1.465967	-0.606107
C	-4.278054	-2.158730	-0.378635
C	-1.957188	-2.342140	-0.729901
S	-3.997927	-3.861182	-0.400813
C	-2.307379	-3.677508	-0.699384
C	-5.639565	-1.632228	-0.054924
C	-1.489059	-4.918393	-0.889530
P	-0.214963	-1.749560	-0.696263
C	0.539771	-4.267307	2.437796
C	0.012051	-3.295726	1.592654
C	1.655234	-5.006812	2.042501
C	0.569362	-3.064893	0.330204
C	2.230381	-4.764651	0.796282
C	1.692851	-3.798193	-0.054623
C	2.242325	-1.941853	-3.967832
C	1.736437	-1.738587	-2.685056
C	1.415964	-2.418859	-4.986589
C	0.399668	-2.052331	-2.398541
C	0.079228	-2.706057	-4.713456
C	-0.424825	-2.531101	-3.424236
H	0.619113	3.188455	1.101682
H	0.679137	5.616894	1.593024
H	-1.403037	6.812946	2.256022
H	-3.606446	3.124036	1.984183
H	-3.548950	5.557321	2.440440
H	-3.967645	-2.281589	3.741373
H	-3.081737	-1.264203	1.686599
H	-3.708271	-1.117938	5.936555
H	-2.552470	1.090835	6.022613
H	-1.669673	2.116057	3.969983
H	-2.749582	3.249438	-0.708792
H	-0.763934	1.842141	-1.880700
H	-1.702009	2.898880	-2.956012
H	-1.653629	-0.075813	-2.985920
H	-2.538869	0.986216	-4.082927
H	-4.831407	0.063087	-4.005411
H	-5.567463	-0.552149	-2.510437
H	-4.169628	-1.387153	-3.224827
H	-4.565791	3.859692	-2.774219
H	-5.423173	2.507197	-3.536847
H	-3.706353	2.774757	-3.883142
H	-5.578815	3.049574	-0.709745
H	-5.178173	1.485273	0.019588
H	-6.244377	1.561652	-1.406828
H	-5.675852	-0.546919	-0.201378
H	-5.891929	-1.830070	0.999862
H	-6.423603	-2.091785	-0.675638
H	-1.111915	-5.312433	0.067125
H	-0.624140	-4.724158	-1.535786
H	-2.092993	-5.706810	-1.362575
H	0.080534	-4.441552	3.413842
H	-0.857164	-2.718377	1.918739
H	2.074004	-5.768049	2.705038
H	3.105584	-5.335802	0.477080
H	2.153392	-3.633296	-1.029524
H	3.290614	-1.713138	-4.175767
H	2.378237	-1.334565	-1.897248
H	1.814090	-2.564042	-5.993933
H	-0.578034	-3.074229	-5.504924
H	-1.471398	-2.768113	-3.220016
H	0.681637	1.639782	3.063101
H	2.445464	1.898838	3.026200
O	1.881204	-0.515411	1.924305
C	1.638022	1.329043	3.505461
H	1.613650	1.582241	4.576690
C	1.850966	-0.174269	3.317647
H	-0.236597	-0.771370	3.348819
H	3.997331	-0.036769	3.672964
C	0.682771	-0.949270	3.919606
C	3.137598	-0.623636	4.012848
H	0.890405	-2.027318	3.908827
H	0.508689	-0.639434	4.961128
H	3.325423	-1.688755	3.808572

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 H    3.034690   -0.500573    5.102433
Cu    0.486896    0.266453    0.452052
 H    4.586852    3.608430   -1.799049
 H    4.017022    2.509323   -4.065456
 H    4.326378    1.518299   -2.622253
 C    3.583129    1.757708   -3.389766
 H    3.703067    4.752513   -2.839316
 H    3.394472    0.843153   -3.970334
 C    3.682193    4.223731   -1.873943
 H    3.721018    4.978606   -1.074383
 C    2.405643    3.403540   -1.740581
 C    2.260600    2.238402   -2.791433
 O    2.417413    2.704913   -0.485615
 H    1.710035    3.330693   -4.586601
 B    1.893925    1.426588   -0.633999
 H    1.207514    1.621907   -4.565058
 C    1.311015    2.527487   -3.948209
 O    1.724607    1.176784   -1.993166
 H    1.134520    4.937161   -2.648469
 C    1.204919    4.350473   -1.720762
 H    1.312712    5.053948   -0.882427
 H    0.312181    2.818317   -3.611676
 H    0.262295    3.804361   -1.578979
 H    5.905580   -0.469709    2.720756
 H    4.563685   -2.130956    2.018471
 H    6.324912    1.230403    2.422667
 C    6.174921    0.252437    1.940352
 O    3.875987    0.770981    1.458528
 H    6.119534   -2.374858    1.173576
 C    5.039607   -2.217986    1.032570
 H    7.135137   -0.057617    1.499363
 B    2.802334    0.004740    0.947000
 H    4.623973   -3.110996    0.544202
 C    5.102222    0.376715    0.860492
 C    4.738683   -0.996732    0.158891
 O    3.332439   -0.912628   -0.007588
 H    5.625762    2.418571    0.435378
 C    5.522647    1.471661   -0.114383
 H    6.478039    1.251544   -0.612885
 H    4.745889    1.620373   -0.867630
 H    6.482795   -1.184273   -1.135861
 C    5.384139   -1.194667   -1.208344
 H    5.083571   -2.169732   -1.621585
 H    5.072409   -0.418651   -1.918619
140
Figure 1_prod / electronic energy: -5322.40355860 a.u. / lowest freq: 15.23 cm-1
 P   -2.230426    1.028195    1.095577
 C   -1.651810    3.717648    1.506724
 C   -1.927669    5.042592    1.849269
 C   -2.642103    2.736807    1.630708
 C   -3.191280    5.392861    2.322129
 C   -3.907653    3.093408    2.114707
 C   -4.180813    4.415890    2.457285
 C   -4.875807   -1.381604    3.190170
 C   -4.332201   -0.570419    2.194168
 C   -3.059300   -0.013103    2.353290
 C   -4.158276   -1.633904    4.359084
 C   -2.894254   -1.067796    4.533322
 C   -2.345827   -0.267589    3.533234
 C   -3.362223    1.999052   -1.421041
 C   -3.163433    0.840933   -0.450510
 C   -3.457707   -0.296812   -1.117276
 C   -2.188423    1.894016   -2.429974
 C   -2.509021    0.576531   -3.168501
 C   -3.869120    0.116315   -2.540969
 C   -4.613023   -0.888349   -3.396116
 C   -4.563146    1.491466   -2.259906
 C   -4.854582    2.312581   -3.520255
 C   -5.867202    1.420576   -1.460667
 C   -3.285223   -1.717228   -0.728598
 C   -4.360847   -2.559958   -0.571428
 C   -2.014310   -2.411277   -0.587646
 S   -3.840316   -4.184072   -0.298128
 C   -2.167389   -3.767184   -0.387895
 C   -5.823189   -2.245795   -0.562901
 C   -1.152519   -4.859706   -0.242055
 P   -0.406026   -1.538181   -0.530498
 C    0.503941   -3.274914    3.061593
 C   -0.138368   -2.627199    2.010138
 C    1.800191   -3.765519    2.892641
 C    0.500990   -2.467141    0.772829
 C    2.447972   -3.587971    1.671552
 C    1.806759   -2.936789    0.617875
 C    2.290856   -1.503996   -3.599650
 C    1.623907   -1.270190   -2.398904
 C    1.765286   -2.397399   -4.533835
 C    0.431574   -1.949619   -2.109080
 C    0.568969   -3.060230   -4.260681
 C   -0.094944   -2.839073   -3.053774
 H   -0.662376    3.439033    1.130372
 H   -1.149157    5.802422    1.747054
 H   -3.407651    6.430222    2.588946
 H   -4.687464    2.334422    2.222094
 H   -5.171066    4.687447    2.830952
 H   -5.867545   -1.819087    3.051704
 H   -4.898264   -0.375444    1.282123
 H   -4.584050   -2.273068    5.136199
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 H   -2.328278   -1.258581    5.448147
 H   -1.346635    0.157643    3.664939
 H   -3.480324    2.987989   -0.957109
 H   -1.215700    1.878749   -1.920068
 H   -2.185391    2.756542   -3.112339
 H   -1.735232   -0.192673   -3.028143
 H   -2.617221    0.723673   -4.253764
 H   -4.757222   -0.487024   -4.411401
 H   -5.604940   -1.130840   -2.989954
 H   -4.047699   -1.828850   -3.490178
 H   -5.061508    3.361328   -3.252461
 H   -5.751790    1.922882   -4.026605
 H   -4.040192    2.313054   -4.255552
 H   -6.267236    2.435654   -1.308460
 H   -5.741393    0.967611   -0.468754
 H   -6.635022    0.848382   -2.006108
 H   -5.984987   -1.173574   -0.722411
 H   -6.279376   -2.514762    0.403012
 H   -6.367387   -2.793158   -1.348339
 H   -0.907418   -5.043620    0.816063
 H   -0.219051   -4.606999   -0.759874
 H   -1.531731   -5.800470   -0.667916
 H   -0.012086   -3.396729    4.017153
 H   -1.156112   -2.254109    2.152167
 H    2.306064   -4.276737    3.715203
 H    3.466565   -3.957920    1.533424
 H    2.339627   -2.789416   -0.322864
 H    3.220817   -0.971063   -3.810207
 H    2.031279   -0.552087   -1.683159
 H    2.283201   -2.569327   -5.480529
 H    0.146584   -3.754142   -4.991459
 H   -1.036174   -3.356690   -2.854617
 H    3.230991    2.454062    2.133522
 H    4.765051    1.745681    2.735825
 O    3.151109   -0.134645    1.607842
 C    3.683772    1.830526    2.917676
 H    3.536239    2.318607    3.893500
 C    3.019253    0.455402    2.906546
 H    1.080815    1.243951    2.351415
 H    4.711931   -0.600414    3.781177
 C    1.516302    0.594541    3.127510
 C    3.632202   -0.478018    3.949663
 H    1.034287   -0.391969    3.062443
 H    1.304712    1.029341    4.116303
 H    3.155076   -1.468287    3.897358
 H    3.483175   -0.073413    4.962297
Cu   -0.182724    0.669801    0.125273
 H    4.603410    3.131081   -0.036328
 H    4.675645    2.700111   -2.500258
 H    3.862138    1.466219   -1.487042
 C    3.730756    2.163053   -2.327285
 H    4.620462    4.704423   -0.881007
 H    3.508301    1.563347   -3.222597
 C    4.056139    4.072616   -0.177024
 H    4.027112    4.592807    0.792472
 C    2.640816    3.824086   -0.679749
 C    2.558732    3.112895   -2.071767
 O    1.990373    2.880398    0.177060
 H    3.222141    4.758463   -3.329802
 B    1.159918    2.035075   -0.571021
 H    2.348273    3.469510   -4.192205
 C    2.382030    4.050123   -3.257646
 O    1.392121    2.299585   -1.925755
 H    2.302205    5.930008   -1.200676
 C    1.830985    5.120895   -0.622497
 H    1.756514    5.448026    0.425661
 H    1.446887    4.621359   -3.185934
 H    0.809272    4.968105   -1.001296
 H    7.479042   -2.101103    1.385783
 H    5.473742   -3.020139    0.687429
 H    8.285376   -0.521961    1.509763
 C    7.723057   -1.183640    0.834230
 O    5.570790   -0.283471    1.440639
 H    6.609323   -3.248909   -0.669630
 C    5.643598   -2.810950   -0.379197
 H    8.381351   -1.444386   -0.008233
 B    4.288900   -0.400580    0.949210
 H    4.852615   -3.310834   -0.957692
 C    6.473869   -0.474044    0.338769
 C    5.595047   -1.310336   -0.663449
 O    4.269503   -0.858702   -0.350298
 H    7.236898    1.520241    0.619178
 C    6.831850    0.909264   -0.200900
 H    7.590472    0.852226   -0.994763
 H    5.946239    1.421708   -0.601941
 H    6.940187   -1.275757   -2.360682
 C    5.888410   -1.047016   -2.131135
 H    5.256849   -1.692620   -2.758747
 H    5.688781   -0.003118   -2.405294
105
Figure 1_L-Cu-Bpin_01 / electronic energy: -4678.61224218 a.u. / lowest freq: 16.61 cm-1
 B    2.903937    1.409851   -0.190721
 O    3.654199    1.302372   -1.370038
 O    3.780912    1.706601    0.853711
 C    5.052096    1.265797   -1.054595
 C    5.092458    1.972105    0.343560
 C    5.831949    1.973287   -2.153778
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C	5.469164	-0.204988	-0.989202
C	5.246667	3.490698	0.241145
C	6.125418	1.414257	1.313151
H	4.517756	3.918309	-0.463300
H	6.258290	3.781222	-0.080250
H	5.060897	3.937070	1.229565
H	5.936564	0.356485	1.539522
H	6.084994	1.971592	2.261322
H	7.143717	1.512418	0.905605
H	4.914542	-0.741000	-0.204616
H	6.546600	-0.319166	-0.797494
H	5.244504	-0.688220	-1.951752
H	6.901391	2.041899	-1.900542
H	5.449375	2.986731	-2.333139
H	5.742681	1.410797	-3.095644
P	-1.204385	1.569151	0.529892
C	-0.654849	4.228046	-0.054740
C	-0.949744	5.577953	-0.253750
C	-1.654637	3.339849	0.353330
C	-2.245016	6.046333	-0.040962
C	-2.953804	3.817434	0.570667
C	-3.246757	5.164606	0.373348
C	-3.891682	0.222494	3.377474
C	-3.332209	0.574795	2.150239
C	-2.026775	1.074770	2.086745
C	-3.157387	0.377780	4.553410
C	-1.861108	0.891184	4.500449
C	-1.296846	1.233644	3.272783
C	-2.183931	1.454323	-2.190990
C	-2.105001	0.783487	-0.829220
C	-2.435375	-0.514539	-1.000789
C	-0.966542	0.884846	-2.972695
C	-1.369640	-0.591693	-3.177828
C	-2.771950	-0.694942	-2.492128
C	-3.554231	-1.924546	-2.903995
C	-3.381273	0.707414	-2.830222
C	-3.565271	0.973871	-4.326924
C	-4.718523	1.013362	-2.150602
C	-2.320371	-1.651616	-0.056162
C	-3.416678	-2.331898	0.416370
C	-1.067312	-2.222648	0.413697
S	-2.935103	-3.666378	1.403283
C	-1.250247	-3.343546	1.193605
C	-4.870712	-2.035149	0.229331
C	-0.256710	-4.263284	1.834947
P	0.535809	-1.429013	0.043897
C	1.945753	-1.459225	3.880444
C	1.138188	-1.341371	2.752504
C	3.222450	-2.013879	3.772696
C	1.590008	-1.786799	1.502813
C	3.680541	-2.451725	2.530961
C	2.870854	-2.337390	1.399716
C	2.870213	-2.469336	-3.137808
C	2.290445	-1.799898	-2.061349
C	2.415075	-3.736162	-3.503794
C	1.260198	-2.404223	-1.326225
C	1.378379	-4.334360	-2.786809
C	0.802917	-3.673470	-1.701554
H	0.358933	3.849407	-0.218720
H	-0.163004	6.264763	-0.574381
H	-2.476742	7.102878	-0.195530
H	-3.743250	3.134490	0.895384
H	-4.262149	5.530850	0.542819
H	-4.908793	-0.174813	3.415648
H	-3.912276	0.455983	1.233725
H	-3.597842	0.100006	5.513847
H	-1.283637	1.019973	5.418775
H	-0.275425	1.623361	3.233145
H	-2.248474	2.550831	-2.178354
H	-0.036079	0.999905	-2.393823
H	-0.825760	1.412161	-3.927146
H	-0.661116	-1.300819	-2.730177
H	-1.447119	-0.853729	-4.243595
H	-3.648468	-1.965703	-4.000353
H	-4.569150	-1.934965	-2.482177
H	-3.045489	-2.846508	-2.581412
H	-3.786446	2.040067	-4.495241
H	-4.420470	0.398132	-4.715016
H	-2.692419	0.718487	-4.941148
H	-5.030031	2.044369	-2.381941
H	-4.677726	0.920995	-1.057753
H	-5.509384	0.342029	-2.521709
H	-5.000656	-1.118788	-0.359095
H	-5.372285	-1.885010	1.198505
H	-5.394903	-2.853358	-0.288867
H	0.032360	-3.910873	2.837779
H	0.659281	-4.335778	1.234393
H	-0.674291	-5.275009	1.942559
H	1.575907	-1.110036	4.847645
H	0.141185	-0.903448	2.846822
H	3.859383	-2.102371	4.655854
H	4.677884	-2.888163	2.436620
H	3.244868	-2.687636	0.434834
H	3.673475	-1.989530	-3.702359
H	2.637259	-0.797234	-1.793129
H	2.862587	-4.254375	-4.355296
H	1.011340	-5.322311	-3.075119

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 H   -0.017178   -4.146224   -1.155803
Cu    0.947081    0.898099    0.075579
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Figure 1_L-Cu-Bpin_02 / electronic energy: -4678.61215750 a.u. / lowest freq: 15.20 cm-1
 P    0.470019   -1.480454    0.027699
Cu    0.994592    0.820724    0.173853
 P   -1.136365    1.578912    0.591894
 B    2.958703    1.323387   -0.086736
 O    3.724121    1.007135   -1.220260
 O    3.820374    1.849489    0.877159
 C    5.116755    1.052101   -0.886478
 C    5.123373    2.052368    0.315182
 C    5.915393    1.496980   -2.102553
 C    5.533337   -0.362865   -0.476904
 C    5.208150    3.513644   -0.130450
 C    6.179748    1.774036    1.375082
 H    4.472092    3.732107   -0.918406
 H    6.210142    3.773330   -0.503889
 H    4.982555    4.162866    0.728761
 H    6.034287    0.792617    1.845970
 H    6.125502    2.537352    2.166029
 H    7.190995    1.809824    0.940599
 H    4.980788   -0.693223    0.415193
 H    6.611525   -0.430918   -0.268523
 H    5.300351   -1.060067   -1.295799
 H    6.976412    1.643443   -1.847014
 H    5.524681    2.432624   -2.524460
 H    5.860837    0.726607   -2.886957
 C   -0.445171    4.223742    0.115042
 C   -0.665886    5.593425   -0.037872
 C   -1.494265    3.376223    0.485026
 C   -1.935800    6.122967    0.184126
 C   -2.767402    3.915176    0.712296
 C   -2.986257    5.282522    0.561740
 C   -3.976821    0.234523    3.287832
 C   -3.366862    0.631580    2.099069
 C   -2.028942    1.042416    2.094914
 C   -3.259152    0.253335    4.484162
 C   -1.929042    0.674240    4.490814
 C   -1.315602    1.062997    3.300933
 C   -2.023766    1.629805   -2.166176
 C   -2.027516    0.902979   -0.830928
 C   -2.416925   -0.368001   -1.065887
 C   -0.809624    1.025629   -2.927636
 C   -1.282664   -0.417260   -3.208936
 C   -2.710608   -0.472930   -2.573352
 C   -3.539256   -1.643997   -3.058483
 C   -3.234751    0.971334   -2.874536
 C   -3.352849    1.303307   -4.365046
 C   -4.578183    1.320061   -2.228509
 C   -2.390510   -1.548169   -0.169733
 C   -3.534794   -2.190428    0.236542
 C   -1.183321   -2.209955    0.302271
 S   -3.154348   -3.601025    1.160265
 C   -1.448614   -3.361911    1.010150
 C   -4.964139   -1.802026    0.028553
 C   -0.527128   -4.377375    1.613486
 C    1.671260   -1.856573    3.924389
 C    0.918875   -1.642604    2.772254
 C    2.963881   -2.375464    3.831108
 C    1.443504   -1.954692    1.510698
 C    3.495736   -2.676948    2.578063
 C    2.742468   -2.465840    1.422292
 C    2.880211   -2.518008   -3.100153
 C    2.294701   -1.863263   -2.017386
 C    2.366718   -3.735643   -3.546663
 C    1.199580   -2.436699   -1.354789
 C    1.265616   -4.300772   -2.902525
 C    0.684285   -3.656652   -1.810365
 H    0.548398    3.798231   -0.056327
 H    0.159081    6.247592   -0.329575
 H   -2.110476    7.194919    0.064945
 H   -3.594841    3.264770    1.008129
 H   -3.981526    5.697257    0.738332
 H   -5.020001   -0.090515    3.279967
 H   -3.932302    0.615414    1.165688
 H   -3.738560   -0.061051    5.414214
 H   -1.363088    0.692560    5.425107
 H   -0.267667    1.376711    3.306234
 H   -2.031571    2.726863   -2.110367
 H    0.102514    1.064803   -2.310398
 H   -0.602452    1.581723   -3.853226
 H   -0.627980   -1.181678   -2.770682
 H   -1.338186   -0.630225   -4.286825
 H   -3.600511   -1.637292   -4.158036
 H   -4.566327   -1.619801   -2.667637
 H   -3.086205   -2.602029   -2.758735
 H   -3.525796    2.383209   -4.498353
 H   -4.216188    0.779662   -4.805446
 H   -2.469280    1.036427   -4.958735
 H   -4.830500    2.373037   -2.431432
 H   -4.580179    1.186593   -1.139218
 H   -5.387637    0.703046   -2.650494
 H   -5.026236   -0.863946   -0.536436
 H   -5.476069   -1.647104    0.991697
 H   -5.525297   -2.573028   -0.522130
 H   -0.348670   -4.180684    2.682558
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 H     0.446900   -4.376099    1.109018
 H    -0.953306   -5.387746    1.525343
 H     1.243235   -1.615183    4.900419
 H    -0.093105   -1.238401    2.857204
 H     3.554733   -2.542928    4.734586
 H     4.507178   -3.081895    2.493993
 H     3.176499   -2.703679    0.448515
 H     3.734755   -2.062346   -3.606601
 H     2.691285   -0.896639   -1.690554
 H     2.818700   -4.240562   -4.403831
 H     0.851939   -5.248853   -3.254574
 H    -0.185744   -4.102988   -1.323203
105
Figure 1_L-Cu-Bpin_03 / electronic energy: -4678.60409663 a.u. / lowest freq: 12.84 cm-1
 B     3.115412   -1.378056   -0.250136
 O     3.866910   -0.205100   -0.150229
 O     3.970075   -2.416685   -0.614311
 C     5.191396   -0.425222   -0.648049
 C     5.333150   -1.979736   -0.518298
 C     6.177250    0.381268    0.185450
 C     5.224476    0.058484   -2.098445
 C     5.851205   -2.418144    0.852893
 C     6.153587   -2.642533   -1.615401
 H     5.291749   -1.929151    1.664308
 H     6.920940   -2.195162    0.981284
 H     5.711449   -3.504365    0.957167
 H     5.705751   -2.487599   -2.605865
 H     6.208412   -3.727271   -1.437911
 H     7.182132   -2.249670   -1.629213
 H     4.527155   -0.515556   -2.725340
 H     6.232304   -0.018856   -2.533416
 H     4.917680    1.114457   -2.132393
 H     7.214678    0.172228   -0.119005
 H     6.079635    0.163405    1.257171
 H     5.992660    1.456852    0.042622
 P    -1.028488   -1.656786    0.894231
 C    -0.191640   -0.566121    3.284237
 C    -0.324270    0.029382    4.537907
 C    -1.322468   -0.967438    2.561835
 C    -1.591630    0.224481    5.083816
 C    -2.592570   -0.779259    3.124468
 C    -2.724677   -0.185480    4.377975
 C    -1.659933   -5.514088   -0.251616
 C    -1.260861   -4.182460   -0.172824
 C    -1.582082   -3.406258    0.950828
 C    -2.369321   -6.092309    0.802632
 C    -2.672848   -5.333757    1.932082
 C    -2.282632   -3.995050    2.007836
 C    -3.764777   -1.010652   -0.145030
 C    -2.250882   -0.938984   -0.224629
 C    -1.937054   -0.231319   -1.328876
 C    -4.211550    0.436295    0.215438
 C    -3.867145    1.222345   -1.067530
 C    -3.259021    0.141425   -2.015487
 C    -3.193907    0.570190   -3.466386
 C    -4.138433   -1.107669   -1.650667
 C    -5.631650   -0.938486   -1.946071
 C    -3.698501   -2.418995   -2.303823
 C    -0.608790    0.262662   -1.760890
 C     0.051954   -0.236331   -2.856364
 C     0.110033    1.353325   -1.115126
 S     1.519100    0.635028   -3.132855
 C     1.280610    1.669746   -1.769601
 C    -0.304606   -1.400387   -3.725182
 C     2.331152    2.686971   -1.456075
 P    -0.548983    2.096322    0.426763
 C     2.152095    4.183710    2.784453
 C     1.053307    3.878618    1.979296
 C     3.157580    3.239934    2.993968
 C     0.942476    2.620468    1.372860
 C     3.054404    1.985366    2.392226
 C     1.952984    1.676685    1.598967
 C    -2.816938    5.501480    0.393398
 C    -2.180606    4.313111    0.747072
 C    -2.577443    6.074881   -0.855862
 C    -1.278546    3.692665   -0.130665
 C    -1.696380    5.456738   -1.743315
 C    -1.048548    4.274461   -1.383380
 H     0.801327   -0.708872    2.849499
 H     0.567288    0.349839    5.081559
 H    -1.700105    0.698547    6.062186
 H    -3.487974   -1.093227    2.585060
 H    -3.719035   -0.038722    4.806016
 H    -1.407395   -6.105184   -1.135008
 H    -0.687604   -3.736521   -0.991735
 H    -2.677500   -7.138982    0.745927
 H    -3.216796   -5.785110    2.765172
 H    -2.524996   -3.416479    2.901708
 H    -4.170734   -1.800766    0.502901
 H    -3.671149    0.815194    1.093551
 H    -5.286181    0.472260    0.445897
 H    -3.154577    2.038675   -0.894553
 H    -4.757147    1.673548   -1.530984
 H    -4.196067    0.850269   -3.826903
 H    -2.812298   -0.226954   -4.120977
 H    -2.539989    1.447957   -3.588888
 H    -6.199440   -1.766238   -1.491821
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 H   -5.812123   -0.977753   -3.031984
 H   -6.063873   -0.000662   -1.575281
 H   -4.315015   -3.252619   -1.932019
 H   -2.651755   -2.671357   -2.097438
 H   -3.832890   -2.374230   -3.396403
 H   -1.264984   -1.827273   -3.413469
 H    0.454565   -2.195175   -3.647827
 H   -0.382587   -1.118265   -4.786647
 H    3.094610    2.240684   -0.799226
 H    1.903538    3.558141   -0.943407
 H    2.827624    3.037742   -2.372704
 H    2.223701    5.171817    3.245809
 H    0.284789    4.638655    1.819909
 H    4.020685    3.484647    3.617916
 H    3.838964    1.236940    2.524046
 H    1.910599    0.695749    1.117544
 H   -3.513580    5.973290    1.090426
 H   -2.392733    3.852990    1.716865
 H   -3.084110    7.000006   -1.140734
 H   -1.511521    5.897831   -2.725798
 H   -0.367595    3.795774   -2.091122
Cu    1.127770   -1.477533    0.170380
105
Figure 1_L-Cu-Bpin_04 / electronic energy: -4678.60278859 a.u. / lowest freq: 10.28 cm-1
 B   -2.989900    1.565349   -0.254751
 O   -3.804667    0.434136   -0.185608
 O   -3.784836    2.656898   -0.601055
 C   -5.105204    0.733493   -0.704497
 C   -5.170216    2.289268   -0.538533
 C   -6.149227   -0.042775    0.085272
 C   -5.130614    0.289589   -2.167904
 C   -5.690877    2.721326    0.833482
 C   -5.934467    3.018816   -1.633845
 H   -5.165308    2.192614    1.642777
 H   -6.770910    2.541243    0.940978
 H   -5.507374    3.798320    0.963136
 H   -5.478196    2.861072   -2.619978
 H   -5.933210    4.101035   -1.433566
 H   -6.982314    2.682726   -1.673388
 H   -4.386501    0.838054   -2.763366
 H   -6.121876    0.435345   -2.622959
 H   -4.884512   -0.781055   -2.223923
 H   -7.167138    0.220853   -0.241931
 H   -6.070520    0.146491    1.163920
 H   -6.010311   -1.122521   -0.077048
 P    1.216586    1.811837    0.601177
 C    0.823048    0.635857    3.095792
 C    1.164800    0.274487    4.399357
 C    1.679290    1.440942    2.337162
 C    2.360681    0.725303    4.955610
 C    2.875270    1.898819    2.906026
 C    3.213301    1.541792    4.208933
 C    2.881698    5.323953   -0.808776
 C    2.561105    3.973386   -0.658665
 C    1.757925    3.551382    0.404305
 C    2.400235    6.263717    0.100159
 C    1.590867    5.850267    1.160684
 C    1.267703    4.504292    1.309672
 C    3.877819    0.720249   -0.221699
 C    2.368093    0.817547   -0.371672
 C    1.987362   -0.152961   -1.227242
 C    4.110982   -0.582343    0.598666
 C    3.700992   -1.684328   -0.401909
 C    3.258362   -0.891087   -1.671642
 C    3.148253   -1.736599   -2.922633
 C    4.300485    0.282182   -1.654890
 C    5.763269   -0.160895   -1.768521
 C    4.076528    1.334095   -2.741821
 C    0.616430   -0.535540   -1.644622
 C    0.044162   -0.022464   -2.783287
 C   -0.239728   -1.492424   -0.965779
 S   -1.511141   -0.720342   -3.048242
 C   -1.430098   -1.700676   -1.632247
 C    0.574121    1.024577   -3.713672
 C   -2.602045   -2.565130   -1.290977
 P    0.286891   -2.226210    0.627315
 C   -2.776866   -3.882370    2.888896
 C   -1.613086   -3.746829    2.131043
 C   -3.629871   -2.794314    3.074667
 C   -1.282812   -2.515927    1.548877
 C   -3.305726   -1.564654    2.501288
 C   -2.137212   -1.425341    1.756871
 C    2.027610   -5.928186    0.831858
 C    1.560240   -4.645802    1.112604
 C    1.776107   -6.505116   -0.413708
 C    0.813364   -3.930065    0.164224
 C    1.052131   -5.794733   -1.370829
 C    0.570782   -4.516538   -1.083708
 H   -0.119132    0.288593    2.664559
 H    0.489715   -0.357618    4.980693
 H    2.627828    0.446887    5.977901
 H    3.547485    2.538864    2.329074
 H    4.147358    1.903049    4.645528
 H    3.513645    5.639063   -1.642479
 H    2.940974    3.247747   -1.378035
 H    2.650523    7.320523   -0.018252
 H    1.206149    6.582013    1.874912
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 H    0.628587    4.191282    2.140496
 H    4.374792    1.612868    0.182933
 H    3.497216   -0.593898    1.509767
 H    5.161862   -0.672768    0.909334
 H    2.892768   -2.322208   -0.028282
 H    4.537096   -2.352168   -0.656866
 H    4.119565   -2.193966   -3.166936
 H    2.819950   -1.147817   -3.792610
 H    2.424112   -2.554106   -2.780370
 H    6.427442    0.704501   -1.615150
 H    5.965958   -0.551995   -2.778137
 H    6.062911   -0.933998   -1.050753
 H    4.762243    2.184367   -2.599221
 H    3.052490    1.721485   -2.763341
 H    4.291179    0.908080   -3.734640
 H    1.515350    0.707573   -4.186698
 H    0.767536    1.962509   -3.170451
 H   -0.143601    1.249191   -4.514974
 H   -3.293865   -2.006168   -0.641457
 H   -2.288057   -3.475669   -0.764775
 H   -3.145914   -2.866311   -2.198477
 H   -3.020846   -4.851925    3.330301
 H   -0.971033   -4.617976    1.983440
 H   -4.547141   -2.907391    3.657507
 H   -3.969033   -0.704708    2.616080
 H   -1.925071   -0.460821    1.285417
 H    2.601998   -6.474176    1.584031
 H    1.781758   -4.189312    2.082029
 H    2.151619   -7.505736   -0.640463
 H    0.858880   -6.238310   -2.350533
 H    0.007636   -3.969469   -1.843603
Cu   -0.988377    1.573185    0.115351
105
Figure 1_L-Cu-Bpin_05 / electronic energy: -4678.60699442 a.u. / lowest freq: 13.79 cm-1
 P    0.020853   -2.542593    0.323468
Cu   -0.569564    1.622856    0.208707
 P    1.583095    1.100309    0.712983
 B   -2.463257    2.269028   -0.143186
 O   -2.935228    3.138127   -1.123435
 O   -3.558111    1.786106    0.582212
 C   -4.334946    3.383353   -0.929878
 C   -4.775874    2.140326   -0.084856
 C   -5.011691    3.506254   -2.287761
 C   -4.464132    4.701914   -0.164717
 C   -5.179941    0.943289   -0.946688
 C   -5.856348    2.418639    0.950085
 H   -4.412375    0.731421   -1.705245
 H   -6.143599    1.102894   -1.453080
 H   -5.272986    0.056847   -0.301469
 H   -5.529795    3.162799    1.688224
 H   -6.102153    1.492396    1.491403
 H   -6.776902    2.783403    0.468517
 H   -3.991727    4.633413    0.826499
 H   -5.514747    5.000788   -0.033075
 H   -3.949240    5.494702   -0.727821
 H   -6.103039    3.601979   -2.177636
 H   -4.796373    2.639598   -2.926727
 H   -4.643782    4.404619   -2.806107
 C    1.007478    1.178518    3.397000
 C    1.160946    0.897341    4.752425
 C    1.867108    0.605869    2.449088
 C    2.160421    0.021044    5.174480
 C    2.869163   -0.270536    2.880658
 C    3.009781   -0.565437    4.236755
 C    3.028161    4.623346   -0.763943
 C    2.235786    3.515132   -0.470472
 C    2.645463    2.583823    0.492624
 C    4.233799    4.815010   -0.088892
 C    4.640884    3.899398    0.882460
 C    3.850465    2.787622    1.174371
 C    3.878304   -0.433814   -0.480867
 C    2.410063   -0.048110   -0.409166
 C    1.807123   -0.577730   -1.493966
 C    3.910224   -1.967589   -0.212984
 C    3.238003   -2.547583   -1.475107
 C    2.892448   -1.283812   -2.320128
 C    2.573602   -1.583826   -3.769709
 C    4.128701   -0.364555   -2.013306
 C    5.476281   -0.938133   -2.461649
 C    4.031525    1.051803   -2.584280
 C    0.361719   -0.652765   -1.800807
 C   -0.241200    0.043415   -2.820803
 C   -0.556502   -1.527587   -1.091416
 S   -1.906254   -0.399209   -2.952920
 C   -1.829441   -1.494843   -1.620223
 C    0.324949    1.109999   -3.702816
 C   -3.059962   -2.261130   -1.244115
 C   -0.959371   -1.807947    4.220865
 C   -0.385400   -2.289256    3.046591
 C   -1.942471   -0.817666    4.162959
 C   -0.810622   -1.816985    1.794238
 C   -2.343359   -0.314492    2.927383
 C   -1.787324   -0.816663    1.749671
 C   -1.245219   -6.047467   -1.387938
 C   -0.620268   -4.830353   -1.125243
 C   -2.142265   -6.588526   -0.464647
 C   -0.895567   -4.122440    0.054767
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 C   -2.406066   -5.902188    0.719533
 C   -1.787810   -4.677810    0.978002
 H    0.204735    1.844764    3.067326
 H    0.483311    1.350331    5.479555
 H    2.275627   -0.208376    6.236452
 H    3.551164   -0.726422    2.163139
 H    3.791668   -1.256009    4.560994
 H    2.699185    5.342104   -1.517832
 H    1.286802    3.365048   -0.994712
 H    4.855395    5.684573   -0.315489
 H    5.581636    4.050961    1.416963
 H    4.176770    2.077415    1.938404
 H    4.559055    0.161445    0.143528
 H    3.358288   -2.229767    0.699906
 H    4.942862   -2.324897   -0.090480
 H    2.331944   -3.125062   -1.242502
 H    3.909725   -3.208419   -2.042852
 H    3.420812   -2.099585   -4.248137
 H    2.366674   -0.670626   -4.346120
 H    1.693728   -2.240742   -3.855669
 H    6.297762   -0.339638   -2.036560
 H    5.569088   -0.883670   -3.557889
 H    5.645513   -1.982340   -2.170475
 H    4.888740    1.656053   -2.246718
 H    3.121369    1.580457   -2.276733
 H    4.060287    1.030108   -3.685467
 H    1.393529    1.248205   -3.497865
 H   -0.175951    2.074097   -3.518608
 H    0.206112    0.872679   -4.771233
 H   -3.965074   -1.772207   -1.630168
 H   -3.158066   -2.346143   -0.154015
 H   -3.028548   -3.283488   -1.653821
 H   -0.622245   -2.193207    5.186064
 H    0.402374   -3.046646    3.102570
 H   -2.381875   -0.427182    5.084176
 H   -3.091266    0.478031    2.851884
 H   -2.122724   -0.396871    0.799623
 H   -1.028925   -6.577833   -2.318565
 H    0.080031   -4.417732   -1.858416
 H   -2.632440   -7.543591   -0.667800
 H   -3.107451   -6.315734    1.448499
 H   -2.021416   -4.146296    1.903262
105
Figure 1_L-Cu-Bpin_06 / electronic energy: -4678.60363299 a.u. / lowest freq: 17.34 cm-1
 B   -2.283125    2.392153   -0.404573
 O   -3.423006    1.607390   -0.212615
 O   -2.687819    3.666696   -0.796243
 C   -4.582524    2.307127   -0.680223
 C   -4.105919    3.797740   -0.622095
 C   -5.763202    1.971142    0.219413
 C   -4.866549    1.833170   -2.106246
 C   -4.336044    4.442380    0.746447
 C   -4.667541    4.696228   -1.714331
 H   -3.956041    3.801945    1.556183
 H   -5.401128    4.647293    0.931394
 H   -3.790289    5.396666    0.789061
 H   -4.389258    4.342438   -2.715876
 H   -4.271602    5.716382   -1.596975
 H   -5.765653    4.750056   -1.653600
 H   -4.028172    2.067758   -2.778009
 H   -5.782120    2.287711   -2.513508
 H   -5.002176    0.741307   -2.105234
 H   -6.653005    2.557147   -0.059135
 H   -5.536052    2.161330    1.276798
 H   -6.014747    0.904468    0.117713
 P    1.677728    1.073326    0.614733
 C    2.082866   -0.463586    2.958599
 C    2.199338   -0.625470    4.339732
 C    1.925123    0.809671    2.406147
 C    2.145075    0.482192    5.182372
 C    1.852446    1.919742    3.261787
 C    1.965410    1.756370    4.639463
 C    3.366012    4.287676   -1.261223
 C    2.482983    3.301947   -0.821590
 C    2.854809    2.421205    0.201568
 C    4.623946    4.408145   -0.671914
 C    4.995382    3.544598    0.360463
 C    4.116131    2.554522    0.795951
 C    3.859320   -0.810861   -0.243459
 C    2.425166   -0.305418   -0.284873
 C    1.816715   -0.916415   -1.323575
 C    3.780737   -2.300209    0.194283
 C    3.084775   -2.973918   -1.006961
 C    2.867522   -1.799591   -2.011087
 C    2.569984   -2.247705   -3.426770
 C    4.164793   -0.944905   -1.764507
 C    5.471946   -1.673784   -2.091717
 C    4.208420    0.396515   -2.498841
 C    0.384758   -0.868935   -1.698442
 C   -0.091950   -0.191877   -2.795162
 C   -0.665922   -1.545950   -0.955647
 S   -1.803375   -0.390062   -2.936866
 C   -1.911737   -1.360066   -1.514935
 C    0.635938    0.689809   -3.759639
 C   -3.251256   -1.865100   -1.080999
 P   -0.287642   -2.578611    0.511265
 C   -2.228295    0.168588    2.942598
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 C   -1.787530   -0.511849    1.807103
 C   -1.982653   -0.349325    4.212510
 C   -1.071668   -1.707504    1.927132
 C   -1.289597   -1.554468    4.343782
 C   -0.823737   -2.218137    3.211252
 C   -3.035514   -5.689349    0.860952
 C   -2.307997   -4.529530    1.135085
 C   -2.833141   -6.384061   -0.330350
 C   -1.365811   -4.048428    0.219558
 C   -1.890295   -5.915419   -1.247295
 C   -1.157837   -4.763779   -0.969836
 H    2.099078   -1.340752    2.310037
 H    2.325212   -1.627279    4.756819
 H    2.237243    0.354358    6.263373
 H    1.711355    2.921953    2.847130
 H    1.912198    2.629124    5.294482
 H    3.065749    4.968032   -2.061312
 H    1.492110    3.209261   -1.276955
 H    5.316630    5.181404   -1.012494
 H    5.976815    3.643032    0.830256
 H    4.415169    1.884824    1.606218
 H    4.562465   -0.199969    0.338159
 H    3.218904   -2.425285    1.127997
 H    4.787634   -2.706186    0.367139
 H    2.127702   -3.439997   -0.734986
 H    3.708547   -3.755146   -1.466090
 H    3.372983   -2.903464   -3.797739
 H    2.481553   -1.399753   -4.121370
 H    1.628364   -2.817037   -3.473758
 H    6.328640   -1.103445   -1.698382
 H    5.603814   -1.745828   -3.182897
 H    5.539889   -2.690980   -1.686207
 H    5.118676    0.950171   -2.218703
 H    3.353998    1.044150   -2.270369
 H    4.242678    0.243483   -3.589333
 H    1.705273    0.721220   -3.520326
 H    0.253496    1.722100   -3.714438
 H    0.527289    0.340546   -4.798218
 H   -3.272723   -2.041461    0.001042
 H   -3.503775   -2.814723   -1.580415
 H   -4.034687   -1.131106   -1.314616
 H   -2.766202    1.111264    2.817655
 H   -2.007503   -0.085082    0.826317
 H   -2.327127    0.184197    5.101572
 H   -1.089413   -1.967727    5.335214
 H   -0.245135   -3.139675    3.328477
 H   -3.772458   -6.045992    1.584799
 H   -2.494772   -3.990726    2.066878
 H   -3.406269   -7.289210   -0.544790
 H   -1.722156   -6.450807   -2.184926
 H   -0.423226   -4.407692   -1.698456
Cu   -0.425176    1.667715   -0.014443
105
Figure 1_L-Cu-Bpin_07 / electronic energy: -4678.60209838 a.u. / lowest freq: 15.70 cm-1
 P   -0.343282   -2.533097    0.593076
Cu   -0.450680    1.628010    0.109411
 P    1.758239    1.218384    0.454426
 B   -2.332775    2.314180   -0.267966
 O   -2.703772    3.583578   -0.704869
 O   -3.493982    1.545586   -0.124592
 C   -4.129058    3.729474   -0.634340
 C   -4.615305    2.241965   -0.684580
 C   -4.602107    4.596824   -1.791800
 C   -4.449128    4.417477    0.694154
 C   -4.810694    1.728858   -2.112256
 C   -5.855174    1.940891    0.145102
 H   -3.925433    1.931889   -2.731992
 H   -5.689526    2.183982   -2.593045
 H   -4.964181    0.639628   -2.088532
 H   -5.696859    2.160052    1.209318
 H   -6.111827    0.874282    0.056187
 H   -6.717979    2.526414   -0.208617
 H   -4.131014    3.801129    1.548262
 H   -5.522778    4.633488    0.799088
 H   -3.900659    5.369789    0.744984
 H   -5.701562    4.648125   -1.823170
 H   -4.241442    4.216149   -2.756458
 H   -4.217981    5.621074   -1.671568
 C    3.618925    1.095956    2.597381
 C    3.989417    0.814992    3.910105
 C    2.291702    0.916590    2.184753
 C    3.036839    0.359434    4.824427
 C    1.339263    0.475821    3.109357
 C    1.712054    0.194405    4.424451
 C    2.812054    5.155699    0.316366
 C    2.187363    3.941134    0.585231
 C    2.677130    2.748951    0.030403
 C    3.925919    5.197857   -0.525035
 C    4.409166    4.020416   -1.091790
 C    3.789160    2.800118   -0.814751
 C    3.941322   -0.673546   -0.368068
 C    2.524873   -0.127835   -0.474491
 C    1.839435   -0.963760   -1.281617
 C    3.803909   -1.972624    0.478015
 C    3.063468   -2.925545   -0.485924
 C    2.816980   -2.049944   -1.754058
 C    2.407863   -2.830221   -2.985443
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 C    4.158467   -1.235599   -1.803502
 C    5.422480   -2.088952   -1.953381
 C    4.212689   -0.178893   -2.907878
 C    0.402281   -0.915166   -1.645519
 C   -0.028509   -0.247678   -2.766051
 C   -0.680737   -1.553544   -0.919507
 S   -1.734913   -0.419317   -2.958964
 C   -1.906548   -1.362147   -1.524572
 C    0.764883    0.581289   -3.728002
 C   -3.279165   -1.780675   -1.102602
 C   -2.673696    0.014607    2.900431
 C   -2.101337   -0.611045    1.791986
 C   -2.433166   -0.469255    4.184789
 C   -1.263968   -1.718300    1.955659
 C   -1.602000   -1.578409    4.359709
 C   -1.008623   -2.186068    3.255483
 C   -1.704577   -5.968805   -1.202334
 C   -1.057034   -4.767065   -0.924737
 C   -2.606306   -6.509729   -0.283949
 C   -1.308278   -4.075978    0.270851
 C   -2.852757   -5.837397    0.911596
 C   -2.208832   -4.630174    1.188225
 H    4.367174    1.463582    1.890672
 H    5.026712    0.955829    4.222838
 H    3.328124    0.141825    5.854796
 H    0.297930    0.355621    2.801686
 H    0.959218   -0.150603    5.136659
 H    2.420518    6.075345    0.757175
 H    1.302967    3.917053    1.229566
 H    4.413422    6.151408   -0.741033
 H    5.275991    4.045784   -1.756482
 H    4.180193    1.889594   -1.266688
 H    4.702469    0.027755   -0.000839
 H    3.237811   -1.781647    1.401033
 H    4.789225   -2.361905    0.772673
 H    2.118953   -3.297409   -0.071035
 H    3.671954   -3.801836   -0.754220
 H    3.184124   -3.561310   -3.259324
 H    2.238168   -2.171402   -3.850673
 H    1.474449   -3.386534   -2.806039
 H    6.315159   -1.455731   -1.827871
 H    5.473697   -2.524464   -2.963897
 H    5.504847   -2.913839   -1.235360
 H    5.154603    0.389461   -2.846525
 H    3.383518    0.535709   -2.868761
 H    4.194798   -0.662118   -3.897871
 H    1.568040   -0.004110   -4.199159
 H    1.229224    1.435432   -3.210321
 H    0.130353    0.985087   -4.529228
 H   -3.839534   -0.900551   -0.750344
 H   -3.239386   -2.510920   -0.286482
 H   -3.835651   -2.233399   -1.937526
 H   -3.308592    0.888865    2.740596
 H   -2.301532   -0.195648    0.805002
 H   -2.885027    0.018848    5.051652
 H   -1.399268   -1.960448    5.363156
 H   -0.325579   -3.027365    3.406813
 H   -1.503375   -6.486296   -2.143503
 H   -0.355624   -4.355707   -1.656621
 H   -3.114627   -7.452225   -0.500581
 H   -3.559491   -6.248283    1.636869
 H   -2.428676   -4.112622    2.124520
105
Figure 1_L-Cu-Bpin_08 / electronic energy: -4678.60272089 a.u. / lowest freq: 15.21 cm-1
 B   -2.559138    2.042317   -0.338181
 O   -3.459678    1.095660   -0.825104
 O   -3.250379    3.236709   -0.129886
 C   -4.706892    1.716421   -1.144806
 C   -4.660693    3.014211   -0.268727
 C   -5.842655    0.759278   -0.808738
 C   -4.700376    2.003591   -2.647602
 C   -5.228281    2.800177    1.135685
 C   -5.302677    4.238816   -0.904776
 H   -4.792066    1.906119    1.604492
 H   -6.323011    2.690322    1.125458
 H   -4.974172    3.668722    1.761753
 H   -4.808506    4.512517   -1.846347
 H   -5.224680    5.098201   -0.221588
 H   -6.370750    4.062860   -1.106393
 H   -3.889432    2.696089   -2.917566
 H   -5.655181    2.429166   -2.991294
 H   -4.530304    1.060797   -3.188609
 H   -6.821110    1.252488   -0.919000
 H   -5.754863    0.373877    0.216006
 H   -5.822069   -0.101677   -1.494105
 P    1.595967    1.466357    0.654974
 C    2.247763    2.621696    3.169522
 C    2.360102    2.587018    4.560303
 C    1.889924    1.468402    2.461604
 C    2.109261    1.406075    5.257403
 C    1.617521    0.290058    3.171608
 C    1.733518    0.257508    4.559272
 C    2.617106    4.665730   -1.663227
 C    1.921581    3.649297   -1.007673
 C    2.551788    2.874653   -0.025888
 C    3.947579    4.920276   -1.335901
 C    4.579690    4.162119   -0.347835
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 C    3.888004    3.143178    0.303373
 C    3.940401   -0.391063    0.350980
 C    2.526652    0.056045    0.016219
 C    2.071698   -0.750108   -0.961862
 C    3.788158   -1.766634    1.058552
 C    3.274401   -2.677335   -0.077131
 C    3.203707   -1.724780   -1.311417
 C    3.098267   -2.449406   -2.637127
 C    4.454043   -0.805731   -1.059027
 C    5.795374   -1.544841   -1.056029
 C    4.593057    0.368837   -2.030346
 C    0.720724   -0.786999   -1.562853
 C    0.430484   -0.185156   -2.763122
 C   -0.418551   -1.472257   -0.982307
 S   -1.214471   -0.475073   -3.199273
 C   -1.542260   -1.392595   -1.779103
 C    1.301753    0.687922   -3.612068
 C   -2.914813   -1.942198   -1.563831
 P   -0.283302   -2.275760    0.658330
 C   -3.073012   -0.171501    2.778384
 C   -1.929518   -0.586933    2.099092
 C   -4.164736   -1.030930    2.896347
 C   -1.864698   -1.855771    1.508012
 C   -4.102094   -2.306643    2.333127
 C   -2.960912   -2.716213    1.644633
 C   -0.471046   -6.332846    1.182539
 C   -0.413996   -4.955718    1.380995
 C   -0.543503   -6.851014   -0.112205
 C   -0.453965   -4.070096    0.291704
 C   -0.560165   -5.981967   -1.201671
 C   -0.517583   -4.600658   -1.002129
 H    2.439744    3.557630    2.639974
 H    2.643932    3.493278    5.100572
 H    2.201278    1.381413    6.345758
 H    1.304541   -0.609722    2.633398
 H    1.524258   -0.670282    5.096702
 H    2.114314    5.260324   -2.429325
 H    0.875010    3.448212   -1.256939
 H    4.494468    5.715946   -1.847474
 H    5.621294    4.363108   -0.086809
 H    4.393685    2.557363    1.074252
 H    4.557086    0.332966    0.899521
 H    3.090666   -1.709493    1.903357
 H    4.754614   -2.109389    1.455822
 H    2.290969   -3.117793    0.136043
 H    3.959503   -3.513161   -0.283298
 H    3.974611   -3.097915   -2.792006
 H    3.036390   -1.754789   -3.487745
 H    2.203185   -3.090790   -2.664452
 H    6.581516   -0.891258   -0.644991
 H    6.090915   -1.799533   -2.086156
 H    5.802300   -2.475749   -0.474980
 H    5.473435    0.975855   -1.765429
 H    3.722230    1.036143   -2.033906
 H    4.749074    0.004032   -3.058539
 H    2.302610    0.253164   -3.736979
 H    1.428261    1.681011   -3.151029
 H    0.871699    0.837178   -4.612700
 H   -3.462985   -1.302027   -0.857448
 H   -2.872208   -2.964740   -1.164818
 H   -3.482231   -1.966823   -2.505478
 H   -3.104565    0.826813    3.220656
 H   -1.076115    0.093850    2.021696
 H   -5.061841   -0.709998    3.431388
 H   -4.950633   -2.989035    2.424669
 H   -2.933807   -3.713319    1.199249
 H   -0.449715   -7.006930    2.042278
 H   -0.341667   -4.560783    2.398988
 H   -0.582160   -7.931325   -0.270319
 H   -0.612101   -6.379377   -2.218212
 H   -0.537849   -3.929741   -1.864283
Cu   -0.606574    1.642979    0.079796
105
Figure 1_L-Cu-Bpin_09 / electronic energy: -4678.60328369 a.u. / lowest freq: 16.25 cm-1
 P    0.139809    2.292587    0.637600
Cu    0.709666   -1.621976    0.115754
 P   -1.492492   -1.512605    0.713110
 B    2.672513   -1.948524   -0.313643
 O    3.331575   -3.172064   -0.434782
 O    3.609556   -0.928661   -0.483539
 C    4.749918   -2.959676   -0.461994
 C    4.851436   -1.472044   -0.940749
 C    5.392676   -3.977375   -1.393154
 C    5.267889   -3.160545    0.963154
 C    4.878391   -1.332927   -2.463779
 C    5.998380   -0.679329   -0.329157
 H    4.059094   -1.899725   -2.929928
 H    5.831760   -1.677398   -2.891958
 H    4.746874   -0.273052   -2.727370
 H    5.898694   -0.602497    0.761534
 H    6.005685    0.343279   -0.736209
 H    6.969005   -1.143403   -0.563534
 H    4.827001   -2.425123    1.652453
 H    6.363656   -3.078591    1.018970
 H    4.979962   -4.163524    1.312116
 H    6.471325   -3.785141   -1.503313
 H    4.931554   -3.962811   -2.389462
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 H     5.269772   -4.990073   -0.979953
 C    -2.059293   -2.614798    3.267757
 C    -2.176725   -2.537733    4.656110
 C    -1.787504   -1.464348    2.517539
 C    -2.014478   -1.316460    5.308793
 C    -1.601792   -0.244108    3.182951
 C    -1.721035   -0.170094    4.568904
 C    -2.462770   -4.703605   -1.628205
 C    -1.787438   -3.669838   -0.979497
 C    -2.398845   -2.969108    0.067698
 C    -3.752182   -5.050635   -1.228133
 C    -4.364191   -4.365078   -0.176673
 C    -3.694351   -3.326253    0.466483
 C    -3.925647    0.202776    0.319417
 C    -2.486255   -0.176431    0.012152
 C    -2.074587    0.597169   -1.010636
 C    -3.855449    1.626850    0.940636
 C    -3.400047    2.495310   -0.252928
 C    -3.265537    1.471897   -1.423175
 C    -3.197252    2.105552   -2.796895
 C    -4.460512    0.498201   -1.111434
 C    -5.841684    1.159759   -1.152112
 C    -4.536873   -0.744857   -2.001134
 C    -0.715291    0.706152   -1.587398
 C    -0.358943    0.125730   -2.779799
 C     0.368396    1.460731   -0.978759
 S     1.280434    0.509270   -3.174730
 C     1.514803    1.444026   -1.743790
 C    -1.166194   -0.754241   -3.680383
 C     2.851933    2.060294   -1.488510
 C     3.871247    2.670533    2.457438
 C     2.719536    2.979621    1.734786
 C     4.052118    1.389243    2.980745
 C     1.728823    2.011453    1.528958
 C     3.067103    0.421342    2.789104
 C     1.909382    0.737266    2.082081
 C     0.217724    5.951129   -1.333881
 C     0.283197    4.578686   -1.086909
 C     0.054395    6.848587   -0.280243
 C     0.181544    4.083922    0.218711
 C    -0.054973    6.366157    1.025659
 C    -0.004382    4.996015    1.270528
 H    -2.181181   -3.580545    2.772050
 H    -2.395443   -3.442033    5.228950
 H    -2.110542   -1.258120    6.395517
 H    -1.351490    0.655118    2.611831
 H    -1.578833    0.788806    5.072510
 H    -1.976615   -5.239546   -2.446596
 H    -0.773450   -3.395679   -1.287312
 H    -4.282126   -5.861659   -1.733417
 H    -5.373717   -4.637315    0.140113
 H    -4.186323   -2.792349    1.282996
 H    -4.497949   -0.524417    0.911065
 H    -3.152475    1.664585    1.782270
 H    -4.839819    1.933960    1.322391
 H    -2.446969    3.010167   -0.070350
 H    -4.136319    3.271054   -0.510855
 H    -4.115300    2.677367   -3.004086
 H    -3.077839    1.354619   -3.592253
 H    -2.349135    2.804563   -2.866496
 H    -6.593332    0.483474   -0.714397
 H    -6.142593    1.348308   -2.194840
 H    -5.905217    2.114248   -0.615165
 H    -5.398164   -1.365368   -1.707213
 H    -3.645656   -1.381453   -1.938883
 H    -4.686583   -0.462876   -3.055635
 H    -2.164994   -0.912329   -3.257603
 H    -0.695005   -1.742008   -3.804603
 H    -1.285557   -0.316005   -4.683853
 H     3.427034    1.415144   -0.806531
 H     2.747988    3.056556   -1.039119
 H     3.422953    2.167073   -2.422261
 H     4.637738    3.435562    2.604327
 H     2.602319    3.982274    1.316857
 H     4.959610    1.147958    3.539661
 H     3.193929   -0.585230    3.194515
 H     1.140181   -0.029970    1.946771
 H     0.299516    6.319379   -2.359470
 H     0.415577    3.886105   -1.921253
 H     0.005211    7.922538   -0.474725
 H    -0.191124    7.061975    1.857057
 H    -0.109279    4.628267    2.295961
121
Figure 1_pc1_major01_01 / electronic energy: -4987.95820018 a.u. / lowest freq: 20.32 cm-1
 P     0.926344   -0.829104    0.735849
 C     0.677302    1.516633    2.221345
 C     0.751347    2.314653    3.361450
 C     1.197844    0.217931    2.227107
 C     1.370600    1.830921    4.513805
 C     1.826476   -0.257754    3.383497
 C     1.916322    0.546804    4.518990
 C     3.130335   -4.322361    0.818039
 C     2.059892   -3.427322    0.803697
 C     2.288695   -2.049899    0.842966
 C     4.439043   -3.847187    0.872411
 C     4.674847   -2.471248    0.895219
 C     3.609595   -1.574735    0.870173
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C	-0.814968	-2.249149	2.666999
C	-0.571130	-1.726868	1.255498
C	-1.744110	-1.818554	0.595056
C	-1.665739	-1.146105	3.360111
C	-3.008477	-1.245707	2.607146
C	-2.778333	-2.398670	1.577280
C	-4.066261	-2.940356	0.992423
C	-1.873667	-3.362044	2.418066
C	-2.524952	-3.904233	3.695535
C	-1.357943	-4.575821	1.645339
C	-2.083165	-1.400288	-0.786362
C	-2.153871	-2.313568	-1.811956
C	-2.442210	-0.057968	-1.200186
S	-2.650367	-1.542511	-3.274309
C	-2.770795	0.013899	-2.538013
C	-1.842323	-3.778728	-1.796312
C	-3.216323	1.175112	-3.373073
P	-2.500122	1.296233	0.033964
C	-2.648152	4.941752	-1.973320
C	-3.049909	3.799408	-1.281427
C	-1.307761	5.123767	-2.318150
C	-2.114026	2.820028	-0.925598
C	-0.366089	4.162489	-1.951360
C	-0.767831	3.026898	-1.251035
C	-6.022725	2.494223	1.740113
C	-4.682241	2.334780	1.396735
C	-7.007652	1.766446	1.069488
C	-4.304599	1.464679	0.361780
C	-6.641701	0.884863	0.053794
C	-5.299369	0.736174	-0.300480
H	0.210178	1.909989	1.318485
H	0.329167	3.321832	3.342912
H	1.435202	2.457123	5.406900
H	2.249227	-1.264795	3.405191
H	2.410821	0.164233	5.414917
H	2.935898	-5.396920	0.785363
H	1.039921	-3.809582	0.764940
H	5.276359	-4.549002	0.886384
H	5.698601	-2.090056	0.921588
H	3.806211	-0.498550	0.853395
H	0.085483	-2.550035	3.220157
H	-1.200061	-0.158057	3.261984
H	-1.776460	-1.349525	4.434728
H	-3.287733	-0.312841	2.102730
H	-3.842977	-1.508489	3.274103
H	-4.719383	-3.322361	1.792302
H	-3.894442	-3.758551	0.278634
H	-4.620991	-2.147246	0.466885
H	-1.773677	-4.442211	4.295682
H	-3.315640	-4.627644	3.441265
H	-2.975162	-3.141337	4.342071
H	-0.614851	-5.125026	2.245000
H	-0.896113	-4.313133	0.688760
H	-2.182642	-5.274051	1.431312
H	-0.812272	-3.953986	-1.454354
H	-1.944222	-4.223616	-2.796233
H	-2.515721	-4.327332	-1.122072
H	-2.402613	1.901842	-3.518257
H	-4.052849	1.704935	-2.895584
H	-3.551123	0.841761	-4.365685
H	-3.391084	5.693675	-2.250234
H	-4.105985	3.667878	-1.034595
H	-0.998098	6.020007	-2.861244
H	0.692931	4.294554	-2.183502
H	-0.005031	2.300380	-0.952844
H	-6.299613	3.182502	2.542189
H	-3.915845	2.895792	1.940496
H	-8.059020	1.884292	1.342185
H	-7.405834	0.307591	-0.472433
H	-5.028493	0.042477	-1.099687
H	3.853348	-5.273228	-2.867955
H	4.984522	-3.113144	-2.339501
C	3.293006	-4.335782	-2.896968
C	3.924207	-3.126384	-2.603116
H	1.428109	-5.271304	-3.464673
C	1.936930	-4.333702	-3.225965
H	6.569500	2.212888	0.543010
C	3.211269	-1.930480	-2.628631
H	5.010684	1.424814	2.246803
H	3.723722	-0.999439	-2.374010
C	1.224496	-3.137192	-3.254001
C	1.841238	-1.913469	-2.949286
C	5.929895	3.062916	0.260472
C	4.420157	2.343684	2.112570
H	6.040917	3.221784	-0.820335
O	4.001736	1.671209	-0.138162
H	0.167451	-3.140896	-3.526584
H	4.828908	3.112365	2.785297
H	6.302906	3.955837	0.785490
C	4.486861	2.770981	0.645675
C	1.047333	-0.668112	-2.971210
B	2.655638	1.867312	-0.447585
H	2.650708	0.721185	-3.438697
C	1.598053	0.591216	-3.172412
C	3.466173	3.908585	0.286723
H	4.150358	4.105820	-1.777853
O	2.303365	3.165791	-0.104092

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 H    4.759205    5.385504   -0.689059
 H    3.989365    5.351744    1.826722
 C    3.894911    4.744782   -0.919310
 H    0.943264    1.431083   -3.424871
 C    3.101480    4.823152    1.446839
 H    3.059747    5.395391   -1.219370
 H    2.374226    5.577293    1.110236
Cu    1.438783    0.375232   -1.154580
 H   -0.034315   -0.794147   -3.066252
 H    3.386657    2.127770    2.415952
 H    2.645559    4.262569    2.273304
121
Figure 1_pc1_major01_02 / electronic energy: -4987.95729960 a.u. / lowest freq: 12.21 cm-1
 B    2.149764    1.721002   -0.563761
 O    1.984447    3.078978   -0.289313
 O    3.484503    1.389779   -0.334324
 C    3.257161    3.690170   -0.031134
 C    4.134216    2.455077    0.367336
 C    3.093016    4.736831    1.060491
 C    3.713930    4.354185   -1.330326
 C    4.057968    2.121988    1.858914
 C    5.589367    2.531832   -0.069925
 H    3.014178    2.085230    2.201743
 H    4.605946    2.850845    2.474493
 H    4.499755    1.127746    2.023977
 H    5.684095    2.605903   -1.161414
 H    6.121035    1.623879    0.252840
 H    6.092364    3.398994    0.385625
 H    3.841480    3.611395   -2.131991
 H    4.661436    4.898618   -1.203066
 H    2.946292    5.071986   -1.656001
 H    4.067235    5.160607    1.349761
 H    2.614718    4.315006    1.954400
 H    2.459961    5.560490    0.696947
 C    1.819761   -3.137137   -2.891439
 C    2.833317   -4.083027   -2.767977
 C    2.109826   -1.767876   -3.024028
 C    4.172221   -3.687983   -2.790440
 C    3.463905   -1.387712   -3.055254
 C    4.478882   -2.335664   -2.943328
 C    1.008716   -0.788697   -3.111281
 C    1.189250    0.577554   -3.219197
 H    5.522314   -2.010807   -2.967181
 H    3.732990   -0.334275   -3.150880
 H    4.968698   -4.429371   -2.693245
 H    2.575758   -5.138733   -2.651935
 H    0.776911   -3.462178   -2.873348
 P    0.681152   -1.241327    0.549731
 C    3.397153   -1.754271    0.451001
 C    4.635004   -2.200591    0.913793
 C    2.267625   -1.809272    1.272666
 C    4.759940   -2.690033    2.212367
 C    2.403853   -2.294740    2.581480
 C    3.641719   -2.730832    3.048419
 C   -1.288691   -4.844270    1.202616
 C   -0.457486   -3.741142    1.387167
 C   -0.312725   -2.786265    0.372898
 C   -1.992052   -5.003968    0.006934
 C   -1.850041   -4.061333   -1.009431
 C   -1.008920   -2.965298   -0.823538
 C    0.526753    0.446119    2.975371
 C   -0.159973   -0.412635    1.925524
 C   -1.489995   -0.271228    2.100198
 C    0.247634    1.915487    2.551913
 C   -1.266862    2.056210    2.804622
 C   -1.686605    0.648085    3.325127
 C   -3.037998    0.646324    4.009494
 C   -0.432496    0.259431    4.183120
 C   -0.148239    1.197228    5.361043
 C   -0.457337   -1.163175    4.747580
 C   -2.617282   -0.730660    1.250034
 C   -3.536889   -1.648584    1.694187
 C   -2.959260   -0.183543   -0.060382
 S   -4.846723   -1.799438    0.578109
 C   -4.182319   -0.631251   -0.513641
 C   -3.517770   -2.494913    2.927235
 C   -5.016747   -0.256275   -1.702398
 P   -1.747176    0.852925   -0.979669
 C   -2.650717   -0.540023   -4.753604
 C   -2.405083   -0.464287   -3.385448
 C   -2.748924    0.625423   -5.515149
 C   -2.264940    0.776117   -2.745812
 C   -2.603996    1.863471   -4.892894
 C   -2.363483    1.939413   -3.520032
 C   -1.496471    4.846904   -0.092979
 C   -1.196625    3.537968   -0.473390
 C   -2.800727    5.196993    0.253012
 C   -2.205951    2.569332   -0.514220
 C   -3.811397    4.234275    0.213139
 C   -3.516022    2.927501   -0.168766
 H    3.310444   -1.339598   -0.553057
 H    5.504565   -2.155298    0.253592
 H    5.729622   -3.035536    2.579300
 H    1.542977   -2.319140    3.251954
 H    3.734712   -3.103999    4.071100
 H   -1.393704   -5.582219    2.001545
 H    0.070048   -3.626372    2.335740
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 H   -2.649914   -5.865399   -0.130592
 H   -2.392677   -4.178375   -1.950636
 H   -0.891158   -2.219742   -1.610165
 H    1.586979    0.223872    3.153238
 H    0.528785    2.086745    1.505314
 H    0.834481    2.615675    3.165057
 H   -1.832242    2.324188    1.905797
 H   -1.491609    2.822298    3.561768
 H   -3.056692    1.405667    4.806706
 H   -3.276950   -0.323461    4.467194
 H   -3.842768    0.893352    3.299452
 H    0.844275    0.976059    5.785415
 H   -0.887209    1.039549    6.162858
 H   -0.165432    2.264239    5.106444
 H    0.484718   -1.377087    5.277168
 H   -0.588730   -1.931041    3.974763
 H   -1.272222   -1.276331    5.480665
 H   -2.595071   -2.322001    3.493140
 H   -3.554249   -3.564709    2.669427
 H   -4.373568   -2.282038    3.586965
 H   -4.938059   -0.995043   -2.515288
 H   -4.723205    0.718839   -2.107103
 H   -6.077143   -0.195465   -1.414238
 H   -2.765908   -1.517223   -5.228527
 H   -2.348238   -1.386579   -2.803532
 H   -2.937770    0.566384   -6.589473
 H   -2.679382    2.784338   -5.476147
 H   -2.251682    2.920476   -3.053947
 H   -0.698629    5.592507   -0.054077
 H   -0.160389    3.271163   -0.698019
 H   -3.031580    6.220378    0.558949
 H   -4.835157    4.501114    0.486472
 H   -4.309381    2.176716   -0.177660
Cu    0.836417    0.267955   -1.177705
 H    0.349737    1.211874   -3.517726
 H    2.176488    1.019000   -3.365121
 H    0.015975   -1.205255   -3.294761
121
Figure 1_pc1_major01_03 / electronic energy: -4987.95729939 a.u. / lowest freq: 12.42 cm-1
 B    2.149838    1.721012   -0.563473
 O    1.984580    3.079009   -0.289083
 O    3.484526    1.389704   -0.333868
 C    3.257314    3.690127   -0.030827
 C    4.134248    2.454996    0.367794
 C    3.093153    4.736867    1.060719
 C    3.714245    4.354028   -1.330021
 C    4.057841    2.121998    1.859383
 C    5.589446    2.531625   -0.069334
 H    3.014019    2.085350    2.202124
 H    4.605829    2.850843    2.474969
 H    4.499533    1.127729    2.024538
 H    5.684290    2.605564   -1.160821
 H    6.121033    1.623679    0.253586
 H    6.092445    3.398809    0.386171
 H    3.841818    3.611178   -2.131627
 H    4.661774    4.898410   -1.202713
 H    2.946681    5.071856   -1.655813
 H    4.067382    5.160572    1.350061
 H    2.614728    4.315139    1.954605
 H    2.460213    5.560565    0.697063
 C    1.819806   -3.136828   -2.891817
 C    2.833353   -4.082744   -2.768474
 C    2.109885   -1.767549   -3.024195
 C    4.172261   -3.687706   -2.790845
 C    3.463969   -1.387390   -3.055327
 C    4.478936   -2.335366   -2.943516
 C    1.008786   -0.788348   -3.111333
 C    1.189340    0.577913   -3.219086
 H    5.522371   -2.010512   -2.967289
 H    3.733066   -0.333941   -3.150784
 H    4.968729   -4.429115   -2.693743
 H    2.575783   -5.138465   -2.652598
 H    0.776952   -3.461863   -2.873800
 P    0.681091   -1.241436    0.549600
 C    3.397058   -1.754560    0.450874
 C    4.634866   -2.201019    0.913645
 C    2.267509   -1.809566    1.272509
 C    4.759736   -2.690613    2.212169
 C    2.403671   -2.295186    2.581272
 C    3.641494   -2.731423    3.048191
 C   -1.289002   -4.844326    1.202012
 C   -0.457737   -3.741269    1.386721
 C   -0.312862   -2.786300    0.372554
 C   -1.992306   -5.003859    0.006274
 C   -1.850173   -4.061136   -1.009992
 C   -1.008993   -2.965172   -0.823942
 C    0.526737    0.445768    2.975401
 C   -0.160020   -0.412859    1.925471
 C   -1.490037   -0.271419    2.100158
 C    0.247660    1.915187    2.552084
 C   -1.266827    2.055939    2.804822
 C   -1.686614    0.647775    3.325184
 C   -3.038005    0.645988    4.009557
 C   -0.432516    0.258996    4.183134
 C   -0.148214    1.196666    5.361146
 C   -0.457411   -1.163663    4.747457
 C   -2.617337   -0.730717    1.249940
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 C   -3.536983   -1.648647    1.693995
 C   -2.959285   -0.183450   -0.060422
 S   -4.846820   -1.799332    0.577897
 C   -4.182360   -0.631063   -0.513732
 C   -3.517902   -2.495088    2.926966
 C   -5.016758   -0.255944   -1.702464
 P   -1.747150    0.853064   -0.979591
 C   -2.650688   -0.539514   -4.753660
 C   -2.405063   -0.463907   -3.385495
 C   -2.748853    0.626002   -5.515103
 C   -2.264890    0.776437   -2.745747
 C   -2.603892    1.863991   -4.892737
 C   -2.363389    1.939803   -3.519866
 C   -1.496304    4.846948   -0.092516
 C   -1.196507    3.538040   -0.473061
 C   -2.800546    5.197049    0.253520
 C   -2.205868    2.569444   -0.513983
 C   -3.811251    4.234371    0.213553
 C   -3.515925    2.927625   -0.168488
 H    3.310401   -1.339781   -0.553146
 H    5.504446   -2.155718    0.253471
 H    5.729385   -3.036229    2.579086
 H    1.542775   -2.319598    3.251719
 H    3.734436   -3.104714    4.070831
 H   -1.394109   -5.582345    2.000863
 H    0.069755   -3.626626    2.335334
 H   -2.650219   -5.865232   -0.131374
 H   -2.392761   -4.178052   -1.951240
 H   -0.891129   -2.219552   -1.610493
 H    1.586957    0.223473    3.153239
 H    0.528803    2.086525    1.505495
 H    0.834539    2.615299    3.165282
 H   -1.832208    2.324034    1.906031
 H   -1.491536    2.821953    3.562054
 H   -3.056683    1.405278    4.806820
 H   -3.276969   -0.323823    4.467195
 H   -3.842775    0.893076    3.299538
 H    0.844284    0.975396    5.785504
 H   -0.887199    1.038959    6.162942
 H   -0.165338    2.263702    5.106646
 H    0.484643   -1.377674    5.277007
 H   -0.588857   -1.931446    3.974566
 H   -1.272288   -1.276853    5.480546
 H   -2.595176   -2.322291    3.492862
 H   -3.554469   -3.564858    2.669068
 H   -4.373668   -2.282205    3.586736
 H   -4.938081   -0.994637   -2.515423
 H   -4.723173    0.719199   -2.107070
 H   -6.077156   -0.195125   -1.414316
 H   -2.765904   -1.516669   -5.228669
 H   -2.348253   -1.386252   -2.803662
 H   -2.937693    0.567065   -6.589434
 H   -2.679246    2.784912   -5.475909
 H   -2.251564    2.920822   -3.053694
 H   -0.698435    5.592519   -0.053542
 H   -0.160281    3.271220   -0.697720
 H   -3.031360    6.220409    0.559566
 H   -4.834999    4.501219    0.486920
 H   -4.309310    2.176868   -0.177452
Cu    0.836500    0.268056   -1.177634
 H    0.349835    1.212282   -3.517533
 H    2.176583    1.019365   -3.364964
 H    0.016039   -1.204870   -3.294861
121
Figure 1_ts(CuBadd)_major01_01 / electronic energy: -4987.95489151 a.u. / lowest freq: -155.31 cm-1
 B    2.321262    0.631883   -1.431413
 O    2.236361    1.650687   -2.361791
 O    3.575633    0.635534   -0.840652
 C    3.532311    2.254119   -2.527748
 C    4.255090    1.849455   -1.193871
 C    3.355686    3.750445   -2.728955
 C    4.163848    1.624444   -3.767707
 C    4.019220    2.843440   -0.056636
 C    5.742063    1.564723   -1.335809
 H    2.949281    3.066264    0.059066
 H    4.560088    3.787590   -0.216824
 H    4.372108    2.396563    0.884727
 H    5.933806    0.735567   -2.029572
 H    6.162292    1.290170   -0.356718
 H    6.277356    2.456013   -1.697285
 H    4.306372    0.540915   -3.640620
 H    5.137639    2.077652   -4.003695
 H    3.495293    1.779083   -4.627570
 H    4.331478    4.258305   -2.764321
 H    2.755403    4.197726   -1.926050
 H    2.840649    3.940770   -3.682552
 C    1.716080   -4.558749   -0.259989
 C    2.477408   -5.353208    0.589672
 C    2.201168   -3.326874   -0.758752
 C    3.763177   -4.958475    0.973488
 C    3.509028   -2.954346   -0.371454
 C    4.269012   -3.755344    0.478401
 C    1.361447   -2.503798   -1.618191
 C    1.844952   -1.349624   -2.319555
 H    5.273620   -3.428788    0.762910
 H    3.928345   -2.009224   -0.726726
 H    4.361114   -5.581374    1.642805
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 H    2.062660   -6.294978    0.960552
 H    0.712327   -4.884661   -0.550359
 P    0.522358   -0.224412    1.468033
 C    3.200345   -0.451589    2.169343
 C    4.317581   -0.320552    2.995625
 C    1.951863    0.012751    2.590031
 C    4.194880    0.287087    4.243461
 C    1.834673    0.623377    3.846865
 C    2.951063    0.762174    4.667546
 C   -1.941129   -2.169360    4.175700
 C   -1.166345   -1.187065    3.564360
 C   -0.519250   -1.453221    2.351189
 C   -2.077919   -3.427032    3.582683
 C   -1.430963   -3.700277    2.379343
 C   -0.655683   -2.714924    1.766998
 C    0.292170    2.698411    1.609437
 C   -0.383178    1.335739    1.595234
 C   -1.702121    1.545305    1.412533
 C    0.199970    3.212220    0.144372
 C   -1.311688    3.465712   -0.027746
 C   -1.912442    3.072115    1.357677
 C   -3.311687    3.611242    1.572914
 C   -0.782509    3.558071    2.328881
 C   -0.511931    5.065403    2.288747
 C   -0.995886    3.184585    3.797524
 C   -2.787049    0.581732    1.111898
 C   -3.843869    0.387918    1.966363
 C   -2.943908   -0.133985   -0.148945
 S   -5.056736   -0.595608    1.230161
 C   -4.165861   -0.768981   -0.243411
 C   -4.022033    0.858694    3.374114
 C   -4.836775   -1.512898   -1.359788
 P   -1.568969   -0.234553   -1.366279
 C   -2.175944   -4.205280   -2.230218
 C   -2.098155   -2.984253   -1.568824
 C   -2.020304   -4.264425   -3.617438
 C   -1.881530   -1.796433   -2.282969
 C   -1.792188   -3.091327   -4.332569
 C   -1.724554   -1.862974   -3.670714
 C   -1.098690    2.704957   -4.177354
 C   -0.872460    1.686960   -3.250155
 C   -2.398634    3.124851   -4.454066
 C   -1.948786    1.072829   -2.598774
 C   -3.475623    2.521591   -3.801595
 C   -3.253024    1.501757   -2.878597
 H    3.299950   -0.902721    1.182423
 H    5.287275   -0.691815    2.655291
 H    5.069584    0.395009    4.889474
 H    0.868423    1.005209    4.184090
 H    2.850783    1.244136    5.642892
 H   -2.446654   -1.952705    5.119817
 H   -1.080242   -0.201820    4.027852
 H   -2.690616   -4.193651    4.063086
 H   -1.530412   -4.681494    1.908917
 H   -0.155159   -2.916147    0.816825
 H    1.303588    2.725079    2.037033
 H    0.593697    2.472786   -0.564565
 H    0.786914    4.133594    0.016031
 H   -1.761852    2.870477   -0.831008
 H   -1.531614    4.520177   -0.252787
 H   -3.322090    4.702588    1.425465
 H   -3.691681    3.407962    2.583688
 H   -4.020579    3.175839    0.851102
 H    0.419342    5.293813    2.831607
 H   -1.324809    5.612691    2.791935
 H   -0.413101    5.482679    1.278775
 H   -0.123295    3.488056    4.397703
 H   -1.146375    2.108621    3.950032
 H   -1.872372    3.709960    4.209394
 H   -3.161565    1.462495    3.686115
 H   -4.095078    0.004466    4.065735
 H   -4.933654    1.463884    3.496703
 H   -4.781461   -2.603369   -1.217616
 H   -4.383870   -1.281929   -2.330263
 H   -5.901433   -1.238574   -1.410390
 H   -2.353121   -5.119768   -1.658973
 H   -2.210473   -2.953271   -0.482793
 H   -2.074802   -5.224067   -4.136404
 H   -1.664761   -3.126239   -5.417158
 H   -1.545660   -0.952556   -4.247817
 H   -0.248353    3.180587   -4.672075
 H    0.155318    1.401726   -3.012721
 H   -2.575046    3.927543   -5.174223
 H   -4.496598    2.851151   -4.008322
 H   -4.103457    1.051687   -2.362124
Cu    0.852673   -0.603089   -0.734959
 H    1.288901   -1.052166   -3.215993
 H    2.927464   -1.247084   -2.465049
 H    0.440771   -2.968525   -1.973342
121
Figure 1_ts(CuBadd)_major01_02 / electronic energy: -4987.95448195 a.u. / lowest freq: -142.45 cm-1
 B    2.264962   -0.470333    1.549168
 O    2.179272   -1.453554    2.517362
 O    3.534675   -0.464838    0.993858
 C    3.481098   -2.031314    2.726582
 C    4.220109   -1.660570    1.392293
 C    3.322924   -3.522533    2.976178
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C	4.082700	-1.350172	3.953811
C	4.007409	-2.690535	0.282284
C	5.702611	-1.359073	1.545314
H	2.941598	-2.932162	0.167137
H	4.560338	-3.621945	0.473382
H	4.360662	-2.265480	-0.669178
H	5.877932	-0.505911	2.213824
H	6.133829	-1.113616	0.563289
H	6.239856	-2.233523	1.943215
H	4.213572	-0.270087	3.790194
H	5.057422	-1.782621	4.222629
H	3.400618	-1.482367	4.806784
H	4.305289	-4.014252	3.044612
H	2.742393	-4.006424	2.179948
H	2.795421	-3.688399	3.927600
C	1.454308	4.601768	-0.000121
C	2.196926	5.389275	-0.872154
C	2.008405	3.460105	0.624721
C	3.530883	5.077249	-1.154291
C	3.360820	3.169682	0.335441
C	4.102549	3.963509	-0.537458
C	1.190134	2.647352	1.516295
C	1.709462	1.569103	2.305863
H	5.145430	3.703685	-0.741113
H	3.833717	2.295090	0.789593
H	4.114978	5.695505	-1.839918
H	1.730295	6.261100	-1.339488
H	0.412103	4.861437	0.210063
P	0.622222	0.155808	-1.436344
C	3.309063	0.512770	-1.998591
C	4.497966	0.356967	-2.710913
C	2.140871	-0.128230	-2.419044
C	4.530441	-0.454334	-3.843917
C	2.178561	-0.937875	-3.562918
C	3.368545	-1.103023	-4.268458
C	-1.553377	1.837542	-4.533991
C	-0.753968	0.963162	-3.802434
C	-0.384890	1.277577	-2.488567
C	-1.994618	3.032304	-3.959707
C	-1.620979	3.355980	-2.656945
C	-0.814228	2.482050	-1.927265
C	0.400832	-2.785701	-1.430549
C	-0.262614	-1.420689	-1.519578
C	-1.591254	-1.614737	-1.402449
C	0.213829	-3.233778	0.047284
C	-1.306329	-3.481880	0.133225
C	-1.817112	-3.137190	-1.299469
C	-3.205177	-3.671703	-1.585051
C	-0.634240	-3.668043	-2.180030
C	-0.379155	-5.173776	-2.061926
C	-0.756392	-3.354118	-3.673674
C	-2.687405	-0.636583	-1.197799
C	-3.690054	-0.466445	-2.119602
C	-2.929658	0.100332	0.038385
S	-4.958959	0.512379	-1.475224
C	-4.165188	0.715152	0.049086
C	-3.784194	-0.978552	-3.521283
C	-4.919249	1.448841	1.118246
P	-1.622720	0.269455	1.321243
C	-2.418859	4.229137	2.117379
C	-2.274234	3.006183	1.470631
C	-2.297313	4.308372	3.506656
C	-2.024266	1.834344	2.200458
C	-2.035858	3.152677	4.238429
C	-1.901353	1.922313	3.590858
C	-1.204798	-2.612168	4.201001
C	-0.961329	-1.603100	3.268345
C	-2.505970	-3.056025	4.430101
C	-2.022144	-1.023738	2.562539
C	-3.567636	-2.485129	3.725189
C	-3.327999	-1.475197	2.795795
H	3.288036	1.124855	-1.097326
H	5.402947	0.865434	-2.370024
H	5.463588	-0.586470	-4.396924
H	1.278997	-1.456417	-3.899712
H	3.389253	-1.742414	-5.154276
H	-1.838435	1.584446	-5.557969
H	-0.426347	0.026186	-4.258648
H	-2.627822	3.712373	-4.534543
H	-1.956650	4.291998	-2.203992
H	-0.516696	2.721032	-0.902910
H	1.436818	-2.838482	-1.789676
H	0.563683	-2.461981	0.745569
H	0.790984	-4.147255	0.254090
H	-1.805806	-2.859689	0.884333
H	-1.541793	-4.528004	0.380068
H	-3.239626	-4.756214	-1.396366
H	-3.512186	-3.503864	-2.626883
H	-3.955293	-3.199398	-0.931493
H	0.571051	-5.432445	-2.556108
H	-1.175946	-5.737347	-2.572882
H	-0.324169	-5.545143	-1.031028
H	0.144644	-3.694796	-4.207991
H	-0.883473	-2.283749	-3.879843
H	-1.614175	-3.886998	-4.114441
H	-2.886102	-1.554049	-3.776314
H	-3.860309	-0.146920	-4.239118

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 H   -4.663732   -1.624858   -3.667204
 H   -4.927425    2.536442    0.946777
 H   -4.488904    1.271609    2.109804
 H   -5.965887    1.108735    1.139521
 H   -2.622212    5.129441    1.532533
 H   -2.365556    2.961221    0.383302
 H   -2.404631    5.269615    4.014290
 H   -1.934313    3.202767    5.325151
 H   -1.697140    1.026663    4.182446
 H   -0.366180   -3.062646    4.737464
 H    0.068945   -1.297379    3.070473
 H   -2.695310   -3.852201    5.154195
 H   -4.589013   -2.833911    3.895107
 H   -4.164698   -1.052110    2.235880
Cu    0.779523    0.682017    0.754710
 H    1.152433    1.308052    3.212803
 H    2.792832    1.516730    2.467669
 H    0.236777    3.085214    1.814284
121
Figure 1_ts(CuBadd)_major01_03 / electronic energy: -4987.95448188 a.u. / lowest freq: -142.46 cm-1
 B    2.264996   -0.470245    1.549137
 O    2.179336   -1.453444    2.517357
 O    3.534691   -0.464764    0.993787
 C    3.481167   -2.031208    2.726541
 C    4.220134   -1.660491    1.392219
 C    3.322993   -3.522422    2.976169
 C    4.082818   -1.350047    3.953736
 C    4.007394   -2.690476    0.282235
 C    5.702642   -1.358997    1.545184
 H    2.941579   -2.932108    0.167133
 H    4.560332   -3.621881    0.473330
 H    4.360611   -2.265437   -0.669246
 H    5.877987   -0.505820    2.213671
 H    6.133828   -1.113562    0.563139
 H    6.239897   -2.233439    1.943086
 H    4.213689   -0.269966    3.790094
 H    5.057547   -1.782498    4.222525
 H    3.400766   -1.482224    4.806736
 H    4.305356   -4.014150    3.044558
 H    2.742413   -4.006320    2.179979
 H    2.795540   -3.688268    3.927622
 C    3.360793    3.169749    0.335258
 C    4.102486    3.963553   -0.537694
 C    2.008374    3.460147    0.624544
 C    3.530778    5.077243   -1.154575
 C    1.454233    4.601760   -0.000352
 C    2.196816    5.389244   -0.872436
 C    1.190144    2.647418    1.516179
 C    1.709522    1.569208    2.305771
 H    1.730152    6.261031   -1.339809
 H    0.412024    4.861409    0.209833
 H    4.114845    5.695481   -1.840243
 H    5.145372    3.703748   -0.741350
 H    3.833723    2.295195    0.789448
 P    0.622212    0.155785   -1.436347
 C    3.309036    0.512775   -1.998646
 C    4.497933    0.356966   -2.710976
 C    2.140855   -0.128278   -2.419049
 C    4.530417   -0.454397   -3.843935
 C    2.178552   -0.937984   -3.562880
 C    3.368532   -1.103141   -4.268425
 C   -1.553373    1.837341   -4.534094
 C   -0.753922    0.963035   -3.802495
 C   -0.384925    1.277490   -2.488616
 C   -1.994742    3.032068   -3.959837
 C   -1.621186    3.355784   -2.657061
 C   -0.814387    2.481932   -1.927341
 C    0.400810   -2.785734   -1.430486
 C   -0.262624   -1.420715   -1.519519
 C   -1.591264   -1.614748   -1.402364
 C    0.213824   -3.233795    0.047354
 C   -1.306335   -3.481888    0.133316
 C   -1.817136   -3.137198   -1.299370
 C   -3.205212   -3.671695   -1.584928
 C   -0.634283   -3.668069   -2.179946
 C   -0.379212   -5.173805   -2.061834
 C   -0.756450   -3.354154   -3.673591
 C   -2.687397   -0.636573   -1.197712
 C   -3.690049   -0.466429   -2.119510
 C   -2.929627    0.100364    0.038464
 S   -4.958930    0.512430   -1.475138
 C   -4.165146    0.715205    0.049165
 C   -3.784212   -0.978554   -3.521184
 C   -4.919199    1.448902    1.118327
 P   -1.622675    0.269484    1.321310
 C   -2.418833    4.229141    2.117570
 C   -2.274178    3.006212    1.470782
 C   -2.297329    4.308327    3.506853
 C   -2.024227    1.834346    2.200574
 C   -2.035883    3.152608    4.238591
 C   -1.901351    1.922268    3.590980
 C   -1.204714   -2.612202    4.201000
 C   -0.961254   -1.603112    3.268366
 C   -2.505883   -3.056064    4.430103
 C   -2.022076   -1.023736    2.562583
 C   -3.567557   -2.485149    3.725219
 C   -3.327930   -1.475195    2.795847
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 H     3.288005    1.124909   -1.097414
 H     5.402906    0.865477   -2.370128
 H     5.463559   -0.586539   -4.396947
 H     1.278998   -1.456565   -3.899636
 H     3.389245   -1.742582   -5.154207
 H    -1.838367    1.584212   -5.558081
 H    -0.426205    0.026080   -4.258686
 H    -2.627980    3.712079   -4.534703
 H    -1.956959    4.291777   -2.204130
 H    -0.516913    2.720950   -0.902977
 H     1.436790   -2.838529   -1.789627
 H     0.563689   -2.461991    0.745626
 H     0.790977   -4.147272    0.254163
 H    -1.805798   -2.859693    0.884429
 H    -1.541802   -4.528010    0.380165
 H    -3.239674   -4.756204   -1.396237
 H    -3.512236   -3.503855   -2.626755
 H    -3.955311   -3.199375   -0.931360
 H     0.570982   -5.432488   -2.556032
 H    -1.176018   -5.737370   -2.572772
 H    -0.324211   -5.545164   -1.030934
 H     0.144570   -3.694859   -4.207918
 H    -0.883508   -2.283785   -3.879770
 H    -1.614251   -3.887020   -4.114341
 H    -2.886139   -1.554082   -3.776211
 H    -3.860303   -0.146929   -4.239029
 H    -4.663771   -1.624834   -3.667090
 H    -4.927359    2.536504    0.946865
 H    -4.488862    1.271656    2.109885
 H    -5.965842    1.108813    1.139594
 H    -2.622174    5.129465    1.532751
 H    -2.365468    2.961291    0.383450
 H    -2.404669    5.269551    4.014519
 H    -1.934368    3.202659    5.325319
 H    -1.697147    1.026601    4.182544
 H    -0.366090   -3.062693    4.737444
 H     0.069017   -1.297381    3.070493
 H    -2.695216   -3.852258    5.154180
 H    -4.588934   -2.833931    3.895143
 H    -4.164635   -1.052090    2.235953
Cu     0.779519    0.682066    0.754689
 H     1.152540    1.308190    3.212749
 H     2.792901    1.516859    2.467528
 H     0.236795    3.085281    1.814190
121
Figure 1_ts(CuBadd)_major01_04 / electronic energy: -4987.94957683 a.u. / lowest freq: -183.19 cm-1
 P     0.834443   -0.920921    0.907577
 C     0.510961    1.363039    2.467311
 C     0.534232    2.118688    3.638379
 C     0.959172    0.037260    2.469328
 C     1.026618    1.561208    4.818167
 C     1.451997   -0.516781    3.656497
 C     1.489943    0.244708    4.823710
 C     3.133915   -4.346279    0.787601
 C     2.039075   -3.480816    0.784536
 C     2.218867   -2.115006    1.013329
 C     4.416303   -3.852834    1.017963
 C     4.603763   -2.485724    1.230255
 C     3.514143   -1.619582    1.220791
 C    -1.077207   -2.588533    2.440653
 C    -0.676439   -1.880764    1.154935
 C    -1.747854   -1.899042    0.337379
 C    -2.053402   -1.601888    3.144562
 C    -3.286282   -1.637013    2.215332
 C    -2.874669   -2.632801    1.083481
 C    -4.036660   -3.123001    0.245367
 C    -2.049676   -3.680761    1.906987
 C    -2.838336   -4.400908    3.006569
 C    -1.391001   -4.768943    1.059031
 C    -1.911861   -1.288556   -1.003468
 C    -1.725236   -2.020771   -2.151086
 C    -2.330167    0.074643   -1.265669
 S    -2.076515   -1.064168   -3.542001
 C    -2.465570    0.336131   -2.613743
 C    -1.246646   -3.431637   -2.298452
 C    -2.888015    1.582803   -3.329095
 P    -2.620868    1.236398    0.119997
 C    -2.716203    5.154403   -1.276531
 C    -3.132858    3.912299   -0.796485
 C    -1.368151    5.391227   -1.546273
 C    -2.204188    2.886796   -0.582970
 C    -0.433165    4.380033   -1.321975
 C    -0.850449    3.142725   -0.837195
 C    -6.382020    1.959991    1.567206
 C    -5.003146    1.914888    1.372952
 C    -7.237757    1.356871    0.643768
 C    -4.457849    1.286732    0.242532
 C    -6.705517    0.715847   -0.473993
 C    -5.324653    0.682271   -0.675361
 H     0.151002    1.815022    1.541832
 H     0.175561    3.150329    3.622640
 H     1.054607    2.154050    5.735577
 H     1.817831   -1.546284    3.673270
 H     1.884018   -0.194004    5.743334
 H     2.978567   -5.412200    0.606570
 H     1.040726   -3.877133    0.601295
 H     5.272249   -4.531846    1.020634
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 H     5.607849   -2.086928    1.393122
 H     3.674807   -0.547520    1.352298
 H    -0.246100   -2.940363    3.067700
 H    -1.614824   -0.598265    3.227080
 H    -2.290477   -1.939585    4.163649
 H    -3.540788   -0.653065    1.805556
 H    -4.186702   -2.009084    2.725767
 H    -4.769889   -3.652192    0.873572
 H    -3.713682   -3.809905   -0.551075
 H    -4.557948   -2.278086   -0.231369
 H    -2.150268   -4.994098    3.630173
 H    -3.559202   -5.104817    2.561569
 H    -3.399848   -3.738881    3.676709
 H    -0.693908   -5.363251    1.670935
 H    -0.839437   -4.370949    0.201660
 H    -2.151904   -5.463216    0.668799
 H    -0.241330   -3.546445   -1.865480
 H    -1.189337   -3.729546   -3.354375
 H    -1.918723   -4.137806   -1.789066
 H    -2.083407    2.334477   -3.336575
 H    -3.762721    2.038931   -2.845613
 H    -3.152576    1.366027   -4.373919
 H    -3.455182    5.941894   -1.444111
 H    -4.194542    3.742394   -0.603915
 H    -1.045862    6.365054   -1.922843
 H     0.631291    4.545560   -1.499357
 H    -0.098812    2.368482   -0.658157
 H    -6.790609    2.456251    2.450641
 H    -4.338191    2.371186    2.112673
 H    -8.318768    1.381669    0.800233
 H    -7.368768    0.236835   -1.198275
 H    -4.920841    0.175133   -1.554594
 H     4.076256   -4.742328   -3.224369
 H     5.077942   -2.851425   -1.933199
 C     3.572824   -3.773949   -3.177281
 C     4.128197   -2.714452   -2.457786
 H     1.906625   -4.377535   -4.418437
 C     2.358629   -3.565493   -3.840994
 H     6.479323    1.907555    0.792493
 C     3.490023   -1.478149   -2.389339
 H     4.810409    1.233077    2.423604
 H     3.948721   -0.681021   -1.797433
 C     1.715020   -2.335908   -3.777279
 C     2.246041   -1.254044   -3.033722
 C     5.902681    2.786933    0.469117
 C     4.255260    2.164864    2.239170
 H     6.079783    2.929650   -0.604851
 O     3.934766    1.491136   -0.034865
 H     0.763608   -2.195433   -4.297948
 H     4.645870    2.931239    2.924368
 H     6.289770    3.664530    1.008779
 C     4.429052    2.572840    0.776024
 C     1.521629    0.002010   -2.923516
 B     2.627899    1.768059   -0.392359
 H     3.242034    1.301485   -2.527391
 C     2.151529    1.214894   -2.417988
 C     3.489249    3.759346    0.351642
 H     4.263177    3.863055   -1.687582
 O     2.302003    3.067644   -0.077646
 H     4.901806    5.130984   -0.605102
 H     4.014283    5.202394    1.886762
 C     4.010667    4.536947   -0.855229
 H     1.641947    2.148842   -2.683371
 C     3.118274    4.714043    1.474641
 H     3.228619    5.227638   -1.204305
 H     2.449607    5.498144    1.089090
Cu     1.305052    0.290822   -0.885408
 H     0.596183    0.097057   -3.496694
 H     3.198472    1.983527    2.483136
 H     2.593624    4.196063    2.288331
121
Figure 1_ts(CuBadd)_major01_05 / electronic energy: -4987.94957683 a.u. / lowest freq: -183.19 cm-1
 P     0.834441   -0.920913    0.907581
 C     0.510951    1.363043    2.467318
 C     0.534232    2.118695    3.638384
 C     0.959184    0.037272    2.469328
 C     1.026650    1.561224    4.818163
 C     1.452041   -0.516760    3.656489
 C     1.489996    0.244732    4.823700
 C     4.603765   -2.485714    1.230229
 C     3.514142   -1.619574    1.220774
 C     2.218866   -2.115000    1.013322
 C     4.416307   -3.852823    1.017934
 C     3.133918   -4.346271    0.787580
 C     2.039076   -3.480810    0.784527
 C    -1.077208   -2.588498    2.440686
 C    -0.676443   -1.880747    1.154957
 C    -1.747859   -1.899038    0.337403
 C    -2.053403   -1.601846    3.144583
 C    -3.286283   -1.636983    2.215355
 C    -2.874673   -2.632787    1.083517
 C    -4.036668   -3.123000    0.245415
 C    -2.049676   -3.680735    1.907036
 C    -2.838333   -4.400868    3.006628
 C    -1.390998   -4.768926    1.059094
 C    -1.911866   -1.288569   -1.003452
 C    -1.725239   -2.020800   -2.151060
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 C   -2.330162    0.074629   -1.265671
 S   -2.076505   -1.064212   -3.541988
 C   -2.465556    0.336101   -2.613750
 C   -1.246648   -3.431668   -2.298398
 C   -2.887993    1.582767   -3.329118
 P   -2.620876    1.236392    0.119984
 C   -2.716206    5.154388   -1.276571
 C   -3.132865    3.912286   -0.796526
 C   -1.368150    5.391217   -1.546287
 C   -2.204194    2.886788   -0.582984
 C   -0.433164    4.380029   -1.321963
 C   -0.850451    3.142723   -0.837183
 C   -6.382038    1.959984    1.567169
 C   -5.003162    1.914882    1.372922
 C   -7.237769    1.356863    0.643727
 C   -4.457859    1.286726    0.242505
 C   -6.705523    0.715842   -0.474032
 C   -5.324658    0.682266   -0.675393
 H    0.150965    1.815018    1.541845
 H    0.175543    3.150330    3.622650
 H    1.054646    2.154068    5.735572
 H    1.817892   -1.546256    3.673257
 H    1.884095   -0.193972    5.743317
 H    5.607851   -2.086915    1.393089
 H    3.674805   -0.547512    1.352282
 H    5.272254   -4.531834    1.020597
 H    2.978571   -5.412191    0.606547
 H    1.040726   -3.877130    0.601295
 H   -0.246100   -2.940317    3.067736
 H   -1.614826   -0.598221    3.227089
 H   -2.290477   -1.939530    4.163674
 H   -3.540788   -0.653041    1.805565
 H   -4.186703   -2.009045    2.725795
 H   -4.769886   -3.652192    0.873631
 H   -3.713695   -3.809906   -0.551027
 H   -4.557966   -2.278091   -0.231320
 H   -2.150266   -4.994056    3.630235
 H   -3.559205   -5.104779    2.561638
 H   -3.399839   -3.738833    3.676765
 H   -0.693902   -5.363223    1.671004
 H   -0.839438   -4.370940    0.201717
 H   -2.151899   -5.463207    0.668872
 H   -1.918649   -4.137808   -1.788873
 H   -0.241279   -3.546440   -1.865539
 H   -1.189472   -3.729650   -3.354308
 H   -2.083378    2.334434   -3.336613
 H   -3.762692    2.038910   -2.845637
 H   -3.152561    1.365978   -4.373938
 H   -3.455185    5.941875   -1.444171
 H   -4.194552    3.742378   -0.603975
 H   -1.045858    6.365043   -1.922857
 H    0.631296    4.545559   -1.499323
 H   -0.098815    2.368486   -0.658121
 H   -6.790631    2.456243    2.450603
 H   -4.338211    2.371179    2.112647
 H   -8.318781    1.381661    0.800187
 H   -7.368770    0.236830   -1.198318
 H   -4.920843    0.175132   -1.554627
 H    4.076276   -4.742315   -3.224405
 H    5.077954   -2.851415   -1.933225
 C    3.572836   -3.773940   -3.177307
 C    4.128205   -2.714445   -2.457806
 H    1.906638   -4.377529   -4.418463
 C    2.358638   -3.565487   -3.841016
 H    6.479327    1.907575    0.792450
 C    3.490023   -1.478146   -2.389348
 H    4.810430    1.233050    2.423567
 H    3.948718   -0.681018   -1.797440
 C    1.715022   -2.335907   -3.777291
 C    2.246040   -1.254044   -3.033729
 C    5.902671    2.786953    0.469097
 C    4.255277    2.164839    2.239158
 H    6.079761    2.929691   -0.604871
 O    3.934768    1.491141   -0.034884
 H    0.763607   -2.195435   -4.297956
 H    4.645896    2.931203    2.924362
 H    6.289758    3.664545    1.008769
 C    4.429048    2.572839    0.776016
 C    1.521624    0.002008   -2.923519
 B    2.627896    1.768056   -0.392368
 H    3.242027    1.301486   -2.527398
 C    2.151523    1.214894   -2.417991
 C    3.489228    3.759342    0.351657
 H    4.263130    3.863103   -1.687573
 O    2.301990    3.067633   -0.077640
 H    4.901779    5.130999   -0.605068
 H    4.014241    5.202393    1.886783
 C    4.010634    4.536973   -0.855198
 H    1.641939    2.148841   -2.683372
 C    3.118241    4.714016    1.474672
 H    3.228585    5.227677   -1.204246
 H    2.449543    5.498098    1.089136
Cu    1.305057    0.290813   -0.885412
 H    0.596171    0.097051   -3.496687
 H    3.198493    1.983496    2.483137
 H    2.593616    4.196018    2.288366
121
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Figure 1_ts(CuBadd)_major01_06 / electronic energy: -4987.94669284 a.u. / lowest freq: -34.62 cm-1

B	-2.851463	0.511325	-0.393898
O	-3.557503	-0.683320	-0.495222
O	-3.702134	1.502676	0.066142
C	-4.957598	-0.427804	-0.321209
C	-4.935237	0.905632	0.500469
C	-5.594516	-1.613265	0.387153
C	-5.567024	-0.258436	-1.713003
C	-4.825341	0.666074	2.006337
C	-6.081214	1.861568	0.208413
H	-4.008816	-0.033121	2.239648
H	-5.758274	0.260224	2.424235
H	-4.615577	1.620986	2.509049
H	-6.091832	2.172941	-0.844441
H	-5.977076	2.767011	0.824905
H	-7.050033	1.396470	0.447016
H	-5.125267	0.598551	-2.242999
H	-6.656451	-0.113727	-1.667040
H	-5.367685	-1.164199	-2.305551
H	-6.651405	-1.411260	0.620000
H	-5.068313	-1.861031	1.318442
H	-5.554711	-2.499649	-0.263952
C	1.147258	2.390647	-4.109661
C	1.806949	3.592474	-4.356899
C	0.027306	2.330556	-3.256119
C	1.370542	4.777019	-3.759809
C	-0.402652	3.538667	-2.665626
C	0.259983	4.737128	-2.912875
C	-0.647593	1.053315	-3.011067
C	-1.985444	0.985553	-2.555273
H	-0.090724	5.652128	-2.428118
H	-1.246148	3.533092	-1.970489
H	1.890570	5.719014	-3.948336
H	2.673746	3.603260	-5.023443
H	1.506553	1.470357	-4.578786
P	-0.289351	-1.736342	-0.638395
C	-2.072498	-2.830294	-2.448540
C	-2.567716	-3.768858	-3.353278
C	-0.823067	-3.016652	-1.841000
C	-1.819403	-4.903241	-3.666379
C	-0.086696	-4.169784	-2.147703
C	-0.580026	-5.103784	-3.057671
C	-0.933146	-4.340097	2.518398
C	-0.551701	-3.817302	1.283952
C	-0.821360	-2.481073	0.964998
C	-1.584162	-3.530424	3.450503
C	-1.857692	-2.199160	3.139372
C	-1.483831	-1.682098	1.900061
C	2.448259	-2.084853	-1.728977
C	1.510327	-1.862173	-0.554338
C	2.270092	-1.503396	0.501212
C	3.004550	-0.673471	-2.078187
C	3.941853	-0.378899	-0.889492
C	3.744317	-1.604047	0.048493
C	4.810375	-1.714834	1.119194
C	3.647527	-2.761662	-1.010900
C	4.892252	-2.929272	-1.888813
C	3.328683	-4.141981	-0.430035
C	1.813330	-0.984896	1.819141
C	2.005634	-1.714160	2.968258
C	1.173543	0.308491	2.080755
S	1.489534	-0.834573	4.355677
C	0.987948	0.534914	3.428919
C	2.522554	-3.108079	3.131833
C	0.498094	1.716038	4.216721
P	0.689736	1.450778	0.708710
C	-2.306344	3.637736	2.503060
C	-1.537032	2.597322	1.991679
C	-1.833159	4.949544	2.462164
C	-0.266003	2.842817	1.457468
C	-0.583424	5.209617	1.904311
C	0.196483	4.164245	1.408260
C	3.774685	3.421174	-1.166256
C	2.563180	2.786907	-0.893144
C	4.734488	3.556187	-0.164884
C	2.298218	2.282950	0.382062
C	4.474995	3.061341	1.114665
C	3.263385	2.430503	1.387712
H	-2.673633	-1.959656	-2.175448
H	-3.544566	-3.610922	-3.816932
H	-2.203336	-5.635409	-4.380896
H	0.877216	-4.349609	-1.669578
H	0.006589	-5.996299	-3.288503
H	-0.717969	-5.385105	2.754079
H	-0.037582	-4.461676	0.566924
H	-1.878235	-3.939272	4.420279
H	-2.363230	-1.557670	3.865310
H	-1.693797	-0.640657	1.650826
H	2.028171	-2.620920	-2.588977
H	2.185005	0.055501	-2.163753
H	3.540604	-0.682892	-3.038548
H	3.705830	0.549658	-0.367490
H	4.994375	-0.308400	-1.201620
H	5.812256	-1.649115	0.666864
H	4.755156	-2.664738	1.668596
H	4.726060	-0.896519	1.851806
H	4.691352	-3.661632	-2.686829

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 H    5.732049   -3.320617   -1.292460
 H    5.234012   -2.006599   -2.373336
 H    3.234395   -4.883392   -1.239606
 H    2.397819   -4.162299    0.150620
 H    4.145305   -4.486350    0.224678
 H    2.678630   -3.574244    2.152507
 H    1.800974   -3.729107    3.684448
 H    3.474998   -3.133254    3.684242
 H   -0.599781    1.748469    4.275889
 H    0.836291    2.664135    3.781728
 H    0.882032    1.666057    5.246039
 H   -3.289191    3.424413    2.928952
 H   -1.934148    1.581880    2.012946
 H   -2.442418    5.766842    2.855249
 H   -0.204857    6.233285    1.853472
 H    1.174112    4.393290    0.982042
 H    3.966542    3.801849   -2.171929
 H    1.826380    2.664500   -1.684253
 H    5.687555    4.045592   -0.379404
 H    5.223728    3.161669    1.904001
 H    3.078542    2.033314    2.388224
Cu   -0.859444    0.542672   -0.912529
 H   -2.572208    0.106446   -2.834487
 H   -2.576503    1.905447   -2.503498
 H   -0.230693    0.184107   -3.528946
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Figure 1_L-Cu-alkyl_major01_01 / electronic energy: -4988.00639632 a.u. / lowest freq: 5.96 cm-1
 B    3.707947    1.488549   -0.882638
 O    3.385854    2.655812   -0.227835
 O    4.520227    0.690176   -0.113354
 C    4.205254    2.745051    0.951960
 C    4.559961    1.238251    1.216542
 C    3.421492    3.421389    2.062469
 C    5.427784    3.584882    0.583161
 C    3.496849    0.505393    2.032100
 C    5.936430    1.005316    1.816900
 H    2.503651    0.618907    1.573820
 H    3.451880    0.867042    3.069417
 H    3.733234   -0.567674    2.052201
 H    6.734802    1.376330    1.161107
 H    6.097965   -0.071634    1.972476
 H    6.022941    1.505218    2.793591
 H    6.022827    3.103640   -0.207423
 H    6.077479    3.759182    1.452803
 H    5.089743    4.561095    0.205272
 H    3.979995    3.385773    3.010154
 H    2.446124    2.944659    2.210463
 H    3.247624    4.478536    1.812463
 C    1.832627   -2.292114   -3.273286
 C    2.218956   -3.621015   -3.402981
 C    2.608859   -1.344772   -2.558104
 C    3.417719   -4.074268   -2.841659
 C    3.829072   -1.821664   -2.024252
 C    4.217717   -3.155120   -2.162166
 C    2.123946    0.040871   -2.395812
 C    3.200339    1.149368   -2.324095
 H    5.165580   -3.481173   -1.722739
 H    4.464206   -1.139977   -1.455583
 H    3.723201   -5.118359   -2.943247
 H    1.579858   -4.313549   -3.959154
 H    0.896967   -1.956174   -3.732589
 P   -0.040530   -1.480133    0.748012
 C    2.340305   -2.819071    1.160925
 C    3.234656   -3.666792    1.815653
 C    1.084673   -2.553169    1.715836
 C    2.881044   -4.243801    3.034002
 C    0.730310   -3.143061    2.936364
 C    1.628363   -3.979966    3.594883
 C   -3.230509   -4.091242    0.370436
 C   -2.351629   -3.143682    0.889859
 C   -1.271725   -2.689103    0.124605
 C   -3.034143   -4.600817   -0.914480
 C   -1.951175   -4.164117   -1.676128
 C   -1.074229   -3.210202   -1.159056
 C   -0.193481    0.166530    3.148956
 C   -0.910289   -0.479402    1.975510
 C   -2.119161    0.114055    1.875886
 C    0.121300    1.610961    2.662076
 C   -1.272797    2.265067    2.608355
 C   -2.230556    1.114254    3.044107
 C   -3.607606    1.602611    3.442853
 C   -1.368304    0.393655    4.135547
 C   -1.013249    1.263980    5.344632
 C   -1.977194   -0.901343    4.679230
 C   -3.118088    0.075176    0.781772
 C   -4.387087   -0.417540    0.961976
 C   -2.932429    0.675805   -0.533307
 S   -5.368977   -0.111131   -0.426940
 C   -4.092031    0.683307   -1.279892
 C   -4.953940   -1.171714    2.122194
 C   -4.396454    1.247501   -2.634406
 P   -1.276896    1.179375   -1.138762
 C   -1.570423   -0.693342   -4.762413
 C   -1.663643   -0.382528   -3.408715
 C   -1.149514    0.274261   -5.677008
 C   -1.350785    0.905061   -2.950811
 C   -0.829450    1.553793   -5.226003
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 C   -0.927086    1.869255   -3.869739
 C    0.265262    4.911108   -0.573769
 C    0.107453    3.540744   -0.775486
 C   -0.854249    5.740488   -0.507511
 C   -1.173053    2.991616   -0.926823
 C   -2.132712    5.197429   -0.647525
 C   -2.293318    3.828845   -0.857057
 H    2.622164   -2.354105    0.212253
 H    4.211534   -3.868762    1.370185
 H    3.581757   -4.902905    3.552189
 H   -0.249774   -2.942801    3.377436
 H    1.350172   -4.433018    4.549306
 H   -4.074464   -4.435560    0.973065
 H   -2.513995   -2.744956    1.892950
 H   -3.726881   -5.342265   -1.319716
 H   -1.786396   -4.564039   -2.679446
 H   -0.224359   -2.870487   -1.756978
 H    0.675891   -0.378341    3.540927
 H    0.614394    1.597335    1.679657
 H    0.794220    2.124659    3.362714
 H   -1.538298    2.642126    1.612850
 H   -1.356257    3.115678    3.301124
 H   -3.522776    2.374712    4.223575
 H   -4.241413    0.797041    3.838649
 H   -4.132176    2.055997    2.587306
 H   -0.274626    0.744712    5.975836
 H   -1.906476    1.439033    5.964891
 H   -0.593798    2.244885    5.088436
 H   -1.274218   -1.387646    5.373931
 H   -2.224495   -1.626857    3.893975
 H   -2.897963   -0.689664    5.245889
 H   -4.192219   -1.303740    2.900611
 H   -5.290909   -2.173700    1.812144
 H   -5.818461   -0.656837    2.569195
 H   -4.335147    0.477106   -3.419259
 H   -3.695084    2.047401   -2.899379
 H   -5.413456    1.666423   -2.657410
 H   -1.820222   -1.701043   -5.103387
 H   -1.988026   -1.149666   -2.700287
 H   -1.067345    0.029755   -6.738480
 H   -0.496762    2.316413   -5.934019
 H   -0.666038    2.875021   -3.531731
 H    1.268455    5.327102   -0.457802
 H    0.990418    2.895246   -0.798303
 H   -0.731427    6.813076   -0.339681
 H   -3.011542    5.843989   -0.589983
 H   -3.297630    3.408688   -0.949907
Cu    0.753203   -0.095427   -0.892432
 H    2.765642    2.077342   -2.733281
 H    4.067186    0.911852   -2.977974
 H    1.456107    0.258092   -3.247441
121
Figure 1_L-Cu-alkyl_major01_02 / electronic energy: -4988.00658408 a.u. / lowest freq: 16.00 cm-1
 B    3.725315    1.294016   -1.152703
 O    3.387250    2.561231   -0.735471
 O    4.545009    0.670078   -0.242853
 C    4.184217    2.881902    0.418729
 C    4.558013    1.456280    0.962098
 C    3.364298    3.735063    1.370252
 C    5.398338    3.665403   -0.077816
 C    3.493395    0.869881    1.887564
 C    5.928972    1.358819    1.610262
 H    2.501533    0.899231    1.413439
 H    3.442451    1.404918    2.846761
 H    3.732685   -0.183324    2.092481
 H    6.731869    1.619201    0.908358
 H    6.103278    0.329826    1.958011
 H    5.993252    2.026751    2.482601
 H    6.021225    3.060304   -0.753373
 H    6.024701    4.012150    0.756831
 H    5.050793    4.547421   -0.635683
 H    3.897248    3.881217    2.321986
 H    2.391733    3.275972    1.578251
 H    3.184457    4.725873    0.927082
 C    1.860479   -2.879796   -2.781317
 C    2.242878   -4.209500   -2.641740
 C    2.618497   -1.813189   -2.235476
 C    3.421546   -4.546092   -1.968217
 C    3.821689   -2.178707   -1.586694
 C    4.207591   -3.513047   -1.455720
 C    2.136159   -0.421329   -2.348765
 C    3.216952    0.676287   -2.498263
 H    5.141948   -3.747497   -0.936283
 H    4.444921   -1.399321   -1.144116
 H    3.723417   -5.590209   -1.856501
 H    1.615218   -4.996175   -3.071358
 H    0.940549   -2.639294   -3.324482
 P   -0.025541   -1.287471    1.042785
 C    2.287606   -2.627549    1.735318
 C    3.140644   -3.368364    2.553927
 C    1.053384   -2.182790    2.220983
 C    2.769893   -3.656899    3.866564
 C    0.681582   -2.483529    3.537716
 C    1.540434   -3.211392    4.358530
 C   -3.207731   -3.937918    0.994736
 C   -2.341917   -2.920166    1.388375
 C   -1.242512   -2.583537    0.590591
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 C   -2.979143   -4.635140   -0.193461
 C   -1.875802   -4.316568   -0.983433
 C   -1.012306   -3.293157   -0.592630
 C   -0.234335    0.776012    3.083963
 C   -0.928727   -0.084590    2.041457
 C   -2.136818    0.472085    1.808050
 C    0.090402    2.100222    2.334941
 C   -1.302349    2.726519    2.130339
 C   -2.269348    1.678018    2.761096
 C   -3.652486    2.232329    3.033086
 C   -1.427700    1.183014    3.986074
 C   -1.096405    2.270501    5.012319
 C   -2.047793    0.013648    4.755466
 C   -3.121039    0.212930    0.730073
 C   -4.390225   -0.241215    0.992324
 C   -2.922436    0.533799   -0.678527
 S   -5.356929   -0.231191   -0.439288
 C   -4.074368    0.385652   -1.422102
 C   -4.964792   -0.756175    2.273393
 C   -4.372014    0.676907   -2.861798
 P   -1.260990    0.907931   -1.356513
 C   -1.520159   -1.541368   -4.621843
 C   -1.622250   -1.013125   -3.338003
 C   -1.104686   -0.732894   -5.682012
 C   -1.323424    0.334964   -3.097047
 C   -0.799281    0.606465   -5.446790
 C   -0.905854    1.139649   -4.161033
 C    0.308616    4.670035   -1.383130
 C    0.140910    3.286342   -1.368543
 C   -0.804349    5.506405   -1.470385
 C   -1.141806    2.728613   -1.452212
 C   -2.085234    4.956226   -1.549333
 C   -2.255277    3.572854   -1.541199
 H    2.583773   -2.389968    0.709434
 H    4.099217   -3.716196    2.161638
 H    3.438828   -4.232406    4.510940
 H   -0.281562   -2.143165    3.926359
 H    1.248626   -3.436662    5.387075
 H   -4.067657   -4.190346    1.619911
 H   -2.529208   -2.377667    2.317570
 H   -3.663045   -5.429894   -0.500724
 H   -1.684901   -4.860569   -1.911591
 H   -0.147671   -3.044348   -1.212879
 H    0.626890    0.318449    3.588924
 H    0.602068    1.898327    1.383070
 H    0.750006    2.741952    2.935749
 H   -1.547702    2.902328    1.075845
 H   -1.400401    3.694280    2.644174
 H   -3.578940    3.148521    3.639404
 H   -4.290424    1.523286    3.578657
 H   -4.166114    2.498033    2.095953
 H   -0.366647    1.886458    5.742966
 H   -2.000466    2.554719    5.573863
 H   -0.675976    3.187777    4.581408
 H   -1.358314   -0.330348    5.542664
 H   -2.280099   -0.848076    4.116508
 H   -2.978644    0.327068    5.254416
 H   -4.214446   -0.714651    3.072111
 H   -5.279960   -1.806354    2.166754
 H   -5.844842   -0.178415    2.595839
 H   -4.278763   -0.223235   -3.489525
 H   -3.686985    1.432781   -3.264118
 H   -5.398376    1.057412   -2.972478
 H   -1.758141   -2.593914   -4.793574
 H   -1.941966   -1.656873   -2.514105
 H   -1.015435   -1.148819   -6.688152
 H   -0.471753    1.246567   -6.269407
 H   -0.657810    2.190178   -3.992550
 H    1.314207    5.090524   -1.312797
 H    1.017906    2.639891   -1.272878
 H   -0.674898    6.591316   -1.471049
 H   -2.958378    5.609961   -1.611872
 H   -3.261529    3.148783   -1.584431
Cu    0.779464   -0.252362   -0.834516
 H    2.783180    1.507020   -3.080660
 H    4.081035    0.311153   -3.093557
 H    1.470188   -0.374534   -3.227731
121
Figure 1_L-Cu-alkyl_major01_03 / electronic energy: -4988.00414970 a.u. / lowest freq: 20.39 cm-1
 P    0.474095   -1.054978    1.076352
 C    0.266777    1.237146    2.620360
 C    0.095959    1.979123    3.788786
 C    0.359063   -0.157304    2.667348
 C    0.022404    1.329566    5.019017
 C    0.287998   -0.802615    3.910148
 C    0.122900   -0.062300    5.078091
 C    2.755393   -4.388217    0.458398
 C    1.764308   -3.412766    0.395039
 C    1.727641   -2.370819    1.331847
 C    3.735448   -4.325039    1.449993
 C    3.718284   -3.280297    2.372213
 C    2.720590   -2.306063    2.314759
 C   -1.737859   -2.787529    2.056227
 C   -1.091428   -1.949246    0.967531
 C   -1.980668   -1.837462   -0.039338
 C   -2.819519   -1.855525    2.673476
 C   -3.844417   -1.736306    1.525444
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C	-3.237057	-2.614703	0.382907
C	-4.237438	-2.965319	-0.698476
C	-2.590878	-3.777439	1.213653
C	-3.585200	-4.605144	2.033372
C	-1.759157	-4.762702	0.390793
C	-1.871643	-1.052092	-1.290703
C	-1.578282	-1.647005	-2.494892
C	-2.101849	0.376004	-1.408126
S	-1.604887	-0.480972	-3.767346
C	-1.997603	0.823778	-2.708519
C	-1.220238	-3.073358	-2.779228
C	-2.163695	2.196894	-3.282642
P	-2.471285	1.370609	0.084638
C	-2.027456	5.462322	-0.477055
C	-2.600099	4.204943	-0.280715
C	-0.655759	5.587036	-0.691988
C	-1.809242	3.048766	-0.299719
C	0.143430	4.443132	-0.707619
C	-0.428865	3.188640	-0.507499
C	-6.319071	2.280781	1.151416
C	-4.937796	2.097769	1.132370
C	-7.081272	1.958129	0.027617
C	-4.294379	1.613563	-0.016919
C	-6.454164	1.456379	-1.112167
C	-5.068942	1.287603	-1.136340
H	0.329454	1.750004	1.659142
H	0.022125	3.067433	3.731034
H	-0.111743	1.905830	5.937478
H	0.361613	-1.890483	3.971583
H	0.067472	-0.575111	6.040960
H	2.769015	-5.192340	-0.280070
H	1.019200	-3.450624	-0.403371
H	4.517394	-5.086404	1.496967
H	4.487894	-3.218365	3.145172
H	2.727500	-1.491256	3.041102
H	-1.047286	-3.243658	2.778805
H	-2.392916	-0.885057	2.961017
H	-3.258208	-2.301482	3.577721
H	-3.996292	-0.702859	1.190881
H	-4.833236	-2.127123	1.807687
H	-5.104557	-3.485350	-0.262609
H	-3.809119	-3.618553	-1.472217
H	-4.612619	-2.056803	-1.195142
H	-3.037919	-5.288489	2.702359
H	-4.204796	-5.227315	1.368389
H	-4.266020	-4.011311	2.655863
H	-1.214896	-5.449607	1.058299
H	-1.021256	-4.270355	-0.251302
H	-2.409720	-5.378043	-0.251148
H	-0.281627	-3.347577	-2.274214
H	-1.078848	-3.247625	-3.854940
H	-1.999929	-3.763825	-2.428718
H	-1.248670	2.795162	-3.148994
H	-2.985914	2.733022	-2.790205
H	-2.381630	2.150513	-4.359295
H	-2.664161	6.350611	-0.464764
H	-3.678369	4.131675	-0.124036
H	-0.208879	6.572286	-0.845455
H	1.221998	4.505770	-0.863454
H	0.220236	2.306101	-0.541852
H	-6.803220	2.667045	2.051464
H	-4.349756	2.332217	2.025007
H	-8.165462	2.092513	0.043691
H	-7.045379	1.195260	-1.993326
H	-4.589953	0.891330	-2.034602
H	4.345582	-4.550916	-2.927285
H	5.548570	-2.722389	-1.720635
C	3.905068	-3.554078	-2.848399
C	4.573869	-2.528037	-2.178047
H	2.120229	-4.053058	-3.965083
C	2.662012	-3.272775	-3.421808
H	6.591037	1.127285	1.365277
C	4.018900	-1.253760	-2.073596
H	4.445738	-0.047891	1.503094
H	4.559794	-0.479642	-1.525739
C	2.107293	-2.000726	-3.319956
C	2.755414	-0.947975	-2.631188
C	6.118040	2.119050	1.311990
C	3.947071	0.921852	1.642708
H	6.718521	2.745993	0.639770
O	4.682223	1.528209	-0.538683
H	1.139547	-1.798529	-3.787244
H	3.938057	1.157475	2.716764
H	6.143328	2.560782	2.319616
C	4.685375	1.981334	0.826932
C	2.096012	0.375179	-2.488358
B	3.585290	2.072965	-1.162490
H	3.833756	1.483324	-3.280715
C	3.010801	1.625262	-2.549785
C	3.891884	3.330967	0.718529
H	5.411209	4.281590	-0.531410
O	3.026014	3.073728	-0.401035
H	5.431910	4.814802	1.172487
H	3.687489	3.774259	2.829809
C	4.780077	4.514756	0.339248
H	2.407198	2.466711	-2.930141
C	3.052209	3.674333	1.936646

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 H     4.143189    5.372688    0.077227
 H     2.533682    4.631871    1.779517
Cu     1.124009   -0.000889   -0.788641
 H     1.323502    0.456759   -3.271937
 H     2.906617    0.815735    1.299242
 H     2.295495    2.906338    2.133294
121
Figure 1_pc1_major02_01 / electronic energy: -4987.94730466 a.u. / lowest freq: 7.19 cm-1
 B    -0.026408    2.452894   -0.023464
 O    -0.790343    3.392663   -0.704117
 O     0.062454    2.843092    1.312386
 C    -1.024880    4.535797    0.124512
 C    -0.799358    3.960743    1.567737
 C    -2.426208    5.069371   -0.134929
 C     0.012668    5.588941   -0.270081
 C    -2.079558    3.430179    2.212186
 C    -0.099593    4.910170    2.531277
 H    -2.626713    2.764284    1.531412
 H    -2.750017    4.247308    2.517667
 H    -1.816087    2.847521    3.108066
 H     0.906665    5.175981    2.180771
 H     0.004558    4.431167    3.516793
 H    -0.680088    5.836055    2.664274
 H     1.035986    5.232020   -0.080571
 H    -0.132352    6.537175    0.268577
 H    -0.078683    5.789991   -1.347971
 H    -3.184569    4.282606   -0.030377
 H    -2.492757    5.465246   -1.159492
 H    -2.668734    5.888111    0.560363
 C     5.033581    0.705713   -2.283110
 C     6.278125    0.894080   -1.685829
 C     3.915042    1.458911   -1.888033
 C     6.439060    1.846375   -0.678938
 C     4.094483    2.414382   -0.869616
 C     5.339218    2.605438   -0.276757
 C     2.599192    1.233681   -2.520253
 C     1.579173    2.172139   -2.509145
 H     5.446942    3.348440    0.517007
 H     3.243309    3.003603   -0.520489
 H     7.413215    1.992295   -0.206374
 H     7.130291    0.292815   -2.012835
 H     4.925688   -0.037139   -3.078231
 P    -2.596111    0.276766    0.201257
 C    -3.060541    1.900391   -2.066321
 C    -3.759087    2.840551   -2.820499
 C    -3.592024    1.396008   -0.870264
 C    -4.992158    3.322289   -2.381007
 C    -4.824860    1.902162   -0.430541
 C    -5.517850    2.855264   -1.177428
 C    -5.960156   -1.918234    1.289192
 C    -5.029440   -1.219319    0.524083
 C    -3.918296   -0.613998    1.131082
 C    -5.790586   -2.024840    2.672449
 C    -4.694364   -1.422148    3.286244
 C    -3.766560   -0.715493    2.517942
 C    -2.231438   -1.215271   -2.423379
 C    -2.003847   -1.035043   -0.930396
 C    -1.157920   -2.012630   -0.538905
 C    -0.889991   -0.811139   -3.096328
 C     0.057084   -1.951324   -2.665796
 C    -0.841011   -2.868118   -1.777360
 C    -0.267659   -4.247178   -1.527294
 C    -2.202504   -2.764203   -2.554194
 C    -2.155462   -3.270897   -4.000204
 C    -3.385912   -3.458526   -1.881351
 C    -0.651795   -2.236541    0.843952
 C    -1.343765   -3.032539    1.728653
 C     0.540981   -1.654853    1.443959
 S    -0.594539   -3.023045    3.279555
 C     0.693038   -1.992870    2.772574
 C    -2.584048   -3.844725    1.521419
 C     1.757684   -1.674871    3.781219
 P     1.784263   -0.814619    0.396291
 C     3.485968    1.830852    3.023256
 C     2.585154    1.146985    2.209868
 C     4.808168    1.397591    3.131513
 C     2.995612    0.004088    1.508496
 C     5.227146    0.280095    2.411969
 C     4.327817   -0.412709    1.601466
 C     4.090781   -3.277681   -1.958268
 C     3.356481   -2.202630   -1.460512
 C     4.194570   -4.452257   -1.214929
 C     2.722797   -2.280862   -0.217422
 C     3.563670   -4.543248    0.026498
 C     2.831375   -3.465831    0.522191
 H    -2.078760    1.572237   -2.407177
 H    -3.325188    3.212550   -3.751890
 H    -5.536421    4.064605   -2.969768
 H    -5.258169    1.552595    0.509140
 H    -6.476525    3.232515   -0.812642
 H    -6.820418   -2.387252    0.805520
 H    -5.168358   -1.139249   -0.557039
 H    -6.517263   -2.579547    3.271021
 H    -4.556199   -1.503302    4.367017
 H    -2.902032   -0.249771    2.998774
 H    -3.118998   -0.716807   -2.834618
 H    -0.539589    0.164444   -2.730732
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 H   -0.994484   -0.738292   -4.188574
 H    0.919393   -1.580287   -2.105135
 H    0.453063   -2.516405   -3.522792
 H   -0.120348   -4.784572   -2.477311
 H   -0.926422   -4.857146   -0.890339
 H    0.711220   -4.182332   -1.028885
 H   -3.074662   -2.971753   -4.529166
 H   -2.114465   -4.371695   -4.019191
 H   -1.304818   -2.901258   -4.586048
 H   -4.303864   -3.296325   -2.468741
 H   -3.572244   -3.093343   -0.867045
 H   -3.221352   -4.546839   -1.828577
 H   -3.438138   -3.210862    1.249412
 H   -2.856113   -4.394226    2.433546
 H   -2.443368   -4.581264    0.716866
 H    1.595517   -2.246295    4.706254
 H    1.760697   -0.607399    4.043626
 H    2.759070   -1.923203    3.404213
 H    3.150464    2.715839    3.569659
 H    1.560380    1.516697    2.118815
 H    5.513680    1.938529    3.766793
 H    6.264424   -0.056962    2.475676
 H    4.675339   -1.285618    1.045985
 H    4.577450   -3.196996   -2.932980
 H    3.265864   -1.289493   -2.046662
 H    4.762638   -5.300369   -1.604339
 H    3.635876   -5.463241    0.611200
 H    2.329925   -3.559654    1.487504
Cu    1.132827    0.987507   -0.902084
 H    1.740272    3.190720   -2.148776
 H    0.720440    2.051325   -3.175322
 H    2.521347    0.377226   -3.198241
121
Figure 1_pc1_major02_02 / electronic energy: -4987.94730699 a.u. / lowest freq: 9.81 cm-1
 B   -0.026560   -2.453708    0.025569
 O   -0.793185   -3.391851    0.705423
 O    0.065185   -2.845560   -1.309595
 C   -1.026519   -4.535821   -0.122458
 C   -0.797238   -3.962566   -1.565753
 C   -2.428741   -5.068431    0.134119
 C    0.009505   -5.589084    0.275784
 C   -2.075399   -3.431227   -2.213590
 C   -0.096363   -4.913750   -2.526734
 H   -2.623168   -2.763769   -1.534826
 H   -2.746221   -4.247886   -2.519533
 H   -1.809297   -2.849974   -3.109609
 H    0.908706   -5.180544   -2.173562
 H    0.010682   -4.435813   -3.512458
 H   -0.677729   -5.839020   -2.660210
 H    1.033464   -5.232997    0.088163
 H   -0.134853   -6.537884   -0.262060
 H   -0.084436   -5.788796    1.353695
 H   -3.186479   -4.281369    0.027329
 H   -2.497946   -5.463648    1.158761
 H   -2.670038   -5.887464   -0.561259
 C    5.035178   -0.706976    2.280302
 C    6.278872   -0.894334    1.680947
 C    3.916322   -1.460271    1.886277
 C    6.438641   -1.845647    0.672937
 C    4.094667   -2.414958    0.866930
 C    5.338525   -2.604909    0.271887
 C    2.601142   -1.235655    2.520138
 C    1.581102   -2.174146    2.509416
 H    5.445316   -3.347198   -0.522672
 H    3.243208   -3.004278    0.518660
 H    7.412114   -1.990709    0.198713
 H    7.131288   -0.292975    2.007131
 H    4.928218    0.035285    3.076095
 P   -2.595931   -0.276504   -0.203619
 C   -3.064023   -1.900920    2.062578
 C   -3.764010   -2.840819    2.815708
 C   -3.593765   -1.395887    0.866029
 C   -4.996794   -3.321776    2.374571
 C   -4.826322   -1.901262    0.424634
 C   -5.520732   -2.854195    1.170438
 C   -5.957686    1.920993   -1.293393
 C   -5.028120    1.220962   -0.527912
 C   -3.916573    0.615717   -1.134252
 C   -5.786521    2.028858   -2.676355
 C   -4.689876    1.426274   -3.289503
 C   -3.763260    0.718440   -2.520844
 C   -2.233005    1.212883    2.422801
 C   -2.004462    1.034214    0.929783
 C   -1.158295    2.012232    0.539907
 C   -0.891983    0.807999    3.096209
 C    0.055376    1.948673    2.667539
 C   -0.842145    2.866416    1.779490
 C   -0.268653    4.245758    1.531331
 C   -2.204129    2.761657    2.555289
 C   -2.158089    3.266661    4.001923
 C   -3.387029    3.456811    1.882408
 C   -0.651195    2.237149   -0.842409
 C   -1.341949    3.034328   -1.726997
 C    0.541185    1.654588   -1.442197
 S   -0.592111    3.024724   -3.277639
 C    0.694074    1.992861   -2.770633
 C   -2.581886    3.847083   -1.519983
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 C    1.759875    1.675040   -3.778108
 P    1.784181    0.813924   -0.394631
 C    5.226325   -0.273235   -2.415797
 C    4.326764    0.417568   -1.603853
 C    4.808945   -1.392344   -3.133754
 C    2.995914   -0.002747   -1.507917
 C    3.488221   -1.829278   -3.022342
 C    2.587209   -1.147379   -2.207519
 C    3.560428    4.543726   -0.020639
 C    2.829029    3.466270   -0.517580
 C    4.191578    4.451762    1.220588
 C    2.721671    2.280257    0.220542
 C    4.088938    3.276171    1.962481
 C    3.355576    2.201077    1.463455
 H   -2.082461   -1.573516    2.404697
 H   -3.331425   -3.213289    3.747521
 H   -5.542200   -4.063931    2.962478
 H   -5.258306   -1.551183   -0.515470
 H   -6.479148   -3.230866    0.804374
 H   -6.818271    2.389934   -0.810219
 H   -5.168226    1.139968    0.552988
 H   -6.512259    2.584487   -3.275210
 H   -4.550475    1.508409   -4.370042
 H   -2.898448    0.252722   -3.001178
 H   -3.120849    0.714087    2.832989
 H   -0.541281   -0.167217    2.729877
 H   -0.997217    0.734025    4.188307
 H    0.918132    1.578305    2.107097
 H    0.450706    2.512838    3.525441
 H   -0.121927    4.782067    2.482051
 H   -0.927044    4.856456    0.894693
 H    0.710507    4.181484    1.033421
 H   -3.077746    2.967052    4.529821
 H   -2.116859    4.367426    4.022284
 H   -1.307964    2.896108    4.587944
 H   -4.305543    3.293442    2.468605
 H   -3.572254    3.093381    0.867267
 H   -3.222643    4.545248    1.831688
 H   -2.852921    4.397611   -2.431796
 H   -2.441422    4.582779   -0.714630
 H   -3.436535    3.213427   -1.249215
 H    1.590714    2.235255   -4.708727
 H    1.773716    0.604909   -4.028576
 H    2.759374    1.937214   -3.405017
 H    6.262490    0.066759   -2.481980
 H    4.672973    1.291814   -1.049658
 H    5.514619   -1.931684   -3.770210
 H    3.154049   -2.715573   -3.567435
 H    1.563597   -1.519803   -2.114278
 H    3.631690    5.464528   -0.604181
 H    2.327293    3.560869   -1.482664
 H    4.758880    5.299922    1.611008
 H    4.575742    3.194729    2.937063
 H    3.265734    1.287166    2.048507
Cu    1.133322   -0.988628    0.903450
 H    1.741981   -3.192555    2.148432
 H    0.723154   -2.053734    3.176681
 H    2.523905   -0.379728    3.198857
121
Figure 1_pc1_major02_03 / electronic energy: -4987.95173049 a.u. / lowest freq: 15.25 cm-1
 B   -2.770952    0.046218    0.622504
 O   -3.450149    1.075955    1.264194
 O   -3.638723   -0.563314   -0.280078
 C   -4.848671    1.007707    0.959103
 C   -4.861928    0.179969   -0.374945
 C   -5.401764    2.420210    0.837089
 C   -5.525991    0.279627    2.120909
 C   -4.774860    1.052510   -1.626911
 C   -6.020239   -0.797912   -0.514245
 H   -3.954371    1.779267   -1.554542
 H   -5.710928    1.602129   -1.804729
 H   -4.583421    0.412471   -2.500526
 H   -6.018432   -1.547206    0.288151
 H   -5.939929   -1.331762   -1.473337
 H   -6.986023   -0.269692   -0.500404
 H   -5.133918   -0.742527    2.232407
 H   -6.617283    0.224591    1.994206
 H   -5.315880    0.822400    3.054586
 H   -4.821651    3.020302    0.123386
 H   -5.351673    2.923407    1.814416
 H   -6.454529    2.406458    0.514983
 C    1.829726   -2.523224    3.551117
 C    2.633081   -3.662052    3.504860
 C    0.540635   -2.515203    2.988541
 C    2.170454   -4.826023    2.890077
 C    0.085669   -3.701455    2.383502
 C    0.890094   -4.835474    2.330625
 C   -0.272157   -1.289167    3.066677
 C   -1.643972   -1.218688    2.859723
 H    0.513292   -5.736528    1.840026
 H   -0.903453   -3.732341    1.923472
 H    2.800374   -5.717458    2.845206
 H    3.630357   -3.637228    3.951549
 H    2.204234   -1.615024    4.031450
 P    0.396724    1.529560    0.986830
 C    0.035633    2.769161    3.476644
 C    0.311516    2.980245    4.827398
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 C    0.898661    2.000818    2.682709
 C    1.448306    2.420603    5.409449
 C    2.022235    1.417129    3.285598
 C    2.300096    1.633950    4.633754
 C   -0.568844    5.438047    0.002065
 C    0.015439    4.334169    0.619897
 C   -0.415361    3.036799    0.309606
 C   -1.578795    5.257454   -0.944973
 C   -2.001619    3.969195   -1.269360
 C   -1.425177    2.865402   -0.641128
 C    3.314499    1.925621    0.362214
 C    1.900145    1.539150   -0.039737
 C    1.910865    1.222992   -1.355765
 C    4.120216    0.600355    0.355961
 C    4.168067    0.262478   -1.146826
 C    3.372128    1.419946   -1.830633
 C    3.639507    1.501183   -3.320326
 C    3.815105    2.628674   -0.928195
 C    5.320323    2.918649   -0.953203
 C    3.110918    3.962213   -1.178315
 C    0.748220    0.823519   -2.210655
 C    0.279148    1.665835   -3.197311
 C   -0.073420   -0.389763   -2.101969
 S   -1.107651    1.007383   -3.980382
 C   -1.116003   -0.413016   -3.000076
 C    0.705704    3.042053   -3.599321
 C   -2.234322   -1.388117   -3.227823
 P    0.153217   -1.602808   -0.738904
 C   -2.850175   -4.417143   -0.714971
 C   -2.067056   -3.286578   -0.487912
 C   -2.407072   -5.414146   -1.582433
 C   -0.835780   -3.122163   -1.134333
 C   -1.171555   -5.273271   -2.214252
 C   -0.391404   -4.140335   -1.988239
 C    3.859708   -3.296736   -0.261657
 C    2.617446   -2.706839   -0.027055
 C    4.329884   -3.442269   -1.565989
 C    1.835264   -2.253183   -1.092077
 C    3.558384   -2.986075   -2.637039
 C    2.321804   -2.389182   -2.401011
 H   -0.867609    3.203240    3.040940
 H   -0.370805    3.585687    5.428688
 H    1.663773    2.587707    6.467256
 H    2.677676    0.763282    2.708426
 H    3.184485    1.175082    5.082205
 H   -0.229102    6.444851    0.256439
 H    0.814977    4.487948    1.348800
 H   -2.034337    6.123648   -1.430922
 H   -2.784019    3.818918   -2.017439
 H   -1.752712    1.855224   -0.896494
 H    3.400513    2.517222    1.282638
 H    3.617928   -0.182957    0.941768
 H    5.122547    0.742164    0.786253
 H    3.719054   -0.702220   -1.378943
 H    5.197580    0.237227   -1.532301
 H    4.724205    1.502619   -3.509677
 H    3.223999    2.407605   -3.779605
 H    3.215175    0.630811   -3.845110
 H    5.579460    3.624180   -0.147655
 H    5.596422    3.398911   -1.905600
 H    5.959281    2.035227   -0.834117
 H    3.461877    4.708015   -0.447272
 H    2.021212    3.899012   -1.077399
 H    3.348616    4.355434   -2.179595
 H    1.474443    3.427725   -2.927227
 H   -0.145110    3.739860   -3.553882
 H    1.100119    3.066668   -4.627417
 H   -2.866447   -1.055778   -4.064202
 H   -2.864915   -1.456241   -2.329399
 H   -1.864493   -2.392821   -3.471919
 H   -3.812924   -4.516554   -0.207761
 H   -2.428522   -2.502483    0.177409
 H   -3.017269   -6.302845   -1.761018
 H   -0.808179   -6.051284   -2.889925
 H    0.570828   -4.062153   -2.494182
 H    4.460529   -3.642234    0.582987
 H    2.257766   -2.591691    0.996016
 H    5.301559   -3.906935   -1.749510
 H    3.926123   -3.088044   -3.660755
 H    1.728968   -2.022399   -3.242969
Cu   -0.838689   -0.442832    1.110625
 H   -2.232851   -2.116306    2.646448
 H   -2.207099   -0.385970    3.286106
 H    0.205234   -0.456003    3.590253
121
Figure 1_ts(CuBadd)_major02_01 / electronic energy: -4987.94649355 a.u. / lowest freq: -62.89 cm-1
 B   -2.895459    0.403111    0.628571
 O   -3.465953    1.574472    1.121393
 O   -3.842044   -0.261248   -0.140558
 C   -4.876702    1.581503    0.867056
 C   -5.006747    0.559189   -0.317420
 C   -5.313736    3.001314    0.537650
 C   -5.565391    1.110323    2.148211
 C   -4.901240    1.216325   -1.693602
 C   -6.243530   -0.326352   -0.268793
 H   -3.996627    1.836525   -1.773832
 H   -5.777317    1.844118   -1.913718
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H	-4.843212	0.432772	-2.463151
H	-6.283319	-0.920479	0.653601
H	-6.230282	-1.026133	-1.117833
H	-7.163211	0.274943	-0.337410
H	-5.265130	0.085151	2.411569
H	-6.661652	1.141070	2.061087
H	-5.268929	1.770724	2.976952
H	-4.726556	3.426125	-0.287364
H	-5.170313	3.646545	1.417180
H	-6.379579	3.032402	0.263760
C	1.219172	-2.486198	3.807053
C	1.677476	-3.791185	3.973917
C	-0.070227	-2.219967	3.312415
C	0.854931	-4.873739	3.658463
C	-0.888722	-3.324208	3.004491
C	-0.432684	-4.628379	3.175880
C	-0.519167	-0.824202	3.170283
C	-1.846273	-0.451143	2.969645
H	-1.088280	-5.463978	2.918032
H	-1.892842	-3.164904	2.605729
H	1.212565	-5.897924	3.787170
H	2.686964	-3.963047	4.356168
H	1.871435	-1.648097	4.065780
P	0.545013	1.658626	0.682911
C	-0.069585	2.893934	3.105393
C	0.071210	3.827057	4.134667
C	0.834620	2.867640	2.038944
C	1.122573	4.740342	4.107814
C	1.884193	3.797642	2.016578
C	2.029577	4.724282	3.045295
C	-1.690052	3.832730	-2.008078
C	-1.274006	2.922091	-1.035725
C	0.073860	2.821063	-0.680712
C	-0.760941	4.654063	-2.642130
C	0.587811	4.559994	-2.296277
C	0.999192	3.652079	-1.323613
C	3.392118	0.955286	1.200353
C	2.217614	1.088740	0.245180
C	2.572464	0.489122	-0.913782
C	3.453346	-0.559566	1.549238
C	3.970581	-1.182141	0.238023
C	4.034996	0.020985	-0.750074
C	4.821188	-0.282480	-2.009869
C	4.590657	1.126192	0.223671
C	5.955490	0.810196	0.847424
C	4.714857	2.522670	-0.385507
C	1.640483	0.350452	-2.069640
C	1.789043	1.097759	-3.214403
C	0.334419	-0.310639	-2.015102
S	0.349143	1.076186	-4.164802
C	-0.491809	0.054342	-3.051115
C	2.926888	1.960489	-3.661214
C	-1.947566	-0.207415	-3.298150
P	-0.130241	-1.485317	-0.677497
C	-3.474288	-3.852399	-0.978209
C	-2.520932	-2.924508	-0.552580
C	-3.351063	-4.458454	-2.225436
C	-1.434290	-2.600765	-1.366416
C	-2.263245	-4.143276	-3.044881
C	-1.308052	-3.229213	-2.613268
C	2.426000	-4.576339	0.200765
C	1.466120	-3.567735	0.274946
C	3.158874	-4.759923	-0.971154
C	1.228710	-2.729700	-0.818345
C	2.920676	-3.934621	-2.071336
C	1.960601	-2.927395	-1.996972
H	-0.899009	2.184778	3.124916
H	-0.646786	3.837040	4.957930
H	1.235504	5.471218	4.912168
H	2.598215	3.798147	1.189890
H	2.852419	5.442499	3.017070
H	-2.750038	3.898018	-2.266791
H	-2.009878	2.296835	-0.530925
H	-1.084463	5.366599	-3.404668
H	1.327081	5.197264	-2.787688
H	2.057566	3.586000	-1.073106
H	3.380536	1.620120	2.073106
H	2.457581	-0.934133	1.824847
H	4.126864	-0.752023	2.397417
H	3.330790	-1.975886	-0.140804
H	4.975369	-1.612880	0.355799
H	5.776800	-0.768898	-1.759930
H	5.050882	0.622692	-2.588744
H	4.262610	-0.970088	-2.664224
H	6.222830	1.597058	1.570366
H	6.737242	0.803176	0.071028
H	6.007474	-0.147876	1.378045
H	5.001087	3.253482	0.387043
H	3.787470	2.874017	-0.848179
H	5.502571	2.539725	-1.155542
H	3.568380	2.229903	-2.815018
H	2.561770	2.893275	-4.116159
H	3.551503	1.448593	-4.410630
H	-2.412810	0.681185	-3.750494
H	-2.472535	-0.415230	-2.356639
H	-2.117595	-1.053967	-3.981012
H	-4.320085	-4.094190	-0.330016

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 H   -2.631526   -2.432027    0.413972
 H   -4.098566   -5.180935   -2.562132
 H   -2.156567   -4.619043   -4.022706
 H   -0.458124   -2.997834   -3.259508
 H    2.604561   -5.212918    1.070628
 H    0.908406   -3.420997    1.199189
 H    3.917292   -5.544313   -1.027805
 H    3.488764   -4.072246   -2.994476
 H    1.794710   -2.281731   -2.861823
Cu   -0.977764   -0.157313    1.120391
 H   -2.637009   -1.206479    2.944848
 H   -2.190704    0.542368    3.264345
 H    0.187326   -0.069144    3.530069
121
Figure 1_ts(CuBadd)_major02_02 / electronic energy: -4987.94870159 a.u. / lowest freq: -97.75 cm-1
 B   -2.209108   -1.757502    0.314879
 O   -3.363618   -1.022929    0.525868
 O   -2.525697   -2.949127   -0.318769
 C   -4.507979   -1.828172    0.212289
 C   -3.896677   -2.907443   -0.750554
 C   -5.575678   -0.946791   -0.417245
 C   -5.018889   -2.418269    1.526272
 C   -3.897392   -2.475785   -2.216712
 C   -4.502161   -4.296433   -0.619755
 H   -3.474874   -1.467972   -2.337734
 H   -4.910653   -2.483491   -2.644287
 H   -3.275442   -3.174352   -2.796225
 H   -4.358529   -4.711736    0.386306
 H   -4.025118   -4.980842   -1.337400
 H   -5.580582   -4.274402   -0.839518
 H   -4.270574   -3.077512    1.990883
 H   -5.946748   -2.991517    1.383606
 H   -5.227197   -1.597219    2.228551
 H   -5.176896   -0.376549   -1.266281
 H   -5.949836   -0.225596    0.324920
 H   -6.429079   -1.549644   -0.763936
 C    2.262496   -1.795569    3.891445
 C    3.495089   -2.428655    4.032115
 C    1.300995   -2.249534    2.964027
 C    3.814649   -3.540486    3.249749
 C    1.634417   -3.388194    2.198717
 C    2.869798   -4.013749    2.335030
 C    0.032762   -1.534147    2.816697
 C   -1.146906   -2.132436    2.277280
 H    3.101797   -4.879804    1.708919
 H    0.928114   -3.764141    1.454764
 H    4.784798   -4.032148    3.351611
 H    4.217479   -2.045890    4.758525
 H    2.033014   -0.917344    4.502468
 P   -0.991194    1.289230    0.777149
 C   -0.852658    1.860957    3.524951
 C   -1.387927    2.045340    4.798437
 C   -1.691694    1.735049    2.407255
 C   -2.770396    2.082884    4.980639
 C   -3.079430    1.750142    2.604218
 C   -3.612880    1.926348    3.880598
 C   -3.686552    3.668273   -1.263532
 C   -2.799054    3.191706   -0.300799
 C   -2.212325    1.926425   -0.440527
 C   -3.984686    2.890869   -2.384608
 C   -3.386932    1.640624   -2.540646
 C   -2.508051    1.160691   -1.569974
 C    1.073986    3.394758    1.372224
 C    0.404806    2.399318    0.443323
 C    1.096853    2.376191   -0.717727
 C    2.403919    2.716566    1.797733
 C    3.211051    2.744780    0.483857
 C    2.243450    3.401548   -0.553036
 C    2.972461    3.868903   -1.797405
 C    1.548449    4.474623    0.362852
 C    2.503408    5.518734    0.951712
 C    0.383966    5.246396   -0.258480
 C    0.799017    1.569088   -1.942162
 C    0.301451    2.186722   -3.069403
 C    0.907063    0.115987   -2.125864
 S    0.007129    1.054134   -4.331159
 C    0.515378   -0.293781   -3.381500
 C   -0.158943    3.593677   -3.280739
 C    0.439685   -1.641707   -4.040068
 P    1.356159   -1.004874   -0.737572
 C    0.580152   -4.891453   -1.823490
 C    0.468903   -3.577060   -1.373999
 C    1.801914   -5.372661   -2.293056
 C    1.573252   -2.715745   -1.405327
 C    2.913020   -4.529871   -2.304482
 C    2.800912   -3.212153   -1.861638
 C    5.023394   -0.456566    1.024124
 C    3.675446   -0.738091    0.803335
 C    5.819030    0.018924   -0.017613
 C    3.110819   -0.545328   -0.460116
 C    5.262518    0.212646   -1.283378
 C    3.915605   -0.067247   -1.504068
 H    0.230847    1.795907    3.408107
 H   -0.717000    2.148985    5.654407
 H   -3.190578    2.222388    5.979417
 H   -3.752142    1.608118    1.756770
 H   -4.697217    1.937644    4.014445
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 H   -4.146467    4.651519   -1.139115
 H   -2.567643    3.809067    0.571251
 H   -4.681244    3.263737   -3.139481
 H   -3.606164    1.033080   -3.421951
 H   -2.034821    0.184111   -1.693551
 H    0.452579    3.764185    2.197893
 H    2.231406    1.693179    2.163471
 H    2.898751    3.276889    2.604798
 H    3.515443    1.753207    0.150284
 H    4.126641    3.346858    0.575591
 H    3.796134    4.545472   -1.520774
 H    2.324784    4.407518   -2.502845
 H    3.415045    3.014563   -2.333395
 H    1.989750    6.094741    1.738167
 H    2.809205    6.234931    0.172505
 H    3.417772    5.104552    1.393806
 H   -0.061650    5.915209    0.495453
 H   -0.414277    4.594207   -0.631576
 H    0.730038    5.883922   -1.087972
 H    0.323138    4.286554   -2.588663
 H   -1.246214    3.664137   -3.111111
 H    0.043799    3.938137   -4.305771
 H    0.192112   -1.530565   -5.105496
 H   -0.337760   -2.269905   -3.582094
 H    1.389988   -2.186728   -3.973557
 H   -0.295958   -5.544125   -1.796870
 H   -0.495752   -3.222897   -1.004980
 H    1.892246   -6.405093   -2.639366
 H    3.878289   -4.899139   -2.659182
 H    3.686103   -2.575080   -1.878226
 H    5.449496   -0.606877    2.018809
 H    3.056941   -1.098707    1.625202
 H    6.874351    0.241892    0.156246
 H    5.879976    0.588350   -2.102628
 H    3.485358    0.091887   -2.495852
Cu   -0.388277   -0.945841    0.810856
 H   -1.145082   -3.209061    2.072280
 H   -2.099916   -1.772878    2.678940
 H   -0.105832   -0.686955    3.494478
121
Figure 1_ts(CuBadd)_major02_03 / electronic energy: -4987.94870162 a.u. / lowest freq: -97.74 cm-1
 B   -2.209124   -1.757493    0.314894
 O   -3.363630   -1.022911    0.525878
 O   -2.525721   -2.949119   -0.318749
 C   -4.507996   -1.828147    0.212299
 C   -3.896698   -2.907425   -0.750539
 C   -5.575687   -0.946759   -0.417240
 C   -5.018913   -2.418237    1.526282
 C   -3.897405   -2.475769   -2.216698
 C   -4.502194   -4.296409   -0.619739
 H   -3.474872   -1.467961   -2.337721
 H   -4.910666   -2.483460   -2.644274
 H   -3.275465   -3.174346   -2.796210
 H   -4.358560   -4.711714    0.386321
 H   -4.025163   -4.980822   -1.337388
 H   -5.580617   -4.274367   -0.839495
 H   -4.270601   -3.077482    1.990897
 H   -5.946773   -2.991483    1.383614
 H   -5.227221   -1.597185    2.228558
 H   -5.176896   -0.376518   -1.266271
 H   -5.949845   -0.225564    0.324924
 H   -6.429088   -1.549608   -0.763937
 C    2.262501   -1.795589    3.891438
 C    3.495090   -2.428687    4.032098
 C    1.300989   -2.249545    2.964027
 C    3.814633   -3.540519    3.249727
 C    1.634393   -3.388207    2.198715
 C    2.869769   -4.013774    2.335016
 C    0.032761   -1.534145    2.816706
 C   -1.146916   -2.132424    2.277299
 H    3.101755   -4.879831    1.708903
 H    0.928079   -3.764148    1.454769
 H    4.784779   -4.032190    3.351580
 H    4.217489   -2.045930    4.758502
 H    2.033033   -0.917363    4.502464
 P   -0.991180    1.289240    0.777154
 C   -0.852617    1.860967    3.524952
 C   -1.387873    2.045367    4.798441
 C   -1.691664    1.735080    2.407262
 C   -2.770340    2.082951    4.980652
 C   -3.079398    1.750214    2.604233
 C   -3.612835    1.926438    3.880616
 C   -3.686512    3.668297   -1.263544
 C   -2.799017    3.191729   -0.300808
 C   -2.212309    1.926437   -0.440522
 C   -3.984662    2.890882   -2.384608
 C   -3.386930    1.640626   -2.540632
 C   -2.508052    1.160692   -1.569958
 C    1.074020    3.394749    1.372214
 C    0.404829    2.399314    0.443317
 C    1.096867    2.376185   -0.717738
 C    2.403954    2.716552    1.797713
 C    3.211075    2.744763    0.483831
 C    2.243469    3.401537   -0.553055
 C    2.972477    3.868891   -1.797426
 C    1.548480    4.474614    0.362840
 C    2.503447    5.518721    0.951694
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 C    0.383994    5.246392   -0.258481
 C    0.799017    1.569082   -1.942171
 C    0.301455    2.186715   -3.069413
 C    0.907049    0.115978   -2.125866
 S    0.007117    1.054125   -4.331163
 C    0.515355   -0.293791   -3.381499
 C   -0.158921    3.593675   -3.280757
 C    0.439646   -1.641719   -4.040060
 P    1.356140   -1.004882   -0.737573
 C    2.912981   -4.529892   -2.304477
 C    2.800879   -3.212171   -1.861642
 C    1.801873   -5.372680   -2.293036
 C    1.573223   -2.715757   -1.405326
 C    0.580116   -4.891465   -1.823466
 C    0.468872   -3.577069   -1.373984
 C    5.262510    0.212595   -1.283396
 C    3.915593   -0.067284   -1.504082
 C    5.819023    0.018875   -0.017631
 C    3.110805   -0.545349   -0.460124
 C    5.023384   -0.456598    1.024111
 C    3.675432   -0.738109    0.803327
 H    0.230886    1.795885    3.408102
 H   -0.716937    2.148994    5.654407
 H   -3.190511    2.222468    5.979432
 H   -3.752121    1.608211    1.756790
 H   -4.697171    1.937767    4.014470
 H   -4.146410    4.651552   -1.139139
 H   -2.567593    3.809098    0.571232
 H   -4.681218    3.263752   -3.139483
 H   -3.606175    1.033073   -3.421927
 H   -2.034839    0.184102   -1.693522
 H    0.452622    3.764178    2.197889
 H    2.231441    1.693166    2.163452
 H    2.898794    3.276874    2.604773
 H    3.515460    1.753190    0.150253
 H    4.126669    3.346837    0.575557
 H    3.796138    4.545475   -1.520798
 H    2.324796    4.407490   -2.502875
 H    3.415077    3.014553   -2.333405
 H    1.989797    6.094726    1.738155
 H    2.809239    6.234919    0.172486
 H    3.417814    5.104535    1.393778
 H   -0.061615    5.915204    0.495458
 H   -0.414254    4.594206   -0.631570
 H    0.730060    5.883919   -1.087973
 H    0.323126    4.286541   -2.588646
 H   -1.246201    3.664138   -3.111184
 H    0.043875    3.938148   -4.305774
 H    0.192053   -1.530581   -5.105484
 H   -0.337791   -2.269913   -3.582068
 H    1.389950   -2.186743   -3.973565
 H    3.878246   -4.899164   -2.659181
 H    3.686071   -2.575100   -1.878240
 H    1.892201   -6.405116   -2.639338
 H   -0.295995   -5.544136   -1.796834
 H   -0.495780   -3.222903   -1.004961
 H    5.879971    0.588286   -2.102649
 H    3.485347    0.091848   -2.495865
 H    6.874347    0.241832    0.156225
 H    5.449486   -0.606909    2.018796
 H    3.056925   -1.098714    1.625197
Cu   -0.388287   -0.945838    0.810864
 H   -1.145103   -3.209049    2.072303
 H   -2.099920   -1.772854    2.678963
 H   -0.105818   -0.686948    3.494484
121
Figure 1_ts(CuBadd)_major02_04 / electronic energy: -4987.94870153 a.u. / lowest freq: -97.74 cm-1
 B   -2.209089   -1.757533    0.314888
 O   -3.363609   -1.022974    0.525877
 O   -2.525662   -2.949159   -0.318766
 C   -4.507960   -1.828229    0.212290
 C   -3.896641   -2.907489   -0.750556
 C   -5.575667   -0.946859   -0.417245
 C   -5.018868   -2.418338    1.526269
 C   -3.897356   -2.475822   -2.216711
 C   -4.502109   -4.296485   -0.619767
 H   -3.474854   -1.468000   -2.337725
 H   -4.910615   -2.483543   -2.644291
 H   -3.275392   -3.174375   -2.796226
 H   -4.358476   -4.711793    0.386293
 H   -4.025057   -4.980885   -1.337415
 H   -5.580530   -4.274466   -0.839533
 H   -4.270548   -3.077577    1.990878
 H   -5.946721   -2.991593    1.383596
 H   -5.227185   -1.597293    2.228551
 H   -5.176886   -0.376603   -1.266271
 H   -5.949842   -0.225676    0.324923
 H   -6.429054   -1.549723   -0.763949
 C    2.262527   -1.795557    3.891445
 C    3.495128   -2.428631    4.032108
 C    1.301029   -2.249526    2.964027
 C    3.814697   -3.540453    3.249733
 C    1.634459   -3.388178    2.198710
 C    2.869848   -4.013720    2.335013
 C    0.032789   -1.534150    2.816704
 C   -1.146877   -2.132452    2.277293
 H    3.101854   -4.879769    1.708896
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 H    0.928157   -3.764126    1.454756
 H    4.784851   -4.032106    3.351588
 H    4.217516   -2.045865    4.758519
 H    2.033038   -0.917339    4.502476
 P   -0.991208    1.289215    0.777151
 C   -3.079445    1.750126    2.604222
 C   -3.612894    1.926334    3.880603
 C   -1.691710    1.735031    2.407258
 C   -2.770409    2.082868    4.980643
 C   -0.852672    1.860938    3.524953
 C   -1.387940    2.045322    4.798440
 C   -3.686579    3.668239   -1.263532
 C   -2.799078    3.191677   -0.300799
 C   -2.212347    1.926396   -0.440523
 C   -3.984714    2.890829   -2.384603
 C   -3.386959    1.640584   -2.540637
 C   -2.508074    1.160657   -1.569967
 C    1.073947    3.394764    1.372226
 C    0.404778    2.399320    0.443324
 C    1.096821    2.376207   -0.717729
 C    2.403892    2.716588    1.797726
 C    3.211018    2.744821    0.483848
 C    2.243403    3.401580   -0.553039
 C    2.972405    3.868952   -1.797407
 C    1.548390    4.474641    0.362856
 C    2.503338    5.518763    0.951714
 C    0.383892    5.246398   -0.258466
 C    0.798993    1.569101   -1.942165
 C    0.301424    2.186729   -3.069407
 C    0.907056    0.116001   -2.125865
 S    0.007116    1.054138   -4.331163
 C    0.515378   -0.293772   -3.381502
 C   -0.158982    3.593680   -3.280746
 C    0.439706   -1.641698   -4.040070
 P    1.356164   -1.004855   -0.737573
 C    0.580207   -4.891446   -1.823485
 C    0.468940   -3.577054   -1.373996
 C    1.801974   -5.372638   -2.293053
 C    1.573277   -2.715724   -1.405331
 C    2.913068   -4.529832   -2.304487
 C    2.800942   -3.212115   -1.861645
 C    5.023393   -0.456504    1.024123
 C    3.675447   -0.738039    0.803335
 C    5.819026    0.018984   -0.017617
 C    3.110819   -0.545291   -0.460118
 C    5.262513    0.212695   -1.283384
 C    3.915602   -0.067209   -1.504073
 H   -3.752158    1.608104    1.756775
 H   -4.697230    1.937631    4.014450
 H   -3.190589    2.222373    5.979421
 H    0.230833    1.795888    3.408109
 H   -0.717012    2.148967    5.654410
 H   -4.146494    4.651485   -1.139118
 H   -2.567666    3.809042    0.571248
 H   -4.681275    3.263693   -3.139476
 H   -3.606193    1.033035   -3.421939
 H   -2.034844    0.184077   -1.693541
 H    0.452539    3.764179    2.197900
 H    2.231394    1.693197    2.163459
 H    2.898719    3.276913    2.604793
 H    3.515422    1.753255    0.150267
 H    4.126599    3.346913    0.575581
 H    3.796063    4.545539   -1.520774
 H    2.324719    4.407553   -2.502848
 H    3.415010    3.014622   -2.333396
 H    1.989671    6.094774    1.738160
 H    2.809135    6.234955    0.172503
 H    3.417701    5.104590    1.393817
 H   -0.061742    5.915188    0.495477
 H   -0.414336    4.594196   -0.631573
 H    0.729949    5.883945   -1.087946
 H    0.323067    4.286559   -2.588649
 H   -1.246259    3.664124   -3.111151
 H    0.043786    3.938152   -4.305769
 H    0.192124   -1.530561   -5.105497
 H   -0.337721   -2.269914   -3.582091
 H    1.390023   -2.186700   -3.973566
 H   -0.295893   -5.544132   -1.796859
 H   -0.495719   -3.222904   -1.004975
 H    1.892320   -6.405070   -2.639360
 H    3.878341   -4.899086   -2.659190
 H    3.686121   -2.575028   -1.878238
 H    5.449496   -0.606806    2.018808
 H    3.056944   -1.098655    1.625204
 H    6.874346    0.241959    0.156241
 H    5.879969    0.588397   -2.102636
 H    3.485355    0.091916   -2.495857
Cu   -0.388266   -0.945850    0.810862
 H   -1.145042   -3.209077    2.072296
 H   -2.099888   -1.772902    2.678957
 H   -0.105809   -0.686958    3.494485
121
Figure 1_ts(CuBadd)_major02_05 / electronic energy: -4987.93948747 a.u. / lowest freq: -189.59 cm-1
 B    0.468913    2.551837   -0.193809
 O   -0.737498    3.157495   -0.443269
 O    1.135490    3.200791    0.833143
 C   -0.823236    4.374256    0.317092
```

C	0.225779	4.121302	1.458764
C	-2.252483	4.567712	0.797214
C	-0.428071	5.511495	-0.623017
C	-0.374111	3.411746	2.672495
C	0.999226	5.352761	1.902225
H	-0.930086	2.510317	2.372707
H	-1.048968	4.070309	3.238294
H	0.438740	3.103441	3.346998
H	1.562954	5.799738	1.072926
H	1.717889	5.075226	2.687760
H	0.319368	6.113385	2.315724
H	0.602880	5.394331	-0.989759
H	-0.514591	6.493290	-0.135322
H	-1.099946	5.501280	-1.494307
H	-2.614964	3.695758	1.355905
H	-2.919905	4.713286	-0.065366
H	-2.326536	5.457203	1.441884
C	4.963907	0.773438	-2.460704
C	6.242918	0.760334	-1.914353
C	3.899205	1.472599	-1.844033
C	6.523179	1.455424	-0.733827
C	4.206869	2.177642	-0.653516
C	5.491323	2.164707	-0.115943
C	2.552858	1.433178	-2.396758
C	1.538705	2.392461	-1.990974
H	5.682980	2.708640	0.813290
H	3.418728	2.715972	-0.119905
H	7.527048	1.442069	-0.302991
H	7.036894	0.203217	-2.420320
H	4.770359	0.227662	-3.389388
P	-2.644119	0.468481	0.292261
C	-3.107504	2.215393	-1.886307
C	-3.783653	3.222842	-2.570431
C	-3.625102	1.673096	-0.701085
C	-4.982906	3.731871	-2.070706
C	-4.825899	2.200976	-0.204613
C	-5.497493	3.220102	-0.880773
C	-6.082689	-1.630795	1.334429
C	-5.134340	-0.933995	0.589439
C	-3.977622	-0.427152	1.202092
C	-5.884479	-1.837442	2.702352
C	-4.740873	-1.336923	3.321246
C	-3.796237	-0.629933	2.574049
C	-2.358155	-0.864748	-2.425396
C	-2.125808	-0.809191	-0.921486
C	-1.355299	-1.873760	-0.605340
C	-0.990596	-0.506994	-3.071339
C	-0.126099	-1.738766	-2.725092
C	-1.090534	-2.652655	-1.905489
C	-0.615436	-4.082786	-1.758132
C	-2.437438	-2.397646	-2.670845
C	-2.419419	-2.799489	-4.150474
C	-3.671724	-3.053043	-2.052867
C	-0.866065	-2.265853	0.745121
C	-1.605026	-3.097261	1.556808
C	0.384351	-1.863278	1.370342
S	-0.821014	-3.336289	3.071512
C	0.540202	-2.370005	2.644966
C	-2.910859	-3.781472	1.300613
C	1.659084	-2.270166	3.640310
P	1.672227	-0.994169	0.416053
C	3.369940	1.367246	3.287943
C	2.478202	0.778686	2.395734
C	4.677836	0.889716	3.388480
C	2.881270	-0.306588	1.608165
C	5.090421	-0.173259	2.586488
C	4.197834	-0.768617	1.695753
C	3.970284	-3.184913	-2.181503
C	3.250494	-2.162978	-1.565179
C	4.016522	-4.452724	-1.602602
C	2.575102	-2.395610	-0.362787
C	3.342114	-4.693798	-0.404996
C	2.623615	-3.671135	0.212619
H	-2.149903	1.869244	-2.272782
H	-3.359783	3.623362	-3.494651
H	-5.509311	4.527878	-2.602989
H	-5.248977	1.822129	0.728329
H	-6.430100	3.615102	-0.470254
H	-6.978247	-2.022200	0.846042
H	-5.295647	-0.778158	-0.480089
H	-6.625631	-2.390095	3.284792
H	-4.579997	-1.495862	4.390110
H	-2.898329	-0.240460	3.061533
H	-3.208723	-0.280490	-2.798774
H	-0.575765	0.419234	-2.646916
H	-1.088550	-0.352532	-4.155516
H	0.762795	-1.467490	-2.145806
H	0.232371	-2.265504	-3.621638
H	-0.497954	-4.556149	-2.745603
H	-1.319343	-4.692172	-1.171087
H	0.361988	-4.124542	-1.254077
H	-3.313900	-2.400916	-4.655483
H	-2.453315	-3.896316	-4.248427
H	-1.543012	-2.448041	-4.708667
H	-4.572676	-2.768140	-2.619777
H	-3.832046	-2.766881	-1.009128
H	-3.593276	-4.151253	-2.098467

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 H   -3.705741   -3.057101    1.084359
 H   -3.227037   -4.373136    2.171158
 H   -2.837079   -4.464623    0.441736
 H    1.472961   -2.935825    4.495005
 H    1.771044   -1.248000    4.029495
 H    2.620665   -2.560027    3.195037
 H    3.044401    2.211502    3.900487
 H    1.465775    1.174350    2.301956
 H    5.379440    1.354461    4.085308
 H    6.117002   -0.541486    2.647790
 H    4.536018   -1.597685    1.071417
 H    4.492068   -2.989330   -3.121111
 H    3.199817   -1.171773   -2.020824
 H    4.574080   -5.257501   -2.087684
 H    3.370842   -5.685930    0.051150
 H    2.088028   -3.877093    1.141866
Cu    1.242135    0.773601   -0.883446
 H    1.897135    3.358691   -1.606206
 H    0.707858    2.530408   -2.692330
 H    2.418881    0.915221   -3.351375
121
Figure 1_ts(CuBadd)_major02_06 / electronic energy: -4987.94647940 a.u. / lowest freq: -60.64 cm-1
 B   -2.871225    0.536110    0.599881
 O   -3.452270    1.674784    1.154448
 O   -3.798478   -0.066795   -0.241548
 C   -4.860494    1.685342    0.885697
 C   -4.964936    0.757828   -0.375944
 C   -5.316578    3.120328    0.667299
 C   -5.555365    1.100812    2.116170
 C   -4.844931    1.518658   -1.696140
 C   -6.196406   -0.136715   -0.412752
 H   -3.948567    2.155429   -1.713417
 H   -5.726458    2.149301   -1.883589
 H   -4.762322    0.795713   -2.520697
 H   -6.225928   -0.823597    0.443274
 H   -6.184738   -0.746329   -1.328902
 H   -7.120574    0.461801   -0.415323
 H   -5.243337    0.061168    2.295268
 H   -6.651002    1.124032    2.020011
 H   -5.275914    1.692596    3.000814
 H   -4.722326    3.622722   -0.107418
 H   -5.200595    3.690965    1.600896
 H   -6.377774    3.156883    0.376583
 C    1.117436   -2.546472    3.785219
 C    1.509032   -3.873773    3.948140
 C   -0.161193   -2.214310    3.303226
 C    0.628621   -4.912037    3.640928
 C   -1.038314   -3.274630    3.003405
 C   -0.649090   -4.600628    3.170322
 C   -0.543728   -0.797662    3.167395
 C   -1.850313   -0.362679    2.971837
 H   -1.349932   -5.400905    2.919850
 H   -2.037711   -3.064372    2.617285
 H    0.932874   -5.953551    3.767620
 H    2.511990   -4.097759    4.320362
 H    1.814606   -1.743595    4.037941
 P    0.630428    1.640017    0.694948
 C    0.046952    2.900832    3.108153
 C    0.214935    3.826336    4.140031
 C    0.969616    2.826150    2.059817
 C    1.312404    4.684186    4.134347
 C    2.066588    3.700156    2.059095
 C    2.238888    4.619166    3.090786
 C   -1.502288    3.922730   -1.989728
 C   -1.127507    2.983566   -1.027810
 C    0.211412    2.834150   -0.657712
 C   -0.539334    4.724065   -2.598158
 C    0.801352    4.581872   -2.237183
 C    1.171045    3.646434   -1.274240
 C    3.445768    0.805806    1.197022
 C    2.273633    0.997842    0.248897
 C    2.594978    0.389814   -0.915477
 C    3.441762   -0.711801    1.537462
 C    3.923236   -1.349400    0.220037
 C    4.036173   -0.144420   -0.761883
 C    4.801184   -0.474059   -2.027944
 C    4.645341    0.929833    0.215058
 C    5.998917    0.551005    0.828485
 C    4.826988    2.322960   -0.387397
 C    1.653300    0.299226   -2.068821
 C    1.830398    1.048200   -3.208515
 C    0.321936   -0.311048   -2.018452
 S    0.391493    1.086707   -4.159902
 C   -0.489046    0.092151   -3.052236
 C    3.000934    1.868328   -3.650982
 C   -1.953307   -0.111664   -3.303225
 P   -0.189994   -1.467731   -0.682243
 C   -3.625439   -3.701092   -0.945952
 C   -2.632426   -2.809943   -0.533587
 C   -3.542109   -4.309615   -2.195391
 C   -1.545372   -2.526261   -1.361763
 C   -2.454701   -4.034325   -3.029547
 C   -1.459447   -3.157718   -2.610393
 C    2.220032   -4.675301    0.185084
 C    1.305799   -3.625341    0.260187
 C    2.948174   -4.886358   -0.985208
 C    1.110230   -2.772174   -0.829816
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 C    2.749877   -4.047203   -2.082748
 C    1.835022   -2.998636   -2.007574
 H   -0.819638    2.237089    3.110207
 H   -0.518245    3.874228    4.948436
 H    1.446584    5.409461    4.940483
 H    2.796230    3.664552    1.247109
 H    3.098536    5.293504    3.078936
 H   -2.555926    4.026021   -2.261131
 H   -1.887233    2.367860   -0.546250
 H   -0.830537    5.458411   -3.352943
 H    1.566412    5.204002   -2.708080
 H    2.223111    3.545660   -1.008364
 H    3.468615    1.464361    2.074228
 H    2.431884   -1.042754    1.817464
 H    4.111159   -0.938058    2.380597
 H    3.245884   -2.110906   -0.159670
 H    4.908064   -1.825972    0.329711
 H    5.737458   -1.000973   -1.786853
 H    5.064447    0.423774   -2.604126
 H    4.210123   -1.134268   -2.682057
 H    6.303992    1.320725    1.554914
 H    6.775118    0.516789    0.047231
 H    6.014117   -0.411791    1.352674
 H    5.148752    3.036851    0.387124
 H    3.913538    2.716652   -0.843442
 H    5.611279    2.310108   -1.161138
 H    3.659273    2.097163   -2.806073
 H    2.673205    2.822607   -4.089662
 H    3.598060    1.341715   -4.412610
 H   -2.379673    0.793597   -3.760850
 H   -2.490338   -0.293124   -2.362817
 H   -2.154766   -0.952739   -3.984317
 H   -4.470262   -3.912627   -0.286021
 H   -2.710058   -2.315188    0.435118
 H   -4.320101   -5.003969   -2.522103
 H   -2.379155   -4.512847   -4.008882
 H   -0.609216   -2.959010   -3.267137
 H    2.366171   -5.323590    1.052339
 H    0.750028   -3.459521    1.182634
 H    3.672488   -5.702352   -1.042458
 H    3.314205   -4.206457   -3.004743
 H    1.700630   -2.343419   -2.870683
Cu   -0.979252   -0.096579    1.114412
 H   -2.677353   -1.077797    2.943734
 H   -2.146905    0.648109    3.258915
 H    0.199953   -0.076696    3.522193
121
Figure 1_ts(CuBadd)_major02_07 / electronic energy: -4987.93946936 a.u. / lowest freq: -190.13 cm-1
 B    0.470200   -2.558350    0.200683
 O   -0.739543   -3.158318    0.447611
 O    1.136952   -3.212319   -0.823153
 C   -0.828885   -4.375479   -0.312134
 C    0.224516   -4.128552   -1.450908
 C   -2.257284   -4.562821   -0.797140
 C   -0.441989   -5.513682    0.630221
 C   -0.368169   -3.416603   -2.666877
 C    0.993005   -5.364109   -1.891638
 H   -0.920033   -2.511853   -2.369540
 H   -1.044826   -4.071913   -3.234296
 H    0.448215   -3.113037   -3.339297
 H    1.553130   -5.812889   -1.060876
 H    1.714353   -5.090802   -2.676188
 H    0.310336   -6.121923   -2.305663
 H    0.588019   -5.400392    1.000855
 H   -0.530832   -6.495478    0.142934
 H   -1.117227   -5.500028    1.498838
 H   -2.614039   -3.689330   -1.357082
 H   -2.928601   -4.705942    0.062773
 H   -2.332486   -5.451872   -1.442289
 C    4.961706   -0.762852    2.460996
 C    6.238966   -0.741373    1.910823
 C    3.899561   -1.468308    1.847070
 C    6.520027   -1.433835    0.728940
 C    4.208639   -2.172370    0.656286
 C    5.491055   -2.150018    0.114177
 C    2.553885   -1.434529    2.401692
 C    1.541910   -2.396607    1.996526
 H    5.683589   -2.692784   -0.815534
 H    3.422606   -2.716514    0.125426
 H    7.522271   -1.413151    0.294641
 H    7.030802   -0.179257    2.414597
 H    4.767292   -0.218005    3.390056
 P   -2.643975   -0.464514   -0.297586
 C   -3.119611   -2.214165    1.875959
 C   -3.800600   -3.221313    2.555714
 C   -3.631699   -1.668359    0.690000
 C   -4.999125   -3.726704    2.050704
 C   -4.831939   -2.192531    0.188174
 C   -5.508257   -3.211492    0.859867
 C   -6.073091    1.649022   -1.341944
 C   -5.129019    0.946454   -0.596903
 C   -3.971898    0.438741   -1.208095
 C   -5.870020    1.860841   -2.708360
 C   -4.725866    1.359696   -3.325749
 C   -3.785682    0.646763   -2.578601
 C   -2.358904    0.859490    2.424404
 C   -2.124119    0.808320    0.920798
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 C   -1.349690    1.871510    0.609140
 C   -0.993754    0.494469    3.071023
 C   -0.124375    1.724239    2.729881
 C   -1.084409    2.644895    1.912488
 C   -0.604275    4.074072    1.772319
 C   -2.433226    2.391622    2.675140
 C   -2.415470    2.788083    4.156240
 C   -3.664860    3.052903    2.058189
 C   -0.860254    2.263174   -0.741716
 C   -1.598475    3.097035   -1.551519
 C    0.382478    1.847681   -1.374520
 S   -0.826447    3.319216   -3.074597
 C    0.529870    2.342973   -2.654563
 C   -2.898219    3.790465   -1.289394
 C    1.637487    2.228374   -3.660930
 P    1.674116    0.985925   -0.417916
 C    5.100198    0.205892   -2.592193
 C    4.199330    0.795544   -1.705846
 C    4.706932   -0.877772   -3.375927
 C    2.893593    0.306556   -1.604112
 C    3.410441   -1.382292   -3.260808
 C    2.510885   -0.799666   -2.372648
 C    3.316839    4.698074    0.399120
 C    2.608015    3.668855   -0.218772
 C    3.986895    4.465069    1.600790
 C    2.564955    2.394968    0.360683
 C    3.946990    3.198546    2.183018
 C    3.237093    2.169988    1.566268
 H   -2.162548   -1.871212    2.266390
 H   -3.380875   -3.624579    3.480633
 H   -5.529177   -4.522583    2.579543
 H   -5.250823   -1.810770   -0.745502
 H   -6.440239   -3.603642    0.445226
 H   -6.968991    2.041031   -0.854666
 H   -5.293939    0.786884    0.471535
 H   -6.607669    2.418143   -3.290809
 H   -4.561158    1.522668   -4.393425
 H   -2.887591    0.256445   -3.065030
 H   -3.212268    0.277124    2.794291
 H   -0.581965   -0.431846    2.643815
 H   -1.093690    0.336702    4.154536
 H    0.763653    1.451485    2.150048
 H    0.235606    2.246259    3.628581
 H   -0.488457    4.543069    2.762066
 H   -1.304337    4.688143    1.185587
 H    0.374807    4.114826    1.271650
 H   -3.311340    2.389940    4.659124
 H   -2.446614    3.884624    4.258161
 H   -1.540357    2.432327    4.713741
 H   -4.567041    2.769666    2.623989
 H   -3.825773    2.769838    1.013692
 H   -3.582621    4.150712    2.106620
 H   -3.208328    4.393913   -2.154034
 H   -2.818849    4.463784   -0.423506
 H   -3.699754    3.071032   -1.080927
 H    1.409086    2.828178   -4.553401
 H    1.789140    1.189690   -3.985457
 H    2.592056    2.589820   -3.252972
 H    6.117932    0.595947   -2.665037
 H    4.522580    1.641835   -1.096953
 H    5.415050   -1.337549   -4.069458
 H    3.100360   -2.243392   -3.857769
 H    1.508590   -1.217072   -2.266813
 H    3.341239    5.689043   -0.059783
 H    2.075997    3.868010   -1.151616
 H    4.536467    5.275100    2.086252
 H    4.465998    3.009106    3.125422
 H    3.191692    1.179569    2.024220
Cu    1.245066   -0.779241    0.886237
 H    1.902472   -3.362325    1.612451
 H    0.711689   -2.535762    2.698370
 H    2.418630   -0.916095    3.355861
121
Figure 1_ts(CuBadd)_major02_08 / electronic energy: -4987.93238186 a.u. / lowest freq: -166.41 cm-1
 B    0.880801   -2.686146   -0.038970
 O   -0.194235   -3.478505    0.281255
 O    1.521677   -3.183748   -1.166044
 C   -0.225072   -4.617832   -0.588527
 C    0.633384   -4.120452   -1.802510
 C   -1.672750   -4.942938   -0.921425
 C    0.421479   -5.777659    0.166570
 C   -0.186041   -3.333354   -2.826367
 C    1.449251   -5.198418   -2.496193
 H   -0.780875   -2.545677   -2.339179
 H   -0.862131   -3.985889   -3.397670
 H    0.498861   -2.847093   -3.537148
 H    2.169378   -5.666868   -1.812804
 H    2.011924   -4.760508   -3.334331
 H    0.790241   -5.980425   -2.903467
 H    1.476858   -5.567290    0.396238
 H    0.368360   -6.718085   -0.401472
 H   -0.108566   -5.919834    1.120069
 H   -2.209287   -4.055315   -1.282920
 H   -2.189177   -5.310152   -0.022113
 H   -1.730802   -5.728982   -1.689792
 C    4.392118    0.399520    2.991783
 C    5.656010    0.942454    2.789547
```

C	3.873000	-0.617930	2.155551
C	6.470297	0.486521	1.748718
C	4.721814	-1.076449	1.120241
C	5.988110	-0.531606	0.923334
C	2.524650	-1.125750	2.369013
C	2.013620	-2.339585	1.751300
H	6.606321	-0.906707	0.102844
H	4.374028	-1.857052	0.439554
H	7.461642	0.915940	1.586428
H	6.013212	1.732114	3.457000
H	3.773297	0.771771	3.814333
P	-2.148616	-0.798837	0.256473
C	-1.031952	-1.113519	2.813307
C	-0.771095	-1.788936	4.005610
C	-1.966577	-1.605037	1.895565
C	-1.437164	-2.978373	4.295057
C	-2.616741	-2.810958	2.190074
C	-2.359362	-3.488340	3.379269
C	-6.305229	-1.104228	0.445219
C	-4.969903	-1.037128	0.837098
C	-3.945414	-1.018615	-0.120252
C	-6.638486	-1.143707	-0.910324
C	-5.629183	-1.127424	-1.871547
C	-4.291216	-1.072951	-1.476876
C	-2.779470	1.661434	1.902877
C	-2.196802	0.979433	0.673360
C	-1.872767	1.946152	-0.211806
C	-1.603361	2.407597	2.592055
C	-1.286330	3.531050	1.585953
C	-2.295643	3.292100	0.423280
C	-2.428930	4.486838	-0.499031
C	-3.559922	2.841313	1.249506
C	-4.077074	3.891450	2.241315
C	-4.774826	2.395667	0.436047
C	-1.286503	1.764295	-1.574378
C	-2.053807	1.934826	-2.705091
C	0.099374	1.411457	-1.900770
S	-1.120225	1.698365	-4.134124
C	0.328732	1.362735	-3.260939
C	-3.511144	2.233444	-2.864120
C	1.540937	1.085500	-4.104076
P	1.342272	1.022021	-0.604804
C	4.410097	-0.894653	-2.554395
C	3.193330	-0.589666	-1.949163
C	5.415164	0.068268	-2.636739
C	2.956498	0.692258	-1.435337
C	5.199417	1.335021	-2.096344
C	3.979263	1.645955	-1.497199
C	2.449221	3.874497	2.102109
C	2.138889	2.663618	1.486199
C	2.284307	5.072421	1.406466
C	1.668320	2.644643	0.170462
C	1.821897	5.057591	0.089045
C	1.519071	3.846806	-0.530869
H	-0.474221	-0.200772	2.588354
H	-0.036281	-1.385726	4.706845
H	-1.236063	-3.509360	5.228529
H	-3.327385	-3.236592	1.477863
H	-2.878870	-4.426562	3.589807
H	-7.092215	-1.115452	1.203128
H	-4.727273	-0.988990	1.901311
H	-7.686731	-1.191259	-1.215221
H	-5.880786	-1.163662	-2.934333
H	-3.502301	-1.060741	-2.234654
H	-3.359836	1.007797	2.568868
H	-0.741935	1.749714	2.764486
H	-1.910633	2.801013	3.571950
H	-0.259996	3.498773	1.222721
H	-1.439389	4.530661	2.017959
H	-2.699482	5.385413	0.077636
H	-3.197286	4.342795	-1.271499
H	-1.474813	4.697128	-1.007593
H	-4.806141	3.429649	2.926236
H	-4.603667	4.695363	1.702383
H	-3.303994	4.364719	2.858075
H	-5.585839	2.092070	1.116001
H	-4.571148	1.542254	-0.218766
H	-5.160193	3.226441	-0.176542
H	-4.001927	2.316050	-1.892450
H	-4.019282	1.433531	-3.425071
H	-3.674062	3.175106	-3.411480
H	1.334186	1.338426	-5.153941
H	1.822603	0.023880	-4.071354
H	2.410737	1.673208	-3.785403
H	4.572768	-1.897627	-2.956375
H	2.428994	-1.366166	-1.878158
H	6.371403	-0.171554	-3.107848
H	5.986933	2.090991	-2.134974
H	3.836787	2.642986	-1.078740
H	2.815357	3.881629	3.131260
H	2.252673	1.720249	2.025259
H	2.515751	6.022959	1.892814
H	1.692439	5.995299	-0.456128
H	1.153877	3.837698	-1.560993
Cu	1.292972	-0.809153	0.707654
H	2.749629	-3.019945	1.301017
H	1.259006	-2.883544	2.328111

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 H    2.031446   -0.791365    3.287562
121
Figure 1_L-Cu-alkyl_major02_01 / electronic energy: -4988.01015868 a.u. / lowest freq: 10.11 cm-1
 B   -3.456763   -2.149240   -0.061304
 O   -4.288896   -1.527545    0.833345
 O   -3.828231   -1.902597   -1.361677
 C   -5.424493   -1.018234    0.115291
 C   -4.871001   -0.911498   -1.354942
 C   -5.851297    0.306081    0.726192
 C   -6.542019   -2.050822    0.261130
 C   -4.210704    0.432980   -1.645583
 C   -5.880730   -1.241077   -2.443038
 H   -3.470941    0.681253   -0.872764
 H   -4.945253    1.249110   -1.697671
 H   -3.692001    0.376913   -2.613120
 H   -6.261965   -2.266487   -2.351986
 H   -5.406511   -1.142397   -3.430958
 H   -6.731593   -0.544082   -2.406232
 H   -6.259060   -3.016194   -0.184629
 H   -7.475727   -1.709524   -0.208753
 H   -6.735636   -2.217724    1.330908
 H   -5.017345    1.016940    0.771106
 H   -6.215798    0.144423    1.751353
 H   -6.667687    0.758174    0.142532
 C    0.301117   -3.120523    3.190729
 C    1.273522   -3.960202    3.721698
 C   -0.296990   -3.362695    1.928255
 C    1.701442   -5.093620    3.019656
 C    0.150453   -4.516670    1.243459
 C    1.128469   -5.357215    1.775715
 C   -1.312082   -2.446945    1.373560
 C   -2.267910   -3.080764    0.349274
 H    1.445434   -6.235413    1.205289
 H   -0.270918   -4.755891    0.264631
 H    2.463773   -5.755869    3.436948
 H    1.705378   -3.731410    4.700453
 H   -0.015857   -2.240613    3.760476
 P   -0.910036    1.379425    0.281927
 C   -3.091662    3.113262    1.004384
 C   -4.120006    3.505260    1.862571
 C   -2.294063    2.006537    1.316035
 C   -4.360853    2.799809    3.040554
 C   -2.568594    1.280149    2.483689
 C   -3.584748    1.681698    3.347505
 C   -0.750443    4.508685   -2.406832
 C   -0.754819    3.774927   -1.223599
 C   -0.934776    2.384744   -1.249685
 C   -0.906744    3.859828   -3.633067
 C   -1.069253    2.476510   -3.670237
 C   -1.085662    1.744207   -2.482905
 C    0.740170    2.057880    2.643919
 C    0.579230    1.972590    1.137237
 C    1.808722    2.080706    0.590764
 C    1.425643    0.718977    3.038570
 C    2.840233    0.884574    2.441699
 C    2.795927    2.286088    1.752131
 C    4.164892    2.840454    1.418263
 C    1.899257    3.082996    2.762458
 C    2.487026    3.208850    4.171667
 C    1.506120    4.493614    2.317316
 C    2.185222    1.893739   -0.834220
 C    2.588036    2.942197   -1.626492
 C    2.143067    0.631759   -1.561134
 S    2.911783    2.407192   -3.235107
 C    2.522704    0.763313   -2.878144
 C    2.709439    4.394692   -1.292304
 C    2.668107   -0.247746   -3.976020
 P    1.648210   -0.909710   -0.706209
 C   -0.589647   -2.997041   -3.422901
 C   -0.141154   -2.081224   -2.473976
 C    0.268233   -3.995910   -3.884591
 C    1.175166   -2.132479   -1.994977
 C    1.567873   -4.077998   -3.384519
 C    2.020014   -3.152678   -2.444318
 C    4.408745   -3.034679    1.440848
 C    3.221443   -2.527317    0.917580
 C    5.636932   -2.564450    0.974452
 C    3.250615   -1.553546   -0.087956
 C    5.673195   -1.589996   -0.022837
 C    4.485430   -1.087192   -0.554207
 H   -2.926223    3.674222    0.083449
 H   -4.736493    4.369754    1.604760
 H   -5.163964    3.111256    3.712536
 H   -1.986874    0.382204    2.709155
 H   -3.780715    1.108727    4.256592
 H   -0.612763    5.591953   -2.372390
 H   -0.604888    4.287149   -0.270347
 H   -0.893543    4.434351   -4.562338
 H   -1.180201    1.960701   -4.626636
 H   -1.205945    0.660528   -2.521063
 H   -0.170418    2.294942    3.209789
 H    0.884766   -0.140485    2.610382
 H    1.446857    0.584698    4.129817
 H    3.098378    0.103194    1.719668
 H    3.619695    0.866616    3.217457
 H    4.795749    2.877777    2.320147
 H    4.111889    3.856857    1.002881
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 H    4.678588    2.201856    0.682258
 H    1.716902    3.577278    4.868340
 H    3.308019    3.943219    4.177785
 H    2.881752    2.272683    4.585719
 H    0.839176    4.951164    3.065169
 H    0.978708    4.509072    1.355644
 H    2.393938    5.140591    2.233261
 H    2.302655    4.591181   -0.293542
 H    2.151032    5.015079   -2.009787
 H    3.758248    4.731233   -1.308659
 H    3.081936    0.216981   -4.882157
 H    1.701225   -0.699494   -4.242222
 H    3.344333   -1.061635   -3.678925
 H   -1.619203   -2.941302   -3.783037
 H   -0.837774   -1.336819   -2.076189
 H   -0.082250   -4.722005   -4.621801
 H    2.238567   -4.868874   -3.728494
 H    3.041365   -3.226633   -2.064227
 H    4.368475   -3.793937    2.225054
 H    2.263632   -2.882526    1.302783
 H    6.567458   -2.955719    1.392690
 H    6.631326   -1.215079   -0.390663
 H    4.523857   -0.317795   -1.328763
Cu   -0.377947   -0.871256    0.485279
 H   -1.743518   -3.380640   -0.573456
 H   -2.716803   -4.022203    0.743545
 H   -1.895844   -2.015877    2.205543
121
Figure 1_L-Cu-alkyl_major02_02 / electronic energy: -4988.00339175 a.u. / lowest freq: 16.37 cm-1
 B   -3.919598   -0.018109   -1.084677
 O   -3.819820   -1.320076   -0.662895
 O   -4.682183    0.730317   -0.214026
 C   -4.682300   -1.500906    0.469853
 C   -4.836101   -0.030713    0.994564
 C   -4.035831   -2.459648    1.455599
 C   -5.992639   -2.088905   -0.051389
 C   -3.691282    0.386110    1.916761
 C   -6.177975    0.285599    1.631743
 H   -2.721882    0.184145    1.436452
 H   -3.724609   -0.134476    2.884631
 H   -3.754902    1.468033    2.102067
 H   -7.005083    0.149479    0.922691
 H   -6.193141    1.331105    1.973895
 H   -6.352914   -0.360757    2.505138
 H   -6.498373   -1.396420   -0.740715
 H   -6.683535   -2.334701    0.768209
 H   -5.769975   -3.013998   -0.603616
 H   -3.005298   -2.164465    1.690846
 H   -4.006251   -3.472263    1.028721
 H   -4.613282   -2.500758    2.391978
 C   -1.279684    3.663200   -2.690340
 C   -1.311883    5.025675   -2.395272
 C   -1.979975    2.706972   -1.922394
 C   -2.078763    5.501309   -1.331804
 C   -2.759713    3.219139   -0.859739
 C   -2.809515    4.580693   -0.575880
 C   -1.881692    1.253141   -2.223693
 C   -3.249670    0.524729   -2.394793
 H   -3.425119    4.928840    0.258797
 H   -3.344102    2.527838   -0.251013
 H   -2.112173    6.568546   -1.099056
 H   -0.741375    5.723140   -3.015839
 H   -0.698943    3.321840   -3.553235
 P   -0.248350   -1.737061   -0.156662
 C   -1.449996   -2.748363   -2.421900
 C   -2.193720   -3.633156   -3.195870
 C   -1.166845   -3.031215   -1.078267
 C   -2.693133   -4.806890   -2.628189
 C   -1.671419   -4.207058   -0.517410
 C   -2.434032   -5.087256   -1.288347
 C    0.777185   -4.040004    3.114264
 C    0.584033   -3.606108    1.805618
 C   -0.047147   -2.381199    1.548047
 C    0.356889   -3.247122    4.184259
 C   -0.266059   -2.025422    3.939088
 C   -0.469339   -1.599200    2.626417
 C    1.837647   -2.272507   -2.214015
 C    1.451819   -1.865327   -0.802533
 C    2.559877   -1.371082   -0.209721
 C    2.080964   -0.928747   -2.959318
 C    3.379303   -0.415533   -2.298667
 C    3.709072   -1.502416   -1.229697
 C    5.127998   -1.414941   -0.707000
 C    3.279557   -2.802573   -1.992192
 C    4.054364   -3.070550   -3.286607
 C    3.337296   -4.090796   -1.169093
 C    2.689783   -0.701945    1.111867
 C    3.365022   -1.283749    2.158320
 C    2.185584    0.626491    1.447844
 S    3.416628   -0.228744    3.523681
 C    2.542375    1.025198    2.718278
 C    3.987968   -2.639746    2.261239
 C    2.335804    2.312208    3.460512
 P    1.133600    1.557200    0.268349
 C   -1.417530    3.384584    2.907222
 C   -0.702440    2.447069    2.167614
 C   -1.183795    4.747465    2.719271
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 C    0.271887    2.853272    1.246766
 C   -0.239098    5.160610    1.782173
 C    0.482345    4.220899    1.045643
 C    2.863774    3.568628   -2.838581
 C    1.986309    2.847034   -2.031793
 C    4.108434    3.953866   -2.340635
 C    2.338423    2.516525   -0.719495
 C    4.469700    3.620412   -1.033874
 C    3.588290    2.905949   -0.224037
 H   -1.098869   -1.811031   -2.862764
 H   -2.400397   -3.396979   -4.242349
 H   -3.290808   -5.496247   -3.229291
 H   -1.494109   -4.441099    0.533365
 H   -2.830283   -5.997798   -0.832326
 H    1.269425   -4.997351    3.300487
 H    0.933892   -4.224194    0.975692
 H    0.518930   -3.583142    5.211159
 H   -0.592540   -1.396350    4.770278
 H   -0.956801   -0.641697    2.440710
 H    1.151237   -2.962099   -2.720922
 H    1.232693   -0.240341   -2.821143
 H    2.200383   -1.088357   -4.040660
 H    3.270001    0.567285   -1.830864
 H    4.202968   -0.332237   -3.023141
 H    5.846081   -1.447520   -1.541350
 H    5.374318   -2.238124   -0.021890
 H    5.291799   -0.467629   -0.169257
 H    3.576393   -3.892201   -3.843625
 H    5.083985   -3.388339   -3.057366
 H    4.118840   -2.210060   -3.964000
 H    2.950337   -4.935015   -1.761339
 H    2.747884   -4.041165   -0.246002
 H    4.377504   -4.332682   -0.898092
 H    3.587624   -3.192027    3.124852
 H    5.080786   -2.577917    2.384821
 H    3.776195   -3.228404    1.361792
 H    3.089119    2.422759    4.253858
 H    1.343502    2.362435    3.933834
 H    2.424654    3.176218    2.790261
 H   -2.162435    3.048852    3.632310
 H   -0.891295    1.383832    2.325425
 H   -1.745933    5.485583    3.295993
 H   -0.062151    6.225437    1.614587
 H    1.217767    4.564282    0.315693
 H    2.578975    3.819140   -3.863135
 H    1.022194    2.519458   -2.423775
 H    4.802078    4.512638   -2.973400
 H    5.445567    3.917812   -0.642801
 H    3.879791    2.640574    0.795323
Cu   -0.635986    0.461300   -0.816590
 H   -3.972195    1.166924   -2.940726
 H   -3.085466   -0.355768   -3.038347
 H   -1.348583    1.163986   -3.188645
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Figure 1_pc1_minor01_01 / electronic energy: -4987.94988378 a.u. / lowest freq: 16.56 cm-1
 B   -3.113030    0.177224   -1.612038
 O   -4.335610   -0.238872   -1.093727
 O   -3.340308    1.165973   -2.563035
 C   -5.408647    0.364126   -1.827755
 C   -4.703570    1.604550   -2.476580
 C   -6.539488    0.702773   -0.867440
 C   -5.887160   -0.659001   -2.858422
 C   -4.721287    2.839805   -1.573931
 C   -5.203451    1.973077   -3.865438
 H   -4.378684    2.592302   -0.558333
 H   -5.724427    3.286469   -1.504218
 H   -4.037569    3.596244   -1.987459
 H   -5.044574    1.158615   -4.584603
 H   -4.662546    2.857797   -4.234112
 H   -6.276900    2.217579   -3.843945
 H   -5.088826   -0.908176   -3.573311
 H   -6.761753   -0.299047   -3.420523
 H   -6.173291   -1.584874   -2.337033
 H   -6.183672    1.311851   -0.026460
 H   -6.964802   -0.223014   -0.451031
 H   -7.347050    1.245630   -1.383192
 C   -0.317467   -4.503284    0.232466
 C   -0.832879   -5.379088    1.184829
 C   -1.145802   -3.594473   -0.447772
 C   -2.195996   -5.373087    1.483122
 C   -2.522027   -3.607527   -0.143650
 C   -3.035517   -4.483596    0.810119
 C   -0.572662   -2.641844   -1.418047
 C   -1.305680   -2.078527   -2.462140
 H   -4.104961   -4.462862    1.035469
 H   -3.194627   -2.898153   -0.634566
 H   -2.600364   -6.055893    2.234009
 H   -0.161988   -6.069009    1.702907
 H    0.753175   -4.518158    0.013513
 P   -1.023871   -0.058603    1.205868
 C    0.729334   -2.006782    2.086237
 C    1.435812   -2.769687    3.014196
 C   -0.269950   -1.124622    2.499295
 C    1.134550   -2.661013    4.370681
 C   -0.570238   -1.021107    3.863754
 C    0.128230   -1.788996    4.793182
 C   -4.458329    1.915873    2.365145
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 C   -3.159512    1.656643    1.925744
 C   -2.663484    0.350412    1.912366
 C   -5.277348    0.869406    2.785599
 C   -4.793136   -0.439637    2.760687
 C   -3.497051   -0.698220    2.322839
 C    0.143456    2.281251    2.629185
 C   -0.022909    1.440630    1.370860
 C    0.872106    1.889782    0.466435
 C    1.515742    1.857743    3.227397
 C    2.519017    2.421146    2.198104
 C    1.607741    3.075129    1.112278
 C    2.321536    4.016943    0.165744
 C    0.472395    3.673293    2.019431
 C    0.954086    4.710370    3.040029
 C   -0.679095    4.322738    1.251006
 C    1.146259    1.373268   -0.901227
 C    0.414896    1.829350   -1.973900
 C    2.184293    0.429514   -1.290634
 S    0.961993    1.103780   -3.438342
 C    2.194021    0.188586   -2.649460
 C   -0.693571    2.834105   -1.998116
 C    3.083384   -0.671924   -3.496658
 P    3.357596   -0.231802   -0.042364
 C    3.638736   -4.150834   -1.229849
 C    3.205876   -2.927009   -0.724082
 C    4.923255   -4.268847   -1.760853
 C    4.026677   -1.792323   -0.766099
 C    5.764184   -3.156124   -1.775329
 C    5.320956   -1.928309   -1.283532
 C    6.879082    1.696970    0.754794
 C    5.760022    0.868270    0.800441
 C    7.045504    2.586186   -0.308072
 C    4.800676    0.901511   -0.222506
 C    6.092771    2.634576   -1.324951
 C    4.978248    1.795025   -1.284897
 H    0.946753   -2.088393    1.020945
 H    2.217354   -3.453387    2.674313
 H    1.682586   -3.258844    5.102862
 H   -1.345840   -0.331949    4.206028
 H   -0.108507   -1.700682    5.856118
 H   -4.831386    2.942824    2.372493
 H   -2.534424    2.482629    1.584975
 H   -6.295638    1.071405    3.126033
 H   -5.432228   -1.266972    3.078043
 H   -3.133619   -1.729441    2.294797
 H   -0.694054    2.243718    3.339632
 H    1.587901    0.766814    3.328376
 H    1.659292    2.290368    4.228125
 H    3.156373    1.642135    1.767983
 H    3.188955    3.178704    2.631038
 H    2.763394    4.861415    0.717232
 H    1.637549    4.426428   -0.593565
 H    3.140011    3.503874   -0.360676
 H    0.132554    4.963739    3.728979
 H    1.246554    5.641131    2.528519
 H    1.806358    4.391540    3.652175
 H   -1.476099    4.628263    1.947301
 H   -1.119802    3.662403    0.497998
 H   -0.332620    5.233406    0.736951
 H   -1.487095    2.544726   -1.297487
 H   -1.157310    2.896128   -2.990427
 H   -0.323688    3.834232   -1.724003
 H    2.898930   -0.488090   -4.564755
 H    2.914822   -1.742937   -3.308691
 H    4.143621   -0.463509   -3.298595
 H    2.970809   -5.015428   -1.202324
 H    2.206805   -2.852449   -0.293514
 H    5.271152   -5.226440   -2.155160
 H    6.774728   -3.240451   -2.182401
 H    5.991395   -1.067031   -1.322113
 H    7.619554    1.656503    1.557125
 H    5.628529    0.184123    1.644439
 H    7.915895    3.246021   -0.340056
 H    6.214357    3.332807   -2.156583
 H    4.236601    1.844607   -2.085525
Cu   -1.430553   -0.761906   -0.930391
 H   -2.305733   -2.442939   -2.713544
 H   -0.777842   -1.564856   -3.271787
 H    0.517159   -2.558634   -1.439575
121
Figure 1_pc1_minor01_02 / electronic energy: -4987.95193410 a.u. / lowest freq: 12.40 cm-1
 B   -3.268968    0.265179   -1.663715
 O   -4.570821   -0.037402   -1.262075
 O   -3.334033    1.131320   -2.753753
 C   -5.505898    0.467419   -2.225059
 C   -4.678317    1.604674   -2.912340
 C   -6.762854    0.934258   -1.505872
 C   -5.845596   -0.681156   -3.176154
 C   -4.780384    2.942655   -2.176740
 C   -4.969933    1.804274   -4.391779
 H   -4.581614    2.822783   -1.100975
 H   -5.771348    3.404978   -2.299160
 H   -4.029124    3.636951   -2.582080
 H   -4.742379    0.901590   -4.974008
 H   -4.352133    2.624385   -4.787702
 H   -6.026907    2.067379   -4.552546
 H   -4.952117   -1.027429   -3.716911
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H	-6.610561	-0.392961	-3.912292
H	-6.234279	-1.527789	-2.590681
H	-6.529714	1.646766	-0.703816
H	-7.273665	0.072371	-1.050688
H	-7.464054	1.412171	-2.207466
C	-0.185549	-4.441889	0.113402
C	-0.676603	-5.527970	0.833452
C	-1.053185	-3.501247	-0.463227
C	-2.050641	-5.695405	1.006691
C	-2.436380	-3.676146	-0.271030
C	-2.926482	-4.758806	0.456149
C	-0.516072	-2.379617	-1.261192
C	-1.195544	-1.843624	-2.344473
H	-4.004684	-4.870249	0.595620
H	-3.137467	-2.946657	-0.686186
H	-2.436726	-6.545976	1.573332
H	0.022654	-6.248027	1.265825
H	0.891840	-4.324678	-0.015112
P	-1.046098	-0.140170	1.408639
C	0.998461	-1.781539	2.403930
C	1.515647	-2.901031	3.056008
C	-0.381679	-1.552566	2.371600
C	0.657820	-3.805146	3.680868
C	-1.240342	-2.484482	2.969942
C	-0.720822	-3.596659	3.629544
C	-3.510330	0.958584	4.561944
C	-2.477671	0.374783	3.831211
C	-2.443336	0.486811	2.433477
C	-4.518861	1.668884	3.908392
C	-4.493220	1.785028	2.520025
C	-3.464738	1.191666	1.787429
C	0.372112	1.991651	2.940310
C	0.148568	1.207665	1.651473
C	0.914565	1.780692	0.700550
C	1.818420	1.672921	3.402385
C	2.675318	2.357994	2.316400
C	1.619283	2.982280	1.351813
C	2.179997	4.022425	0.404327
C	0.518446	3.434320	2.381838
C	0.996393	4.471214	3.403591
C	-0.774222	3.980144	1.773697
C	1.084817	1.388936	-0.721868
C	0.268321	1.892561	-1.708823
C	2.127943	0.521775	-1.242144
S	0.751072	1.298493	-3.255274
C	2.054267	0.369566	-2.611179
C	-0.877194	2.848125	-1.594760
C	2.906904	-0.426527	-3.551652
P	3.435577	-0.115350	-0.125397
C	3.628743	-4.066259	-1.162433
C	3.246378	-2.824740	-0.657806
C	4.825217	-4.191765	-1.868940
C	4.030387	-1.684952	-0.880892
C	5.632079	-3.070430	-2.064062
C	5.237907	-1.825142	-1.575494
C	6.994678	1.865420	0.288031
C	5.912228	1.001028	0.437705
C	7.004462	2.798612	-0.749913
C	4.830636	1.043046	-0.455505
C	5.930065	2.856496	-1.636286
C	4.850572	1.983354	-1.492017
H	1.680816	-1.081279	1.913886
H	2.596286	-3.062228	3.074119
H	1.061891	-4.680248	4.195105
H	-2.322922	-2.342050	2.927658
H	-1.401749	-4.311917	4.096384
H	-3.524928	0.860150	5.649934
H	-1.690807	-0.167837	4.359855
H	-5.326892	2.127910	4.483068
H	-5.282832	2.331963	1.999427
H	-3.462274	1.260095	0.697754
H	-0.392483	1.859475	3.715228
H	1.992451	0.591025	3.467833
H	2.006247	2.093311	4.401010
H	3.328142	1.655796	1.786752
H	3.322167	3.147158	2.727301
H	2.600791	4.870780	0.966402
H	1.411016	4.414074	-0.278821
H	2.990100	3.600109	-0.209591
H	0.250322	4.573287	4.207891
H	1.094521	5.458485	2.924795
H	1.959212	4.240780	3.875582
H	-1.491494	4.219164	2.574927
H	-1.265383	3.273561	1.097310
H	-0.583743	4.911380	1.216405
H	-1.544868	2.541759	-0.779766
H	-1.482542	2.848761	-2.509282
H	-0.527107	3.873295	-1.394722
H	2.647176	-0.211317	-4.597868
H	2.778846	-1.507559	-3.389004
H	3.971939	-0.193166	-3.414703
H	2.996895	-4.941247	-0.990421
H	2.325515	-2.738672	-0.075019
H	5.133655	-5.164490	-2.259193
H	6.576040	-3.163789	-2.606373
H	5.874259	-0.954883	-1.751707
H	7.828046	1.818638	0.993077

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 H    5.905348    0.282755    1.263209
 H    7.845948    3.486401   -0.862094
 H    5.927698    3.588917   -2.447056
 H    4.014143    2.045279   -2.191618
Cu   -1.641201   -0.598926   -0.772993
 H   -2.112982   -2.303924   -2.722169
 H   -0.668358   -1.193166   -3.048000
 H    0.544623   -2.146582   -1.132158
121
Figure 1_pc1_minor01_03 / electronic energy: -4987.95470336 a.u. / lowest freq: 27.07 cm-1
 B   -3.564333    0.051732   -1.050160
 O   -4.746168   -0.664252   -0.874788
 O   -3.884646    1.345258   -1.453115
 C   -5.845798    0.073935   -1.424983
 C   -5.304268    1.545757   -1.400614
 C   -7.085591   -0.165160   -0.575634
 C   -6.074806   -0.455462   -2.841957
 C   -5.620683    2.282827   -0.099723
 C   -5.724890    2.403306   -2.586198
 H   -5.343157    1.684442    0.779262
 H   -6.689016    2.532935   -0.022285
 H   -5.046198    3.220444   -0.068604
 H   -5.366393    1.987254   -3.536896
 H   -5.300239    3.413329   -2.481774
 H   -6.820495    2.500046   -2.635563
 H   -5.191937   -0.286563   -3.476403
 H   -6.946438    0.012584   -3.323191
 H   -6.251136   -1.540323   -2.792479
 H   -6.896619    0.048320    0.484865
 H   -7.395110   -1.218096   -0.656189
 H   -7.924170    0.461254   -0.917093
 C    0.552731   -4.232502   -1.357412
 C    0.556949   -5.500319   -0.780973
 C   -0.634584   -3.493084   -1.479025
 C   -0.628863   -6.060353   -0.303865
 C   -1.826548   -4.077028   -1.010284
 C   -1.820088   -5.341202   -0.425547
 C   -0.597462   -2.146766   -2.076650
 C   -1.684938   -1.567242   -2.722866
 H   -2.755430   -5.767531   -0.054223
 H   -2.768206   -3.526251   -1.080446
 H   -0.626625   -7.050392    0.157820
 H    1.496217   -6.053415   -0.697708
 H    1.486002   -3.798495   -1.724386
 P   -0.774447   -0.441639    1.226396
 C    0.268283   -2.936522    1.820327
 C    1.145465   -3.849512    2.403464
 C    0.466974   -1.558361    1.980456
 C    2.240240   -3.396233    3.139019
 C    1.557185   -1.113649    2.734306
 C    2.444329   -2.026561    3.302445
 C   -4.222697    0.453558    3.271319
 C   -3.233421    0.338548    2.298704
 C   -2.061193   -0.387019    2.548306
 C   -4.062634   -0.172753    4.508297
 C   -2.904706   -0.904777    4.763596
 C   -1.907546   -1.009730    3.791929
 C   -0.364615    2.307246    2.351058
 C   -0.159099    1.272305    1.250019
 C    0.395769    1.918972    0.201413
 C    1.047314    2.691811    2.870545
 C    1.667536    3.419732    1.660656
 C    0.527821    3.397626    0.595534
 C    0.727673    4.394325   -0.526961
 C   -0.742692    3.558588    1.508092
 C   -0.791318    4.871324    2.296956
 C   -2.086858    3.425803    0.788181
 C    0.890532    1.362191   -1.082407
 C    0.227189    1.515356   -2.278479
 C    2.158152    0.665617   -1.231238
 S    1.120210    0.784666   -3.565933
 C    2.409637    0.286681   -2.532123
 C   -1.055956    2.217438   -2.587451
 C    3.585113   -0.425298   -3.128164
 P    3.311890    0.503294    0.181379
 C    6.134858   -2.484186   -0.457543
 C    5.551576   -1.225365   -0.309097
 C    5.346133   -3.633642   -0.430526
 C    4.168715   -1.096809   -0.133940
 C    3.967427   -3.515306   -0.249855
 C    3.384760   -2.259122   -0.096973
 C    5.592191    3.556014   -1.502399
 C    4.619737    2.567207   -1.342324
 C    6.561476    3.755766   -0.520759
 C    4.600419    1.766716   -0.193918
 C    6.547465    2.969451    0.632460
 C    5.566470    1.994502    0.799583
 H   -0.581256   -3.303791    1.240056
 H    0.975329   -4.919929    2.268668
 H    2.937979   -4.111353    3.581112
 H    1.722351   -0.047185    2.874186
 H    3.300571   -1.662635    3.874864
 H   -5.126941    1.029396    3.058080
 H   -3.365698    0.827060    1.332288
 H   -4.840380   -0.091386    5.271334
 H   -2.769700   -1.399222    5.728491
 H   -1.003999   -1.579537    4.017045
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 H   -1.075755    2.023633    3.137569
 H    1.628696    1.814969    3.180397
 H    0.967481    3.347750    3.749310
 H    2.572331    2.928520    1.280624
 H    1.944098    4.458385    1.895448
 H    0.822762    5.412627   -0.118779
 H   -0.109830    4.391877   -1.238796
 H    1.650121    4.177764   -1.088795
 H   -1.567827    4.811896    3.076405
 H   -1.065275    5.703849    1.629707
 H    0.150173    5.144564    2.789213
 H   -2.906710    3.509951    1.519050
 H   -2.218759    2.475946    0.257263
 H   -2.219767    4.239838    0.057239
 H   -1.605637    2.448099   -1.670168
 H   -1.722982    1.597223   -3.202519
 H   -0.871601    3.156030   -3.135186
 H    3.598842   -0.318634   -4.222176
 H    3.565062   -1.500859   -2.892573
 H    4.527533   -0.019076   -2.735592
 H    7.215157   -2.564388   -0.601319
 H    6.185995   -0.336988   -0.346104
 H    5.804421   -4.618475   -0.547549
 H    3.337275   -4.407322   -0.218193
 H    2.303755   -2.184002    0.051140
 H    5.590670    4.172281   -2.404843
 H    3.867746    2.424141   -2.121387
 H    7.323185    4.528513   -0.648803
 H    7.297096    3.124382    1.412180
 H    5.550051    1.400014    1.718294
Cu   -1.711968   -0.799730   -0.840945
 H   -2.606404   -2.130463   -2.897563
 H   -1.522381   -0.721745   -3.396776
 H    0.398242   -1.717130   -2.228493
121
Figure 1_pc1_minor01_04 / electronic energy: -4987.95276732 a.u. / lowest freq: 16.33 cm-1
 B   -2.842609    1.042824   -0.194489
 O   -3.713008    0.310657    0.620661
 O   -3.448463    2.251762   -0.510663
 C   -5.002051    0.937120    0.632115
 C   -4.639218    2.416743    0.272600
 C   -5.641295    0.745454    1.999054
 C   -5.848464    0.251934   -0.442539
 C   -4.271553    3.252523    1.499256
 C   -5.684840    3.149178   -0.554990
 H   -3.516757    2.742625    2.116683
 H   -5.149299    3.469121    2.126168
 H   -3.845283    4.208118    1.162251
 H   -5.855407    2.657711   -1.521849
 H   -5.346673    4.176961   -0.756064
 H   -6.643309    3.207551   -0.016111
 H   -5.407668    0.387787   -1.441735
 H   -6.879465    0.635609   -0.462332
 H   -5.888923   -0.827876   -0.234140
 H   -4.976446    1.080740    2.805998
 H   -5.856836   -0.321159    2.164076
 H   -6.590815    1.298234    2.071499
 C   -0.939154   -3.311566   -2.963513
 C   -1.465933   -4.587458   -2.784073
 C   -1.716073   -2.162049   -2.730212
 C   -2.791740   -4.752932   -2.377783
 C   -3.050188   -2.346232   -2.321859
 C   -3.578796   -3.623460   -2.154675
 C   -1.120719   -0.824219   -2.890108
 C   -1.850473    0.358923   -2.845733
 H   -4.615827   -3.736512   -1.828290
 H   -3.677164   -1.479878   -2.101639
 H   -3.206132   -5.753259   -2.232905
 H   -0.836006   -5.462315   -2.964849
 H    0.099028   -3.193844   -3.284078
 P   -0.211085   -1.308498    0.608057
 C   -2.476679   -2.820097    0.989786
 C   -3.225007   -3.953279    1.303791
 C   -1.077708   -2.891573    0.932589
 C   -2.590406   -5.171726    1.542337
 C   -0.444880   -4.113171    1.193014
 C   -1.198940   -5.249161    1.486064
 C   -0.561251    1.213212    3.840385
 C   -0.647738    0.651731    2.565907
 C   -0.134023   -0.619769    2.314864
 C    0.026780    0.493898    4.878518
 C    0.515963   -0.793284    4.641530
 C    0.436930   -1.347298    3.366836
 C    1.981851   -2.780668   -0.710950
 C    1.518969   -1.716077    0.273221
 C    2.607130   -0.989016    0.607178
 C    2.357892   -1.997064   -2.001616
 C    3.634799   -1.242152   -1.585818
 C    3.820127   -1.641135   -0.092076
 C    5.204177   -1.332648    0.441707
 C    3.371564   -3.143303   -0.122059
 C    4.216959   -4.044388   -1.027552
 C    3.316924   -3.816316    1.252118
 C    2.711317    0.314965    1.309591
 C    3.373537    0.448241    2.504515
 C    2.292322    1.600332    0.754398
 S    3.551614    2.113755    2.929419
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 C    2.743181    2.667399    1.502557
 C    3.893879   -0.611281    3.422557
 C    2.697037    4.147429    1.266019
 P    1.170915    1.677862   -0.701778
 C   -1.057630    4.851140    0.719125
 C   -0.304407    3.684043    0.640349
 C   -1.261226    5.637613   -0.415392
 C    0.289294    3.291585   -0.567254
 C   -0.698034    5.243589   -1.626944
 C    0.073495    4.082898   -1.702208
 C    2.723703    1.712213   -4.497153
 C    1.886733    1.569563   -3.390790
 C    4.001687    2.246794   -4.339143
 C    2.311829    1.965936   -2.116330
 C    4.434694    2.645686   -3.073763
 C    3.595444    2.507307   -1.969621
 H   -2.981922   -1.867066    0.800992
 H   -4.314548   -3.883375    1.351013
 H   -3.179192   -6.061991    1.776758
 H    0.642822   -4.185634    1.182010
 H   -0.693012   -6.198086    1.679526
 H   -0.958066    2.215595    4.020029
 H   -1.117199    1.196665    1.744484
 H    0.099388    0.931620    5.877041
 H    0.967106   -1.365481    5.455675
 H    0.832400   -2.350914    3.188968
 H    1.286438   -3.611545   -0.884184
 H    1.546418   -1.316917   -2.284660
 H    2.532944   -2.680625   -2.845399
 H    3.550092   -0.155626   -1.694031
 H    4.511337   -1.551356   -2.174601
 H    5.969666   -1.769898   -0.218279
 H    5.364144   -1.738121    1.450326
 H    5.384295   -0.246986    0.480798
 H    3.733470   -5.028719   -1.132982
 H    5.209231   -4.214344   -0.580299
 H    4.375182   -3.647184   -2.037880
 H    2.926530   -4.842498    1.158802
 H    2.683714   -3.280945    1.970749
 H    4.326759   -3.896204    1.685304
 H    3.640929   -1.606487    3.036460
 H    3.445225   -0.516710    4.423418
 H    4.987163   -0.553107    3.542051
 H    3.663279    4.602313    1.531843
 H    1.920434    4.641053    1.870387
 H    2.496067    4.376309    0.213154
 H   -1.491913    5.146463    1.677147
 H   -0.148566    3.090904    1.542288
 H   -1.856045    6.552001   -0.354280
 H   -0.851153    5.844933   -2.526302
 H    0.515811    3.805154   -2.661328
 H    2.377907    1.394148   -5.483423
 H    0.892694    1.136659   -3.520591
 H    4.664019    2.349257   -5.202014
 H    5.435599    3.064108   -2.943792
 H    3.955175    2.800811   -0.981142
Cu   -1.172515    0.109296   -0.927226
 H   -2.942263    0.359864   -2.869662
 H   -1.392527    1.294289   -3.182269
 H   -0.091120   -0.802299   -3.254606
121
Figure 1_pc1_minor01_05 / electronic energy: -4987.95012928 a.u. / lowest freq: 21.46 cm-1
 B   -1.614375   -1.861202   -0.310978
 O   -1.540463   -3.244361   -0.226675
 O   -2.835229   -1.443874    0.210568
 C   -2.823492   -3.776664    0.126566
 C   -3.515801   -2.549607    0.817478
 C   -2.631416   -4.988638    1.025513
 C   -3.507412   -4.190441   -1.177377
 C   -3.248925   -2.475698    2.319697
 C   -5.007930   -2.414359    0.550125
 H   -2.174917   -2.569964    2.530049
 H   -3.787007   -3.259971    2.872996
 H   -3.584291   -1.495150    2.687858
 H   -5.222783   -2.304687   -0.521351
 H   -5.393854   -1.520511    1.063238
 H   -5.557790   -3.288961    0.930492
 H   -3.655827   -3.324057   -1.839710
 H   -4.482595   -4.668610   -1.001261
 H   -2.863399   -4.908803   -1.706403
 H   -2.007524   -4.747239    1.896076
 H   -2.128609   -5.792384    0.466290
 H   -3.599788   -5.375603    1.379267
 C    2.797239   -0.807454   -4.174953
 C    4.061815   -1.366933   -4.352293
 C    1.827309   -1.434985   -3.374344
 C    4.396932   -2.567066   -3.725507
 C    2.180377   -2.648021   -2.754080
 C    3.445138   -3.201968   -2.924130
 C    0.491035   -0.831941   -3.223301
 C   -0.659153   -1.566083   -2.924043
 H    3.694049   -4.138852   -2.418842
 H    1.457139   -3.151916   -2.108013
 H    5.390131   -3.003091   -3.855182
 H    4.794143   -0.855673   -4.982763
 H    2.550341    0.136888   -4.669100
 P    1.447236   -0.751465    0.497081
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 C    3.697630   -0.065441   -0.960209
 C    5.054730   -0.003925   -1.270353
 C    3.243653   -0.846902    0.107303
 C    5.973299   -0.747156   -0.530331
 C    4.172424   -1.588669    0.847191
 C    5.528327   -1.543585    0.525217
 C    1.248310   -4.609894    1.880115
 C    1.522203   -3.476951    1.120335
 C    1.175628   -2.202513    1.590338
 C    0.611296   -4.489534    3.117254
 C    0.245025   -3.228490    3.581644
 C    0.521643   -2.092527    2.818510
 C    2.697666    1.417416    2.046959
 C    1.425909    0.695953    1.610786
 C    0.376494    1.436786    2.031698
 C    2.783568    2.656045    1.115612
 C    1.592881    3.507866    1.600923
 C    0.976989    2.664901    2.764723
 C    0.074661    3.485575    3.663450
 C    2.268224    2.046380    3.394857
 C    3.253654    3.080397    3.952508
 C    2.046381    1.013653    4.500242
 C   -1.098985    1.337691    1.837743
 C   -1.931774    1.132357    2.910685
 C   -1.838331    1.727648    0.634935
 S   -3.569751    1.510920    2.511985
 C   -3.177208    1.927555    0.878458
 C   -1.618132    0.645084    4.289567
 C   -4.295239    2.438343    0.020254
 P   -1.052852    1.524377   -1.008057
 C   -4.314242    0.396586   -3.243359
 C   -3.366829    0.511689   -2.230568
 C   -4.289572    1.265312   -4.336467
 C   -2.384425    1.513839   -2.281506
 C   -3.307749    2.250730   -4.404869
 C   -2.361230    2.375852   -3.384945
 C   -0.111024    5.536040   -1.300458
 C   -0.784279    4.351408   -1.015140
 C    1.134264    5.496833   -1.933427
 C   -0.218219    3.116218   -1.358587
 C    1.697727    4.272605   -2.288882
 C    1.021462    3.085495   -2.003003
 H    2.977864    0.500430   -1.556179
 H    5.392244    0.616231   -2.103685
 H    7.037021   -0.708071   -0.776962
 H    3.843569   -2.198539    1.691261
 H    6.241967   -2.128707    1.110215
 H    1.526781   -5.595719    1.500393
 H    2.010989   -3.587173    0.148900
 H    0.393392   -5.380374    3.711091
 H   -0.266013   -3.121542    4.541481
 H    0.204757   -1.113153    3.177037
 H    3.605830    0.803308    2.073778
 H    2.697747    2.368337    0.060083
 H    3.745085    3.176073    1.235836
 H    0.847544    3.692660    0.821127
 H    1.913237    4.491544    1.975105
 H    0.623078    4.361523    4.043732
 H   -0.288018    2.918915    4.532055
 H   -0.803267    3.859474    3.114356
 H    4.229354    2.605177    4.142887
 H    2.888787    3.473286    4.914947
 H    3.429398    3.940238    3.294677
 H    3.017701    0.647557    4.868828
 H    1.481132    0.136820    4.166246
 H    1.521329    1.460695    5.359572
 H   -0.536945    0.635494    4.463740
 H   -1.987650   -0.384173    4.429138
 H   -2.084660    1.270426    5.066056
 H   -4.928300    3.125520    0.602239
 H   -4.941553    1.625905   -0.346428
 H   -3.917514    2.986177   -0.850289
 H   -5.077781   -0.382914   -3.179897
 H   -3.390448   -0.175610   -1.381784
 H   -5.032322    1.171801   -5.132383
 H   -3.274284    2.935531   -5.255808
 H   -1.603367    3.157913   -3.460053
 H   -0.555181    6.495048   -1.023906
 H   -1.751998    4.383957   -0.507286
 H    1.665528    6.426853   -2.149457
 H    2.671105    4.238604   -2.783519
 H    1.464171    2.122104   -2.271112
Cu   -0.157491   -0.686128   -1.143719
 H   -0.618455   -2.653822   -2.821163
 H   -1.634977   -1.165630   -3.209350
 H    0.365460    0.152733   -3.685987
121
Figure 1_ts(CuBadd)_minor01_01 / electronic energy: -4987.94730051 a.u. / lowest freq: -107.88 cm-1
 B   -2.786277    0.887420   -0.117073
 O   -3.724278    0.112202    0.553111
 O   -3.251756    2.176492   -0.257473
 C   -4.958460    0.843803    0.647856
 C   -4.475458    2.330725    0.477569
 C   -5.615559    0.533189    1.984203
 C   -5.857215    0.366969   -0.492539
 C   -4.137995    3.007944    1.804404
 C   -5.413090    3.219800   -0.326501
```

H	-3.435573	2.404056	2.397583
H	-5.039478	3.190623	2.407254
H	-3.659869	3.975468	1.599398
H	-5.573470	2.829766	-1.340218
H	-4.974936	4.224891	-0.419292
H	-6.389652	3.317594	0.172021
H	-5.403178	0.559416	-1.476022
H	-6.841931	0.855895	-0.466697
H	-6.012969	-0.718017	-0.397814
H	-4.938782	0.728019	2.826622
H	-5.897364	-0.529769	2.019488
H	-6.529369	1.131486	2.120409
C	-1.314715	-3.194477	-3.374557
C	-1.837593	-4.481757	-3.439116
C	-2.003529	-2.145633	-2.723494
C	-3.079403	-4.777947	-2.868189
C	-3.256985	-2.467198	-2.151653
C	-3.782384	-3.754918	-2.229645
C	-1.430758	-0.806574	-2.651149
C	-2.201299	0.325952	-2.234673
H	-4.752422	-3.962858	-1.769295
H	-3.813995	-1.703238	-1.604238
H	-3.491865	-5.788079	-2.923191
H	-1.271235	-5.266370	-3.948867
H	-0.347539	-2.983082	-3.838614
P	-0.077796	-1.208096	1.054292
C	-1.658861	-3.470239	0.746016
C	-2.195793	-4.708673	1.097296
C	-0.803285	-2.795439	1.620883
C	-1.885250	-5.277677	2.331115
C	-0.496786	-3.369594	2.861246
C	-1.036098	-4.605389	3.213040
C	-0.996736	1.299091	4.147423
C	-1.025924	0.555177	2.969648
C	0.065218	-0.244586	2.606724
C	0.129127	1.258411	4.970490
C	1.213937	0.453295	4.622906
C	1.179296	-0.302255	3.451366
C	1.823805	-2.972193	-0.226264
C	1.594907	-1.692479	0.565575
C	2.724346	-0.958617	0.479612
C	1.820513	-2.519933	-1.711463
C	3.110609	-1.679197	-1.802571
C	3.721687	-1.776186	-0.364645
C	5.189580	-1.405078	-0.315570
C	3.326334	-3.234628	0.043619
C	3.946039	-4.323665	-0.836608
C	3.622598	-3.607673	1.498576
C	3.001227	0.435860	0.893322
C	3.951407	0.736350	1.841187
C	2.424546	1.624155	0.285626
S	4.185486	2.442202	1.956330
C	3.016701	2.787624	0.734181
C	4.702495	-0.175400	2.758793
C	2.844999	4.215456	0.311890
P	1.015822	1.551655	-0.889769
C	-0.968411	4.492863	1.143880
C	-0.284114	3.335692	0.791605
C	-1.283975	5.445046	0.172240
C	0.131239	3.126343	-0.530315
C	-0.905054	5.226845	-1.150159
C	-0.194942	4.076033	-1.500457
C	1.566118	1.886518	-4.945287
C	1.009140	1.729591	-3.677289
C	2.931980	2.132677	-5.083958
C	1.804484	1.835115	-2.526455
C	3.733956	2.228188	-3.947156
C	3.174764	2.083640	-2.677747
H	-1.906003	-3.025800	-0.219600
H	-2.860595	-5.224658	0.400500
H	-2.307616	-6.245911	2.610309
H	0.164446	-2.852480	3.560799
H	-0.793504	-5.047070	4.182411
H	-1.854499	1.919420	4.418450
H	-1.904192	0.592359	2.320213
H	0.159153	1.849869	5.888680
H	2.093275	0.409948	5.269921
H	2.025892	-0.939564	3.192027
H	1.137746	-3.799222	0.000303
H	0.915356	-1.942423	-1.936058
H	1.841835	-3.387440	-2.386137
H	2.923516	-0.631500	-2.073261
H	3.815809	-2.077652	-2.547704
H	5.753602	-2.000846	-1.050045
H	5.636651	-1.587748	0.671463
H	5.343507	-0.343250	-0.563839
H	3.448781	-5.288848	-0.649066
H	5.012158	-4.453302	-0.591512
H	3.880800	-4.123839	-1.913628
H	3.260773	-4.627641	1.703616
H	3.140082	-2.937750	2.221933
H	4.707057	-3.601055	1.693601
H	4.429551	-1.220718	2.572006
H	4.469761	0.047084	3.812476
H	5.792359	-0.078495	2.635989
H	3.762813	4.787435	0.511612
H	2.018106	4.707290	0.846506

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 H    2.634078    4.284342   -0.763220
 H   -1.261450    4.649255    2.184747
 H   -0.049109    2.594609    1.559749
 H   -1.826904    6.352969    0.445990
 H   -1.150116    5.963217   -1.919348
 H    0.118798    3.938812   -2.537583
 H    0.928763    1.806140   -5.828802
 H   -0.059956    1.527686   -3.587801
 H    3.372230    2.246647   -6.077298
 H    4.805357    2.417369   -4.046737
 H    3.815986    2.157484   -1.796800
Cu   -1.055612   -0.069771   -0.647854
 H   -3.292346    0.219474   -2.222719
 H   -1.904553    1.318506   -2.591299
 H   -0.517811   -0.640095   -3.229435
121
Figure 1_ts(CuBadd)_minor01_02 / electronic energy: -4987.94593447 a.u. / lowest freq: -131.74 cm-1
 B   -3.036591   -0.190902   -1.602248
 O   -4.219584   -0.448510   -0.935792
 O   -3.272704    0.554485   -2.739989
 C   -5.316742   -0.019949   -1.759460
 C   -4.627297    1.040330   -2.686536
 C   -6.417810    0.528813   -0.867078
 C   -5.813734   -1.245809   -2.523710
 C   -4.582218    2.434023   -2.060390
 C   -5.187483    1.115937   -4.097560
 H   -4.193002    2.393437   -1.032263
 H   -5.576506    2.903401   -2.037853
 H   -3.915289    3.075606   -2.655163
 H   -5.075754    0.161834   -4.629176
 H   -4.654093    1.888538   -4.671546
 H   -6.254929    1.384220   -4.077952
 H   -5.040489   -1.641583   -3.199173
 H   -6.710944   -1.020409   -3.118827
 H   -6.070151   -2.036080   -1.802567
 H   -6.035197    1.295181   -0.180283
 H   -6.842268   -0.283773   -0.258584
 H   -7.230453    0.962673   -1.469898
 C   -0.550834   -4.495064    0.495645
 C   -0.939887   -5.213263    1.620522
 C   -1.400337   -3.543366   -0.113172
 C   -2.203082   -5.021207    2.187171
 C   -2.685810   -3.380373    0.461666
 C   -3.068764   -4.102310    1.590655
 C   -0.943127   -2.738948   -1.240411
 C   -1.865716   -2.020001   -2.093779
 H   -4.063630   -3.938092    2.015021
 H   -3.383661   -2.651426    0.039160
 H   -2.507128   -5.579829    3.075354
 H   -0.245596   -5.933219    2.063216
 H    0.443284   -4.658536    0.074420
 P   -0.993848    0.322717    1.243570
 C    0.461448   -1.749998    2.361069
 C    1.064501   -2.480569    3.384147
 C   -0.336177   -0.642281    2.656919
 C    0.863482   -2.109417    4.712313
 C   -0.539425   -0.275090    3.993686
 C    0.058930   -1.008032    5.016031
 C   -4.273584    2.704699    1.985872
 C   -2.997264    2.274970    1.620212
 C   -2.601640    0.954460    1.851578
 C   -5.167361    1.816029    2.580735
 C   -4.782172    0.492720    2.803285
 C   -3.509506    0.062559    2.436704
 C    0.352913    2.780958    2.269403
 C    0.099775    1.755685    1.175261
 C    0.992194    1.985399    0.191384
 C    1.707982    2.360640    2.908533
 C    2.720622    2.674789    1.786192
 C    1.829781    3.201588    0.617793
 C    2.580578    3.911459   -0.489156
 C    0.763763    4.024744    1.428267
 C    1.341945    5.176970    2.257298
 C   -0.351467    4.624997    0.572427
 C    1.173172    1.234206   -1.077324
 C    0.382759    1.498733   -2.171938
 C    2.185850    0.226223   -1.345477
 S    0.874592    0.544540   -3.522769
 C    2.147621   -0.227393   -2.647766
 C   -0.740448    2.477607   -2.315806
 C    3.004884   -1.223927   -3.368026
 P    3.321590   -0.323521   -0.014742
 C    3.153779   -4.352381   -0.779282
 C    2.831749   -3.028926   -0.486035
 C    4.474533   -4.709512   -1.054911
 C    3.818752   -2.033143   -0.490527
 C    5.466627   -3.731062   -1.038106
 C    5.142115   -2.402631   -0.760255
 C    6.998142    1.419970    0.481217
 C    5.808711    0.716749    0.664462
 C    7.246205    2.067323   -0.729803
 C    4.859011    0.632985   -0.364447
 C    6.301489    2.004147   -1.753579
 C    5.115995    1.290768   -1.572969
 H    0.598822   -2.040167    1.317831
 H    1.685778   -3.344775    3.138085
 H    1.331100   -2.680888    5.517690
```

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 H   -1.164542    0.587254    4.239660
 H   -0.102388   -0.719163    6.057220
 H   -4.567320    3.740636    1.800880
 H   -2.311077    2.976921    1.144970
 H   -6.167526    2.151261    2.865405
 H   -5.481343   -0.213024    3.257735
 H   -3.225068   -0.980620    2.600596
 H   -0.467630    2.922644    2.986416
 H    1.702982    1.296345    3.180015
 H    1.909108    2.932318    3.825965
 H    3.294680    1.793463    1.484413
 H    3.448284    3.446208    2.077219
 H    3.093184    4.805539   -0.101318
 H    1.905849    4.227492   -1.299932
 H    3.347288    3.255044   -0.927432
 H    0.546859    5.623667    2.875367
 H    1.722804    5.970307    1.594844
 H    2.158052    4.891846    2.932158
 H   -1.126667    5.073135    1.214089
 H   -0.833875    3.895135   -0.084382
 H    0.046700    5.430306   -0.064885
 H   -1.410248    2.418774   -1.447661
 H   -1.350463    2.251186   -3.198886
 H   -0.364313    3.509710   -2.400962
 H    2.919889   -1.095716   -4.456643
 H    2.717385   -2.259188   -3.127831
 H    4.061759   -1.104584   -3.094900
 H    2.370240   -5.113893   -0.791089
 H    1.792501   -2.762093   -0.277164
 H    4.727127   -5.748664   -1.278213
 H    6.505002   -3.997894   -1.249541
 H    5.932671   -1.649622   -0.770042
 H    7.730887    1.469387    1.290100
 H    5.615914    0.223499    1.622047
 H    8.175385    2.623715   -0.873848
 H    6.485949    2.513980   -2.702234
 H    4.380862    1.256377   -2.380015
Cu   -1.311565   -0.753640   -0.681349
 H   -2.899370   -2.387792   -2.156898
 H   -1.473707   -1.715908   -3.071116
 H    0.056780   -2.947334   -1.630797
121
Figure 1_ts(CuBadd)_minor01_03 / electronic energy: -4987.94518213 a.u. / lowest freq: -182.92 cm-1
 B   -2.939052   -0.058017   -1.795830
 O   -4.229269   -0.224193   -1.318691
 O   -2.947299    0.675761   -2.964838
 C   -5.151740    0.201898   -2.337005
 C   -4.272279    1.200745   -3.168036
 C   -6.371563    0.818764   -1.672713
 C   -5.555080   -1.038850   -3.132064
 C   -4.299960    2.622397   -2.606681
 C   -4.571894    1.227214   -4.658439
 H   -4.081150    2.634570   -1.528430
 H   -5.276648    3.101638   -2.767858
 H   -3.537058    3.229549   -3.114870
 H   -4.408294    0.247338   -5.125627
 H   -3.913324    1.953312   -5.157865
 H   -5.613607    1.532584   -4.840465
 H   -4.691126   -1.493969   -3.639205
 H   -6.317444   -0.806314   -3.889548
 H   -5.973353   -1.786275   -2.441496
 H   -6.090731    1.606147   -0.961205
 H   -6.923267    0.045457   -1.117592
 H   -7.052553    1.247755   -2.423548
 C   -0.949197   -4.312466    0.689557
 C   -1.549494   -5.087719    1.672714
 C   -1.679409   -3.356879   -0.057651
 C   -2.907888   -4.938867    1.974318
 C   -3.049817   -3.207256    0.277069
 C   -3.642938   -3.983994    1.271887
 C   -1.043378   -2.563027   -1.095697
 C   -1.828189   -1.797795   -2.054698
 H   -4.703406   -3.837377    1.497162
 H   -3.660212   -2.464791   -0.244447
 H   -3.378274   -5.548387    2.749507
 H   -0.945901   -5.816573    2.221038
 H    0.114374   -4.445182    0.479580
 P   -0.945088    0.278675    1.445205
 C    0.908079   -1.380429    2.729437
 C    1.296736   -2.448531    3.536753
 C   -0.442157   -1.028000    2.624615
 C    0.340059   -3.173290    4.247319
 C   -1.401961   -1.782033    3.310556
 C   -1.008741   -2.839657    4.128841
 C   -3.429254    2.094534    4.213212
 C   -2.397980    1.345035    3.651215
 C   -2.339764    1.148224    2.264224
 C   -4.411435    2.658425    3.396707
 C   -4.365477    2.459305    2.018141
 C   -3.338156    1.701636    1.455691
 C    0.661272    2.504065    2.619951
 C    0.340060    1.549781    1.479214
 C    1.104936    1.909376    0.428558
 C    2.101223    2.153434    3.082167
 C    2.959230    2.601870    1.879150
 C    1.911270    3.144425    0.858646
 C    2.502370    3.979199   -0.257874
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 C    0.881308    3.827284    1.835067
 C    1.459228    4.974101    2.670583
 C   -0.391759    4.360462    1.174864
 C    1.196256    1.265312   -0.904889
 C    0.389658    1.647288   -1.952154
 C    2.136587    0.223186   -1.270154
 S    0.760857    0.733695   -3.367192
 C    2.010356   -0.164886   -2.587732
 C   -0.677375    2.695170   -1.978780
 C    2.770094   -1.185087   -3.380029
 P    3.370047   -0.374490   -0.056737
 C    2.818639   -4.388635   -0.595750
 C    2.652736   -3.038757   -0.291935
 C    4.027975   -4.846744   -1.120945
 C    3.684646   -2.121283   -0.537982
 C    5.068351   -3.944935   -1.341000
 C    4.898125   -2.590521   -1.053692
 C    7.185622    1.108359    0.017616
 C    5.993615    0.449685    0.312271
 C    7.305250    1.839180   -1.165444
 C    4.909178    0.493858   -0.577588
 C    6.228330    1.904490   -2.048373
 C    5.037979    1.235764   -1.757785
 H    1.663151   -0.823716    2.167620
 H    2.354902   -2.710848    3.609776
 H    0.644603   -4.006561    4.885004
 H   -2.464277   -1.545744    3.211682
 H   -1.766269   -3.415815    4.664581
 H   -3.465493    2.240797    5.295193
 H   -1.635819    0.908374    4.301155
 H   -5.218530    3.246951    3.839385
 H   -5.137887    2.886995    1.374679
 H   -3.319963    1.518990    0.379099
 H   -0.079505    2.545621    3.427886
 H    2.202910    1.082636    3.301798
 H    2.359615    2.700606    4.000319
 H    3.545059    1.782885    1.447221
 H    3.671307    3.396660    2.145470
 H    3.018889    4.861425    0.151294
 H    1.731337    4.331491   -0.959951
 H    3.241437    3.400185   -0.833863
 H    0.744811    5.254775    3.460909
 H    1.611811    5.864501    2.040354
 H    2.416147    4.749008    3.157334
 H   -1.079483    4.747729    1.943554
 H   -0.935199    3.599451    0.604574
 H   -0.157643    5.194722    0.494103
 H   -1.430343    2.490840   -1.204307
 H   -1.199833    2.702153   -2.942604
 H   -0.256825    3.695952   -1.797282
 H    2.585008   -1.063644   -4.456843
 H    2.480433   -2.210581   -3.102619
 H    3.851213   -1.089958   -3.209785
 H    2.001870   -5.091767   -0.415877
 H    1.705323   -2.688554    0.129893
 H    4.159992   -5.906305   -1.351963
 H    6.019726   -4.295444   -1.748696
 H    5.717109   -1.895145   -1.251264
 H    8.020017    1.060596    0.721385
 H    5.901902   -0.104750    1.251172
 H    8.236019    2.363672   -1.394192
 H    6.312651    2.478509   -2.974273
 H    4.202075    1.300748   -2.457816
Cu   -1.390172   -0.581013   -0.551817
 H   -2.838992   -2.172611   -2.277510
 H   -1.294066   -1.511604   -2.967983
 H   -0.006203   -2.796659   -1.347127
121
Figure 1_ts(CuBadd)_minor01_04 / electronic energy: -4987.94747424 a.u. / lowest freq: -174.36 cm-1
 B    3.349062    0.004295   -1.272019
 O    4.439890    0.522514   -0.597899
 O    3.739216   -1.027231   -2.101677
 C    5.640952   -0.034484   -1.163610
 C    5.111129   -1.357954   -1.824048
 C    6.660494   -0.241135   -0.055378
 C    6.164720    0.973918   -2.184443
 C    5.108729   -2.554217   -0.872005
 C    5.801364   -1.738541   -3.124777
 H    4.636637   -2.309474    0.089928
 H    6.127720   -2.917526   -0.674972
 H    4.533978   -3.373640   -1.328460
 H    5.679650   -0.964375   -3.893487
 H    5.371777   -2.672815   -3.516342
 H    6.876852   -1.903620   -2.959857
 H    5.441338    1.135306   -2.997981
 H    7.117571    0.649576   -2.627221
 H    6.328935    1.939324   -1.683152
 H    6.244176   -0.832087    0.770956
 H    6.972231    0.732340    0.351245
 H    7.556627   -0.752068   -0.439079
 C    0.262964    4.391714   -1.138997
 C    0.439649    5.551174   -0.394089
 C    1.283465    3.418136   -1.254796
 C    1.646778    5.799701    0.269421
 C    2.505908    3.697414   -0.591882
 C    2.674414    4.861122    0.155615
 C    1.058793    2.185362   -1.986174
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 C    2.161666    1.327926   -2.391421
 H    3.628106    5.033777    0.662771
 H    3.325035    2.973812   -0.635795
 H    1.784793    6.711757    0.854566
 H   -0.375842    6.277838   -0.329748
 H   -0.688798    4.214926   -1.647773
 P    0.679216    0.069942    1.333683
 C   -1.546994    0.983286    2.873867
 C   -2.307246    1.990253    3.468434
 C   -0.395629    1.304527    2.149477
 C   -1.912356    3.323007    3.359360
 C   -0.004748    2.646913    2.041131
 C   -0.754654    3.649015    2.652094
 C    2.684803   -0.354449    4.932064
 C    1.727288    0.003518    3.983058
 C    1.943732   -0.265934    2.626622
 C    3.863587   -0.987497    4.537358
 C    4.088965   -1.250543    3.186172
 C    3.136997   -0.883097    2.237726
 C   -0.132033   -2.665242    2.234730
 C   -0.133062   -1.545677    1.203749
 C   -0.657458   -2.052267    0.066708
 C   -1.619137   -2.914095    2.605522
 C   -2.201439   -3.489727    1.298253
 C   -0.976247   -3.529276    0.332668
 C   -1.187736   -4.419893   -0.874089
 C    0.187740   -3.888396    1.327749
 C    0.035241   -5.251519    2.008339
 C    1.597000   -3.841406    0.728144
 C   -0.985656   -1.335432   -1.188063
 C   -0.281064   -1.486787   -2.359901
 C   -2.118724   -0.435300   -1.326066
 S   -0.977517   -0.521358   -3.614426
 C   -2.233810    0.085428   -2.595490
 C    0.900434   -2.350271   -2.664829
 C   -3.238498    1.037370   -3.167278
 P   -3.288891   -0.198963    0.059638
 C   -5.529344    3.289048   -0.096721
 C   -5.177562    1.938687   -0.102137
 C   -4.542376    4.272923   -0.095027
 C   -3.831746    1.551782   -0.113651
 C   -3.198799    3.896082   -0.106855
 C   -2.844401    2.548697   -0.117589
 C   -6.026139   -2.587746   -1.982884
 C   -4.904061   -1.804973   -1.706928
 C   -7.022567   -2.753750   -1.021837
 C   -4.761453   -1.178133   -0.462892
 C   -6.886160   -2.144179    0.226065
 C   -5.757825   -1.376103    0.506802
 H   -1.858508   -0.056237    2.969809
 H   -3.214626    1.729579    4.018039
 H   -2.511329    4.110800    3.822163
 H    0.887854    2.916816    1.469870
 H   -0.439413    4.690423    2.557073
 H    2.505190   -0.139812    5.988083
 H    0.805502    0.490507    4.308764
 H    4.609982   -1.270289    5.283237
 H    5.013804   -1.736975    2.866774
 H    3.321251   -1.065714    1.178561
 H    0.535877   -2.517002    3.093486
 H   -2.123539   -1.991244    2.918526
 H   -1.697553   -3.625001    3.440460
 H   -3.010554   -2.875449    0.881617
 H   -2.608118   -4.502763    1.434490
 H   -1.461287   -5.437733   -0.555175
 H   -0.287225   -4.495523   -1.499465
 H   -2.006099   -4.039989   -1.505974
 H    0.763466   -5.345558    2.829778
 H    0.248565   -6.059125    1.290265
 H   -0.961217   -5.440378    2.427178
 H    2.343707   -4.046754    1.511410
 H    1.846729   -2.870048    0.282624
 H    1.718475   -4.614995   -0.047073
 H    1.274291   -2.819506   -1.748312
 H    1.736249   -1.776715   -3.087834
 H    0.634735   -3.147227   -3.377554
 H   -3.309440    0.930352   -4.259218
 H   -2.968862    2.082530   -2.946428
 H   -4.235310    0.860253   -2.741791
 H   -6.585664    3.569510   -0.094288
 H   -5.967782    1.184965   -0.106378
 H   -4.816612    5.330478   -0.084936
 H   -2.415322    4.656394   -0.100430
 H   -1.785002    2.274466   -0.134538
 H   -6.120939   -3.070720   -2.958421
 H   -4.130976   -1.690022   -2.469893
 H   -7.901573   -3.364272   -1.241813
 H   -7.655670   -2.277719    0.990267
 H   -5.646261   -0.923512    1.496844
Cu    1.490654    0.625633   -0.663786
 H    3.144359    1.806879   -2.519652
 H    1.937654    0.646147   -3.219823
 H    0.101342    2.073230   -2.502047
121
Figure 1_ts(CuBadd)_minor01_05 / electronic energy: -4987.94747424 a.u. / lowest freq: -174.36 cm-1
 B   -3.349062   -0.004299   -1.272018
 O   -4.439887   -0.522518   -0.597894
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O	-3.739218	1.027228	-2.101674
C	-5.640951	0.034481	-1.163600
C	-5.111130	1.357952	-1.824039
C	-6.660489	0.241133	-0.055364
C	-6.164724	-0.973920	-2.184431
C	-5.108725	2.554214	-0.871995
C	-5.801371	1.738540	-3.124765
H	-4.636627	2.309471	0.089935
H	-6.127716	2.917522	-0.674956
H	-4.533978	3.373638	-1.328454
H	-5.679661	0.964375	-3.893476
H	-5.371785	2.672814	-3.516331
H	-6.876858	1.903620	-2.959839
H	-5.441346	-1.135306	-2.997974
H	-7.117577	-0.649578	-2.627204
H	-6.328935	-1.939326	-1.683140
H	-6.244167	0.832084	0.770969
H	-6.972225	-0.732342	0.351260
H	-7.556623	0.752066	-0.439061
C	-0.262965	-4.391713	-1.139000
C	-0.439648	-5.551175	-0.394094
C	-1.283467	-3.418135	-1.254795
C	-1.646774	-5.799704	0.269418
C	-2.505908	-3.697416	-0.591879
C	-2.674412	-4.861124	0.155615
C	-1.058797	-2.185358	-1.986170
C	-2.161672	-1.327921	-2.391413
H	-3.628103	-5.033782	0.662773
H	-3.325036	-2.973814	-0.635789
H	-1.784788	-6.711761	0.854562
H	0.375845	-6.277838	-0.329756
H	0.688796	-4.214923	-1.647777
P	-0.679214	-0.069941	1.333687
C	0.004750	-2.646913	2.041135
C	0.754657	-3.649015	2.652097
C	0.395632	-1.304527	2.149480
C	1.912361	-3.323007	3.359361
C	1.546998	-0.983286	2.873867
C	2.307251	-1.990253	3.468434
C	-4.088962	1.250540	3.186182
C	-3.136997	0.883091	2.237735
C	-1.943727	0.265937	2.626629
C	-3.863575	0.987506	4.537370
C	-2.684785	0.354468	4.932075
C	-1.727274	-0.003502	3.983067
C	0.132039	2.665243	2.234729
C	0.133065	1.545676	1.203749
C	0.657456	2.052266	0.066706
C	1.619144	2.914097	2.605515
C	2.201441	3.489725	1.298243
C	0.976245	3.529276	0.332662
C	1.187729	4.419891	-0.874096
C	-0.187737	3.888396	1.327748
C	-0.035237	5.251520	2.008335
C	-1.597000	3.841404	0.728149
C	0.985652	1.335430	-1.188066
C	0.281058	1.486785	-2.359903
C	2.118720	0.435298	-1.326071
S	0.977509	0.521356	-3.614429
C	2.233803	-0.085430	-2.595495
C	-0.900439	2.350271	-2.664828
C	3.238490	-1.037374	-3.167283
P	3.288889	0.198961	0.059630
C	5.529345	-3.289048	-0.096731
C	5.177562	-1.938687	-0.102146
C	4.542377	-4.272923	-0.095037
C	3.831745	-1.551783	-0.113659
C	3.198800	-3.896084	-0.106863
C	2.844401	-2.548699	-0.117596
C	6.026133	2.587745	-1.982896
C	4.904056	1.804971	-1.706939
C	7.022561	2.753754	-1.021850
C	4.761450	1.178134	-0.462902
C	6.886154	2.144185	0.226054
C	5.757820	1.376108	0.506793
H	-0.887853	-2.916816	1.469876
H	0.439415	-4.690423	2.557077
H	2.511334	-4.110799	3.822164
H	1.858513	0.056237	2.969808
H	3.214632	-1.729579	4.018036
H	-5.013806	1.736963	2.866785
H	-3.321258	1.065697	1.178569
H	-4.609968	1.270300	5.283250
H	-2.505166	0.139840	5.988094
H	-0.805483	-0.490483	4.308771
H	-0.535868	2.517003	3.093488
H	2.123548	1.991247	2.918521
H	1.697562	3.625006	3.440451
H	3.010551	2.875443	0.881605
H	2.608126	4.502760	1.434475
H	1.461297	5.437727	-0.555185
H	0.287210	4.495530	-1.499460
H	2.006078	4.039977	-1.505993
H	-0.763457	5.345560	2.829776
H	-0.248564	6.059124	1.290260
H	0.961224	5.440380	2.427168
H	-2.343704	4.046753	1.511417

```
 H   -1.846731    2.870045    0.282632
 H   -1.718480    4.614990   -0.047069
 H   -1.274295    2.819505   -1.748311
 H   -1.736255    1.776717   -3.087834
 H   -0.634740    3.147228   -3.377552
 H    3.309427   -0.930362   -4.259224
 H    2.968856   -2.082534   -2.946427
 H    4.235303   -0.860253   -2.741800
 H    6.585665   -3.569509   -0.094299
 H    5.967781   -1.184964   -0.106388
 H    4.816614   -5.330478   -0.084946
 H    2.415323   -4.656396   -0.100437
 H    1.785002   -2.274468   -0.134544
 H    6.120933    3.070716   -2.958434
 H    4.130972    1.690016   -2.469904
 H    7.901566    3.364277   -1.241826
 H    7.655664    2.277729    0.990256
 H    5.646257    0.923519    1.496835
Cu   -1.490653   -0.625632   -0.663779
 H   -3.144363   -1.806877   -2.519647
 H   -1.937661   -0.646143   -3.219817
 H   -0.101348   -2.073226   -2.502046
121
Figure 1_ts(CuBadd)_minor01_06 / electronic energy: -4987.94708758 a.u. / lowest freq: -81.68 cm-1
 B    2.440749   -1.296524    0.236237
 O    3.431975   -0.468565    0.739666
 O    2.718351   -2.611544    0.565823
 C    4.530614   -1.264460    1.211387
 C    3.858981   -2.670046    1.439452
 C    5.101681   -0.621274    2.466504
 C    5.588611   -1.274493    0.108756
 C    3.337475   -2.867461    2.860688
 C    4.719024   -3.859665    1.037978
 H    2.726468   -2.015168    3.184620
 H    4.158716   -2.999143    3.580267
 H    2.707431   -3.769223    2.891412
 H    4.982801   -3.829660   -0.027384
 H    4.169088   -4.794890    1.222405
 H    5.647122   -3.891350    1.629080
 H    5.207877   -1.730087   -0.817233
 H    6.491911   -1.822126    0.414878
 H    5.878740   -0.238065   -0.119432
 H    4.324411   -0.442206    3.221341
 H    5.553095    0.349369    2.212310
 H    5.885207   -1.254079    2.910605
 C    1.949697    1.976184   -4.091338
 C    2.678613    3.123687   -4.395222
 C    2.328176    1.122366   -3.034968
 C    3.809483    3.463759   -3.649797
 C    3.447874    1.507646   -2.263420
 C    4.178780    2.649239   -2.576922
 C    1.608640   -0.128026   -2.790170
 C    2.205916   -1.205282   -2.073106
 H    5.042722    2.916227   -1.961933
 H    3.735232    0.910296   -1.394088
 H    4.383925    4.361735   -3.889883
 H    2.364026    3.756419   -5.230093
 H    1.076623    1.714303   -4.697287
 P    0.354898    1.323010    0.582130
 C    2.425623    3.200580    1.032879
 C    3.183679    4.326685    0.709067
 C    1.322295    2.840140    0.250347
 C    2.850812    5.103750   -0.398547
 C    1.037142    3.589758   -0.900993
 C    1.779581    4.725624   -1.208422
 C    0.615125   -0.568332    4.218368
 C    0.604769   -0.293436    2.850371
 C    0.521012    1.022454    2.390660
 C    0.551491    0.474376    5.140367
 C    0.461849    1.793687    4.690325
 C    0.436545    2.065539    3.324531
 C   -1.981972    3.132638    0.036403
 C   -1.397236    1.820628    0.535910
 C   -2.427385    1.016508    0.880967
 C   -2.609812    2.793389   -1.341540
 C   -3.808980    1.909111   -0.939964
 C   -3.718905    1.828532    0.617686
 C   -5.006881    1.347172    1.254688
 C   -3.227204    3.281132    0.948226
 C   -4.193214    4.392092    0.521968
 C   -2.859550    3.556342    2.406390
 C   -2.422620   -0.381989    1.404440
 C   -2.812361   -0.644364    2.698117
 C   -2.108178   -1.611397    0.669175
 S   -2.871327   -2.339146    3.005313
 C   -2.357466   -2.749299    1.406405
 C   -3.078841    0.289850    3.834045
 C   -2.284073   -4.213776    1.084692
 P   -1.243680   -1.538137   -0.949832
 C    0.592781   -5.190882   -1.274500
 C    0.218357   -3.910136   -0.876716
 C   -0.102930   -5.842425   -2.293604
 C   -0.872445   -3.265209   -1.476914
 C   -1.171618   -5.198443   -2.915068
 C   -1.553574   -3.917815   -2.512124
 C   -4.884306   -1.181294   -2.859233
 C   -3.895884   -1.528027   -1.941394
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 C   -4.565547   -0.382757   -3.960056
 C   -2.579252   -1.080342   -2.116601
 C   -3.256977    0.062669   -4.142265
 C   -2.266844   -0.285876   -3.223244
 H    2.700932    2.603795    1.904509
 H    4.038357    4.597754    1.333654
 H    3.438570    5.991325   -0.644693
 H    0.235065    3.280772   -1.574780
 H    1.533663    5.305006   -2.100869
 H    0.670979   -1.604174    4.560977
 H    0.651981   -1.110871    2.126401
 H    0.565467    0.261552    6.212041
 H    0.404850    2.614832    5.408697
 H    0.350308    3.100472    2.984264
 H   -1.297942    3.989531    0.037106
 H   -1.892652    2.266092   -1.986726
 H   -2.923048    3.704693   -1.871688
 H   -3.772897    0.910955   -1.381134
 H   -4.767850    2.356816   -1.239258
 H   -5.854253    1.956187    0.902613
 H   -4.985935    1.411470    2.351497
 H   -5.216574    0.300464    0.983507
 H   -3.686849    5.369165    0.574890
 H   -5.051136    4.433932    1.211961
 H   -4.594912    4.283913   -0.492937
 H   -2.477827    4.584891    2.506435
 H   -2.081441    2.883565    2.785221
 H   -3.741511    3.473143    3.061483
 H   -3.065992    1.328917    3.496999
 H   -2.297040    0.187330    4.603912
 H   -4.049362    0.092394    4.314853
 H   -2.942439   -4.781640    1.758278
 H   -1.265750   -4.612669    1.205286
 H   -2.601656   -4.420572    0.055855
 H    1.444711   -5.675132   -0.790862
 H    0.796043   -3.410185   -0.096918
 H    0.194531   -6.844848   -2.610956
 H   -1.714659   -5.692824   -3.724230
 H   -2.394429   -3.435597   -3.013329
 H   -5.909591   -1.528496   -2.712075
 H   -4.150886   -2.140873   -1.072555
 H   -5.342219   -0.103586   -4.675866
 H   -3.005357    0.692869   -4.998393
 H   -1.246187    0.080915   -3.351109
Cu    0.892532   -0.416186   -0.770505
 H    3.285396   -1.162413   -1.889074
 H    1.853672   -2.220425   -2.283481
 H    0.810229   -0.368881   -3.497008
121
Figure 1_ts(CuBadd)_minor01_07 / electronic energy: -4987.94846380 a.u. / lowest freq: -106.29 cm-1
 B   -0.993713   -2.333504   -0.157268
 O   -0.334271   -3.450929    0.317379
 O   -2.328824   -2.384083    0.214329
 C   -1.302160   -4.383382    0.823532
 C   -2.501380   -3.440211    1.174758
 C   -0.711564   -5.127429    2.008921
 C   -1.627556   -5.358512   -0.307683
 C   -2.374853   -2.809115    2.560685
 C   -3.879729   -4.055083    0.997153
 H   -1.372207   -2.381701    2.705761
 H   -2.568481   -3.537462    3.362045
 H   -3.106663   -1.992732    2.644838
 H   -4.058488   -4.358749   -0.042908
 H   -4.652634   -3.322430    1.274211
 H   -3.999942   -4.936133    1.645977
 H   -2.072321   -4.838825   -1.169849
 H   -2.323386   -6.144955    0.019538
 H   -0.698303   -5.840609   -0.645924
 H   -0.332449   -4.432563    2.768203
 H    0.128863   -5.755149    1.676522
 H   -1.463979   -5.785363    2.470965
 C    2.447422   -0.908002   -4.350651
 C    3.793690   -1.159871   -4.600461
 C    1.751433   -1.566060   -3.314590
 C    4.502748   -2.077326   -3.822147
 C    2.483575   -2.499300   -2.546123
 C    3.831143   -2.743128   -2.793362
 C    0.342530   -1.267696   -3.061724
 C   -0.527903   -2.183169   -2.379865
 H    4.369374   -3.461018   -2.167861
 H    1.990471   -3.017303   -1.718389
 H    5.561739   -2.267926   -4.010493
 H    4.298122   -0.629445   -5.413318
 H    1.910816   -0.181163   -4.968199
 P    1.574447   -0.255645    0.463331
 C    3.341017    0.694223   -1.442979
 C    4.572794    1.068256   -1.977065
 C    3.261728    0.093306   -0.183057
 C    5.744638    0.821442   -1.264210
 C    4.443652   -0.147158    0.529437
 C    5.677459    0.208426   -0.012180
 C    2.828645   -3.654856    2.415739
 C    2.650971   -2.653416    1.464525
 C    1.856529   -1.535659    1.750121
 C    2.200075   -3.563956    3.658805
 C    1.377570   -2.473647    3.935765
 C    1.203475   -1.469217    2.983175
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 C    2.307334    2.319248    1.680832
 C    1.238427    1.264860    1.414083
 C    0.057207    1.764212    1.841055
 C    2.036998    3.422666    0.625710
 C    0.693734    4.005244    1.111774
 C    0.364588    3.179693    2.398952
 C   -0.668868    3.853331    3.278241
 C    1.799424    2.972944    2.988671
 C    2.519227    4.272936    3.366424
 C    1.900256    2.050038    4.203718
 C   -1.351816    1.270940    1.788838
 C   -2.037644    1.006269    2.950261
 C   -2.240249    1.289701    0.622174
 S   -3.739600    0.903502    2.666363
 C   -3.567881    1.174146    0.963365
 C   -1.526647    0.787621    4.338409
 C   -4.829733    1.258246    0.158077
 P   -1.531200    1.082473   -1.056374
 C   -4.524899   -1.007882   -2.939271
 C   -3.560863   -0.584136   -2.028910
 C   -4.828034   -0.231673   -4.059185
 C   -2.894713    0.637325   -2.212256
 C   -4.157452    0.972881   -4.259387
 C   -3.196265    1.405969   -3.343534
 C   -1.585209    5.145088   -1.764574
 C   -1.933542    3.871473   -1.324157
 C   -0.407120    5.333917   -2.491961
 C   -1.109412    2.774317   -1.610683
 C    0.409748    4.245054   -2.791738
 C    0.057145    2.967316   -2.354571
 H    2.423780    0.857449   -2.012970
 H    4.616250    1.538421   -2.961745
 H    6.712690    1.101603   -1.686270
 H    4.405903   -0.608050    1.518702
 H    6.592916    0.011433    0.550805
 H    3.458688   -4.516199    2.181462
 H    3.142427   -2.741796    0.492598
 H    2.340427   -4.350060    4.404491
 H    0.863438   -2.400455    4.897151
 H    0.543212   -0.629319    3.201218
 H    3.339822    1.951033    1.701108
 H    1.978629    2.999635   -0.385558
 H    2.839759    4.173871    0.621265
 H   -0.108530    3.907075    0.374880
 H    0.771945    5.074629    1.357292
 H   -0.341871    4.876660    3.520733
 H   -0.828754    3.323229    4.227149
 H   -1.640711    3.932119    2.766987
 H    3.589598    4.073393    3.535011
 H    2.111596    4.675070    4.307682
 H    2.448096    5.067953    2.614204
 H    2.949456    1.979179    4.531185
 H    1.560668    1.028329    4.001758
 H    1.322626    2.449141    5.052781
 H   -0.465557    1.047308    4.411237
 H   -1.630538   -0.272764    4.621743
 H   -2.079308    1.381756    5.082104
 H   -5.600206    1.802100    0.725547
 H   -5.236588    0.263690   -0.081156
 H   -4.670799    1.791094   -0.786064
 H   -5.039012   -1.958139   -2.774486
 H   -3.327770   -1.205399   -1.160604
 H   -5.580173   -0.568370   -4.776565
 H   -4.380326    1.586196   -5.135865
 H   -2.686657    2.354533   -3.521499
 H   -2.227929    5.997079   -1.531082
 H   -2.847033    3.728208   -0.740663
 H   -0.127563    6.335654   -2.827043
 H    1.331957    4.390026   -3.358970
 H    0.697817    2.111705   -2.582967
Cu   -0.055440   -0.747240   -1.041889
 H   -0.160094   -3.199194   -2.201428
 H   -1.585745   -2.158127   -2.661182
 H   -0.119196   -0.546289   -3.744070
121
Figure 1_ts(CuBadd)_minor01_08 / electronic energy: -4987.94719470 a.u. / lowest freq: -103.80 cm-1
 B   -2.504839    1.208274    0.235413
 O   -3.521217    0.386008    0.697330
 O   -2.752893    2.514714    0.618875
 C   -4.611137    1.195210    1.169186
 C   -3.901792    2.562931    1.482897
 C   -5.246008    0.514629    2.372433
 C   -5.629538    1.295565    0.034108
 C   -3.394362    2.659426    2.919401
 C   -4.717510    3.800776    1.139476
 H   -2.841875    1.756672    3.210002
 H   -4.219749    2.804644    3.631619
 H   -2.712186    3.518751    3.003064
 H   -4.951493    3.849705    0.067991
 H   -4.147570    4.705381    1.401038
 H   -5.660148    3.820098    1.707420
 H   -5.206003    1.790617   -0.852182
 H   -6.527315    1.851698    0.341124
 H   -5.940263    0.282202   -0.261009
 H   -4.501842    0.279382    3.144577
 H   -5.715900   -0.429131    2.057856
 H   -6.026250    1.151254    2.816803
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C	-1.934349	-2.050981	-4.059187
C	-2.625369	-3.224592	-4.351079
C	-2.332912	-1.204219	-3.003237
C	-3.738629	-3.600064	-3.595764
C	-3.436393	-1.622929	-2.224614
C	-4.128857	-2.791538	-2.525939
C	-1.648876	0.065486	-2.761490
C	-2.271890	1.123333	-2.027872
H	-4.979112	-3.083780	-1.903354
H	-3.739951	-1.031092	-1.356994
H	-4.282636	-4.519255	-3.826087
H	-2.294789	-3.850702	-5.184837
H	-1.074503	-1.763875	-4.672664
P	-0.300004	-1.343795	0.602053
C	-0.939915	-3.632980	-0.865492
C	-1.650635	-4.793536	-1.155587
C	-1.220620	-2.895264	0.294663
C	-2.685822	-5.210185	-0.318175
C	-2.286486	-3.297890	1.107651
C	-3.013587	-4.449054	0.801851
C	-0.309066	-1.778830	4.714977
C	-0.300711	-2.063419	3.351837
C	-0.444645	-1.033630	2.410168
C	-0.440587	-0.459141	5.154266
C	-0.564536	0.570709	4.224332
C	-0.571490	0.282660	2.858773
C	2.080447	-3.076795	0.012656
C	1.466774	-1.783131	0.523777
C	2.478432	-0.946399	0.845524
C	2.665019	-2.719452	-1.379649
C	3.846244	-1.800307	-1.005620
C	3.788740	-1.717909	0.553128
C	5.076423	-1.194475	1.156568
C	3.350664	-3.184814	0.896366
C	4.340977	-4.265593	0.448233
C	3.025574	-3.469441	2.362681
C	2.435819	0.449127	1.375567
C	2.841041	0.718983	2.663072
C	2.053817	1.669343	0.656864
S	2.829625	2.411643	2.984011
C	2.263433	2.811209	1.400289
C	3.170840	-0.207494	3.788901
C	2.109603	4.273540	1.097397
P	1.171977	1.569939	-0.951723
C	-0.771322	5.168526	-1.278143
C	-0.361422	3.898069	-0.881650
C	-0.091645	5.841892	-2.293746
C	0.748717	3.285482	-1.479672
C	0.996734	5.229721	-2.913104
C	1.413667	3.959705	-2.511766
C	3.200652	0.055548	-4.176692
C	2.210459	0.361215	-3.242517
C	4.495664	0.543192	-4.005909
C	2.509768	1.154811	-2.131772
C	4.801188	1.340506	-2.900489
C	3.812891	1.644167	-1.967355
H	-0.165968	-3.296855	-1.558791
H	-1.408952	-5.362425	-2.055869
H	-3.248763	-6.117197	-0.550991
H	-2.558120	-2.714202	1.989323
H	-3.839218	-4.751974	1.450239
H	-0.205859	-2.589776	5.439782
H	-0.181646	-3.097653	3.019508
H	-0.440913	-0.236361	6.224008
H	-0.656601	1.606903	4.557763
H	-0.667173	1.090360	2.128533
H	1.423915	-3.954817	0.029818
H	1.917036	-2.212835	-2.006352
H	2.991997	-3.620776	-1.918427
H	3.771997	-0.805100	-1.447465
H	4.811024	-2.220772	-1.324739
H	5.931555	-1.786141	0.793897
H	5.081624	-1.243006	2.254229
H	5.253400	-0.147027	0.865810
H	3.868350	-5.258369	0.518662
H	5.218408	-4.276707	1.114631
H	4.711185	-4.149223	-0.577682
H	2.677907	-4.509008	2.472256
H	2.237267	-2.819905	2.760303
H	3.920502	-3.358858	2.995695
H	3.239079	-1.240912	3.441818
H	2.380319	-0.172408	4.555709
H	4.121447	0.058289	4.276350
H	2.744363	4.867747	1.770986
H	1.072806	4.615772	1.233785
H	2.404731	4.509042	0.068076
H	-1.637502	5.627893	-0.795508
H	-0.925205	3.382438	-0.102066
H	-0.416732	6.835970	-2.610275
H	1.528324	5.740791	-3.719522
H	2.269009	3.503212	-3.012060
H	2.959716	-0.573651	-5.036606
H	1.200945	-0.037617	-3.362572
H	5.272125	0.298496	-4.734466
H	5.815495	1.721991	-2.762328
H	4.057484	2.257598	-1.095959
Cu	-0.918861	0.363240	-0.751866

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 H   -3.351050    1.048378   -1.851052
 H   -1.954266    2.148704   -2.245926
 H   -0.872861    0.337693   -3.481766
121
Figure 1_L-Cu-alkyl_minor01_01 / electronic energy: -4988.00887570 a.u. / lowest freq: 18.81 cm-1
 B   -3.575252    1.605115   -0.485813
 O   -3.441344    0.404444    0.169565
 O   -4.656551    2.314891   -0.012934
 C   -4.655420    0.170959    0.908951
 C   -5.164938    1.634615    1.147125
 C   -4.355264   -0.621769    2.169709
 C   -5.586019   -0.639478    0.007042
 C   -4.532066    2.292280    2.373306
 C   -6.676839    1.782810    1.195950
 H   -3.438811    2.169192    2.374573
 H   -4.931998    1.876625    3.309569
 H   -4.749027    3.370416    2.353775
 H   -7.146881    1.467258    0.255545
 H   -6.943672    2.835502    1.371999
 H   -7.098225    1.183522    2.017228
 H   -5.874926   -0.076981   -0.893202
 H   -6.502714   -0.934488    0.537733
 H   -5.062422   -1.551522   -0.312329
 H   -3.602810   -0.135285    2.800727
 H   -3.979509   -1.620569    1.901687
 H   -5.274052   -0.751165    2.761853
 C   -1.242113   -0.536321   -4.014132
 C   -1.637881   -1.651579   -4.739511
 C   -2.116790    0.141712   -3.124127
 C   -2.943405   -2.149845   -4.631336
 C   -3.437752   -0.356978   -3.069366
 C   -3.836490   -1.480515   -3.796495
 C   -1.623074    1.261898   -2.302641
 C   -2.664063    2.167550   -1.636167
 H   -4.868311   -1.833993   -3.705380
 H   -4.171774    0.132928   -2.429214
 H   -3.254399   -3.032154   -5.195734
 H   -0.919024   -2.144812   -5.400641
 H   -0.212566   -0.175018   -4.110332
 P   -0.304255   -1.185683    0.671187
 C   -2.306925   -2.671354   -0.511757
 C   -3.230926   -3.708791   -0.631661
 C   -1.505918   -2.566998    0.630054
 C   -3.373658   -4.638017    0.398008
 C   -1.648941   -3.505135    1.659412
 C   -2.582635   -4.534022    1.544472
 C   -1.023079    0.849521    4.129547
 C   -1.023215    0.398944    2.810297
 C   -0.223668   -0.683956    2.426852
 C   -0.211963    0.224750    5.076575
 C    0.589120   -0.855394    4.702290
 C    0.582007   -1.310590    3.384861
 C    1.385304   -3.070704   -0.761449
 C    1.276140   -1.981958    0.293195
 C    2.523384   -1.520224    0.524981
 C    1.729902   -2.307177   -2.071878
 C    3.165531   -1.809603   -1.796316
 C    3.475642   -2.344268   -0.359421
 C    4.950875   -2.331877   -0.017451
 C    2.738108   -3.725545   -0.383342
 C    3.276622   -4.711922   -1.424363
 C    2.697026   -4.465251    0.956672
 C    2.961693   -0.331667    1.296133
 C    3.700485   -0.436993    2.449126
 C    2.741400    1.052641    0.902813
 S    4.145872    1.125259    3.041599
 C    3.357251    1.952392    1.745114
 C    4.082814   -1.660684    3.219206
 C    3.441217    3.446887    1.688941
 P    1.674927    1.473325   -0.517806
 C   -0.575586    4.294673    1.419064
 C    0.209622    3.180808    1.133313
 C   -0.710019    5.317582    0.478419
 C    0.878100    3.073420   -0.094603
 C   -0.045331    5.219045   -0.742908
 C    0.742868    4.103771   -1.031099
 C    3.118499    2.034332   -4.296628
 C    2.297683    1.800359   -3.194997
 C    4.474998    2.301505   -4.110742
 C    2.819880    1.852134   -1.894873
 C    5.005298    2.338484   -2.820848
 C    4.182813    2.116531   -1.716561
 H   -2.220794   -1.924456   -1.304250
 H   -3.846971   -3.779883   -1.531329
 H   -4.105881   -5.444465    0.311044
 H   -1.037305   -3.431638    2.562249
 H   -2.692499   -5.260716    2.353032
 H   -1.652823    1.695792    4.414889
 H   -1.648798    0.888289    2.059739
 H   -0.201064    0.581390    6.109262
 H    1.226128   -1.346270    5.441898
 H    1.219544   -2.149048    3.096241
 H    0.523633   -3.747583   -0.838923
 H    1.017634   -1.487310   -2.249647
 H    1.680909   -2.974540   -2.944390
 H    3.262297   -0.717088   -1.834782
 H    3.889078   -2.213761   -2.520135
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 H    5.523591   -2.886835   -0.776812
 H    5.156622   -2.792838    0.959095
 H    5.344446   -1.303444    0.006649
 H    2.573986   -5.551927   -1.544462
 H    4.236775   -5.134811   -1.088434
 H    3.440366   -4.276039   -2.417931
 H    2.134045   -5.405827    0.848887
 H    2.216086   -3.885708    1.755157
 H    3.713270   -4.731207    1.289311
 H    3.672098   -2.557130    2.739005
 H    3.687604   -1.620391    4.246583
 H    5.175176   -1.779929    3.290575
 H    4.405066    3.798868    2.085163
 H    2.642682    3.920432    2.281831
 H    3.346061    3.810176    0.657680
 H   -1.086101    4.362861    2.382835
 H    0.312476    2.389950    1.879800
 H   -1.330061    6.189540    0.698592
 H   -0.141852    6.014397   -1.485707
 H    1.247130    4.039953   -1.997853
 H    2.697336    1.993628   -5.303668
 H    1.239982    1.567685   -3.342909
 H    5.122306    2.474714   -4.973647
 H    6.068776    2.538533   -2.670974
 H    4.611569    2.134821   -0.712049
Cu   -0.413594    0.454154   -0.891631
 H   -3.360843    2.632056   -2.371463
 H   -2.144152    3.036522   -1.187028
 H   -0.948659    1.878338   -2.924481
121
Figure 1_L-Cu-alkyl_minor01_02 / electronic energy: -4987.99955082 a.u. / lowest freq: 14.44 cm-1
 B    3.817626    0.051599   -2.225777
 O    3.744744   -0.623994   -1.027641
 O    4.931589   -0.312922   -2.940185
 C    4.982328   -1.337392   -0.835590
 C    5.517828   -1.462710   -2.307526
 C    4.702021   -2.668998   -0.156692
 C    5.868512   -0.463603    0.049378
 C    4.980393   -2.695742   -3.033181
 C    7.030240   -1.394757   -2.441745
 H    3.888112   -2.778227   -2.930260
 H    5.437210   -3.621194   -2.654473
 H    5.213167   -2.609847   -4.104636
 H    7.430757   -0.443107   -2.068905
 H    7.313702   -1.490804   -3.500293
 H    7.506258   -2.217897   -1.887679
 H    6.116281    0.488585   -0.441794
 H    6.805695   -0.974650    0.312682
 H    5.330747   -0.226416    0.978248
 H    3.923286   -3.238427   -0.680921
 H    4.366867   -2.508808    0.877648
 H    5.617050   -3.279578   -0.119789
 C    1.944385    4.023966   -0.476865
 C    2.583971    5.001748    0.273172
 C    2.647845    2.950543   -1.080319
 C    3.971962    4.965324    0.459037
 C    4.048933    2.958705   -0.905848
 C    4.692602    3.936817   -0.144365
 C    1.917983    1.890313   -1.814051
 C    2.748386    1.050219   -2.788493
 H    5.779706    3.892112   -0.029350
 H    4.660407    2.184867   -1.376232
 H    4.477154    5.730000    1.053689
 H    1.993970    5.806319    0.722270
 H    0.857144    4.066374   -0.597267
 P    0.209818    0.122816    1.586856
 C   -2.092225    1.277258    2.848444
 C   -2.811332    2.376858    3.321738
 C   -0.794237    1.441783    2.363386
 C   -2.233887    3.644449    3.324839
 C   -0.216656    2.721097    2.372617
 C   -0.928835    3.813736    2.856357
 C    2.230473   -0.473809    5.142818
 C    1.239514   -0.130757    4.224613
 C    1.487175   -0.234027    2.850341
 C    3.473745   -0.923594    4.695119
 C    3.728386   -1.017807    3.327296
 C    2.741577   -0.666907    2.405917
 C   -0.950413   -2.457125    2.605437
 C   -0.689255   -1.442221    1.503375
 C   -1.070258   -2.011610    0.339427
 C   -2.493154   -2.555945    2.750123
 C   -2.919308   -3.186835    1.408553
 C   -1.567449   -3.424439    0.663624
 C   -1.680014   -4.404248   -0.486461
 C   -0.614699   -3.783469    1.861587
 C   -1.003864   -5.056195    2.619209
 C    0.867126   -3.911137    1.498537
 C   -1.123169   -1.393161   -1.003533
 C   -0.220432   -1.672280   -2.002105
 C   -2.134496   -0.436674   -1.409902
 S   -0.610459   -0.785590   -3.433948
 C   -1.975369   -0.015035   -2.712268
 C    1.024170   -2.499419   -1.943617
 C   -2.766637    0.971835   -3.512822
 P   -3.445772    0.096379   -0.252807
 C   -2.352810    4.028180   -0.625241
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 C   -2.347430    2.642066   -0.493236
 C   -3.551676    4.709653   -0.840805
 C   -3.541049    1.908435   -0.580815
 C   -4.742084    3.990282   -0.925772
 C   -4.738314    2.600307   -0.794783
 C   -7.374083   -0.984943   -0.699929
 C   -6.174801   -0.436475   -0.248904
 C   -7.400514   -1.739619   -1.873536
 C   -4.987075   -0.602690   -0.980368
 C   -6.220816   -1.942510   -2.588011
 C   -5.023468   -1.378239   -2.146467
 H   -2.559644    0.293708    2.834973
 H   -3.832140    2.237634    3.684880
 H   -2.801179    4.504594    3.687815
 H    0.793839    2.868619    1.978471
 H   -0.468091    4.804237    2.852441
 H    2.031311   -0.388105    6.213546
 H    0.268669    0.222290    4.582229
 H    4.249049   -1.193743    5.415799
 H    4.704923   -1.357499    2.973470
 H    2.945915   -0.717996    1.331727
 H   -0.411172   -2.285919    3.546648
 H   -2.956257   -1.576490    2.920645
 H   -2.760058   -3.191463    3.606674
 H   -3.582432   -2.538201    0.818788
 H   -3.446355   -4.142466    1.547075
 H   -2.048411   -5.376341   -0.123268
 H   -0.717485   -4.575530   -0.989852
 H   -2.394192   -4.042695   -1.243090
 H   -0.462681   -5.103501    3.577812
 H   -0.715525   -5.947221    2.039289
 H   -2.075590   -5.143469    2.838118
 H    1.459852   -4.102315    2.407332
 H    1.275608   -3.010041    1.023845
 H    1.030640   -4.761036    0.816376
 H    1.886280   -1.873998   -1.662020
 H    1.242441   -2.977849   -2.909602
 H    0.932355   -3.286329   -1.185066
 H   -2.708953    0.750349   -4.588447
 H   -2.385773    1.994626   -3.359614
 H   -3.824536    0.966423   -3.219692
 H   -1.411618    4.579180   -0.558795
 H   -1.395381    2.125709   -0.335336
 H   -3.555667    5.797115   -0.945365
 H   -5.686933    4.510987   -1.099885
 H   -5.683404    2.059009   -0.876787
 H   -8.290790   -0.832521   -0.125307
 H   -6.161686    0.126673    0.689254
 H   -8.337701   -2.177681   -2.224728
 H   -6.229083   -2.542842   -3.501091
 H   -4.108096   -1.549900   -2.716938
Cu    1.060666    0.881711   -0.333328
 H    3.252055    1.670618   -3.560517
 H    2.060592    0.401526   -3.365669
 H    1.069840    2.356560   -2.348819
121
Figure 1_L-Cu-alkyl_minor01_03 / electronic energy: -4988.00110311 a.u. / lowest freq: 19.62 cm-1
 B   -3.729150   -0.361378   -2.376538
 O   -5.021038   -0.435472   -1.917782
 O   -3.284431    0.940942   -2.407526
 C   -5.523242    0.896048   -1.720682
 C   -4.197603    1.733910   -1.626179
 C   -6.378289    0.926521   -0.463364
 C   -6.367453    1.245799   -2.944267
 C   -3.625860    1.781777   -0.212992
 C   -4.306906    3.136248   -2.203177
 H   -3.591717    0.779374    0.238112
 H   -4.209525    2.439729    0.445855
 H   -2.593341    2.160888   -0.257779
 H   -4.493316    3.117249   -3.285052
 H   -3.379980    3.699379   -2.023990
 H   -5.127824    3.683628   -1.715624
 H   -5.763234    1.249036   -3.863778
 H   -6.848491    2.228624   -2.837722
 H   -7.157029    0.488919   -3.061680
 H   -5.844550    0.510360    0.401189
 H   -7.291583    0.333221   -0.618110
 H   -6.680493    1.958057   -0.226724
 C   -1.711064   -3.884194    0.115193
 C   -2.194643   -4.600209    1.203157
 C   -2.517975   -2.973831   -0.615417
 C   -3.525973   -4.462970    1.612925
 C   -3.866219   -2.878728   -0.200622
 C   -4.351670   -3.603552    0.889246
 C   -1.920671   -2.147789   -1.695354
 C   -2.862634   -1.602587   -2.792170
 H   -5.401203   -3.486928    1.176186
 H   -4.545545   -2.206003   -0.724823
 H   -3.909192   -5.021953    2.469819
 H   -1.523292   -5.276011    1.740951
 H   -0.665003   -4.011684   -0.177776
 P   -0.359918    0.122616    1.431017
 C    0.963783   -2.209710    2.198868
 C    1.682621   -3.041562    3.056864
 C    0.570756   -0.933445    2.608963
 C    2.008955   -2.600725    4.337794
 C    0.881256   -0.505035    3.906222
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 C    1.602518   -1.333388    4.762965
 C   -3.523938    1.884801    3.467160
 C   -2.300986    1.727174    2.811113
 C   -1.880950    0.460538    2.400105
 C   -4.336277    0.780705    3.715686
 C   -3.921699   -0.489568    3.307146
 C   -2.703816   -0.648227    2.653524
 C    1.009989    2.634726    2.368168
 C    0.555958    1.667674    1.284997
 C    1.106286    2.086402    0.123880
 C    2.527389    2.345160    2.552801
 C    3.128549    2.853037    1.225999
 C    1.889846    3.369996    0.429544
 C    2.245655    4.260058   -0.742657
 C    1.019954    3.977625    1.583796
 C    1.680906    5.138489    2.333110
 C   -0.366748    4.458676    1.148153
 C    1.150059    1.413319   -1.197849
 C    0.430995    1.858287   -2.279871
 C    2.023061    0.294187   -1.526790
 S    0.808125    0.931497   -3.689643
 C    1.956035   -0.055753   -2.857997
 C   -0.585390    2.948859   -2.371892
 C    2.694081   -1.100552   -3.637258
 P    3.042223   -0.508352   -0.234148
 C    1.907933   -4.291865   -1.390189
 C    1.915218   -2.934788   -1.076860
 C    3.098417   -5.020579   -1.385171
 C    3.112576   -2.273227   -0.766470
 C    4.292375   -4.375671   -1.067861
 C    4.300748   -3.014000   -0.760367
 C    7.009892    0.382354    0.263084
 C    5.710071   -0.095879    0.420488
 C    7.358689    1.092031   -0.886651
 C    4.745936    0.104235   -0.579823
 C    6.402293    1.315500   -1.876640
 C    5.105421    0.824178   -1.725663
 H    0.709171   -2.556569    1.196604
 H    1.988497   -4.033765    2.716801
 H    2.576563   -3.246760    5.011767
 H    0.556659    0.478964    4.253881
 H    1.846020   -0.990274    5.771232
 H   -3.843110    2.882283    3.778669
 H   -1.692957    2.606638    2.601844
 H   -5.295110    0.907952    4.223546
 H   -4.552209   -1.362585    3.490494
 H   -2.399023   -1.646494    2.322480
 H    0.432105    2.621802    3.301884
 H    2.710761    1.274133    2.715107
 H    2.926966    2.885638    3.423014
 H    3.657982    2.072764    0.666211
 H    3.848074    3.671049    1.377171
 H    2.805982    5.142511   -0.396540
 H    1.354004    4.615099   -1.279397
 H    2.882101    3.724656   -1.464295
 H    1.121160    5.356248    3.256876
 H    1.660626    6.052219    1.718263
 H    2.725093    4.958494    2.617173
 H   -0.924398    4.845912    2.015803
 H   -0.974305    3.669152    0.688222
 H   -0.280459    5.285089    0.424722
 H   -0.710302    3.441940   -1.400458
 H   -1.556447    2.529504   -2.670310
 H   -0.296988    3.713246   -3.110160
 H    2.866294   -0.766272   -4.670948
 H    2.129000   -2.045145   -3.680206
 H    3.668675   -1.317904   -3.182598
 H    0.964600   -4.782508   -1.643385
 H    0.972606   -2.376903   -1.095229
 H    3.093819   -6.085436   -1.629176
 H    5.232617   -4.932551   -1.063204
 H    5.251727   -2.529722   -0.528054
 H    7.749758    0.213071    1.049050
 H    5.437353   -0.625735    1.338232
 H    8.373325    1.479210   -1.006514
 H    6.665027    1.878070   -2.775809
 H    4.364790    1.017045   -2.504894
Cu   -0.997983   -0.853317   -0.483873
 H   -3.521051   -2.400533   -3.193466
 H   -2.229885   -1.270296   -3.633210
 H   -1.112665   -2.730602   -2.171826
121
Figure 1_L-Cu-alkyl_minor01_04 / electronic energy: -4987.99975913 a.u. / lowest freq: 21.32 cm-1
 B   -3.711598   -0.758206   -2.021836
 O   -4.465843   -0.889740   -0.883057
 O   -3.943220    0.448120   -2.640936
 C   -5.390576    0.207254   -0.808785
 C   -4.718407    1.272869   -1.753356
 C   -5.519446    0.638405    0.642326
 C   -6.732004   -0.299131   -1.334695
 C   -3.734768    2.183377   -1.021809
 C   -5.692464    2.107141   -2.569481
 H   -2.972521    1.594009   -0.489666
 H   -4.242330    2.834863   -0.297222
 H   -3.221817    2.822320   -1.753869
 H   -6.326449    1.482900   -3.212430
 H   -5.133512    2.800202   -3.215586
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H	-6.339709	2.705080	-1.910130
H	-6.658681	-0.619491	-2.384741
H	-7.513997	0.470007	-1.257399
H	-7.045538	-1.168190	-0.737667
H	-4.535652	0.829358	1.087737
H	-6.005814	-0.156860	1.226394
H	-6.130887	1.549165	0.729813
C	-1.003064	-4.554390	-0.603624
C	-1.271661	-5.695670	0.147983
C	-1.959947	-3.531263	-0.788540
C	-2.523745	-5.876682	0.739963
C	-3.225209	-3.747262	-0.196730
C	-3.496372	-4.892406	0.550907
C	-1.618499	-2.311872	-1.565532
C	-2.699287	-1.822775	-2.566740
H	-4.487537	-5.016313	0.997689
H	-3.998328	-2.984316	-0.309271
H	-2.740516	-6.772852	1.326415
H	-0.498515	-6.462265	0.259050
H	-0.025440	-4.443801	-1.082047
P	-0.562560	0.566531	1.371644
C	0.705310	-1.521697	2.707711
C	1.490848	-2.108469	3.700751
C	0.456278	-0.146756	2.720072
C	2.023421	-1.321565	4.718888
C	0.963617	0.632675	3.768411
C	1.750249	0.048558	4.757177
C	-3.643715	2.888386	2.906724
C	-2.526021	2.488442	2.172272
C	-1.994896	1.205221	2.331561
C	-4.247775	2.008570	3.802112
C	-3.732739	0.720275	3.956960
C	-2.616699	0.321376	3.226835
C	0.658414	3.321968	1.439229
C	0.313644	2.016032	0.736706
C	0.883657	2.067283	-0.487778
C	2.186597	3.235988	1.727591
C	2.802752	3.334805	0.318143
C	1.562648	3.439381	-0.620550
C	1.897445	3.908831	-2.021070
C	0.605485	4.325831	0.250714
C	1.147704	5.719500	0.582585
C	-0.785263	4.526533	-0.355474
C	1.025728	0.998698	-1.507840
C	0.305689	0.987543	-2.678049
C	1.995388	-0.085036	-1.433373
S	0.807107	-0.319363	-3.691180
C	1.993135	-0.873397	-2.563872
C	-0.807341	1.883470	-3.114618
C	2.829864	-2.060257	-2.929539
P	3.069885	-0.269770	0.038908
C	4.795495	-3.972128	0.718167
C	4.627589	-2.611391	0.460527
C	3.696979	-4.829128	0.712225
C	3.359184	-2.084444	0.184079
C	2.429844	-4.314807	0.435824
C	2.261265	-2.957317	0.171408
C	6.251790	1.184170	-2.220630
C	5.010991	0.645609	-1.878201
C	7.201718	1.446282	-1.233961
C	4.701910	0.365755	-0.541637
C	6.901512	1.179959	0.102441
C	5.656286	0.656264	0.445769
H	0.278915	-2.140719	1.915375
H	1.688230	-3.182398	3.669582
H	2.645621	-1.775752	5.493697
H	0.741277	1.700987	3.818368
H	2.150811	0.664656	5.565567
H	-4.044865	3.895513	2.771066
H	-2.079221	3.185515	1.465060
H	-5.123276	2.322132	4.375305
H	-4.203554	0.019340	4.649896
H	-2.224538	-0.690827	3.359391
H	0.047533	3.571925	2.316903
H	2.444902	2.293548	2.227903
H	2.509957	4.058106	2.382283
H	3.424341	2.470787	0.057612
H	3.437274	4.225116	0.199179
H	2.369452	4.902982	-1.986826
H	1.006915	3.977387	-2.662654
H	2.607986	3.221524	-2.506117
H	0.503600	6.197683	1.337797
H	1.129626	6.360862	-0.312852
H	2.172854	5.729350	0.972717
H	-1.415895	5.127697	0.318637
H	-1.309094	3.584907	-0.556519
H	-0.712803	5.079783	-1.305400
H	-0.898464	2.734434	-2.429276
H	-1.771563	1.350905	-3.112871
H	-0.640477	2.277779	-4.128774
H	3.005441	-2.096992	-4.014785
H	2.339041	-3.002810	-2.638801
H	3.804283	-2.026303	-2.426384
H	5.795462	-4.361669	0.924051
H	5.504347	-1.960541	0.470779
H	3.825920	-5.894181	0.917932
H	1.562143	-4.976851	0.429811

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 H    1.262618   -2.573004   -0.059974
 H    6.475604    1.399228   -3.268288
 H    4.274563    0.455237   -2.662017
 H    8.172515    1.868122   -1.504639
 H    7.635139    1.393628    0.883351
 H    5.418529    0.476572    1.498547
Cu   -1.096148   -0.926465   -0.231198
 H   -3.265237   -2.679856   -2.991766
 H   -2.188077   -1.356676   -3.426285
 H   -0.700645   -2.532732   -2.138238
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Figure 1_L-Cu-alkyl_minor01_05 / electronic energy: -4987.99842918 a.u. / lowest freq: 21.17 cm-1
 B    3.403019   -1.957775   -0.448326
 O    4.272409   -1.188418    0.283907
 O    2.726654   -2.846292    0.358934
 C    4.297367   -1.677589    1.636813
 C    2.938628   -2.460382    1.727233
 C    4.403568   -0.494550    2.582507
 C    5.520590   -2.581671    1.766627
 C    1.766430   -1.565956    2.116863
 C    2.965037   -3.704046    2.599817
 H    1.733276   -0.665764    1.486789
 H    1.820405   -1.252852    3.169206
 H    0.829684   -2.119046    1.967171
 H    3.692660   -4.442161    2.237589
 H    1.971165   -4.176376    2.600205
 H    3.215078   -3.444652    3.639745
 H    5.453539   -3.448709    1.092494
 H    5.646668   -2.947894    2.795867
 H    6.419679   -2.009968    1.493058
 H    3.624613    0.247667    2.372722
 H    5.380781   -0.003620    2.462343
 H    4.310443   -0.819214    3.629986
 C    2.356989    1.346219   -3.825154
 C    2.889658    2.604269   -4.090642
 C    2.793918    0.555309   -2.736569
 C    3.903967    3.133092   -3.288645
 C    3.842450    1.100500   -1.959158
 C    4.377881    2.358723   -2.227742
 C    2.173374   -0.757725   -2.445208
 C    3.172199   -1.862897   -1.995240
 H    5.179388    2.742674   -1.588873
 H    4.224134    0.534918   -1.107075
 H    4.322766    4.121365   -3.493071
 H    2.507255    3.181027   -4.937978
 H    1.562419    0.957417   -4.470993
 P    0.316986    1.586452    0.125421
 C   -0.264077    2.631062   -2.356080
 C   -0.482274    3.614644   -3.318653
 C    0.226915    2.962790   -1.088683
 C   -0.180772    4.944374   -3.031611
 C    0.525292    4.301743   -0.808317
 C    0.331848    5.283711   -1.778355
 C    3.632018    3.141583    2.011684
 C    2.707393    2.762692    1.040076
 C    1.499617    2.154013    1.408800
 C    3.372024    2.904624    3.361944
 C    2.190383    2.263891    3.733201
 C    1.263719    1.886153    2.762175
 C   -2.201400    2.978454    0.812874
 C   -1.315073    1.743576    0.921401
 C   -2.036546    0.774802    1.525793
 C   -3.241718    2.622088   -0.282551
 C   -4.074945    1.526034    0.411856
 C   -3.425242    1.392267    1.827960
 C   -4.327263    0.691072    2.822525
 C   -3.043378    2.885941    2.110188
 C   -4.240432    3.843107    2.160584
 C   -2.228785    3.147624    3.377063
 C   -1.727936   -0.652329    1.839501
 C   -1.628846   -1.062740    3.149098
 C   -1.708072   -1.785299    0.906845
 S   -1.614154   -2.783946    3.269108
 C   -1.704679   -3.002196    1.555116
 C   -1.506886   -0.258184    4.404309
 C   -1.760679   -4.420873    1.069267
 P   -1.386019   -1.520915   -0.883656
 C    0.512841   -4.979436   -1.965187
 C    0.176820   -3.760342   -1.382735
 C   -0.378988   -5.613252   -2.832171
 C   -1.068090   -3.169351   -1.637077
 C   -1.607738   -5.017502   -3.111233
 C   -1.952416   -3.801859   -2.518129
 C   -5.425662   -1.332045   -1.675009
 C   -4.200115   -1.663723   -1.103674
 C   -5.479170   -0.422696   -2.733822
 C   -3.015760   -1.092970   -1.589889
 C   -4.303971    0.140419   -3.229012
 C   -3.074968   -0.197939   -2.661749
 H   -0.467653    1.581753   -2.589687
 H   -0.870297    3.336010   -4.301094
 H   -0.337048    5.718221   -3.786988
 H    0.904344    4.587765    0.175398
 H    0.573412    6.324468   -1.550074
 H    4.564267    3.623380    1.707803
 H    2.928749    2.944433   -0.013735
 H    4.096809    3.205689    4.121700
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 H    1.985879    2.053857    4.785782
 H    0.351197    1.367174    3.059655
 H   -1.674746    3.926979    0.651260
 H   -2.753047    2.268050   -1.199974
 H   -3.847875    3.498767   -0.553545
 H   -4.047458    0.569535   -0.115247
 H   -5.134445    1.805372    0.507434
 H   -5.302960    1.199537    2.865949
 H   -3.913303    0.685217    3.840179
 H   -4.511623   -0.353788    2.527584
 H   -3.888485    4.884739    2.087783
 H   -4.763497    3.742920    3.124900
 H   -4.983748    3.690958    1.368427
 H   -2.028608    4.226099    3.475323
 H   -1.258027    2.641287    3.379024
 H   -2.785991    2.839282    4.276179
 H   -1.641886    0.808189    4.200761
 H   -0.508816   -0.388759    4.853063
 H   -2.247435   -0.559767    5.160716
 H   -2.231229   -5.059612    1.831125
 H   -0.757624   -4.827717    0.870205
 H   -2.346382   -4.512763    0.147680
 H    1.482898   -5.431687   -1.745068
 H    0.891515   -3.275985   -0.712469
 H   -0.112823   -6.565492   -3.296981
 H   -2.308190   -5.499527   -3.797404
 H   -2.921783   -3.356209   -2.747709
 H   -6.344592   -1.776545   -1.286195
 H   -4.163329   -2.361883   -0.263092
 H   -6.441708   -0.154552   -3.175521
 H   -4.341906    0.851939   -4.056903
 H   -2.156108    0.244389   -3.054264
Cu    0.630310   -0.337090   -1.157758
 H    4.143858   -1.753523   -2.519809
 H    2.765052   -2.838123   -2.310676
 H    1.675777   -1.105974   -3.367949
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Figure 1_pc1_minor02_01 / electronic energy: -4987.96129307 a.u. / lowest freq: 14.50 cm-1
 B   -2.113803    1.774171    0.474850
 O   -2.096608    3.170392    0.435813
 O   -3.296122    1.375002    1.113072
 C   -3.135958    3.692147    1.274347
 C   -4.156489    2.506119    1.300177
 C   -3.670817    4.983294    0.674409
 C   -2.510443    3.967516    2.643459
 C   -5.135077    2.534466    0.125227
 C   -4.917136    2.348398    2.608249
 H   -4.607335    2.663699   -0.831495
 H   -5.878175    3.339786    0.227139
 H   -5.672271    1.575631    0.081858
 H   -4.238841    2.147333    3.448234
 H   -5.623670    1.507684    2.534261
 H   -5.496993    3.256207    2.837254
 H   -2.130176    3.040279    3.098113
 H   -3.224570    4.433373    3.338904
 H   -1.658929    4.652275    2.514973
 H   -3.973243    4.846806   -0.372275
 H   -2.890907    5.759309    0.700914
 H   -4.536958    5.352798    1.244905
 C   -4.944596   -2.025904   -3.156584
 C   -5.885582   -2.563978   -2.278618
 C   -3.972908   -1.120141   -2.705674
 C   -5.868893   -2.207123   -0.930854
 C   -3.962267   -0.778145   -1.343931
 C   -4.900847   -1.312428   -0.468527
 C   -3.002988   -0.560067   -3.668406
 C   -2.087576    0.384846   -3.420072
 H   -4.862309   -1.023278    0.584143
 H   -3.211526   -0.090968   -0.947997
 H   -6.604496   -2.627623   -0.240638
 H   -6.635426   -3.266650   -2.650610
 H   -4.964939   -2.307924   -4.213303
 P    1.280916    0.838744   -1.419543
 C    0.423822    3.375966   -2.156725
 C    0.478806    4.593755   -2.835206
 C    1.401251    2.397841   -2.383675
 C    1.499331    4.839120   -3.753681
 C    2.423199    2.649942   -3.307289
 C    2.470804    3.864922   -3.989241
 C    1.932691   -2.039090   -4.249896
 C    1.352740   -1.091452   -3.407830
 C    2.133092   -0.387801   -2.480454
 C    3.301143   -2.296763   -4.171591
 C    4.087362   -1.593111   -3.259024
 C    3.508293   -0.641722   -2.420690
 C    2.504010    2.497698    0.669803
 C    2.369838    1.134722    0.004983
 C    2.883137    0.218798    0.855107
 C    1.464836    2.493194    1.822605
 C    2.044942    1.433265    2.783715
 C    3.377876    0.988161    2.091799
 C    4.335658    0.286422    3.031981
 C    3.843977    2.332066    1.434752
 C    4.144077    3.451116    2.436808
 C    5.057428    2.225793    0.508040
 C    2.865918   -1.262187    0.766437
 C    4.014750   -1.998680    0.596551
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 C    1.685301   -2.102338    0.898002
 S    3.669537   -3.691220    0.611619
 C    1.978549   -3.448078    0.860492
 C    5.417291   -1.536510    0.359611
 C    1.094931   -4.648478    1.013201
 P    0.009082   -1.387852    1.027691
 C   -2.972608   -4.137244    0.161454
 C   -2.134671   -3.279264    0.874933
 C   -2.780486   -4.338823   -1.204224
 C   -1.091672   -2.615974    0.223623
 C   -1.743335   -3.673894   -1.860207
 C   -0.911212   -2.812336   -1.151951
 C    0.042513   -2.130794    5.099634
 C    0.379817   -2.154322    3.745972
 C   -1.082402   -1.427480    5.529079
 C   -0.403458   -1.468428    2.810646
 C   -1.867882   -0.741862    4.601009
 C   -1.526847   -0.750912    3.249514
 H   -0.377971    3.187219   -1.435317
 H   -0.285853    5.351320   -2.647628
 H    1.537858    5.790801   -4.289162
 H    3.188684    1.894301   -3.500114
 H    3.270472    4.051107   -4.710188
 H    1.309939   -2.583009   -4.963825
 H    0.278155   -0.899194   -3.471758
 H    3.756309   -3.045135   -4.824633
 H    5.161511   -1.784326   -3.199084
 H    4.131843   -0.093144   -1.713403
 H    2.436822    3.361277   -0.005772
 H    0.459721    2.242865    1.454021
 H    1.399357    3.485231    2.292525
 H    1.375901    0.574251    2.930652
 H    2.251630    1.848135    3.781767
 H    4.544866    0.921724    3.906784
 H    5.296928    0.052264    2.553322
 H    3.905539   -0.656458    3.405278
 H    4.213171    4.417663    1.912339
 H    5.116412    3.275926    2.924101
 H    3.395600    3.560396    3.231839
 H    5.282438    3.212017    0.072154
 H    4.900770    1.530069   -0.325708
 H    5.952620    1.902453    1.063163
 H    5.456721   -0.442179    0.315194
 H    5.807045   -1.925083   -0.594634
 H    6.101656   -1.871258    1.154830
 H    1.681089   -5.530657    1.308640
 H    0.573761   -4.890188    0.073804
 H    0.330420   -4.478860    1.783155
 H   -3.788233   -4.647617    0.679202
 H   -2.297346   -3.134360    1.945272
 H   -3.443571   -5.005416   -1.760072
 H   -1.587408   -3.816830   -2.932122
 H   -0.103310   -2.292082   -1.670929
 H    0.664816   -2.665198    5.821346
 H    1.267776   -2.701532    3.420246
 H   -1.343661   -1.407886    6.589905
 H   -2.747507   -0.184645    4.932166
 H   -2.134464   -0.189097    2.532643
Cu   -0.611373    0.532717   -0.118835
 H   -3.074876   -0.966600   -4.684263
 H   -1.957816    0.838568   -2.430787
 H   -1.426369    0.742329   -4.214164
121
Figure 1_pc1_minor02_02 / electronic energy: -4987.94484714 a.u. / lowest freq: 4.40 cm-1
 B   -3.003931    1.201832   -0.893950
 O   -2.949543    2.589522   -0.917297
 O   -4.338697    0.801919   -0.941141
 C   -4.265134    3.125368   -0.721042
 C   -5.172093    1.941895   -1.202191
 C   -4.405814    4.410396   -1.523057
 C   -4.414386    3.423436    0.771595
 C   -5.439456    1.970999   -2.707469
 C   -6.482289    1.790465   -0.444497
 H   -4.505464    2.100747   -3.274259
 H   -6.133342    2.777761   -2.986591
 H   -5.888107    1.013017   -3.010004
 H   -6.312024    1.612560    0.625578
 H   -7.047769    0.935141   -0.844027
 H   -7.105292    2.691384   -0.555036
 H   -4.311343    2.506884    1.370933
 H   -5.383298    3.890295    1.002687
 H   -3.618342    4.117175    1.079950
 H   -4.171006    4.256395   -2.584500
 H   -3.711589    5.169292   -1.131377
 H   -5.427434    4.813634   -1.444977
 C    0.173117   -3.284746   -3.223507
 C   -0.113364   -4.627834   -3.455821
 C   -0.836499   -2.379430   -2.853266
 C   -1.415617   -5.107197   -3.307586
 C   -2.141027   -2.882198   -2.685952
 C   -2.424317   -4.226527   -2.912109
 C   -0.514356   -0.951771   -2.700673
 C   -1.442470    0.063613   -2.936123
 H   -3.444504   -4.592735   -2.771006
 H   -2.943299   -2.211124   -2.366469
 H   -1.640690   -6.161128   -3.486998
 H    0.688507   -5.307531   -3.756016
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 H    1.195833   -2.916404   -3.345951
 P    2.696344   -0.016254   -1.026227
 C    1.980202    1.444825   -3.334526
 C    2.136644    1.886797   -4.646749
 C    2.988305    0.707377   -2.694297
 C    3.302824    1.591440   -5.352272
 C    4.149672    0.404113   -3.420628
 C    4.305978    0.845284   -4.734591
 C    6.582554    0.768887    0.210851
 C    5.327759    0.911853   -0.376389
 C    4.404047   -0.143919   -0.345595
 C    6.928576   -0.429849    0.840513
 C    6.020222   -1.485988    0.872087
 C    4.764929   -1.343555    0.277022
 C    1.730468    2.820676   -0.417505
 C    2.024746    1.374760   -0.042568
 C    1.616599    1.215364    1.232501
 C    0.181690    2.905857   -0.520476
 C   -0.266770    2.736982    0.946935
 C    1.073102    2.565977    1.722932
 C    0.941071    2.750862    3.220074
 C    2.001698    3.551072    0.929217
 C    1.548371    5.015366    0.952026
 C    3.470080    3.537037    1.352472
 C    1.660847   -0.017087    2.054203
 C    2.708543   -0.263905    2.913202
 C    0.639955   -1.046606    2.113835
 S    2.446279   -1.721623    3.792830
 C    0.926093   -2.027891    3.045501
 C    3.959668    0.523298    3.151517
 C    0.144908   -3.217845    3.518263
 P   -0.911862   -1.013815    1.138751
 C   -0.369699   -4.897690    0.000619
 C   -0.218640   -3.533558    0.224238
 C   -1.556155   -5.540355    0.358921
 C   -1.237273   -2.800122    0.848121
 C   -2.589487   -4.806512    0.936816
 C   -2.431481   -3.441576    1.183522
 C   -4.455967    0.076042    2.919244
 C   -3.489668   -0.339289    2.004985
 C   -4.098037    0.376999    4.233533
 C   -2.152093   -0.489331    2.399433
 C   -2.767975    0.249704    4.629479
 C   -1.802489   -0.186223    3.721335
 H    1.053365    1.677949   -2.808281
 H    1.337317    2.462453   -5.119538
 H    3.427592    1.937541   -6.380989
 H    4.947980   -0.181881   -2.959217
 H    5.222338    0.602412   -5.278225
 H    7.294640    1.597098    0.182813
 H    5.062783    1.852530   -0.865653
 H    7.910844   -0.538722    1.306586
 H    6.285195   -2.425100    1.363409
 H    4.049811   -2.170036    0.310014
 H    2.272449    3.210445   -1.289138
 H   -0.233825    2.116890   -1.162245
 H   -0.144246    3.864944   -0.945799
 H   -0.933994    1.876941    1.088133
 H   -0.813269    3.616456    1.316210
 H    0.548413    3.753434    3.451333
 H    1.902997    2.635244    3.741153
 H    0.237734    2.017036    3.644363
 H    2.127439    5.598576    0.218003
 H    1.741529    5.458795    1.941922
 H    0.485786    5.169885    0.727809
 H    4.058615    4.202867    0.700733
 H    3.921257    2.541360    1.300115
 H    3.583913    3.909111    2.383500
 H    4.478793    0.728561    2.206179
 H    4.655658   -0.025248    3.801503
 H    3.745569    1.488706    3.633878
 H    0.517525   -3.559355    4.494795
 H    0.219912   -4.061596    2.816110
 H   -0.919976   -2.974707    3.633510
 H    0.439574   -5.459663   -0.470160
 H    0.709162   -3.035296   -0.070256
 H   -1.677789   -6.610496    0.176236
 H   -3.525935   -5.298424    1.210070
 H   -3.241013   -2.891821    1.667288
 H   -5.494521    0.177942    2.595613
 H   -3.783442   -0.525301    0.970303
 H   -4.853697    0.715309    4.946318
 H   -2.474677    0.488263    5.654510
 H   -0.767510   -0.285239    4.053128
Cu   -1.391423   -0.061539   -0.920522
 H    0.550134   -0.708348   -2.717259
 H   -2.441663   -0.171842   -3.314856
 H   -1.095129    1.073477   -3.173225
121
Figure 1_pc1_minor02_03 / electronic energy: -4987.95227656 a.u. / lowest freq: 8.20 cm-1
 B    1.549476    2.284059   -0.076041
 O    0.933588    3.528602    0.009866
 O    2.798639    2.450322   -0.676052
 C    1.678953    4.498382   -0.743061
 C    3.104542    3.848995   -0.784807
 C    1.606743    5.840938   -0.031377
 C    1.033014    4.605906   -2.124217
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C	3.962719	4.221031	0.423690
C	3.881972	4.089316	-2.069451
H	3.414002	4.077490	1.366185
H	4.303946	5.265840	0.377306
H	4.850591	3.571317	0.447259
H	3.357444	3.681973	-2.944081
H	4.863914	3.596831	-2.005662
H	4.051990	5.164619	-2.232368
H	1.065966	3.643888	-2.657165
H	1.525538	5.369548	-2.744122
H	-0.022705	4.889666	-2.006965
H	1.911513	5.759641	1.020237
H	0.573884	6.220211	-0.054746
H	2.250643	6.583544	-0.527221
C	3.438098	-1.915206	3.365635
C	4.617567	-2.655036	3.317121
C	3.209489	-0.850442	2.476249
C	5.594842	-2.362073	2.365435
C	4.193449	-0.583968	1.503181
C	5.368723	-1.327477	1.454107
C	2.007440	-0.019800	2.615163
C	1.991439	1.323044	2.251564
H	6.115619	-1.101981	0.688569
H	4.024810	0.211022	0.770748
H	6.520790	-2.940685	2.325284
H	4.775437	-3.466911	4.032228
H	2.682759	-2.147673	4.122074
P	-1.321019	0.421043	1.512106
C	-2.409886	1.563449	3.902786
C	-2.640168	2.634923	4.767607
C	-1.769795	1.767317	2.674582
C	-2.234550	3.921430	4.416913
C	-1.337938	3.062222	2.340440
C	-1.581828	4.130780	3.200860
C	-1.626654	-3.387572	2.984522
C	-1.145554	-2.167870	2.507333
C	-2.020046	-1.109851	2.244145
C	-2.991580	-3.555517	3.208523
C	-3.873087	-2.500870	2.959163
C	-3.391305	-1.287672	2.474246
C	-2.870616	1.995454	-0.488831
C	-2.366270	0.668811	0.053190
C	-2.590230	-0.270979	-0.887971
C	-1.871028	2.386274	-1.609689
C	-2.145509	1.315563	-2.685914
C	-3.285508	0.442966	-2.065759
C	-4.011668	-0.405115	-3.089466
C	-4.111020	1.536879	-1.301265
C	-4.713199	2.616014	-2.207937
C	-5.248869	1.020770	-0.418668
C	-2.189910	-1.703702	-0.906435
C	-3.143483	-2.693746	-0.857700
C	-0.839319	-2.240816	-1.078149
S	-2.438277	-4.247902	-1.090241
C	-0.841114	-3.610923	-1.256771
C	-4.614101	-2.596013	-0.605166
C	0.222402	-4.605581	-1.623063
P	0.664599	-1.169692	-1.005818
C	4.149571	-3.334499	-1.589784
C	3.096818	-2.437537	-1.777343
C	4.189519	-4.144733	-0.457274
C	2.074603	-2.337837	-0.827859
C	3.188566	-4.028879	0.507896
C	2.153460	-3.116901	0.333614
C	0.323524	-0.859662	-5.116028
C	0.211085	-1.316417	-3.803849
C	1.060420	0.291345	-5.396305
C	0.828167	-0.622368	-2.755141
C	1.695973	0.973875	-4.359332
C	1.579881	0.522359	-3.044755
H	-2.730106	0.562519	4.198673
H	-3.140155	2.458821	5.723112
H	-2.416850	4.758259	5.095421
H	-0.785923	3.236219	1.411127
H	-1.244292	5.132698	2.923917
H	-0.931276	-4.208467	3.174658
H	-0.078603	-2.034400	2.315577
H	-3.373210	-4.510073	3.578952
H	-4.943844	-2.629894	3.133571
H	-4.090366	-0.474653	2.263871
H	-3.051026	2.777649	0.260323
H	-0.840112	2.376403	-1.238282
H	-2.077609	3.402159	-1.977019
H	-1.267580	0.701832	-2.911991
H	-2.476744	1.758450	-3.637253
H	-4.375999	0.225428	-3.915593
H	-4.878477	-0.928496	-2.662545
H	-3.340907	-1.163220	-3.523451
H	-5.053703	3.470946	-1.601746
H	-5.596327	2.218974	-2.733249
H	-4.027232	3.005325	-2.970403
H	-5.745408	1.867122	0.081979
H	-4.905808	0.333981	0.363986
H	-6.014319	0.504643	-1.020084
H	-4.900606	-1.557934	-0.409797
H	-4.898759	-3.191013	0.276540
H	-5.204076	-2.964868	-1.458836

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 H    0.978297   -4.167073   -2.285036
 H   -0.230218   -5.456768   -2.152388
 H    0.742551   -5.004519   -0.740332
 H    4.936730   -3.404932   -2.344273
 H    3.069403   -1.830888   -2.684583
 H    5.006181   -4.856980   -0.318295
 H    3.220115   -4.644270    1.409223
 H    1.377272   -3.034242    1.097741
 H   -0.173591   -1.402825   -5.923238
 H   -0.380017   -2.210893   -3.595157
 H    1.141439    0.654789   -6.423551
 H    2.280942    1.872287   -4.571651
 H    2.076392    1.070535   -2.240944
Cu    0.907769    0.485070    0.667798
 H    1.237361   -0.387987    3.299336
 H    2.922241    1.805264    1.941019
 H    1.253841    1.995309    2.698645
121
Figure 1_pc1_minor02_04 / electronic energy: -4987.93892719 a.u. / lowest freq: 7.92 cm-1
 B   -2.299604    2.033898   -1.056048
 O   -1.684610    3.281847   -1.075177
 O   -3.682332    2.215644   -1.109403
 C   -2.667126    4.303898   -0.863741
 C   -3.981086    3.599886   -1.345562
 C   -2.282529    5.545600   -1.653982
 C   -2.672547    4.621808    0.632993
 C   -4.230782    3.760903   -2.845294
 C   -5.231077    3.981250   -0.566873
 H   -3.334354    3.502242   -3.428576
 H   -4.533352    4.786636   -3.103557
 H   -5.037886    3.077658   -3.148761
 H   -5.138884    3.728515    0.497951
 H   -6.101955    3.441227   -0.967989
 H   -5.432467    5.060238   -0.653515
 H   -2.945381    3.736958    1.227805
 H   -3.368080    5.438150    0.878478
 H   -1.660803    4.930735    0.935423
 H   -2.105517    5.315228   -2.712785
 H   -1.356439    5.976766   -1.244582
 H   -3.069996    6.312444   -1.589607
 C   -0.157174   -3.291746   -3.004646
 C   -0.767803   -4.370271   -3.640935
 C   -0.819627   -2.060725   -2.872003
 C   -2.063728   -4.248362   -4.144225
 C   -2.130623   -1.957099   -3.368249
 C   -2.743991   -3.038859   -3.994946
 C   -0.114229   -0.912303   -2.272797
 C   -0.336764    0.394037   -2.685650
 H   -3.766306   -2.936650   -4.367715
 H   -2.680737   -1.019599   -3.250303
 H   -2.545355   -5.095185   -4.638881
 H   -0.228661   -5.315660   -3.742839
 H    0.856335   -3.396541   -2.606645
 P    3.373090   -0.494238   -0.542382
 C    2.916935   -0.451208   -3.284324
 C    2.759036    0.099579   -4.556456
 C    3.146014    0.363855   -2.168590
 C    2.822502    1.480318   -4.729107
 C    3.242850    1.749103   -2.362593
 C    3.070079    2.303806   -3.628955
 C    7.088175    0.632486    0.976180
 C    5.710292    0.452639    0.836688
 C    5.173745   -0.129571   -0.315589
 C    7.954335    0.230208   -0.037448
 C    7.431972   -0.357736   -1.191778
 C    6.058110   -0.539607   -1.327213
 C    2.643335    2.053236    0.937910
 C    2.541335    0.548620    0.710314
 C    1.617178    0.090712    1.590643
 C    1.303718    2.628112    0.386381
 C    0.273256    2.142667    1.430001
 C    1.126488    1.300921    2.417938
 C    0.478238    0.998121    3.752293
 C    2.429319    2.169981    2.473013
 C    2.230166    3.614460    2.951645
 C    3.512424    1.574796    3.373179
 C    1.188273   -1.302282    1.886746
 C    2.082085   -2.206059    2.418652
 C   -0.181042   -1.823383    1.883441
 S    1.274701   -3.632038    2.970278
 C   -0.280476   -3.060436    2.487432
 C    3.565898   -2.135357    2.596891
 C   -1.453052   -3.942723    2.798704
 P   -1.571158   -1.015892    0.998149
 C   -2.805713   -4.524558   -0.786603
 C   -2.017639   -3.527021   -0.220655
 C   -4.192326   -4.380899   -0.841187
 C   -2.608366   -2.385681    0.335336
 C   -4.784592   -3.231231   -0.323115
 C   -3.998608   -2.239280    0.264211
 C   -4.327706    1.346420    2.923235
 C   -3.482376    0.776132    1.970543
 C   -4.328806    0.873076    4.233789
 C   -2.635153   -0.284120    2.314782
 C   -3.479738   -0.175897    4.588382
 C   -2.639542   -0.750025    3.636616
 H    2.842192   -1.534161   -3.155897
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 H    2.570823   -0.554642   -5.410876
 H    2.685823    1.918013   -5.720866
 H    3.462022    2.408858   -1.523055
 H    3.136484    3.386522   -3.759042
 H    7.481891    1.094299    1.885006
 H    5.049240    0.775631    1.637986
 H    9.032178    0.373045    0.069145
 H    8.101458   -0.679927   -1.993087
 H    5.669323   -1.002871   -2.238654
 H    3.550877    2.532153    0.546152
 H    1.086611    2.237585   -0.615630
 H    1.331201    3.723691    0.302685
 H   -0.534072    1.556989    0.977024
 H   -0.207898    2.976378    1.961326
 H    0.291432    1.931286    4.306442
 H    1.113972    0.350799    4.376403
 H   -0.488600    0.496848    3.630325
 H    3.188629    4.154141    2.887307
 H    1.918639    3.632745    4.007921
 H    1.494033    4.191225    2.379562
 H    4.470199    2.101129    3.237107
 H    3.678317    0.504842    3.210901
 H    3.229218    1.700372    4.429823
 H    3.964575   -1.185053    2.230320
 H    4.066173   -2.936148    2.030070
 H    3.854021   -2.244023    3.654270
 H   -1.410839   -4.263646    3.851195
 H   -1.455640   -4.850966    2.176303
 H   -2.408676   -3.431722    2.642104
 H   -2.330026   -5.415906   -1.200405
 H   -0.932875   -3.649818   -0.195306
 H   -4.808250   -5.161829   -1.293160
 H   -5.868428   -3.101602   -0.368694
 H   -4.482830   -1.351774    0.677039
 H   -4.986332    2.169262    2.634680
 H   -3.488651    1.161484    0.948445
 H   -4.987415    1.322346    4.980860
 H   -3.465579   -0.548822    5.615105
 H   -1.964360   -1.550580    3.942242
Cu   -1.306472    0.253092   -0.909500
 H    0.805192   -1.150091   -1.732325
 H   -1.025821    0.617647   -3.504923
 H    0.409423    1.167482   -2.480847
121
Figure 1_ts(CuBadd)_minor02_01 / electronic energy: -4987.94770508 a.u. / lowest freq: -69.30 cm-1
 B   -1.458715    2.422573   -0.112285
 O   -0.772971    3.615568   -0.252665
 O   -2.657999    2.652433    0.557587
 C   -1.426240    4.637671    0.521303
 C   -2.881393    4.067897    0.659307
 C   -1.324206    5.960919   -0.222165
 C   -0.700733    4.739537    1.862190
 C   -3.790406    4.469733   -0.501674
 C   -3.567321    4.363251    1.983997
 H   -3.311589    4.281206   -1.473903
 H   -4.063762    5.534081   -0.453779
 H   -4.715348    3.875221   -0.458728
 H   -3.007345    3.949298    2.833127
 H   -4.570401    3.911336    1.989732
 H   -3.683172    5.447221    2.135814
 H   -0.757213    3.794372    2.422119
 H   -1.115886    5.544417    2.486242
 H    0.360619    4.960206    1.679964
 H   -1.700235    5.879995   -1.250357
 H   -0.271791    6.278142   -0.272841
 H   -1.890759    6.748392    0.298278
 C   -3.398691   -1.660472   -3.462047
 C   -4.598910   -2.365905   -3.497354
 C   -3.188267   -0.612047   -2.542875
 C   -5.628490   -2.058702   -2.605851
 C   -4.226830   -0.340635   -1.624230
 C   -5.425179   -1.046763   -1.664115
 C   -1.963490    0.183046   -2.596964
 C   -1.931502    1.528079   -2.144782
 H   -6.210124   -0.809062   -0.941055
 H   -4.085402    0.434396   -0.865286
 H   -6.572614   -2.607734   -2.635375
 H   -4.733940   -3.161056   -4.236028
 H   -2.608171   -1.903479   -4.178579
 P    1.405884    0.353194   -1.472394
 C    1.417140    1.872240   -3.795932
 C    1.962680    2.671518   -4.800216
 C    2.198183    1.454608   -2.710187
 C    3.297074    3.069255   -4.728999
 C    3.542651    1.848250   -2.656545
 C    4.086183    2.653873   -3.655850
 C    3.589718   -2.922138   -2.766414
 C    3.253094   -1.644801   -2.326272
 C    1.913357   -1.305282   -2.099342
 C    2.592224   -3.876669   -2.980815
 C    1.256005   -3.542488   -2.769860
 C    0.920913   -2.259088   -2.335969
 C    2.883661    1.855439    0.613077
 C    2.382960    0.539904    0.035769
 C    2.531105   -0.398481    0.992272
 C    1.848588    2.246790    1.702347
 C    2.083613    1.182723    2.791609
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 C    3.212304    0.287569    2.194305
 C    3.888283   -0.590670    3.226429
 C    4.088583    1.363511    1.460166
 C    4.688247    2.429102    2.383687
 C    5.243327    0.801160    0.627279
 C    2.029019   -1.795377    1.026632
 C    2.901511   -2.856365    1.031921
 C    0.636236   -2.214006    1.185593
 S    2.069302   -4.339897    1.308140
 C    0.524490   -3.571231    1.418448
 C    4.379435   -2.874963    0.805921
 C   -0.624165   -4.458266    1.803526
 P   -0.777952   -1.032356    1.029464
 C   -3.412833   -3.784255   -0.508929
 C   -2.318491   -2.949531   -0.311763
 C   -4.489169   -3.750361    0.378109
 C   -2.262265   -2.094714    0.796237
 C   -4.465617   -2.865104    1.453258
 C   -3.358595   -2.041555    1.663404
 C   -1.767511    1.260625    4.295404
 C   -1.618071    0.780838    2.994127
 C   -1.289746    0.520700    5.376185
 C   -0.989372   -0.446879    2.761513
 C   -0.676806   -0.712691    5.151900
 C   -0.529814   -1.195850    3.852946
 H    0.371512    1.564195   -3.867269
 H    1.338691    2.986780   -5.639717
 H    3.723580    3.701883   -5.511041
 H    4.177168    1.521778   -1.831088
 H    5.134861    2.954689   -3.596147
 H    4.638208   -3.177640   -2.937344
 H    4.043778   -0.911556   -2.149075
 H    2.859839   -4.881286   -3.317172
 H    0.469596   -4.281893   -2.939631
 H   -0.123472   -1.988302   -2.166137
 H    3.088129    2.652096   -0.113449
 H    0.831303    2.230566    1.292639
 H    2.037531    3.264959    2.070839
 H    1.192094    0.588133    3.011681
 H    2.410994    1.626407    3.743830
 H    4.253273    0.023062    4.064782
 H    4.747679   -1.137468    2.814401
 H    3.184247   -1.330134    3.639636
 H    5.093928    3.259751    1.784210
 H    5.525494    2.005323    2.960762
 H    3.978747    2.857784    3.102328
 H    5.777712    1.620828    0.120704
 H    4.913802    0.091718   -0.141942
 H    5.975799    0.287851    1.270831
 H    4.748245   -1.865171    0.594151
 H    4.634150   -3.510227   -0.056664
 H    4.924513   -3.266928    1.678774
 H   -0.269196   -5.258322    2.469943
 H   -1.090818   -4.936578    0.929560
 H   -1.404888   -3.903637    2.336061
 H   -3.428723   -4.460537   -1.366206
 H   -1.480975   -2.991737   -1.009969
 H   -5.351410   -4.402215    0.220121
 H   -5.309802   -2.817815    2.145352
 H   -3.349934   -1.370054    2.524082
 H   -2.256937    2.223646    4.461451
 H   -1.996756    1.371024    2.157419
 H   -1.396737    0.903418    6.394007
 H   -0.303614   -1.301143    5.993328
 H   -0.031576   -2.154160    3.691327
Cu   -0.853529    0.552421   -0.712431
 H   -1.224513   -0.131439   -3.340034
 H   -2.886933    1.991154   -1.878097
 H   -1.244437    2.225260   -2.632589
121
Figure 1_ts(CuBadd)_minor02_02 / electronic energy: -4987.95176996 a.u. / lowest freq: -106.00 cm-1
 B    1.661237    2.191684    0.031274
 O    1.130545    3.467516    0.138046
 O    2.842974    2.244943   -0.700597
 C    1.860541    4.365230   -0.716623
 C    3.228921    3.617606   -0.884503
 C    1.957498    5.724489   -0.041416
 C    1.085407    4.489021   -2.027284
 C    4.236481    3.953892    0.214010
 C    3.876586    3.771353   -2.251567
 H    3.783660    3.887434    1.214284
 H    4.654248    4.963687    0.090363
 H    5.064574    3.230882    0.170454
 H    3.230582    3.386886   -3.052126
 H    4.822807    3.210631   -2.280800
 H    4.101347    4.828422   -2.460651
 H    0.994439    3.517812   -2.536411
 H    1.564193    5.202587   -2.713553
 H    0.070462    4.851880   -1.811813
 H    2.374052    5.647255    0.971449
 H    0.956697    6.174873    0.038262
 H    2.589682    6.406477   -0.630361
 C    3.379682   -1.841866    3.420086
 C    4.543417   -2.606392    3.414634
 C    3.174794   -0.806295    2.484401
 C    5.541473   -2.373902    2.465944
 C    4.183825   -0.603139    1.515754
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 C    5.344694   -1.370316    1.513709
 C    1.985499    0.037105    2.555764
 C    1.997708    1.378509    2.075898
 H    6.105388   -1.188270    0.749508
 H    4.045082    0.162344    0.746358
 H    6.455946   -2.971901    2.461720
 H    4.674408   -3.391713    4.164618
 H    2.612916   -2.029649    4.177976
 P   -1.341937    0.466347    1.507555
 C   -2.414792    1.633618    3.891140
 C   -2.622008    2.709793    4.755737
 C   -1.756821    1.821737    2.670052
 C   -2.175916    3.984625    4.411244
 C   -1.286279    3.104006    2.341492
 C   -1.507086    4.177948    3.201392
 C   -1.687509   -3.311187    3.047747
 C   -1.190769   -2.103917    2.555388
 C   -2.056977   -1.051006    2.247797
 C   -3.057845   -3.470267    3.244283
 C   -3.930296   -2.419348    2.951274
 C   -3.433728   -1.218880    2.450067
 C   -2.846508    2.073162   -0.492467
 C   -2.382844    0.733378    0.051876
 C   -2.610484   -0.197931   -0.896487
 C   -1.812379    2.441839   -1.588886
 C   -2.092387    1.383430   -2.676540
 C   -3.266027    0.535824   -2.083615
 C   -3.990478   -0.293071   -3.123799
 C   -4.080044    1.647044   -1.331712
 C   -4.636686    2.742899   -2.247260
 C   -5.247296    1.156655   -0.473038
 C   -2.239480   -1.638506   -0.907112
 C   -3.214330   -2.607241   -0.852768
 C   -0.899602   -2.206749   -1.061305
 S   -2.539315   -4.179114   -1.050519
 C   -0.928249   -3.579676   -1.214329
 C   -4.685568   -2.473400   -0.621221
 C    0.117155   -4.603665   -1.550726
 P    0.627731   -1.171096   -1.016460
 C    4.072473   -3.405895   -1.564263
 C    3.029387   -2.501993   -1.772007
 C    4.112420   -4.178605   -0.405967
 C    2.018175   -2.358529   -0.816784
 C    3.118920   -4.022302    0.561416
 C    2.094352   -3.102611    0.367307
 C    0.278581   -0.914367   -5.127272
 C    0.153856   -1.345362   -3.807513
 C    1.053562    0.206117   -5.427935
 C    0.796343   -0.654038   -2.772669
 C    1.712665    0.885730   -4.403611
 C    1.583380    0.461663   -3.081271
 H   -2.766773    0.641541    4.180960
 H   -3.134911    2.546526    5.706602
 H   -2.339101    4.824853    5.090387
 H   -0.721292    3.263171    1.417707
 H   -1.137775    5.170002    2.929921
 H   -0.999588   -4.129206    3.273846
 H   -0.118641   -1.974416    2.389160
 H   -3.450755   -4.415079    3.627607
 H   -5.004970   -2.541250    3.105479
 H   -4.124345   -0.408590    2.204009
 H   -3.022753    2.856071    0.257052
 H   -0.789943    2.397970   -1.194878
 H   -1.979051    3.464842   -1.956149
 H   -1.225703    0.749494   -2.889188
 H   -2.393445    1.839707   -3.631356
 H   -4.326525    0.346882   -3.954684
 H   -4.875629   -0.799735   -2.714419
 H   -3.327565   -1.063604   -3.547829
 H   -4.972050    3.602865   -1.645381
 H   -5.516029    2.367696   -2.794493
 H   -3.924238    3.119697   -2.991518
 H   -5.736981    2.014201    0.014933
 H   -4.934811    0.465668    0.318763
 H   -6.009919    0.654485   -1.089572
 H   -4.950841   -1.426930   -0.441866
 H   -4.996292   -3.052001    0.262578
 H   -5.271294   -2.838004   -1.479677
 H    0.878504   -4.199283   -2.228064
 H   -0.351150   -5.463307   -2.051971
 H    0.632557   -4.983141   -0.656796
 H    4.853054   -3.509714   -2.321744
 H    3.001727   -1.923932   -2.697580
 H    4.922684   -4.894506   -0.249516
 H    3.150632   -4.608502    1.481898
 H    1.327237   -2.982774    1.135578
 H   -0.237147   -1.454634   -5.924666
 H   -0.465355   -2.216519   -3.582136
 H    1.146205    0.547516   -6.461706
 H    2.329183    1.758833   -4.632614
 H    2.099291    1.005275   -2.286266
Cu    0.877075    0.406739    0.678335
 H    1.257180   -0.220366    3.330461
 H    2.974366    1.808806    1.826517
 H    1.331959    2.095969    2.566784
121
Figure 1_ts(CuBadd)_minor02_03 / electronic energy: -4987.95176079 a.u. / lowest freq: -108.47 cm-1
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B	-1.717898	2.139919	-0.012296
O	-1.220474	3.431223	-0.084201
O	-2.914856	2.147223	0.698300
C	-1.990399	4.290657	0.775066
C	-3.342807	3.505422	0.894565
C	-2.105291	5.663575	0.131058
C	-1.247577	4.400844	2.105722
C	-4.329908	3.836518	-0.224255
C	-4.031294	3.619541	2.245230
H	-3.850414	3.803058	-1.213645
H	-4.776957	4.832597	-0.091458
H	-5.139836	3.092107	-0.216198
H	-3.403762	3.226676	3.056003
H	-4.969606	3.045059	2.235261
H	-4.277688	4.668616	2.469730
H	-1.141628	3.419646	2.592363
H	-1.761755	5.083173	2.798125
H	-0.238383	4.796691	1.923320
H	-2.497702	5.603211	-0.892443
H	-1.113626	6.138092	0.084467
H	-2.764643	6.316656	0.722918
C	-3.414334	-1.871782	-3.389124
C	-4.576846	-2.637432	-3.362024
C	-3.191610	-0.838310	-2.455667
C	-5.555768	-2.407521	-2.393048
C	-4.180554	-0.637894	-1.465412
C	-5.340469	-1.406709	-1.441662
C	-2.004684	0.006674	-2.548693
C	-2.016699	1.348456	-2.071763
H	-6.086258	-1.227195	-0.662328
H	-4.026186	0.126916	-0.698029
H	-6.469664	-3.006061	-2.372077
H	-4.722369	-3.421325	-4.110822
H	-2.662208	-2.057630	-4.162009
P	1.336803	0.513067	-1.508681
C	1.209951	3.159542	-2.306865
C	1.401124	4.250055	-3.152844
C	1.716265	1.895125	-2.651464
C	2.075425	4.090898	-4.364692
C	2.379856	1.741150	-3.874324
C	2.557060	2.833569	-4.725154
C	4.007736	-2.283610	-2.977454
C	3.477408	-1.102031	-2.466156
C	2.096163	-0.974307	-2.265053
C	3.165388	-3.355567	-3.282262
C	1.790676	-3.236064	-3.087986
C	1.260040	-2.047720	-2.585156
C	2.790977	2.137050	0.515111
C	2.364913	0.791646	-0.045885
C	2.619307	-0.144433	0.890903
C	1.747546	2.462355	1.617234
C	2.061289	1.401160	2.692840
C	3.255609	0.592622	2.086656
C	4.003137	-0.229279	3.116174
C	4.037365	1.734807	1.347430
C	4.564675	2.834839	2.275150
C	5.216070	1.286549	0.481608
C	2.289784	-1.595033	0.882376
C	3.290500	-2.536410	0.818316
C	0.965594	-2.201592	1.025940
S	2.657525	-4.128337	0.995482
C	1.030518	-3.574919	1.162353
C	4.758445	-2.361600	0.592711
C	0.011415	-4.629502	1.485213
P	-0.588671	-1.207189	0.992983
C	-3.011031	-4.098156	-0.618809
C	-2.004880	-3.160924	-0.412596
C	-4.002923	-4.285140	0.344315
C	-1.947170	-2.427606	0.779031
C	-3.980637	-3.524735	1.511381
C	-2.956965	-2.601735	1.730705
C	-1.674698	0.813642	4.402283
C	-1.555780	0.396387	3.076830
C	-1.003530	0.131947	5.417235
C	-0.763620	-0.711761	2.755113
C	-0.226463	-0.983670	5.104245
C	-0.109432	-1.405697	3.780982
H	0.640591	3.291632	-1.381415
H	1.004020	5.227744	-2.868960
H	2.215035	4.944042	-5.032883
H	2.759823	0.763247	-4.176618
H	3.074323	2.696275	-5.677745
H	5.085690	-2.374511	-3.130314
H	4.144949	-0.275218	-2.211301
H	3.585028	-4.285495	-3.673443
H	1.126166	-4.070545	-3.323911
H	0.184223	-1.948881	-2.421370
H	2.944283	2.933668	-0.224929
H	0.726267	2.392008	1.223862
H	1.883762	3.485946	1.995512
H	1.213715	0.741321	2.903630
H	2.355278	1.856473	3.650311
H	4.322819	0.409249	3.954641
H	4.900829	-0.708204	2.700787
H	3.360894	-1.021794	3.531411
H	4.885765	3.706516	1.682335
H	5.447989	2.474089	2.825778

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 H    3.838732    3.190872    3.016426
 H    5.676384    2.161493   -0.003941
 H    4.921506    0.590233   -0.312284
 H    5.996857    0.805828    1.092450
 H    4.997238   -1.306807    0.425212
 H    5.086411   -2.922646   -0.296114
 H    5.350991   -2.720335    1.448992
 H    0.499756   -5.480111    1.982852
 H   -0.489186   -5.015624    0.585695
 H   -0.764253   -4.249965    2.160656
 H   -3.028696   -4.676203   -1.544833
 H   -1.238173   -3.018081   -1.177188
 H   -4.798714   -5.014915    0.178137
 H   -4.760634   -3.652383    2.265807
 H   -2.943397   -2.031531    2.661509
 H   -2.290181    1.684397    4.641903
 H   -2.081755    0.940238    2.288812
 H   -1.088099    0.468238    6.453356
 H    0.298306   -1.525937    5.894330
 H    0.514556   -2.270669    3.545330
Cu   -0.881727    0.385843   -0.679173
 H   -1.284597   -0.252628   -3.330406
 H   -2.993673    1.777675   -1.822495
 H   -1.351516    2.066285   -2.562867
121
Figure 1_ts(CuBadd)_minor02_04 / electronic energy: -4987.94109714 a.u. / lowest freq: -155.05 cm-1
 B   -2.732017    1.664795    0.017914
 O   -2.645153    2.836994    0.740174
 O   -4.052155    1.257021   -0.085979
 C   -3.923583    3.104406    1.341992
 C   -4.899284    2.314966    0.400628
 C   -4.152414    4.607228    1.379351
 C   -3.876720    2.547686    2.764325
 C   -5.341590    3.127788   -0.814848
 C   -6.104022    1.704717    1.096646
 H   -4.483476    3.599122   -1.317235
 H   -6.057899    3.915465   -0.539929
 H   -5.828344    2.455512   -1.536858
 H   -5.801168    0.986984    1.870341
 H   -6.728376    1.170639    0.364871
 H   -6.721711    2.485814    1.565373
 H   -3.711941    1.460364    2.764156
 H   -4.802103    2.763534    3.318289
 H   -3.038607    3.015260    3.301551
 H   -4.027410    5.065563    0.389593
 H   -3.428704    5.076061    2.062728
 H   -5.163844    4.836980    1.747844
 C   -0.692658   -0.552093   -4.564434
 C   -1.238160   -1.465661   -5.459451
 C   -1.458161    0.003069   -3.513273
 C   -2.569098   -1.876772   -5.338117
 C   -2.797629   -0.440807   -3.395303
 C   -3.335886   -1.361074   -4.291851
 C   -0.877788    0.988625   -2.613493
 C   -1.709167    1.900187   -1.854656
 H   -4.373521   -1.683298   -4.166361
 H   -3.423421   -0.065991   -2.579796
 H   -2.995938   -2.596398   -6.040794
 H   -0.615876   -1.863155   -6.266577
 H    0.350026   -0.239924   -4.677177
 P    2.620981    0.501609   -1.059226
 C    1.815247    3.084977   -1.889448
 C    1.863475    4.217005   -2.701015
 C    2.787356    2.079379   -1.992489
 C    2.881500    4.362934   -3.642434
 C    3.800714    2.233715   -2.950871
 C    3.847570    3.364498   -3.765738
 C    6.655982    0.456203   -0.077466
 C    5.355477    0.898597   -0.306455
 C    4.383724    0.020522   -0.809337
 C    7.001890   -0.870358   -0.349015
 C    6.046187   -1.748415   -0.856085
 C    4.743077   -1.302507   -1.087920
 C    2.011910    2.392639    1.275165
 C    2.162493    1.016351    0.639587
 C    1.824931    0.115184    1.584505
 C    0.481609    2.607096    1.432210
 C    0.101697    1.575289    2.515906
 C    1.460000    0.888719    2.860219
 C    1.438409    0.103389    4.154849
 C    2.441283    2.107926    2.743772
 C    2.147734    3.254768    3.717637
 C    3.922956    1.768863    2.897493
 C    1.814963   -1.362802    1.466486
 C    2.903129   -2.114829    1.849219
 C    0.707504   -2.183488    1.015701
 S    2.574917   -3.797221    1.676261
 C    0.973307   -3.537330    1.100146
 C    4.239458   -1.674270    2.361158
 C    0.117129   -4.739419    0.835391
 P   -0.898027   -1.502980    0.474042
 C   -1.068251   -3.838273   -2.870237
 C   -0.688175   -2.921777   -1.895482
 C   -2.277512   -4.526664   -2.753070
 C   -1.497622   -2.712622   -0.770423
 C   -3.102874   -4.291336   -1.655871
 C   -2.714253   -3.389273   -0.664291
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 C   -4.131404   -1.399063    2.998137
 C   -3.278397   -1.238553    1.907810
 C   -3.684309   -2.043628    4.151863
 C   -1.972746   -1.748039    1.947295
 C   -2.381803   -2.536573    4.204887
 C   -1.531518   -2.396195    3.107168
 H    0.998444    2.985680   -1.174233
 H    1.094161    4.986094   -2.598005
 H    2.918913    5.248282   -4.281590
 H    4.566232    1.462440   -3.067038
 H    4.646409    3.462703   -4.504923
 H    7.404079    1.148244    0.316706
 H    5.092133    1.937663   -0.092472
 H    8.021831   -1.216984   -0.165632
 H    6.311212   -2.786520   -1.070062
 H    3.991531   -1.996616   -1.474251
 H    2.542327    3.212571    0.772463
 H   -0.053553    2.427269    0.492589
 H    0.248714    3.637014    1.736485
 H   -0.641532    0.846666    2.166170
 H   -0.322457    2.050987    3.412210
 H    1.193151    0.762501    5.002408
 H    2.405422   -0.376038    4.367364
 H    0.672582   -0.687114    4.120295
 H    2.710544    4.153861    3.418871
 H    2.480563    2.985718    4.732787
 H    1.089665    3.535878    3.784542
 H    4.531183    2.677802    2.764198
 H    4.271040    1.028863    2.170668
 H    4.131871    1.381861    3.907826
 H    4.701335   -0.949732    1.677602
 H    4.928374   -2.524870    2.459258
 H    4.154340   -1.197438    3.348888
 H    0.542806   -5.630016    1.319323
 H    0.027808   -4.950161   -0.240773
 H   -0.897111   -4.594834    1.231580
 H   -0.423579   -4.004861   -3.735509
 H    0.252277   -2.373697   -2.001962
 H   -2.579652   -5.238717   -3.524415
 H   -4.055386   -4.817903   -1.561088
 H   -3.359218   -3.236712    0.203203
 H   -5.148897   -1.004000    2.948799
 H   -3.633289   -0.699538    1.025849
 H   -4.350495   -2.157110    5.010261
 H   -2.019248   -3.036223    5.106142
 H   -0.516220   -2.793363    3.164377
Cu   -1.199765    0.448965   -0.599508
 H    0.147494    1.295502   -2.831426
 H   -2.744746    2.038810   -2.196050
 H   -1.244133    2.854113   -1.580075
121
Figure 1_ts(CuBadd)_minor02_05 / electronic energy: -4987.94907131 a.u. / lowest freq: -186.32 cm-1
 B   -1.623807    2.237244   -0.105564
 O   -1.166091    3.540078   -0.227424
 O   -2.791934    2.231033    0.645943
 C   -1.960968    4.417328    0.589964
 C   -3.271055    3.576496    0.804210
 C   -2.159745    5.730501   -0.152036
 C   -1.200406    4.669896    1.889749
 C   -4.324400    3.818707   -0.275937
 C   -3.903578    3.714718    2.180812
 H   -3.899394    3.748516   -1.287858
 H   -4.791459    4.808733   -0.170105
 H   -5.113289    3.056752   -0.188534
 H   -3.224553    3.377593    2.974682
 H   -4.817772    3.104351    2.232352
 H   -4.184614    4.760343    2.378577
 H   -1.054449    3.741060    2.458458
 H   -1.730207    5.391576    2.528298
 H   -0.209690    5.084465    1.653529
 H   -2.575504    5.574293   -1.156078
 H   -1.192614    6.243543   -0.263284
 H   -2.833649    6.396783    0.407600
 C   -3.625362   -1.706538   -3.101571
 C   -4.846595   -2.351452   -2.934420
 C   -3.255413   -0.606540   -2.298518
 C   -5.746430   -1.935325   -1.948882
 C   -4.170562   -0.212771   -1.293280
 C   -5.389965   -0.865076   -1.127290
 C   -2.006122    0.109789   -2.524815
 C   -1.861383    1.467753   -2.102785
 H   -6.072262   -0.529847   -0.340604
 H   -3.916946    0.617231   -0.629156
 H   -6.705157   -2.443231   -1.819907
 H   -5.100695   -3.195090   -3.582545
 H   -2.938490   -2.046528   -3.882242
 P    1.543541    0.572831   -1.352201
 C    1.480304    3.229289   -2.162875
 C    1.865897    4.349096   -2.898784
 C    2.119872    1.996062   -2.362403
 C    2.879070    4.248683   -3.852897
 C    3.133052    1.901845   -3.323856
 C    3.508556    3.022636   -4.065249
 C    2.173329   -2.721958   -3.693474
 C    1.609738   -1.619611   -3.050352
 C    2.358298   -0.869886   -2.135745
 C    3.491650   -3.086590   -3.424204
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 C    4.246762   -2.341478   -2.516871
 C    3.683890   -1.239453   -1.877164
 C    2.667008    2.143494    0.878681
 C    2.388356    0.793672    0.235942
 C    2.549199   -0.146253    1.188175
 C    1.455882    2.402443    1.810372
 C    1.622122    1.309202    2.885915
 C    2.951974    0.589228    2.480113
 C    3.568494   -0.209578    3.609136
 C    3.782445    1.780236    1.893460
 C    4.099799    2.882733    2.909446
 C    5.105292    1.398114    1.225972
 C    2.248749   -1.596444    1.171176
 C    3.253789   -2.523865    1.321771
 C    0.924087   -2.203194    1.178989
 S    2.605255   -4.102812    1.558360
 C    0.972386   -3.559366    1.447753
 C    4.736549   -2.336329    1.272006
 C   -0.099855   -4.579306    1.694727
 P   -0.645879   -1.323016    0.771259
 C   -3.475731   -4.170660   -0.300913
 C   -2.850512   -3.108971    0.356825
 C   -2.854120   -4.795625   -1.378699
 C   -1.592235   -2.670825   -0.057072
 C   -1.613427   -4.332862   -1.822050
 C   -0.992871   -3.270924   -1.172158
 C   -1.607775   -1.391564    4.800993
 C   -0.951995   -1.618294    3.591217
 C   -2.789149   -0.650966    4.830101
 C   -1.468615   -1.099781    2.397411
 C   -3.306419   -0.127252    3.645149
 C   -2.644793   -0.339764    2.436892
 H    0.676107    3.321773   -1.426087
 H    1.362535    5.304219   -2.729996
 H    3.174432    5.125122   -4.434887
 H    3.636578    0.949273   -3.501781
 H    4.299148    2.934949   -4.814384
 H    1.574645   -3.302200   -4.399428
 H    0.570211   -1.346738   -3.247167
 H    3.933079   -3.954322   -3.920093
 H    5.282113   -2.619909   -2.306333
 H    4.279726   -0.663261   -1.167359
 H    2.895788    2.963849    0.185755
 H    0.512798    2.325121    1.259398
 H    1.506228    3.412312    2.239372
 H    0.785940    0.595903    2.903882
 H    1.702567    1.730722    3.899433
 H    3.721052    0.436996    4.487321
 H    4.543585   -0.637495    3.338131
 H    2.911828   -1.037478    3.919349
 H    4.433331    3.793846    2.387095
 H    4.923620    2.565928    3.568704
 H    3.257801    3.162141    3.555367
 H    5.597717    2.300032    0.829579
 H    4.978034    0.702740    0.387468
 H    5.797616    0.941811    1.951699
 H    4.984124   -1.274745    1.162664
 H    5.168943   -2.869649    0.410430
 H    5.232423   -2.716131    2.178577
 H    0.273515   -5.363220    2.369866
 H   -0.430974   -5.067428    0.765621
 H   -0.979309   -4.126077    2.167671
 H   -4.456524   -4.510407    0.039767
 H   -3.340744   -2.649775    1.217771
 H   -3.342355   -5.631666   -1.884984
 H   -1.123286   -4.803805   -2.677682
 H   -0.013501   -2.928472   -1.513093
 H   -1.190433   -1.797771    5.725355
 H   -0.024935   -2.195500    3.582845
 H   -3.302566   -0.475628    5.778515
 H   -4.225316    0.463591    3.659964
 H   -3.035062    0.112753    1.523923
Cu   -0.748389    0.456831   -0.730442
 H   -1.371520   -0.248860   -3.339671
 H   -2.789641    2.016378   -1.898149
 H   -1.133467    2.084596   -2.640713
121
Figure 1_ts(CuBadd)_minor02_06 / electronic energy: -4987.93299261 a.u. / lowest freq: -157.28 cm-1
 B   -1.511900    2.150747    0.936081
 O   -0.697609    2.989332    1.666130
 O   -2.835345    2.302644    1.327902
 C   -1.456483    3.526870    2.762066
 C   -2.923193    3.433762    2.215818
 C   -0.972272    4.937135    3.057386
 C   -1.209422    2.621898    3.969292
 C   -3.317800    4.642177    1.369322
 C   -3.981570    3.157816    3.270816
 H   -2.553319    4.866135    0.610300
 H   -3.466721    5.540381    1.986136
 H   -4.260862    4.424184    0.846324
 H   -3.801841    2.204597    3.785826
 H   -4.974181    3.104602    2.799494
 H   -4.002508    3.962243    4.021558
 H   -1.563553    1.596978    3.782270
 H   -1.703552    3.005059    4.874052
 H   -0.127808    2.573594    4.163270
 H   -0.985725    5.568315    2.159102
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H	0.061672	4.903392	3.432235
H	-1.597512	5.410543	3.829615
C	-2.535915	0.947501	-4.305042
C	-3.749619	0.758110	-4.957826
C	-2.476573	1.291706	-2.936491
C	-4.957337	0.888747	-4.267204
C	-3.709249	1.412282	-2.253137
C	-4.921714	1.210362	-2.908682
C	-1.194630	1.527021	-2.281530
C	-1.085565	2.445205	-1.168753
H	-5.855623	1.303700	-2.347200
H	-3.713022	1.652387	-1.185239
H	-5.911066	0.737184	-4.778192
H	-3.754339	0.505001	-6.022031
H	-1.599951	0.841168	-4.861928
P	3.085821	0.086432	-1.379646
C	2.063574	2.201058	-2.856302
C	1.739253	3.525698	-3.156980
C	2.584653	1.853291	-1.604603
C	1.925589	4.520774	-2.201017
C	2.797401	2.871523	-0.662365
C	2.458185	4.190444	-0.952622
C	7.157320	-0.244867	-0.608846
C	5.770737	-0.382741	-0.527953
C	4.922358	0.340108	-1.374704
C	7.723064	0.617057	-1.546181
C	6.889347	1.338657	-2.401990
C	5.505153	1.200866	-2.318714
C	3.137678	0.400158	1.631442
C	2.720081	-0.330275	0.360593
C	1.931767	-1.359603	0.749984
C	1.847288	1.118125	2.120550
C	0.964553	-0.055503	2.597887
C	1.834140	-1.309866	2.291067
C	1.408728	-2.587963	2.981957
C	3.257592	-0.761733	2.657034
C	3.418642	-0.285043	4.106173
C	4.379129	-1.770762	2.415304
C	1.318157	-2.462919	-0.036640
C	2.096722	-3.474459	-0.552235
C	-0.107511	-2.753847	-0.161761
S	1.122075	-4.785686	-1.111963
C	-0.355826	-4.005680	-0.688710
C	3.584181	-3.621761	-0.637250
C	-1.627214	-4.758050	-0.947123
P	-1.409614	-1.505384	0.139897
C	-3.494910	-2.288736	-3.295977
C	-2.489021	-1.995810	-2.382110
C	-4.805362	-2.484825	-2.857403
C	-2.774209	-1.932441	-1.012934
C	-5.101098	-2.388516	-1.499803
C	-4.089829	-2.115043	-0.577996
C	-3.372480	-1.109704	3.715039
C	-2.777193	-0.858536	2.479262
C	-3.312101	-2.385039	4.275716
C	-2.122672	-1.885471	1.788578
C	-2.662188	-3.412624	3.591744
C	-2.073531	-3.165887	2.352203
H	1.912211	1.424580	-3.611045
H	1.326142	3.773540	-4.137331
H	1.662408	5.556718	-2.427350
H	3.249876	2.644237	0.302709
H	2.617084	4.967305	-0.201023
H	7.795511	-0.817063	0.069107
H	5.348564	-1.057836	0.214555
H	8.807942	0.728633	-1.611165
H	7.318790	2.019171	-3.141429
H	4.873830	1.780938	-2.996646
H	4.021050	1.046661	1.534412
H	1.364659	1.684662	1.316897
H	2.064081	1.834816	2.925590
H	0.002455	-0.083376	2.074203
H	0.741448	-0.006349	3.673973
H	1.478393	-2.475726	4.075336
H	2.039596	-3.439927	2.683695
H	0.368483	-2.845190	2.746481
H	4.409972	0.180070	4.230313
H	3.373319	-1.137511	4.802209
H	2.672977	0.448310	4.434854
H	5.364550	-1.287594	2.506255
H	4.320285	-2.255127	1.436503
H	4.338362	-2.566093	3.175703
H	4.075347	-2.645299	-0.710986
H	3.868803	-4.195476	-1.531348
H	3.992082	-4.151596	0.238243
H	-1.473401	-5.832287	-0.766936
H	-1.968304	-4.637767	-1.986924
H	-2.438573	-4.420486	-0.292630
H	-3.258471	-2.347785	-4.360319
H	-1.468757	-1.823332	-2.735470
H	-5.596664	-2.702124	-3.578485
H	-6.126216	-2.529568	-1.149299
H	-4.334452	-2.057560	0.484462
H	-3.883472	-0.300569	4.242492
H	-2.829564	0.144650	2.048310
H	-3.772655	-2.578887	5.247309
H	-2.608472	-4.413212	4.026609

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 H   -1.559633   -3.977582    1.832573
Cu   -1.030791    0.645561   -0.358308
 H   -0.308347    1.377953   -2.899229
 H   -1.914798    3.150600   -1.014615
 H   -0.109627    2.923544   -1.030352
121
Figure 1_L-Cu-alkyl_minor02_01 / electronic energy: -4988.00284447 a.u. / lowest freq: 18.49 cm-1
 B   -3.578268    1.551810   -1.214751
 O   -3.156644    2.597694   -0.431966
 O   -4.781004    1.050351   -0.774457
 C   -4.043185    2.722389    0.694406
 C   -5.327774    1.966158    0.189676
 C   -4.255365    4.198256    0.994274
 C   -3.377943    2.041484    1.886392
 C   -6.301432    2.872437   -0.563558
 C   -6.068516    1.187659    1.263448
 H   -5.790460    3.448508   -1.349548
 H   -6.806715    3.576495    0.113021
 H   -7.068691    2.249721   -1.046580
 H   -5.425420    0.431173    1.728623
 H   -6.935896    0.675254    0.821076
 H   -6.437725    1.866012    2.047427
 H   -3.160005    0.985101    1.676616
 H   -4.005240    2.097610    2.787525
 H   -2.429967    2.547810    2.104261
 H   -4.581119    4.753525    0.104999
 H   -3.313651    4.645188    1.346377
 H   -5.008790    4.328799    1.785899
 C   -1.670843   -2.493996   -3.142153
 C   -2.166175   -3.789365   -3.202870
 C   -2.400768   -1.431897   -2.549476
 C   -3.421205   -4.100122   -2.666012
 C   -3.668800   -1.769237   -2.025695
 C   -4.160130   -3.076125   -2.077484
 C   -1.829329   -0.068294   -2.507587
 C   -2.837930    1.102003   -2.527638
 H   -5.146795   -3.289505   -1.654704
 H   -4.285137   -0.993440   -1.567487
 H   -3.811595   -5.119786   -2.710254
 H   -1.566282   -4.571625   -3.676389
 H   -0.685931   -2.279071   -3.570597
 P    1.787282    0.765872   -1.344448
 C    3.284802    2.663744   -2.854451
 C    3.396203    3.720870   -3.755213
 C    2.030268    2.107201   -2.573864
 C    2.256893    4.231188   -4.382038
 C    0.894440    2.617718   -3.210905
 C    1.006296    3.678950   -4.110010
 C    4.376685   -2.015704   -2.820922
 C    3.272740   -1.197912   -2.591370
 C    3.289162   -0.256179   -1.552072
 C    5.505044   -1.909336   -2.005972
 C    5.530030   -0.972304   -0.973675
 C    4.429624   -0.144222   -0.750558
 C    1.398727    3.053179    0.398790
 C    1.935799    1.640420    0.232804
 C    2.103805    1.127493    1.469618
 C   -0.059453    2.850491    0.891606
 C    0.150715    2.270963    2.308391
 C    1.705071    2.228351    2.467705
 C    2.159397    2.096651    3.906196
 C    2.131667    3.512592    1.682995
 C    1.600770    4.820229    2.277501
 C    3.640853    3.682837    1.490055
 C    2.384641   -0.258356    1.908926
 C    3.544825   -0.582603    2.572674
 C    1.454500   -1.375161    1.837362
 S    3.493584   -2.210845    3.144667
 C    1.917663   -2.491960    2.502796
 C    4.767607    0.247004    2.805768
 C    1.288761   -3.833413    2.722915
 P   -0.079596   -1.373122    0.830810
 C   -0.845346   -5.271978   -0.424505
 C   -0.991697   -4.037510    0.208465
 C    0.269657   -5.531703   -1.218414
 C   -0.016415   -3.048548    0.060019
 C    1.241188   -4.543172   -1.383140
 C    1.096105   -3.311552   -0.751277
 C   -2.401884   -1.326560    4.255186
 C   -1.293156   -1.304572    3.407343
 C   -3.680299   -1.525919    3.735418
 C   -1.460135   -1.452831    2.026572
 C   -3.852003   -1.675916    2.358507
 C   -2.753209   -1.608155    1.505996
 H    4.181255    2.271398   -2.366891
 H    4.377171    4.152343   -3.967931
 H    2.347042    5.059038   -5.089456
 H   -0.084113    2.181895   -2.993078
 H    0.112388    4.072610   -4.599241
 H    4.351908   -2.746627   -3.632388
 H    2.383929   -1.297825   -3.221868
 H    6.367298   -2.557714   -2.178207
 H    6.414172   -0.880679   -0.338298
 H    4.458484    0.595480    0.050759
 H    1.499196    3.708676   -0.476351
 H   -0.623824    2.177518    0.229193
 H   -0.607524    3.803003    0.908407
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 H   -0.284541    1.268790    2.434782
 H   -0.294117    2.908702    3.087412
 H    1.732306    2.910215    4.513269
 H    3.252831    2.145200    4.006603
 H    1.822636    1.144977    4.346290
 H    1.752210    5.646603    1.564707
 H    2.154045    5.075625    3.195227
 H    0.533692    4.798444    2.532900
 H    3.844244    4.585673    0.892725
 H    4.105638    2.834906    0.970406
 H    4.148667    3.812983    2.459228
 H    4.645309    1.241673    2.359932
 H    5.654904   -0.218432    2.347884
 H    4.979924    0.376922    3.878276
 H    0.200814   -3.745006    2.839416
 H    1.687781   -4.305523    3.632412
 H    1.483385   -4.513135    1.878331
 H   -1.615668   -6.035665   -0.294945
 H   -1.868755   -3.865826    0.834105
 H    0.380753   -6.500040   -1.711891
 H    2.121118   -4.730780   -2.003346
 H    1.871766   -2.552308   -0.874449
 H   -2.260666   -1.198706    5.330876
 H   -0.292975   -1.172502    3.827223
 H   -4.544092   -1.559031    4.403568
 H   -4.848539   -1.829855    1.939091
 H   -2.902014   -1.682749    0.425056
Cu   -0.354592   -0.123317   -1.105101
 H   -1.190832    0.034866   -3.404309
 H   -3.617822    0.929544   -3.301109
 H   -2.292550    2.004588   -2.857285
121
Figure 1_L-Cu-alkyl_minor02_02 / electronic energy: -4988.00460427 a.u. / lowest freq: 19.49 cm-1
 B    3.635258   -1.383737   -1.047351
 O    4.512845   -2.443076   -1.073882
 O    3.390843   -0.967894    0.240420
 C    4.721887   -2.884610    0.277871
 C    4.365879   -1.595138    1.096302
 C    6.155270   -3.363199    0.437785
 C    3.747839   -4.034432    0.531110
 C    5.543719   -0.627884    1.216755
 C    3.764619   -1.852569    2.466476
 H    6.021275   -0.446442    0.242397
 H    6.305861   -1.004325    1.914101
 H    5.177726    0.335771    1.599557
 H    2.843137   -2.441001    2.404981
 H    3.524685   -0.898301    2.957012
 H    4.482943   -2.392437    3.102095
 H    2.704764   -3.699055    0.437305
 H    3.885771   -4.475390    1.529131
 H    3.919559   -4.821126   -0.218404
 H    6.875820   -2.612359    0.088192
 H    6.311208   -4.281231   -0.147988
 H    6.370101   -3.593245    1.492518
 C    2.331692    2.902608   -2.841163
 C    2.924647    4.147072   -2.661078
 C    2.756696    1.753323   -2.131116
 C    3.977491    4.313898   -1.755946
 C    3.834255    1.947635   -1.236748
 C    4.422132    3.197742   -1.047174
 C    2.108141    0.441595   -2.349543
 C    3.059445   -0.768396   -2.368832
 H    5.246174    3.296138   -0.333650
 H    4.204879    1.098728   -0.661620
 H    4.442680    5.292143   -1.611710
 H    2.558816    5.002620   -3.235887
 H    1.511282    2.802428   -3.559368
 P   -1.335052   -1.206640   -1.338737
 C    0.064161   -3.314371   -2.463533
 C    0.233253   -4.551236   -3.085120
 C   -1.217574   -2.791336   -2.256496
 C   -0.881307   -5.269082   -3.518485
 C   -2.331547   -3.514940   -2.697957
 C   -2.162186   -4.747250   -3.327818
 C   -3.935291    1.039490   -3.540363
 C   -2.793867    0.424616   -3.028072
 C   -2.888067   -0.453143   -1.939586
 C   -5.180563    0.789188   -2.963562
 C   -5.282713   -0.088526   -1.883872
 C   -4.143178   -0.710468   -1.376769
 C   -0.956461   -3.004232    0.916232
 C   -1.638733   -1.767667    0.355153
 C   -2.120272   -1.063546    1.400740
 C    0.339551   -2.472552    1.579454
 C   -0.209875   -1.658772    2.771203
 C   -1.761252   -1.853349    2.671804
 C   -2.489028   -1.511465    3.955281
 C   -1.851521   -3.323667    2.140331
 C   -1.272838   -4.371193    3.096955
 C   -3.251749   -3.799706    1.745053
 C   -2.734202    0.284246    1.435816
 C   -4.051919    0.466116    1.784130
 C   -2.038892    1.540891    1.201898
 S   -4.439450    2.145163    1.864936
 C   -2.840809    2.639468    1.438210
 C   -5.122993   -0.551886    2.015761
 C   -2.554149    4.111244    1.418483
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 P   -0.312092    1.597805    0.579849
 C    0.543878    5.455141   -0.677768
 C    0.558812    4.271714    0.060380
 C   -0.263280    5.571050   -1.808157
 C   -0.244830    3.195637   -0.322884
 C   -1.042475    4.486254   -2.214390
 C   -1.026253    3.303196   -1.480738
 C    1.043228    2.599708    4.358142
 C    0.195460    2.363662    3.276850
 C    2.414664    2.373888    4.233727
 C    0.713798    1.889430    2.065681
 C    2.933031    1.890384    3.032395
 C    2.085997    1.631210    1.955342
 H    0.935882   -2.745855   -2.128837
 H    1.238896   -4.951023   -3.235063
 H   -0.752371   -6.235811   -4.010969
 H   -3.338954   -3.117465   -2.550965
 H   -3.036997   -5.304793   -3.670833
 H   -3.849650    1.724572   -4.386939
 H   -1.817593    0.630612   -3.476729
 H   -6.074465    1.277758   -3.358246
 H   -6.256690   -0.290125   -1.431597
 H   -4.227867   -1.397223   -0.532880
 H   -0.803064   -3.827230    0.205734
 H    0.944239   -1.868047    0.886987
 H    0.967463   -3.310869    1.912707
 H    0.052365   -0.593719    2.723598
 H    0.164779   -2.034545    3.735280
 H   -2.077797   -2.094935    4.793686
 H   -3.565985   -1.723177    3.896951
 H   -2.368166   -0.445451    4.204409
 H   -1.121227   -5.325492    2.567561
 H   -1.979601   -4.564414    3.919423
 H   -0.314544   -4.087990    3.550210
 H   -3.200659   -4.833682    1.368382
 H   -3.706413   -3.188684    0.954784
 H   -3.929789   -3.802087    2.613688
 H   -4.713735   -1.564342    1.924682
 H   -5.929612   -0.450321    1.271849
 H   -5.580170   -0.452052    3.012457
 H   -3.299098    4.656582    2.015741
 H   -2.578545    4.521778    0.397604
 H   -1.564365    4.326263    1.839933
 H    1.173062    6.291854   -0.365503
 H    1.190282    4.199856    0.948479
 H   -0.275641    6.501628   -2.380513
 H   -1.667965    4.560622   -3.107261
 H   -1.649172    2.462267   -1.796967
 H    0.630582    2.968263    5.300241
 H   -0.877055    2.544670    3.380618
 H    3.080486    2.569203    5.077751
 H    4.005011    1.704186    2.935170
 H    2.487462    1.210464    1.029137
Cu    0.489316    0.209984   -1.141418
 H    1.613250    0.490959   -3.337785
 H    3.953909   -0.573173   -3.004796
 H    2.564919   -1.609864   -2.888839
121
Figure 1_L-Cu-alkyl_minor02_03 / electronic energy: -4987.99535033 a.u. / lowest freq: 13.37 cm-1
 B   -3.622429   -2.108342    0.741907
 O   -3.241674   -2.816677   -0.371116
 O   -4.838119   -1.495903    0.553915
 C   -4.136149   -2.489631   -1.449226
 C   -5.405029   -1.962850   -0.681273
 C   -4.374058   -3.731811   -2.293148
 C   -3.457718   -1.411663   -2.289043
 C   -6.397555   -3.069521   -0.329658
 C   -6.124316   -0.809359   -1.360836
 H   -5.898002   -3.917111    0.162982
 H   -6.919704   -3.443595   -1.222068
 H   -7.149007   -2.670156    0.367373
 H   -5.465356    0.060266   -1.478568
 H   -6.990289   -0.501468   -0.755983
 H   -6.492581   -1.108963   -2.353614
 H   -3.204823   -0.530074   -1.682359
 H   -4.088985   -1.088438   -3.129060
 H   -2.525479   -1.815086   -2.703194
 H   -4.721613   -4.579268   -1.688261
 H   -3.437046   -4.030614   -2.786298
 H   -5.119365   -3.530411   -3.077489
 C   -1.711441    1.283126    3.618890
 C   -2.228702    2.478272    4.101326
 C   -2.472049    0.405079    2.808303
 C   -3.540972    2.860228    3.802229
 C   -3.799039    0.803953    2.533545
 C   -4.315683    2.008398    3.016702
 C   -1.853916   -0.837402    2.276322
 C   -2.786868   -2.053301    2.070456
 H   -5.348557    2.278360    2.775824
 H   -4.434613    0.165615    1.917463
 H   -3.948894    3.800978    4.180032
 H   -1.599759    3.123402    4.721081
 H   -0.677785    1.012105    3.858522
 P    2.238695   -0.783753    1.246153
 C    0.896627   -3.035672    2.251120
 C    0.679836   -4.087820    3.138307
 C    2.068920   -2.266273    2.318093
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 C    1.623767   -4.382816    4.122413
 C    3.003629   -2.563715    3.319927
 C    2.783064   -3.613790    4.211765
 C    6.342122   -1.249587    0.803410
 C    4.983261   -1.533710    0.915345
 C    4.060213   -0.508630    1.173628
 C    6.796225    0.065196    0.937823
 C    5.887750    1.090579    1.191385
 C    4.526982    0.802457    1.314809
 C    1.465637   -2.757821   -0.945701
 C    1.934996   -1.397654   -0.450370
 C    2.001294   -0.591203   -1.528879
 C   -0.029020   -2.562177   -1.324852
 C    0.058957   -1.625043   -2.550878
 C    1.591142   -1.420261   -2.753836
 C    1.952884   -0.879736   -4.121236
 C    2.144353   -2.826696   -2.343434
 C    1.657976   -3.983699   -3.222194
 C    3.669563   -2.919958   -2.282004
 C    2.321650    0.852020   -1.594177
 C    3.551849    1.305959   -2.009780
 C    1.396662    1.935620   -1.321497
 S    3.565826    3.027998   -2.115946
 C    1.932488    3.179736   -1.590349
 C    4.794145    0.528339   -2.315037
 C    1.332293    4.546566   -1.470807
 P   -0.225679    1.698119   -0.523864
 C    0.834338    3.995510    2.681078
 C    0.763453    3.014320    1.696741
 C   -0.117873    5.015510    2.722035
 C   -0.250220    3.049086    0.728618
 C   -1.142566    5.038970    1.778545
 C   -1.209923    4.061664    0.784440
 C   -3.846049    2.367015   -2.299276
 C   -2.838986    2.093055   -1.377288
 C   -3.523100    2.644612   -3.628723
 C   -1.491588    2.133937   -1.768534
 C   -2.187699    2.661370   -4.028562
 C   -1.174197    2.416059   -3.101202
 H    0.132159   -2.802059    1.507935
 H   -0.239631   -4.673323    3.063156
 H    1.452221   -5.203983    4.822290
 H    3.917475   -1.972806    3.414017
 H    3.526385   -3.829233    4.983160
 H    7.051702   -2.055889    0.603107
 H    4.634464   -2.563375    0.801994
 H    7.861706    0.287402    0.841957
 H    6.235934    2.120926    1.295039
 H    3.816943    1.611406    1.507159
 H    1.663430   -3.605778   -0.277570
 H   -0.614734   -2.127770   -0.501190
 H   -0.506728   -3.521062   -1.568364
 H   -0.445699   -0.660108   -2.395572
 H   -0.387341   -2.075465   -3.450319
 H    1.581150   -1.553022   -4.909374
 H    3.038987   -0.774505   -4.255453
 H    1.497098    0.108732   -4.290298
 H    1.899658   -4.946334   -2.743607
 H    2.173037   -3.965258   -4.195616
 H    0.578960   -3.977832   -3.421794
 H    3.973746   -3.912706   -1.912872
 H    4.116856   -2.169084   -1.621365
 H    4.110068   -2.796441   -3.284425
 H    5.008841   -0.183408   -1.506016
 H    5.665486    1.190354   -2.416470
 H    4.701272   -0.044634   -3.249559
 H    1.815045    5.248105   -2.166550
 H    1.449531    4.949580   -0.452166
 H    0.259158    4.529872   -1.702284
 H    1.633163    3.958747    3.425377
 H    1.505866    2.211194    1.678876
 H   -0.066935    5.784438    3.496333
 H   -1.898798    5.826648    1.808889
 H   -2.008951    4.111333    0.042552
 H   -4.890501    2.349331   -1.980150
 H   -3.102834    1.842775   -0.344831
 H   -4.314701    2.844301   -4.354595
 H   -1.929570    2.871990   -5.068955
 H   -0.128980    2.443305   -3.418765
Cu   -0.841470   -0.046613    0.746386
 H   -1.054759   -1.132316    2.978596
 H   -3.474928   -2.167924    2.934217
 H   -2.156913   -2.960015    2.068100
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Figure 1_L-Cu-alkyl_minor02_04 / electronic energy: -4987.99700051 a.u. / lowest freq: -32.38 cm-1
 B   -3.016917    2.583386   -0.985420
 O   -2.514319    2.473527    0.286403
 O   -4.245688    3.199846   -0.991871
 C   -3.559355    2.804412    1.216383
 C   -4.521973    3.681069    0.334042
 C   -2.977597    3.533967    2.416993
 C   -4.176754    1.483445    1.666974
 C   -4.164340    5.166185    0.353226
 C   -5.999683    3.491237    0.636931
 H   -3.093715    5.323414    0.154230
 H   -4.412066    5.633398    1.317011
 H   -4.733380    5.681889   -0.434328
```

H	-6.316557	2.453269	0.469764
H	-6.603827	4.139446	-0.015251
H	-6.219107	3.759790	1.681455
H	-4.614688	0.933505	0.821511
H	-4.952856	1.630456	2.432368
H	-3.384061	0.854801	2.097886
H	-2.337950	4.374345	2.116265
H	-2.375493	2.842774	3.023781
H	-3.786256	3.920888	3.055663
C	-2.688417	-1.727810	-2.761398
C	-3.654680	-2.723237	-2.729471
C	-2.963642	-0.391793	-2.366815
C	-4.960387	-2.441918	-2.304352
C	-4.297657	-0.126740	-1.982768
C	-5.267120	-1.132442	-1.940541
C	-1.876483	0.611955	-2.333193
C	-2.292733	2.088901	-2.288340
H	-6.283261	-0.878387	-1.623481
H	-4.592426	0.887111	-1.705073
H	-5.719662	-3.226653	-2.270882
H	-3.385573	-3.739925	-3.030575
H	-1.668650	-1.982192	-3.070354
P	3.044801	-0.144247	-1.075530
C	1.733389	-0.814474	-3.413396
C	1.050177	-0.617734	-4.614024
C	2.068271	0.266802	-2.585620
C	0.687392	0.669215	-5.004600
C	1.687932	1.556557	-2.989691
C	1.006699	1.755292	-4.188210
C	6.919292	1.076162	-0.561762
C	5.654391	0.512934	-0.412087
C	4.672860	0.668613	-1.404271
C	7.233998	1.789598	-1.720040
C	6.276412	1.928582	-2.722895
C	5.004860	1.371818	-2.567875
C	2.177867	2.449428	0.237796
C	2.429369	0.946321	0.248845
C	2.110354	0.503122	1.483299
C	0.634239	2.596984	0.250183
C	0.265095	2.068485	1.654018
C	1.642674	1.716920	2.297013
C	1.595442	1.568678	3.803400
C	2.548125	2.846298	1.692364
C	2.127238	4.265077	2.093687
C	4.044002	2.733043	1.983265
C	2.110500	-0.881433	2.017023
C	3.102854	-1.333563	2.855900
C	1.079392	-1.881629	1.800439
S	2.782543	-2.948540	3.381475
C	1.313970	-3.053961	2.490004
C	4.358119	-0.655000	3.304080
C	0.536025	-4.332790	2.533318
P	-0.329388	-1.697556	0.658661
C	1.095432	-4.635267	-1.791698
C	0.944318	-3.501085	-0.998332
C	0.048835	-5.551250	-1.909797
C	-0.251898	-3.267007	-0.305817
C	-1.142807	-5.324158	-1.224165
C	-1.294766	-4.188902	-0.426440
C	-4.254817	-1.918561	1.815171
C	-3.081968	-1.878030	1.065860
C	-4.201536	-1.831322	3.206467
C	-1.834373	-1.795400	1.702746
C	-2.967919	-1.705717	3.843709
C	-1.788327	-1.694833	3.098112
H	2.014127	-1.828727	-3.119443
H	0.797156	-1.475676	-5.241177
H	0.148907	0.827838	-5.941644
H	1.938527	2.423460	-2.378108
H	0.719882	2.766787	-4.484881
H	7.665944	0.952296	0.226484
H	5.422354	-0.056313	0.493537
H	8.226025	2.230866	-1.842221
H	6.515956	2.476651	-3.637510
H	4.270050	1.491963	-3.366484
H	2.702183	3.011477	-0.547229
H	0.162376	2.019987	-0.557785
H	0.327047	3.642946	0.110844
H	-0.399448	1.193688	1.618115
H	-0.252548	2.828030	2.253373
H	1.242771	2.502417	4.268743
H	2.579775	1.329594	4.232389
H	0.897895	0.769707	4.100241
H	2.619679	5.003626	1.440887
H	2.448901	4.477617	3.125612
H	1.046809	4.448972	2.044611
H	4.579933	3.570446	1.509009
H	4.488442	1.810197	1.594722
H	4.242093	2.790625	3.065630
H	5.248553	-1.123773	2.855281
H	4.478350	-0.700088	4.397366
H	4.350059	0.398513	3.008119
H	0.722835	-4.873846	3.472054
H	0.819053	-4.995573	1.699880
H	-0.543822	-4.150015	2.461235
H	2.037504	-4.803294	-2.319065
H	1.772068	-2.791045	-0.909496

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 H    0.164414   -6.441741   -2.531920
 H   -1.965922   -6.038138   -1.303824
 H   -2.235216   -4.041920    0.106297
 H   -5.215849   -1.997331    1.302106
 H   -3.144407   -1.904614   -0.025004
 H   -5.123255   -1.849249    3.792753
 H   -2.917577   -1.621863    4.931848
 H   -0.826879   -1.612530    3.610317
Cu   -0.750176   -0.094879   -0.841388
 H   -1.221276    0.436634   -3.202032
 H   -2.920363    2.370006   -3.159896
 H   -1.377509    2.704436   -2.375082
121
Figure 1_L-Cu-alkyl_major_01 / electronic energy: -4988.00213073 a.u. / lowest freq: 5.51 cm-1
 B   -4.786516   -0.332462   -0.765204
 O   -5.624676   -0.957398    0.124943
 O   -5.444896    0.616008   -1.507697
 C   -6.968114   -0.509271   -0.121271
 C   -6.733526    0.834091   -0.909911
 C   -7.684787   -0.345352    1.210402
 C   -7.654850   -1.586856   -0.958589
 C   -6.600853    2.051778    0.004573
 C   -7.753172    1.111321   -2.003631
 H   -5.863992    1.877991    0.803020
 H   -7.562331    2.323466    0.463842
 H   -6.248167    2.907323   -0.589999
 H   -7.756794    0.322566   -2.767021
 H   -7.515408    2.062826   -2.502067
 H   -8.765138    1.195871   -1.579249
 H   -7.156238   -1.721297   -1.930043
 H   -8.713287   -1.350001   -1.139832
 H   -7.605215   -2.544128   -0.418826
 H   -8.681784    0.098280    1.066853
 H   -7.113027    0.290650    1.898900
 H   -7.815961   -1.328382    1.687164
 C   -2.173292    2.802800    0.502298
 C   -2.312654    3.588612    1.637505
 C   -2.598586    1.449419    0.459344
 C   -2.892831    3.069458    2.802657
 C   -3.209240    0.961017    1.638275
 C   -3.341923    1.750513    2.783060
 C   -2.358472    0.619422   -0.737264
 C   -3.249349   -0.632368   -0.888856
 H   -3.814173    1.321879    3.672306
 H   -3.604449   -0.056389    1.660656
 H   -2.997915    3.684842    3.699268
 H   -1.961957    4.624845    1.617074
 H   -1.703831    3.231380   -0.388019
 P    1.550067    1.384865   -1.068561
 C    0.424418    3.676308   -2.173401
 C    0.375568    5.022485   -2.540767
 C    1.539889    3.166974   -1.501990
 C    1.440582    5.866719   -2.232363
 C    2.612102    4.019353   -1.204816
 C    2.559936    5.363663   -1.564299
 C    5.090415    0.281056   -2.911443
 C    4.186417    0.767785   -1.969412
 C    2.811730    0.736101   -2.228936
 C    4.631238   -0.231628   -4.125778
 C    3.264177   -0.249208   -4.399600
 C    2.358474    0.231642   -3.454146
 C    1.843978    2.318993    1.668210
 C    2.273029    1.338899    0.587573
 C    2.906855    0.317358    1.203277
 C    0.708600    1.584809    2.437392
 C    1.471402    0.452868    3.155363
 C    2.953099    0.657444    2.704207
 C    3.949896   -0.081436    3.573089
 C    3.040242    2.221327    2.650755
 C    2.806669    2.914092    3.996499
 C    4.348894    2.774781    2.079497
 C    3.318467   -0.993077    0.644562
 C    4.636280   -1.366764    0.541641
 C    2.407406   -2.034022    0.187691
 S    4.775106   -2.969207   -0.087133
 C    3.063931   -3.177088   -0.215202
 C    5.871751   -0.578613    0.840751
 C    2.548816   -4.496002   -0.707525
 P    0.597848   -1.763932    0.151421
 C   -0.094181   -3.391103   -3.538038
 C    0.440241   -2.672419   -2.472281
 C   -1.130247   -4.301237   -3.319397
 C   -0.043840   -2.862024   -1.170760
 C   -1.623659   -4.486263   -2.028794
 C   -1.085609   -3.770357   -0.958236
 C   -1.725734   -2.486500    3.425854
 C   -1.200543   -1.985332    2.236423
 C   -1.059926   -3.507623    4.103668
 C   -0.014669   -2.507675    1.707464
 C    0.131149   -4.023320    3.589643
 C    0.654129   -3.525977    2.396709
 H   -0.414248    3.013688   -2.404892
 H   -0.501959    5.412242   -3.061642
 H    1.399830    6.922540   -2.510646
 H    3.489224    3.631440   -0.679901
 H    3.395459    6.024355   -1.321136
 H    6.161603    0.303461   -2.697006
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 H    4.552170    1.167082   -1.021391
 H    5.342495   -0.614885   -4.861255
 H    2.897780   -0.643878   -5.350187
 H    1.286213    0.212849   -3.669855
 H    1.577998    3.327051    1.323011
 H   -0.061696    1.212854    1.744881
 H    0.205826    2.261615    3.142481
 H    1.117063   -0.549818    2.887518
 H    1.391390    0.532445    4.249860
 H    3.785267    0.164747    4.633667
 H    4.991043    0.173519    3.329853
 H    3.834732   -1.171735    3.467204
 H    2.693221    3.999378    3.845051
 H    3.672962    2.764734    4.660266
 H    1.916546    2.563426    4.533225
 H    4.297891    3.873381    2.015296
 H    4.573802    2.394153    1.074891
 H    5.198034    2.526563    2.736471
 H    5.612622    0.452499    1.109994
 H    6.539504   -0.539848   -0.034281
 H    6.444518   -1.016453    1.673265
 H    2.390118   -4.487079   -1.797217
 H    1.590697   -4.750339   -0.237349
 H    3.262778   -5.300339   -0.478669
 H    0.301880   -3.238749   -4.544991
 H    1.255011   -1.966475   -2.650321
 H   -1.553737   -4.862682   -4.155358
 H   -2.435008   -5.195494   -1.848713
 H   -1.484666   -3.927470    0.046520
 H   -2.649413   -2.066089    3.830435
 H   -1.700846   -1.163168    1.720486
 H   -1.464939   -3.898174    5.040329
 H    0.659385   -4.817090    4.123220
 H    1.594780   -3.925759    2.011007
Cu   -0.374823    0.213803   -0.620787
 H   -2.981048   -1.421788   -0.164886
 H   -3.056104   -1.085134   -1.878456
 H   -2.468249    1.255722   -1.632745
121
Figure 1_L-Cu-alkyl_major_02 / electronic energy: -4988.00326436 a.u. / lowest freq: 12.36 cm-1
 B   -4.711635    0.088273    1.441576
 O   -5.563565    1.140317    1.216158
 O   -5.361493   -1.120036    1.373267
 C   -6.902401    0.624904    1.108625
 C   -6.647991   -0.892202    0.775538
 C   -7.645044    1.394219    0.027143
 C   -7.576160    0.836754    2.463272
 C   -6.497458   -1.156544   -0.723285
 C   -7.659346   -1.854247    1.377977
 H   -5.780759   -0.460882   -1.184874
 H   -7.459889   -1.072786   -1.248724
 H   -6.110029   -2.175709   -0.868528
 H   -7.678510   -1.791837    2.474084
 H   -7.400100   -2.887511    1.102688
 H   -8.670293   -1.646029    0.996065
 H   -7.062381    0.278431    3.260150
 H   -8.631922    0.529342    2.445220
 H   -7.534627    1.905982    2.718895
 H   -8.636588    0.951819   -0.153268
 H   -7.086335    1.404359   -0.917869
 H   -7.792271    2.437570    0.344024
 C   -2.646938   -1.228770   -1.857871
 C   -2.943009   -0.957855   -3.188440
 C   -2.785778   -0.251927   -0.840163
 C   -3.405090    0.304670   -3.577368
 C   -3.271216    1.011280   -1.258099
 C   -3.568399    1.281145   -2.593069
 C   -2.392376   -0.546516    0.553439
 C   -3.160581    0.220889    1.654310
 H   -3.935094    2.275124   -2.866419
 H   -3.422020    1.799105   -0.517800
 H   -3.636794    0.518239   -4.623563
 H   -2.814468   -1.746862   -3.935635
 H   -2.283488   -2.223726   -1.582515
 P    0.738742    1.669217   -0.461058
 C    0.745679    4.461663   -1.031233
 C    0.207647    5.744350   -0.946483
 C    0.085887    3.381721   -0.431618
 C   -0.992350    5.958489   -0.264241
 C   -1.115450    3.603168    0.248733
 C   -1.653293    4.887545    0.335521
 C    0.952938    0.841954   -4.436459
 C    0.526302    1.017126   -3.121699
 C    1.416567    1.486220   -2.145440
 C    2.276833    1.116284   -4.782269
 C    3.166494    1.586539   -3.815600
 C    2.736450    1.781090   -2.503234
 C    1.909223    2.438975    2.052484
 C    2.104185    1.726587    0.721833
 C    3.165479    0.904068    0.859726
 C    1.372325    1.336000    3.008354
 C    2.599642    0.411414    3.162589
 C    3.699795    1.102060    2.289729
 C    5.102793    0.625147    2.601486
 C    3.373834    2.614428    2.524050
 C    3.522737    3.072094    3.978165
 C    4.172827    3.593596    1.659400
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 C     3.666383   -0.171280   -0.028032
 C     4.895420   -0.098171   -0.637757
 C     2.999293   -1.441088   -0.269256
 S     5.256838   -1.567067   -1.471851
 C     3.767903   -2.313292   -1.011648
 C     5.854981    1.047735   -0.695489
 C     3.520427   -3.726927   -1.443225
 P     1.280287   -1.748626    0.275578
 C     0.065186   -3.142710   -3.376644
 C     0.674833   -2.414895   -2.359098
 C    -0.654583   -4.300453   -3.075727
 C     0.587231   -2.841864   -1.027262
 C    -0.755464   -4.723633   -1.750994
 C    -0.138493   -3.999219   -0.729506
 C     0.338954   -3.588609    3.797158
 C     0.301155   -2.840529    2.621874
 C     1.496736   -4.285516    4.143867
 C     1.414761   -2.797441    1.771404
 C     2.614325   -4.234089    3.310239
 C     2.575015   -3.494496    2.128702
 H     1.684536    4.302852   -1.568448
 H     0.725405    6.583218   -1.417681
 H    -1.413985    6.964637   -0.202738
 H    -1.629565    2.757550    0.712523
 H    -2.594313    5.048009    0.866702
 H     0.248935    0.476380   -5.187612
 H    -0.506629    0.776360   -2.850981
 H     2.616632    0.964345   -5.809581
 H     4.202526    1.806147   -4.084254
 H     3.433500    2.158017   -1.752690
 H     1.300778    3.353008    2.018889
 H     0.498543    0.823954    2.572635
 H     1.053512    1.766771    3.968375
 H     2.416461   -0.613798    2.815421
 H     2.930829    0.334434    4.209010
 H     5.321043    0.764408    3.671866
 H     5.865852    1.173600    2.030988
 H     5.219538   -0.446874    2.378081
 H     3.040429    4.052896    4.117169
 H     4.588124    3.195257    4.229104
 H     3.091090    2.383296    4.715465
 H     3.872528    4.628440    1.888166
 H     4.022459    3.440398    0.583148
 H     5.251310    3.513622    1.870655
 H     5.448008    1.911316   -0.155553
 H     6.039158    1.358734   -1.736102
 H     6.829631    0.793819   -0.250526
 H     3.043061   -3.771330   -2.434622
 H     2.862160   -4.248959   -0.737543
 H     4.466675   -4.284573   -1.500700
 H     0.146497   -2.796485   -4.409756
 H     1.231627   -1.507558   -2.606423
 H    -1.139468   -4.868936   -3.872723
 H    -1.318635   -5.627262   -1.505871
 H    -0.227574   -4.345412    0.302845
 H    -0.535679   -3.615344    4.451192
 H    -0.596533   -2.272709    2.360525
 H     1.531487   -4.862133    5.071286
 H     3.526536   -4.770342    3.582104
 H     3.461679   -3.447967    1.492428
Cu    -0.421707   -0.151943    0.294664
 H    -2.881579    1.287707    1.705306
 H    -2.879501   -0.196747    2.637167
 H    -2.511123   -1.629468    0.727648
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Figure 1_L-Cu-alkyl_major_03 / electronic energy: -4988.00032240 a.u. / lowest freq: 13.63 cm-1
 B    -4.701898   -0.559022   -0.655350
 O    -5.470086   -0.963108    0.407775
 O    -5.430223    0.170544   -1.563085
 C    -6.834979   -0.587515    0.158563
 C    -6.681865    0.520669   -0.951885
 C    -7.453366   -0.097960    1.459408
 C    -7.565103   -1.836928   -0.330868
 C    -6.520730    1.927710   -0.375072
 C    -7.774161    0.514036   -2.009929
 H    -5.739475    1.959186    0.398005
 H    -7.461061    2.300069    0.057364
 H    -6.219168    2.611431   -1.182176
 H    -7.810236   -0.438932   -2.553985
 H    -7.587555    1.314063   -2.741754
 H    -8.759188    0.694713   -1.553534
 H    -7.130505   -2.217121   -1.267411
 H    -8.635375   -1.644972   -0.495155
 H    -7.471299   -2.626624    0.429381
 H    -8.471918    0.283285    1.290906
 H    -6.851603    0.698272    1.916687
 H    -7.515573   -0.929340    2.177541
 C    -2.869752    2.910838   -0.187138
 C    -3.240690    3.885760    0.733258
 C    -2.800274    1.538235    0.152243
 C    -3.581177    3.537832    2.044136
 C    -3.181051    1.213142    1.475073
 C    -3.555634    2.187810    2.398298
 C    -2.365769    0.519929   -0.830255
 C    -3.157313   -0.815433   -0.780583
 H    -3.838747    1.884482    3.410736
 H    -3.206626    0.165624    1.781323
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 H   -3.876370    4.301321    2.767617
 H   -3.281070    4.933217    0.419463
 H   -2.639242    3.206081   -1.215584
 P    1.615186    1.414408   -1.033781
 C    2.750148    3.924086   -1.804022
 C    2.685669    5.305002   -1.984503
 C    1.621958    3.219492   -1.367055
 C    1.497821    5.993026   -1.727847
 C    0.433996    3.913988   -1.118509
 C    0.371337    5.296200   -1.292532
 C    3.187718   -0.187757   -4.442801
 C    2.325750    0.319529   -3.471548
 C    2.823259    0.750625   -2.234511
 C    4.555739   -0.271757   -4.184408
 C    5.060161    0.167456   -2.959973
 C    4.199676    0.680146   -1.990744
 C    2.008027    2.317943    1.692966
 C    2.373551    1.317735    0.608003
 C    2.977950    0.271797    1.211580
 C    0.843710    1.636208    2.466427
 C    1.561734    0.466714    3.173919
 C    3.050051    0.605351    2.713008
 C    4.017446   -0.180285    3.573947
 C    3.205919    2.162699    2.663226
 C    3.019764    2.859628    4.014062
 C    4.526001    2.667785    2.073949
 C    3.352281   -1.040846    0.633188
 C    4.660435   -1.444926    0.515846
 C    2.414717   -2.041123    0.144114
 S    4.756446   -3.026055   -0.170496
 C    3.040652   -3.183745   -0.305737
 C    5.916648   -0.697631    0.833569
 C    2.491682   -4.468213   -0.850255
 P    0.612107   -1.727037    0.163443
 C   -0.340292   -3.237237   -3.513131
 C    0.247597   -2.530925   -2.467253
 C   -1.295301   -4.219871   -3.244399
 C   -0.097817   -2.807875   -1.137460
 C   -1.652192   -4.491292   -1.924355
 C   -1.058130   -3.789436   -0.874689
 C   -1.605532   -2.462272    3.510489
 C   -1.110854   -1.948802    2.313536
 C   -0.935162   -3.506858    4.146772
 C    0.045911   -2.481042    1.733127
 C    0.228668   -4.032728    3.583159
 C    0.719313   -3.523091    2.381392
 H    3.685825    3.397172   -2.006711
 H    3.569401    5.848073   -2.327886
 H    1.450970    7.075053   -1.872385
 H   -0.446132    3.363724   -0.777822
 H   -0.562980    5.825707   -1.091317
 H    2.786917   -0.524732   -5.401561
 H    1.252897    0.380740   -3.676258
 H    5.232542   -0.676837   -4.940389
 H    6.132164    0.109680   -2.757242
 H    4.600512    1.025763   -1.036234
 H    1.794441    3.338996    1.349891
 H    0.055584    1.301402    1.773103
 H    0.375309    2.331302    3.177916
 H    1.161277   -0.517338    2.903649
 H    1.492372    0.544320    4.269207
 H    3.861872    0.058850    4.637438
 H    5.067055    0.040508    3.333824
 H    3.863337   -1.264292    3.454622
 H    2.943858    3.948795    3.867276
 H    3.892435    2.676826    4.661079
 H    2.127952    2.540303    4.567633
 H    4.519862    3.768452    2.029687
 H    4.710686    2.301402    1.055927
 H    5.378203    2.372237    2.707033
 H    5.686193    0.337686    1.111817
 H    6.593663   -0.669880   -0.034643
 H    6.469028   -1.160922    1.666181
 H    2.239087   -4.376846   -1.918005
 H    1.578931   -4.768936   -0.320405
 H    3.226800   -5.279302   -0.747680
 H   -0.055641   -3.014966   -4.544335
 H    0.992101   -1.761575   -2.686024
 H   -1.763439   -4.769090   -4.064569
 H   -2.401680   -5.255406   -1.705213
 H   -1.349050   -4.014221    0.153923
 H   -2.509217   -2.035797    3.951923
 H   -1.612343   -1.110178    1.827121
 H   -1.315810   -3.908326    5.089006
 H    0.760011   -4.845502    4.084002
 H    1.637427   -3.933577    1.954522
Cu   -0.358161    0.292332   -0.614884
 H   -2.832173   -1.475654    0.041240
 H   -2.942404   -1.384262   -1.702687
 H   -2.495623    0.955255   -1.836981
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Figure 1_pc3_major_01 / electronic energy: -5826.83109267 a.u. / lowest freq: 13.73 cm-1
 P    0.558075    0.782223   -1.701306
 C   -0.143736   -0.685577   -3.939604
 C   -0.538554   -0.904606   -5.258694
 C    0.005795    0.615526   -3.443227
 C   -0.802127    0.179073   -6.094869
```

C	-0.270939	1.697230	-4.290390
C	-0.671867	1.480161	-5.606810
C	3.988278	2.847132	-2.787018
C	2.682116	2.362203	-2.778655
C	2.286606	1.406642	-1.833695
C	4.912023	2.393984	-1.844173
C	4.527522	1.441501	-0.903054
C	3.225421	0.944446	-0.907733
C	-1.738477	2.642788	-1.457716
C	-0.318830	2.246604	-1.075779
C	0.078987	3.095036	-0.103526
C	-2.616493	2.266819	-0.229648
C	-2.166267	3.289773	0.832027
C	-1.062557	4.112104	0.104256
C	-0.723655	5.413111	0.802299
C	-1.653341	4.190572	-1.345817
C	-3.007503	4.899397	-1.447553
C	-0.730549	4.846368	-2.376009
C	1.272787	3.062861	0.779681
C	2.268091	4.004897	0.708356
C	1.457871	2.134533	1.891149
S	3.403954	3.800241	1.995423
C	2.554097	2.448332	2.664888
C	2.483578	5.084788	-0.303872
C	3.065839	1.852993	3.941585
P	0.350908	0.680984	2.043873
C	3.305475	-2.029027	3.060567
C	2.636790	-0.931950	2.522009
C	2.667263	-2.861850	3.980110
C	1.320992	-0.629684	2.903608
C	1.358221	-2.576174	4.364277
C	0.693943	-1.469451	3.835541
C	-3.161595	0.940877	4.134702
C	-2.157581	0.587621	3.234254
C	-2.909585	1.893877	5.120871
C	-0.884189	1.168392	3.319002
C	-1.648933	2.487044	5.205781
C	-0.641521	2.125797	4.312034
H	0.031874	-1.537552	-3.276377
H	-0.651005	-1.925930	-5.629220
H	-1.116834	0.010640	-7.127408
H	-0.185770	2.719107	-3.918606
H	-0.888044	2.333168	-6.254130
H	4.284677	3.589478	-3.531503
H	1.973933	2.735545	-3.520130
H	5.932900	2.783007	-1.846364
H	5.244115	1.084860	-0.161589
H	2.927089	0.192862	-0.177905
H	-2.107684	2.244090	-2.411372
H	-2.446426	1.229084	0.079926
H	-3.685853	2.354453	-0.466937
H	-1.771664	2.827983	1.743028
H	-2.987049	3.952024	1.145405
H	-1.636432	6.010504	0.952516
H	-0.014388	6.024571	0.226709
H	-0.282764	5.228290	1.794370
H	-3.434176	4.751750	-2.452658
H	-2.882690	5.984199	-1.302936
H	-3.753778	4.554310	-0.721576
H	-1.192533	4.811377	-3.375453
H	0.252617	4.363238	-2.444349
H	-0.569601	5.909040	-2.133696
H	1.725011	5.022066	-1.092773
H	3.469980	4.986019	-0.781971
H	2.429883	6.087768	0.147938
H	3.949269	1.216367	3.775126
H	2.299324	1.236180	4.425398
H	3.357938	2.646255	4.646180
H	4.335132	-2.233704	2.758183
H	3.159922	-0.290116	1.810055
H	3.188723	-3.726258	4.397212
H	0.845094	-3.216125	5.086039
H	-0.328675	-1.262752	4.159136
H	-4.148212	0.479255	4.052086
H	-2.377928	-0.131963	2.442236
H	-3.697868	2.182039	5.820310
H	-1.449074	3.240435	5.971489
H	0.335053	2.610504	4.379790
C	0.867610	-3.106158	-0.256968
C	1.942691	-2.317385	-0.611612
C	2.626393	-2.409438	-1.941723
O	3.670022	-3.407057	-1.914503
P	5.124321	-3.253226	-1.286706
O	6.258251	-3.080862	-2.212843
O	4.911406	-2.051444	-0.230296
O	5.282415	-4.580031	-0.404260
C	6.032355	-1.548977	0.484246
H	0.609146	-3.260220	0.795414
H	0.410158	-3.803741	-0.968370
H	2.530737	-1.854570	0.183317
H	1.936339	-2.749972	-2.724849
H	3.056920	-1.446319	-2.252571
B	-4.294943	-1.136305	-1.175987
O	-5.292771	-1.815114	-1.827469
O	-4.756189	-0.517080	-0.039456
C	-6.539663	-1.534303	-1.165889
C	-6.061550	-1.037354	0.249416

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 C   -7.382807   -2.799631   -1.143965
 C   -7.245609   -0.446824   -1.973626
 C   -5.874601   -2.175034    1.254102
 C   -6.912318    0.064348    0.861603
 H   -5.251845   -2.981069    0.838160
 H   -6.837260   -2.600451    1.573209
 H   -5.359897   -1.782544    2.143327
 H   -6.934212    0.962585    0.230311
 H   -6.496122    0.350303    1.839132
 H   -7.945212   -0.281146    1.019276
 H   -6.654949    0.481101   -2.002879
 H   -8.238342   -0.216922   -1.560422
 H   -7.377716   -0.796526   -3.008295
 H   -8.310640   -2.639879   -0.573960
 H   -6.837524   -3.643298   -0.700895
 H   -7.660099   -3.077974   -2.171760
 C   -1.969580   -2.984409    1.613685
 C   -2.267447   -4.185650    2.244183
 C   -2.220418   -2.769741    0.237823
 C   -2.834813   -5.245270    1.526095
 C   -2.784652   -3.856023   -0.465299
 C   -3.083926   -5.065421    0.166390
 C   -1.882840   -1.478222   -0.399431
 C   -2.781626   -1.102108   -1.596353
 H   -3.524990   -5.878421   -0.418070
 H   -3.004505   -3.751399   -1.530212
 H   -3.072272   -6.190828    2.019270
 H   -2.057728   -4.299190    3.311967
 H   -1.515817   -2.175070    2.192445
Cu    0.122437   -1.259346   -0.691425
 H   -2.611145   -1.744492   -2.477414
 H   -2.527644   -0.084488   -1.939378
 H   -1.996545   -0.697309    0.369549
 H    5.660355   -0.798979    1.193722
 H    6.757197   -1.081464   -0.198570
 H    6.536067   -2.351205    1.046747
 C    4.256779   -4.991418    0.492673
 H    4.654094   -5.836136    1.069114
 H    3.360884   -5.314966   -0.057902
 H    3.980371   -4.180678    1.184565
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Figure 1_pc3_major_02 / electronic energy: -5826.83024921 a.u. / lowest freq: 19.64 cm-1
 C    0.855304    3.120995    0.980769
 C    1.984661    2.541541    0.439823
 C    2.794982    1.550791    1.218151
 O    3.643299    2.227695    2.171287
 P    5.229721    2.135086    2.104779
 O    5.877567    0.808724    2.153777
 O    5.536298    2.991857    0.775638
 O    5.661394    3.059348    3.335258
 C    6.850936    3.025201    0.237718
 H    0.426824    4.031399    0.551007
 H    0.522508    2.861055    1.992596
 H    2.463723    3.000246   -0.432385
 H    2.138927    0.900736    1.807589
 H    3.408661    0.917506    0.565666
 B   -3.751962    1.333297    1.715476
 O   -4.337435    1.730681    2.891411
 O   -4.688321    1.071131    0.744452
 C   -5.761128    1.558199    2.764835
 C   -5.957738    1.555178    1.203956
 C   -6.467041    2.692980    3.489406
 C   -6.109289    0.220049    3.414837
 C   -6.141002    2.955501    0.618440
 C   -7.057140    0.631461    0.703803
 H   -5.354707    3.642967    0.964304
 H   -7.121915    3.379780    0.877859
 H   -6.069034    2.895591   -0.477310
 H   -6.854377   -0.418021    0.954523
 H   -7.138429    0.707557   -0.390915
 H   -8.029417    0.914496    1.134916
 H   -5.614957   -0.616645    2.898542
 H   -7.193938    0.039046    3.417906
 H   -5.759308    0.227837    4.457853
 H   -7.553777    2.642600    3.323122
 H   -6.105056    3.673679    3.153902
 H   -6.285308    2.615914    4.571787
 C   -2.948465    3.326607   -1.534776
 C   -3.474315    4.576534   -1.850809
 C   -2.374033    3.049572   -0.273319
 C   -3.465443    5.610934   -0.911026
 C   -2.390701    4.108795    0.661812
 C   -2.922468    5.359654    0.350064
 C   -1.823894    1.713253    0.049408
 C   -2.205256    1.224350    1.462924
 H   -2.916367    6.148384    1.108015
 H   -1.980499    3.945496    1.661490
 H   -3.886388    6.589681   -1.153166
 H   -3.917249    4.739420   -2.837909
 H   -3.005121    2.522250   -2.274503
 P    1.050691    0.247521   -1.882153
 C    3.370885   -1.134907   -1.136703
 C    4.738325   -1.265509   -0.903257
 C    2.864051   -0.010093   -1.799248
 C    5.618902   -0.268190   -1.319197
 C    3.754948    0.992363   -2.206192
 C    5.122287    0.860984   -1.969172
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 C   -0.523293    2.958935   -4.517183
 C   -0.216995    2.207264   -3.383067
 C    0.810727    1.257485   -3.405854
 C    0.204027    2.773784   -5.690861
 C    1.247185    1.845998   -5.719579
 C    1.551212    1.094737   -4.586244
 C    0.856039   -2.088967   -3.664567
 C    0.371249   -1.348014   -2.421742
 C   -0.682707   -2.038717   -1.933573
 C    1.496027   -3.410177   -3.161322
 C    0.280398   -4.179001   -2.607827
 C   -0.919123   -3.223570   -2.897113
 C   -2.264854   -3.916724   -2.846870
 C   -0.487973   -2.581643   -4.260627
 C   -0.347662   -3.579265   -5.414011
 C   -1.385611   -1.444341   -4.755904
 C   -1.470740   -1.958427   -0.677195
 C   -2.807487   -1.632258   -0.660865
 C   -1.014323   -2.499898    0.595402
 S   -3.517810   -2.037026    0.861169
 C   -2.033449   -2.619434    1.517703
 C   -3.655150   -1.007537   -1.722661
 C   -2.041746   -3.167978    2.912217
 P    0.733284   -2.976907    0.855495
 C    1.152105   -0.192884    3.935416
 C    0.573377   -0.985240    2.942771
 C    2.527201   -0.240951    4.162640
 C    1.361027   -1.847414    2.169532
 C    3.328455   -1.068160    3.376044
 C    2.749071   -1.857196    2.383662
 C    1.187445   -6.185933    3.461481
 C    1.303260   -4.921976    2.880756
 C    0.338049   -7.142231    2.907502
 C    0.565426   -4.592636    1.737409
 C   -0.392068   -6.828038    1.760096
 C   -0.275006   -5.567810    1.177761
 H    2.685254   -1.904481   -0.773163
 H    5.115867   -2.147654   -0.381277
 H    6.689403   -0.368036   -1.128048
 H    3.383877    1.892432   -2.701146
 H    5.803495    1.651477   -2.291080
 H   -1.329846    3.694682   -4.474557
 H   -0.785862    2.363456   -2.464678
 H   -0.032776    3.358422   -6.583057
 H    1.829264    1.705291   -6.633283
 H    2.381064    0.386458   -4.625153
 H    1.496795   -1.514509   -4.342655
 H    2.267145   -3.228047   -2.404023
 H    1.978464   -3.944147   -3.992692
 H    0.365222   -4.388885   -1.532777
 H    0.129344   -5.144491   -3.113440
 H   -2.282903   -4.750207   -3.566228
 H   -3.091326   -3.238356   -3.099923
 H   -2.466358   -4.334914   -1.848528
 H    0.193955   -3.111048   -6.251750
 H   -1.341203   -3.868134   -5.791922
 H    0.183095   -4.503721   -5.153042
 H   -0.983746   -1.028451   -5.693531
 H   -1.468113   -0.615104   -4.041660
 H   -2.400839   -1.814207   -4.971165
 H   -4.459017   -1.681898   -2.058264
 H   -3.042226   -0.742046   -2.593099
 H   -4.127438   -0.092317   -1.333255
 H   -2.663527   -2.548434    3.575987
 H   -1.033229   -3.211121    3.338085
 H   -2.450881   -4.191387    2.928288
 H    0.519919    0.472156    4.528688
 H   -0.500975   -0.918437    2.770134
 H    2.980109    0.391079    4.929596
 H    4.412264   -1.064500    3.503201
 H    3.389097   -2.491254    1.763307
 H    1.762917   -6.419254    4.360771
 H    1.965765   -4.185172    3.340475
 H    0.243298   -8.128285    3.368211
 H   -1.061982   -7.568264    1.315807
 H   -0.862273   -5.334630    0.284949
Cu    0.186165    1.597813   -0.201144
 H   -1.659378    1.751468    2.265775
 H   -1.911547    0.166806    1.568799
 H   -2.234774    0.999634   -0.678625
 H    6.793696    3.538868   -0.730055
 H    7.248999    2.009976    0.094007
 H    7.530240    3.588251    0.897788
 C    5.164047    4.383221    3.489475
 H    5.710153    4.839150    4.324791
 H    4.088357    4.373041    3.719679
 H    5.333462    4.978599    2.579254
142
Figure 1_pc3_major_03 / electronic energy: -5826.82859981 a.u. / lowest freq: 5.22 cm-1
 P   -0.611888   -1.368369    1.360996
 C    0.251262   -1.198982    3.980939
 C    0.269468   -1.470578    5.347954
 C   -0.751647   -1.731440    3.157345
 C   -0.725030   -2.266611    5.915128
 C   -1.741237   -2.535526    3.737333
 C   -1.731254   -2.796069    5.107031
 C    0.552113   -5.283901    0.653958
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C	-0.064459	-4.167648	1.217600
C	0.191065	-2.890202	0.707052
C	1.419771	-5.136955	-0.429479
C	1.676805	-3.866598	-0.943796
C	1.070452	-2.752911	-0.368109
C	-3.572299	-1.050715	1.350981
C	-2.295456	-1.538383	0.678373
C	-2.655360	-2.000517	-0.540150
C	-4.015779	0.207772	0.544276
C	-4.467119	-0.382353	-0.802745
C	-4.194650	-1.902597	-0.635144
C	-4.891200	-2.749368	-1.680354
C	-4.593369	-2.119617	0.864426
C	-6.050701	-1.784772	1.199157
C	-4.339106	-3.539558	1.376289
C	-1.841821	-2.372933	-1.723844
C	-1.796184	-3.652159	-2.217919
C	-1.156618	-1.412119	-2.582439
S	-0.973621	-3.694007	-3.737364
C	-0.684182	-1.987784	-3.742618
C	-2.309075	-4.923605	-1.620040
C	-0.038904	-1.390320	-4.956715
P	-0.895305	0.315139	-2.012820
C	3.022254	0.441657	-3.360748
C	1.800199	-0.001836	-2.861830
C	3.165337	1.755563	-3.804481
C	0.688636	0.851247	-2.803526
C	2.074285	2.620409	-3.736329
C	0.849084	2.174486	-3.238858
C	-3.485669	3.324462	-3.017954
C	-2.513932	2.537592	-2.399260
C	-4.129766	2.865082	-4.166099
C	-2.155017	1.292803	-2.934481
C	-3.793373	1.617646	-4.694972
C	-2.811518	0.837627	-4.085425
H	1.033474	-0.566922	3.550914
H	1.065439	-1.053579	5.968967
H	-0.716317	-2.474300	6.987757
H	-2.525925	-2.971319	3.120135
H	-2.512830	-3.423028	5.542498
H	0.351724	-6.276335	1.064540
H	-0.742991	-4.301890	2.062545
H	1.897928	-6.014893	-0.870314
H	2.358874	-3.739254	-1.787536
H	1.278384	-1.754734	-0.749288
H	-3.513316	-0.888150	2.435349
H	-3.188799	0.910819	0.416556
H	-4.821174	0.743645	1.065271
H	-3.917738	0.025579	-1.659061
H	-5.535186	-0.207508	-1.000277
H	-5.974239	-2.550377	-1.664382
H	-4.747036	-3.825754	-1.515388
H	-4.526256	-2.511056	-2.691475
H	-6.197907	-1.808672	2.290808
H	-6.726668	-2.538643	0.765149
H	-6.385573	-0.801605	0.845799
H	-4.582704	-3.613473	2.448003
H	-3.300786	-3.868384	1.241202
H	-4.990142	-4.256650	0.851618
H	-2.744944	-4.733444	-0.631769
H	-1.495904	-5.653651	-1.489740
H	-3.078739	-5.393553	-2.252519
H	1.042623	-1.593607	-4.993380
H	-0.174672	-0.302887	-4.985379
H	-0.486322	-1.810821	-5.870406
H	3.870410	-0.244351	-3.386531
H	1.710123	-1.039636	-2.539385
H	4.123019	2.106163	-4.196454
H	2.171461	3.654824	-4.074640
H	0.011131	2.874121	-3.202421
H	-3.740160	4.291024	-2.577479
H	-2.051183	2.915166	-1.483171
H	-4.899408	3.474145	-4.646491
H	-4.299966	1.246363	-5.589122
H	-2.571062	-0.143217	-4.500919
C	0.821821	2.492160	1.851750
C	-0.313504	1.997569	2.449771
C	-1.678480	2.283629	1.919932
O	-2.109971	3.602068	2.328392
P	-3.045692	4.431619	1.336823
O	-2.525299	4.717988	-0.017171
O	-4.404419	3.570824	1.373737
O	-3.334714	5.757789	2.168864
C	-5.318690	3.587315	0.282709
H	1.767363	2.542301	2.397504
H	0.755380	3.090073	0.934761
H	-0.255086	1.614529	3.474643
H	-1.673216	2.235539	0.820006
H	-2.409044	1.560016	2.304795
B	4.803806	1.410403	-0.386488
O	5.800445	2.328473	-0.160732
O	5.297306	0.241703	-0.913866
C	7.020976	1.812210	-0.720092
C	6.726357	0.268790	-0.785500
C	8.186067	2.196721	0.178027
C	7.186936	2.446172	-2.100303
C	7.069035	-0.463156	0.512311

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 C    7.354534   -0.446294   -1.971141
 H    6.631729    0.041503    1.387045
 H    8.155513   -0.549416    0.659639
 H    6.643748   -1.476652    0.469886
 H    6.991842   -0.046023   -2.927243
 H    7.105962   -1.517523   -1.935160
 H    8.450793   -0.351993   -1.945268
 H    6.357169    2.170945   -2.768509
 H    8.132812    2.147860   -2.574973
 H    7.185717    3.541092   -1.993996
 H    9.117378    1.725381   -0.171080
 H    8.009965    1.897864    1.219716
 H    8.330504    3.287333    0.158142
 C    3.315351   -1.487540    2.146138
 C    3.858122   -1.959854    3.334583
 C    3.303612   -0.109809    1.816308
 C    4.430148   -1.078673    4.259286
 C    3.914815    0.755259    2.753848
 C    4.457263    0.280754    3.949860
 C    2.649270    0.377584    0.581045
 C    3.289564    1.630399   -0.039774
 H    4.913864    0.989564    4.647175
 H    3.972131    1.825963    2.543026
 H    4.857210   -1.449366    5.194227
 H    3.836313   -3.033400    3.543205
 H    2.874557   -2.198346    1.442950
Cu    0.702148    0.555778    1.198212
 H    3.196481    2.523809    0.600179
 H    2.748600    1.896397   -0.963995
 H    2.679895   -0.428665   -0.166138
 H   -6.230340    3.079771    0.622136
 H   -4.905348    3.052490   -0.584214
 H   -5.575639    4.616639   -0.011619
 C   -3.887924    5.731890    3.480511
 H   -4.124617    6.769274    3.747539
 H   -3.162875    5.326711    4.201820
 H   -4.809974    5.131597    3.508783
142
Figure 1_pc3_major_04 / electronic energy: -5826.82790049 a.u. / lowest freq: 12.27 cm-1
 C    1.326535    1.894445   -1.827356
 C    0.414642    2.339057   -0.896143
 C   -1.062814    2.160390   -1.039596
 O   -1.653387    3.251044   -1.783698
 P   -2.039547    4.682936   -1.206848
 O   -3.475834    5.009080   -1.093949
 O   -1.214393    4.712793    0.174673
 O   -1.305334    5.708414   -2.190878
 C   -1.449892    5.748167    1.122121
 H    2.331829    2.320826   -1.880854
 H    0.992519    1.311808   -2.693989
 H    0.733378    3.094844   -0.168569
 H   -1.297512    1.265417   -1.623417
 H   -1.555516    2.082962   -0.063045
 B    5.451024   -0.836696   -1.597764
 O    6.396284   -0.191833   -2.353392
 O    6.020849   -1.651850   -0.649541
 C    7.693306   -0.689618   -1.977331
 C    7.412365   -1.305284   -0.556629
 C    8.685984    0.461902   -1.981935
 C    8.093356   -1.735199   -3.016354
 C    7.540522   -0.281074    0.571838
 C    8.220451   -2.550420   -0.229417
 H    6.981649    0.639674    0.345895
 H    8.590760   -0.018867    0.765901
 H    7.115202   -0.710160    1.491265
 H    8.025138   -3.362611   -0.941947
 H    7.956019   -2.911354    0.775722
 H    9.298368   -2.328267   -0.237387
 H    7.392396   -2.583243   -3.023244
 H    9.107234   -2.120992   -2.836668
 H    8.073810   -1.273200   -4.014366
 H    9.664589    0.132766   -1.600568
 H    8.333590    1.300860   -1.367661
 H    8.827805    0.830251   -3.008986
 C    3.949409    1.510284    1.504058
 C    4.480133    2.697267    1.995305
 C    3.991104    1.178880    0.125341
 C    5.087287    3.619616    1.135627
 C    4.620831    2.123450   -0.719747
 C    5.153572    3.314234   -0.223543
 C    3.357861   -0.061621   -0.371215
 C    3.899282   -0.621333   -1.701340
 H    5.634792    4.011724   -0.915635
 H    4.715669    1.913597   -1.787031
 H    5.508178    4.550936    1.522024
 H    4.425612    2.902024    3.068545
 H    3.493578    0.802551    2.200528
 P    0.235634   -0.411443    1.492956
 C   -2.187357   -0.151897    2.954972
 C   -3.148268    0.586304    3.643595
 C   -1.116064    0.493188    2.330799
 C   -3.047798    1.974626    3.713189
 C   -1.020527    1.889723    2.404613
 C   -1.980694    2.626020    3.094740
 C    3.456802   -1.805935    3.628283
 C    2.475950   -1.621169    2.658315
 C    1.412651   -0.730977    2.871584
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 C    3.399212   -1.091838    4.825936
 C    2.347945   -0.204599    5.047681
 C    1.357503   -0.027372    4.079540
 C   -0.087564   -3.382768    1.776666
 C   -0.368779   -2.070569    1.044733
 C   -1.018614   -2.396058   -0.093349
 C   -1.455474   -3.930048    2.263340
 C   -2.160042   -4.310469    0.945324
 C   -1.113208   -3.932208   -0.146144
 C   -1.382107   -4.547910   -1.504316
 C    0.229264   -4.318079    0.577487
 C    0.352436   -5.802452    0.936017
 C    1.507897   -3.936292   -0.174090
 C   -1.589350   -1.549586   -1.171178
 C   -0.886917   -1.291048   -2.325488
 C   -2.964773   -1.080174   -1.236151
 S   -1.889187   -0.499879   -3.488171
 C   -3.267051   -0.493712   -2.448124
 C    0.535685   -1.613466   -2.659249
 C   -4.558464    0.054741   -2.970626
 P   -4.159961   -1.397420    0.124076
 C   -4.953068    2.657356    0.656253
 C   -4.413766    1.470833    0.153946
 C   -5.935550    2.613881    1.643454
 C   -4.841443    0.229880    0.634293
 C   -6.368660    1.381557    2.136128
 C   -5.815418    0.201694    1.645986
 C   -7.837036   -2.240790   -1.665649
 C   -6.827127   -1.576628   -0.968300
 C   -7.600585   -3.496466   -2.222797
 C   -5.564269   -2.159529   -0.812005
 C   -6.346619   -4.089807   -2.069577
 C   -5.342516   -3.431110   -1.362739
 H   -2.278199   -1.237131    2.900370
 H   -3.983759    0.072488    4.122961
 H   -3.805821    2.551738    4.247378
 H   -0.184161    2.405142    1.925279
 H   -1.896217    3.712807    3.150963
 H    4.275930   -2.503527    3.439937
 H    2.545749   -2.173100    1.720161
 H    4.173512   -1.226842    5.584702
 H    2.291009    0.355173    5.984125
 H    0.543459    0.673039    4.275422
 H    0.670897   -3.340162    2.565544
 H   -2.011628   -3.184325    2.845954
 H   -1.307077   -4.800428    2.918772
 H   -3.101436   -3.767593    0.796959
 H   -2.390306   -5.384779    0.890434
 H   -1.482938   -5.640783   -1.417149
 H   -0.573892   -4.339451   -2.220529
 H   -2.313860   -4.160269   -1.943973
 H    1.181062   -5.948822    1.647303
 H    0.589357   -6.391542    0.035747
 H   -0.547901   -6.240305    1.384591
 H    2.391053   -4.242566    0.408866
 H    1.593305   -2.860009   -0.365404
 H    1.565723   -4.460488   -1.141264
 H    0.689019   -2.695518   -2.787224
 H    1.205881   -1.272252   -1.857369
 H    0.854455   -1.120914   -3.588483
 H   -4.383210    0.900208   -3.651950
 H   -5.204725    0.406399   -2.158533
 H   -5.113040   -0.718587   -3.527019
 H   -4.602809    3.609454    0.248494
 H   -3.662028    1.522739   -0.634651
 H   -6.363622    3.540890    2.032640
 H   -7.134003    1.338368    2.914830
 H   -6.148994   -0.756950    2.055547
 H   -8.813717   -1.764493   -1.781137
 H   -7.028924   -0.585848   -0.556103
 H   -8.391125   -4.012970   -2.772372
 H   -6.149651   -5.075212   -2.498661
 H   -4.368986   -3.914351   -1.242861
Cu    1.417932    0.599212   -0.231439
 H    3.644517    0.017216   -2.565077
 H    3.416626   -1.594785   -1.897724
 H    3.463579   -0.833746    0.403344
 H   -0.689647    5.646665    1.906452
 H   -2.452661    5.656112    1.564116
 H   -1.347151    6.741449    0.658098
 C    0.070912    5.567353   -2.523526
 H    0.330833    6.408727   -3.177975
 H    0.250747    4.622288   -3.057664
 H    0.703679    5.603376   -1.623068
142
Figure 1_ts(AS)_major_01 / electronic energy: -5826.79676454 a.u. / lowest freq: -342.36 cm-1
 P   -0.324270    1.952480    0.257176
 C    0.435040    3.932915   -1.523402
 C    0.455822    5.209031   -2.083527
 C   -0.418483    3.639876   -0.451010
 C   -0.384177    6.204045   -1.585202
 C   -1.249118    4.649374    0.051295
 C   -1.235871    5.921911   -0.516889
 C    1.901862    3.500506    3.384701
 C    1.013444    3.400516    2.313491
 C    0.782155    2.161771    1.706848
 C    2.561614    2.367454    3.860533
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C	2.332864	1.128647	3.260682
C	1.452428	1.033637	2.187443
C	-3.289365	2.042783	0.369527
C	-1.959034	1.621112	0.985416
C	-2.256417	0.888231	2.080079
C	-3.941834	0.736050	-0.172726
C	-4.300670	-0.030828	1.113485
C	-3.789491	0.906073	2.244971
C	-4.340196	0.559685	3.612852
C	-4.133031	2.314475	1.648818
C	-5.621814	2.550492	1.372653
C	-3.655407	3.490133	2.504866
C	-1.409770	0.026946	2.939303
C	-1.097845	0.355175	4.233309
C	-0.946840	-1.303080	2.564492
S	-0.282333	-0.950206	5.016740
C	-0.351657	-1.966095	3.616981
C	-1.291405	1.655688	4.943989
C	0.166009	-3.367871	3.737199
P	-1.123087	-1.876999	0.829931
C	2.767486	-3.360522	0.757770
C	1.631848	-2.628837	1.100437
C	2.700379	-4.344587	-0.226257
C	0.397925	-2.876992	0.484056
C	1.487399	-4.578559	-0.873578
C	0.349855	-3.850816	-0.525735
C	-4.103707	-4.462056	-0.282985
C	-3.073029	-3.520670	-0.279262
C	-4.545591	-5.030343	0.910758
C	-2.448058	-3.160793	0.924390
C	-3.953615	-4.647986	2.115104
C	-2.912332	-3.720728	2.122684
H	1.101208	3.161835	-1.921136
H	1.131994	5.421804	-2.914484
H	-0.374824	7.201851	-2.029835
H	-1.908502	4.447267	0.894612
H	-1.894756	6.697340	-0.119563
H	2.080818	4.473652	3.847571
H	0.518198	4.300281	1.943834
H	3.261851	2.451247	4.694931
H	2.849885	0.236212	3.619671
H	1.286637	0.071046	1.706965
H	-3.243649	2.857432	-0.364725
H	-3.252671	0.164115	-0.799619
H	-4.819758	0.959172	-0.793433
H	-3.828513	-1.018719	1.174212
H	-5.383592	-0.193781	1.218256
H	-5.439689	0.621018	3.602777
H	-3.972116	1.235026	4.398726
H	-4.069957	-0.468777	3.898646
H	-5.749160	3.478686	0.793234
H	-6.168698	2.680877	2.319881
H	-6.115709	1.745294	0.815593
H	-3.888472	4.446008	2.009687
H	-2.577564	3.470269	2.709898
H	-4.181262	3.496031	3.472680
H	-1.917562	2.326300	4.343338
H	-0.324166	2.159147	5.104286
H	-1.768760	1.524835	5.927270
H	1.260276	-3.392735	3.857559
H	-0.087098	-3.963281	2.852447
H	-0.272741	-3.864605	4.616593
H	3.712241	-3.144838	1.260279
H	1.712260	-1.875594	1.884642
H	3.590936	-4.915581	-0.499200
H	1.420288	-5.337010	-1.657067
H	-0.587413	-4.057548	-1.047575
H	-4.577719	-4.730665	-1.230348
H	-2.797563	-3.037365	-1.224810
H	-5.359235	-5.759781	0.906399
H	-4.306148	-5.072415	3.058389
H	-2.475580	-3.420950	3.076683
C	0.550563	-0.223916	-3.225611
C	-0.367797	0.841118	-3.331782
C	-1.613859	0.790630	-2.697783
O	-3.019936	0.324561	-4.097548
P	-3.669149	-1.019978	-3.774014
O	-2.900638	-2.066953	-3.031852
O	-5.059604	-0.636569	-3.000035
O	-4.211549	-1.680341	-5.160465
C	-5.737774	-1.617380	-2.248411
H	1.475889	-0.202467	-3.801733
H	0.189877	-1.221545	-2.944624
H	-0.073690	1.757731	-3.852309
H	-1.857482	-0.098937	-2.115170
H	-2.169063	1.705084	-2.495750
B	4.611780	-1.324521	-1.208933
O	5.623391	-1.949122	-1.891679
O	4.997104	-0.946105	0.051006
C	6.712637	-2.167433	-0.975492
C	6.422665	-1.098826	0.143483
C	8.029866	-1.974914	-1.709312
C	6.597878	-3.604582	-0.470743
C	7.034486	0.268918	-0.157919
C	6.786885	-1.534486	1.553577
H	6.778356	0.609884	-1.172270
H	8.129412	0.255938	-0.056806

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 H    6.631211    1.004677    0.553333
 H    6.243583   -2.439480    1.855792
 H    6.532877   -0.734146    2.264382
 H    7.866579   -1.730987    1.635005
 H    5.662717   -3.758569    0.086581
 H    7.440831   -3.874667    0.181494
 H    6.595676   -4.289962   -1.331241
 H    8.875018   -2.038636   -1.007325
 H    8.072799   -1.005726   -2.223046
 H    8.155868   -2.764375   -2.465261
 C    3.494482    2.359957   -0.374981
 C    4.014770    3.624127   -0.640561
 C    3.141166    1.472273   -1.410704
 C    4.222599    4.042217   -1.956094
 C    3.381779    1.906650   -2.730092
 C    3.911080    3.167741   -2.998657
 C    2.510487    0.150906   -1.117594
 C    3.182388   -1.041693   -1.798566
 H    4.078379    3.470903   -4.035753
 H    3.134470    1.248235   -3.566362
 H    4.631543    5.033379   -2.165857
 H    4.267617    4.286722    0.191473
 H    3.357160    2.044485    0.660643
Cu    0.575270    0.622523   -1.421841
 H    3.274833   -0.911679   -2.889023
 H    2.572217   -1.952405   -1.673042
 H    2.529372   -0.015095   -0.031851
 H   -6.692630   -1.182907   -1.918613
 H   -5.161761   -1.917470   -1.358512
 H   -5.956384   -2.518699   -2.846634
 C   -4.942963   -0.889453   -6.071734
 H   -5.227886   -1.529985   -6.918512
 H   -4.340125   -0.047054   -6.448072
 H   -5.860199   -0.484648   -5.611296
142
Figure 1_ts(AS)_major_02 / electronic energy: -5826.79516945 a.u. / lowest freq: -325.10 cm-1
 C    1.329593    2.025287   -1.722547
 C    0.396762    2.522587   -0.786183
 C   -0.887668    1.990736   -0.651337
 O   -2.276655    3.181384   -1.606989
 P   -2.547753    4.590679   -1.077607
 O   -3.932813    5.082227   -0.830684
 O   -1.626748    4.680551    0.281197
 O   -1.810239    5.666168   -2.063185
 C   -1.702409    5.836803    1.082343
 H    2.284757    2.535557   -1.856541
 H    0.971808    1.442256   -2.579920
 H    0.707391    3.302818   -0.084834
 H   -1.219772    1.189139   -1.305169
 H   -1.442966    2.150840    0.268405
 B    5.370015   -0.432486   -1.698714
 O    6.374319    0.253015   -2.323819
 O    5.845496   -1.335700   -0.782733
 C    7.633569   -0.299892   -1.891037
 C    7.233930   -1.031631   -0.555323
 C    8.635586    0.830414   -1.717534
 C    8.101295   -1.259693   -2.982536
 C    7.291632   -0.116894    0.668620
 C    7.991211   -2.320324   -0.281485
 H    6.767662    0.833797    0.489056
 H    8.328805    0.103425    0.960000
 H    6.793848   -0.617364    1.512254
 H    7.836773   -3.063496   -1.074799
 H    7.644140   -2.759000    0.665963
 H    9.069989   -2.124488   -0.188417
 H    7.391208   -2.088980   -3.119007
 H    9.091277   -1.680651   -2.755697
 H    8.171501   -0.714141   -3.935108
 H    9.576914    0.451921   -1.291299
 H    8.245330    1.619927   -1.062148
 H    8.861192    1.282579   -2.694657
 C    3.861172    1.549668    1.528107
 C    4.444605    2.633597    2.176829
 C    3.892128    1.420518    0.123411
 C    5.089249    3.633994    1.445169
 C    4.548814    2.439844   -0.594157
 C    5.138090    3.524433    0.055843
 C    3.244192    0.253469   -0.538389
 C    3.829884   -0.168758   -1.889881
 H    5.646549    4.291329   -0.534748
 H    4.626916    2.375993   -1.681231
 H    5.552617    4.483731    1.951791
 H    4.403084    2.691730    3.267848
 H    3.380988    0.769112    2.121469
 P    0.365776   -0.667271    1.413115
 C   -0.737762    1.558669    2.632257
 C   -1.649682    2.262778    3.412920
 C   -0.888643    0.178684    2.435424
 C   -2.721112    1.593083    4.005483
 C   -1.957169   -0.487383    3.039899
 C   -2.869276    0.219692    3.822953
 C    3.825701   -2.193454    2.984602
 C    2.735186   -1.927933    2.162215
 C    1.684527   -1.111883    2.606379
 C    3.885579   -1.639169    4.264117
 C    2.841638   -0.834911    4.717240
 C    1.743859   -0.572565    3.895494
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 C    0.022643   -3.639270    1.457552
 C   -0.262853   -2.270650    0.842220
 C   -0.964455   -2.488883   -0.291033
 C   -1.337182   -4.191792    1.961751
 C   -2.109173   -4.446150    0.650304
 C   -1.099451   -4.011990   -0.456791
 C   -1.437318   -4.511374   -1.846601
 C    0.258951   -4.488445    0.177066
 C    0.349849   -5.998750    0.418670
 C    1.514051   -4.095746   -0.605678
 C   -1.544654   -1.528459   -1.262988
 C   -0.864401   -1.174310   -2.404103
 C   -2.886429   -0.967728   -1.210860
 S   -1.846773   -0.184923   -3.420523
 C   -3.183127   -0.208684   -2.325272
 C    0.539787   -1.505462   -2.801722
 C   -4.393774    0.596619   -2.674780
 P   -4.034757   -1.403049    0.158519
 C   -4.872278    2.559471    1.136058
 C   -4.318447    1.447443    0.495734
 C   -5.806701    2.389406    2.155578
 C   -4.699435    0.154231    0.863542
 C   -6.182840    1.101676    2.543151
 C   -5.625359   -0.004578    1.908646
 C   -7.776308   -2.074116   -1.575605
 C   -6.736358   -1.467742   -0.868879
 C   -7.576883   -3.297387   -2.213325
 C   -5.478002   -2.076846   -0.788142
 C   -6.328753   -3.916761   -2.135244
 C   -5.294051   -3.315185   -1.422395
 H    0.095676    2.089329    2.163176
 H   -1.530359    3.339720    3.547773
 H   -3.445429    2.146111    4.607366
 H   -2.091133   -1.558783    2.889497
 H   -3.707261   -0.306599    4.283534
 H    4.635562   -2.828107    2.618175
 H    2.704534   -2.363331    1.162003
 H    4.745247   -1.837834    4.908105
 H    2.878083   -0.402164    5.719482
 H    0.939493    0.065783    4.266421
 H    0.819266   -3.667836    2.210052
 H   -1.846060   -3.482562    2.626866
 H   -1.185153   -5.116058    2.537118
 H   -3.036664   -3.864378    0.590405
 H   -2.375324   -5.505398    0.520355
 H   -1.562222   -5.605160   -1.842854
 H   -0.650567   -4.263658   -2.574320
 H   -2.373851   -4.068598   -2.217843
 H    1.222428   -6.225041    1.052019
 H    0.495949   -6.525261   -0.537624
 H   -0.531152   -6.438085    0.902109
 H    2.413230   -4.432683   -0.066153
 H    1.606678   -3.016069   -0.768985
 H    1.528074   -4.587777   -1.590871
 H    0.669052   -2.578993   -3.003492
 H    1.231961   -1.229261   -1.992379
 H    0.847269   -0.956470   -3.702674
 H   -4.157905    1.670302   -2.595208
 H   -5.226668    0.378246   -1.998223
 H   -4.726871    0.390943   -3.703332
 H   -4.588663    3.558271    0.791745
 H   -3.600609    1.619725   -0.307767
 H   -6.246175    3.260969    2.646982
 H   -6.911237    0.957846    3.345084
 H   -5.918163   -1.010311    2.226565
 H   -8.748649   -1.578766   -1.631828
 H   -6.912054   -0.504595   -0.384783
 H   -8.392378   -3.769091   -2.766650
 H   -6.160649   -4.878312   -2.626340
 H   -4.326390   -3.819410   -1.360184
Cu    1.275980    0.657380   -0.277946
 H    3.649389    0.570546   -2.687059
 H    3.347514   -1.102795   -2.221648
 H    3.308152   -0.598284    0.151040
 H   -0.913312    5.772892    1.845337
 H   -2.678991    5.919941    1.586412
 H   -1.538606    6.754184    0.491453
 C   -0.488325    5.429660   -2.486970
 H   -0.228326    6.200177   -3.226913
 H   -0.384794    4.437084   -2.956497
 H    0.227845    5.496407   -1.649647
142
Figure 1_ts(AS)_major_03 / electronic energy: -5826.79145442 a.u. / lowest freq: -196.64 cm-1
 P    0.332795   -0.761161    1.750044
 C   -0.106823    0.991213    3.842466
 C   -0.449210    1.380894    5.135974
 C   -0.164575   -0.356205    3.463910
 C   -0.867977    0.425562    6.060922
 C   -0.597125   -1.307311    4.397060
 C   -0.945973   -0.917213    5.688407
 C    3.476432   -3.186375    2.886924
 C    2.244757   -2.535459    2.871821
 C    1.965509   -1.583113    1.884926
 C    4.432929   -2.904237    1.910552
 C    4.159855   -1.956821    0.925535
 C    2.934301   -1.294609    0.921060
 C   -2.240488   -2.194804    1.570610
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C	-0.755772	-2.120627	1.243579
C	-0.483116	-3.142571	0.402971
C	-2.965732	-1.798212	0.252401
C	-2.664361	-2.996515	-0.669137
C	-1.793491	-3.934713	0.219286
C	-1.688191	-5.346273	-0.319622
C	-2.460977	-3.731895	1.621360
C	-3.933512	-4.148560	1.693372
C	-1.743110	-4.439954	2.772643
C	0.716937	-3.455136	-0.413519
C	1.498567	-4.560270	-0.190596
C	1.085747	-2.741375	-1.630945
S	2.647326	-4.766806	-1.466802
C	2.091477	-3.373786	-2.329969
C	1.476716	-5.523043	0.953415
C	2.706926	-3.073806	-3.663226
P	0.310651	-1.118970	-1.965270
C	3.910668	0.738180	-2.900962
C	2.985989	-0.206275	-2.456807
C	3.485888	1.873871	-3.588334
C	1.615793	-0.045795	-2.707249
C	2.124531	2.052015	-3.835072
C	1.201821	1.101867	-3.401415
C	-2.947809	-0.704326	-4.407273
C	-1.976220	-0.543719	-3.420578
C	-2.835488	-1.743561	-5.329810
C	-0.868158	-1.400917	-3.353953
C	-1.751987	-2.620140	-5.256194
C	-0.775108	-2.451972	-4.275174
H	0.195456	1.745631	3.109806
H	-0.395501	2.434954	5.416713
H	-1.141053	0.727832	7.074611
H	-0.676022	-2.358239	4.115102
H	-1.283607	-1.666819	6.407480
H	3.688046	-3.924342	3.663901
H	1.504764	-2.777884	3.636682
H	5.395294	-3.420732	1.922009
H	4.904773	-1.724553	0.161274
H	2.723245	-0.549285	0.154331
H	-2.564816	-1.630344	2.455109
H	-2.584181	-0.851509	-0.147856
H	-4.042109	-1.657803	0.419459
H	-2.130411	-2.717933	-1.585438
H	-3.579410	-3.517453	-0.987150
H	-2.692384	-5.782965	-0.435979
H	-1.110578	-6.005501	0.343337
H	-1.205945	-5.357105	-1.309510
H	-4.374102	-3.802521	2.641970
H	-4.021696	-5.246316	1.674271
H	-4.555625	-3.755653	0.879919
H	-2.232164	-4.203361	3.730825
H	-0.683737	-4.166543	2.857694
H	-1.798760	-5.532570	2.644588
H	0.731555	-5.211869	1.695226
H	2.453976	-5.561524	1.458115
H	1.232345	-6.545734	0.625613
H	3.778080	-2.833583	-3.576973
H	2.210407	-2.226219	-4.149551
H	2.619623	-3.944936	-4.331281
H	4.972743	0.584500	-2.701959
H	3.345360	-1.081791	-1.915231
H	4.211351	2.615329	-3.929792
H	1.772936	2.938121	-4.368817
H	0.141482	1.266468	-3.607161
H	-3.801332	-0.023099	-4.441461
H	-2.098024	0.244635	-2.674278
H	-3.598950	-1.879113	-6.099540
H	-1.666933	-3.444374	-5.968320
H	0.052884	-3.160915	-4.220825
C	1.062273	2.963922	-0.122381
C	2.233306	2.210687	0.179114
C	2.674012	2.021552	1.474426
O	4.327982	3.473717	1.927726
P	5.624242	3.329910	1.155451
O	6.963052	3.428640	1.803199
O	5.467421	1.885618	0.359431
O	5.620661	4.389709	-0.104352
C	6.545107	1.430938	-0.417394
H	0.811867	3.161376	-1.167201
H	0.709319	3.718464	0.590228
H	2.770560	1.707918	-0.629365
H	2.174814	2.503991	2.315532
H	3.431314	1.274881	1.699285
B	-3.942427	1.722144	0.906391
O	-4.872207	2.389905	1.653391
O	-4.466576	1.214033	-0.251208
C	-6.162285	2.190879	1.040181
C	-5.772696	1.788102	-0.432172
C	-6.966379	3.475352	1.155746
C	-6.854809	1.064780	1.804694
C	-5.604027	2.989650	-1.361661
C	-6.685299	0.755511	-1.073649
H	-4.929399	3.744140	-0.929530
H	-6.568686	3.466644	-1.587006
H	-5.159756	2.647530	-2.307786
H	-6.710784	-0.181985	-0.502931
H	-6.324071	0.523902	-2.086759

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 H   -7.711208    1.144037   -1.159662
 H   -6.294355    0.120798    1.730301
 H   -7.875278    0.894101    1.432540
 H   -6.918476    1.337317    2.868469
 H   -7.924609    3.381936    0.622754
 H   -6.419403    4.335462    0.748300
 H   -7.185703    3.681983    2.213862
 C   -1.792019    3.200486   -2.013597
 C   -2.067927    4.400511   -2.662548
 C   -1.799853    3.098807   -0.610773
 C   -2.365683    5.548845   -1.925500
 C   -2.094627    4.268079    0.112730
 C   -2.375267    5.472277   -0.533465
 C   -1.530767    1.798677    0.066425
 C   -2.423222    1.565378    1.292229
 H   -2.604162    6.360911    0.060782
 H   -2.108335    4.241284    1.204808
 H   -2.586483    6.491483   -2.431505
 H   -2.059257    4.437758   -3.755130
 H   -1.573808    2.309630   -2.607233
Cu    0.354455    1.255792    0.566153
 H   -2.183451    2.243288    2.126783
 H   -2.279018    0.552377    1.698443
 H   -1.668311    0.985420   -0.662344
 H    6.389366    0.363867   -0.636763
 H    7.501740    1.543440    0.119025
 H    6.622203    1.980682   -1.372708
 C    4.439277    4.585777   -0.837907
 H    4.611652    5.406405   -1.550974
 H    3.593563    4.856096   -0.183221
 H    4.156396    3.685197   -1.411452
142
Figure 1_ts(AS)_major_04 / electronic energy: -5826.79527463 a.u. / lowest freq: -325.32 cm-1
 C   -1.351100   -2.038180   -1.771235
 C   -0.395605   -2.535792   -0.858146
 C    0.882880   -1.985633   -0.739384
 O    2.269638   -3.166418   -1.718520
 P    2.607855   -4.540081   -1.136749
 O    4.016428   -4.968914   -0.905151
 O    1.727266   -4.604727    0.251022
 O    1.889297   -5.684405   -2.055224
 C    1.944538   -5.664762    1.153437
 H   -2.304519   -2.555095   -1.892617
 H   -1.015555   -1.440924   -2.628153
 H   -0.683954   -3.325994   -0.158358
 H    1.193601   -1.179049   -1.397633
 H    1.456122   -2.143883    0.169242
 B   -5.375458    0.472050   -1.672399
 O   -6.387059   -0.181664   -2.319188
 O   -5.840896    1.350563   -0.727729
 C   -7.640775    0.366215   -1.865274
 C   -7.232175    1.054254   -0.508628
 C   -8.649127   -0.762875   -1.722004
 C   -8.107458    1.360883   -2.925503
 C   -7.299338    0.104318    0.687654
 C   -7.976938    2.341826   -0.197649
 H   -6.781157   -0.844039    0.481043
 H   -8.338756   -0.117334    0.969827
 H   -6.800211    0.575739    1.546983
 H   -7.816654    3.104968   -0.970525
 H   -7.625087    2.751679    0.760946
 H   -9.057334    2.153183   -0.108615
 H   -7.391129    2.187550   -3.044494
 H   -9.091772    1.783904   -2.678747
 H   -8.189912    0.843145   -3.892490
 H   -9.586036   -0.392246   -1.279521
 H   -8.260392   -1.574979   -1.093843
 H   -8.882561   -1.182813   -2.711586
 C   -3.857315   -1.649106    1.481122
 C   -4.445941   -2.752201    2.091661
 C   -3.906153   -1.460220    0.083715
 C   -5.114063   -3.712270    1.327663
 C   -4.585198   -2.440264   -0.666915
 C   -5.180193   -3.543740   -0.054897
 C   -3.252498   -0.274626   -0.538580
 C   -3.838348    0.198334   -1.873354
 H   -5.706715   -4.278236   -0.670320
 H   -4.675763   -2.329951   -1.749187
 H   -5.581215   -4.576765    1.805042
 H   -4.389277   -2.857851    3.178390
 H   -3.357417   -0.901589    2.100345
 P   -0.361056    0.601678    1.402258
 C    1.962365    0.433323    3.025113
 C    2.887524   -0.268508    3.796980
 C    0.918364   -0.245750    2.392694
 C    2.777895   -1.650212    3.939597
 C    0.805256   -1.634282    2.550403
 C    1.731891   -2.333600    3.318169
 C   -3.823514    2.013720    3.082677
 C   -2.743061    1.799575    2.232119
 C   -1.670903    0.985873    2.627422
 C   -3.852220    1.410489    4.340919
 C   -2.786908    0.608679    4.745815
 C   -1.699616    0.397699    3.896226
 C   -0.077572    3.577529    1.519621
 C    0.233684    2.230543    0.870220
 C    0.924445    2.490253   -0.260763
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 C    1.272289    4.148490    2.029041
 C    2.030971    4.449354    0.719865
 C    1.024668    4.018968   -0.392031
 C    1.345248    4.559357   -1.770361
 C   -0.341093    4.449403    0.260209
 C   -0.465129    5.951517    0.535101
 C   -1.592417    4.042384   -0.521694
 C    1.522318    1.562491   -1.253036
 C    0.853071    1.226962   -2.406177
 C    2.869091    1.013602   -1.204334
 S    1.850936    0.268915   -3.436860
 C    3.179795    0.281046   -2.332523
 C   -0.555225    1.543182   -2.800668
 C    4.400016   -0.505473   -2.691631
 P    4.008151    1.439530    0.175727
 C    4.919915   -2.526549    1.072945
 C    4.339122   -1.412726    0.459983
 C    5.859070   -2.358432    2.088393
 C    4.699670   -0.119821    0.849632
 C    6.212829   -1.071839    2.499860
 C    5.630175    0.035760    1.891156
 C    7.737774    2.198333   -1.548355
 C    6.707565    1.564896   -0.851300
 C    7.519641    3.429042   -2.165162
 C    5.440341    2.153543   -0.758821
 C    6.262349    4.028159   -2.075501
 C    5.237129    3.399315   -1.372399
 H    2.065306    1.512159    2.907225
 H    3.705840    0.268731    4.279904
 H    3.512375   -2.198699    4.533229
 H   -0.012806   -2.174142    2.065815
 H    1.642123   -3.416496    3.424297
 H   -4.650272    2.647425    2.754260
 H   -2.738266    2.272932    1.248815
 H   -4.703706    1.569036    5.006490
 H   -2.797809    0.138315    5.731498
 H   -0.878008   -0.239061    4.230046
 H   -0.869874    3.571561    2.277020
 H    1.801359    3.436428    2.675091
 H    1.102434    5.056017    2.625830
 H    2.970530    3.889459    0.641465
 H    2.273763    5.516763    0.612967
 H    1.456971    5.654026   -1.737700
 H    0.556061    4.321967   -2.498865
 H    2.284369    4.138015   -2.160110
 H   -1.330898    6.142806    1.188983
 H   -0.641694    6.494216   -0.406960
 H    0.414029    6.402362    1.011448
 H   -2.495002    4.355934    0.026294
 H   -1.664991    2.962454   -0.695938
 H   -1.621556    4.545290   -1.501063
 H   -0.708126    2.620769   -2.958326
 H   -1.245900    1.217706   -2.008525
 H   -0.843899    1.025209   -3.725808
 H    4.174155   -1.582845   -2.635423
 H    5.227578   -0.293027   -2.006730
 H    4.736385   -0.276353   -3.714149
 H    4.654624   -3.522864    0.706989
 H    3.617736   -1.579857   -0.341757
 H    6.319082   -3.231051    2.558758
 H    6.944151   -0.930051    3.299495
 H    5.906837    1.040377    2.226455
 H    8.717030    1.717970   -1.613920
 H    6.898168    0.596488   -0.383775
 H    8.327407    3.921979   -2.711314
 H    6.079508    4.994940   -2.550828
 H    4.261814    3.887687   -1.301961
Cu   -1.282472   -0.689081   -0.308949
 H   -3.666246   -0.516322   -2.694532
 H   -3.347658    1.138185   -2.174938
 H   -3.309717    0.552370    0.180850
 H    1.149562   -5.629987    1.912216
 H    2.920936   -5.575836    1.656643
 H    1.897760   -6.645896    0.651161
 C    0.551516   -5.515880   -2.461729
 H    0.322531   -6.294912   -3.203163
 H    0.391773   -4.527724   -2.924460
 H   -0.148845   -5.625238   -1.615795
142
Figure 1_ts(AS)_major_05 / electronic energy: -5826.77845892 a.u. / lowest freq: -202.70 cm-1
 C    0.582252    0.907119    2.589417
 C    1.863737    1.256630    2.108384
 C    2.580355    0.459023    1.220636
 O    4.147139   -0.624533    2.215802
 P    5.347902    0.157059    2.733074
 O    6.748296   -0.277024    2.478581
 O    5.080964    1.688510    2.179342
 O    5.178368    0.360679    4.354005
 C    6.080294    2.663613    2.343841
 H    0.101045    1.546591    3.330402
 H    0.266101   -0.140566    2.580551
 H    2.283467    2.235752    2.357874
 H    2.197371   -0.507665    0.891162
 H    3.407145    0.892737    0.669950
 B   -3.917760    0.208000    1.449028
 O   -4.764324   -0.305610    2.394355
 O   -4.591359    0.734806    0.378458
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C	-6.101592	-0.291959	1.858370
C	-5.990144	0.776417	0.703074
C	-7.074833	0.072385	2.968379
C	-6.395129	-1.702373	1.351272
C	-6.296369	2.199354	1.167114
C	-6.796067	0.444495	-0.543006
H	-5.717698	2.466057	2.064325
H	-7.365909	2.334562	1.384434
H	-6.017255	2.902152	0.368879
H	-6.458509	-0.493704	-1.002804
H	-6.680947	1.246711	-1.287285
H	-7.866797	0.354753	-0.305600
H	-5.699438	-1.991841	0.550883
H	-7.422452	-1.792438	0.970226
H	-6.273404	-2.414770	2.180652
H	-8.096691	0.169923	2.571721
H	-6.798419	1.013174	3.461638
H	-7.080746	-0.720556	3.730753
C	-2.912868	3.724528	0.798284
C	-3.446979	4.880008	1.365502
C	-2.269064	2.742188	1.574055
C	-3.375919	5.085666	2.743065
C	-2.240977	2.957133	2.965107
C	-2.778738	4.107633	3.539718
C	-1.748006	1.486529	0.944229
C	-2.350946	0.227607	1.575980
H	-2.734162	4.238634	4.624134
H	-1.805900	2.200413	3.621160
H	-3.797219	5.987545	3.193354
H	-3.942412	5.615231	0.725620
H	-3.034069	3.555560	-0.273703
P	1.089653	1.624124	-1.496190
C	3.939222	1.507788	-1.630920
C	5.212134	2.061721	-1.501247
C	2.798074	2.306061	-1.499391
C	5.362352	3.421675	-1.239593
C	2.957495	3.672810	-1.229150
C	4.230276	4.225231	-1.101549
C	-1.409034	4.701946	-2.523268
C	-0.744441	3.685722	-1.835985
C	0.227475	2.913768	-2.472709
C	-1.099168	4.951639	-3.857994
C	-0.109053	4.199384	-4.495702
C	0.558675	3.191322	-3.806090
C	1.977822	-0.111124	-3.759521
C	1.076283	0.152497	-2.555133
C	0.191690	-0.867714	-2.503224
C	2.822991	-1.369439	-3.389664
C	1.781246	-2.506582	-3.410272
C	0.456930	-1.763997	-3.738316
C	-0.689966	-2.650842	-4.178888
C	0.961191	-0.700297	-4.775730
C	1.604033	-1.285585	-6.037996
C	-0.123462	0.267941	-5.247449
C	-0.917880	-1.269990	-1.598926
C	-2.204986	-0.851670	-1.838710
C	-0.861963	-2.437514	-0.724560
S	-3.341912	-1.943279	-1.131473
C	-2.113425	-2.941082	-0.439361
C	-2.693058	0.312722	-2.639340
C	-2.534379	-4.169969	0.308711
P	0.739841	-2.986574	-0.015113
C	-0.532211	-2.426296	3.934614
C	-0.577371	-2.636131	2.557370
C	0.694859	-2.299545	4.588411
C	0.604646	-2.724135	1.807855
C	1.876459	-2.375174	3.854411
C	1.829389	-2.582594	2.476034
C	1.124124	-7.049265	0.710592
C	1.106858	-5.664106	0.877994
C	0.711103	-7.619758	-0.492444
C	0.671455	-4.825932	-0.156867
C	0.285678	-6.792761	-1.532711
C	0.270977	-5.409406	-1.368110
H	3.845540	0.437541	-1.807724
H	6.089384	1.418324	-1.595639
H	6.359435	3.854725	-1.133268
H	2.083443	4.319333	-1.115958
H	4.336555	5.292115	-0.892299
H	-2.166140	5.298517	-2.008797
H	-0.970229	3.498069	-0.786843
H	-1.619130	5.743268	-4.402639
H	0.147414	4.403785	-5.537663
H	1.347059	2.627799	-4.307895
H	2.575252	0.742832	-4.104494
H	3.289748	-1.273308	-2.401010
H	3.631212	-1.527276	-4.117739
H	1.721549	-3.038090	-2.452950
H	1.993090	-3.257845	-4.184800
H	-0.402435	-3.234240	-5.067462
H	-1.584722	-2.062378	-4.432435
H	-0.982821	-3.361053	-3.392506
H	2.043688	-0.474194	-6.639449
H	0.840557	-1.775212	-6.662847
H	2.397201	-2.019045	-5.850858
H	0.308359	1.039233	-5.903477
H	-0.638607	0.777548	-4.426556

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 H   -0.880151   -0.270405   -5.839752
 H   -2.977305    0.025824   -3.664926
 H   -1.913629    1.083517   -2.703172
 H   -3.571821    0.763872   -2.154787
 H   -3.323777   -3.949610    1.043404
 H   -1.690771   -4.629592    0.835217
 H   -2.934254   -4.921230   -0.391536
 H   -1.466294   -2.349490    4.496299
 H   -1.549566   -2.703179    2.072933
 H    0.727042   -2.125488    5.666699
 H    2.846724   -2.242524    4.337062
 H    2.769909   -2.582066    1.920910
 H    1.460987   -7.686225    1.532105
 H    1.429629   -5.239359    1.831273
 H    0.721869   -8.704611   -0.620723
 H   -0.040316   -7.226806   -2.481009
 H   -0.070612   -4.777789   -2.190886
Cu    0.258476    1.381597    0.680076
 H   -2.071629    0.113947    2.635670
 H   -1.955464   -0.670642    1.075579
 H   -2.032122    1.503281   -0.119558
 H    5.695957    3.612576    1.941902
 H    7.003698    2.394645    1.805049
 H    6.332247    2.814336    3.408560
 C    3.952828    0.811217    4.873628
 H    3.958461    0.639827    5.960635
 H    3.097353    0.268493    4.437097
 H    3.806062    1.891177    4.694904
142
Figure 1_ts(AS)_major_06 / electronic energy: -5826.78081695 a.u. / lowest freq: -282.89 cm-1
 C   -0.145356   -0.154924    2.972086
 C    0.810654    0.893286    2.947781
 C    1.842055    0.955715    2.008715
 O    3.577700    0.354908    2.963525
 P    4.870598    0.166233    2.178748
 O    5.299488   -1.166792    1.660604
 O    4.779665    1.275886    0.967271
 O    6.100742    0.759384    3.081160
 C    5.815946    1.302262    0.011669
 H   -0.880064   -0.193627    3.779381
 H    0.096233   -1.112849    2.502261
 H    0.699424    1.721552    3.655531
 H    1.950340    0.175487    1.251760
 H    2.357277    1.893658    1.814195
 B   -3.817456   -1.819851    0.317417
 O   -4.581307   -2.886908    0.702988
 O   -4.387636   -1.117287   -0.713421
 C   -5.667763   -3.024023   -0.235305
 C   -5.736382   -1.587697   -0.879283
 C   -6.920504   -3.440144    0.518107
 C   -5.263986   -4.110139   -1.229449
 C   -6.635084   -0.623833   -0.106498
 C   -6.093351   -1.569207   -2.356567
 H   -6.397801   -0.623166    0.968084
 H   -7.699304   -0.870293   -0.230839
 H   -6.470791    0.395147   -0.486946
 H   -5.358332   -2.117716   -2.960165
 H   -6.125460   -0.531036   -2.719576
 H   -7.085648   -2.015910   -2.520847
 H   -4.356309   -3.829698   -1.783897
 H   -6.065813   -4.317123   -1.952733
 H   -5.050071   -5.038576   -0.679767
 H   -7.786892   -3.474362   -0.159546
 H   -7.146847   -2.751888    1.342806
 H   -6.782079   -4.444827    0.944282
 C   -3.192794    1.736761    3.149779
 C   -3.918561    2.101190    4.278580
 C   -3.243726    0.429482    2.621147
 C   -4.716620    1.161255    4.937528
 C   -4.042984   -0.501931    3.306837
 C   -4.768605   -0.140396    4.445273
 C   -2.461442    0.084297    1.396188
 C   -2.460680   -1.382846    0.973500
 H   -5.381739   -0.891571    4.950398
 H   -4.119301   -1.528498    2.943237
 H   -5.281757    1.441214    5.829649
 H   -3.849996    3.124054    4.658303
 H   -2.540276    2.477824    2.675712
 P   -0.498263    2.435679   -0.355431
 C    0.726323    4.222565    1.432427
 C    1.244431    5.448640    1.851764
 C    0.198589    4.068676    0.146419
 C    1.231043    6.542028    0.990017
 C    0.162232    5.185828   -0.702004
 C    0.681225    6.408696   -0.286352
 C   -4.427915    3.488937   -0.939674
 C   -3.228749    3.058565   -0.371997
 C   -2.065422    2.979018   -1.145474
 C   -4.475269    3.851093   -2.284763
 C   -3.314533    3.797859   -3.057322
 C   -2.117572    3.367236   -2.490149
 C    1.614411    2.699760   -2.392011
 C    0.578794    1.827952   -1.692095
 C    0.784861    0.552576   -2.103522
 C    2.959177    2.354319   -1.699984
 C    3.214232    0.908113   -2.184001
 C    1.977262    0.597277   -3.089664
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 C    2.113588   -0.574839   -4.040881
 C    1.757670    1.993716   -3.763355
 C    2.939959    2.499837   -4.598401
 C    0.526296    2.068095   -4.667227
 C    0.064263   -0.734507   -1.883301
 C   -1.171354   -0.951326   -2.457292
 C    0.673107   -1.980664   -1.405070
 S   -1.548387   -2.637705   -2.503480
 C   -0.074579   -3.090815   -1.726587
 C   -2.162695   -0.003852   -3.046914
 C    0.214179   -4.550523   -1.560420
 P    2.153558   -1.962622   -0.310243
 C    0.038918   -3.889984    2.738661
 C    0.354485   -3.363251    1.485058
 C    0.978840   -3.862977    3.766551
 C    1.613626   -2.804640    1.239208
 C    2.237993   -3.308127    3.531564
 C    2.555502   -2.780316    2.282159
 C    4.466594   -5.339780   -1.089139
 C    3.501087   -4.492168   -0.547948
 C    5.300126   -4.892429   -2.113821
 C    3.347252   -3.182781   -1.022470
 C    5.173112   -3.584584   -2.580382
 C    4.215536   -2.734189   -2.028704
 H    0.724439    3.379978    2.122160
 H    1.655722    5.545082    2.858977
 H    1.637662    7.502517    1.314767
 H   -0.282000    5.111039   -1.696235
 H    0.651445    7.264925   -0.963982
 H   -5.328966    3.535347   -0.323918
 H   -3.211639    2.790774    0.685048
 H   -5.415845    4.181905   -2.731130
 H   -3.340341    4.089082   -4.109807
 H   -1.218099    3.324279   -3.105528
 H    1.390361    3.771786   -2.430112
 H    2.884832    2.422495   -0.606032
 H    3.752033    3.047550   -2.015185
 H    3.293761    0.201469   -1.350145
 H    4.140459    0.825206   -2.771854
 H    2.979925   -0.432147   -4.705358
 H    1.214984   -0.679983   -4.668717
 H    2.251024   -1.528912   -3.515466
 H    2.762362    3.546978   -4.892100
 H    3.032861    1.914120   -5.526201
 H    3.909285    2.462250   -4.087238
 H    0.307303    3.115470   -4.931245
 H   -0.372563    1.634395   -4.217909
 H    0.711117    1.531175   -5.610400
 H   -1.790023    1.020360   -2.996489
 H   -3.107571   -0.046010   -2.482449
 H   -2.380892   -0.242401   -4.099677
 H    0.883756   -4.740340   -0.716360
 H    0.701999   -4.946253   -2.466001
 H   -0.708571   -5.126398   -1.397767
 H   -0.952981   -4.315818    2.908946
 H   -0.407708   -3.370438    0.707571
 H    0.730619   -4.269171    4.750141
 H    2.981401   -3.272181    4.331507
 H    3.540270   -2.328296    2.117910
 H    4.569735   -6.356292   -0.701782
 H    2.868872   -4.860259    0.263195
 H    6.056683   -5.557678   -2.536783
 H    5.836098   -3.214690   -3.366146
 H    4.156371   -1.702591   -2.379209
Cu   -0.649802    0.947576    1.405313
 H   -2.183169   -2.045870    1.807094
 H   -1.687821   -1.525856    0.200101
 H   -2.853244    0.683483    0.559929
 H    5.614431    2.127790   -0.684578
 H    5.869948    0.356868   -0.551499
 H    6.797131    1.477537    0.486783
 C    5.950519    2.010974    3.709024
 H    6.899910    2.255618    4.207114
 H    5.147507    1.991381    4.464067
 H    5.722711    2.808180    2.980015
142
Figure 1_pi-allyl_major_01 / electronic energy: -5826.81392270 a.u. / lowest freq: 20.43 cm-1
 P   -0.073699    2.006942   -0.786878
 C    0.932353    2.738799   -3.265460
 C    1.191523    3.596536   -4.333493
 C    0.179411    3.175952   -2.169340
 C    0.690884    4.897217   -4.318744
 C   -0.321943    4.484487   -2.163339
 C   -0.068211    5.338917   -3.233654
 C    2.392440    4.276236    1.640595
 C    1.528005    3.905694    0.610492
 C    1.025460    2.601619    0.552275
 C    2.760656    3.352742    2.619377
 C    2.259616    2.052045    2.568211
 C    1.401692    1.683470    1.536920
 C   -2.931365    2.639681   -1.106187
 C   -1.752803    2.333717   -0.189677
 C   -2.243948    2.222984    1.062164
 C   -3.777460    1.334806   -1.136658
 C   -4.345602    1.261215    0.294398
 C   -3.752983    2.526802    0.984030
 C   -4.448612    2.903045    2.275380
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C	-3.789135	3.559886	-0.193727
C	-5.188527	3.852692	-0.745733
C	-3.151441	4.912199	0.129272
C	-1.638347	1.742122	2.326938
C	-1.333494	2.587636	3.362920
C	-1.471363	0.337706	2.673867
S	-0.892023	1.692102	4.773383
C	-1.118808	0.163637	3.995589
C	-1.271062	4.080968	3.374611
C	-0.985394	-1.082750	4.817369
P	-1.625055	-0.961065	1.385091
C	1.958043	-2.714251	2.633420
C	0.914400	-1.803833	2.467626
C	1.892659	-3.974396	2.044199
C	-0.219919	-2.132139	1.711589
C	0.789232	-4.298309	1.254649
C	-0.248037	-3.383964	1.073360
C	-4.765865	-3.616912	1.359524
C	-3.603059	-2.912458	1.047133
C	-5.484686	-3.318615	2.516835
C	-3.124686	-1.912759	1.909678
C	-5.034024	-2.304580	3.361389
C	-3.863946	-1.606616	3.060860
H	1.325547	1.719417	-3.281834
H	1.785322	3.242404	-5.178871
H	0.890121	5.570181	-5.155937
H	-0.915443	4.839597	-1.319995
H	-0.466761	6.355756	-3.219592
H	2.786263	5.294563	1.673226
H	1.267592	4.638321	-0.154744
H	3.444056	3.646937	3.419219
H	2.548054	1.316286	3.321735
H	1.023115	0.663652	1.493572
H	-2.678118	3.038518	-2.097224
H	-3.158682	0.465858	-1.376532
H	-4.567610	1.395717	-1.898405
H	-4.056165	0.345782	0.825979
H	-5.444709	1.300663	0.312351
H	-5.515282	3.100725	2.086450
H	-4.014939	3.802708	2.736718
H	-4.389356	2.087076	3.012055
H	-5.107301	4.417429	-1.688265
H	-5.755293	4.478486	-0.038573
H	-5.792373	2.960229	-0.949863
H	-3.162030	5.561630	-0.760419
H	-2.113156	4.831747	0.474591
H	-3.726022	5.430478	0.913376
H	-1.718413	4.488706	2.460512
H	-0.225504	4.427453	3.415579
H	-1.799771	4.511714	4.238475
H	0.027286	-1.198658	5.233452
H	-1.211562	-1.975664	4.223255
H	-1.689061	-1.057656	5.664441
H	2.826741	-2.427264	3.229683
H	0.987380	-0.833462	2.958456
H	2.707774	-4.690151	2.175270
H	0.738241	-5.267789	0.753404
H	-1.058130	-3.636567	0.385709
H	-5.116469	-4.395483	0.677558
H	-3.078299	-3.124443	0.108001
H	-6.400587	-3.865579	2.754150
H	-5.595030	-2.051822	4.264702
H	-3.535992	-0.809943	3.730306
C	0.608457	-1.768988	-2.708482
C	-0.159290	-0.863180	-3.500982
C	-1.300490	-0.311371	-2.967420
O	-1.717749	-4.054778	-4.036663
P	-2.534336	-3.671793	-2.847377
O	-1.915143	-3.179522	-1.557331
O	-3.640472	-2.557851	-3.360707
O	-3.528263	-4.904596	-2.386234
C	-4.560712	-2.035549	-2.437605
H	1.543832	-2.158730	-3.105739
H	0.054126	-2.418255	-2.013854
H	0.284349	-0.430706	-4.404801
H	-1.805660	-0.841925	-2.151687
H	-1.823629	0.507354	-3.466281
B	4.165394	-1.939955	0.109235
O	5.197124	-2.831033	0.000516
O	4.395940	-0.988326	1.065923
C	6.133411	-2.564676	1.063982
C	5.774359	-1.083304	1.461457
C	7.547080	-2.752874	0.536758
C	5.851800	-3.571569	2.176596
C	6.539892	-0.039717	0.648761
C	5.890896	-0.776454	2.945675
H	6.469898	-0.238813	-0.431061
H	7.602316	-0.003444	0.929996
H	6.099427	0.950620	0.835295
H	5.224728	-1.407321	3.548753
H	5.621594	0.274452	3.129054
H	6.924070	-0.926858	3.293296
H	4.843378	-3.440157	2.594249
H	6.583404	-3.485478	2.992880
H	5.917866	-4.588468	1.762560
H	8.285848	-2.444008	1.291492
H	7.719350	-2.175296	-0.380652

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 H     7.721081   -3.814469    0.306880
 C     3.680911    1.560601   -1.318192
 C     4.454721    2.421796   -2.093343
 C     3.206269    0.341910   -1.833323
 C     4.785493    2.083271   -3.405281
 C     3.570894    0.006198   -3.149058
 C     4.345650    0.864791   -3.925851
 C     2.344776   -0.550325   -0.995629
 C     2.875518   -1.961047   -0.792783
 H     4.605600    0.580927   -4.948821
 H     3.233559   -0.938450   -3.580995
 H     5.388643    2.758704   -4.016511
 H     4.805070    3.364059   -1.664482
 H     3.442509    1.830380   -0.288282
Cu     0.484424   -0.089266   -1.636044
 H     3.112009   -2.471686   -1.738888
 H     2.118314   -2.587395   -0.295283
 H     2.210358   -0.092583   -0.008685
 H    -5.117716   -1.223704   -2.929693
 H    -4.062811   -1.627445   -1.541865
 H    -5.285689   -2.799267   -2.103087
 C    -4.228319   -5.602799   -3.384667
 H    -4.772118   -6.431898   -2.907407
 H    -3.543621   -6.016031   -4.144353
 H    -4.961400   -4.956865   -3.901224
142
Figure 1_pi-allyl_major_02 / electronic energy: -5826.80177164 a.u. / lowest freq: 15.50 cm-1
 C     0.093530    1.897507    2.580760
 C     1.178549    2.673278    2.064492
 C     2.276090    2.063877    1.507012
 O     4.553634    0.148020    2.233954
 P     5.816027    0.939768    2.020601
 O     7.082968    0.333657    1.508294
 O     5.377486    2.222294    1.063663
 O     6.191872    1.736543    3.417314
 C     6.378143    2.970810    0.427441
 H    -0.776387    2.409645    2.988655
 H     0.308699    0.908601    3.005324
 H     1.004451    3.741156    1.886752
 H     2.595315    1.049356    1.778212
 H     3.022057    2.631707    0.945697
 B    -4.059256    0.417125    1.558945
 O    -4.912652    0.308757    2.621488
 O    -4.718024    0.591041    0.373724
 C    -6.259063    0.231741    2.109474
 C    -6.103465    0.845516    0.665723
 C    -7.182994    1.012453    3.030466
 C    -6.650335   -1.244022    2.099457
 C    -6.290939    2.361125    0.630171
 C    -6.967823    0.187718   -0.397721
 H    -5.681540    2.861392    1.396516
 H    -7.343432    2.642641    0.777456
 H    -5.964428    2.738522   -0.350133
 H    -6.739828   -0.880287   -0.510426
 H    -6.802044    0.677906   -1.368657
 H    -8.034596    0.292326   -0.148234
 H    -5.997913   -1.829985    1.435928
 H    -7.692913   -1.384989    1.780025
 H    -6.546130   -1.648839    3.116997
 H    -8.196598    1.067382    2.605745
 H    -6.818320    2.033822    3.199898
 H    -7.250890    0.509414    4.006397
 C    -2.305198    3.558620   -0.391843
 C    -2.790719    4.863655   -0.395755
 C    -2.316036    2.773816    0.773922
 C    -3.307569    5.425918    0.772182
 C    -2.853009    3.353807    1.938352
 C    -3.338201    4.660512    1.937789
 C    -1.820799    1.367466    0.741282
 C    -2.489085    0.394974    1.697118
 H    -3.754181    5.080594    2.856955
 H    -2.915818    2.773339    2.861857
 H    -3.692476    6.448275    0.771604
 H    -2.771242    5.440863   -1.323566
 H    -1.919655    3.129289   -1.318395
 P     0.951657    1.009190   -1.501806
 C     3.549445    0.171764   -0.893622
 C     4.914636    0.023306   -1.129171
 C     2.766673    0.949064   -1.751559
 C     5.505233    0.651492   -2.222856
 C     3.369027    1.594491   -2.840454
 C     4.733413    1.443299   -3.074353
 C     0.548841    4.987899   -2.322365
 C     0.951495    3.767671   -1.788900
 C     0.470817    2.566237   -2.330240
 C    -0.343035    5.022410   -3.396889
 C    -0.821608    3.831658   -3.939238
 C    -0.413704    2.605790   -3.409482
 C     1.072261   -0.651168   -3.898823
 C     0.384641   -0.338100   -2.571094
 C    -0.449688   -1.363663   -2.304788
 C     2.069921   -1.798347   -3.571466
 C     1.123011   -2.972584   -3.247821
 C    -0.303692   -2.372030   -3.466794
 C    -1.385627   -3.421037   -3.618337
 C    -0.044053   -1.408433   -4.669525
 C     0.442519   -2.096300   -5.950214
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 C   -1.250554   -0.556548   -5.063705
 C   -1.347668   -1.723583   -1.179947
 C   -2.708322   -1.567181   -1.297823
 C   -0.973105   -2.597593   -0.081123
 S   -3.531952   -2.570709   -0.158991
 C   -2.067113   -3.179296    0.526001
 C   -3.487513   -0.738942   -2.269952
 C   -2.162036   -4.230746    1.590231
 P    0.783073   -2.700032    0.431522
 C   -0.051771   -1.395343    4.322106
 C   -0.238850   -1.904641    3.038900
 C    1.209360   -0.953752    4.729996
 C    0.832260   -1.988597    2.135993
 C    2.275441   -1.005171    3.836209
 C    2.084379   -1.513127    2.549769
 C    1.987502   -6.348784    1.981496
 C    1.757977   -4.981195    1.826240
 C    1.487396   -7.257986    1.050483
 C    1.017296   -4.503645    0.737918
 C    0.757501   -6.790061   -0.043219
 C    0.527831   -5.424854   -0.200665
 H    3.104769   -0.315115   -0.024905
 H    5.527110   -0.550282   -0.432127
 H    6.576576    0.536326   -2.403353
 H    2.773325    2.214854   -3.513655
 H    5.195273    1.947025   -3.926755
 H    0.928495    5.917698   -1.893374
 H    1.647950    3.749192   -0.945751
 H   -0.665000    5.980873   -3.810275
 H   -1.518808    3.850803   -4.779832
 H   -0.796090    1.679931   -3.837273
 H    1.516557    0.210323   -4.414935
 H    2.724664   -1.539068   -2.731586
 H    2.715653   -2.011641   -4.434705
 H    1.245177   -3.345658   -2.222277
 H    1.272890   -3.830213   -3.920131
 H   -1.159863   -4.074980   -4.474697
 H   -2.377686   -2.976813   -3.782616
 H   -1.450288   -4.057476   -2.721876
 H    0.794337   -1.338554   -6.668696
 H   -0.387436   -2.637787   -6.430503
 H    1.258715   -2.813769   -5.802969
 H   -0.955432    0.205604   -5.802033
 H   -1.717955   -0.050045   -4.213581
 H   -2.023029   -1.184014   -5.535199
 H   -3.600268   -1.240636   -3.243964
 H   -2.986962    0.225211   -2.437764
 H   -4.486491   -0.518328   -1.874595
 H   -2.905228   -3.966317    2.357531
 H   -1.197727   -4.393416    2.084228
 H   -2.470608   -5.191504    1.147305
 H   -0.901184   -1.338839    5.007254
 H   -1.237671   -2.222767    2.747325
 H    1.350747   -0.550541    5.735755
 H    3.267585   -0.625643    4.086703
 H    2.945491   -1.510014    1.876884
 H    2.561065   -6.703611    2.841219
 H    2.154576   -4.285499    2.569612
 H    1.665725   -8.328373    1.176628
 H    0.361599   -7.493500   -0.779807
 H   -0.055306   -5.074445   -1.056785
Cu    0.225738    1.380947    0.663724
 H   -2.228827    0.577941    2.751336
 H   -2.135774   -0.623813    1.479056
 H   -1.893227    0.985600   -0.287004
 H    5.892151    3.669532   -0.271238
 H    7.070901    2.326635   -0.137626
 H    6.974324    3.560171    1.148602
 C    5.173652    2.425156    4.092004
 H    5.590131    2.825560    5.029360
 H    4.321812    1.767859    4.339959
 H    4.787047    3.273465    3.497936
142
Figure 1_pi-allyl_major_03 / electronic energy: -5826.80299964 a.u. / lowest freq: 13.04 cm-1
 C   -1.411603   -1.919227   -2.109234
 C   -0.389358   -2.578018   -1.350087
 C    0.757083   -1.916936   -0.987979
 O    3.247883   -3.292303   -1.731570
 P    3.214159   -4.603215   -0.995113
 O    4.402506   -5.203699   -0.311182
 O    1.974013   -4.452760    0.103223
 O    2.600098   -5.772679   -1.979495
 C    1.786679   -5.470166    1.051084
 H   -2.333935   -2.457204   -2.329373
 H   -1.110564   -1.175314   -2.857422
 H   -0.633495   -3.519184   -0.845399
 H    1.094538   -1.038778   -1.540537
 H    1.444905   -2.364022   -0.273612
 B   -5.311993    0.362189   -1.579696
 O   -6.411640   -0.115430   -2.229384
 O   -5.629919    1.120360   -0.484892
 C   -7.580267    0.463233   -1.608048
 C   -7.025415    0.899100   -0.200480
 C   -8.679851   -0.584454   -1.558445
 C   -8.009983    1.644871   -2.473877
 C   -7.092141   -0.217029    0.841696
 C   -7.631925    2.175147    0.358172
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H	-6.666192	-1.156197	0.457543
H	-8.125849	-0.406497	1.164504
H	-6.503172	0.080298	1.721796
H	-7.451076	3.036433	-0.298026
H	-7.188707	2.395491	1.340723
H	-8.717177	2.058827	0.496622
H	-7.231485	2.421218	-2.511764
H	-8.938715	2.100050	-2.101000
H	-8.188373	1.291946	-3.500161
H	-9.548814	-0.207533	-0.998588
H	-8.332446	-1.513408	-1.088149
H	-9.012372	-0.824375	-2.579231
C	-3.612117	-2.120821	1.217367
C	-4.189909	-3.252765	1.783814
C	-3.785439	-1.813650	-0.144443
C	-4.963114	-4.113253	1.001649
C	-4.561802	-2.692556	-0.918084
C	-5.145574	-3.825190	-0.350228
C	-3.168042	-0.576003	-0.703876
C	-3.815616	0.022699	-1.944099
H	-5.753762	-4.485669	-0.973327
H	-4.737178	-2.482993	-1.975048
H	-5.422648	-4.999760	1.444655
H	-4.042421	-3.458301	2.846911
H	-3.026201	-1.446214	1.845120
P	-0.445407	0.546222	1.283946
C	1.704478	0.522385	3.122198
C	2.620095	-0.119288	3.953007
C	0.845498	-0.227739	2.313453
C	2.685086	-1.511508	3.981582
C	0.910172	-1.626390	2.351888
C	1.828923	-2.265673	3.180181
C	-4.105183	1.598873	2.792297
C	-2.958491	1.521079	2.007244
C	-1.844041	0.788857	2.442124
C	-4.152765	0.947154	4.025033
C	-3.043104	0.231800	4.472512
C	-1.892687	0.151269	3.686927
C	-0.394853	3.529349	1.472461
C	0.025522	2.226205	0.797159
C	0.730099	2.560643	-0.305636
C	0.899374	4.167859	2.042891
C	1.681100	4.548361	0.769601
C	0.738565	4.096233	-0.389768
C	1.076128	4.709367	-1.733107
C	-0.671183	4.420512	0.228769
C	-0.899136	5.902953	0.541393
C	-1.866960	3.962296	-0.609989
C	1.420949	1.687699	-1.286340
C	0.848258	1.381595	-2.498356
C	2.765405	1.150115	-1.144280
S	1.934911	0.456196	-3.469545
C	3.172096	0.447073	-2.261000
C	-0.526946	1.698561	-2.997294
C	4.425400	-0.320034	-2.537653
P	3.799177	1.611020	0.306228
C	4.927907	-2.288548	1.254019
C	4.288759	-1.220461	0.615634
C	5.812147	-2.052625	2.304481
C	4.539337	0.093682	1.020122
C	6.050874	-0.745087	2.732466
C	5.409776	0.316129	2.101697
C	7.572007	2.546031	-1.230088
C	6.539667	1.868495	-0.579158
C	7.326651	3.761140	-1.867017
C	5.242733	2.395841	-0.554295
C	6.039254	4.299754	-1.844415
C	5.011051	3.626469	-1.188123
H	1.664786	1.611219	3.102028
H	3.293281	0.474753	4.574234
H	3.412863	-2.011682	4.624047
H	0.240284	-2.224589	1.731287
H	1.884281	-3.355930	3.188892
H	-4.966881	2.161495	2.428059
H	-2.936974	2.038246	1.046047
H	-5.056027	0.998290	4.637277
H	-3.070231	-0.273537	5.440358
H	-1.036627	-0.422317	4.048013
H	-1.210186	3.448405	2.201168
H	1.452275	3.472466	2.686289
H	0.654728	5.046228	2.657039
H	2.653440	4.044891	0.708470
H	1.865608	5.630309	0.699549
H	1.142207	5.804712	-1.647066
H	0.318959	4.478112	-2.496065
H	2.043475	4.344561	-2.110872
H	-1.799918	6.019241	1.164834
H	-1.074170	6.462564	-0.390962
H	-0.068835	6.392942	1.064325
H	-2.807301	4.197944	-0.087236
H	-1.863105	2.886762	-0.822768
H	-1.893322	4.495073	-1.573538
H	-0.692448	2.780985	-3.092442
H	-1.281819	1.310190	-2.298522
H	-0.717003	1.243838	-3.979291
H	4.231720	-1.400583	-2.412993
H	5.223630	-0.031304	-1.844821

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 H     4.782860   -0.141883   -3.563090
 H     4.754191   -3.308731    0.896737
 H     3.620657   -1.448545   -0.217391
 H     6.316450   -2.890829    2.792085
 H     6.736130   -0.550693    3.561413
 H     5.596446    1.338003    2.447051
 H     8.574483    2.111472   -1.243560
 H     6.752277    0.912374   -0.096423
 H     8.136020    4.287935   -2.378143
 H     5.834492    5.253679   -2.336531
 H     4.010407    4.066520   -1.173230
Cu    -1.157537   -0.806721   -0.473526
 H    -3.761455   -0.632436   -2.826852
 H    -3.303539    0.959689   -2.215819
 H    -3.172640    0.181133    0.087348
 H     0.856559   -5.261263    1.602023
 H     2.622687   -5.524634    1.768239
 H     1.683878   -6.461240    0.573928
 C     1.478454   -5.477164   -2.770679
 H     1.404577   -6.237953   -3.563106
 H     1.566316   -4.483468   -3.241043
 H     0.543013   -5.504143   -2.182330
64
Figure 2_L-Cu-OtBu_dimer / electronic energy: -4357.97211601 a.u. / lowest freq: -19.85 cm-1
 H    -1.057876   -2.823794   -2.825878
 H    -1.980246   -2.667714   -1.312041
 O     0.078207   -1.017819   -1.258789
 C    -1.048228   -3.061420   -1.749889
 H    -1.045898   -4.158508   -1.636503
 C     0.158516   -2.389922   -1.074836
 H     1.475367   -2.665464   -2.785121
 H    -0.759805   -2.350911    0.894993
 C     1.458383   -2.909326   -1.710688
 C     0.156991   -2.742073    0.424044
 H     2.324017   -2.413213   -1.241845
 H     1.581586   -3.999730   -1.600580
 H     1.020173   -2.268300    0.919277
 H     0.205803   -3.828385    0.609487
Cu     1.378579    0.329330   -0.465065
 H     2.131666   -0.991227    3.381390
 H     4.682348   -1.405429    2.732758
 H     5.481708   -1.718565    0.494438
 H     4.675857   -1.081458   -2.009653
 C     2.171292   -0.117226    2.712040
 C     4.582052   -0.512693    2.098216
 H     1.198856   -0.010984    2.213049
 N     3.192040   -0.289898    1.712946
 C     3.045354   -0.000511    0.406199
 C     5.265779   -0.663084    0.738250
 N     4.251927   -0.137199   -0.170576
 H     3.612584    0.354358   -2.080687
 C     4.493554   -0.077568   -1.587637
 H     2.354764    0.782239    3.326204
 H     4.963659    0.354622    2.665833
 H     6.206045   -0.097525    0.661498
 H     5.369453    0.553572   -1.807185
 H    -0.378809    4.066234    1.363434
 H    -1.215620    2.487467    1.315536
 C    -0.309944    3.028560    0.996342
 H    -1.542344    4.628000   -0.917965
 H    -2.304280    3.010119   -0.908883
 H     0.559090    2.547332    1.474899
 C    -1.400215    3.570787   -1.196882
 C    -0.167055    2.941122   -0.531923
 H     1.054762    4.773347   -0.703921
 H    -1.305843    3.511187   -2.293040
 C     1.092639    3.703570   -0.968950
 O    -0.065048    1.615388   -0.935560
 H     1.981855    3.258646   -0.494162
 H     1.220534    3.621154   -2.060206
Cu    -1.382126    0.156912   -0.516840
 H    -2.351582    0.600724    3.422431
 H    -4.934218   -0.004844    2.870939
 H    -6.034910    0.158807    0.756762
 H    -5.219728    0.475454   -1.806850
 C    -2.122775   -0.170906    2.668848
 C    -4.523985   -0.695038    2.117592
 H    -1.198578    0.107935    2.144915
 N    -3.185413   -0.283990    1.706499
 C    -3.039380   -0.179163    0.373767
 C    -5.297331   -0.660916    0.794239
 N    -4.235455   -0.434437   -0.181200
 H    -3.591154   -0.191053   -2.134929
 C    -4.528168   -0.356233   -1.586950
 H    -1.956896   -1.128121    3.192726
 H    -4.493762   -1.703279    2.564902
 H    -5.829131   -1.601827    0.585031
 H    -4.988412   -1.291515   -1.945367
32
Figure 2_L-Cu-OtBu / electronic energy: -2178.96309100 a.u. / lowest freq: 32.39 cm-1
 H     4.562030   -0.987762   -1.171425
 H     4.380081   -1.687590    0.453032
 O     2.059982   -0.792706   -0.375405
 C     4.412589   -0.739884   -0.108257
 H     5.285124   -0.160867    0.237784
 C     3.083853    0.016444    0.070903
 H     3.239088    1.094749   -1.813757
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 H    2.816631   -0.564871    2.149701
 C    3.141678    1.325832   -0.740702
 C    2.905653    0.363686    1.562854
 H    2.203830    1.891377   -0.606175
 H    3.980920    1.980488   -0.449346
 H    1.973161    0.937231    1.704528
 H    3.740138    0.957642    1.973285
Cu    0.281496   -0.385007   -0.217334
 H   -2.761249   -2.831320    0.955264
 H   -4.389467   -0.710878    1.073176
 H   -3.900683    1.628760    1.086134
 H   -1.572215    2.982676    0.893515
 C   -2.368865   -2.376101    0.031132
 C   -3.894740   -0.371839    0.149702
 H   -1.295333   -2.593746   -0.043339
 N   -2.556823   -0.949305    0.044007
 C   -1.588253   -0.032817   -0.058431
 C   -3.606305    1.135384    0.145880
 N   -2.155228    1.178072   -0.017727
 H   -0.385003    2.236847   -0.219836
 C   -1.452620    2.433488   -0.055287
 H   -2.885552   -2.835640   -0.827649
 H   -4.517059   -0.688565   -0.702765
 H   -4.103640    1.662997   -0.682992
 H   -1.827633    3.068788   -0.873938
74
Figure 2_ed / electronic energy: -3000.72395415 a.u. / lowest freq: -18.37 cm-1
 H   -4.229726    2.326034   -0.150745
 H   -5.967249    0.343716    0.271356
 H   -3.598722   -3.318573    1.735428
 H   -5.751654   -1.943746    0.936556
 H   -2.602038    1.801266   -0.690477
 H   -2.058957   -2.801506    0.982474
 C   -3.680511    1.617234   -0.792634
 C   -3.082739   -0.631120    0.042698
 N   -3.970093    0.257841   -0.410861
 N   -3.731163   -1.761591    0.333175
 C   -3.126225   -2.981981    0.798743
 C   -5.341967   -0.246351   -0.418210
 C   -5.161926   -1.699720    0.039540
 H   -3.978015    1.799131   -1.838489
 H   -5.779726   -0.163645   -1.424914
 H   -3.228038   -3.784690    0.049042
 H   -5.421195   -2.428940   -0.745075
 H   -1.082452    3.518912    1.603248
 H    0.421000    3.855965    0.726137
 O    0.362799    1.259831    1.681643
 C    0.000087    3.675244    1.723920
 H    0.157069    4.577191    2.336829
 C    0.647440    2.454235    2.386838
 H   -1.041587    2.096285    3.707116
 H    2.616865    2.798759    1.517328
 C    0.046175    2.252029    3.779325
 C    2.162870    2.651821    2.505931
 H    0.485762    1.362278    4.255566
 H    0.231377    3.121792    4.428639
 H    2.624169    1.758465    2.954414
 H    2.399418    3.521663    3.139641
Cu   -1.156351   -0.318937    0.168491
 H    3.647599   -2.084771   -1.808356
 H    4.667626   -2.150948    0.441562
 H    3.655695   -0.715072    0.059525
 C    3.791806   -1.560284    0.748890
 H    3.766971   -3.811735   -1.373951
 H    3.989671   -1.143848    1.747863
 C    3.071698   -3.006853   -1.658071
 H    2.610722   -3.279576   -2.619431
 C    1.991855   -2.826667   -0.601374
 C    2.522294   -2.409985    0.814491
 O    1.169976   -1.706527   -0.954041
 H    3.446123   -4.284636    1.408303
 B    0.804805   -1.023733    0.203641
 H    3.081088   -3.176114    2.752087
 C    2.709243   -3.561359    1.790696
 O    1.472302   -1.555242    1.289645
 H    1.649931   -4.980210   -0.367044
 C    1.084847   -4.057441   -0.565083
 H    0.586842   -4.163168   -1.540589
 H    1.766043   -4.089918    1.981929
 H    0.303393   -3.954382    0.202674
 H    0.142553    4.036318   -1.814791
 H    2.021822    3.781526   -0.667704
 H   -1.142136    3.179841   -2.691591
 C   -0.059830    3.194506   -2.489871
 O   -0.270892    1.738450   -0.614242
 H    2.659078    3.660530   -2.329825
 C    2.572105    3.136225   -1.366163
 H    0.457094    3.377402   -3.444530
 B    0.601562    1.008532    0.304352
 H    3.586208    2.995173   -0.962469
 C    0.360180    1.861111   -1.877169
 C    1.904481    1.766240   -1.514568
 O    1.926733    1.143401   -0.240157
 H   -1.221585    0.778172   -2.863054
 C   -0.123344    0.730502   -2.793547
 H    0.281161    0.832229   -3.811835
 H    0.157572   -0.257891   -2.407175
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 H    2.663210    1.336698   -3.516069
 C    2.714992    0.923238   -2.496709
 H    3.773217    0.915775   -2.191785
 H    2.356419   -0.113387   -2.509049
74
Figure 2_ts(TB) / electronic energy: -3000.72314236 a.u. / lowest freq: -71.58 cm-1
 H   -4.448283    1.831801   -0.546545
 H   -6.034945   -0.274227   -0.136759
 H   -3.216551   -3.476593    1.843614
 H   -5.506494   -2.318901    0.990513
 H   -2.733610    1.438777   -0.890484
 H   -1.787148   -3.089113    0.837440
 C   -3.773199    1.128838   -1.061090
 C   -2.995601   -1.009119   -0.092528
 N   -3.958927   -0.208011   -0.557112
 N   -3.547831   -2.188579    0.211178
 C   -2.863967   -3.303706    0.812657
 C   -5.261789   -0.864729   -0.651030
 C   -4.996322   -2.217748    0.017945
 H   -3.991266    1.174517   -2.142029
 H   -5.558704   -0.964972   -1.708457
 H   -3.032398   -4.223784    0.230395
 H   -5.289878   -3.073253   -0.608926
 H   -1.889619    3.082951    1.743967
 H   -0.475447    3.841768    0.978387
 O    0.012370    1.213800    1.663904
 C   -0.874460    3.464722    1.930869
 H   -0.944087    4.308818    2.634747
 C    0.013393    2.358438    2.507367
 H   -1.580508    1.488051    3.697900
 H    1.869593    3.236060    1.766788
 C   -0.558425    1.872271    3.838323
 C    1.443340    2.866966    2.709358
 H    0.060226    1.055179    4.239327
 H   -0.588936    2.683719    4.581426
 H    2.086995    2.051714    3.072839
 H    1.463920    3.684030    3.447489
Cu   -1.064796   -0.614475    0.066837
 H    4.152179   -1.222790   -1.601625
 H    4.926631   -1.208560    0.732258
 H    3.609618   -0.050027    0.333136
 C    3.901707   -0.891709    0.976936
 H    4.666629   -2.898230   -1.268204
 H    3.893798   -0.529670    2.016219
 C    3.817631   -2.267672   -1.575410
 H    3.534087   -2.557519   -2.598835
 C    2.634973   -2.459067   -0.637358
 C    2.900430   -2.039896    0.849730
 O    1.576663   -1.571157   -1.014383
 H    4.231911   -3.656063    1.429621
 B    0.913650   -1.122778    0.130318
 H    3.464389   -2.800114    2.789141
 C    3.297763   -3.183901    1.771368
 O    1.621543   -1.531095    1.251149
 H    2.864132   -4.640428   -0.558217
 C    2.093462   -3.884147   -0.768821
 H    1.733821   -4.037022   -1.797388
 H    2.516389   -3.953389    1.826435
 H    1.245776   -4.049768   -0.087193
 H   -0.420230    4.054241   -1.831844
 H    1.344645    4.063200   -0.458545
 H   -1.457836    3.001197   -2.817127
 C   -0.416657    3.197554   -2.518434
 O   -0.527086    1.723785   -0.642973
 H    2.129607    4.141849   -2.060330
 C    2.062456    3.564957   -1.125973
 H    0.146515    3.473608   -3.422999
 B    0.378612    1.188218    0.318412
 H    3.048455    3.588701   -0.638400
 C    0.169014    1.950819   -1.865317
 C    1.669377    2.108377   -1.380171
 O    1.690769    1.442805   -0.120721
 H   -1.129452    0.602593   -2.935045
 C   -0.047937    0.753365   -2.794138
 H    0.399213    0.929741   -3.783876
 H    0.379967   -0.167761   -2.378157
 H    2.645391    1.898337   -3.314327
 C    2.688765    1.457115   -2.306623
 H    3.703702    1.618116   -1.911727
 H    2.515077    0.376425   -2.376759
74
Figure 2_prod / electronic energy: -3000.74272641 a.u. / lowest freq: 20.41 cm-1
 H   -3.886200    1.904460    0.040425
 H   -5.783170   -0.000028    0.231301
 H   -3.671290   -4.009664    0.712028
 H   -5.779110   -2.391811    0.307129
 H   -2.431530    1.418920   -0.867743
 H   -2.156883   -3.467472   -0.075581
 C   -3.521445    1.318515   -0.819820
 C   -3.044171   -1.083929   -0.477400
 N   -3.884978   -0.068040   -0.690769
 N   -3.774686   -2.199854   -0.351226
 C   -3.248139   -3.529587   -0.185304
 C   -5.293235   -0.458612   -0.643950
 C   -5.207063   -1.984777   -0.540404
 H   -3.958179    1.745967   -1.737311
 H   -5.823136   -0.116425   -1.545676
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 H   -3.484024   -4.160187   -1.059528
 H   -5.550488   -2.493752   -1.456806
 H   -0.953241    3.764861    3.357981
 H    0.759299    3.428938    2.975556
 O   -0.875512    1.986080    1.406417
 C   -0.148430    3.018702    3.444873
 H    0.062558    2.860737    4.513442
 C   -0.552175    1.706030    2.774674
 H   -2.662097    1.885852    3.254227
 H    1.522396    1.080215    2.546667
 C   -1.843289    1.160855    3.378161
 C    0.563820    0.669955    2.888868
 H   -2.130100    0.224690    2.875511
 H   -1.717424    0.955828    4.451620
 H    0.344931   -0.216712    2.276614
 H    0.673948    0.353697    3.937508
Cu   -1.061912   -1.136593   -0.315311
 H    4.402647   -0.650240   -0.989617
 H    4.621398   -1.002509    1.402523
 H    3.160136   -0.085512    0.918287
 C    3.522073   -0.979220    1.447740
 H    5.192444   -2.244337   -0.885959
 H    3.226802   -0.887955    2.503535
 C    4.303465   -1.709747   -1.255594
 H    4.297891   -1.782907   -2.353926
 C    3.032949   -2.326933   -0.689967
 C    2.899711   -2.248976    0.864652
 O    1.888776   -1.577832   -1.121179
 H    4.481998   -3.631811    1.423538
 B    0.903669   -1.611522   -0.123564
 H    3.275879   -3.326507    2.696880
 C    3.409346   -3.471239    1.614104
 O    1.480199   -2.146878    1.031772
 H    3.743816   -4.379616   -1.009699
 C    2.869341   -3.749566   -1.231268
 H    2.746510   -3.702507   -2.323658
 H    2.863688   -4.380535    1.328701
 H    1.973529   -4.232021   -0.812859
 H    0.385110    4.774697   -2.173196
 H    1.496802    4.695314   -0.164989
 H   -0.507126    3.734422   -3.303777
 C    0.419699    3.821781   -2.717391
 O   -0.524972    2.690348   -0.813439
 H    2.757526    4.544486   -1.420219
 C    2.313155    4.059293   -0.539290
 H    1.265214    3.846315   -3.421248
 B   -0.030339    2.224887    0.383639
 H    3.082788    4.000577    0.244528
 C    0.538550    2.632846   -1.776365
 C    1.822046    2.649090   -0.858748
 O    1.334459    2.085967    0.372262
 H   -0.612874    1.326243   -3.039970
 C    0.375562    1.330242   -2.556106
 H    1.139110    1.225440   -3.340341
 H    0.434150    0.455202   -1.891068
 H    3.294722    2.132517   -2.363615
 C    2.962520    1.788006   -1.372089
 H    3.820345    1.859265   -0.686128
 H    2.658330    0.735648   -1.440404
39
Figure 2_L-Cu-Bpin / electronic energy: -2356.95154150 a.u. / lowest freq: 22.11 cm-1
 H   -4.270736   -2.604302    0.699216
 H   -3.469511   -2.304962   -1.601614
 C   -4.343959   -1.520428    0.875987
 H   -4.082488   -1.334048    1.925984
 H   -5.392484   -1.222875    0.718439
 C   -3.691752   -1.230867   -1.514808
 O   -2.057742   -1.109903    0.223326
 H   -4.742108   -1.073870   -1.802677
 C   -3.418948   -0.778798   -0.078579
 H   -3.048558   -0.694945   -2.228327
 B   -1.238080   -0.000001   -0.000001
 H   -3.048552    0.694945    2.228328
 C   -3.418947    0.778799    0.078581
 H   -4.742104    1.073871    1.802681
 O   -2.057741    1.109902   -0.223328
 C   -3.691747    1.230867    1.514810
 H   -5.392484    1.222879   -0.718433
 H   -4.082491    1.334050   -1.925981
 C   -4.343959    1.520430   -0.875984
 H   -3.469505    2.304963    1.601615
 H   -4.270733    2.604304   -0.699213
Cu    0.797333   -0.000001   -0.000002
 H    3.463333   -3.022428   -0.742996
 H    5.468944   -1.227903   -0.850209
 H    5.489479    1.160908   -0.929040
 H    3.459252    2.934328   -1.042286
 C    3.103330   -2.441738    0.122397
 C    4.991258   -0.767023    0.029199
 H    2.005088   -2.444141    0.118745
 N    3.563409   -1.079451    0.055881
 C    2.777376    0.000000    0.000000
 C    4.991258    0.767025   -0.029195
 N    3.563409    1.079451   -0.055879
 H    2.005087    2.444141   -0.118746
 C    3.103329    2.441739   -0.122398
 H    3.459253   -2.934329    1.042284
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 H    5.489478   -1.160906    0.929045
 H    5.468941    1.227905    0.850214
 H    3.463332    3.022430    0.742995
63
Figure 2_para-NMe2_pc1 / electronic energy: -2800.13914226 a.u. / lowest freq: 11.78 cm-1
 H   -1.333971    0.243414    3.056739
 H   -1.893376    2.829609    3.069201
 H   -0.688071    4.552383    1.916772
 H    0.998491    4.702807   -0.211619
 C   -1.373470    0.282834    1.956552
 C   -1.944602    2.741995    1.973929
 H   -0.596041   -0.378332    1.551730
 N   -1.133518    1.624953    1.495244
 C   -0.349919    1.950940    0.461461
 C   -1.310196    3.932532    1.247769
 N   -0.473028    3.268081    0.252315
 H    0.856454    3.322226   -1.337625
 C    0.287785    4.020402   -0.708683
 H   -2.359725   -0.087483    1.627340
 H   -3.001033    2.588891    1.692196
 H   -2.050980    4.589107    0.767875
 H   -0.374671    4.621842   -1.352210
 H   -2.767736   -3.170397   -0.236803
 C   -4.120942   -1.463589   -0.294555
 C   -2.899880   -2.132180   -0.540668
 H   -5.106753    0.465927   -0.533520
 C   -4.197617   -0.111173   -0.702935
 H    3.717471   -3.695181    1.377144
 C   -1.838147   -1.491617   -1.169100
 H    3.285411   -1.815466    2.900357
 H   -0.913655   -2.054844   -1.319349
 C   -3.124255    0.511400   -1.329702
 C   -1.915640   -0.153276   -1.586486
 C    4.320631   -3.077535    0.694244
 C    4.021795   -1.222272    2.337804
 H    4.133536   -3.430286   -0.328621
 O    2.597283   -1.412067    0.430536
 H   -3.227248    1.561189   -1.621345
 H    5.016188   -1.413817    2.768306
 H    5.382390   -3.245359    0.933266
 C    3.949569   -1.610813    0.859570
 C   -0.785244    0.562879   -2.210379
 B    2.470938   -0.152892   -0.164855
 H    0.542092   -1.112693   -2.610797
 C    0.406322   -0.028055   -2.607354
 C    4.734524   -0.624609   -0.068691
 H    4.257146   -1.740107   -1.883431
 O    3.749650    0.381869   -0.336700
 H    5.928935   -1.991280   -1.304900
 H    6.691896   -0.741314    0.869901
 C    5.121596   -1.250897   -1.410052
 H    1.096954    0.529823   -3.246568
 C    5.956199    0.020768    0.569083
 H    5.469354   -0.457086   -2.088064
 H    6.442648    0.693807   -0.153274
Cu    0.681519    0.693168   -0.683351
 H   -0.995746    1.590413   -2.524773
 H    3.777844   -0.159236    2.481159
 H    5.687948    0.615842    1.452278
 H   -6.119227   -0.535626    1.429040
 H   -6.819271   -0.854368   -0.180933
 C   -6.347580   -1.331593    0.694020
 H   -7.093407   -2.000394    1.141173
 N   -5.181931   -2.096442    0.319083
 H   -4.702808   -4.146160    0.102454
 H   -5.943667   -3.765430    1.307360
 C   -4.998037   -3.416586    0.874669
 H   -4.229590   -3.441734    1.670846
63
Figure 2_para-NMe2_ts(CuBadd) / electronic energy: -2800.12649875 a.u. / lowest freq: -191.73 cm-1
 H   -1.551574    1.994754    2.672223
 H   -0.200802    4.242581    2.701214
 H    1.905508    4.675068    1.631952
 H    3.365644    3.587764   -0.362832
 C   -1.402513    1.921070    1.584675
 C   -0.233413    4.159777    1.605332
 H   -1.174414    0.877306    1.332011
 N   -0.306042    2.764055    1.180794
 C    0.523000    2.494237    0.163758
 C    1.055544    4.630811    0.928231
 N    1.279673    3.577750   -0.058623
 H    2.390718    2.736914   -1.596977
 C    2.421166    3.612158   -0.934160
 H   -2.343839    2.202978    1.081594
 H   -1.120504    4.709888    1.245231
 H    0.956536    5.614340    0.446722
 H    2.411123    4.524756   -1.550299
 H   -2.966489   -2.118374    1.279676
 C   -4.293856   -0.989585   -0.019006
 C   -3.043752   -1.491091    0.390857
 H   -5.233609    0.197215   -1.584699
 C   -4.297687   -0.206187   -1.195709
 H    2.121481   -3.603603    2.400097
 C   -1.872308   -1.206837   -0.312281
 H    2.597044   -1.294161    3.071466
 H   -0.934148   -1.616848    0.073508
 C   -3.125770    0.072321   -1.888153
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 C   -1.862994   -0.405428   -1.475179
 C    2.758348   -3.542611    1.504790
 C    3.387472   -1.260430    2.307353
 H    2.276693   -4.124531    0.708007
 O    1.686440   -1.558049    0.656242
 H   -3.188149    0.688874   -2.790664
 H    4.313275   -1.651976    2.753962
 H    3.726254   -4.008705    1.744685
 C    2.944944   -2.088418    1.100990
 C   -0.636920   -0.062985   -2.190627
 B    1.927599   -0.653832   -0.366579
 H    0.509849   -1.823575   -1.561546
 C    0.609073   -0.788441   -1.924348
 C    3.854147   -1.870348   -0.159048
 H    2.708780   -3.256704   -1.400066
 O    3.246965   -0.717078   -0.771054
 H    4.250620   -3.926112   -0.800316
 H    5.776714   -2.395563    0.699429
 C    3.756889   -3.014729   -1.167504
 H    1.351333   -0.727884   -2.729973
 C    5.310928   -1.564210    0.148469
 H    4.248569   -2.710013   -2.103206
 H    5.867929   -1.425893   -0.790316
Cu    0.603258    0.840843   -0.803408
 H   -0.749360    0.429002   -3.161127
 H    3.546986   -0.206575    2.034535
 H    5.416374   -0.646179    0.741438
 H   -6.857765    0.076178   -0.183514
 H   -6.872327   -1.561352   -0.890596
 C   -6.733372   -0.993433    0.051692
 H   -7.547647   -1.267338    0.735133
 N   -5.465717   -1.252418    0.691384
 H   -5.154768   -3.265937    1.342722
 H   -6.419124   -2.337038    2.193497
 C   -5.430417   -2.260750    1.722455
 H   -4.713094   -1.998563    2.516830
63
Figure 2_para-NMe2_L-Cu-alkyl_01 / electronic energy: -2800.18197688 a.u. / lowest freq: 12.08 cm-1
 H   -0.028887    1.982339    2.652630
 H    2.469256    2.874769    2.768118
 H    4.338951    2.970242    1.272695
 H    4.665374    1.639086   -0.967794
 C   -0.112551    2.528145    1.697680
 C    2.246584    3.410824    1.829686
 H   -0.740475    1.943888    1.012191
 N    1.184615    2.719297    1.101779
 C    1.607282    2.149812   -0.032312
 C    3.410127    3.363071    0.832681
 N    2.899545    2.456551   -0.193486
 H    3.177209    1.312595   -1.900948
 C    3.713991    2.070964   -1.316355
 H   -0.601008    3.496388    1.892182
 H    1.944522    4.436450    2.088708
 H    3.631440    4.349852    0.392656
 H    3.941158    2.934363   -1.964650
 H   -3.666436   -1.802720    1.107518
 C   -4.357864   -0.014310    0.085923
 C   -3.449825   -1.059845    0.338552
 H   -4.668198    1.698107   -1.225112
 C   -4.002545    0.879214   -0.949021
 H    0.777921   -3.601718    2.649645
 C   -2.253148   -1.184801   -0.372156
 H    0.113249   -1.289560    2.277937
 H   -1.584367   -2.005737   -0.106208
 C   -2.806577    0.741599   -1.645032
 C   -1.874207   -0.285208   -1.385783
 C    1.718261   -3.490432    2.089680
 C    1.095493   -1.081375    1.829057
 H    1.920825   -4.440826    1.578871
 O    0.615964   -2.655661    0.110115
 H   -2.581076    1.469230   -2.432504
 H    1.779510   -0.762012    2.628611
 H    2.524606   -3.301593    2.814592
 C    1.596728   -2.335059    1.110248
 C   -0.581359   -0.347272   -2.131818
 B    0.998944   -2.047978   -1.063843
 H   -0.709226   -2.549778   -2.412437
 C    0.056142   -1.757824   -2.280247
 C    2.877597   -2.069923    0.235558
 H    3.033800   -4.144318   -0.427966
 O    2.311156   -1.638029   -1.011902
 H    4.201978   -3.700062    0.848101
 H    4.164052   -1.237100    1.772644
 C    3.679956   -3.338387   -0.049564
 H    0.675035   -1.761812   -3.193609
 C    3.792143   -0.978462    0.769497
 H    4.433597   -3.119135   -0.820279
 H    4.661046   -0.864116    0.104543
Cu    0.557371    0.937086   -1.132869
 H   -0.760827    0.069031   -3.139685
 H    0.968131   -0.250757    1.116920
 H    3.273860   -0.012382    0.820973
 H   -6.157517    2.076365    0.262121
 H   -6.939137    0.773597   -0.672971
 C   -6.544544    1.046647    0.327006
 H   -7.387907    1.065520    1.029657
 N   -5.538552    0.134471    0.814243
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 H   -6.156319   -1.895319    1.091228
 H   -6.906658   -0.677829    2.158471
 C   -5.973027   -0.956321    1.652247
 H   -5.234120   -1.179697    2.438954
63
Figure 2_para-NMe2_L-Cu-alkyl_02 / electronic energy: -2800.17645420 a.u. / lowest freq: 21.44 cm-1
 B   -1.676356   -2.051381    0.255057
 O   -2.470196   -1.866668    1.359581
 O   -2.419586   -2.147310   -0.896319
 C   -3.846682   -1.965860    0.957721
 C   -3.760645   -1.727773   -0.597361
 C   -4.655132   -0.921550    1.712906
 C   -4.324194   -3.369178    1.327129
 C   -3.866429   -0.251539   -0.980101
 C   -4.735234   -2.552107   -1.424093
 H   -3.167254    0.365876   -0.397647
 H   -4.885639    0.134206   -0.831187
 H   -3.608392   -0.137329   -2.043023
 H   -4.581014   -3.629824   -1.282446
 H   -4.594468   -2.328770   -2.492121
 H   -5.775928   -2.308389   -1.161335
 H   -3.757386   -4.142178    0.786978
 H   -5.394033   -3.505548    1.112306
 H   -4.167448   -3.528569    2.404260
 H   -5.697339   -0.903448    1.359652
 H   -4.225116    0.081881    1.594545
 H   -4.663841   -1.160913    2.786931
 C   -0.485567    1.162474   -1.590393
 C   -1.150067    2.380274   -1.477347
 C   -0.182897    0.347021   -0.484082
 C   -1.564365    2.878594   -0.223524
 C   -0.593367    0.859694    0.760418
 C   -1.265465    2.074674    0.894306
 C    0.500974   -0.975984   -0.632536
 C   -0.103889   -2.080020    0.283085
 H   -1.563290    2.388497    1.895368
 H   -0.401810    0.281624    1.668503
 H   -1.361010    2.938026   -2.390516
 H   -0.206983    0.815887   -2.591347
Cu    2.418990   -0.641341   -0.324998
 H    0.241310   -1.997979    1.328618
 H    0.259566   -3.065344   -0.060516
 H    0.352407   -1.298267   -1.679442
 H    5.791517   -2.888400   -0.999615
 H    7.235666   -1.176163    0.500929
 C    5.306987   -1.980570   -1.394610
 H    4.256883   -2.207453   -1.622318
 H    6.443023    0.421696    2.095541
 N    5.350805   -0.913564   -0.429313
 C    6.625989   -0.380472    0.046137
 H    5.819980   -1.691911   -2.327213
 C    4.287842   -0.265145    0.058097
 C    6.179613    0.683392    1.057218
 H    4.045176    1.393311    2.749760
 H    7.197897    0.045930   -0.794478
 N    4.727640    0.682454    0.892613
 C    3.896429    1.563957    1.670372
 H    6.597165    1.679327    0.844503
 H    2.843568    1.372884    1.423804
 H    4.127550    2.619192    1.451712
 H   -3.537445    4.053905   -1.796087
 H   -3.275978    5.644210   -1.028079
 C   -2.787880    4.696124   -1.289640
 H   -2.001208    4.932026   -2.023447
 N   -2.236486    4.096136   -0.098121
 H   -3.689926    3.627365    1.399558
 H   -3.392091    5.360747    1.087355
 C   -2.910594    4.375992    1.147714
 H   -2.201072    4.414345    1.989292
63
Figure 2_para-NMe2_L-Cu-alkyl_03 / electronic energy: -2800.17710480 a.u. / lowest freq: -13.53 cm-1
 B   -1.929369   -1.810779   -0.266173
 O   -2.840197   -2.358973   -1.137932
 O   -2.545338   -1.272590    0.837438
 C   -4.160702   -2.007738   -0.692289
 C   -3.920887   -1.691935    0.829296
 C   -5.106659   -3.168242   -0.957410
 C   -4.594270   -0.781800   -1.495100
 C   -4.012235   -2.931898    1.717922
 C   -4.792716   -0.581803    1.393163
 H   -3.400676   -3.756068    1.321497
 H   -5.048434   -3.284687    1.821793
 H   -3.632096   -2.681669    2.719221
 H   -4.630745    0.370648    0.872786
 H   -4.561709   -0.428514    2.457813
 H   -5.857795   -0.847283    1.311997
 H   -3.930468    0.074297   -1.305074
 H   -5.626541   -0.485288   -1.258791
 H   -4.541485   -1.018558   -2.567986
 H   -6.098480   -2.968083   -0.524551
 H   -4.723986   -4.107200   -0.536167
 H   -5.231973   -3.310079   -2.041101
 C    2.813128   -0.656732    1.271017
 C    4.196232   -0.758739    1.183152
 C    1.938170   -1.116098    0.263148
 C    4.821313   -1.346360    0.059587
 C    2.573707   -1.693037   -0.849810
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 C     3.963943   -1.794787   -0.961373
 C     0.459841   -0.953663    0.394115
 C    -0.382694   -1.853125   -0.515569
 H     4.373635   -2.247901   -1.865130
 H     1.970025   -2.074560   -1.677319
 H     4.794702   -0.377364    2.011562
 H     2.383280   -0.187661    2.163081
Cu     0.014475    0.956879    0.164687
 H    -0.091953   -2.928294   -0.437606
 H    -0.230458   -1.621279   -1.586296
 H     0.187971   -1.157935    1.447595
 H    -3.409233    2.616440   -1.047020
 H    -2.160420    5.013023   -1.306927
 C    -2.876640    2.564607   -0.082268
 H    -2.622675    1.517289    0.131472
 H     0.133815    5.678611   -1.194454
 N    -1.663997    3.339386   -0.116416
 C    -1.694794    4.783777   -0.334398
 H    -3.553836    2.932797    0.705384
 C    -0.426971    2.835676   -0.057329
 C    -0.205774    5.153756   -0.288467
 H     2.345637    4.138642   -1.011926
 H    -2.284715    5.283517    0.449280
 N     0.439024    3.846670   -0.176062
 C     1.872410    3.730659   -0.104148
 H     0.050230    5.780493    0.581752
 H     2.139136    2.669675   -0.010248
 H     2.269502    4.275232    0.768756
 H     6.418291   -2.815540   -1.644984
 H     6.592785   -1.098005   -2.093788
 C     6.790731   -1.840041   -1.293014
 H     7.878739   -1.934335   -1.180376
 N     6.208348   -1.480114   -0.023244
 H     6.892289    0.368811    0.807664
 H     8.088700   -0.950699    0.700970
 C     7.030936   -0.728464    0.893982
 H     6.830264   -1.007252    1.940825
63
Figure 2_para-NMe2_ts(BHE) / electronic energy: -2800.13027722 a.u. / lowest freq: -940.79 cm-1
 B    -2.399371   -1.248071   -0.278252
 O    -3.333919   -1.845078   -1.079852
 O    -2.952836   -0.644696    0.818737
 C    -4.630874   -1.400636   -0.634192
 C    -4.347845   -0.997017    0.860553
 C    -5.636494   -2.526532   -0.807116
 C    -5.014802   -0.208715   -1.509294
 C    -4.487602   -2.164255    1.835365
 C    -5.147376    0.197523    1.356062
 H    -3.933638   -3.049190    1.488699
 H    -5.540537   -2.445055    1.981856
 H    -4.072613   -1.866456    2.809439
 H    -4.928279    1.102733    0.774720
 H    -4.899738    0.401979    2.408315
 H    -6.227171   -0.006052    1.295752
 H    -4.292787    0.615007   -1.402743
 H    -6.018317    0.168774   -1.266449
 H    -5.011365   -0.523037   -2.563379
 H    -6.609518   -2.244040   -0.377755
 H    -5.296527   -3.452736   -0.325806
 H    -5.785252   -2.734086   -1.877067
 C     2.345986   -1.354435    1.495195
 C     3.718478   -1.545550    1.397186
 C     1.492399   -1.345685    0.370136
 C     4.349036   -1.764337    0.151738
 C     2.132746   -1.559759   -0.868997
 C     3.509777   -1.754814   -0.979028
 C     0.065675   -1.070901    0.503070
 C    -0.871366   -1.211565   -0.595747
 H     3.927377   -1.901280   -1.975905
 H     1.545654   -1.546644   -1.791751
 H     4.305149   -1.527368    2.316585
 H     1.912641   -1.183624    2.485828
Cu    -0.207539    0.734406   -0.506988
 H    -0.580402   -1.869005   -1.426158
 H    -1.098749   -0.052016   -1.609617
 H    -0.334772   -0.977430    1.516654
 H    -2.292309    4.357734   -0.206466
 H     0.025304    5.653647   -0.082679
 C    -1.792420    3.517777    0.301068
 H    -2.173942    2.575049   -0.113469
 H     2.152930    4.876964   -0.868038
 N    -0.370147    3.577400    0.092102
 C     0.393717    4.767754    0.455326
 H    -2.044597    3.559566    1.374903
 C     0.407541    2.526871   -0.206107
 C     1.817547    4.370913    0.053718
 H     3.298350    2.481936   -1.453119
 H     0.299491    4.962894    1.537552
 N     1.681960    2.935966   -0.182411
 C     2.827639    2.131536   -0.518677
 H     2.559608    4.571602    0.840546
 H     2.515631    1.087147   -0.647495
 H     3.580593    2.171662    0.284447
 H     5.935939   -2.648057   -1.940755
 H     6.209151   -0.897819   -1.729909
 C     6.339588   -1.890107   -1.250374
 H     7.416587   -2.082399   -1.158134
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 N    5.725380   -1.978289    0.052197
 H    6.490675   -0.601894    1.500543
 H    7.599560   -1.891380    0.958317
 C    6.551093   -1.666651    1.194120
 H    6.280413   -2.280369    2.068138
63
Figure 2_para-NMe2_pc2 / electronic energy: -2800.16816835 a.u. / lowest freq: 25.36 cm-1
 B   -2.482731   -1.189180   -0.010090
 O   -3.504937   -1.834429   -0.653971
 O   -2.939733   -0.235351    0.872636
 C   -4.711823   -1.090053   -0.400494
 C   -4.370581   -0.354348    0.948451
 C   -5.885026   -2.052717   -0.321177
 C   -4.897956   -0.124435   -1.569167
 C   -4.688768   -1.194891    2.183988
 C   -4.976113    1.033177    1.089346
 H   -4.261755   -2.205626    2.102016
 H   -5.772568   -1.285044    2.345896
 H   -4.248187   -0.712991    3.069276
 H   -4.638094    1.709238    0.293226
 H   -4.679924    1.471267    2.054186
 H   -6.075230    0.982266    1.063563
 H   -4.061269    0.586403   -1.640239
 H   -5.838747    0.438078   -1.482417
 H   -4.925558   -0.698663   -2.506905
 H   -6.805087   -1.519997   -0.036899
 H   -5.706514   -2.856692    0.404990
 H   -6.051551   -2.516662   -1.304758
 C    2.282675   -0.289449    1.324924
 C    3.664450   -0.424677    1.303681
 C    1.442456   -1.044653    0.493383
 C    4.291503   -1.345572    0.429150
 C    2.064619   -1.956633   -0.371541
 C    3.444384   -2.111323   -0.408290
 C   -0.014236   -0.814123    0.526768
 C   -0.978746   -1.464882   -0.232206
 H    3.865740   -2.837889   -1.102686
 H    1.458144   -2.567718   -1.044570
 H    4.260155    0.192654    1.975934
 H    1.836753    0.441954    2.006022
Cu   -0.562650    0.368305   -1.144502
 H   -0.681768   -2.248462   -0.937663
 H   -1.378507    0.349308   -2.520914
 H   -0.355807   -0.192322    1.362724
 H   -1.660359    3.766209    0.684200
 H    0.844834    4.796376    0.217981
 C   -1.101553    2.878916    1.028891
 H   -1.683230    1.977205    0.790731
 H    2.858006    4.034538   -0.844578
 N    0.190361    2.795578    0.397657
 C    1.204650    3.827305    0.605728
 H   -0.989990    2.945340    2.122763
 C    0.512544    1.938671   -0.578072
 C    2.385168    3.278360   -0.201107
 H    3.013757    2.069815   -2.659403
 H    1.430977    3.950912    1.674911
 N    1.748117    2.230728   -0.995513
 C    2.512295    1.429788   -1.916546
 H    3.167015    2.837021    0.441972
 H    1.832788    0.745438   -2.441569
 H    3.279239    0.835871   -1.389845
 H    5.925807   -3.476271   -0.298594
 H    6.038954   -2.223564   -1.563734
 C    6.261241   -2.444276   -0.504261
 H    7.350453   -2.419852   -0.380429
 N    5.657017   -1.486518    0.392161
 H    6.344568    0.408211    1.054944
 H    7.544500   -0.901155    1.052449
 C    6.489815   -0.670521    1.243990
 H    6.295869   -0.852407    2.316328
63
Figure 2_para-NMe2_ts(H>B) / electronic energy: -2800.15510862 a.u. / lowest freq: -383.35 cm-1
 B   -2.469004   -0.851366   -0.356664
 O   -3.516283   -1.653883   -0.846044
 O   -2.950072   -0.042072    0.707329
 C   -4.740499   -1.080589   -0.395594
 C   -4.309487   -0.388326    0.952736
 C   -5.773368   -2.187859   -0.231231
 C   -5.230787   -0.076851   -1.442649
 C   -4.330606   -1.353968    2.140819
 C   -5.097499    0.868315    1.297905
 H   -3.785430   -2.280561    1.907095
 H   -5.354937   -1.615897    2.445859
 H   -3.830075   -0.876169    2.996563
 H   -4.982931    1.642206    0.527181
 H   -4.734699    1.286184    2.249685
 H   -6.169358    0.644977    1.414948
 H   -4.524441    0.756274   -1.564521
 H   -6.217930    0.334033   -1.184179
 H   -5.315949   -0.588753   -2.413208
 H   -6.697831   -1.799730    0.223771
 H   -5.391655   -3.007050    0.392475
 H   -6.030621   -2.607593   -1.215620
 C    2.261540   -0.346932    1.310874
 C    3.645732   -0.462397    1.269337
 C    1.419046   -1.134759    0.513965
 C    4.271753   -1.397177    0.410333
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 C    2.040620   -2.068920   -0.327915
 C    3.421391   -2.204883   -0.384579
 C   -0.036076   -0.897444    0.542421
 C   -0.982338   -1.392492   -0.310112
 H    3.841132   -2.950970   -1.059130
 H    1.430151   -2.714281   -0.965020
 H    4.243234    0.181391    1.914650
 H    1.816381    0.397871    1.978004
Cu   -0.802902    0.634145   -1.033245
 H   -0.655522   -2.055582   -1.123940
 H   -2.243977    0.248474   -1.650177
 H   -0.378870   -0.272676    1.377948
 H   -1.161140    4.044360    1.089814
 H    1.458878    4.674228    0.486102
 C   -0.757935    3.025739    1.219350
 H   -1.520285    2.296751    0.910880
 H    3.104192    3.744036   -0.979327
 N    0.430661    2.827446    0.430787
 C    1.644217    3.603438    0.673223
 H   -0.541473    2.872589    2.289035
 C    0.530497    2.001365   -0.616232
 C    2.628554    2.991617   -0.332241
 H    2.806185    1.815491   -2.915484
 H    1.973811    3.494806    1.717983
 N    1.769632    2.100920   -1.108724
 C    2.329288    1.232892   -2.110967
 H    3.427267    2.408252    0.156731
 H    1.527164    0.620470   -2.543485
 H    3.085197    0.560134   -1.670057
 H    5.990270   -2.252411   -1.612914
 H    7.335939   -2.406871   -0.462297
 C    6.244912   -2.460908   -0.557907
 H    5.943588   -3.500218   -0.337818
 H    6.308160    0.416160    0.928781
 N    5.639114   -1.514139    0.348826
 H    7.527241   -0.876629    0.957116
 C    6.472113   -0.653289    1.154790
 H    6.296104   -0.798039    2.235522
63
Figure 2_para-NMe2_int1 / electronic energy: -2800.15704127 a.u. / lowest freq: 23.81 cm-1
 B   -2.570648   -0.395195   -0.420380
 O   -3.569660   -1.094475   -1.184665
 O   -3.144713   -0.092360    0.874060
 C   -4.815596   -0.881274   -0.546227
 C   -4.393433   -0.752398    0.962848
 C   -5.737210   -2.056338   -0.848291
 C   -5.442690    0.411682   -1.082132
 C   -4.172948   -2.121719    1.617297
 C   -5.343476    0.076295    1.819113
 H   -3.526063   -2.755585    0.992360
 H   -5.117093   -2.656950    1.802490
 H   -3.667279   -1.974781    2.583949
 H   -5.412992    1.110820    1.456149
 H   -4.978317    0.109398    2.857530
 H   -6.354548   -0.360617    1.830673
 H   -4.829424    1.289473   -0.830283
 H   -6.458135    0.573434   -0.689507
 H   -5.506083    0.347869   -2.179273
 H   -6.675344   -1.985816   -0.275336
 H   -5.253963   -3.014840   -0.615899
 H   -5.995332   -2.064193   -1.918798
 C    2.164556   -0.509498    1.304883
 C    3.537029   -0.715896    1.236339
 C    1.260685   -1.208806    0.492702
 C    4.086079   -1.664197    0.339802
 C    1.803950   -2.159434   -0.383080
 C    3.171865   -2.388740   -0.464007
 C   -0.172931   -0.862017    0.534508
 C   -1.100026   -1.052161   -0.440448
 H    3.530753   -3.143813   -1.163085
 H    1.139165   -2.745015   -1.023828
 H    4.184140   -0.132666    1.891091
 H    1.780656    0.242700    2.001191
Cu   -0.828695    1.113085   -0.715154
 H   -0.762111   -1.534822   -1.371342
 H   -2.420567    0.868756   -1.068909
 H   -0.502017   -0.380099    1.465983
 H   -0.133881    4.658914    1.337061
 H    2.397253    4.638390    0.362423
 C   -0.003241    3.569295    1.446336
 H   -0.961656    3.075579    1.237437
 H    3.567761    3.336939   -1.267891
 N    0.988757    3.071400    0.530140
 C    2.366408    3.556570    0.573168
 H    0.284074    3.357038    2.488901
 C    0.760708    2.213513   -0.469133
 C    3.042196    2.721846   -0.521964
 H    2.529382    1.522866   -3.071368
 H    2.805703    3.393323    1.569299
 N    1.910662    2.021255   -1.123671
 C    2.116830    1.049702   -2.165667
 H    3.760023    1.988828   -0.116260
 H    1.153935    0.583205   -2.414029
 H    2.814294    0.263005   -1.832379
 H    5.736054   -2.566240   -1.733197
 H    7.061180   -2.875755   -0.587485
 C    5.969847   -2.831697   -0.685747
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 H     5.579656   -3.848183   -0.503316
 H     6.241542    0.004514    0.846876
 N     5.441775   -1.872385    0.255747
 H     7.377523   -1.361494    0.834547
 C     6.342227   -1.076358    1.055864
 H     6.178768   -1.225101    2.137946
63
Figure 2_para-NMe2_ts(Cu>O) / electronic energy: -2800.15146860 a.u. / lowest freq: -49.96 cm-1
 B    -1.835064   -1.329527   -0.712392
 O    -2.723358   -2.405153   -1.038545
 O    -2.284635   -0.788004    0.574009
 C    -3.937152   -2.178779   -0.342243
 C    -3.444867   -1.494570    0.989274
 C    -4.645576   -3.512167   -0.136297
 C    -4.835820   -1.254598   -1.174665
 C    -3.003669   -2.516468    2.040385
 C    -4.441617   -0.520171    1.604534
 H    -2.297817   -3.241174    1.608344
 H    -3.853290   -3.064985    2.474903
 H    -2.485768   -1.988113    2.855496
 H    -4.678249    0.302952    0.916762
 H    -4.018050   -0.081008    2.521050
 H    -5.380608   -1.028106    1.875291
 H    -4.386350   -0.259712   -1.304600
 H    -5.830037   -1.129475   -0.720315
 H    -4.967891   -1.696229   -2.174134
 H    -5.528925   -3.396348    0.510894
 H    -3.975223   -4.257358    0.312133
 H    -4.986373   -3.908365   -1.105334
 C     2.779002   -0.887385    1.320885
 C     4.166930   -0.802224    1.347559
 C     2.066660   -1.221689    0.159817
 C     4.932478   -1.050185    0.184551
 C     2.831473   -1.472239   -0.991152
 C     4.217425   -1.392942   -0.989710
 C     0.593441   -1.244035    0.182585
 C    -0.254733   -1.563011   -0.813807
 H     4.749722   -1.596247   -1.918973
 H     2.330551   -1.727382   -1.928701
 H     4.656117   -0.540839    2.285849
 H     2.224867   -0.681824    2.242095
Cu    -1.526199    0.923531   -0.843576
 H     0.167230   -1.877690   -1.780147
 H    -2.084921   -0.354047   -1.705795
 H     0.149957   -0.923556    1.134489
 H    -3.348453    4.414141    0.231038
 H     1.998733    2.756709   -1.929937
 H     1.226250    4.974620   -0.628544
 H    -0.933001    5.645822    0.146265
 H    -3.248265    2.636956    0.427650
 H     1.057646    1.288011   -1.523896
 C    -0.785891    2.628137   -0.314169
 C    -2.803426    3.594321    0.728102
 N    -1.412972    3.598027    0.357228
 C     1.513106    2.198480   -1.113347
 N     0.486358    2.995614   -0.492142
 C     0.806042    4.284123    0.118816
 C    -0.556377    4.743938    0.655537
 H    -2.919159    3.711994    1.817672
 H     2.285407    1.907705   -0.381957
 H     1.555726    4.151410    0.915820
 H    -0.544387    4.946362    1.737601
 H     6.784129   -0.593294   -1.843807
 H     8.124330   -1.123458   -0.808339
 C     7.054350   -1.259916   -1.005904
 H     6.904890   -2.301390   -1.344168
 N     6.304069   -0.957407    0.190309
 H     8.077062   -0.587184    1.219685
 H     6.688515    0.338476    1.824161
 C     6.999191   -0.638948    1.414941
 H     6.836679   -1.398551    2.201485
63
Figure 2_para-NMe2_int2 / electronic energy: -2800.15550685 a.u. / lowest freq: 11.28 cm-1
 B     0.501602    1.212973   -0.830967
 O     0.850698    2.578275   -1.146188
 O     1.051412    0.967415    0.527350
 C     1.861574    3.016960   -0.263188
 C     1.563527    2.190698    1.042767
 C     1.741127    4.526176   -0.082006
 C     3.239790    2.698373   -0.860418
 C     0.468524    2.830902    1.899455
 C     2.787497    1.901731    1.901758
 H    -0.414837    3.077868    1.292798
 H     0.819046    3.745297    2.401522
 H     0.156920    2.113931    2.674000
 H     3.514485    1.278615    1.363006
 H     2.491363    1.362133    2.814340
 H     3.283939    2.835266    2.209225
 H     3.403623    1.613787   -0.971818
 H     4.060084    3.104037   -0.249655
 H     3.303169    3.144854   -1.864061
 H     2.434618    4.893365    0.690832
 H     0.718339    4.814430    0.194289
 H     1.987367    5.035215   -1.026392
 C    -3.913824   -0.334450    1.123987
 C    -5.264597   -0.664509    1.153439
 C    -3.244288   -0.001143   -0.062774
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 C   -6.034391   -0.681709   -0.032475
 C   -4.010322   -0.032306   -1.239608
 C   -5.359450   -0.361614   -1.236094
 C   -1.814219    0.362925   -0.024021
 C   -1.048067    0.852750   -1.013512
 H   -5.894217   -0.369977   -2.186070
 H   -3.538682    0.202529   -2.197622
 H   -5.721831   -0.907401    2.112624
 H   -3.356939   -0.329574    2.066354
Cu    2.189279   -0.451317   -0.732872
 H   -1.508383    1.012346   -2.000558
 H    1.139098    0.385554   -1.719046
 H   -1.337414    0.221496    0.955531
 H    3.089135   -1.654588    3.053319
 H    5.238847   -2.973614    2.151692
 C    2.590517   -1.988150    2.129472
 H    1.897725   -1.203504    1.796702
 H    6.382351   -2.632268    0.074782
 N    3.560890   -2.231346    1.092078
 C    4.624413   -3.217530    1.272315
 H    2.016816   -2.902690    2.356040
 C    3.504324   -1.741872   -0.151074
 C    5.395459   -3.109011   -0.048547
 H    5.832059   -1.391025   -2.253812
 H    4.188308   -4.218541    1.427971
 N    4.522526   -2.252389   -0.849318
 C    4.860875   -1.911434   -2.206319
 H    5.546993   -4.081701   -0.539481
 H    4.083272   -1.248331   -2.608090
 H    4.920771   -2.815491   -2.833272
 H   -7.738560   -1.747876   -1.972859
 H   -9.170104   -1.262330   -1.039198
 C   -8.125491   -1.005202   -1.251843
 H   -8.120378   -0.020194   -1.751823
 H   -7.599241   -2.207407    1.710201
 N   -7.373495   -0.994874   -0.019596
 H   -9.090465   -1.510642    1.040665
 C   -8.028414   -1.310798    1.227228
 H   -7.968104   -0.480228    1.953281
63
Figure 2_para-NMe2_ts(C-Brot) / electronic energy: -2800.15035858 a.u. / lowest freq: -85.14 cm-1
 B    0.412849    0.837493   -0.808667
 O    0.529683    2.205182   -1.249875
 O    1.063944    0.819746    0.538237
 C    1.563609    2.843634   -0.530598
 C    1.493930    2.135039    0.872580
 C    1.285049    4.341997   -0.482789
 C    2.906527    2.613722   -1.238420
 C    0.440145    2.758968    1.789956
 C    2.824597    2.059635    1.612245
 H   -0.511933    2.906412    1.261649
 H    0.767284    3.729098    2.193737
 H    0.256850    2.077911    2.634581
 H    3.559314    1.460439    1.056870
 H    2.683393    1.588819    2.597376
 H    3.244436    3.064437    1.775694
 H    3.195117    1.549533   -1.245744
 H    3.724426    3.181286   -0.770055
 H    2.814424    2.936373   -2.286280
 H    1.993612    4.858115    0.183806
 H    0.263175    4.547297   -0.137354
 H    1.390959    4.775444   -1.489206
 C   -4.438789    0.778068    0.712684
 C   -5.753881    0.336095    0.806003
 C   -3.512370    0.207459   -0.172771
 C   -6.224551   -0.720628   -0.006965
 C   -3.985542   -0.839464   -0.980735
 C   -5.294550   -1.296607   -0.907219
 C   -2.125118    0.710274   -0.211407
 C   -1.071634    0.209144   -0.877858
 H   -5.597167   -2.112402   -1.563971
 H   -3.311918   -1.315869   -1.698067
 H   -6.419056    0.824226    1.518248
 H   -4.116654    1.599381    1.360520
Cu    2.327724   -0.539832   -0.626273
 H   -1.239858   -0.696128   -1.480389
 H    1.139448    0.035238   -1.645838
 H   -1.965309    1.602562    0.408227
 H    3.444413   -1.381257    3.200129
 H    5.750776   -2.369312    2.338159
 C    2.983209   -1.824933    2.303490
 H    2.191988   -1.153402    1.943628
 H    6.818961   -1.992413    0.228016
 N    3.965983   -1.992361    1.262886
 C    5.181704   -2.771684    1.486915
 H    2.533989   -2.791443    2.587188
 C    3.830078   -1.580250   -0.001710
 C    5.916096   -2.620846    0.148816
 H    6.038803   -0.916873   -2.128974
 H    4.926076   -3.820177    1.713653
 N    4.914859   -1.957788   -0.684664
 C    5.197078   -1.626292   -2.056789
 H    6.212353   -3.585130   -0.290153
 H    4.305187   -1.164452   -2.500457
 H    5.454865   -2.530772   -2.630381
 H   -7.418405   -3.199383   -0.545720
 H   -9.029305   -2.448065   -0.582182
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 C   -7.963320   -2.261669   -0.760181
 H   -7.839965   -2.041246   -1.834935
 N   -7.523156   -1.165712    0.070470
 H   -9.403618   -1.077805    0.961701
 H   -8.064929   -0.723083    2.076796
 C   -8.424777   -0.589903    1.040194
 H   -8.577743    0.491351    0.874609
63
Figure 2_para-NMe2_int3 / electronic energy: -2800.15493149 a.u. / lowest freq: 16.63 cm-1
 B    0.326870    0.592902   -0.417959
 O    0.313060    1.908467   -1.009758
 O    1.169005    0.729432    0.816162
 C    1.295890    2.719687   -0.404292
 C    1.407515    2.113458    1.043087
 C    0.831538    4.171672   -0.431210
 C    2.606830    2.600329   -1.193491
 C    0.307579    2.628695    1.974773
 C    2.768440    2.288696    1.703657
 H   -0.681899    2.535295    1.504227
 H    0.466315    3.678737    2.262705
 H    0.302298    2.018982    2.891077
 H    3.559224    1.777469    1.137208
 H    2.752050    1.861504    2.718176
 H    3.031229    3.354311    1.791553
 H    3.021249    1.578424   -1.151234
 H    3.378430    3.295473   -0.830100
 H    2.404738    2.828687   -2.250613
 H    1.514963    4.820591    0.138587
 H   -0.179221    4.275123   -0.014214
 H    0.804784    4.536411   -1.469462
 C   -4.741039    0.891201   -0.692516
 C   -6.064190    0.486895   -0.549833
 C   -3.658808    0.079096   -0.322224
 C   -6.382369   -0.782777   -0.015418
 C   -3.980365   -1.182776    0.203890
 C   -5.293050   -1.609346    0.355013
 C   -2.277405    0.569669   -0.495029
 C   -1.124687   -0.048857   -0.188054
 H   -5.470542   -2.602051    0.768622
 H   -3.180177   -1.863047    0.507473
 H   -6.853214    1.172113   -0.859569
 H   -4.540576    1.882213   -1.111471
Cu    2.400526   -0.559612   -0.377242
 H   -1.176152   -1.058041    0.249479
 H    0.955554   -0.290047   -1.229125
 H   -2.204494    1.574857   -0.932288
 H    4.624786   -0.910899    2.974288
 H    6.699331   -1.766370    1.524655
 C    4.006705   -1.552298    2.324759
 H    3.033087   -1.067984    2.173149
 H    7.100880   -1.686527   -0.830483
 N    4.640215   -1.744287    1.045831
 C    5.966399   -2.350061    0.945945
 H    3.851769   -2.516646    2.836094
 C    4.118515   -1.410150   -0.138713
 C    6.233986   -2.312656   -0.565029
 H    5.579769   -0.812266   -2.894967
 H    5.952439   -3.373603    1.352802
 N    5.002700   -1.725243   -1.089547
 C    4.827185   -1.516314   -2.502913
 H    6.395401   -3.313113   -0.996161
 H    3.825939   -1.100557   -2.676922
 H    4.921018   -2.467114   -3.052400
 H   -7.540735   -2.679728    1.646473
 H   -9.053280   -2.657088    0.720177
 H   -9.723367   -0.849404   -0.115601
 H   -8.782107    0.616615    0.227630
 C   -7.967914   -2.520454    0.641027
 C   -8.766186   -0.349707   -0.306636
 N   -7.685117   -1.197076    0.137622
 H   -7.575789   -3.315426   -0.019903
 H   -8.711831   -0.133635   -1.389395
44
Figure 2_para-NMe2-alkenylBpin / electronic energy: -853.456934437 a.u. / lowest freq: 23.23 cm-1
 B   -2.187170   -0.365211    0.009480
 O   -3.150062   -1.308190    0.256850
 O   -2.719971    0.871376   -0.253825
 C   -4.429772   -0.720739   -0.045141
 C   -4.122547    0.819094    0.064576
 C   -5.461729   -1.234491    0.945780
 C   -4.799537   -1.155667   -1.462554
 C   -4.280376    1.361085    1.484676
 C   -4.893795    1.689895   -0.914167
 H   -3.742396    0.739095    2.215571
 H   -5.337156    1.416990    1.783044
 H   -3.856508    2.375071    1.528609
 H   -4.661526    1.436198   -1.956775
 H   -4.636808    2.747934   -0.756642
 H   -5.977402    1.578257   -0.758380
 H   -4.071062   -0.786727   -2.199959
 H   -5.798937   -0.798203   -1.749417
 H   -4.801313   -2.254633   -1.510976
 H   -6.427272   -0.727499    0.798153
 H   -5.140704   -1.082014    1.984379
 H   -5.619453   -2.312545    0.794328
 C    2.524789    1.319156   -0.116960
 C    3.911059    1.255250   -0.091630
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 C     1.719306    0.170822   -0.054482
 C     4.579018    0.009600   -0.003909
 C     2.385000   -1.064718    0.028476
 C     3.767329   -1.153399    0.052138
 C     0.259119    0.304712   -0.075142
 C    -0.668799   -0.668118    0.038170
 H     4.224495   -2.140270    0.117856
 H     1.807980   -1.991876    0.074166
 H     4.477072    2.184934   -0.144841
 H     2.045955    2.300298   -0.188373
 H    -0.341817   -1.706766    0.171089
 H    -0.096635    1.336458   -0.193713
 H     6.587387    1.699032   -0.957837
 H     6.513293    1.810645    0.822063
 C     6.741153    1.134989   -0.020836
 H     7.804145    0.873333    0.040392
 N     5.945699   -0.071055    0.023558
 H     6.334805   -1.911285    1.011367
 H     7.683963   -1.215909    0.088537
 C     6.597253   -1.359645    0.091378
 H     6.341286   -1.999507   -0.771386
63
Figure 2_para-NMe2_pc2_rev / electronic energy: -2800.16441697 a.u. / lowest freq: 18.93 cm-1
 B    -1.404452    1.193477    0.493136
 O    -2.307444    1.083008    1.521247
 O    -1.936369    1.825644   -0.603843
 C    -3.594291    1.493963    1.027891
 C    -3.209140    2.374520   -0.221238
 C    -4.332963    2.241061    2.127228
 C    -4.357294    0.225974    0.649657
 C    -2.975245    3.842614    0.131380
 C    -4.170665    2.265215   -1.393828
 H    -2.284103    3.947149    0.981047
 H    -3.915241    4.356339    0.379305
 H    -2.524692    4.349718   -0.734510
 H    -4.222784    1.238849   -1.780338
 H    -3.834067    2.917806   -2.212906
 H    -5.181988    2.584143   -1.099352
 H    -3.843452   -0.315313   -0.155866
 H    -5.384955    0.449043    0.328929
 H    -4.406220   -0.436150    1.527000
 H    -5.281161    2.651512    1.748157
 H    -3.731919    3.064745    2.533776
 H    -4.566743    1.552359    2.952792
 C     3.400701    1.402724   -0.992957
 C     4.772922    1.226763   -0.864913
 C     2.480845    0.734450   -0.174083
 C     5.307393    0.345012    0.103798
 C     3.011769   -0.135247    0.789950
 C     4.379016   -0.331925    0.932053
 C     1.030785    0.961261   -0.354592
 C     0.045606    0.675451    0.588515
 H     4.726377   -1.026998    1.696237
 H     2.340991   -0.693594    1.448507
 H     5.431352    1.781206   -1.533094
 H     3.029363    2.086632   -1.761767
Cu     0.023667   -0.785448   -0.889842
 H     0.344697    0.200152    1.530463
 H     0.790510   -1.130110   -2.263021
 H     0.776678    1.646068   -1.172115
 H     7.481506    1.975649   -0.479767
 H     8.607599    0.607481   -0.359855
 C     7.576706    0.883023   -0.612338
 H     7.423422    0.660762   -1.683609
 N     6.661996    0.152504    0.232990
 H     6.920989   -0.483534    2.245410
 H     8.263625   -0.829304    1.133561
 C     7.170731   -0.780448    1.210495
 H     6.779883   -1.801160    1.051443
 H    -4.486942   -2.792274   -0.421683
 H    -3.792921   -1.125413   -2.407872
 H    -3.383037   -3.076137    1.681948
 C    -3.470767   -3.205211   -0.518279
 C    -2.825311   -1.653639   -2.400037
 H    -1.005054   -2.245043    2.674061
 N    -2.564753   -2.218380   -1.101854
 C    -2.810608   -3.490806    0.835191
 H    -2.027381   -0.942461   -2.648178
 C    -1.448412   -2.036211   -0.387336
 N    -1.531630   -2.794671    0.709211
 H    -3.524788   -4.099291   -1.161764
 H    -2.853805   -2.438479   -3.174465
 C    -0.592882   -2.777139    1.799559
 H    -2.657771   -4.564275    1.021285
 H     0.323228   -2.269246    1.473239
 H    -0.337461   -3.804044    2.104386
63
Figure 2_para-NMe2_ts(CuHadd_rev) / electronic energy: -2800.14106095 a.u. / lowest freq: -810.46 cm-1
 B    -1.240346    1.451404    0.484642
 O    -2.045037    1.694654    1.590324
 O    -1.890277    1.830458   -0.690998
 C    -3.360289    1.994945    1.115625
 C    -3.070735    2.553032   -0.323766
 C    -4.020442    2.987571    2.060366
 C    -4.151231    0.685164    1.092822
 C    -2.714279    4.040565   -0.319303
 C    -4.168559    2.287443   -1.341911
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 H   -1.942736    4.264063    0.432732
 H   -3.591746    4.672717   -0.118437
 H   -2.311819    4.313174   -1.306259
 H   -4.351936    1.213543   -1.472005
 H   -3.880150    2.702199   -2.319536
 H   -5.109397    2.768643   -1.033824
 H   -3.702128   -0.041583    0.399430
 H   -5.201989    0.843267    0.808720
 H   -4.131951    0.240721    2.099110
 H   -4.996379    3.312935    1.668345
 H   -3.392750    3.874646    2.217585
 H   -4.188083    2.515942    3.040385
 C    3.388192    1.356564   -1.107838
 C    4.764153    1.261028   -0.912298
 C    2.483765    0.548142   -0.415345
 C    5.307780    0.331262    0.002517
 C    3.021524   -0.380463    0.483374
 C    4.389946   -0.495648    0.694508
 C    1.007372    0.697363   -0.613316
 C    0.154367    0.866777    0.547644
 H    4.745533   -1.243275    1.403429
 H    2.349292   -1.046096    1.033168
 H    5.415506    1.923203   -1.482367
 H    3.011022    2.091725   -1.825016
Cu   -0.293955   -0.876040   -0.461526
 H    0.576872    0.596597    1.523169
 H    0.833646   -0.666099   -1.565086
 H    0.759845    1.333488   -1.470963
 H    7.405938    2.136644   -0.362152
 H    8.604462    0.828866   -0.264034
 C    7.570994    1.060085   -0.548851
 H    7.479899    0.891769   -1.637294
 N    6.665469    0.230147    0.208655
 H    6.782871   -0.559781    2.173865
 H    8.274533   -0.628501    1.214724
 C    7.183514   -0.725498    1.157896
 H    6.954108   -1.769503    0.875164
 H   -4.569436   -3.343668   -0.506235
 H   -4.203138   -1.183911   -1.967851
 H   -3.310719   -4.027649    1.422971
 C   -3.508882   -3.543125   -0.716727
 C   -3.124948   -1.402157   -2.002706
 H   -0.940671   -3.527725    2.510410
 N   -2.771754   -2.301387   -0.933898
 C   -2.762619   -4.152361    0.472824
 H   -2.571802   -0.460622   -1.880366
 C   -1.602320   -2.273335   -0.278424
 N   -1.535839   -3.358529    0.500707
 H   -3.451898   -4.179886   -1.616923
 H   -2.891497   -1.834948   -2.991390
 C   -0.520537   -3.597378    1.492592
 H   -2.543013   -5.221776    0.342215
 H    0.265226   -2.837699    1.387376
 H   -0.072296   -4.595638    1.367052
63
Figure 2_para-NMe2_L-Cu-alkyl_rev / electronic energy: -2800.19059809 a.u. / lowest freq: 17.92 cm-1
 B    1.691100   -1.551271    0.519713
 O    2.702162   -1.506734    1.484186
 O    2.255701   -1.757016   -0.746608
 C    3.951749   -1.365448    0.810690
 C    3.649820   -2.016935   -0.587425
 C    5.042435   -2.061787    1.611291
 C    4.257091    0.131426    0.710187
 C    3.841283   -3.534644   -0.585674
 C    4.414404   -1.401753   -1.750870
 H    3.321791   -4.001047    0.264714
 H    4.903972   -3.816225   -0.542844
 H    3.413243   -3.949289   -1.510601
 H    4.185386   -0.334549   -1.867674
 H    4.141395   -1.909737   -2.688292
 H    5.500493   -1.513482   -1.609121
 H    3.481393    0.655037    0.131642
 H    5.235349    0.324833    0.246048
 H    4.264888    0.562917    1.722376
 H    5.999113   -2.046448    1.066510
 H    4.781398   -3.105819    1.829774
 H    5.190692   -1.544364    2.571206
 C   -3.252826   -2.434514   -0.583288
 C   -4.595248   -2.070764   -0.595342
 C   -2.244794   -1.596304   -0.085658
 C   -5.014656   -0.816741   -0.092141
 C   -2.667687   -0.364485    0.419565
 C   -4.006479    0.027072    0.421570
 C   -0.790562   -2.042994   -0.135493
 C    0.209551   -1.345348    0.784760
 H   -4.260984    1.001460    0.839870
 H   -1.922294    0.322131    0.832424
 H   -5.322942   -2.776616   -0.996903
 H   -2.978408   -3.417548   -0.980727
Cu    0.448142    0.592583    0.388959
 H   -0.054259   -1.449226    1.852888
 H   -0.443556   -1.943243   -1.180633
 H   -0.798248   -3.137353    0.043575
 H   -7.376184   -2.298828   -0.015544
 H   -8.334584   -0.885584   -0.507843
 C   -7.346383   -1.354459   -0.589825
 H   -7.189181   -1.614921   -1.652012
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 N   -6.342181   -0.441892   -0.099868
 H   -6.500855    0.916666    1.529527
 H   -7.814137    0.966406    0.331944
 C   -6.732054    0.832242    0.451225
 H   -6.236210    1.675921   -0.061737
 H    2.719358    4.564823   -1.394725
 H    3.215536    2.069073   -2.245188
 H    1.651468    5.253969    0.635498
 C    1.671810    4.236493   -1.322821
 C    2.140504    1.877936   -2.099462
 H    0.140081    4.100084    2.527781
 N    1.591473    2.790003   -1.128335
 C    0.958899    4.772869   -0.075153
 H    2.005308    0.848008   -1.739932
 C    0.818334    2.439819   -0.094085
 N    0.404602    3.554744    0.513645
 H    1.160812    4.521490   -2.257702
 H    1.635925    1.984785   -3.074858
 C   -0.402311    3.605874    1.704692
 H    0.161477    5.492815   -0.312323
 H   -0.648250    2.580589    2.011077
 H   -1.338041    4.159422    1.524241
84
Figure 2_para-NMe2_pc3_01 / electronic energy: -3639.01987332 a.u. / lowest freq: 17.29 cm-1
 C    1.578826    0.473364   -0.560801
 C    1.674011    0.800156    0.793789
 C    1.429642    2.192356    1.290484
 O    2.641029    2.989021    1.266016
 P    3.135061    3.647826   -0.101672
 O    2.097770    4.154144   -1.024245
 O    4.143822    4.724216    0.530269
 O    4.082575    2.581509   -0.839862
 C    4.920287    5.538823   -0.340739
 H    2.096525   -0.393891   -0.981087
 H    1.275136    1.233825   -1.288985
 H    2.273988    0.166619    1.458229
 H    0.665042    2.707531    0.688849
 H    1.113767    2.202872    2.341385
 B    0.467058   -3.141033   -0.878527
 O    0.923831   -3.886970    0.182783
 O    1.461809   -2.898595   -1.791703
 C    2.355621   -3.980814    0.091705
 C    2.611454   -3.684944   -1.433939
 C    2.797810   -5.359539    0.556070
 C    2.931905   -2.909295    1.015244
 C    2.581610   -4.944064   -2.298866
 C    3.873440   -2.886222   -1.720578
 H    1.676319   -5.539721   -2.108880
 H    3.461948   -5.578444   -2.122374
 H    2.575895   -4.650897   -3.358934
 H    3.861419   -1.907575   -1.223415
 H    3.968149   -2.714247   -2.802837
 H    4.765091   -3.437205   -1.384953
 H    2.622799   -1.904073    0.696793
 H    4.030458   -2.944385    1.045343
 H    2.555938   -3.071113    2.036353
 H    3.879797   -5.491240    0.405314
 H    2.270190   -6.159059    0.019696
 H    2.588023   -5.476846    1.629638
 C   -2.574959    0.732419   -2.016315
 C   -3.799963    1.388975   -2.065839
 C   -2.374012   -0.470584   -1.309377
 C   -4.938774    0.871900   -1.409179
 C   -3.513987   -0.971548   -0.656142
 C   -4.751157   -0.325894   -0.691262
 C   -1.028607   -1.094460   -1.220494
 C   -1.004252   -2.614072   -0.997146
 H   -5.582934   -0.783337   -0.153942
 H   -3.439934   -1.897183   -0.079258
 H   -3.864773    2.318461   -2.632758
 H   -1.723929    1.181951   -2.539663
Cu   -0.065839   -0.198246    0.339343
 H   -1.532827   -3.161582   -1.809415
 H   -1.526047   -2.893645   -0.065661
 H   -0.463601   -0.856456   -2.136510
 H    5.544643    6.183099    0.290806
 H    4.275191    6.166764   -0.974255
 H    5.571745    4.925631   -0.983914
 C    5.051586    1.824629   -0.129830
 H    5.759145    1.425602   -0.868260
 H    4.575397    0.986822    0.402078
 H    5.603517    2.446486    0.592284
 H   -0.176307   -2.538190    3.744263
 H   -2.265825   -1.045803    4.622864
 C   -0.734945   -2.554460    2.791652
 H   -0.022827   -2.598048    1.959187
 H   -1.343921   -3.471662    2.766438
 C   -2.664342   -1.147850    3.598407
 N   -1.571427   -1.390758    2.658395
 H   -3.382639   -1.980495    3.592795
 H   -3.432912    0.906455    3.857223
 C   -1.310110   -0.335225    1.878296
 C   -3.256992    0.160077    3.068702
 N   -2.223661    0.606708    2.139021
 H   -4.205372    0.004962    2.525052
 H   -2.376300    2.701914    2.087210
 C   -2.381072    1.835535    1.406152
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 H   -1.553903    1.937889    0.691717
 H   -3.328044    1.835409    0.840647
 H   -5.626472    3.567760   -1.302411
 H   -5.865928    2.974451   -2.967451
 C   -6.226359    2.877954   -1.930906
 H   -7.266687    3.228585   -1.920605
 N   -6.177957    1.509199   -1.475317
 H   -7.469129    0.005120   -0.753304
 H   -8.142151    1.639395   -0.794853
 C   -7.227548    1.067370   -0.590499
 H   -6.979618    1.194216    0.484021
84
Figure 2_para-NMe2_pc3_02 / electronic energy: -3639.01951463 a.u. / lowest freq: 15.61 cm-1
 C    0.576687   -1.050059   -1.110766
 C    0.599460   -1.909252   -0.012696
 C    1.745611   -1.976272    0.947550
 O    2.765088   -2.895775    0.475578
 P    4.212419   -2.338090    0.104301
 O    4.886591   -1.471410    1.092316
 O    4.907025   -3.739886   -0.238404
 O    4.063546   -1.568910   -1.301093
 C    6.311820   -3.785438   -0.467022
 H   -0.068802   -1.268862   -1.967926
 H    1.394810   -0.346394   -1.300167
 H   -0.053367   -2.790631   -0.020518
 H    2.196307   -0.986245    1.108430
 H    1.425592   -2.363463    1.924423
 B    0.650108    2.510254   -1.311613
 O    1.897629    2.068648   -1.681942
 O    0.724267    3.497032   -0.357203
 C    2.855448    2.616942   -0.756510
 C    2.101805    3.887118   -0.221101
 C    4.154374    2.902358   -1.491317
 C    3.086132    1.564115    0.324278
 C    2.310746    5.120367   -1.098458
 C    2.387283    4.227807    1.232780
 H    2.128562    4.895833   -2.160036
 H    3.328554    5.523972   -0.996337
 H    1.599193    5.900956   -0.791720
 H    2.108898    3.408608    1.908035
 H    1.815131    5.120563    1.526588
 H    3.456280    4.447063    1.375653
 H    2.151205    1.334039    0.858744
 H    3.837557    1.887955    1.057964
 H    3.452888    0.641607   -0.145238
 H    4.871470    3.409762   -0.828603
 H    3.991730    3.527661   -2.378960
 H    4.608475    1.955973   -1.820568
 C   -3.817126    0.753519    0.036116
 C   -5.044087    0.125035   -0.148253
 C   -2.789154    0.731856   -0.929180
 C   -5.333543   -0.587733   -1.333186
 C   -3.107397    0.056460   -2.122021
 C   -4.332312   -0.580767   -2.325189
 C   -1.458569    1.332105   -0.649528
 C   -0.702130    1.929113   -1.844614
 H   -4.499292   -1.081721   -3.279704
 H   -2.370783    0.021028   -2.929680
 H   -5.786853    0.196915    0.647333
 H   -3.641326    1.287283    0.976317
Cu   -0.571662   -0.236792    0.306738
 H   -1.291108    2.719722   -2.358304
 H   -0.474591    1.168388   -2.609692
 H   -1.583516    2.112588    0.120315
 H    6.561736   -4.825243   -0.711469
 H    6.866200   -3.479228    0.432650
 H    6.603195   -3.138576   -1.309830
 C    3.511904   -2.207327   -2.446146
 H    3.250143   -1.420027   -3.163894
 H    2.604971   -2.775655   -2.191551
 H    4.248643   -2.884833   -2.904673
 H   -2.756953   -3.060206    2.518841
 H   -2.872532   -1.335207    4.640887
 C   -2.850705   -2.132002    1.932105
 H   -2.339234   -2.263208    0.970277
 H   -3.920086   -1.950531    1.733452
 C   -2.842554   -0.537776    3.884228
 N   -2.263584   -1.019245    2.631488
 H   -3.876531   -0.192415    3.710148
 H   -1.209261    0.336623    5.075064
 C   -1.332989   -0.196186    2.136519
 C   -1.896802    0.608004    4.255398
 N   -1.150211    0.798491    3.013547
 H   -2.425019    1.528491    4.543229
 H    0.753808    1.597810    3.473195
 C   -0.155060    1.833379    2.892086
 H    0.114344    1.960265    1.834701
 H   -0.560582    2.789237    3.256840
 H   -6.967031   -0.910691   -3.576632
 H   -6.161630   -2.457648   -3.207063
 C   -6.893487   -1.725141   -2.828226
 H   -7.865316   -2.233507   -2.785595
 N   -6.541419   -1.256023   -1.510595
 H   -7.282578   -1.353065    0.463974
 H   -8.455806   -1.690399   -0.816754
 C   -7.598527   -1.058311   -0.550522
 H   -7.953785   -0.009177   -0.497049
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Figure 2_para-NMe2_ts(AS)_01 / electronic energy: -3638.99054294 a.u. / lowest freq: -333.16 cm-1
 C    1.173855    1.196094   -0.383305
 C    1.247783    1.505878    1.007529
 C    0.148421    2.015574    1.704439
 O    0.191071    4.066615    1.672520
 P   -0.169159    4.540002    0.263419
 O   -1.095800    3.740804   -0.595631
 O   -0.693190    6.071963    0.483773
 O    1.211818    4.764935   -0.588365
 C   -1.133936    6.804115   -0.637869
 H    2.079662    0.906234   -0.922675
 H    0.408768    1.705996   -0.979723
 H    2.184040    1.354362    1.553665
 H   -0.824966    2.066168    1.215396
 H    0.158949    2.045637    2.793401
 B    2.383288   -2.230438   -1.046740
 O    3.210702   -2.751767   -0.085145
 O    3.042707   -1.364586   -1.878301
 C    4.457042   -2.029043   -0.128846
 C    4.451320   -1.449955   -1.592050
 C    5.600038   -2.982101    0.177213
 C    4.372821   -0.944001    0.941887
 C    5.058709   -2.407396   -2.615656
 C    5.072222   -0.069481   -1.731071
 H    4.618705   -3.412734   -2.535457
 H    6.148013   -2.492692   -2.494427
 H    4.853630   -2.027691   -3.627262
 H    4.567772    0.673362   -1.099276
 H    4.997305    0.267760   -2.775343
 H    6.137880   -0.095773   -1.457471
 H    3.552276   -0.243601    0.730574
 H    5.308625   -0.372189    1.017232
 H    4.178850   -1.413080    1.917766
 H    6.569035   -2.473903    0.061060
 H    5.585087   -3.861691   -0.479516
 H    5.523610   -3.334254    1.216668
 C   -2.230595   -0.377439   -1.905882
 C   -3.615947   -0.441507   -1.990021
 C   -1.453753   -1.414845   -1.359209
 C   -4.325832   -1.576762   -1.536621
 C   -2.165550   -2.536576   -0.906829
 C   -3.554318   -2.622412   -0.984412
 C    0.024097   -1.268113   -1.231976
 C    0.851639   -2.552187   -1.159713
 H   -4.036497   -3.525201   -0.608443
 H   -1.624915   -3.377089   -0.464203
 H   -4.146785    0.408651   -2.418499
 H   -1.730523    0.527072   -2.266545
Cu    0.247128   -0.281258    0.516371
 H    0.681217   -3.167022   -2.068568
 H    0.557413   -3.185715   -0.307151
 H    0.395688   -0.638780   -2.050830
 H   -1.490336    7.781915   -0.283051
 H   -1.959941    6.290196   -1.156593
 H   -0.319182    6.970356   -1.363981
 C    2.309696    5.397520    0.025871
 H    3.147580    5.385289   -0.686215
 H    2.613457    4.874825    0.947532
 H    2.085060    6.447994    0.281777
 H    1.625227   -2.691361    3.522249
 H   -0.881063   -2.872247    4.496362
 C    1.147917   -2.894331    2.548071
 H    1.714545   -2.387201    1.758583
 H    1.197075   -3.977950    2.359371
 C   -1.202340   -3.021389    3.452001
 N   -0.218655   -2.441843    2.537709
 H   -1.305448   -4.102675    3.278529
 H   -2.958230   -1.792637    3.989429
 C   -0.681932   -1.372320    1.886327
 C   -2.472357   -2.235497    3.107457
 N   -1.961640   -1.196283    2.217017
 H   -3.220236   -2.846965    2.575197
 H   -3.166208    0.511241    2.470950
 C   -2.839354   -0.187535    1.683721
 H   -2.315652    0.374722    0.901348
 H   -3.730075   -0.652818    1.232876
 H   -6.332001    0.349766   -1.244400
 H   -6.170220   -0.088546   -2.966466
 C   -6.458027   -0.473622   -1.974927
 H   -7.525942   -0.721619   -2.022975
 N   -5.705809   -1.655756   -1.625076
 H   -6.067965   -3.717898   -1.338964
 H   -7.469553   -2.654249   -1.145243
 C   -6.391552   -2.735641   -0.957371
 H   -6.235606   -2.734026    0.140049
84
Figure 2_para-NMe2_ts(AS)_02 / electronic energy: -3638.99039008 a.u. / lowest freq: -339.36 cm-1
 C    0.424023   -0.962412   -1.267192
 C    0.379024   -2.023710   -0.324030
 C    1.178822   -2.055824    0.823904
 O    2.772440   -3.297414    0.465123
 P    4.036718   -2.476391    0.210798
 O    4.529104   -1.484626    1.210179
 O    5.161650   -3.596410   -0.173337
 O    3.852092   -1.666119   -1.208268
 C    6.494787   -3.173867   -0.357082
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 H   -0.163039   -1.049016   -2.185184
 H    1.318783   -0.334389   -1.339322
 H   -0.341871   -2.835126   -0.465662
 H    1.838443   -1.221029    1.071425
 H    0.910621   -2.714331    1.648391
 B    0.694405    2.481133   -1.354559
 O    1.913660    1.982076   -1.731309
 O    0.811246    3.468713   -0.408623
 C    2.896589    2.482961   -0.800191
 C    2.209541    3.796513   -0.282133
 C    4.214333    2.690046   -1.526526
 C    3.058256    1.427542    0.289937
 C    2.472439    5.004887   -1.178933
 C    2.514725    4.145956    1.164955
 H    2.279726    4.773133   -2.237152
 H    3.508106    5.361481   -1.083101
 H    1.799081    5.823173   -0.883985
 H    2.217907    3.344943    1.853051
 H    1.973253    5.060359    1.449994
 H    3.591034    4.333100    1.296885
 H    2.104982    1.253619    0.814552
 H    3.811546    1.723178    1.033042
 H    3.387755    0.478645   -0.154069
 H    4.954774    3.154876   -0.858318
 H    4.095868    3.322248   -2.416175
 H    4.613676    1.717393   -1.849229
 C   -3.781622    0.817600    0.041616
 C   -5.036197    0.241235   -0.124654
 C   -2.761699    0.708922   -0.920104
 C   -5.352969   -0.495732   -1.289361
 C   -3.089131   -0.013434   -2.079261
 C   -4.337694   -0.600271   -2.267108
 C   -1.409821    1.288251   -0.669897
 C   -0.690563    1.941100   -1.854523
 H   -4.521085   -1.141275   -3.195882
 H   -2.341175   -0.128309   -2.868934
 H   -5.778453    0.374490    0.662961
 H   -3.581823    1.378479    0.960630
Cu   -0.541453   -0.250635    0.290531
 H   -1.303213    2.772609   -2.256657
 H   -0.533021    1.235840   -2.685003
 H   -1.489461    2.025450    0.144383
 H    7.087361   -4.052326   -0.650644
 H    6.917149   -2.751008    0.569041
 H    6.577016   -2.414188   -1.153735
 C    3.411214   -2.351201   -2.357254
 H    3.059939   -1.606308   -3.086005
 H    2.583545   -3.040531   -2.125574
 H    4.230373   -2.931344   -2.816862
 H   -2.642777   -2.953790    2.578161
 H   -2.722204   -1.201318    4.671122
 C   -2.740932   -2.042249    1.967700
 H   -2.219541   -2.192990    1.013494
 H   -3.810025   -1.872046    1.758733
 C   -2.728304   -0.416738    3.900970
 N   -2.165408   -0.908605    2.644534
 H   -3.773277   -0.100150    3.741369
 H   -1.095769    0.521680    5.044967
 C   -1.258372   -0.078360    2.126874
 C   -1.801405    0.757619    4.230664
 N   -1.072405    0.935076    2.974500
 H   -2.343817    1.674676    4.501502
 H    0.812434    1.772150    3.428381
 C   -0.088167    1.977142    2.824582
 H    0.197820    2.064062    1.768462
 H   -0.509964    2.941495    3.144723
 H   -6.838917   -1.162541   -3.574296
 H   -6.180682   -2.644216   -2.832958
 C   -6.881356   -1.804975   -2.674820
 H   -7.891879   -2.227513   -2.614193
 N   -6.590709   -1.079153   -1.462760
 H   -7.322507   -1.324575    0.514972
 H   -8.531341   -1.410018   -0.783262
 C   -7.614629   -0.900327   -0.463166
 H   -7.863258    0.164833   -0.302469
84
Figure 2_para-NMe2_pi-allyl_01 / electronic energy: -3639.01658157 a.u. / lowest freq: 26.65 cm-1
 C    1.038181    1.960407   -1.003317
 C    1.580404    2.438469    0.220008
 C    0.810472    2.475599    1.372660
 O   -2.261328    3.193993    1.274047
 P   -2.883071    2.843393   -0.047145
 O   -2.112057    2.170182   -1.150381
 O   -4.223496    1.947848    0.310092
 O   -3.571709    4.177421   -0.723748
 C   -4.936152    1.345691   -0.739848
 H    1.713451    1.809466   -1.846867
 H   -0.036880    2.110487   -1.207353
 H    2.670758    2.508957    0.309192
 H   -0.286520    2.597414    1.329898
 H    1.295618    2.643814    2.338779
 B    3.404171   -0.898160   -0.793056
 O    4.457440   -1.202579    0.026640
 O    3.676163    0.156539   -1.620088
 C    5.444619   -0.160934   -0.106589
 C    5.078377    0.468752   -1.503493
 C    6.833170   -0.773981   -0.030019
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 C    5.231898    0.800898    1.060648
 C    5.784106   -0.215166   -2.672458
 C    5.260932    1.974943   -1.589658
 H    5.662292   -1.307900   -2.633224
 H    6.858638    0.016433   -2.687896
 H    5.341407    0.140714   -3.614221
 H    4.632322    2.506372   -0.863305
 H    4.986563    2.326826   -2.595005
 H    6.311684    2.247163   -1.409451
 H    4.229518    1.251832    1.029624
 H    5.977556    1.608290    1.061847
 H    5.324388    0.247438    2.006688
 H    7.603689   -0.008745   -0.207642
 H    6.964925   -1.580680   -0.762646
 H    6.998148   -1.196330    0.972196
 C   -1.574093   -1.073656   -1.867585
 C   -2.807086   -1.709525   -1.916690
 C   -0.495565   -1.582194   -1.125424
 C   -3.043720   -2.908782   -1.204608
 C   -0.734846   -2.768763   -0.417157
 C   -1.965692   -3.418061   -0.445234
 C    0.810071   -0.864584   -1.102899
 C    2.049396   -1.691031   -0.780784
 H   -2.080159   -4.338243    0.128080
 H    0.060029   -3.207973    0.190598
 H   -3.599199   -1.256261   -2.512169
 H   -1.458695   -0.121123   -2.390922
Cu    0.751199    0.515715    0.367723
 H    2.152707   -2.495073   -1.540666
 H    1.959213   -2.218131    0.181488
 H    0.948817   -0.339493   -2.053864
 H   -5.730391    0.722635   -0.301110
 H   -4.281370    0.712445   -1.359797
 H   -5.409725    2.096332   -1.398488
 C   -4.342881    5.021281    0.093445
 H   -4.619652    5.910925   -0.492530
 H   -3.781979    5.343623    0.987029
 H   -5.270600    4.526385    0.433171
 H    2.640647   -0.658879    3.734381
 H    0.294033   -1.535241    4.698495
 C    2.362738   -1.233943    2.834154
 H    2.791209   -0.742632    1.953681
 H    2.806329   -2.237863    2.912329
 C    0.126080   -2.003493    3.713745
 N    0.931775   -1.324281    2.697844
 H    0.400901   -3.065432    3.787106
 H   -1.988908   -1.412370    3.968580
 C    0.180264   -0.591245    1.871395
 C   -1.300381   -1.785109    3.196860
 N   -1.101138   -0.787054    2.149526
 H   -1.737295   -2.697118    2.755879
 H   -2.790971    0.465720    2.076025
 C   -2.212963   -0.212216    1.432706
 H   -1.839744    0.362159    0.575408
 H   -2.873553   -1.009269    1.056928
 H   -5.623187   -1.913238   -1.439277
 H   -5.201171   -2.735115   -2.964400
 C   -5.385468   -2.895744   -1.888689
 H   -6.275327   -3.530840   -1.799713
 N   -4.267464   -3.542125   -1.242087
 H   -3.790351   -5.509013   -0.629351
 H   -5.509586   -5.081958   -0.587525
 C   -4.499742   -4.694447   -0.405395
 H   -4.414186   -4.464317    0.674395
84
Figure 2_para-NMe2_pi-allyl_02 / electronic energy: -3639.01320290 a.u. / lowest freq: 11.59 cm-1
 C    0.100664   -0.378414   -2.118302
 C   -0.621887   -1.599517   -2.202091
 C   -0.391313   -2.641485   -1.317479
 O    2.404002   -3.174043    0.294282
 P    3.153005   -2.104875   -0.444503
 O    2.812787   -0.641479   -0.311267
 O    4.746655   -2.338868   -0.126819
 O    3.085558   -2.396072   -2.065943
 C    5.684701   -1.414641   -0.621844
 H   -0.195210    0.449025   -2.764420
 H    1.138959   -0.380606   -1.752144
 H   -1.556615   -1.603850   -2.776193
 H    0.572903   -2.794658   -0.811349
 H   -1.111346   -3.462508   -1.257608
 B    1.191130    2.557344   -0.275378
 O    2.125194    3.164276   -1.064379
 O    1.657690    2.259778    0.969615
 C    3.391988    3.160883   -0.377776
 C    2.988747    2.784311    1.112640
 C    4.023013    4.538940   -0.530719
 C    4.267755    2.111768   -1.056994
 C    2.882968    3.992569    2.041555
 C    3.864397    1.709175    1.742038
 H    2.213581    4.762879    1.630800
 H    3.865686    4.447893    2.230976
 H    2.465516    3.666045    3.005743
 H    3.777902    0.767388    1.182739
 H    3.540743    1.529045    2.778851
 H    4.916732    2.030909    1.773060
 H    3.824830    1.109120   -0.965092
 H    5.278530    2.099378   -0.622585
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 H     4.362546    2.364563   -2.124247
 H     4.968239    4.600073    0.029223
 H     3.357604    5.339855   -0.182264
 H     4.246358    4.723562   -1.592126
 C    -3.431085    1.008116    0.834410
 C    -4.801768    0.889955    0.640932
 C    -2.529125    1.162816   -0.231083
 C    -5.359774    0.905727   -0.659530
 C    -3.091079    1.201180   -1.518451
 C    -4.457540    1.077614   -1.736991
 C    -1.059016    1.245823    0.006019
 C    -0.308972    2.362309   -0.704434
 H    -4.825743    1.116821   -2.762212
 H    -2.435874    1.324047   -2.385285
 H    -5.442169    0.782295    1.516439
 H    -3.041400    0.978340    1.856485
Cu    -0.692250   -0.701906   -0.305741
 H    -0.799178    3.320334   -0.425828
 H    -0.391814    2.317109   -1.799701
 H    -0.855100    1.307035    1.083773
 H     6.688522   -1.843395   -0.481614
 H     5.636001   -0.453348   -0.083520
 H     5.540968   -1.217180   -1.698254
 C     3.194927   -3.716825   -2.530826
 H     3.006055   -3.714050   -3.614954
 H     2.464044   -4.383410   -2.043076
 H     4.204104   -4.131807   -2.356128
 H    -3.343688   -3.487566    1.005229
 H    -2.271667   -3.373838    3.484220
 C    -3.279849   -2.387882    1.061358
 H    -3.139318   -1.987033    0.049896
 H    -4.231431   -2.001249    1.458064
 C    -2.170468   -2.288721    3.326958
 N    -2.181953   -1.979962    1.897977
 H    -3.014556   -1.791785    3.830486
 H    -0.143784   -2.529424    4.176962
 C    -1.065240   -1.373500    1.496136
 C    -0.804638   -1.746703    3.773897
 N    -0.250119   -1.211418    2.530935
 H    -0.886841   -0.948714    4.528055
 H     1.804997   -1.306446    2.903254
 C     1.060537   -0.605972    2.494568
 H     1.345849   -0.376781    1.458929
 H     1.074788    0.320207    3.089985
 H    -7.075843    1.846086   -2.662846
 H    -6.817146    0.094620   -2.878492
 C    -7.249444    0.854774   -2.204830
 H    -8.332608    0.685951   -2.173287
 N    -6.711095    0.759776   -0.868055
 H    -7.369221   -0.203565    0.901122
 H    -8.634344    0.529232   -0.104197
 C    -7.608239    0.662125    0.259108
 H    -7.590523    1.567005    0.894512
64
Figure 2_L-Cu-OtBu_dimer / electronic energy: -4357.97211601 a.u. / lowest freq: -19.85 cm-1
 H    -1.057876   -2.823794   -2.825878
 H    -1.980246   -2.667714   -1.312041
 O     0.078207   -1.017819   -1.258789
 C    -1.048228   -3.061420   -1.749889
 H    -1.045898   -4.158508   -1.636503
 C     0.158516   -2.389922   -1.074836
 H     1.475367   -2.665464   -2.785121
 H    -0.759805   -2.350911    0.894993
 C     1.458383   -2.909326   -1.710688
 C     0.156991   -2.742073    0.424044
 H     2.324017   -2.413213   -1.241845
 H     1.581586   -3.999730   -1.600580
 H     1.020173   -2.268300    0.919277
 H     0.205803   -3.828385    0.609487
Cu     1.378579    0.329330   -0.465065
 H     2.131666   -0.991227    3.381390
 H     4.682348   -1.405429    2.732758
 H     5.481708   -1.718565    0.494438
 H     4.675857   -1.081458   -2.009653
 C     2.171292   -0.117226    2.712040
 C     4.582052   -0.512693    2.098216
 H     1.198856   -0.010984    2.213049
 N     3.192040   -0.289898    1.712946
 C     3.045354   -0.000511    0.406199
 C     5.265779   -0.663084    0.738250
 N     4.251927   -0.137199   -0.170576
 H     3.612584    0.354358   -2.080687
 C     4.493554   -0.077568   -1.587637
 H     2.354764    0.782239    3.326204
 H     4.963659    0.354622    2.665833
 H     6.206045   -0.097525    0.661498
 H     5.369453    0.553572   -1.807185
 H    -0.378809    4.066234    1.363434
 H    -1.215620    2.487467    1.315536
 C    -0.309944    3.028560    0.996342
 H    -1.542344    4.628000   -0.917965
 H    -2.304280    3.010119   -0.908883
 H     0.559090    2.547332    1.474899
 C    -1.400215    3.570787   -1.196882
 C    -0.167055    2.941122   -0.531923
 H     1.054762    4.773347   -0.703921
 H    -1.305843    3.511187   -2.293040
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 C    1.092639    3.703570   -0.968950
 O   -0.065048    1.615388   -0.935560
 H    1.981855    3.258646   -0.494162
 H    1.220534    3.621154   -2.060206
Cu   -1.382126    0.156912   -0.516840
 H   -2.351582    0.600724    3.422431
 H   -4.934218   -0.004844    2.870939
 H   -6.034910    0.158807    0.756762
 H   -5.219728    0.475454   -1.806850
 C   -2.122775   -0.170906    2.668848
 C   -4.523985   -0.695038    2.117592
 H   -1.198578    0.107935    2.144915
 N   -3.185413   -0.283990    1.706499
 C   -3.039380   -0.179163    0.373767
 C   -5.297331   -0.660916    0.794239
 N   -4.235455   -0.434437   -0.181200
 H   -3.591154   -0.191053   -2.134929
 C   -4.528168   -0.356233   -1.586950
 H   -1.956896   -1.128121    3.192726
 H   -4.493762   -1.703279    2.564902
 H   -5.829131   -1.601827    0.585031
 H   -4.988412   -1.291515   -1.945367
32
Figure 2_L-Cu-OtBu / electronic energy: -2178.96309100 a.u. / lowest freq: 32.39 cm-1
 H    4.562030   -0.987762   -1.171425
 H    4.380081   -1.687590    0.453032
 O    2.059982   -0.792706   -0.375405
 C    4.412589   -0.739884   -0.108257
 H    5.285124   -0.160867    0.237784
 C    3.083853    0.016444    0.070903
 H    3.239088    1.094749   -1.813757
 H    2.816631   -0.564871    2.149701
 C    3.141678    1.325832   -0.740702
 C    2.905653    0.363686    1.562854
 H    2.203830    1.891377   -0.606175
 H    3.980920    1.980488   -0.449346
 H    1.973161    0.937231    1.704528
 H    3.740138    0.957642    1.973285
Cu    0.281496   -0.385007   -0.217334
 H   -2.761249   -2.831320    0.955264
 H   -4.389467   -0.710878    1.073176
 H   -3.900683    1.628760    1.086134
 H   -1.572215    2.982676    0.893515
 C   -2.368865   -2.376101    0.031132
 C   -3.894740   -0.371839    0.149702
 H   -1.295333   -2.593746   -0.043339
 N   -2.556823   -0.949305    0.044007
 C   -1.588253   -0.032817   -0.058431
 C   -3.606305    1.135384    0.145880
 N   -2.155228    1.178072   -0.017727
 H   -0.385003    2.236847   -0.219836
 C   -1.452620    2.433488   -0.055287
 H   -2.885552   -2.835640   -0.827649
 H   -4.517059   -0.688565   -0.702765
 H   -4.103640    1.662997   -0.682992
 H   -1.827633    3.068788   -0.873938
74
Figure 2_ed / electronic energy: -3000.72395415 a.u. / lowest freq: -18.37 cm-1
 H   -4.229726    2.326034   -0.150745
 H   -5.967249    0.343716    0.271356
 H   -3.598722   -3.318573    1.735428
 H   -5.751654   -1.943746    0.936556
 H   -2.602038    1.801266   -0.690477
 H   -2.058957   -2.801506    0.982474
 C   -3.680511    1.617234   -0.792634
 C   -3.082739   -0.631120    0.042698
 N   -3.970093    0.257841   -0.410861
 N   -3.731163   -1.761591    0.333175
 C   -3.126225   -2.981981    0.798743
 C   -5.341967   -0.246351   -0.418210
 C   -5.161926   -1.699720    0.039540
 H   -3.978015    1.799131   -1.838489
 H   -5.779726   -0.163645   -1.424914
 H   -3.228038   -3.784690    0.049042
 H   -5.421195   -2.428940   -0.745075
 H   -1.082452    3.518912    1.603248
 H    0.421000    3.855965    0.726137
 O    0.362799    1.259831    1.681643
 C    0.000087    3.675244    1.723920
 H    0.157069    4.577191    2.336829
 C    0.647440    2.454235    2.386838
 H   -1.041587    2.096285    3.707116
 H    2.616865    2.798759    1.517328
 C    0.046175    2.252029    3.779325
 C    2.162870    2.651821    2.505931
 H    0.485762    1.362278    4.255566
 H    0.231377    3.121792    4.428639
 H    2.624169    1.758465    2.954414
 H    2.399418    3.521663    3.139641
Cu   -1.156351   -0.318937    0.168491
 H    3.647599   -2.084771   -1.808356
 H    4.667626   -2.150948    0.441562
 H    3.655695   -0.715072    0.059525
 C    3.791806   -1.560284    0.748890
 H    3.766971   -3.811735   -1.373951
 H    3.989671   -1.143848    1.747863
 C    3.071698   -3.006853   -1.658071
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 H     2.610722   -3.279576   -2.619431
 C     1.991855   -2.826667   -0.601374
 C     2.522294   -2.409985    0.814491
 O     1.169976   -1.706527   -0.954041
 H     3.446123   -4.284636    1.408303
 B     0.804805   -1.023733    0.203641
 H     3.081088   -3.176114    2.752087
 C     2.709243   -3.561359    1.790696
 O     1.472302   -1.555242    1.289645
 H     1.649931   -4.980210   -0.367044
 C     1.084847   -4.057441   -0.565083
 H     0.586842   -4.163168   -1.540589
 H     1.766043   -4.089918    1.981929
 H     0.303393   -3.954382    0.202674
 H     0.142553    4.036318   -1.814791
 H     2.021822    3.781526   -0.667704
 H    -1.142136    3.179841   -2.691591
 C    -0.059830    3.194506   -2.489871
 O    -0.270892    1.738450   -0.614242
 H     2.659078    3.660530   -2.329825
 C     2.572105    3.136225   -1.366163
 H     0.457094    3.377402   -3.444530
 B     0.601562    1.008532    0.304352
 H     3.586208    2.995173   -0.962469
 C     0.360180    1.861111   -1.877169
 C     1.904481    1.766240   -1.514568
 O     1.926733    1.143401   -0.240157
 H    -1.221585    0.778172   -2.863054
 C    -0.123344    0.730502   -2.793547
 H     0.281161    0.832229   -3.811835
 H     0.157572   -0.257891   -2.407175
 H     2.663210    1.336698   -3.516069
 C     2.714992    0.923238   -2.496709
 H     3.773217    0.915775   -2.191785
 H     2.356419   -0.113387   -2.509049
74
Figure 2_ts(TB) / electronic energy: -3000.72314236 a.u. / lowest freq: -71.58 cm-1
 H    -4.448283    1.831801   -0.546545
 H    -6.034945   -0.274227   -0.136759
 H    -3.216551   -3.476593    1.843614
 H    -5.506494   -2.318901    0.990513
 H    -2.733610    1.438777   -0.890484
 H    -1.787148   -3.089113    0.837440
 C    -3.773199    1.128838   -1.061090
 C    -2.995601   -1.009119   -0.092528
 N    -3.958927   -0.208011   -0.557112
 N    -3.547831   -2.188579    0.211178
 C    -2.863967   -3.303706    0.812657
 C    -5.261789   -0.864729   -0.651030
 C    -4.996322   -2.217748    0.017945
 H    -3.991266    1.174517   -2.142029
 H    -5.558704   -0.964972   -1.708457
 H    -3.032398   -4.223784    0.230395
 H    -5.289878   -3.073253   -0.608926
 H    -1.889619    3.082951    1.743967
 H    -0.475447    3.841768    0.978387
 O     0.012370    1.213800    1.663904
 C    -0.874460    3.464722    1.930869
 H    -0.944087    4.308818    2.634747
 C     0.013393    2.358438    2.507367
 H    -1.580508    1.488051    3.697900
 H     1.869593    3.236060    1.766788
 C    -0.558425    1.872271    3.838323
 C     1.443340    2.866966    2.709358
 H     0.060226    1.055179    4.239327
 H    -0.588936    2.683719    4.581426
 H     2.086995    2.051714    3.072839
 H     1.463920    3.684030    3.447489
Cu    -1.064796   -0.614475    0.066837
 H     4.152179   -1.222790   -1.601625
 H     4.926631   -1.208560    0.732258
 H     3.609618   -0.050027    0.333136
 C     3.901707   -0.891709    0.976936
 H     4.666629   -2.898230   -1.268204
 H     3.893798   -0.529670    2.016219
 C     3.817631   -2.267672   -1.575410
 H     3.534087   -2.557519   -2.598835
 C     2.634973   -2.459067   -0.637358
 C     2.900430   -2.039896    0.849730
 O     1.576663   -1.571157   -1.014383
 H     4.231911   -3.656063    1.429621
 B     0.913650   -1.122778    0.130318
 H     3.464389   -2.800114    2.789141
 C     3.297763   -3.183901    1.771368
 O     1.621543   -1.531095    1.251149
 H     2.864132   -4.640428   -0.558217
 C     2.093462   -3.884147   -0.768821
 H     1.733821   -4.037022   -1.797388
 H     2.516389   -3.953389    1.826435
 H     1.245776   -4.049768   -0.087193
 H    -0.420230    4.054241   -1.831844
 H     1.344645    4.063200   -0.458545
 H    -1.457836    3.001197   -2.817127
 C    -0.416657    3.197554   -2.518434
 O    -0.527086    1.723785   -0.642973
 H     2.129607    4.141849   -2.060330
 C     2.062456    3.564957   -1.125973
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 H    0.146515    3.473608   -3.422999
 B    0.378612    1.188218    0.318412
 H    3.048455    3.588701   -0.638400
 C    0.169014    1.950819   -1.865317
 C    1.669377    2.108377   -1.380171
 O    1.690769    1.442805   -0.120721
 H   -1.129452    0.602593   -2.935045
 C   -0.047937    0.753365   -2.794138
 H    0.399213    0.929741   -3.783876
 H    0.379967   -0.167761   -2.378157
 H    2.645391    1.898337   -3.314327
 C    2.688765    1.457115   -2.306623
 H    3.703702    1.618116   -1.911727
 H    2.515077    0.376425   -2.376759
74
Figure 2_prod / electronic energy: -3000.74272641 a.u. / lowest freq: 20.41 cm-1
 H   -3.886200    1.904460    0.040425
 H   -5.783170   -0.000028    0.231301
 H   -3.671290   -4.009664    0.712028
 H   -5.779110   -2.391811    0.307129
 H   -2.431530    1.418920   -0.867743
 H   -2.156883   -3.467472   -0.075581
 C   -3.521445    1.318515   -0.819820
 C   -3.044171   -1.083929   -0.477400
 N   -3.884978   -0.068040   -0.690769
 N   -3.774686   -2.199854   -0.351226
 C   -3.248139   -3.529587   -0.185304
 C   -5.293235   -0.458612   -0.643950
 C   -5.207063   -1.984777   -0.540404
 H   -3.958179    1.745967   -1.737311
 H   -5.823136   -0.116425   -1.545676
 H   -3.484024   -4.160187   -1.059528
 H   -5.550488   -2.493752   -1.456806
 H   -0.953241    3.764861    3.357981
 H    0.759299    3.428938    2.975556
 O   -0.875512    1.986080    1.406417
 C   -0.148430    3.018702    3.444873
 H    0.062558    2.860737    4.513442
 C   -0.552175    1.706030    2.774674
 H   -2.662097    1.885852    3.254227
 H    1.522396    1.080215    2.546667
 C   -1.843289    1.160855    3.378161
 C    0.563820    0.669955    2.888868
 H   -2.130100    0.224690    2.875511
 H   -1.717424    0.955828    4.451620
 H    0.344931   -0.216712    2.276614
 H    0.673948    0.353697    3.937508
Cu   -1.061912   -1.136593   -0.315311
 H    4.402647   -0.650240   -0.989617
 H    4.621398   -1.002509    1.402523
 H    3.160136   -0.085512    0.918287
 C    3.522073   -0.979220    1.447740
 H    5.192444   -2.244337   -0.885959
 H    3.226802   -0.887955    2.503535
 C    4.303465   -1.709747   -1.255594
 H    4.297891   -1.782907   -2.353926
 C    3.032949   -2.326933   -0.689967
 C    2.899711   -2.248976    0.864652
 O    1.888776   -1.577832   -1.121179
 H    4.481998   -3.631811    1.423538
 B    0.903669   -1.611522   -0.123564
 H    3.275879   -3.326507    2.696880
 C    3.409346   -3.471239    1.614104
 O    1.480199   -2.146878    1.031772
 H    3.743816   -4.379616   -1.009699
 C    2.869341   -3.749566   -1.231268
 H    2.746510   -3.702507   -2.323658
 H    2.863688   -4.380535    1.328701
 H    1.973529   -4.232021   -0.812859
 H    0.385110    4.774697   -2.173196
 H    1.496802    4.695314   -0.164989
 H   -0.507126    3.734422   -3.303777
 C    0.419699    3.821781   -2.717391
 O   -0.524972    2.690348   -0.813439
 H    2.757526    4.544486   -1.420219
 C    2.313155    4.059293   -0.539290
 H    1.265214    3.846315   -3.421248
 B   -0.030339    2.224887    0.383639
 H    3.082788    4.000577    0.244528
 C    0.538550    2.632846   -1.776365
 C    1.822046    2.649090   -0.858748
 O    1.334459    2.085967    0.372262
 H   -0.612874    1.326243   -3.039970
 C    0.375562    1.330242   -2.556106
 H    1.139110    1.225440   -3.340341
 H    0.434150    0.455202   -1.891068
 H    3.294722    2.132517   -2.363615
 C    2.962520    1.788006   -1.372089
 H    3.820345    1.859265   -0.686128
 H    2.658330    0.735648   -1.440404
39
Figure 2_L-Cu-Bpin / electronic energy: -2356.95154150 a.u. / lowest freq: 22.11 cm-1
 H   -4.270736   -2.604302    0.699216
 H   -3.469511   -2.304962   -1.601614
 C   -4.343959   -1.520428    0.875987
 H   -4.082488   -1.334048    1.925984
 H   -5.392484   -1.222875    0.718439
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 C   -3.691752   -1.230867   -1.514808
 O   -2.057742   -1.109903    0.223326
 H   -4.742108   -1.073870   -1.802677
 C   -3.418948   -0.778798   -0.078579
 H   -3.048558   -0.694945   -2.228327
 B   -1.238080   -0.000001   -0.000001
 H   -3.048552    0.694945    2.228328
 C   -3.418947    0.778799    0.078581
 H   -4.742104    1.073871    1.802681
 O   -2.057741    1.109902   -0.223328
 C   -3.691747    1.230867    1.514810
 H   -5.392484    1.222879   -0.718433
 H   -4.082491    1.334050   -1.925981
 C   -4.343959    1.520430   -0.875984
 H   -3.469505    2.304963    1.601615
 H   -4.270733    2.604304   -0.699213
Cu    0.797333   -0.000001   -0.000002
 H    3.463333   -3.022428   -0.742996
 H    5.468944   -1.227903   -0.850209
 H    5.489479    1.160908   -0.929040
 H    3.459252    2.934328   -1.042286
 C    3.103330   -2.441738    0.122397
 C    4.991258   -0.767023    0.029199
 H    2.005088   -2.444141    0.118745
 N    3.563409   -1.079451    0.055881
 C    2.777376    0.000000    0.000000
 C    4.991258    0.767025   -0.029195
 N    3.563409    1.079451   -0.055879
 H    2.005087    2.444141   -0.118746
 C    3.103329    2.441739   -0.122398
 H    3.459253   -2.934329    1.042284
 H    5.489478   -1.160906    0.929045
 H    5.468941    1.227905    0.850214
 H    3.463332    3.022430    0.742995
55
Figure 2_para-H_pc1 / electronic energy: -2666.30230457 a.u. / lowest freq: 20.52 cm-1
 H    1.497496   -0.326859    3.292186
 H    2.890504   -2.532612    2.713480
 H    2.465512   -4.090744    0.944336
 H    1.070010   -4.085537   -1.389616
 C    1.651877   -0.024496    2.244220
 C    2.997105   -2.092815    1.710777
 H    0.745545    0.481256    1.886021
 N    1.897628   -1.177265    1.418098
 C    1.337347   -1.393685    0.224107
 C    2.864564   -3.126210    0.586153
 N    1.905301   -2.482362   -0.308166
 H    0.774936   -2.449913   -2.046755
 C    1.517721   -3.090393   -1.552696
 H    2.495375    0.685935    2.204757
 H    3.957787   -1.550477    1.675054
 H    3.815561   -3.322200    0.068585
 H    2.386157   -3.207011   -2.221195
 H    5.122260    2.896464    1.494191
 H    2.931241    4.038088    1.146047
 C    4.386411    2.479658    0.802547
 C    3.160089    3.115294    0.606694
 H    5.619289    0.794422    0.239794
 C    4.662122    1.303689    0.099924
 H   -4.224090    2.362879    2.120738
 C    2.218213    2.584749   -0.273613
 H   -3.358296    0.258406    3.039257
 H    1.264744    3.101212   -0.405757
 C    3.722660    0.775268   -0.780256
 C    2.478524    1.400269   -0.984675
 C   -4.575680    1.885536    1.193494
 C   -3.858525   -0.275142    2.217133
 H   -4.431193    2.600983    0.373004
 O   -2.429952    0.898603    0.705386
 H    3.941837   -0.153639   -1.314987
 H   -4.891913   -0.491119    2.527273
 H   -5.653731    1.689327    1.302267
 C   -3.807817    0.593016    0.958050
 C    1.497634    0.778894   -1.896203
 B   -1.908675   -0.016368   -0.210962
 H   -0.135793    2.216476   -1.755575
 C    0.212357    1.256771   -2.146954
 C   -4.209439   -0.187342   -0.337611
 H   -3.938407    1.554022   -1.623985
 O   -2.959959   -0.769493   -0.734702
 H   -5.650718    1.174446   -1.280926
 H   -6.180463   -0.874848    0.265479
 C   -4.659234    0.736977   -1.471038
 H   -0.334686    0.889777   -3.019996
 C   -5.238964   -1.288260   -0.128726
 H   -4.713811    0.158051   -2.405185
 H   -5.459971   -1.780935   -1.087659
Cu    0.075996   -0.160929   -0.680632
 H    1.899315   -0.008001   -2.543520
 H   -3.331293   -1.228870    2.065691
 H   -4.876695   -2.056365    0.567182
55
Figure 2_para-H_ts(CuBadd) / electronic energy: -2666.29368708 a.u. / lowest freq: -166.19 cm-1
 H    0.996475   -1.288793    3.261287
 H    1.959935   -3.624569    2.587431
 H    1.579873   -4.781718    0.519138
 H    0.787005   -4.074678   -2.019439
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 C    1.381123   -0.872486    2.317415
 C    2.382948   -3.113002    1.710812
 H    0.636879   -0.172541    1.913544
 N    1.597853   -1.930709    1.364808
 C    1.340979   -1.847726    0.054545
 C    2.292418   -3.943466    0.427021
 N    1.790126   -2.963301   -0.532901
 H    1.266827   -2.406685   -2.461225
 C    1.573954   -3.308038   -1.913110
 H    2.312167   -0.320206    2.530824
 H    3.420643   -2.822561    1.950210
 H    3.261894   -4.351495    0.106596
 H    2.500593   -3.696104   -2.363703
 H    4.156558    3.930126    1.867465
 H    1.729312    3.484945    2.267247
 C    3.557859    3.403369    1.120711
 C    2.201890    3.153089    1.337996
 H    5.191316    3.157646   -0.275991
 C    4.131796    2.968495   -0.079799
 H   -3.384870    1.863720    2.629112
 C    1.432753    2.482762    0.388625
 H   -2.665478   -0.467535    2.859602
 H    0.378053    2.288590    0.603582
 C    3.372194    2.299769   -1.031825
 C    1.996487    2.025021   -0.830391
 C   -3.836801    1.690453    1.640966
 C   -3.250868   -0.717613    1.962229
 H   -3.682666    2.594499    1.037507
 O   -1.823604    0.736803    0.715336
 H    3.844409    1.967898   -1.961584
 H   -4.278639   -0.949741    2.277203
 H   -4.918002    1.542328    1.784589
 C   -3.207639    0.466163    0.995793
 C    1.223894    1.289151   -1.816475
 B   -1.477276    0.064623   -0.447421
 H   -0.753453    2.044882   -1.243659
 C   -0.233039    1.216079   -1.745091
 C   -3.763535    0.114089   -0.428724
 H   -3.397141    2.118927   -1.214100
 O   -2.598160   -0.430603   -1.078847
 H   -5.108968    1.793195   -0.830097
 H   -5.747144   -0.567079    0.124761
 C   -4.183217    1.349163   -1.224314
 H   -0.731487    0.947278   -2.684329
 C   -4.874289   -0.923269   -0.443440
 H   -4.359634    1.060007   -2.270875
 H   -5.197184   -1.109090   -1.478710
Cu    0.470780   -0.366854   -0.813045
 H    1.712563    1.068679   -2.769873
 H   -2.808359   -1.619026    1.512320
 H   -4.542906   -1.878784   -0.016344
55
Figure 2_para-H_L-Cu-alkyl_01 / electronic energy: -2666.34950794 a.u. / lowest freq: 22.15 cm-1
 H    0.339344   -1.817615    2.748346
 H   -2.108589   -2.844145    2.488715
 H   -3.694707   -3.077129    0.708339
 H   -3.672137   -1.764181   -1.598009
 C    0.600861   -2.421786    1.862755
 C   -1.710559   -3.402420    1.624157
 H    1.331917   -1.864786    1.261647
 N   -0.564614   -2.691971    1.059896
 C   -0.816931   -2.159207   -0.141633
 C   -2.687657   -3.432860    0.443923
 N   -2.050214   -2.524933   -0.507097
 H   -2.053103   -1.480750   -2.299426
 C   -2.677215   -2.207202   -1.763246
 H    1.062705   -3.360513    2.207225
 H   -1.422116   -4.405431    1.971383
 H   -2.787430   -4.437993    0.000844
 H   -2.798060   -3.108081   -2.388082
 H    5.572884   -0.201789    1.928040
 H    3.972471    1.710127    2.112696
 C    4.788943   -0.057682    1.180623
 C    3.892974    1.005805    1.278943
 H    5.360404   -1.769285   -0.013669
 C    4.663284   -0.933068    0.095135
 H   -0.672135    3.544931    2.768710
 C    2.890226    1.195249    0.325943
 H    0.118845    1.260027    2.467666
 H    2.192919    2.025046    0.451149
 C    3.664464   -0.748601   -0.853465
 C    2.730614    0.315769   -0.769611
 C   -1.478283    3.434587    2.028192
 C   -0.761267    1.044755    1.844193
 H   -1.591561    4.393836    1.506560
 O    0.001823    2.669271    0.281328
 H    3.585120   -1.451789   -1.689346
 H   -1.574567    0.701007    2.499647
 H   -2.410464    3.218481    2.572034
 C   -1.144564    2.305347    1.067937
 C    1.642447    0.437343   -1.768783
 B   -0.138216    2.089405   -0.958162
 H    1.795428    2.646955   -1.923411
 C    1.028719    1.847771   -1.977177
 C   -2.229259    2.038884   -0.040069
 H   -2.319748    4.131151   -0.657793
 O   -1.426390    1.658277   -1.169295
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 H   -3.695811    3.611962    0.355854
 H   -3.737814    1.115803    1.218529
 C   -3.000719    3.296191   -0.435495
 H    0.602941    1.889622   -2.993685
 C   -3.194887    0.909185    0.283597
 H   -3.585500    3.085993   -1.343239
 H   -3.936418    0.809039   -0.523040
Cu    0.360673   -0.901507   -1.045933
 H    2.011507    0.044107   -2.732487
 H   -0.493012    0.230566    1.153375
 H   -2.668550   -0.048884    0.382931
55
Figure 2_para-H_L-Cu-alkyl_02 / electronic energy: -2666.34283721 a.u. / lowest freq: 16.64 cm-1
 B   -2.265439   -1.181273    0.352358
 O   -3.062031   -0.796138    1.400932
 O   -2.967355   -1.248144   -0.826317
 C   -4.421053   -0.723346    0.936317
 C   -4.235238   -0.603745   -0.622360
 C   -5.103780    0.470820    1.584751
 C   -5.112423   -2.018378    1.360062
 C   -4.085491    0.841419   -1.100028
 C   -5.299154   -1.314490   -1.444448
 H   -3.325994    1.384259   -0.518198
 H   -5.037110    1.389033   -1.037386
 H   -3.759588    0.835874   -2.150509
 H   -5.315918   -2.394278   -1.246610
 H   -5.097322   -1.170465   -2.516319
 H   -6.296323   -0.901148   -1.229829
 H   -4.644207   -2.896649    0.891190
 H   -6.181489   -2.012200    1.102083
 H   -5.023549   -2.131434    2.450718
 H   -6.109812    0.619000    1.163525
 H   -4.525092    1.392920    1.443089
 H   -5.210955    0.299538    2.666261
 C   -0.332484    1.690407   -1.660479
 C   -0.690944    3.034084   -1.639744
 C   -0.321965    0.896829   -0.489527
 C   -1.060906    3.655944   -0.442659
 C   -0.698709    1.549216    0.706483
 C   -1.059301    2.896592    0.727933
 C    0.069278   -0.534706   -0.530037
 C   -0.718021   -1.443452    0.451206
 H   -1.348118    3.358127    1.676942
 H   -0.719503    0.984286    1.641600
 H   -1.346755    4.710406   -0.425457
 H   -0.691972    3.603911   -2.573735
 H   -0.058742    1.223149   -2.612039
Cu    2.023063   -0.508455   -0.227807
 H   -0.389286   -1.323109    1.498056
 H   -0.505838   -2.499262    0.204974
 H   -0.107953   -0.902128   -1.556423
 H    5.048663   -3.271556   -0.779903
 H    6.766280   -1.641204    0.501124
 C    4.645897   -2.347059   -1.224557
 H    3.564247   -2.464823   -1.372792
 H    6.262797    0.173077    1.977441
 N    4.876656   -1.220263   -0.359327
 C    6.233857   -0.816253    0.003587
 H    5.126059   -2.197624   -2.206257
 C    3.934680   -0.392782    0.103836
 C    5.982379    0.379575    0.931394
 H    4.032160    1.529497    2.621932
 H    6.802510   -0.541775   -0.900301
 N    4.535734    0.558619    0.825089
 C    3.867020    1.617871    1.535098
 H    6.512820    1.289649    0.612271
 H    2.789328    1.557526    1.333528
 H    4.235551    2.603455    1.207430
55
Figure 2_para-H_L-Cu-alkyl_03 / electronic energy: -2666.34484998 a.u. / lowest freq: 19.00 cm-1
 B   -1.896435   -1.314222   -0.258172
 O   -3.049880   -1.734910   -0.875379
 O   -2.134367   -0.262728    0.595169
 C   -4.081576   -0.772963   -0.596605
 C   -3.560521   -0.113846    0.730262
 C   -5.416558   -1.487764   -0.469835
 C   -4.114110    0.202582   -1.773010
 C   -3.972812   -0.886281    1.982804
 C   -3.908074    1.357070    0.889075
 H   -3.752120   -1.959637    1.884291
 H   -5.045047   -0.768726    2.196048
 H   -3.407014   -0.501294    2.843812
 H   -3.525023    1.963166    0.058679
 H   -3.477219    1.745239    1.823958
 H   -4.999536    1.489735    0.939279
 H   -3.160230    0.742831   -1.871267
 H   -4.923961    0.939532   -1.671580
 H   -4.278676   -0.362077   -2.702411
 H   -6.206534   -0.781158   -0.173721
 H   -5.375232   -2.297771    0.269773
 H   -5.698529   -1.926775   -1.438283
 C    2.897005   -2.308278    1.229954
 C    4.124538   -2.940134    1.076536
 C    1.926706   -2.280591    0.195897
 C    4.451110   -3.586655   -0.122215
 C    2.274041   -2.957261   -0.994955
 C    3.510856   -3.587165   -1.150962
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 C    0.647310   -1.560086    0.380249
 C   -0.503054   -1.975714   -0.538921
 H    3.735990   -4.093848   -2.094344
 H    1.561373   -2.986910   -1.822416
 H    5.416882   -4.082659   -0.245087
 H    4.841117   -2.932913    1.903349
 H    2.668095   -1.803771    2.174738
Cu    1.078943    0.363586    0.188298
 H   -0.669195   -3.076960   -0.548441
 H   -0.285964   -1.741620   -1.600102
 H    0.337765   -1.652488    1.437988
 H   -1.356308    3.348647   -0.903306
 H    0.794565    4.966093   -1.256393
 C   -0.851479    3.048723    0.030878
 H   -1.063763    1.988957    0.227912
 H    3.153264    4.572555   -1.240032
 N    0.573194    3.231030   -0.070188
 C    1.153509    4.552188   -0.299813
 H   -1.265142    3.653106    0.854677
 C    1.480727    2.250218   -0.032816
 C    2.658861    4.252977   -0.309714
 H    4.469982    2.208687   -1.137097
 H    0.860529    5.249603    0.500062
 N    2.690851    2.797145   -0.182485
 C    3.940146    2.081971   -0.178734
 H    3.190748    4.721381    0.534365
 H    3.740675    1.013684   -0.022213
 H    4.597253    2.442420    0.629918
55
Figure 2_para-H_ts(BHE) / electronic energy: -2666.29763823 a.u. / lowest freq: -918.55 cm-1
 B   -2.024988    0.866085    0.278234
 O   -3.082376    1.145392    1.100024
 O   -2.389780    0.143865   -0.826164
 C   -4.193997    0.340737    0.659263
 C   -3.827794    0.066538   -0.847103
 C   -5.486046    1.112075    0.869676
 C   -4.187780   -0.927296    1.511514
 C   -4.321971    1.159051   -1.793087
 C   -4.245188   -1.301657   -1.361740
 H   -4.049257    2.160956   -1.429392
 H   -5.412952    1.118820   -1.923959
 H   -3.852583    1.018339   -2.777839
 H   -3.758097   -2.112362   -0.803919
 H   -3.965793   -1.404532   -2.420797
 H   -5.335542   -1.429108   -1.285473
 H   -3.253463   -1.493078    1.377828
 H   -5.034834   -1.584705    1.268659
 H   -4.262589   -0.647626    2.572519
 H   -6.341096    0.556245    0.456368
 H   -5.449410    2.101987    0.397021
 H   -5.662741    1.257329    1.945634
 C    2.428800    2.542442   -1.465395
 C    3.670372    3.151149   -1.331944
 C    1.647577    2.183431   -0.338057
 C    4.196810    3.440840   -0.067456
 C    2.195941    2.496086    0.931926
 C    3.440957    3.109175    1.057994
 C    0.376916    1.499323   -0.502940
 C   -0.555000    1.288347    0.585952
 H    3.829206    3.325241    2.057660
 H    1.644866    2.234140    1.838896
 H    5.173365    3.919360    0.035854
 H    4.240368    3.405968   -2.230330
 H    2.040889    2.321684   -2.464471
Cu    0.670287   -0.340609    0.434991
 H   -0.459943    1.941408    1.462525
 H   -0.432956    0.000737    1.554103
 H    0.028642    1.333581   -1.526521
 H   -0.245741   -4.400352    0.285965
 H    2.348179   -4.979640    0.142437
 C   -0.012908   -3.487372   -0.284383
 H   -0.653033   -2.670995    0.076136
 H    4.143576   -3.579575    0.900183
 N    1.365032   -3.115241   -0.100767
 C    2.445252   -4.043097   -0.425888
 H   -0.240877   -3.674062   -1.347982
 C    1.801298   -1.872466    0.144679
 C    3.688004   -3.233692   -0.043651
 H    4.510381   -0.905821    1.386035
 H    2.418975   -4.291847   -1.501027
 N    3.138644   -1.890812    0.126012
 C    3.996573   -0.772257    0.418702
 H    4.465820   -3.244752   -0.820979
 H    3.397433    0.146453    0.459228
 H    4.760450   -0.656375   -0.366226
55
Figure 2_para-H_pc2 / electronic energy: -2666.32935168 a.u. / lowest freq: 30.42 cm-1
 B   -1.972778    1.035248    0.009813
 O   -3.085630    1.512288    0.646802
 O   -2.248889   -0.048624   -0.791319
 C   -4.130592    0.533387    0.481017
 C   -3.675799   -0.224724   -0.822579
 C   -5.467419    1.246361    0.363810
 C   -4.110337   -0.356306    1.722154
 C   -4.182128    0.430638   -2.105982
 C   -3.988385   -1.712589   -0.834835
 H   -3.974314    1.510964   -2.116412
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 H   -5.263317    0.281321   -2.237910
 H   -3.667089   -0.021589   -2.966287
 H   -3.501275   -2.236800   -0.002282
 H   -3.631099   -2.159993   -1.774546
 H   -5.073806   -1.881944   -0.769327
 H   -3.144347   -0.871874    1.828659
 H   -4.913609   -1.106510    1.695607
 H   -4.253238    0.270673    2.614406
 H   -6.270729    0.527476    0.142684
 H   -5.453343    2.011373   -0.423333
 H   -5.708482    1.743135    1.315181
 C    2.795097    1.074944   -1.577032
 C    4.126036    1.484463   -1.604555
 C    1.886965    1.617213   -0.652945
 C    4.581217    2.450274   -0.705019
 C    2.359049    2.587633    0.245747
 C    3.689729    2.999071    0.218047
 C    0.495576    1.115753   -0.633082
 C   -0.541342    1.601714    0.157202
 H    4.034848    3.753902    0.928788
 H    1.682326    3.021190    0.985380
 H    5.624605    2.773659   -0.723752
 H    4.813705    1.048185   -2.333433
 H    2.446339    0.312927   -2.279803
Cu    0.256976   -0.083099    1.066855
 H   -0.371627    2.455992    0.820628
 H   -0.500193   -0.169922    2.467373
 H    0.245348    0.429816   -1.450498
 H   -0.411960   -3.700285   -0.424902
 H    2.257246   -4.321893   -0.135614
 C   -0.017385   -2.771968   -0.873082
 H   -0.707814   -1.946993   -0.648362
 H    4.187067   -3.200186    0.738754
 N    1.290465   -2.456144   -0.359224
 C    2.433150   -3.335380   -0.597950
 H    0.023018   -2.906901   -1.965675
 C    1.554880   -1.484630    0.521354
 C    3.573360   -2.568312    0.080002
 H    4.180181   -1.102273    2.398921
 H    2.596070   -3.488384   -1.674866
 N    2.848821   -1.555395    0.844554
 C    3.552237   -0.592586    1.651387
 H    4.244794   -2.079333   -0.647185
 H    2.821490    0.036961    2.175489
 H    4.198459    0.052648    1.031334
55
Figure 2_para-H_ts(H>B) / electronic energy: -2666.31628206 a.u. / lowest freq: -410.68 cm-1
 B   -1.954813   -0.598679   -0.324418
 O   -3.076397   -1.109894   -0.998837
 O   -2.372807    0.173881    0.783688
 C   -4.205425   -0.344959   -0.581502
 C   -3.792709    0.082606    0.875956
 C   -5.448668   -1.220805   -0.652442
 C   -4.367647    0.849569   -1.525312
 C   -4.116398   -0.994110    1.914919
 C   -4.358274    1.422431    1.326295
 H   -3.735499   -1.975908    1.596284
 H   -5.196972   -1.081479    2.102915
 H   -3.623379   -0.733372    2.863519
 H   -4.009810    2.242398    0.684327
 H   -4.033621    1.638262    2.355772
 H   -5.459397    1.410032    1.315284
 H   -3.507346    1.531411   -1.471019
 H   -5.282495    1.420356   -1.306639
 H   -4.435379    0.477140   -2.558829
 H   -6.319921   -0.704119   -0.221068
 H   -5.304943   -2.171375   -0.121808
 H   -5.679728   -1.454033   -1.703126
 C    2.752494   -1.162324    1.419993
 C    4.066997   -1.622060    1.394076
 C    1.759479   -1.754143    0.621864
 C    4.418566   -2.693867    0.571332
 C    2.125363   -2.837770   -0.191768
 C    3.439345   -3.301020   -0.216728
 C    0.393020   -1.187581    0.641520
 C   -0.606709   -1.419320   -0.267558
 H    3.700803   -4.147908   -0.856157
 H    1.372419   -3.331763   -0.810357
 H    4.822469   -1.141827    2.021143
 H    2.485609   -0.314074    2.057154
Cu    0.092750    0.509303   -0.795867
 H   -0.387207   -2.075198   -1.122415
 H   -1.373487    0.579201   -1.473110
 H    0.160935   -0.580800    1.526621
 H    0.717767    4.151954    1.078253
 H    3.328194    4.025660    0.295232
 C    0.815539    3.068365    1.257674
 H   -0.132543    2.579900    0.996140
 H    4.601186    2.574620   -1.117666
 N    1.870115    2.502436    0.458488
 C    3.250337    2.965283    0.586615
 H    1.009676    2.910189    2.331109
 C    1.710402    1.568461   -0.483710
 C    3.999244    2.031323   -0.373610
 H    3.668968    0.648704   -2.862959
 H    3.595462    2.874503    1.627939
 N    2.908145    1.301094   -1.013483
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 C    3.177667    0.251093   -1.960204
 H    4.664144    1.325432    0.152526
 H    2.228786   -0.220094   -2.249463
 H    3.831869   -0.518274   -1.515729
 H    5.447855   -3.059572    0.550047
55
Figure 2_para-H_int1 / electronic energy: -2666.31795715 a.u. / lowest freq: 20.92 cm-1
 B    1.931157    0.230617   -0.432330
 O    3.047512    0.700439   -1.206870
 O    2.442856   -0.222279    0.843943
 C    4.220092    0.169264   -0.616489
 C    3.820444    0.101629    0.903195
 C    5.392992    1.092155   -0.922698
 C    4.494573   -1.219520   -1.206081
 C    3.968083    1.460275    1.597837
 C    4.558279   -0.965339    1.703012
 H    3.481565    2.255341    1.013261
 H    5.020814    1.736920    1.762411
 H    3.470447    1.411396    2.578461
 H    4.352411   -1.971757    1.314259
 H    4.231532   -0.938932    2.754296
 H    5.646753   -0.797045    1.683475
 H    3.695698   -1.930642   -0.949525
 H    5.453089   -1.635469   -0.860223
 H    4.533448   -1.135993   -2.303052
 H    6.297072    0.784977   -0.373661
 H    5.161048    2.134121   -0.663406
 H    5.623563    1.059962   -1.999018
 C   -2.602835    1.494976    1.400656
 C   -3.876556    2.057983    1.350683
 C   -1.581687    1.934267    0.542846
 C   -4.152801    3.084883    0.446756
 C   -1.869978    2.978235   -0.350072
 C   -3.140892    3.546658   -0.397426
 C   -0.273264    1.246348    0.574217
 C    0.650086    1.204502   -0.420303
 H   -3.343919    4.359322   -1.099312
 H   -1.087827    3.353445   -1.014456
 H   -4.657632    1.694187    2.023075
 H   -2.393210    0.685518    2.105745
Cu   -0.114916   -0.848792   -0.671688
 H    0.417545    1.746238   -1.350634
 H    1.475805   -0.940908   -1.102253
 H   -0.054507    0.714022    1.509964
 H   -1.368290   -4.442887    1.126854
 H   -3.868640   -3.882106    0.330029
 C   -1.256247   -3.360485    1.302346
 H   -0.232862   -3.063302    1.037716
 H   -4.787834   -2.284795   -1.193137
 N   -2.185532   -2.613111    0.496657
 C   -3.625678   -2.842327    0.601689
 H   -1.417129   -3.165185    2.375417
 C   -1.862867   -1.666074   -0.388178
 C   -4.197547   -1.818401   -0.388990
 H   -3.567588   -0.450295   -2.808398
 H   -3.967549   -2.674702    1.635121
 N   -2.991148   -1.197530   -0.929225
 C   -3.072767   -0.120533   -1.880304
 H   -4.829474   -1.058409    0.098469
 H   -2.054842    0.216561   -2.119083
 H   -3.638389    0.729110   -1.463039
 H   -5.149069    3.531439    0.406476
55
Figure 2_para-H_ts(Cu>O) / electronic energy: -2666.31305334 a.u. / lowest freq: -46.48 cm-1
 B   -1.327490   -1.078768   -0.725626
 O   -2.441997   -1.893621   -1.112160
 O   -1.648254   -0.515211    0.584512
 C   -3.571480   -1.432037   -0.391168
 C   -2.936803   -0.968459    0.973184
 C   -4.575796   -2.570593   -0.261467
 C   -4.222067   -0.269284   -1.152701
 C   -2.741273   -2.133273    1.948379
 C   -3.684097    0.163415    1.667764
 H   -2.228968   -2.973640    1.456727
 H   -3.693182   -2.495511    2.366422
 H   -2.108367   -1.795357    2.783075
 H   -3.692879    1.075408    1.054972
 H   -3.191230    0.407031    2.621655
 H   -4.725360   -0.119730    1.888408
 H   -3.553673    0.601681   -1.213708
 H   -5.165932    0.050178   -0.686354
 H   -4.439535   -0.596280   -2.180881
 H   -5.408784   -2.292399    0.403047
 H   -4.102076   -3.480207    0.131164
 H   -4.997669   -2.811718   -1.249299
 C    3.145895   -2.156634    1.382706
 C    4.496103   -2.503182    1.416046
 C    2.439333   -2.090905    0.170552
 C    5.175335   -2.787267    0.231579
 C    3.140894   -2.375710   -1.014010
 C    4.489545   -2.720746   -0.983500
 C    1.018491   -1.690067    0.185379
 C    0.143729   -1.705912   -0.836804
 H    5.013495   -2.933764   -1.918771
 H    2.627099   -2.313881   -1.976268
 H    5.020694   -2.550126    2.373675
 H    2.621308   -1.931519    2.315752
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Cu   -0.447472    1.042451   -0.830881
 H    0.484922   -2.077122   -1.814657
 H   -1.324851   -0.039247   -1.673700
 H    0.655828   -1.321086    1.153348
 H    6.234695   -3.054172    0.252915
 H   -1.380776    5.031472   -0.218694
 H    3.598645    1.789895   -1.266592
 H    3.202725    4.250418   -0.310125
 H    1.231486    5.539283    0.106949
 H   -1.822279    3.300832   -0.102635
 H    2.228806    0.663266   -1.031896
 C    0.633155    2.537477   -0.248222
 C   -1.195817    4.092757    0.328500
 N    0.185895    3.704045    0.223308
 C    2.830131    1.447839   -0.555110
 N    1.967048    2.538546   -0.178641
 C    2.515093    3.764119    0.399391
 C    1.253635    4.595037    0.673567
 H   -1.485050    4.242612    1.381824
 H    3.336457    1.017903    0.325079
 H    3.081130    3.534509    1.316173
 H    1.124821    4.837114    1.740196
55
Figure 2_para-H_int2 / electronic energy: -2666.31784905 a.u. / lowest freq: 20.01 cm-1
 B   -0.616210    0.966215   -0.809586
 O   -0.501986    2.366113   -1.141561
 O   -0.016136    0.828642    0.544573
 C    0.427641    2.977795   -0.271688
 C    0.283304    2.127529    1.045410
 C    0.060167    4.447547   -0.100472
 C    1.833234    2.886965   -0.881660
 C   -0.903076    2.576943    1.900474
 C    1.543574    2.061799    1.897670
 H   -1.817766    2.655120    1.294813
 H   -0.719622    3.545434    2.389655
 H   -1.080803    1.827147    2.686309
 H    2.362992    1.562072    1.361752
 H    1.348562    1.493486    2.820028
 H    1.876983    3.070255    2.188176
 H    2.175854    1.844144   -0.984498
 H    2.580631    3.433096   -0.287098
 H    1.807274    3.325295   -1.890485
 H    0.692915    4.929521    0.661133
 H   -0.992517    4.567592    0.188017
 H    0.208921    4.981211   -1.051681
 C   -4.677288   -1.406127    1.106219
 C   -5.952852   -1.969604    1.100169
 C   -4.121314   -0.843646   -0.054676
 C   -6.706200   -1.984893   -0.073139
 C   -4.895612   -0.868175   -1.228372
 C   -6.169042   -1.430535   -1.237493
 C   -2.764868   -0.257590    0.005784
 C   -2.093487    0.368551   -0.974093
 H   -6.748695   -1.437757   -2.164202
 H   -4.494320   -0.442216   -2.151083
 H   -6.360814   -2.400011    2.018307
 H   -4.094264   -1.398340    2.031826
Cu    1.325265   -0.373186   -0.665342
 H   -2.579694    0.472982   -1.955554
 H    0.126176    0.226215   -1.681522
 H   -2.269893   -0.353100    0.981219
 H    2.616174   -1.351521    3.050265
 H    4.929149   -2.223687    2.052513
 C    2.145555   -1.808014    2.164655
 H    1.290091   -1.190494    1.860049
 H    5.903778   -1.727112   -0.076635
 N    3.083488   -1.881753    1.073844
 C    4.341207   -2.613083    1.207764
 H    1.782864   -2.811330    2.443880
 C    2.887230   -1.388509   -0.153104
 C    5.009478   -2.367712   -0.151419
 H    4.999354   -0.518096   -2.311785
 H    4.142472   -3.680944    1.395948
 N    3.958283   -1.677937   -0.897502
 C    4.175109   -1.248875   -2.254314
 H    5.301139   -3.298660   -0.660355
 H    3.256817   -0.777617   -2.628560
 H    4.425619   -2.106067   -2.899468
 H   -7.704967   -2.427707   -0.082907
55
Figure 2_para-H_ts(C-Brot) / electronic energy: -2666.31236794 a.u. / lowest freq: -119.59 cm-1
 B   -0.637241    0.603730   -0.744076
 O   -0.826719    1.953951   -1.207615
 O    0.042819    0.744210    0.577076
 C    0.089783    2.802785   -0.548597
 C    0.226287    2.126920    0.867087
 C   -0.482080    4.215747   -0.508528
 C    1.415444    2.832008   -1.323855
 C   -0.886841    2.554059    1.826324
 C    1.579145    2.328861    1.538737
 H   -1.872544    2.485959    1.345092
 H   -0.747765    3.582850    2.191242
 H   -0.886936    1.878248    2.694873
 H    2.393668    1.891147    0.945580
 H    1.584394    1.844208    2.527045
 H    1.790567    3.399104    1.687960
 H    1.917509    1.851156   -1.337132
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 H    2.121225    3.567457   -0.909605
 H    1.205019    3.105277   -2.368723
 H    0.144795    4.881955    0.104624
 H   -1.503115    4.224057   -0.105390
 H   -0.522208    4.631002   -1.527102
 C   -5.463195   -0.225970    0.610276
 C   -6.688935   -0.889149    0.647604
 C   -4.345936   -0.791267   -0.026225
 C   -6.825021   -2.142220    0.051239
 C   -4.499159   -2.058798   -0.615002
 C   -5.721739   -2.723885   -0.577978
 C   -3.076222   -0.033284   -0.056983
 C   -1.969334   -0.309686   -0.763991
 H   -5.815596   -3.708147   -1.043919
 H   -3.647054   -2.535885   -1.104990
 H   -7.543389   -0.423139    1.144828
 H   -5.365277    0.756957    1.080216
Cu    1.491422   -0.425499   -0.618847
 H   -1.987685   -1.207184   -1.400057
 H    0.205237   -0.042140   -1.600555
 H   -3.082067    0.867203    0.570722
 H    2.931542   -0.847481    3.173817
 H    5.277057   -1.685057    2.234971
 C    2.476663   -1.404618    2.339598
 H    1.585240   -0.863955    1.994073
 H    6.145441   -1.236722    0.044134
 N    3.408721   -1.524392    1.246974
 C    4.706704   -2.170704    1.429735
 H    2.171948   -2.397129    2.712463
 C    3.144676   -1.233643   -0.031476
 C    5.348493   -1.999624    0.048954
 H    5.141627   -0.487173   -2.331416
 H    4.565662   -3.230535    1.701392
 N    4.220080   -1.544343   -0.761978
 C    4.384973   -1.272952   -2.166150
 H    5.769129   -2.933797   -0.350808
 H    3.425363   -0.933093   -2.577555
 H    4.704231   -2.180301   -2.702825
 H   -7.783703   -2.665638    0.078714
55
Figure 2_para-H_int3 / electronic energy: -2666.31707941 a.u. / lowest freq: 15.86 cm-1
 B   -0.693147    0.354395   -0.399671
 O   -0.888411    1.620263   -1.058380
 O    0.154575    0.655675    0.794885
 C    0.020707    2.571343   -0.544813
 C    0.255486    2.069515    0.928125
 C   -0.606507    3.957780   -0.636517
 C    1.305778    2.552523   -1.383740
 C   -0.851451    2.527184    1.880837
 C    1.618744    2.422633    1.507866
 H   -1.845111    2.313958    1.460959
 H   -0.786346    3.602600    2.104829
 H   -0.758827    1.973621    2.827238
 H    2.429583    1.941338    0.942996
 H    1.687445    2.079730    2.551736
 H    1.782179    3.511508    1.498492
 H    1.829995    1.584785   -1.313369
 H    2.010908    3.341209   -1.081856
 H    1.042681    2.708962   -2.440486
 H    0.026625    4.715529   -0.148909
 H   -1.601407    3.978889   -0.172776
 H   -0.723716    4.242564   -1.693277
 C   -5.754429   -0.082859   -0.530671
 C   -6.994109   -0.686587   -0.324003
 C   -4.557497   -0.738619   -0.198278
 C   -7.066538   -1.968020    0.221073
 C   -4.649688   -2.031831    0.346233
 C   -5.886115   -2.637046    0.553740
 C   -3.270276   -0.049524   -0.431956
 C   -2.039215   -0.461203   -0.089545
 H   -5.930618   -3.643170    0.978564
 H   -3.738863   -2.576441    0.606540
 H   -7.909405   -0.152258   -0.591078
 H   -5.706076    0.921534   -0.961076
Cu    1.482280   -0.568936   -0.406570
 H   -1.936122   -1.426179    0.429735
 H    0.003028   -0.494937   -1.196958
 H   -3.357722    0.919151   -0.941257
 H    3.735686   -0.351079    2.999807
 H    5.892934   -1.048696    1.642775
 C    3.176916   -1.062203    2.370766
 H    2.175546   -0.654039    2.179918
 H    6.248293   -0.924392   -0.721852
 N    3.853766   -1.260894    1.114540
 C    5.239101   -1.723800    1.070612
 H    3.078568   -2.011410    2.923765
 C    3.295949   -1.152294   -0.095424
 C    5.537884   -1.716953   -0.433594
 H    4.660032   -0.519064   -2.850783
 H    5.318878   -2.729685    1.515005
 N    4.223066   -1.445873   -1.012387
 C    4.049969   -1.340043   -2.437906
 H    5.935309   -2.676138   -0.797713
 H    2.991829   -1.138078   -2.650939
 H    4.344460   -2.276371   -2.937773
 H   -8.035533   -2.446397    0.382694
36
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Figure 2_para-H-alkenylBpin / electronic energy: -719.616306926 a.u. / lowest freq: 11.87 cm-1
 B     0.922364   -0.365147   -0.028404
 O     1.894117   -1.316245   -0.173823
 O     1.433940    0.892512    0.148584
 C     3.161660   -0.695762    0.122071
 C     2.848301    0.828137   -0.120020
 C     4.227554   -1.277336   -0.792080
 C     3.487647   -1.014695    1.579963
 C     3.048728    1.254565   -1.573413
 C     3.579766    1.781941    0.809984
 H     2.542480    0.568799   -2.269063
 H     4.114997    1.296474   -1.838243
 H     2.618726    2.256986   -1.714756
 H     3.324723    1.603424    1.862628
 H     3.311513    2.820863    0.566919
 H     4.668438    1.676163    0.689783
 H     2.735025   -0.594781    2.263998
 H     4.475038   -0.625732    1.866988
 H     3.496130   -2.106186    1.715677
 H     5.185806   -0.755417   -0.649802
 H     3.942879   -1.205244   -1.849722
 H     4.382907   -2.340283   -0.555288
 C    -3.806743    1.248461    0.192092
 C    -5.197110    1.149758    0.183811
 C    -2.998838    0.113525    0.018524
 C    -5.806490   -0.090352   -0.001273
 C    -3.628094   -1.129019   -0.169041
 C    -5.016012   -1.228789   -0.178362
 C    -1.532965    0.275159    0.038943
 C    -0.597425   -0.686080   -0.066780
 H    -5.487864   -2.203239   -0.325431
 H    -3.028632   -2.030869   -0.311211
 H    -6.895940   -0.172912   -0.008967
 H    -5.805802    2.046357    0.322501
 H    -3.332001    2.222916    0.336640
 H    -0.908917   -1.730947   -0.184153
 H    -1.195659    1.312156    0.158923
55
Figure 2_para-H_pc2_rev / electronic energy: -2666.32621361 a.u. / lowest freq: 23.57 cm-1
 B     0.642761   -1.195883    0.437475
 O     1.569312   -1.077275    1.441695
 O     1.158006   -1.796684   -0.683378
 C     2.851761   -1.456016    0.911437
 C     2.453845   -2.322277   -0.344107
 C     3.627558   -2.208618    1.981002
 C     3.583084   -0.167743    0.540291
 C     2.262370   -3.801644   -0.013464
 C     3.380935   -2.168950   -1.539284
 H     1.597009   -3.937875    0.852009
 H     3.220166   -4.297682    0.199510
 H     1.800456   -4.303319   -0.876498
 H     3.402895   -1.133853   -1.904577
 H     3.035597   -2.810942   -2.363045
 H     4.406010   -2.472764   -1.278561
 H     3.036359    0.382883   -0.236702
 H     4.603692   -0.366690    0.183390
 H     3.648127    0.474966    1.430875
 H     4.574792   -2.594698    1.574986
 H     3.050983   -3.050589    2.385399
 H     3.866565   -1.530234    2.813512
 C    -4.211397   -1.372005   -0.961238
 C    -5.583118   -1.246493   -0.754342
 C    -3.287821   -0.836832   -0.050102
 C    -6.064322   -0.580897    0.373530
 C    -3.786469   -0.173916    1.082809
 C    -5.157832   -0.046412    1.290596
 C    -1.837260   -0.995157   -0.314779
 C    -0.818959   -0.719536    0.597407
 H    -5.523013    0.475652    2.178541
 H    -3.096107    0.253818    1.813552
 H    -7.139462   -0.477418    0.537615
 H    -6.281857   -1.668883   -1.480779
 H    -3.840940   -1.887193   -1.851584
Cu    -0.957012    0.811512   -0.786262
 H    -1.087843   -0.297385    1.573042
 H    -1.814421    1.233796   -2.074586
 H    -1.600681   -1.623627   -1.181214
 H     3.536903    2.876723   -0.426168
 H     2.816639    1.237832   -2.428021
 H     2.486358    3.121841    1.709641
 C     2.509796    3.267740   -0.490909
 C     1.828346    1.722036   -2.367613
 H     0.134700    2.265001    2.764231
 N     1.607956    2.264103   -1.052359
 C     1.883419    3.533483    0.882885
 H     1.052501    0.976521   -2.583335
 C     0.513631    2.064927   -0.309957
 N     0.612257    2.818189    0.787623
 H     2.525133    4.165578   -1.131349
 H     1.784334    2.512533   -3.135706
 C    -0.304698    2.785987    1.896354
 H     1.719180    4.603053    1.080799
 H    -1.217444    2.259515    1.589420
 H    -0.574348    3.808581    2.203347
55
Figure 2_para-H_ts(CuHadd_rev) / electronic energy: -2666.30378750 a.u. / lowest freq: -811.40 cm-1
 B    -0.454039    1.448428    0.489228
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 O   -1.320692    1.641379    1.556053
 O   -1.058301    1.813053   -0.712698
 C   -2.626461    1.869715    1.015613
 C   -2.296745    2.461225   -0.401635
 C   -3.398424    2.806018    1.931656
 C   -3.332028    0.514710    0.935416
 C   -2.031178    3.966835   -0.365866
 C   -3.321881    2.142743   -1.478632
 H   -1.316741    4.228340    0.429018
 H   -2.955607    4.541901   -0.209532
 H   -1.593612    4.274311   -1.327278
 H   -3.436651    1.061384   -1.624916
 H   -3.004955    2.581926   -2.436552
 H   -4.303605    2.567840   -1.219499
 H   -2.793875   -0.173159    0.266959
 H   -4.369431    0.610768    0.582722
 H   -3.350799    0.060761    1.937406
 H   -4.374756    3.061652    1.492331
 H   -2.846495    3.735628    2.123626
 H   -3.580216    2.315819    2.899927
 C    4.160811    1.725110   -0.705727
 C    5.528002    1.685425   -0.426435
 C    3.315423    0.692105   -0.286689
 C    6.069910    0.611508    0.278435
 C    3.871639   -0.385340    0.415198
 C    5.234682   -0.426146    0.698617
 C    1.841710    0.779833   -0.542726
 C    0.959040    0.911279    0.599884
 H    5.651023   -1.277853    1.242306
 H    3.221913   -1.208967    0.725954
 H    7.140380    0.578282    0.494970
 H    6.173613    2.500581   -0.762973
 H    3.741600    2.573413   -1.253580
Cu    0.608858   -0.837424   -0.449322
 H    1.363667    0.633658    1.580875
 H    1.770605   -0.593647   -1.507677
 H    1.594921    1.418608   -1.398528
 H   -3.614501   -3.377487   -0.479004
 H   -3.229433   -1.343230   -2.099186
 H   -2.412657   -3.926710    1.523644
 C   -2.549733   -3.591984   -0.651107
 C   -2.149236   -1.554797   -2.095122
 H   -0.084754   -3.351936    2.647517
 N   -1.811142   -2.369614   -0.956630
 C   -1.828990   -4.097265    0.602677
 H   -1.604677   -0.602920   -2.029397
 C   -0.673677   -2.261239   -0.256966
 N   -0.625149   -3.269218    0.619388
 H   -2.475185   -4.302607   -1.492284
 H   -1.891234   -2.055352   -3.044698
 C    0.371110   -3.425952    1.646043
 H   -1.576137   -5.166371    0.551943
 H    1.116951   -2.626223    1.545178
 H    0.876103   -4.401571    1.562960
55
Figure 2_para-H_L-Cu-alkyl_rev / electronic energy: -2666.35607480 a.u. / lowest freq: 17.86 cm-1
 B   -1.701785    1.209692    0.324652
 O   -2.617071    0.932512    1.344129
 O   -2.240887    0.828773   -0.911840
 C   -3.623233    0.072237    0.813487
 C   -3.600735    0.441988   -0.714456
 C   -4.946155    0.347447    1.513325
 C   -3.183819   -1.370202    1.079064
 C   -4.478876    1.650785   -1.042997
 C   -3.936893   -0.711334   -1.649219
 H   -4.272922    2.488799   -0.360386
 H   -5.550996    1.410478   -0.987750
 H   -4.254906    1.985859   -2.066731
 H   -3.223832   -1.539008   -1.540181
 H   -3.897730   -0.368892   -2.694495
 H   -4.950919   -1.093966   -1.455898
 H   -2.224925   -1.585330    0.584371
 H   -3.930012   -2.103472    0.739337
 H   -3.036217   -1.505063    2.161147
 H   -5.762577   -0.231478    1.054760
 H   -5.208499    1.413213    1.475860
 H   -4.876766    0.055832    2.572283
 C    2.657058    3.187932    0.400993
 C    4.034220    2.990164    0.509911
 C    1.891390    2.463732   -0.521991
 C    4.677720    2.063084   -0.311003
 C    2.555658    1.548884   -1.351297
 C    3.931461    1.345502   -1.247571
 C    0.383734    2.595588   -0.550454
 C   -0.307062    1.762280    0.537125
 H    4.425148    0.624061   -1.904172
 H    1.978164    0.978506   -2.085229
 H    5.755647    1.905228   -0.225588
 H    4.609718    3.565355    1.240067
 H    2.161033    3.912317    1.054155
Cu    0.457449   -0.082326    0.468814
 H   -0.137361    2.172177    1.548046
 H    0.020502    2.282855   -1.543092
 H    0.128573    3.669091   -0.455875
 H    1.005029   -4.841416   -0.279989
 H   -1.179641   -3.407191   -1.120428
 H    2.904314   -4.317099    1.070916
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 C    1.584329   -3.988578   -0.669701
 C   -0.428546   -2.663701   -1.435831
 H    3.370286   -2.050113    2.569048
 N    0.773069   -2.772725   -0.649411
 C    2.764427   -3.611977    0.237465
 H   -0.847268   -1.655593   -1.309362
 C    1.241485   -1.838176    0.182922
 N    2.371345   -2.293783    0.731185
 H    1.893080   -4.231209   -1.698141
 H   -0.210507   -2.825801   -2.503933
 C    3.232157   -1.537336    1.603402
 H    3.718299   -3.542180   -0.310964
 H    2.778034   -0.553057    1.780975
 H    4.222993   -1.388555    1.142604
76
Figure 2_para-H_pc3_01 / electronic energy: -3505.18603597 a.u. / lowest freq: 2.52 cm-1
 C    0.398919   -0.869750   -1.435602
 C    0.427338   -1.915417   -0.518220
 C    1.412939   -1.989963    0.606397
 O    2.635277   -2.639188    0.175574
 P    4.004762   -1.819701    0.207482
 O    4.352269   -1.119615    1.460704
 O    4.978808   -2.997115   -0.270725
 O    3.940457   -0.776713   -1.014930
 C    6.388074   -2.806178   -0.193263
 H   -0.071830   -1.006336   -2.414707
 H    1.082308   -0.018073   -1.347367
 H   -0.045149   -2.867927   -0.786383
 H    1.647716   -0.991506    1.002897
 H    1.024800   -2.596704    1.435661
 B   -0.173720    2.629400   -0.985819
 O    1.170430    2.456431   -1.208592
 O   -0.410509    3.414070    0.116280
 C    1.880022    2.955514   -0.058386
 C    0.843118    3.965866    0.554432
 C    3.190902    3.576464   -0.511675
 C    2.156223    1.759391    0.848604
 C    0.953947    5.368474   -0.040998
 C    0.851356    4.041160    2.072893
 H    0.965543    5.339114   -1.140832
 H    1.861470    5.884207    0.304241
 H    0.081630    5.961371    0.271478
 H    0.627701    3.069333    2.531378
 H    0.092371    4.760782    2.414152
 H    1.831450    4.382042    2.439562
 H    1.218592    1.284898    1.178478
 H    2.734005    2.044054    1.739363
 H    2.743711    1.016438    0.292222
 H    3.711091    4.044977    0.337478
 H    3.037017    4.335041   -1.290473
 H    3.848157    2.795277   -0.921291
 C   -4.367731   -0.044260   -0.677558
 C   -5.423275   -0.799083   -1.175591
 C   -3.250543    0.306700   -1.476397
 C   -5.421569   -1.239111   -2.504127
 C   -3.286137   -0.127827   -2.820963
 C   -4.344240   -0.888637   -3.318828
 C   -2.107487    1.035451   -0.894760
 C   -1.316666    1.965712   -1.824860
 H   -4.327244   -1.207834   -4.365255
 H   -2.461109    0.132430   -3.489262
 H   -6.250343   -1.832542   -2.897412
 H   -6.264473   -1.045657   -0.520615
 H   -4.389089    0.292084    0.364168
Cu   -1.071286   -0.553223   -0.107631
 H   -1.965550    2.746005   -2.277456
 H   -0.860638    1.419382   -2.666582
 H   -2.451651    1.600828   -0.013111
 H    6.857584   -3.728916   -0.555502
 H    6.702770   -2.619151    0.844151
 H    6.713624   -1.965892   -0.826826
 C    3.697841   -1.198255   -2.351868
 H    3.360541   -0.317755   -2.912948
 H    2.917278   -1.972085   -2.393647
 H    4.621561   -1.586013   -2.808175
 H   -3.009081   -4.107084    1.210184
 H   -3.769781   -2.852056    3.471308
 C   -3.102421   -3.116502    0.737297
 H   -2.349449   -3.028336   -0.055873
 H   -4.102757   -3.037927    0.279305
 C   -3.771119   -1.936121    2.862418
 N   -2.889916   -2.071210    1.704121
 H   -4.806096   -1.751577    2.525561
 H   -2.603543   -1.018518    4.490593
 C   -2.080365   -1.019938    1.539279
 C   -3.166697   -0.729478    3.586531
 N   -2.257845   -0.192802    2.575645
 H   -3.917302    0.019392    3.877931
 H   -0.725675    0.842768    3.597437
 C   -1.493309    1.002910    2.820302
 H   -1.004235    1.317916    1.889170
 H   -2.155751    1.817935    3.149958
76
Figure 2_para-H_pc3_02 / electronic energy: -3505.18914182 a.u. / lowest freq: 17.50 cm-1
 C    0.404263   -1.108386   -1.691834
 C    0.469245   -2.025215   -0.647427
 C    1.384751   -1.842439    0.525357
```

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 O    2.648677   -2.521222    0.318008
 P    3.968817   -1.660759    0.080444
 O    4.235513   -0.552351    1.022367
 O    5.020454   -2.867009    0.058163
 O    3.898746   -1.108516   -1.425441
 C    6.412812   -2.575030   -0.012987
 H   -0.012424   -1.399395   -2.661296
 H    1.014265   -0.199745   -1.674524
 H    0.085644   -3.041704   -0.795653
 H    1.568273   -0.772886    0.714251
 H    0.962749   -2.284859    1.437467
 B   -0.402449    2.625523   -0.064022
 O   -0.108437    3.934558    0.219356
 O    0.734464    1.861759   -0.179833
 C    1.307666    4.125209    0.053010
 C    1.868783    2.662742    0.209735
 C    1.805232    5.112201    1.096795
 C    1.515798    4.698831   -1.348461
 C    2.211677    2.298521    1.652597
 C    3.046453    2.335710   -0.694483
 H    1.374946    2.509237    2.335139
 H    3.093381    2.854563    2.002745
 H    2.458480    1.227945    1.704505
 H    2.774393    2.398160   -1.756483
 H    3.409329    1.320258   -0.485891
 H    3.877186    3.033199   -0.505922
 H    1.166046    4.000816   -2.123615
 H    2.573278    4.930899   -1.539409
 H    0.936677    5.628946   -1.444770
 H    2.899261    5.217118    1.041734
 H    1.533487    4.802845    2.114622
 H    1.359962    6.101715    0.914641
 C   -3.773638   -0.311544   -2.526304
 C   -5.049027   -0.828421   -2.719036
 C   -3.430252    0.442366   -1.375776
 C   -6.057500   -0.615847   -1.771380
 C   -4.471981    0.657178   -0.443231
 C   -5.751661    0.135543   -0.636522
 C   -2.050050    0.912389   -1.167947
 C   -1.868858    2.086037   -0.204170
 H   -6.524439    0.324890    0.114851
 H   -4.273798    1.240219    0.459165
 H   -7.060681   -1.021695   -1.922051
 H   -5.264847   -1.402970   -3.624830
 H   -3.000995   -0.494748   -3.280723
Cu   -1.106014   -0.730249   -0.406265
 H   -2.172098    1.801019    0.823541
 H   -2.527245    2.945792   -0.452188
 H   -1.582959    1.131980   -2.142195
 H    6.939722   -3.536031   -0.057468
 H    6.743237   -2.018496    0.876765
 H    6.654784   -1.992232   -0.915886
 C    3.680103   -1.977443   -2.530175
 H    3.309103   -1.363195   -3.360195
 H    2.931984   -2.747959   -2.293053
 H    4.620617   -2.463671   -2.832116
 H   -3.771535   -3.795477    0.728993
 H   -3.855180   -2.820025    3.241909
 C   -3.690283   -2.738247    0.428675
 H   -3.082068   -2.674444   -0.482707
 H   -4.700283   -2.359421    0.201171
 C   -3.691505   -1.833616    2.783352
 N   -3.067377   -1.961656    1.468183
 H   -4.670863   -1.334936    2.684745
 H   -2.103161   -1.561845    4.289642
 C   -2.012145   -1.158546    1.308021
 C   -2.670746   -0.979517    3.543651
 N   -1.783341   -0.536206    2.470676
 H   -3.126154   -0.120061    4.057167
 H    0.062958   -0.162189    3.421687
 C   -0.657179    0.319972    2.738167
 H   -0.150460    0.547459    1.791807
 H   -0.988229    1.264516    3.198824
76
Figure 2_para-H_ts(AS)_01 / electronic energy: -3505.15917847 a.u. / lowest freq: -332.84 cm-1
 C    0.248569   -0.952868   -1.799470
 C    0.238832   -2.166785   -1.069742
 C    0.749358   -2.263899    0.232695
 O    2.643501   -3.087606    0.152322
 P    3.683447   -1.970105    0.129237
 O    3.662626   -0.877692    1.149019
 O    5.113240   -2.756181    0.093654
 O    3.643984   -1.244741   -1.341069
 C    6.301081   -1.994604    0.130398
 H   -0.105273   -0.950619   -2.833617
 H    0.955416   -0.162429   -1.526398
 H   -0.240721   -3.051779   -1.500092
 H    1.148404   -1.381970    0.739168
 H    0.472829   -3.105648    0.864659
 B   -0.217084    2.606099   -0.067916
 O    0.120188    3.906010    0.195942
 O    0.885096    1.801812   -0.187917
 C    1.545295    4.041499    0.020751
 C    2.052604    2.561439    0.195270
 C    2.080690    5.023454    1.049867
 C    1.767791    4.587944   -1.388696
 C    2.379286    2.197631    1.641320
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 C    3.212490    2.162947   -0.702010
 H    1.551156    2.449507    2.320904
 H    3.278690    2.729467    1.985005
 H    2.588326    1.118378    1.693985
 H    2.959371    2.259159   -1.766394
 H    3.479084    1.115412   -0.502014
 H    4.091689    2.792482   -0.494391
 H    1.393131    3.891617   -2.153792
 H    2.832764    4.778861   -1.583709
 H    1.222216    5.536765   -1.497771
 H    3.177577    5.087218    0.990142
 H    1.802059    4.736972    2.072449
 H    1.671117    6.026036    0.855906
 C   -3.710375   -0.237535   -2.476568
 C   -5.016953   -0.666389   -2.686527
 C   -3.351299    0.524122   -1.343853
 C   -6.022999   -0.346564   -1.770026
 C   -4.380757    0.837475   -0.435500
 C   -5.692344    0.410355   -0.646355
 C   -1.935733    0.932293   -1.133899
 C   -1.702650    2.108817   -0.188549
 H   -6.466090    0.676902    0.078941
 H   -4.154718    1.428619    0.454549
 H   -7.050732   -0.678555   -1.934678
 H   -5.256386   -1.251998   -3.578404
 H   -2.935768   -0.497590   -3.204910
Cu   -1.113539   -0.739997   -0.374205
 H   -2.028272    1.865442    0.841029
 H   -2.328110    2.976512   -0.479642
 H   -1.469663    1.130543   -2.109550
 H    7.148224   -2.693260    0.080434
 H    6.374850   -1.407887    1.060594
 H    6.366866   -1.299941   -0.724913
 C    3.597444   -2.027646   -2.510678
 H    3.357145   -1.363822   -3.353769
 H    2.825979   -2.811617   -2.443369
 H    4.568961   -2.512441   -2.710477
 H   -3.991142   -3.543598    0.897318
 H   -3.930397   -2.513112    3.360412
 C   -3.842476   -2.508441    0.551497
 H   -3.250355   -2.525979   -0.372747
 H   -4.826128   -2.064253    0.330304
 C   -3.699543   -1.548372    2.886325
 N   -3.140575   -1.742881    1.549188
 H   -4.634223   -0.966331    2.817930
 H   -2.021939   -1.411610    4.311655
 C   -2.035449   -1.027876    1.346520
 C   -2.578425   -0.781526    3.597276
 N   -1.709245   -0.407065    2.482537
 H   -2.937794    0.108834    4.132590
 H    0.215502   -0.264631    3.329019
 C   -0.479497    0.313014    2.696033
 H   -0.001771    0.498371    1.725636
 H   -0.675521    1.278835    3.186828
76
Figure 2_para-H_ts(AS)_02 / electronic energy: -3505.15468151 a.u. / lowest freq: -321.33 cm-1
 C    0.594816   -1.219165   -0.406893
 C    0.859196   -1.213394    0.990365
 C    1.803066   -0.349035    1.555577
 O    3.633424   -1.313710    1.654517
 P    4.238531   -1.325702    0.251221
 O    3.906680   -0.246118   -0.729971
 O    5.847678   -1.450765    0.510277
 O    3.891971   -2.756788   -0.466539
 C    6.705470   -1.495129   -0.608689
 H   -0.103788   -1.949432   -0.823517
 H    1.377704   -0.859293   -1.084079
 H    0.299685   -1.877905    1.655677
 H    2.292852    0.402525    0.936084
 H    1.833987   -0.203869    2.634765
 B   -3.074655   -0.717268   -0.847413
 O   -3.913805   -1.023841    0.192319
 O   -2.628514   -1.836578   -1.497412
 C   -3.860602   -2.449461    0.400677
 C   -3.363259   -2.970231   -0.998152
 C   -5.234891   -2.945394    0.818027
 C   -2.848083   -2.691816    1.517882
 C   -4.502827   -3.231449   -1.981053
 C   -2.437245   -4.174150   -0.937225
 H   -5.194696   -2.377533   -2.032898
 H   -5.075808   -4.129707   -1.709194
 H   -4.078652   -3.385341   -2.984084
 H   -1.525476   -3.961530   -0.363632
 H   -2.136908   -4.462637   -1.955316
 H   -2.947373   -5.033780   -0.477052
 H   -1.851311   -2.323191    1.234440
 H   -2.765744   -3.758603    1.769498
 H   -3.166973   -2.150529    2.420766
 H   -5.241014   -4.042116    0.906553
 H   -6.010490   -2.646194    0.101438
 H   -5.498697   -2.523767    1.799183
 C    0.672187    2.163047   -2.584396
 C    1.256919    3.368424   -2.958501
 C   -0.564971    2.118370   -1.908093
 C    0.621713    4.580621   -2.675127
 C   -1.191643    3.349564   -1.639031
 C   -0.607253    4.559209   -2.015421
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 C   -1.131487    0.811153   -1.484850
 C   -2.637233    0.738926   -1.234878
 H   -1.122992    5.497667   -1.793204
 H   -2.155045    3.364106   -1.124300
 H    1.078605    5.528510   -2.969055
 H    2.218920    3.362611   -3.477655
 H    1.187030    1.223563   -2.807507
Cu   -0.229163    0.431324    0.280241
 H   -3.195491    1.039884   -2.147132
 H   -2.962242    1.434138   -0.443812
 H   -0.835044    0.038844   -2.206066
 H    7.739510   -1.403912   -0.246372
 H    6.496542   -0.668657   -1.307533
 H    6.607000   -2.448616   -1.156127
 C    3.954658   -3.941868    0.291827
 H    3.753537   -4.786151   -0.383534
 H    3.204822   -3.944902    1.099757
 H    4.950546   -4.087228    0.745780
 H   -2.629682    0.840317    3.511686
 H   -1.538408    3.281784    3.993813
 C   -2.716143    1.216617    2.477794
 H   -2.630415    0.373675    1.783000
 H   -3.715827    1.660050    2.351948
 C   -1.655931    3.463773    2.912413
 N   -1.695539    2.191280    2.192303
 H   -2.589099    4.025388    2.760398
 H    0.279371    4.521073    3.046048
 C   -0.611237    1.989052    1.439584
 C   -0.433078    4.150219    2.294608
 N    0.158731    3.074652    1.501909
 H   -0.705121    4.991591    1.635519
 H    2.248231    3.321013    1.513718
 C    1.404600    3.270990    0.806146
 H    1.570759    2.442605    0.107097
 H    1.375990    4.206643    0.226126
76
Figure 2_para-H_pi-allyl_01 / electronic energy: -3505.17787296 a.u. / lowest freq: 22.64 cm-1
 C   -0.292336   -1.996265   -0.516347
 C   -0.657294   -2.172478    0.840957
 C    0.151939   -1.681744    1.859566
 O    3.278334   -1.795095    1.605959
 P    3.723960   -1.757308    0.172128
 O    2.755212   -1.595906   -0.968927
 O    4.872921   -0.576496    0.088411
 O    4.619275   -3.091944   -0.181980
 C    5.418173   -0.255091   -1.165702
 H   -1.026065   -2.234136   -1.288295
 H    0.778214   -1.969753   -0.790081
 H   -1.699353   -2.425319    1.068105
 H    1.247473   -1.603836    1.735664
 H   -0.241374   -1.627995    2.878946
 B   -3.225774    0.273853   -0.842142
 O   -4.276797    0.558037   -0.012068
 O   -3.289122   -0.995737   -1.345927
 C   -5.009617   -0.660878    0.222479
 C   -4.569864   -1.557377   -0.997750
 C   -6.496647   -0.348648    0.275548
 C   -4.543266   -1.204590    1.571516
 C   -5.472644   -1.394950   -2.218622
 C   -4.390171   -3.031301   -0.672892
 H   -5.622617   -0.334925   -2.471767
 H   -6.456431   -1.858658   -2.058252
 H   -4.998606   -1.885137   -3.081526
 H   -3.624485   -3.191712    0.097257
 H   -4.078520   -3.575163   -1.576685
 H   -5.336111   -3.469932   -0.321668
 H   -3.468378   -1.435685    1.562773
 H   -5.090542   -2.115045    1.853816
 H   -4.718752   -0.444452    2.347013
 H   -7.080877   -1.275638    0.375150
 H   -6.835144    0.184727   -0.622028
 H   -6.713154    0.284793    1.148446
 C    1.534224    1.143907   -2.425841
 C    2.571416    1.995179   -2.795951
 C    0.397058    1.629000   -1.754374
 C    2.513968    3.356735   -2.490347
 C    0.356904    3.000542   -1.450705
 C    1.401549    3.852187   -1.810301
 C   -0.707749    0.693173   -1.394342
 C   -2.089003    1.304916   -1.180431
 H    1.338652    4.915824   -1.565110
 H   -0.505860    3.415869   -0.925640
 H    3.328213    4.024878   -2.780946
 H    3.438835    1.589603   -3.322703
 H    1.622411    0.072560   -2.621675
Cu   -0.258990   -0.180865    0.363671
 H   -2.404428    1.825803   -2.109483
 H   -2.083676    2.084013   -0.402812
 H   -0.763819   -0.096960   -2.151409
 H    6.170489    0.535052   -1.020976
 H    4.647003    0.113169   -1.861866
 H    5.914021   -1.125001   -1.632420
 C    5.579409   -3.523836    0.749124
 H    6.028774   -4.454876    0.372206
 H    5.127453   -3.718613    1.736172
 H    6.384540   -2.778995    0.883368
 H   -2.285352    1.505544    3.488966
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 H   -0.188407    3.093644    3.927761
 C   -2.149425    1.759310    2.424116
 H   -2.425767    0.891579    1.814316
 H   -2.830283    2.586693    2.172939
 C   -0.143498    3.244864    2.836675
 N   -0.782376    2.120060    2.152193
 H   -0.659308    4.187011    2.600571
 H    2.053528    3.178766    3.082891
 C    0.093373    1.386091    1.465178
 C    1.290434    3.191906    2.291302
 N    1.296817    1.936135    1.545175
 H    1.517816    4.027151    1.608402
 H    3.231470    1.113045    1.643330
 C    2.488546    1.438827    0.901721
 H    2.226985    0.576028    0.276268
 H    2.929077    2.218398    0.260513
76
Figure 2_para-H_pi-allyl_02 / electronic energy: -3505.17326116 a.u. / lowest freq: 19.34 cm-1
 C   -0.027072   -0.848331   -2.079244
 C   -0.496060   -2.144766   -1.754368
 C   -0.316033   -2.646033   -0.471715
 O    2.858620   -3.870731   -0.541325
 P    3.154972   -2.502217   -0.020819
 O    2.401886   -1.868267    1.121226
 O    4.772607   -2.445853    0.288354
 O    3.040163   -1.399657   -1.259437
 C    5.324145   -1.283889    0.849089
 H   -0.294675   -0.404094   -3.039935
 H    0.880118   -0.464928   -1.593536
 H   -1.236134   -2.617516   -2.410511
 H    0.516895   -2.308565    0.164654
 H   -0.847592   -3.548297   -0.158527
 B    0.198178    2.546378    0.079855
 O    0.730765    3.697016    0.596333
 O    1.153861    1.709113   -0.420666
 C    2.122957    3.742181    0.211395
 C    2.447809    2.224633   -0.037103
 C    2.930121    4.392534    1.322192
 C    2.204278    4.584178   -1.060593
 C    2.874990    1.485163    1.227855
 C    3.434165    1.945853   -1.157854
 H    2.238405    1.750204    2.085022
 H    3.915426    1.725825    1.492387
 H    2.787540    0.399893    1.060879
 H    3.073472    2.328273   -2.122508
 H    3.567788    0.857395   -1.243623
 H    4.408980    2.408300   -0.940344
 H    1.646394    4.119514   -1.887428
 H    3.245629    4.727659   -1.382854
 H    1.763668    5.573473   -0.868182
 H    4.005959    4.343482    1.095679
 H    2.756420    3.907025    2.291090
 H    2.652242    5.452757    1.418189
 C   -3.678746    0.284092   -2.306342
 C   -5.029323    0.008921   -2.498864
 C   -3.218740    0.931010   -1.142551
 C   -5.967783    0.379626   -1.532964
 C   -4.178074    1.299142   -0.183500
 C   -5.532524    1.030273   -0.378633
 C   -1.758801    1.177319   -0.958840
 C   -1.341717    2.228990    0.058292
 H   -6.256532    1.334901    0.381549
 H   -3.863255    1.809379    0.729001
 H   -7.029075    0.169090   -1.683688
 H   -5.354492   -0.493808   -3.413339
 H   -2.954034   -0.009577   -3.071658
Cu   -1.190876   -0.672743   -0.437452
 H   -1.641216    1.957150    1.086533
 H   -1.875055    3.177963   -0.146998
 H   -1.307546    1.401396   -1.932649
 H    6.389495   -1.473800    1.051494
 H    4.828167   -1.012423    1.796098
 H    5.254611   -0.421472    0.161490
 C    3.421492   -1.785391   -2.553911
 H    3.169445   -0.966252   -3.245234
 H    2.896384   -2.700239   -2.874408
 H    4.508338   -1.973330   -2.622713
 H   -4.148233   -3.106495    0.931266
 H   -3.639203   -2.361102    3.473608
 C   -4.064101   -2.025606    0.731544
 H   -3.707280   -1.879423   -0.295926
 H   -5.062989   -1.572779    0.821970
 C   -3.418783   -1.355261    3.086151
 N   -3.142113   -1.409300    1.650310
 H   -4.294618   -0.715057    3.277347
 H   -1.561600   -1.486657    4.278466
 C   -1.964726   -0.876172    1.340641
 C   -2.117677   -0.768606    3.655152
 N   -1.355018   -0.460993    2.445998
 H   -2.283274    0.143408    4.247221
 H    0.669732   -0.663184    2.989212
 C   -0.009078    0.054147    2.503388
 H    0.359617    0.209728    1.481630
 H    0.014392    1.008157    3.053056
64
Figure 2_L-Cu-OtBu_dimer / electronic energy: -4357.97211601 a.u. / lowest freq: -19.85 cm-1
 H   -1.057876   -2.823794   -2.825878
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```
 H   -1.980246   -2.667714   -1.312041
 O    0.078207   -1.017819   -1.258789
 C   -1.048228   -3.061420   -1.749889
 H   -1.045898   -4.158508   -1.636503
 C    0.158516   -2.389922   -1.074836
 H    1.475367   -2.665464   -2.785121
 H   -0.759805   -2.350911    0.894993
 C    1.458383   -2.909326   -1.710688
 C    0.156991   -2.742073    0.424044
 H    2.324017   -2.413213   -1.241845
 H    1.581586   -3.999730   -1.600580
 H    1.020173   -2.268300    0.919277
 H    0.205803   -3.828385    0.609487
Cu    1.378579    0.329330   -0.465065
 H    2.131666   -0.991227    3.381390
 H    4.682348   -1.405429    2.732758
 H    5.481708   -1.718565    0.494438
 H    4.675857   -1.081458   -2.009653
 C    2.171292   -0.117226    2.712040
 C    4.582052   -0.512693    2.098216
 H    1.198856   -0.010984    2.213049
 N    3.192040   -0.289898    1.712946
 C    3.045354   -0.000511    0.406199
 C    5.265779   -0.663084    0.738250
 N    4.251927   -0.137199   -0.170576
 H    3.612584    0.354358   -2.080687
 C    4.493554   -0.077568   -1.587637
 H    2.354764    0.782239    3.326204
 H    4.963659    0.354622    2.665833
 H    6.206045   -0.097525    0.661498
 H    5.369453    0.553572   -1.807185
 H   -0.378809    4.066234    1.363434
 H   -1.215620    2.487467    1.315536
 C   -0.309944    3.028560    0.996342
 H   -1.542344    4.628000   -0.917965
 H   -2.304280    3.010119   -0.908883
 H    0.559090    2.547332    1.474899
 C   -1.400215    3.570787   -1.196882
 C   -0.167055    2.941122   -0.531923
 H    1.054762    4.773347   -0.703921
 H   -1.305843    3.511187   -2.293040
 C    1.092639    3.703570   -0.968950
 O   -0.065048    1.615388   -0.935560
 H    1.981855    3.258646   -0.494162
 H    1.220534    3.621154   -2.060206
Cu   -1.382126    0.156912   -0.516840
 H   -2.351582    0.600724    3.422431
 H   -4.934218   -0.004844    2.870939
 H   -6.034910    0.158807    0.756762
 H   -5.219728    0.475454   -1.806850
 C   -2.122775   -0.170906    2.668848
 C   -4.523985   -0.695038    2.117592
 H   -1.198578    0.107935    2.144915
 N   -3.185413   -0.283990    1.706499
 C   -3.039380   -0.179163    0.373767
 C   -5.297331   -0.660916    0.794239
 N   -4.235455   -0.434437   -0.181200
 H   -3.591154   -0.191053   -2.134929
 C   -4.528168   -0.356233   -1.586950
 H   -1.956896   -1.128121    3.192726
 H   -4.493762   -1.703279    2.564902
 H   -5.829131   -1.601827    0.585031
 H   -4.988412   -1.291515   -1.945367
32
Figure 2_L-Cu-OtBu / electronic energy: -2178.96309100 a.u. / lowest freq: 32.39 cm-1
 H    4.562030   -0.987762   -1.171425
 H    4.380081   -1.687590    0.453032
 O    2.059982   -0.792706   -0.375405
 C    4.412589   -0.739884   -0.108257
 H    5.285124   -0.160867    0.237784
 C    3.083853    0.016444    0.070903
 H    3.239088    1.094749   -1.813757
 H    2.816631   -0.564871    2.149701
 C    3.141678    1.325832   -0.740702
 C    2.905653    0.363686    1.562854
 H    2.203830    1.891377   -0.606175
 H    3.980920    1.980488   -0.449346
 H    1.973161    0.937231    1.704528
 H    3.740138    0.957642    1.973285
Cu    0.281496   -0.385007   -0.217334
 H   -2.761249   -2.831320    0.955264
 H   -4.389467   -0.710878    1.073176
 H   -3.900683    1.628760    1.086134
 H   -1.572215    2.982676    0.893515
 C   -2.368865   -2.376101    0.031132
 C   -3.894740   -0.371839    0.149702
 H   -1.295333   -2.593746   -0.043339
 N   -2.556823   -0.949305    0.044007
 C   -1.588253   -0.032817   -0.058431
 C   -3.606305    1.135384    0.145880
 N   -2.155228    1.178072   -0.017727
 H   -0.385003    2.236847   -0.219836
 C   -1.452620    2.433488   -0.055287
 H   -2.885552   -2.835640   -0.827649
 H   -4.517059   -0.688565   -0.702765
 H   -4.103640    1.662997   -0.682992
 H   -1.827633    3.068788   -0.873938
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74
Figure 2_ed / electronic energy: -3000.72395415 a.u. / lowest freq: -18.37 cm-1
 H    -4.229726    2.326034   -0.150745
 H    -5.967249    0.343716    0.271356
 H    -3.598722   -3.318573    1.735428
 H    -5.751654   -1.943746    0.936556
 H    -2.602038    1.801266   -0.690477
 H    -2.058957   -2.801506    0.982474
 C    -3.680511    1.617234   -0.792634
 C    -3.082739   -0.631120    0.042698
 N    -3.970093    0.257841   -0.410861
 N    -3.731163   -1.761591    0.333175
 C    -3.126225   -2.981981    0.798743
 C    -5.341967   -0.246351   -0.418210
 C    -5.161926   -1.699720    0.039540
 H    -3.978015    1.799131   -1.838489
 H    -5.779726   -0.163645   -1.424914
 H    -3.228038   -3.784690    0.049042
 H    -5.421195   -2.428940   -0.745075
 H    -1.082452    3.518912    1.603248
 H     0.421000    3.855965    0.726137
 O     0.362799    1.259831    1.681643
 C     0.000087    3.675244    1.723920
 H     0.157069    4.577191    2.336829
 C     0.647440    2.454235    2.386838
 H    -1.041587    2.096285    3.707116
 H     2.616865    2.798759    1.517328
 C     0.046175    2.252029    3.779325
 C     2.162870    2.651821    2.505931
 H     0.485762    1.362278    4.255566
 H     0.231377    3.121792    4.428639
 H     2.624169    1.758465    2.954414
 H     2.399418    3.521663    3.139641
Cu    -1.156351   -0.318937    0.168491
 H     3.647599   -2.084771   -1.808356
 H     4.667626   -2.150948    0.441562
 H     3.655695   -0.715072    0.059525
 C     3.791806   -1.560284    0.748890
 H     3.766971   -3.811735   -1.373951
 H     3.989671   -1.143848    1.747863
 C     3.071698   -3.006853   -1.658071
 H     2.610722   -3.279576   -2.619431
 C     1.991855   -2.826667   -0.601374
 C     2.522294   -2.409985    0.814491
 O     1.169976   -1.706527   -0.954041
 H     3.446123   -4.284636    1.408303
 B     0.804805   -1.023733    0.203641
 H     3.081088   -3.176114    2.752087
 C     2.709243   -3.561359    1.790696
 O     1.472302   -1.555242    1.289645
 H     1.649931   -4.980210   -0.367044
 C     1.084847   -4.057441   -0.565083
 H     0.586842   -4.163168   -1.540589
 H     1.766043   -4.089918    1.981929
 H     0.303393   -3.954382    0.202674
 H     0.142553    4.036318   -1.814791
 H     2.021822    3.781526   -0.667704
 H    -1.142136    3.179841   -2.691591
 C    -0.059830    3.194506   -2.489871
 O    -0.270892    1.738450   -0.614242
 H     2.659078    3.660530   -2.329825
 C     2.572105    3.136225   -1.366163
 H     0.457094    3.377402   -3.444530
 B     0.601562    1.008532    0.304352
 H     3.586208    2.995173   -0.962469
 C     0.360180    1.861111   -1.877169
 C     1.904481    1.766240   -1.514568
 O     1.926733    1.143401   -0.240157
 H    -1.221585    0.778172   -2.863054
 C    -0.123344    0.730502   -2.793547
 H     0.281161    0.832229   -3.811835
 H     0.157572   -0.257891   -2.407175
 H     2.663210    1.336698   -3.516069
 C     2.714992    0.923238   -2.496709
 H     3.773217    0.915775   -2.191785
 H     2.356419   -0.113387   -2.509049
74
Figure 2_ts(TB) / electronic energy: -3000.72314236 a.u. / lowest freq: -71.58 cm-1
 H    -4.448283    1.831801   -0.546545
 H    -6.034945   -0.274227   -0.136759
 H    -3.216551   -3.476593    1.843614
 H    -5.506494   -2.318901    0.990513
 H    -2.733610    1.438777   -0.890484
 H    -1.787148   -3.089113    0.837440
 C    -3.773199    1.128838   -1.061090
 C    -2.995601   -1.009119   -0.092528
 N    -3.958927   -0.208011   -0.557112
 N    -3.547831   -2.188579    0.211178
 C    -2.863967   -3.303706    0.812657
 C    -5.261789   -0.864729   -0.651030
 C    -4.996322   -2.217748    0.017945
 H    -3.991266    1.174517   -2.142029
 H    -5.558704   -0.964972   -1.708457
 H    -3.032398   -4.223784    0.230395
 H    -5.289878   -3.073253   -0.608926
 H    -1.889619    3.082951    1.743967
 H    -0.475447    3.841768    0.978387
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 O    0.012370    1.213800    1.663904
 C   -0.874460    3.464722    1.930869
 H   -0.944087    4.308818    2.634747
 C    0.013393    2.358438    2.507367
 H   -1.580508    1.488051    3.697900
 H    1.869593    3.236060    1.766788
 C   -0.558425    1.872271    3.838323
 C    1.443340    2.866966    2.709358
 H    0.060226    1.055179    4.239327
 H   -0.588936    2.683719    4.581426
 H    2.086995    2.051714    3.072839
 H    1.463920    3.684030    3.447489
Cu   -1.064796   -0.614475    0.066837
 H    4.152179   -1.222790   -1.601625
 H    4.926631   -1.208560    0.732258
 H    3.609618   -0.050027    0.333136
 C    3.901707   -0.891709    0.976936
 H    4.666629   -2.898230   -1.268204
 H    3.893798   -0.529670    2.016219
 C    3.817631   -2.267672   -1.575410
 H    3.534087   -2.557519   -2.598835
 C    2.634973   -2.459067   -0.637358
 C    2.900430   -2.039896    0.849730
 O    1.576663   -1.571157   -1.014383
 H    4.231911   -3.656063    1.429621
 B    0.913650   -1.122778    0.130318
 H    3.464389   -2.800114    2.789141
 C    3.297763   -3.183901    1.771368
 O    1.621543   -1.531095    1.251149
 H    2.864132   -4.640428   -0.558217
 C    2.093462   -3.884147   -0.768821
 H    1.733821   -4.037022   -1.797388
 H    2.516389   -3.953389    1.826435
 H    1.245776   -4.049768   -0.087193
 H   -0.420230    4.054241   -1.831844
 H    1.344645    4.063200   -0.458545
 H   -1.457836    3.001197   -2.817127
 C   -0.416657    3.197554   -2.518434
 O   -0.527086    1.723785   -0.642973
 H    2.129607    4.141849   -2.060330
 C    2.062456    3.564957   -1.125973
 H    0.146515    3.473608   -3.422999
 B    0.378612    1.188218    0.318412
 H    3.048455    3.588701   -0.638400
 C    0.169014    1.950819   -1.865317
 C    1.669377    2.108377   -1.380171
 O    1.690769    1.442805   -0.120721
 H   -1.129452    0.602593   -2.935045
 C   -0.047937    0.753365   -2.794138
 H    0.399213    0.929741   -3.783876
 H    0.379967   -0.167761   -2.378157
 H    2.645391    1.898337   -3.314327
 C    2.688765    1.457115   -2.306623
 H    3.703702    1.618116   -1.911727
 H    2.515077    0.376425   -2.376759
74
Figure 2_prod / electronic energy: -3000.74272641 a.u. / lowest freq: 20.41 cm-1
 H   -3.886200    1.904460    0.040425
 H   -5.783170   -0.000028    0.231301
 H   -3.671290   -4.009664    0.712028
 H   -5.779110   -2.391811    0.307129
 H   -2.431530    1.418920   -0.867743
 H   -2.156883   -3.467472   -0.075581
 C   -3.521445    1.318515   -0.819820
 C   -3.044171   -1.083929   -0.477400
 N   -3.884978   -0.068040   -0.690769
 N   -3.774686   -2.199854   -0.351226
 C   -3.248139   -3.529587   -0.185304
 C   -5.293235   -0.458612   -0.643950
 C   -5.207063   -1.984777   -0.540404
 H   -3.958179    1.745967   -1.737311
 H   -5.823136   -0.116425   -1.545676
 H   -3.484024   -4.160187   -1.059528
 H   -5.550488   -2.493752   -1.456806
 H   -0.953241    3.764861    3.357981
 H    0.759299    3.428938    2.975556
 O   -0.875512    1.986080    1.406417
 C   -0.148430    3.018702    3.444873
 H    0.062558    2.860737    4.513442
 C   -0.552175    1.706030    2.774674
 H   -2.662097    1.885852    3.254227
 H    1.522396    1.080215    2.546667
 C   -1.843289    1.160855    3.378161
 C    0.563820    0.669955    2.888868
 H   -2.130100    0.224690    2.875511
 H   -1.717424    0.955828    4.451620
 H    0.344931   -0.216712    2.276614
 H    0.673948    0.353697    3.937508
Cu   -1.061912   -1.136593   -0.315311
 H    4.402647   -0.650240   -0.989617
 H    4.621398   -1.002509    1.402523
 H    3.160136   -0.085512    0.918287
 C    3.522073   -0.979220    1.447740
 H    5.192444   -2.244337   -0.885959
 H    3.226802   -0.887955    2.503535
 C    4.303465   -1.709747   -1.255594
 H    4.297891   -1.782907   -2.353926
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 C     3.032949   -2.326933   -0.689967
 C     2.899711   -2.248976    0.864652
 O     1.888776   -1.577832   -1.121179
 H     4.481998   -3.631811    1.423538
 B     0.903669   -1.611522   -0.123564
 H     3.275879   -3.326507    2.696880
 C     3.409346   -3.471239    1.614104
 O     1.480199   -2.146878    1.031772
 H     3.743816   -4.379616   -1.009699
 C     2.869341   -3.749566   -1.231268
 H     2.746510   -3.702507   -2.323658
 H     2.863688   -4.380535    1.328701
 H     1.973529   -4.232021   -0.812859
 H     0.385110    4.774697   -2.173196
 H     1.496802    4.695314   -0.164989
 H    -0.507126    3.734422   -3.303777
 C     0.419699    3.821781   -2.717391
 O    -0.524972    2.690348   -0.813439
 H     2.757526    4.544486   -1.420219
 C     2.313155    4.059293   -0.539290
 H     1.265214    3.846315   -3.421248
 B    -0.030339    2.224887    0.383639
 H     3.082788    4.000577    0.244528
 C     0.538550    2.632846   -1.776365
 C     1.822046    2.649090   -0.858748
 O     1.334459    2.085967    0.372262
 H    -0.612874    1.326243   -3.039970
 C     0.375562    1.330242   -2.556106
 H     1.139110    1.225440   -3.340341
 H     0.434150    0.455202   -1.891068
 H     3.294722    2.132517   -2.363615
 C     2.962520    1.788006   -1.372089
 H     3.820345    1.859265   -0.686128
 H     2.658330    0.735648   -1.440404
39
Figure 2_L-Cu-Bpin / electronic energy: -2356.95154150 a.u. / lowest freq: 22.11 cm-1
 H    -4.270736   -2.604302    0.699216
 H    -3.469511   -2.304962   -1.601614
 C    -4.343959   -1.520428    0.875987
 H    -4.082488   -1.334048    1.925984
 H    -5.392484   -1.222875    0.718439
 C    -3.691752   -1.230867   -1.514808
 O    -2.057742   -1.109903    0.223326
 H    -4.742108   -1.073870   -1.802677
 C    -3.418948   -0.778798   -0.078579
 H    -3.048558   -0.694945   -2.228327
 B    -1.238080   -0.000001   -0.000001
 H    -3.048552    0.694945    2.228328
 C    -3.418947    0.778799    0.078581
 H    -4.742104    1.073871    1.802681
 O    -2.057741    1.109902   -0.223328
 C    -3.691747    1.230867    1.514810
 H    -5.392484    1.222879   -0.718433
 H    -4.082491    1.334050   -1.925981
 C    -4.343959    1.520430   -0.875984
 H    -3.469505    2.304963    1.601615
 H    -4.270733    2.604304   -0.699213
Cu     0.797333   -0.000001   -0.000002
 H     3.463333   -3.022428   -0.742996
 H     5.468944   -1.227903   -0.850209
 H     5.489479    1.160908   -0.929040
 H     3.459252    2.934328   -1.042286
 C     3.103330   -2.441738    0.122397
 C     4.991258   -0.767023    0.029199
 H     2.005088   -2.444141    0.118745
 N     3.563409   -1.079451    0.055881
 C     2.777376    0.000000    0.000000
 C     4.991258    0.767025   -0.029195
 N     3.563409    1.079451   -0.055879
 H     2.005087    2.444141   -0.118746
 C     3.103329    2.441739   -0.122398
 H     3.459253   -2.934329    1.042284
 H     5.489478   -1.160906    0.929045
 H     5.468941    1.227905    0.850214
 H     3.463332    3.022430    0.742995
61
Figure 2_para-CO2Me_pc1 / electronic energy: -2893.94952148 a.u. / lowest freq: 9.33 cm-1
 H    -1.142174    0.326395    3.043058
 H    -1.672288    2.930104    2.958728
 H    -0.410778    4.587535    1.772325
 H     1.325376    4.617521   -0.336876
 C    -1.212426    0.337763    1.943701
 C    -1.711049    2.809470    1.866209
 H    -0.480376   -0.371680    1.536378
 N    -0.926823    1.653956    1.436005
 C    -0.110453    1.927965    0.414095
 C    -1.032632    3.957955    1.112749
 N    -0.189267    3.239543    0.160605
 H     1.150212    3.208094   -1.422766
 C     0.599024    3.940252   -0.817532
 H    -2.225259    0.008361    1.655078
 H    -2.766899    2.676062    1.573693
 H    -1.746523    4.612421    0.591241
 H    -0.044230    4.539290   -1.482157
 H    -2.821199   -3.001484   -0.005036
 C    -3.951528   -1.213186   -0.399856
 C    -2.800099   -2.008391   -0.458518
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 H   -4.808328    0.695614   -0.946093
 C   -3.919421    0.063799   -0.980425
 H    3.944068   -3.671481    1.547823
 C   -1.645138   -1.545527   -1.073006
 H    3.553935   -1.740970    3.010175
 H   -0.762791   -2.188488   -1.089740
 C   -2.765666    0.524476   -1.595558
 C   -1.595840   -0.261703   -1.655126
 C    4.529362   -3.082680    0.825300
 C    4.280677   -1.171387    2.411938
 H    4.310395   -3.471360   -0.177935
 O    2.810410   -1.413679    0.543942
 H   -2.753645    1.524553   -2.037177
 H    5.283774   -1.356378    2.824337
 H    5.596665   -3.248067    1.039502
 C    4.172716   -1.608784    0.950122
 C   -0.383471    0.290726   -2.269072
 B    2.689088   -0.178377   -0.087479
 H    0.906515   -1.471785   -2.215757
 C    0.831452   -0.397455   -2.403722
 C    4.942288   -0.659595   -0.028775
 H    4.397518   -1.819490   -1.795866
 O    3.958341    0.350473   -0.300563
 H    6.081778   -2.076921   -1.258094
 H    6.921395   -0.771253    0.858890
 C    5.281639   -1.328820   -1.361922
 H    1.587646   -0.003612   -3.089368
 C    6.186299   -0.009265    0.556866
 H    5.620621   -0.559734   -2.071963
 H    6.660135    0.638253   -0.196393
Cu    0.907932    0.621506   -0.664812
 H   -0.511359    1.245360   -2.789607
 H    4.048013   -0.102353    2.527113
 H    5.947121    0.611885    1.430264
 O   -5.218902   -2.844335    0.798992
 H   -7.203768   -1.524638    1.976330
 C   -5.155737   -1.752978    0.281861
 H   -7.775958   -2.231095    0.435060
 C   -7.376520   -1.322502    0.908973
 O   -6.182131   -0.896940    0.270949
 H   -8.095015   -0.501903    0.799125
61
Figure 2_para-CO2Me_ts(CuBadd) / electronic energy: -2893.94492610 a.u. / lowest freq: -121.71 cm-1
 H   -0.026999    1.140106    3.265072
 H    0.014985    3.738814    3.095139
 H    1.051062    5.100131    1.417880
 H    2.004952    4.687899   -1.115892
 C   -0.362395    1.080737    2.218022
 C   -0.421688    3.605299    2.094447
 H    0.163965    0.250481    1.727676
 N   -0.049969    2.309166    1.532440
 C    0.406907    2.399063    0.279489
 C    0.145466    4.582235    1.058629
 N    0.482583    3.692340   -0.050204
 H    1.153407    3.375470   -1.987482
 C    1.026202    4.205465   -1.279522
 H   -1.446176    0.874745    2.208777
 H   -1.518533    3.679027    2.187354
 H   -0.581350    5.344806    0.742898
 H    0.343454    4.946730   -1.723917
 H   -2.582847   -2.331186    0.985986
 C   -3.886763   -1.142497   -0.248728
 C   -2.634826   -1.651387    0.132010
 H   -4.902677    0.129998   -1.674419
 C   -3.939393   -0.271701   -1.354113
 H    2.554836   -3.496087    2.244144
 C   -1.479242   -1.307693   -0.548973
 H    2.893249   -1.209492    3.061869
 H   -0.524361   -1.712470   -0.204080
 C   -2.789964    0.078382   -2.036994
 C   -1.511146   -0.413611   -1.656905
 C    3.223025   -3.356664    1.381181
 C    3.708755   -1.096414    2.332095
 H    2.801168   -3.915765    0.535830
 O    2.086924   -1.378203    0.599463
 H   -2.857988    0.761491   -2.888517
 H    4.635115   -1.468790    2.793333
 H    4.202002   -3.790240    1.636354
 C    3.354598   -1.875287    1.065792
 C   -0.317973    0.003135   -2.349764
 B    2.325473   -0.404737   -0.356204
 H    0.988943   -1.657112   -1.774052
 C    0.976512   -0.612112   -2.110466
 C    4.296904   -1.540412   -0.143061
 H    3.269405   -2.906778   -1.503105
 O    3.654603   -0.381816   -0.714160
 H    4.823625   -3.531143   -0.886550
 H    6.208983   -2.024480    0.758194
 C    4.294605   -2.626030   -1.218421
 H    1.737300   -0.426084   -2.877427
 C    5.724082   -1.183677    0.238946
 H    4.800753   -2.241265   -2.116017
 H    6.307983   -0.962856   -0.667122
Cu    0.838682    0.880803   -0.838244
 H   -0.443435    0.651998   -3.221307
 H    3.827841   -0.022714    2.123417
 H    5.762785   -0.300290    0.889905
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 O   -5.074107   -2.263259    1.492314
 H   -7.377192   -0.968063    1.771513
 C   -5.081986   -1.535806    0.522972
 H   -7.595197   -2.402569    0.727113
 C   -7.411047   -1.317839    0.728685
 O   -6.213634   -0.998982    0.041768
 H   -8.220581   -0.805506    0.194874
61
Figure 2_para-CO2Me_L-Cu-alkyl_01 / electronic energy: -2894.00090787 a.u. / lowest freq: 16.20 cm-1
 H   -0.563035    1.663586    2.354290
 H    1.603693    3.173507    2.675584
 H    3.521438    3.755636    1.358673
 H    4.401164    2.529675   -0.791014
 C   -0.692409    2.178424    1.387419
 C    1.342365    3.634353    1.707783
 H   -1.093556    1.461548    0.658374
 N    0.564976    2.691680    0.905738
 C    1.235845    2.230171   -0.155286
 C    2.569053    3.881422    0.822620
 N    2.416078    2.855878   -0.207738
 H    3.148621    1.797189   -1.835045
 C    3.406539    2.682059   -1.238406
 H   -1.421115    2.993331    1.522271
 H    0.767191    4.549470    1.911444
 H    2.565334    4.884188    0.363826
 H    3.455368    3.562439   -1.901635
 H   -3.052972   -2.039004    1.211582
 C   -3.887840   -0.550380   -0.098490
 C   -2.880801   -1.434250    0.317614
 H   -4.426803    0.897020   -1.616020
 C   -3.654765    0.211823   -1.260163
 H    1.599352   -3.363935    2.895954
 C   -1.688507   -1.555639   -0.379304
 H    0.460775   -1.282959    2.336220
 H   -0.926399   -2.243937   -0.010540
 C   -2.465299    0.100394   -1.953056
 C   -1.419648   -0.774837   -1.537067
 C    2.514971   -3.082717    2.355038
 C    1.392505   -0.892402    1.901536
 H    2.943103   -3.994267    1.918041
 O    1.341147   -2.645038    0.291919
 H   -2.310697    0.708236   -2.849901
 H    1.954612   -0.379209    2.695356
 H    3.229813   -2.674989    3.085989
 C    2.185941   -2.048506    1.291935
 C   -0.148475   -0.803264   -2.255879
 B    1.640173   -2.057359   -0.913530
 H    0.104093   -3.002211   -2.223401
 C    0.719434   -2.081566   -2.182211
 C    3.414674   -1.565798    0.435009
 H    4.055651   -3.593463   -0.062911
 O    2.821409   -1.358002   -0.858157
 H    5.033614   -2.811620    1.211108
 H    4.408487   -0.360257    1.940528
 C    4.488441   -2.639033    0.271972
 H    1.372151   -2.100205   -3.070684
 C    4.039993   -0.263018    0.908035
 H    5.211225   -2.309412   -0.488842
 H    4.895206   -0.005763    0.265402
Cu    0.623203    0.762399   -1.271416
 H   -0.297181   -0.477407   -3.298249
 H    1.121912   -0.156882    1.128018
 H    3.320019    0.563849    0.862457
 O   -5.358671   -1.077618    1.706296
 H   -7.126850    0.944146    1.824088
 C   -5.135859   -0.467134    0.683028
 H   -7.774067   -0.463069    0.930803
 C   -7.268733    0.508219    0.823459
 O   -6.033914    0.371946    0.142976
 H   -7.885604    1.178869    0.213179
61
Figure 2_para-CO2Me_L-Cu-alkyl_02 / electronic energy: -2893.99404152 a.u. / lowest freq: 8.62 cm-1
 O   -2.300529    4.471530    1.294012
 H   -1.941079    6.754352    0.051792
 C   -1.865274    4.100254    0.225742
 H   -3.528042    6.092778   -0.440142
 C   -2.465274    6.166049   -0.715944
 O   -1.885858    4.881631   -0.864411
 H   -2.370402    6.662630   -1.689052
 B   -1.699597   -2.313396    0.197374
 O   -2.498071   -2.209306    1.306718
 O   -2.432634   -2.361092   -0.961443
 C   -3.870720   -2.331823    0.891830
 C   -3.786554   -1.995596   -0.644707
 C   -4.719651   -1.368694    1.707076
 C   -4.295936   -3.772854    1.169358
 C   -3.925745   -0.502196   -0.939942
 C   -4.736290   -2.792844   -1.524489
 H   -3.248330    0.097167   -0.313947
 H   -4.955389   -0.150329   -0.780791
 H   -3.658365   -0.319607   -1.991056
 H   -4.556379   -3.872961   -1.446302
 H   -4.596901   -2.503202   -2.576655
 H   -5.783451   -2.589930   -1.253470
 H   -3.696151   -4.488115    0.587026
 H   -5.358390   -3.935215    0.936937
 H   -4.140782   -3.991426    2.236251
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 H   -5.760098   -1.366223    1.348373
 H   -4.327424   -0.344372    1.657678
 H   -4.724659   -1.678312    2.762987
 C   -0.255115    1.119702   -1.487850
 C   -0.794390    2.378185   -1.295300
 C   -0.148246    0.171668   -0.434602
 C   -1.265878    2.775191   -0.029699
 C   -0.629970    0.594013    0.832854
 C   -1.172117    1.855315    1.024943
 C    0.434060   -1.154910   -0.657350
 C   -0.126614   -2.298146    0.222257
 H   -1.542445    2.147933    2.010538
 H   -0.587172   -0.094193    1.679318
 H   -0.866289    3.071779   -2.135368
 H    0.094648    0.834563   -2.484760
Cu    2.359222   -0.803852   -0.335320
 H    0.225742   -2.242442    1.266611
 H    0.258767   -3.259333   -0.160675
 H    0.331399   -1.419207   -1.723545
 H    5.700360   -3.085851   -0.987258
 H    7.147803   -1.391894    0.523071
 C    5.231421   -2.174792   -1.393604
 H    4.180064   -2.389763   -1.627081
 H    6.399530    0.258624    2.083064
 N    5.284139   -1.100031   -0.437357
 C    6.563872   -0.587736    0.049330
 H    5.754845   -1.901649   -2.324864
 C    4.227908   -0.444308    0.053472
 C    6.127418    0.497906    1.042005
 H    4.008923    1.233824    2.742290
 H    7.157927   -0.185805   -0.787457
 N    4.673894    0.497528    0.889786
 C    3.851343    1.391774    1.662477
 H    6.543648    1.488732    0.803853
 H    2.795747    1.201088    1.428031
 H    4.083901    2.443493    1.428892
61
Figure 2_para-CO2Me_L-Cu-alkyl_03 / electronic energy: -2893.99568367 a.u. / lowest freq: 9.65 cm-1
 B   -2.273185   -1.754723   -0.315655
 O   -3.225853   -2.267701   -1.161167
 O   -2.836454   -1.156583    0.784762
 C   -4.515204   -1.820473   -0.705637
 C   -4.234549   -1.500493    0.806806
 C   -5.542865   -2.915455   -0.941410
 C   -4.872988   -0.577419   -1.519147
 C   -4.377530   -2.722876    1.712673
 C   -5.036946   -0.340475    1.372141
 H   -3.831437   -3.589384    1.311026
 H   -5.431275   -3.006382    1.847219
 H   -3.956068   -2.486027    2.700509
 H   -4.853661    0.594060    0.827716
 H   -4.768330   -0.177690    2.426486
 H   -6.114177   -0.561713    1.327792
 H   -4.149793    0.234032   -1.347828
 H   -5.879086   -0.207184   -1.274959
 H   -4.850270   -0.829624   -2.589541
 H   -6.514072   -2.633659   -0.507401
 H   -5.226913   -3.870930   -0.502628
 H   -5.685698   -3.069541   -2.021213
 C    2.501773   -0.936814    1.284050
 C    3.874083   -0.940121    1.129961
 C    1.613383   -1.228055    0.208238
 C    4.460220   -1.246578   -0.114349
 C    2.228584   -1.570609   -1.025669
 C    3.606670   -1.568858   -1.179743
 C    0.168777   -1.130086    0.386324
 C   -0.734373   -1.875032   -0.594605
 H    4.049697   -1.824756   -2.145466
 H    1.603564   -1.830888   -1.882665
 H    4.516214   -0.702343    1.980538
 H    2.072657   -0.687278    2.259458
Cu   -0.121125    0.833403    0.224340
 H   -0.507536   -2.965108   -0.637408
 H   -0.584087   -1.536274   -1.636391
 H   -0.109547   -1.337269    1.433966
 H   -3.617938    2.768030   -0.599760
 H   -2.253653    5.081079   -1.001679
 C   -2.906658    2.608797    0.226960
 H   -2.703973    1.533135    0.326186
 H    0.084067    5.356874   -1.429409
 N   -1.666341    3.296117   -0.021938
 C   -1.620394    4.749974   -0.164732
 H   -3.376298    2.966088    1.159022
 C   -0.456777    2.727615   -0.009810
 C   -0.127060    5.007949   -0.405145
 H    2.238919    3.722360   -1.315233
 H   -1.992838    5.233210    0.753729
 N    0.457047    3.684470   -0.193970
 C    1.877605    3.475016   -0.302986
 H    0.300431    5.739433    0.297243
 H    2.099433    2.419770   -0.095797
 H    2.421159    4.102251    0.421590
 O    6.460555   -1.491126   -1.394487
 H    8.324204   -0.111880   -0.113306
 C    5.918134   -1.242480   -0.339355
 H    8.436991   -1.839214    0.331563
 C    8.023586   -0.864544    0.630808
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 O    6.614471   -0.921019    0.762443
 H    8.416348   -0.584835    1.615768
61
Figure 2_para-CO2Me_ts(BHE) / electronic energy: -2893.94910035 a.u. / lowest freq: -771.32 cm-1
 B   -2.603071   -1.261221   -0.270209
 O   -3.524621   -1.865861   -1.079070
 O   -3.158527   -0.724958    0.859803
 C   -4.830951   -1.498769   -0.590803
 C   -4.534208   -1.150124    0.914847
 C   -5.788195   -2.660747   -0.795430
 C   -5.283288   -0.287414   -1.404074
 C   -4.588217   -2.369268    1.833053
 C   -5.381459   -0.024044    1.484161
 H   -3.995877   -3.203691    1.429295
 H   -5.620236   -2.715661    1.986884
 H   -4.166574   -2.097831    2.811938
 H   -5.218731    0.919123    0.946344
 H   -5.124557    0.140062    2.541204
 H   -6.450949   -0.278273    1.431273
 H   -4.603905    0.566547   -1.261942
 H   -6.301981    0.025436   -1.133644
 H   -5.275992   -0.549612   -2.472236
 H   -6.763667   -2.443839   -0.334759
 H   -5.395860   -3.590685   -0.363359
 H   -5.950116   -2.827749   -1.870509
 C    2.186526   -1.178006    1.395686
 C    3.556066   -1.285718    1.249078
 C    1.303611   -1.231668    0.280884
 C    4.135786   -1.467422   -0.021712
 C    1.907032   -1.436047   -0.991247
 C    3.279882   -1.546679   -1.131287
 C   -0.114448   -1.050129    0.458435
 C   -1.083003   -1.168084   -0.610678
 H    3.718273   -1.693670   -2.121228
 H    1.282009   -1.486075   -1.885748
 H    4.200657   -1.228736    2.128429
 H    1.762080   -1.028639    2.392516
Cu   -0.454919    0.768497   -0.529055
 H   -0.791539   -1.745204   -1.496217
 H   -1.452223    0.118200   -1.587763
 H   -0.480174   -0.947178    1.484290
 H   -2.581094    4.327696   -0.208078
 H   -0.297360    5.680685   -0.080382
 C   -2.065625    3.511852    0.322785
 H   -2.422756    2.550665   -0.070766
 H    1.864604    4.971573   -0.832948
 N   -0.643175    3.599069    0.121767
 C    0.092470    4.811971    0.470566
 H   -2.324020    3.575361    1.393708
 C    0.156815    2.574320   -0.196946
 C    1.527244    4.445063    0.075914
 H    3.057180    2.636279   -1.452119
 H   -0.009911    5.019312    1.549268
 N    1.419511    3.011693   -0.187154
 C    2.583097    2.239505   -0.538666
 H    2.258283    4.642525    0.873831
 H    2.291182    1.197302   -0.717220
 H    3.326233    2.261360    0.274104
 O    6.123970   -1.733866   -1.313374
 H    8.107567   -0.803478    0.134703
 C    5.591543   -1.579490   -0.235566
 H    7.999530   -2.570942    0.375084
 C    7.704285   -1.593620    0.785446
 O    6.295923   -1.491366    0.902979
 H    8.109856   -1.480981    1.798024
61
Figure 2_para-CO2Me_pc2 / electronic energy: -2893.97546090 a.u. / lowest freq: 25.51 cm-1
 B   -2.699138   -1.202332   -0.021925
 O   -3.723697   -1.841396   -0.663401
 O   -3.143953   -0.280554    0.897228
 C   -4.934492   -1.118431   -0.364039
 C   -4.573339   -0.416152    0.997927
 C   -6.093566   -2.097870   -0.287156
 C   -5.155387   -0.123903   -1.501968
 C   -4.858485   -1.292644    2.216016
 C   -5.188544    0.961080    1.186823
 H   -4.421613   -2.295819    2.100036
 H   -5.938090   -1.400412    2.394006
 H   -4.407990   -0.828673    3.105839
 H   -4.872532    1.660537    0.402020
 H   -4.877957    1.376602    2.157133
 H   -6.287337    0.899432    1.180790
 H   -4.327819    0.597560   -1.571864
 H   -6.099150    0.426590   -1.378988
 H   -5.199236   -0.673309   -2.453715
 H   -7.013695   -1.584582    0.030217
 H   -5.889487   -2.918514    0.413103
 H   -6.274425   -2.537379   -1.279318
 C    2.082343   -0.298514    1.244787
 C    3.462904   -0.425751    1.173640
 C    1.236728   -1.031645    0.393598
 C    4.040315   -1.300647    0.243778
 C    1.827338   -1.906100   -0.533863
 C    3.208070   -2.038808   -0.605488
 C   -0.221643   -0.818211    0.479917
 C   -1.194622   -1.450010   -0.289866
 H    3.659708   -2.721714   -1.327635
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 H     1.201941   -2.490155   -1.211305
 H     4.101351    0.156256    1.839664
 H     1.639969    0.395361    1.964546
Cu    -0.773979    0.396482   -1.121573
 H    -0.907326   -2.210737   -1.023171
 H    -1.637350    0.425595   -2.457024
 H    -0.546881   -0.241411    1.353074
 H    -1.894177    3.747139    0.750574
 H     0.583232    4.827959    0.277293
 C    -1.318858    2.859469    1.065150
 H    -1.890732    1.956013    0.809947
 H     2.577427    4.125170   -0.853692
 N    -0.033481    2.812251    0.416837
 C     0.966506    3.856411    0.633894
 H    -1.195257    2.898181    2.159075
 C     0.298320    1.972091   -0.568673
 C     2.144879    3.349846   -0.204715
 H     2.729498    2.178631   -2.706780
 H     1.207290    3.956790    1.702426
 N     1.524086    2.287811   -0.993467
 C     2.290447    1.520273   -1.940641
 H     2.956009    2.929793    0.415383
 H     1.626412    0.797982   -2.433523
 H     3.107400    0.971278   -1.441203
 O     6.048085   -2.233755   -0.654122
 H     8.010747   -0.565155   -0.043198
 C     5.514458   -1.478370    0.123345
 H     7.928048   -1.840347    1.210498
 C     7.610851   -0.820277    0.948891
 O     6.195157   -0.707426    0.973384
 H     7.988787   -0.111404    1.694588
61
Figure 2_para-CO2Me_ts(H>B) / electronic energy: -2893.96254522 a.u. / lowest freq: -339.78 cm-1
 B    -2.691157   -0.874132   -0.326803
 O    -3.737405   -1.659424   -0.841052
 O    -3.169335   -0.089544    0.754215
 C    -4.961335   -1.086435   -0.386922
 C    -4.535466   -0.426232    0.979571
 C    -6.002829   -2.189392   -0.253186
 C    -5.434920   -0.058304   -1.417596
 C    -4.578369   -1.414684    2.147602
 C    -5.313398    0.831930    1.340984
 H    -4.039704   -2.341787    1.901324
 H    -5.608577   -1.672301    2.435712
 H    -4.082961   -0.958672    3.018024
 H    -5.185370    1.617749    0.584575
 H    -4.954226    1.229625    2.302712
 H    -6.388153    0.616812    1.445610
 H    -4.719768    0.770120   -1.520584
 H    -6.418883    0.358521   -1.156904
 H    -5.520292   -0.551491   -2.397713
 H    -6.928038   -1.803656    0.202153
 H    -5.631757   -3.023390    0.357247
 H    -6.255089   -2.587429   -1.247799
 C     2.066865   -0.333047    1.234354
 C     3.448559   -0.439851    1.140869
 C     1.217751   -1.125235    0.442207
 C     4.022775   -1.355705    0.250197
 C     1.805928   -2.048936   -0.438231
 C     3.186519   -2.161502   -0.532439
 C    -0.239554   -0.911114    0.531958
 C    -1.202364   -1.411243   -0.307336
 H     3.636323   -2.880157   -1.220301
 H     1.175077   -2.688430   -1.059112
 H     4.089689    0.189843    1.759376
 H     1.626674    0.392923    1.923288
Cu    -0.967180    0.585829   -0.973267
 H    -0.888359   -2.059724   -1.137286
 H    -2.431144    0.243720   -1.574067
 H    -0.562827   -0.320931    1.398836
 H    -1.429194    3.997578    1.149365
 H     1.141014    4.741123    0.465297
 C    -0.987852    2.992052    1.251750
 H    -1.732053    2.243441    0.945716
 H     2.794371    3.873272   -1.028899
 N     0.189173    2.852548    0.433189
 C     1.373470    3.679783    0.652275
 H    -0.743162    2.827672    2.313738
 C     0.309720    2.021977   -0.607005
 C     2.365559    3.105239   -0.367660
 H     2.552597    1.944555   -2.945954
 H     1.725228    3.588308    1.691311
 N     1.533761    2.170862   -1.122545
 C     2.111305    1.334483   -2.141825
 H     3.199557    2.562884    0.109743
 H     1.328625    0.696283   -2.571997
 H     2.901064    0.688424   -1.720812
 O     6.028198   -2.286430   -0.654593
 H     7.954167   -0.506191   -0.192454
 C     5.496899   -1.506206    0.099697
 H     7.956338   -1.751206    1.094088
 C     7.597870   -0.748454    0.819404
 O     6.181110   -0.677644    0.890639
 H     7.978967   -0.010149    1.534346
61
Figure 2_para-CO2Me_int1 / electronic energy: -2893.96426596 a.u. / lowest freq: 12.16 cm-1
 B    -2.801105   -0.407026   -0.409596
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 O   -3.812792   -1.087511   -1.168259
 O   -3.348864   -0.117024    0.895995
 C   -5.049458   -0.868406   -0.511444
 C   -4.606899   -0.761104    0.993602
 C   -5.985792   -2.030904   -0.815097
 C   -5.668209    0.436972   -1.025671
 C   -4.395820   -2.138867    1.632207
 C   -5.534648    0.072455    1.868968
 H   -3.761153   -2.774120    0.996089
 H   -5.344264   -2.665299    1.820023
 H   -3.881148   -2.006818    2.596226
 H   -5.587845    1.112920    1.520712
 H   -5.161115    0.084207    2.904797
 H   -6.553267   -0.346368    1.882290
 H   -5.040123    1.304793   -0.775533
 H   -6.674745    0.607431   -0.614422
 H   -5.750731    0.384354   -2.122066
 H   -6.916771   -1.956768   -0.231219
 H   -5.509460   -2.996295   -0.597398
 H   -6.255525   -2.025124   -1.882697
 C    1.931763   -0.476218    1.247321
 C    3.306348   -0.641141    1.135760
 C    1.043723   -1.184773    0.420678
 C    3.830563   -1.540920    0.199077
 C    1.579714   -2.101915   -0.497924
 C    2.953325   -2.278021   -0.605735
 C   -0.398231   -0.883228    0.508873
 C   -1.330820   -1.061721   -0.462969
 H    3.365872   -2.990717   -1.322622
 H    0.912174   -2.686438   -1.134818
 H    3.979013   -0.067888    1.775090
 H    1.529972    0.237838    1.971119
Cu   -1.044239    1.102216   -0.696719
 H   -0.998800   -1.514967   -1.409946
 H   -2.636051    0.860525   -1.046443
 H   -0.719189   -0.433826    1.458183
 H   -0.244068    4.507237    1.547981
 H    2.267415    4.543546    0.465540
 C   -0.102993    3.413932    1.571441
 H   -1.069833    2.927626    1.384920
 H    3.315982    3.362027   -1.326647
 N    0.837830    2.988742    0.568963
 C    2.224519    3.449612    0.592019
 H    0.246109    3.131426    2.578070
 C    0.563882    2.185360   -0.462405
 C    2.843292    2.693306   -0.591238
 H    2.197679    1.637388   -3.176162
 H    2.698421    3.201670    1.554438
 N    1.685027    2.017172   -1.170391
 C    1.838799    1.110151   -2.277498
 H    3.593040    1.948377   -0.276192
 H    0.866461    0.649722   -2.498992
 H    2.558468    0.312343   -2.029387
 O    5.786541   -2.536062   -0.746005
 H    7.786223   -0.842283   -0.295062
 C    5.296095   -1.744939    0.024130
 H    7.756496   -2.088185    0.990471
 C    7.433731   -1.072001    0.720996
 O    6.021530   -0.947572    0.810019
 H    7.850616   -0.349289    1.431921
61
Figure 2_para-CO2Me_ts(Cu>O) / electronic energy: -2893.95949767 a.u. / lowest freq: -41.11 cm-1
 B   -2.088606   -1.288405   -0.714448
 O   -2.953107   -2.371191   -1.080934
 O   -2.498216   -0.848498    0.617654
 C   -4.133613   -2.247251   -0.305003
 C   -3.587217   -1.653651    1.046243
 C   -4.784045   -3.618191   -0.168056
 C   -5.105318   -1.290518   -1.008053
 C   -3.024925   -2.738053    1.970045
 C   -4.585087   -0.793060    1.810970
 H   -2.319851   -3.385063    1.427746
 H   -3.815282   -3.366242    2.408464
 H   -2.476259   -2.255386    2.793143
 H   -4.896621    0.081603    1.223594
 H   -4.124956   -0.424666    2.740878
 H   -5.483339   -1.368989    2.084395
 H   -4.697636   -0.271186   -1.071465
 H   -6.078372   -1.243298   -0.496856
 H   -5.273278   -1.648755   -2.035153
 H   -5.619281   -3.590804    0.548943
 H   -4.058285   -4.371165    0.167198
 H   -5.182174   -3.945806   -1.140798
 C    2.576304   -0.863948    1.173103
 C    3.964366   -0.785931    1.148981
 C    1.838977   -1.177290    0.018221
 C    4.658946   -1.020647   -0.043004
 C    2.551508   -1.414218   -1.171480
 C    3.936594   -1.336942   -1.201451
 C    0.367855   -1.202002    0.094951
 C   -0.506102   -1.489873   -0.887662
 H    4.480207   -1.518706   -2.130716
 H    2.012855   -1.653085   -2.090844
 H    4.513711   -0.540285    2.058874
 H    2.043000   -0.674224    2.108456
Cu   -1.796319    0.994470   -0.812580
 H   -0.115471   -1.766868   -1.877636
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 H   -2.396983   -0.277044   -1.638500
 H   -0.044266   -0.921227    1.071979
 O    6.775556   -1.111542   -1.147985
 H    8.478234    0.245451    0.401114
 C    6.144131   -0.942219   -0.131672
 H    8.598297   -1.505835    0.749554
 C    8.130273   -0.561317    1.062811
 O    6.713910   -0.662333    1.041591
 H    8.404910   -0.336133    2.099739
 H   -3.606500    4.477452    0.293475
 H    1.717516    2.845238   -1.929186
 H    0.949522    5.051360   -0.620081
 H   -1.203185    5.712845    0.182363
 H   -3.504442    2.699214    0.475438
 H    0.792605    1.368713   -1.518022
 C   -1.044777    2.695596   -0.278024
 C   -3.057570    3.654342    0.780425
 N   -1.670004    3.662711    0.397968
 C    1.246712    2.280315   -1.108721
 N    0.223494    3.068328   -0.470274
 C    0.542758    4.360376    0.134127
 C   -0.815648    4.812995    0.686793
 H   -3.164868    3.763989    1.871638
 H    2.031242    1.992653   -0.389172
 H    1.302938    4.233963    0.922060
 H   -0.792024    5.014843    1.768712
61
Figure 2_para-CO2Me_int2 / electronic energy: -2893.96407343 a.u. / lowest freq: 14.84 cm-1
 B   -0.800035   -1.237700   -0.828636
 O   -1.193418   -2.594659   -1.119670
 O   -1.306884   -0.958810    0.537903
 C   -2.195559   -2.993483   -0.206446
 C   -1.840874   -2.161412    1.081525
 C   -2.115240   -4.503294   -0.009543
 C   -3.577233   -2.641065   -0.774794
 C   -0.743327   -2.824520    1.917013
 C   -3.033312   -1.825648    1.967391
 H    0.114916   -3.108294    1.290616
 H   -1.108911   -3.720854    2.440220
 H   -0.388415   -2.108289    2.673495
 H   -3.750116   -1.179364    1.442229
 H   -2.695993   -1.292843    2.869494
 H   -3.554307   -2.739689    2.292264
 H   -3.713493   -1.554015   -0.896230
 H   -4.393614   -3.015590   -0.139529
 H   -3.677951   -3.097816   -1.770755
 H   -2.796270   -4.838331    0.788466
 H   -1.094198   -4.819672    0.240969
 H   -2.405744   -5.016132   -0.939131
 C    3.703401    0.174172    1.001656
 C    5.062057    0.467771    0.978336
 C    3.002086   -0.151312   -0.172227
 C    5.763026    0.449001   -0.232778
 C    3.719200   -0.160503   -1.382752
 C    5.075085    0.134010   -1.412347
 C    1.563027   -0.463991   -0.082820
 C    0.759572   -0.935286   -1.050755
 H    5.621136    0.125629   -2.357834
 H    3.205677   -0.395833   -2.317418
 H    5.584188    0.713009    1.904196
 H    3.166186    0.191714    1.953715
Cu   -2.432308    0.478410   -0.716035
 H    1.189794   -1.117871   -2.046547
 H   -1.411934   -0.394274   -1.707596
 H    1.120987   -0.298542    0.907919
 H   -3.296937    1.722112    3.060560
 H   -5.433596    3.062486    2.158864
 C   -2.797321    2.046099    2.133884
 H   -2.114054    1.252499    1.802803
 H   -6.586845    2.722875    0.086832
 N   -3.767713    2.295500    1.098099
 C   -4.819167    3.295033    1.276474
 H   -2.213198    2.955396    2.354842
 C   -3.721381    1.798615   -0.142394
 C   -5.595410    3.188665   -0.041609
 H   -6.058532    1.465967   -2.237112
 H   -4.371049    4.291679    1.425842
 N   -4.734377    2.318510   -0.840923
 C   -5.080776    1.974293   -2.195159
 H   -5.738083    4.160540   -0.536703
 H   -4.312988    1.298897   -2.595349
 H   -5.130787    2.875415   -2.827165
 O    7.856421    0.762088   -1.343355
 H    9.357163    2.227558    0.294572
 C    7.218340    0.755530   -0.317089
 H    9.740861    0.494667    0.526437
 C    9.140197    1.336196    0.901221
 O    7.755212    1.024882    0.874333
 H    9.388845    1.532286    1.950585
61
Figure 2_para-CO2Me_ts(C-Brot) / electronic energy: -2893.95849867 a.u. / lowest freq: -111.99 cm-1
 B    0.695163    0.849995   -0.807648
 O    0.820773    2.223504   -1.221682
 O    1.316310    0.801478    0.549402
 C    1.848269    2.842426   -0.474734
 C    1.753185    2.108153    0.913976
 C    1.578294    4.341178   -0.401674
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 C     3.198804    2.616988   -1.168959
 C     0.692961    2.723522    1.829150
 C     3.073464    2.007109    1.668967
 H    -0.250727    2.891532    1.292091
 H     1.024414    3.682097    2.255965
 H     0.492529    2.028042    2.657967
 H     3.809675    1.410166    1.112971
 H     2.915544    1.522190    2.644586
 H     3.500356    3.005134    1.853699
 H     3.478879    1.550837   -1.197556
 H     4.014784    3.166915   -0.676960
 H     3.123552    2.964864   -2.210058
 H     2.280770    4.838346    0.285336
 H     0.552977    4.546732   -0.066818
 H     1.701378    4.793456   -1.397760
 C    -4.160605    0.803350    0.666786
 C    -5.479741    0.366958    0.718428
 C    -3.247808    0.272397   -0.260632
 C    -5.927611   -0.616925   -0.170172
 C    -3.714539   -0.711431   -1.151288
 C    -5.030751   -1.148860   -1.106061
 C    -1.856092    0.765013   -0.260718
 C    -0.801261    0.244693   -0.908203
 H    -5.384987   -1.909358   -1.804865
 H    -3.038791   -1.133104   -1.898337
 H    -6.168494    0.790521    1.450845
 H    -3.821525    1.572471    1.365839
Cu     2.598466   -0.540098   -0.612277
 H    -0.973529   -0.656847   -1.514049
 H     1.420068    0.054798   -1.642105
 H    -1.698485    1.648293    0.370267
 H     3.704465   -1.434455    3.201095
 H     6.006796   -2.426405    2.326226
 C     3.240559   -1.871495    2.302553
 H     2.450536   -1.195906    1.947847
 H     7.079958   -2.062686    0.217096
 N     4.220533   -2.036038    1.258957
 C     5.432782   -2.823026    1.475479
 H     2.789080   -2.838362    2.581197
 C     4.090193   -1.603736    0.000636
 C     6.164033   -2.671263    0.135455
 H     6.309800   -0.943403   -2.123228
 H     5.172602   -3.870750    1.699824
 N     5.172445   -1.979820   -0.686563
 C     5.455792   -1.638359   -2.055990
 H     6.438356   -3.636442   -0.315818
 H     4.570824   -1.156019   -2.491581
 H     5.695696   -2.540835   -2.640476
 O    -7.752404   -1.965462   -0.918286
 H    -9.521274   -2.010587    1.061466
 C    -7.330475   -1.118225   -0.167000
 H    -9.968763   -0.732323   -0.107488
 C    -9.443617   -0.936711    0.837029
 O    -8.085674   -0.528450    0.761098
 H    -9.895722   -0.354138    1.647868
61
Figure 2_para-CO2Me_int3 / electronic energy: -2893.96339570 a.u. / lowest freq: 19.10 cm-1
 B     0.606257    0.579371   -0.456726
 O     0.589795    1.885282   -1.066489
 O     1.423539    0.736713    0.788284
 C     1.562819    2.709479   -0.461070
 C     1.655680    2.126288    0.996930
 C     1.095449    4.159452   -0.518036
 C     2.883784    2.580411   -1.231115
 C     0.542226    2.652962    1.905367
 C     3.007107    2.314952    1.672448
 H    -0.440661    2.554809    1.422132
 H     0.697378    3.706778    2.180794
 H     0.523988    2.055968    2.829721
 H     3.806837    1.798259    1.123927
 H     2.978731    1.903415    2.693119
 H     3.265052    3.382729    1.746987
 H     3.299348    1.560117   -1.168716
 H     3.649416    3.281991   -0.867784
 H     2.695120    2.793232   -2.293871
 H     1.769903    4.818408    0.050745
 H     0.078696    4.268024   -0.117178
 H     1.083271    4.506954   -1.562428
 C    -4.442666    0.984590   -0.541680
 C    -5.763024    0.583645   -0.371788
 C    -3.375570    0.084648   -0.376517
 C    -6.054909   -0.743290   -0.036161
 C    -3.685239   -1.247684   -0.047598
 C    -5.001617   -1.654047    0.120564
 C    -1.994032    0.572408   -0.552218
 C    -0.851868   -0.058554   -0.233862
 H    -5.231974   -2.691249    0.371787
 H    -2.883222   -1.979897    0.068440
 H    -6.573051    1.302866   -0.500923
 H    -4.225945    2.023640   -0.803669
Cu     2.679320   -0.566109   -0.363828
 H    -0.916088   -1.062140    0.212920
 H     1.237778   -0.314134   -1.243042
 H    -1.914016    1.581238   -0.976983
 H     4.854478   -0.884821    3.027229
 H     6.944531   -1.767103    1.618464
 C     4.241758   -1.530081    2.376510
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 H    3.273696   -1.041610    2.204469
 H    7.380074   -1.718215   -0.731752
 N    4.892775   -1.741318    1.109476
 C    6.217380   -2.354630    1.036426
 H    4.073382   -2.487244    2.896970
 C    4.389770   -1.420941   -0.086549
 C    6.507034   -2.337704   -0.470914
 H    5.889057   -0.858240   -2.827035
 H    6.192117   -3.372790    1.456024
 N    5.285588   -1.752517   -1.020590
 C    5.131936   -1.559524   -2.438840
 H    6.670596   -3.344154   -0.886855
 H    4.132622   -1.148388   -2.633704
 H    5.236423   -2.516182   -2.975968
 O   -7.739513   -2.373300    0.427582
 H   -9.906852   -1.051619    1.146173
 C   -7.449143   -1.232527    0.153905
 H  -10.016034   -1.383155   -0.609099
 C   -9.721049   -0.638201    0.144257
 O   -8.358317   -0.269940   -0.010021
 H  -10.303725    0.279742    0.006340
42
Figure 2_para-CO2Me-alkenylBpin / electronic energy: -947.261050912 a.u. / lowest freq: 13.61 cm-1
 B    2.536731   -0.351136   -0.017816
 O    3.507318   -1.307017    0.091467
 O    3.044449    0.917279   -0.089343
 C    4.760349   -0.629615    0.319214
 C    4.471353    0.802509   -0.264709
 C    5.875327   -1.387204   -0.382583
 C    4.996326   -0.622611    1.828498
 C    4.745855    0.900135   -1.764214
 C    5.160646    1.939871    0.470457
 H    4.269808    0.075213   -2.315220
 H    5.823957    0.886700   -1.979228
 H    4.330817    1.845090   -2.144324
 H    4.841247    2.001481    1.518889
 H    4.920642    2.897749   -0.014329
 H    6.253003    1.810310    0.441985
 H    4.207048   -0.068094    2.357891
 H    5.967553   -0.174767    2.082696
 H    4.987792   -1.658529    2.197849
 H    6.823693   -0.833725   -0.309558
 H    5.649454   -1.557045   -1.443307
 H    6.018218   -2.368010    0.094703
 C   -2.207218    1.219150    0.141935
 C   -3.592625    1.099338    0.165560
 C   -1.385376    0.103371   -0.083437
 C   -4.189417   -0.146927   -0.050480
 C   -1.997705   -1.142169   -0.304573
 C   -3.380002   -1.264785   -0.289389
 C    0.078353    0.284197   -0.078553
 C    1.016202   -0.679307   -0.047860
 H   -3.852270   -2.233203   -0.464204
 H   -1.388084   -2.026100   -0.502335
 H   -4.214799    1.975709    0.350685
 H   -1.746933    2.196518    0.307586
 H    0.706356   -1.730832   -0.015627
 H    0.406700    1.330741   -0.083277
 O   -6.220518   -1.390859   -0.242301
 H   -8.075832    0.017569    1.049167
 C   -5.670406   -0.334915   -0.040108
 H   -8.154100    0.388896   -0.700309
 C   -7.745844    0.716413    0.266859
 O   -6.327659    0.794119    0.220526
 H   -8.101542    1.727137    0.496846
61
Figure 2_para-CO2Me_pc2_rev / electronic energy: -2893.97226879 a.u. / lowest freq: 18.35 cm-1
 B   -1.659253    1.162062    0.484585
 O   -2.509790    1.042718    1.552884
 O   -2.239202    1.798463   -0.582136
 C   -3.820265    1.458269    1.125246
 C   -3.495840    2.342385   -0.139420
 C   -4.503028    2.203627    2.261068
 C   -4.602514    0.192095    0.783268
 C   -3.250429    3.810810    0.202028
 C   -4.509522    2.229678   -1.266395
 H   -2.518862    3.918286    1.016777
 H   -4.179210    4.320309    0.496135
 H   -2.845315    4.319658   -0.684912
 H   -4.580412    1.202435   -1.647273
 H   -4.210192    2.879668   -2.101930
 H   -5.505710    2.550840   -0.926508
 H   -4.125519   -0.351758   -0.042562
 H   -5.642436    0.417927    0.507382
 H   -4.615431   -0.468464    1.663109
 H   -5.468663    2.613648    1.928626
 H   -3.883583    3.027350    2.638728
 H   -4.696127    1.513607    3.095957
 C    3.066452    1.461738   -1.209555
 C    4.444828    1.331850   -1.101477
 C    2.203216    0.784784   -0.333000
 C    5.003354    0.515149   -0.111980
 C    2.774726   -0.034125    0.655606
 C    4.152467   -0.170103    0.765041
 C    0.741292    0.970265   -0.471868
 C   -0.201354    0.647250    0.506927
 H    4.574757   -0.814230    1.537332
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 H     2.134128   -0.582818    1.349252
 H     5.106773    1.866841   -1.785117
 H     2.643008    2.101472   -1.987742
Cu    -0.195811   -0.793168   -0.967456
 H     0.144296    0.174336    1.433699
 H     0.539387   -1.164110   -2.337883
 H     0.445055    1.660332   -1.269751
 O     7.251426    1.002240   -0.757667
 H     8.768883    0.413396    1.365471
 C     6.487431    0.414668   -0.028811
 O     6.894624   -0.397516    0.948344
 C     8.297062   -0.547405    1.112473
 H     8.436219   -1.257154    1.936048
 H     8.761756   -0.942649    0.197563
 H    -4.657909   -2.839906   -0.224696
 H    -4.138561   -1.140016   -2.234849
 H    -3.382780   -3.135044    1.781392
 C    -3.645092   -3.230818   -0.405515
 C    -3.155610   -1.634292   -2.296012
 H    -0.867667   -2.389324    2.587248
 N    -2.799774   -2.212549   -1.026148
 C    -2.881982   -3.541341    0.886393
 H    -2.399141   -0.891874   -2.578608
 C    -1.625095   -2.056706   -0.405871
 N    -1.613193   -2.848410    0.668694
 H    -3.729786   -4.107707   -1.069314
 H    -3.204893   -2.406894   -3.081766
 C    -0.565139   -2.894712    1.654178
 H    -2.721228   -4.617827    1.044552
 H     0.327731   -2.398587    1.252740
 H    -0.309236   -3.939096    1.891030
61
Figure 2_para-CO2Me_ts(CuHadd_rev) / electronic energy: -2893.95003715 a.u. / lowest freq: -793.39 cm-1
 B     1.480275   -1.449560    0.479173
 O     2.251616   -1.666607    1.611741
 O     2.173298   -1.822428   -0.671263
 C     3.589030   -1.939954    1.182059
 C     3.359733   -2.513408   -0.262316
 C     4.240888   -2.911589    2.153622
 C     4.350253   -0.612866    1.175304
 C     3.040847   -4.009082   -0.260920
 C     4.482173   -2.224614   -1.246615
 H     2.253627   -4.249559    0.469138
 H     3.928093   -4.617425   -0.031419
 H     2.675916   -4.296202   -1.258296
 H     4.639616   -1.147132   -1.380289
 H     4.238627   -2.655804   -2.229241
 H     5.425267   -2.676454   -0.902958
 H     3.909358    0.098681    0.461114
 H     5.412940   -0.750228    0.927343
 H     4.287509   -0.161424    2.176747
 H     5.235304   -3.216905    1.793176
 H     3.628985   -3.811858    2.297137
 H     4.368748   -2.430665    3.135107
 C    -3.070448   -1.461207   -1.275910
 C    -4.451014   -1.396486   -1.112283
 C    -2.222592   -0.622271   -0.543210
 C    -5.014398   -0.489585   -0.209685
 C    -2.796176    0.290650    0.353803
 C    -4.172540    0.357581    0.524153
 C    -0.737986   -0.727985   -0.697301
 C     0.072341   -0.889565    0.494432
 H    -4.601214    1.073349    1.226780
 H    -2.149427    0.963353    0.922767
 H    -5.107962   -2.053307   -1.685765
 H    -2.642297   -2.176815   -1.982338
Cu     0.498897    0.874712   -0.492452
 H    -0.389535   -0.635141    1.455896
 H    -0.611098    0.666309   -1.615603
 H    -0.444520   -1.345741   -1.553463
 O    -7.257307   -1.164004   -0.687483
 H    -8.716022   -0.434289    1.415169
 C    -6.497570   -0.461391   -0.063788
 O    -6.906995    0.428306    0.841928
 C    -8.306465    0.523511    1.062183
 H    -8.444475    1.291763    1.831821
 H    -8.831547    0.819822    0.142401
 H     4.741558    3.391654   -0.428007
 H     4.440754    1.227258   -1.887770
 H     3.426163    4.059368    1.468939
 C     3.685317    3.582787   -0.665965
 C     3.362541    1.435716   -1.960333
 H     1.034714    3.506196    2.495925
 N     2.965805    2.334837   -0.906721
 C     2.901791    4.181150    0.505165
 H     2.814434    0.489213   -1.853714
 C     1.781900    2.292632   -0.280427
 N     1.682966    3.374534    0.499183
 H     3.646701    4.221703   -1.565486
 H     3.159502    1.864067   -2.957504
 C     0.642655    3.597242    1.468574
 H     2.674256    5.248453    0.371478
 H    -0.143317    2.844010    1.326174
 H     0.201969    4.599573    1.350142
61
Figure 2_para-CO2Me_L-Cu-alkyl_rev / electronic energy: -2894.00374351 a.u. / lowest freq: 15.88 cm-1
 B     2.552577   -1.265434    0.260816
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 O     3.508027   -1.103519    1.267350
 O     3.074147   -0.827731   -0.963940
 C     4.538837   -0.255110    0.764043
 C     4.456296   -0.519217   -0.783945
 C     5.865631   -0.636413    1.403619
 C     4.172619    1.183349    1.138576
 C     5.266286   -1.742264   -1.218493
 C     4.823724    0.678033   -1.649217
 H     5.031960   -2.618108   -0.594832
 H     6.349735   -1.558397   -1.169990
 H     5.007731   -1.989911   -2.259012
 H     4.174261    1.539989   -1.446539
 H     4.716956    0.418014   -2.713286
 H     5.868370    0.979743   -1.476661
 H     3.209860    1.471152    0.690384
 H     4.939560    1.906253    0.824075
 H     4.063340    1.250216    2.231459
 H     6.695246   -0.064410    0.960345
 H     6.076074   -1.707477    1.285237
 H     5.838749   -0.416036    2.481534
 C    -1.931982   -2.876757    0.331166
 C    -3.262805   -2.510275    0.500956
 C    -1.107268   -2.203976   -0.581027
 C    -3.806265   -1.455989   -0.242204
 C    -1.676919   -1.180099   -1.353362
 C    -3.003348   -0.800658   -1.184788
 C     0.375989   -2.488641   -0.638320
 C     1.138019   -1.761966    0.480048
 H    -3.420649    0.012997   -1.779789
 H    -1.055708   -0.654404   -2.083831
 H    -3.895538   -3.030906    1.222756
 H    -1.513725   -3.687466    0.934190
Cu     0.446123    0.114829    0.538964
 H     0.971868   -2.225165    1.468025
 H     0.761982   -2.169011   -1.619616
 H     0.528219   -3.583447   -0.584863
 O    -5.975194   -1.657405    0.743099
 H    -7.120374    0.699368    0.579299
 C    -5.219157   -1.063410    0.011231
 O    -5.571963    0.042414   -0.651576
 C    -6.907635    0.492098   -0.479495
 H    -6.999461    1.414621   -1.064291
 H    -7.626043   -0.255144   -0.847450
 H    -0.116169    4.902683   -0.102661
 H     2.127595    3.487775   -0.898930
 H    -2.049932    4.327127    1.175762
 C    -0.666279    4.045369   -0.523291
 C     1.383379    2.752633   -1.248400
 H    -2.562114    2.033931    2.603738
 N     0.162856    2.842080   -0.488870
 C    -1.872381    3.638671    0.335504
 H     1.797491    1.740814   -1.137998
 C    -0.323557    1.886654    0.308806
 N    -1.480796    2.316661    0.820121
 H    -0.941197    4.295598   -1.559550
 H     1.188761    2.939408   -2.317001
 C    -2.369050    1.534332    1.640563
 H    -2.806227    3.567007   -0.246266
 H    -1.906788    0.556629    1.831324
 H    -3.333622    1.374251    1.130351
82
Figure 2_para-CO2Me_pc3_01 / electronic energy: -3732.83783511 a.u. / lowest freq: 8.90 cm-1
 C     1.616236    0.675759   -0.583120
 C     1.650896    1.007316    0.765651
 C     1.140483    2.323148    1.274792
 O     2.184445    3.324007    1.285906
 P     2.567211    4.077700   -0.071111
 O     1.464357    4.388788   -1.003399
 O     3.347398    5.317053    0.581801
 O     3.701508    3.205463   -0.798950
 C     3.861312    6.336558   -0.268418
 H     2.264907   -0.099366   -1.000633
 H     1.175736    1.367610   -1.309876
 H     2.341716    0.481144    1.435212
 H     0.306326    2.694167    0.659263
 H     0.804878    2.255078    2.317099
 B     1.150180   -3.081908   -0.906914
 O     1.777817   -3.793762    0.086062
 O     2.044044   -2.592041   -1.824468
 C     3.198356   -3.607754   -0.052217
 C     3.331747   -3.176602   -1.560362
 C     3.910496   -4.901842    0.306478
 C     3.597697   -2.501321    0.922137
 C     3.490700   -4.361635   -2.511443
 C     4.416238   -2.145422   -1.831069
 H     2.717136   -5.124940   -2.339085
 H     4.477478   -4.835437   -2.407871
 H     3.386938   -4.004821   -3.546649
 H     4.256981   -1.217693   -1.266120
 H     4.426747   -1.890881   -2.901183
 H     5.405977   -2.548584   -1.568592
 H     3.084579   -1.558459    0.683863
 H     4.682081   -2.320640    0.911776
 H     3.310160   -2.795384    1.942563
 H     4.992039   -4.812371    0.124830
 H     3.526430   -5.752187   -0.271707
 H     3.762345   -5.122878    1.373854
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 C   -2.513980    0.239748   -1.911709
 C   -3.810563    0.716391   -1.860664
 C   -2.111243   -0.941205   -1.227694
 C   -4.798914    0.035882   -1.124337
 C   -3.131816   -1.625865   -0.515669
 C   -4.430322   -1.145222   -0.461724
 C   -0.717759   -1.361071   -1.231182
 C   -0.397195   -2.833439   -0.960554
 H   -5.193426   -1.687976    0.101944
 H   -2.887575   -2.546223    0.018965
 H   -4.074180    1.631140   -2.395302
 H   -1.763373    0.791661   -2.486052
Cu    0.096887   -0.280062    0.333497
 H   -0.839879   -3.500966   -1.732920
 H   -0.824673   -3.174530   -0.002851
 H   -0.202801   -1.001671   -2.134052
 H    4.356896    7.073420    0.375585
 H    3.049896    6.829050   -0.825270
 H    4.596539    5.931569   -0.981871
 C    4.797686    2.651846   -0.085864
 H    5.534111    2.320056   -0.828665
 H    4.476635    1.786644    0.514218
 H    5.265814    3.397107    0.576178
 H    0.546289   -2.652381    3.703952
 H   -1.749183   -1.660868    4.669193
 C   -0.007407   -2.739678    2.752619
 H    0.691112   -2.605308    1.918584
 H   -0.421875   -3.757731    2.687497
 C   -2.151495   -1.770851    3.647440
 N   -1.059273   -1.760021    2.675627
 H   -2.707537   -2.718746    3.600855
 H   -3.233784    0.114698    4.042310
 C   -1.038265   -0.653869    1.923174
 C   -2.985280   -0.562430    3.211852
 N   -2.100426    0.088886    2.249253
 H   -3.926281   -0.852794    2.714257
 H   -2.614194    2.123852    2.314874
 C   -2.505249    1.302174    1.588590
 H   -1.744613    1.580636    0.848340
 H   -3.467037    1.163846    1.067699
 O   -7.064851   -0.040975   -0.378872
 H   -7.996402    2.422715   -0.571744
 C   -6.190727    0.513320   -1.009892
 H   -8.456878    1.500366   -2.033100
 C   -7.715515    2.195313   -1.611005
 O   -6.407646    1.654667   -1.680505
 H   -7.700247    3.120768   -2.199155
82
Figure 2_para-CO2Me_pc3_02 / electronic energy: -3732.83759747 a.u. / lowest freq: 15.28 cm-1
 C    0.533956   -1.103606   -1.001249
 C    0.511174   -1.851190    0.166823
 C    1.673004   -1.940238    1.109905
 O    2.572659   -3.005029    0.718190
 P    4.050461   -2.630076    0.242047
 O    4.834880   -1.727410    1.108883
 O    4.602597   -4.118184    0.036940
 O    3.910470   -2.006594   -1.233906
 C    5.988509   -4.309984   -0.231924
 H   -0.175068   -1.317495   -1.807470
 H    1.406726   -0.499874   -1.274194
 H   -0.241687   -2.641234    0.273436
 H    2.227421   -0.991516    1.157747
 H    1.339122   -2.185004    2.127159
 B    0.968737    2.406241   -1.542108
 O    2.137880    1.794095   -1.919203
 O    1.194519    3.463542   -0.695988
 C    3.201463    2.327830   -1.106089
 C    2.611578    3.716056   -0.665761
 C    4.472553    2.402647   -1.935443
 C    3.393634    1.364569    0.062131
 C    2.891166    4.829853   -1.673329
 C    3.010154    4.162271    0.731382
 H    2.619808    4.526450   -2.695648
 H    3.950463    5.124602   -1.667145
 H    2.287761    5.711484   -1.411116
 H    2.694544    3.441247    1.495817
 H    2.538411    5.129408    0.960164
 H    4.100740    4.290865    0.801452
 H    2.473600    1.282846    0.662295
 H    4.213316    1.678509    0.723563
 H    3.641810    0.368472   -0.327815
 H    5.277754    2.894584   -1.369126
 H    4.315974    2.951628   -2.873256
 H    4.807833    1.385757   -2.187569
 C   -3.555527    1.135891    0.169472
 C   -4.795129    0.531316    0.096882
 C   -2.574921    0.972611   -0.850872
 C   -5.146614   -0.274588   -1.001979
 C   -2.962331    0.179759   -1.964003
 C   -4.205127   -0.431753   -2.031809
 C   -1.244515    1.546341   -0.705458
 C   -0.460999    1.927508   -1.965240
 H   -4.461040   -1.038501   -2.902909
 H   -2.259593    0.037593   -2.788149
 H   -5.528086    0.677515    0.894136
 H   -3.308061    1.758308    1.034610
Cu   -0.463712   -0.030513    0.390546
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 H   -0.977743    2.724428   -2.541072
 H   -0.348410    1.074850   -2.653811
 H   -1.259634    2.378131    0.015774
 H    6.133837   -5.380366   -0.422236
 H    6.601431   -4.007399    0.630245
 H    6.308370   -3.742394   -1.120218
 C    3.265282   -2.714200   -2.286425
 H    2.992889   -1.978689   -3.053392
 H    2.353428   -3.217191   -1.931987
 H    3.947039   -3.458846   -2.725134
 H   -2.668211   -2.421937    3.093035
 H   -2.487762   -0.486276    4.972368
 C   -2.725874   -1.580303    2.383913
 H   -2.266093   -1.880505    1.433930
 H   -3.789067   -1.352369    2.200795
 C   -2.478164    0.221981    4.130846
 N   -2.030757   -0.430731    2.901540
 H   -3.502723    0.609335    3.997871
 H   -0.733034    1.143282    5.116854
 C   -1.077361    0.253589    2.262470
 C   -1.444837    1.341672    4.297705
 N   -0.752361    1.313169    3.010667
 H   -1.902638    2.326041    4.474354
 H    1.171913    2.110910    3.351932
 C    0.290618    2.257934    2.704059
 H    0.591625    2.136727    1.655276
 H   -0.072352    3.288685    2.839076
 O   -7.332406   -0.759676   -0.176394
 H   -8.761474   -1.493348   -2.290899
 C   -6.485541   -0.894824   -1.033000
 H   -8.165314   -2.937685   -1.422518
 C   -7.963221   -2.249585   -2.256919
 O   -6.689552   -1.642427   -2.127821
 H   -7.944925   -2.809157   -3.199818
82
Figure 2_para-CO2Me_ts(AS)_01 / electronic energy: -3732.80314503 a.u. / lowest freq: -348.41 cm-1
 C    1.313085    1.217578   -0.643736
 C    1.615832    1.544177    0.701738
 C    0.638268    2.045441    1.570881
 O    0.701047    4.121974    1.516405
 P    0.029009    4.576391    0.221132
 O   -0.992253    3.709998   -0.446854
 O   -0.555014    6.061858    0.570167
 O    1.185407    4.909425   -0.889543
 C   -1.267010    6.761411   -0.426132
 H    2.102758    0.859836   -1.308221
 H    0.457047    1.713316   -1.116833
 H    2.621213    1.369658    1.097675
 H   -0.396829    2.129490    1.238029
 H    0.825515    2.078570    2.643484
 B    2.454014   -2.331462   -0.968762
 O    3.371989   -2.951954   -0.162523
 O    3.036098   -1.414339   -1.803492
 C    4.625317   -2.252597   -0.298848
 C    4.465762   -1.559901   -1.701717
 C    5.768832   -3.248391   -0.203836
 C    4.697896   -1.252036    0.852959
 C    4.907683   -2.448356   -2.862812
 C    5.115180   -0.190105   -1.811824
 H    4.455199   -3.449231   -2.797770
 H    6.000889   -2.560253   -2.895083
 H    4.580804   -1.989971   -3.807509
 H    4.704854    0.519776   -1.081511
 H    4.947396    0.223825   -2.817032
 H    6.201473   -0.265077   -1.652807
 H    3.877674   -0.520376    0.797384
 H    5.651436   -0.704995    0.858155
 H    4.608238   -1.792069    1.806991
 H    6.732371   -2.749185   -0.385781
 H    5.656693   -4.067597   -0.925693
 H    5.799245   -3.685966    0.804848
 C   -2.201270   -0.545414   -1.788754
 C   -3.584582   -0.632220   -1.790531
 C   -1.395619   -1.506418   -1.137611
 C   -4.231047   -1.693582   -1.137826
 C   -2.062796   -2.568321   -0.490874
 C   -3.448121   -2.657980   -0.490331
 C    0.073787   -1.358362   -1.129307
 C    0.911961   -2.619419   -0.928209
 H   -3.945828   -3.488946    0.014754
 H   -1.483382   -3.335709    0.026276
 H   -4.175432    0.127944   -2.303956
 H   -1.716508    0.291762   -2.299382
Cu    0.446289   -0.171597    0.468113
 H    0.689314   -3.362479   -1.723832
 H    0.676899   -3.130960    0.018841
 H    0.395212   -0.826237   -2.033465
 H   -1.615710    7.708032    0.010870
 H   -2.140504    6.187447   -0.776646
 H   -0.629892    6.991251   -1.297906
 C    2.326653    5.637300   -0.500913
 H    3.025305    5.654627   -1.349954
 H    2.827384    5.170365    0.363012
 H    2.076536    6.679006   -0.233349
 H    2.019455   -2.274412    3.626202
 H   -0.428048   -2.449384    4.712731
 C    1.512385   -2.538761    2.682650
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 H     2.029461   -2.046387    1.851287
 H     1.589899   -3.627167    2.538963
 C    -0.798995   -2.655144    3.695126
 N     0.134649   -2.121460    2.703565
 H    -0.901968   -3.744587    3.583671
 H    -2.527785   -1.391592    4.245347
 C    -0.379004   -1.110456    2.000347
 C    -2.092201   -1.896628    3.370509
 N    -1.642297   -0.923893    2.377684
 H    -2.866777   -2.546567    2.930723
 H    -2.846131    0.789994    2.575164
 C    -2.550757    0.043922    1.819987
 H    -2.063166    0.557524    0.982273
 H    -3.458487   -0.451537    1.441343
 O    -6.300816   -2.721435   -0.532838
 H    -8.172107   -0.826018   -0.790394
 C    -5.708246   -1.833652   -1.102971
 H    -8.107410   -1.847505   -2.258735
 C    -7.751612   -0.911683   -1.803318
 O    -6.334250   -0.862666   -1.774709
 H    -8.076292   -0.058299   -2.410158
82
Figure 2_para-CO2Me_ts(AS)_02 / electronic energy: -3732.80085269 a.u. / lowest freq: -311.21 cm-1
 C     0.260663   -0.186102   -1.846888
 C     0.361464   -1.537649   -1.445495
 C     1.210878   -1.952486   -0.409594
 O     2.933982   -2.760088   -1.264133
 P     4.200118   -2.235803   -0.592380
 O     4.127289   -1.530259    0.723469
 O     5.200353   -3.529342   -0.536982
 O     4.985715   -1.250573   -1.642189
 C     6.465383   -3.375937    0.066462
 H    -0.424232    0.076396   -2.657361
 H     1.097729    0.504453   -1.699838
 H    -0.320295   -2.277323   -1.877255
 H     1.843655   -1.248563    0.134962
 H     1.045279   -2.917892    0.065412
 B     0.636305    2.927968   -0.477912
 O     1.719257    2.823393   -1.309706
 O     0.994352    3.285494    0.796629
 C     2.910178    2.899028   -0.493881
 C     2.385960    3.663995    0.774658
 C     4.002712    3.617361   -1.266398
 C     3.331424    1.466775   -0.184957
 C     2.433923    5.183016    0.619940
 C     3.040600    3.250771    2.082288
 H     1.971772    5.506780   -0.324730
 H     3.466060    5.560202    0.650470
 H     1.875262    5.646432    1.446428
 H     2.911791    2.180900    2.287091
 H     2.596705    3.814761    2.916018
 H     4.118673    3.470004    2.058157
 H     2.555590    0.933632    0.383020
 H     4.260455    1.422601    0.397961
 H     3.509476    0.915257   -1.118385
 H     4.885155    3.773006   -0.627869
 H     3.665247    4.591258   -1.644929
 H     4.311881    3.006298   -2.127334
 C    -3.644298    0.742723    0.862088
 C    -4.932927    0.268935    0.677360
 C    -2.822053    1.098896   -0.230992
 C    -5.464746    0.130607   -0.612790
 C    -3.383565    0.981598   -1.519950
 C    -4.674098    0.503487   -1.708610
 C    -1.420991    1.515303   -0.004403
 C    -0.847199    2.622175   -0.892299
 H    -5.077908    0.413685   -2.718426
 H    -2.788090    1.257510   -2.393423
 H    -5.552258   -0.002581    1.535174
 H    -3.245200    0.842457    1.875420
Cu    -0.536604   -0.301251   -0.032222
 H    -1.448890    3.546400   -0.775944
 H    -0.880408    2.365138   -1.961934
 H    -1.290900    1.788451    1.053912
 H     7.002337   -4.330665   -0.028752
 H     6.374765   -3.122460    1.135625
 H     7.060157   -2.588120   -0.427812
 C     5.119791   -1.641592   -2.989415
 H     5.667261   -0.847916   -3.518157
 H     4.136862   -1.778088   -3.469470
 H     5.686738   -2.583864   -3.085414
 H    -2.543876   -3.711715    1.241968
 H    -1.871803   -3.194464    3.797782
 C    -2.671882   -2.620214    1.165746
 H    -2.432236   -2.306941    0.140904
 H    -3.726802   -2.376438    1.370428
 C    -1.922134   -2.128479    3.533168
 N    -1.795660   -1.944181    2.087354
 H    -2.892817   -1.733485    3.877051
 H     0.088861   -1.961541    4.422747
 C    -0.893531   -1.018424    1.767508
 C    -0.734275   -1.318946    4.067893
 N    -0.310366   -0.575561    2.881538
 H    -1.011184   -0.633742    4.881604
 H     1.765243   -0.214796    3.043824
 C     0.813049    0.327397    2.915711
 H     0.846358    0.897123    1.977361
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 H    0.700427    1.042386    3.744031
 O   -7.552318   -0.728697    0.163761
 H   -9.292781   -0.343020   -1.836952
 C   -6.841531   -0.404891   -0.760187
 H   -8.652465   -2.013719   -1.855195
 C   -8.530924   -1.004555   -2.275258
 O   -7.224567   -0.504275   -2.036734
 H   -8.654937   -1.038091   -3.363877
82
Figure 2_para-CO2Me_pi-allyl_01 / electronic energy: -3732.82691538 a.u. / lowest freq: 24.29 cm-1
 C    1.305599    1.992604   -0.918110
 C    1.877733    2.369817    0.320653
 C    1.096741    2.403695    1.471325
 O   -1.940412    3.182483    1.294652
 P   -2.541794    2.964682   -0.064684
 O   -1.743789    2.409585   -1.214879
 O   -3.879193    2.031793    0.181090
 O   -3.222691    4.356134   -0.617472
 C   -4.682973    1.686538   -0.918831
 H    1.970190    1.800295   -1.761979
 H    0.242796    2.220993   -1.120943
 H    2.969738    2.344958    0.420246
 H    0.011773    2.612418    1.419865
 H    1.579871    2.485650    2.449216
 B    3.464155   -1.041781   -0.845464
 O    4.554679   -1.475569   -0.141851
 O    3.745456    0.050580   -1.618528
 C    5.605172   -0.500368   -0.295692
 C    5.171150    0.258230   -1.606360
 C    6.941598   -1.217376   -0.392206
 C    5.573205    0.386303    0.947605
 C    5.723773   -0.375307   -2.880846
 C    5.453374    1.751497   -1.600271
 H    5.532523   -1.458352   -2.910016
 H    6.805720   -0.208439   -2.978887
 H    5.227136    0.079458   -3.750314
 H    4.940803    2.262020   -0.774377
 H    5.106847    2.199501   -2.543216
 H    6.533560    1.940387   -1.510395
 H    4.615341    0.920556    1.035699
 H    6.383379    1.128988    0.936086
 H    5.695475   -0.242108    1.841981
 H    7.750433   -0.501021   -0.599974
 H    6.937086   -1.980921   -1.180532
 H    7.165828   -1.716193    0.562119
 C   -1.554755   -0.826638   -1.706757
 C   -2.833913   -1.363373   -1.687384
 C   -0.484722   -1.460250   -1.045277
 C   -3.094552   -2.552613   -0.993156
 C   -0.758359   -2.660468   -0.363232
 C   -2.040168   -3.195058   -0.334391
 C    0.865345   -0.836972   -1.061309
 C    2.059279   -1.741059   -0.775699
 H   -2.241498   -4.122621    0.205866
 H    0.042158   -3.181206    0.165281
 H   -3.647608   -0.846670   -2.197314
 H   -1.388425    0.138689   -2.190364
Cu    0.885098    0.534579    0.413907
 H    2.089080   -2.556786   -1.529390
 H    1.971950   -2.255192    0.193927
 H    1.006255   -0.308042   -2.010654
 H   -5.204977    0.744896   -0.690039
 H   -4.082411    1.541955   -1.831597
 H   -5.442618    2.462123   -1.124255
 C   -3.985534    5.130221    0.273531
 H   -4.305723    6.042360   -0.251903
 H   -3.402534    5.418609    1.164396
 H   -4.888140    4.592488    0.616088
 H    2.881793   -0.664852    3.670744
 H    0.581598   -1.490499    4.762054
 C    2.540176   -1.212037    2.775567
 H    2.913094   -0.696817    1.882756
 H    2.977019   -2.221545    2.795510
 C    0.339919   -1.943806    3.786213
 N    1.102201   -1.279336    2.728009
 H    0.586735   -3.014077    3.833786
 H   -1.730998   -1.269272    4.169295
 C    0.320220   -0.542050    1.936689
 C   -1.110428   -1.679891    3.360103
 N   -0.947385   -0.705711    2.283307
 H   -1.608467   -2.581651    2.966687
 H   -2.545813    0.668355    2.273116
 C   -2.077714   -0.090562    1.631018
 H   -1.737689    0.404908    0.714370
 H   -2.821533   -0.856086    1.363490
 O   -4.715920   -4.158841   -0.290055
 H   -7.068298   -2.918309   -0.412569
 C   -4.455075   -3.142940   -0.892083
 H   -6.812611   -3.895266   -1.890432
 C   -6.719225   -2.889526   -1.455202
 O   -5.381057   -2.421624   -1.529674
 H   -7.326024   -2.180472   -2.030036
82
Figure 2_para-CO2Me_pi-allyl_02 / electronic energy: -3732.82458329 a.u. / lowest freq: 17.28 cm-1
 C   -0.474408    1.343438   -2.190320
 C   -0.462405    0.018990   -2.703503
 C    0.504648   -0.876110   -2.279171
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 O    2.097973   -3.170749   -0.684423
 P    3.269952   -2.249633   -0.517378
 O    3.172747   -0.755193   -0.678002
 O    3.920011   -2.597838    0.964856
 O    4.501551   -2.718151   -1.506573
 C    5.069650   -1.901427    1.378493
 H   -1.338854    1.982135   -2.383501
 H    0.472011    1.867190   -2.021030
 H   -1.373132   -0.368321   -3.174925
 H    1.478677   -0.557249   -1.872519
 H    0.410775   -1.946046   -2.473865
 B    0.670668    3.145693    0.321737
 O    1.303579    3.830667   -0.676899
 O    1.547850    2.622713    1.230998
 C    2.726355    3.608537   -0.548452
 C    2.863553    3.146174    0.951527
 C    3.455997    4.898392   -0.886569
 C    3.106411    2.513147   -1.541138
 C    3.088308    4.302893    1.922943
 C    3.895686    2.051597    1.178921
 H    2.341830    5.099752    1.784781
 H    4.090403    4.739891    1.806688
 H    2.994346    3.928320    2.952919
 H    3.672183    1.141000    0.603355
 H    3.925799    1.792838    2.248547
 H    4.896722    2.412262    0.895672
 H    2.654251    1.543326   -1.288907
 H    4.194860    2.361526   -1.567555
 H    2.780739    2.811773   -2.549084
 H    4.535917    4.788942   -0.707357
 H    3.085497    5.746469   -0.295993
 H    3.311385    5.136193   -1.950841
 C   -3.148532    0.010865    1.361367
 C   -4.448944   -0.458078    1.259758
 C   -2.680243    1.063467    0.547668
 C   -5.340306    0.114927    0.343132
 C   -3.594160    1.644676   -0.350665
 C   -4.900308    1.179170   -0.453801
 C   -1.252430    1.471031    0.624984
 C   -0.888120    2.936496    0.404264
 H   -5.587564    1.642455   -1.163397
 H   -3.274236    2.469890   -0.990660
 H   -4.794133   -1.277931    1.893066
 H   -2.464042   -0.448114    2.079274
Cu   -0.439009    0.111051   -0.598580
 H   -1.282500    3.534485    1.249975
 H   -1.350206    3.349398   -0.503999
 H   -0.822905    1.125017    1.574901
 H    5.442039   -2.373540    2.299901
 H    4.856651   -0.838642    1.588560
 H    5.866807   -1.944117    0.616382
 C    4.802937   -4.087105   -1.606700
 H    5.580801   -4.211882   -2.375145
 H    3.916843   -4.676540   -1.896558
 H    5.187925   -4.494139   -0.653939
 H   -1.406307   -3.549395   -1.351890
 H    0.198015   -4.371143    0.641527
 C   -1.807187   -2.840951   -0.607241
 H   -2.078604   -1.905728   -1.115360
 H   -2.719937   -3.276338   -0.170563
 C   -0.319106   -3.632813    1.272043
 N   -0.841844   -2.566113    0.421770
 H   -1.132926   -4.125029    1.825961
 H    1.684974   -3.289170    2.112511
 C   -0.182709   -1.421231    0.588343
 C    0.666401   -2.881066    2.174121
 N    0.654881   -1.533440    1.608206
 H    0.350969   -2.849415    3.230090
 H    2.557162   -0.861361    2.129212
 C    1.515954   -0.512572    2.143489
 H    1.445727    0.398422    1.541483
 H    1.231446   -0.276913    3.183265
 O   -7.125244   -1.363125    0.918354
 H   -9.363737   -0.178992    0.151473
 C   -6.719562   -0.436652    0.256214
 H   -8.829960   -1.305994   -1.132806
 C   -8.809368   -0.259490   -0.794827
 O   -7.474233    0.199802   -0.641510
 H   -9.270891    0.384289   -1.552350
56
Figure 3_L-Cu-OtBu_dimer / electronic energy: -4668.27269506 a.u. / lowest freq: 20.28 cm-1
 H    1.454781    3.185323    2.121955
 H   -1.091667    3.295320    2.232897
 H    1.480610    4.376760    0.788877
 C    1.390257    3.304563    1.028715
 H    2.248895    2.774926    0.584062
 H   -1.141168    4.483981    0.897486
 C   -1.116435    3.408141    1.137329
 C    0.084478    2.685555    0.510787
 O    0.044189    1.344738    0.873648
 H   -2.049560    2.947919    0.774353
 H    0.052315    3.874754   -1.357879
 C    0.025055    2.825701   -1.018825
 H    0.875658    2.290877   -1.472279
 H   -0.901160    2.361194   -1.396152
 H    2.958274    1.006115   -2.657041
 H    3.299551   -1.873435   -2.121429
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 C    3.677359    1.175331   -1.841405
 C    3.978968   -1.600940   -1.299765
 H    4.699652    1.104301   -2.245503
 H    3.518839    2.190392   -1.447525
 H    4.999010   -1.491753   -1.701120
 H    3.968610   -2.417548   -0.562485
 P    3.392482   -0.052886   -0.509011
 C    4.751395    0.319901    0.663359
 H    5.728245    0.345249    0.155766
 H    4.568915    1.292893    1.143584
 H    4.770992   -0.448839    1.450266
Cu    1.387359   -0.047785    0.355891
 H    1.052783   -3.300511    2.261431
 H    2.049259   -2.926990    0.836004
 O   -0.048207   -1.342931    0.876207
 C    1.110810   -3.401807    1.166003
 H    1.154224   -4.474801    0.916365
 C   -0.077761   -2.683448    0.511400
 H   -1.486976   -3.182509    2.088692
 H    0.959296   -2.370999   -1.370977
 C   -1.393184   -3.307099    0.998157
 C    0.017837   -2.822386   -1.016552
 H   -2.243357   -2.784789    0.529205
 H   -1.470986   -4.380974    0.761611
 H   -0.814236   -2.274610   -1.489485
 H   -0.015593   -3.870539   -1.357852
 H   -2.864028   -0.603368   -2.784246
 H   -3.433166    2.132063   -1.768599
 C   -3.581006   -0.953346   -2.026339
 C   -4.101882    1.661026   -1.032388
 H   -4.600512   -0.883806   -2.437656
 H   -3.356876   -2.007230   -1.803518
 H   -5.099460    1.538334   -1.483310
 H   -4.181695    2.333019   -0.164790
 P   -3.397860    0.051973   -0.503299
 C   -4.732552   -0.612373    0.562621
 H   -5.709729   -0.575241    0.056317
 H   -4.504550   -1.654856    0.830705
 H   -4.786261   -0.026266    1.492473
Cu   -1.393433    0.048543    0.362283
28
Figure 3_L-Cu-OtBu / electronic energy: -2334.10735270 a.u. / lowest freq: -39.13 cm-1
 H   -4.105877   -1.332535    0.968255
 H   -4.149740   -1.387400   -0.808196
 O   -1.712519   -0.853226    0.000001
 C   -4.074557   -0.711355    0.058637
 H   -4.956088   -0.048773    0.060108
 C   -2.745372    0.062111    0.000906
 H   -2.638090    0.394148    2.149194
 H   -2.753281    0.265927   -2.166060
 C   -2.653965    0.994061    1.224813
 C   -2.718854    0.919727   -1.279501
 H   -1.712633    1.569392    1.184920
 H   -3.490501    1.710689    1.287963
 H   -1.776368    1.492537   -1.324725
 H   -3.557324    1.634317   -1.340220
 H    2.442116    1.017710   -2.209934
 H    3.078065   -1.733910   -1.400494
 C    2.702639    1.337847   -1.190198
 C    3.315084   -1.349708   -0.397345
 H    3.784909    1.532944   -1.136890
 H    2.155445    2.266931   -0.971809
 H    4.370113   -1.036408   -0.368346
 H    3.157970   -2.162063    0.327594
 P    2.201656    0.043634    0.000306
 C    2.853579    0.661225    1.592861
 H    3.931571    0.875098    1.526895
 H    2.317993    1.579995    1.874683
 H    2.679866   -0.091178    2.376412
Cu    0.062960   -0.408951   -0.003275
70
Figure 3_ed / electronic energy: -3155.87460188 a.u. / lowest freq: 11.42 cm-1
 H   -0.953281   -3.166097   -0.309839
 H   -2.577969   -2.483931   -0.153509
 O   -0.722801   -0.949157    1.165859
 C   -1.784111   -3.004943    0.394843
 H   -2.158222   -3.987377    0.724568
 C   -1.300935   -2.179344    1.589376
 H    0.648291   -3.149536    1.617528
 H   -3.221244   -1.298799    2.101803
 C   -0.183773   -2.938745    2.311306
 C   -2.439912   -1.904482    2.572798
 H    0.208864   -2.337581    3.146164
 H   -0.544498   -3.898139    2.713555
 H   -2.060320   -1.341525    3.439455
 H   -2.878571   -2.846939    2.937460
Cu    1.139839   -0.920846    0.386293
 H    1.056430    4.912258    0.610864
 H    2.420469    3.941746    2.458899
 H    0.701370    3.458516    2.402659
 C    1.735449    3.084044    2.391288
 H    2.707250    4.756558   -0.052951
 H    1.879972    2.458170    3.283891
 C    1.657698    4.452166   -0.184163
 H    1.306082    4.849580   -1.147882
 C    1.534322    2.938372   -0.174971
 C    2.012113    2.248287    1.144500
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 O    0.145692    2.568639   -0.221946
 H    4.143931    2.596400    0.951770
 B   -0.029916    1.375300    0.444402
 H    3.702501    1.320418    2.112925
 C    3.450475    1.762470    1.137384
 O    1.127301    1.108628    1.201500
 H    3.251675    2.634595   -1.503243
 C    2.195444    2.340356   -1.418544
 H    1.664689    2.695001   -2.313853
 H    3.609342    0.994382    0.369926
 H    2.135444    1.240689   -1.404032
 H   -3.741486   -1.478482   -2.045890
 H   -4.291404   -1.318464    0.099435
 H   -2.833922   -0.708588   -3.361743
 C   -3.485339   -0.510025   -2.496037
 O   -1.630269   -0.279491   -1.014975
 H   -5.500527   -0.242437   -0.645178
 C   -4.684450   -0.292834    0.091969
 H   -4.409992   -0.043182   -2.870615
 B   -1.338180    0.190930    0.348230
 H   -5.115024   -0.091914    1.085474
 C   -2.753803    0.399038   -1.508504
 C   -3.582938    0.736127   -0.195713
 O   -2.623638    0.690654    0.835872
 H   -1.601520    1.343872   -3.063483
 C   -2.292899    1.655469   -2.264419
 H   -3.130173    2.197298   -2.730793
 H   -1.740687    2.341103   -1.608781
 H   -4.940611    2.237160   -1.041325
 C   -4.225555    2.125176   -0.210655
 H   -4.773476    2.286728    0.730889
 H   -3.466517    2.914749   -0.291729
 H    4.749033   -1.452497   -0.129415
 C    4.256493   -1.368792   -1.109548
 H    4.274484   -0.314095   -1.421428
 H    4.817512   -1.966521   -1.844659
 H    3.139485   -3.910893    0.308949
 C    2.717087   -3.740696   -0.692506
 P    2.524841   -1.944693   -0.980227
 H    3.382198   -4.194279   -1.443776
 H    1.733374   -4.230143   -0.742993
 C    1.932965   -1.853706   -2.708395
 H    2.575860   -2.437454   -3.385113
 H    1.920774   -0.803126   -3.035062
 H    0.902696   -2.235271   -2.761689
70
Figure 3_ts(TB) / electronic energy: -3155.86594930 a.u. / lowest freq: -80.57 cm-1
 H    3.010276   -2.382916    0.118642
 H    1.683795   -3.550734    0.289052
 O    0.986480   -1.022586    1.231429
 C    2.428017   -2.966919    0.847086
 H    3.108602   -3.663642    1.360560
 C    1.764613   -2.038365    1.865178
 H    3.454412   -0.689234    1.957273
 H    0.067382   -3.345104    2.249766
 C    2.833443   -1.280682    2.648443
 C    0.860433   -2.829879    2.810029
 H    2.364821   -0.587587    3.363520
 H    3.486796   -1.968789    3.205755
 H    0.379103   -2.153513    3.532327
 H    1.437600   -3.583696    3.368135
Cu    1.191646    0.705211   -0.156501
 H   -4.427383    0.766248   -0.614487
 H   -4.518683    0.953062    1.818726
 H   -3.273614   -0.182983    1.196620
 C   -3.444824    0.713535    1.807889
 H   -4.940033    2.443526   -0.292598
 H   -3.136606    0.474696    2.836818
 C   -4.170605    1.821119   -0.775127
 H   -4.205093    2.017783   -1.857471
 C   -2.789480    2.154856   -0.232080
 C   -2.601465    1.882699    1.299916
 O   -1.819873    1.275125   -0.815333
 H   -3.824652    3.498708    2.084955
 B   -0.832690    0.986003    0.123485
 H   -2.656331    2.821205    3.244537
 C   -2.803566    3.100143    2.190308
 O   -1.228345    1.472481    1.363096
 H   -3.133588    4.320679   -0.285336
 C   -2.402291    3.578362   -0.637798
 H   -2.355518    3.636570   -1.735582
 H   -2.091022    3.901305    1.952964
 H   -1.410567    3.846106   -0.243686
 H    0.204209   -4.250825   -1.796312
 H   -0.675749   -4.205721    0.241701
 H    0.503640   -3.256638   -3.237470
 C   -0.244142   -3.509492   -2.470797
 O    0.458693   -1.748160   -1.013589
 H   -2.092610   -4.638531   -0.753443
 C   -1.697902   -3.906637   -0.032981
 H   -1.103862   -3.973045   -2.978655
 B    0.018530   -1.182613    0.206285
 H   -2.317693   -3.950556    0.875196
 C   -0.662553   -2.241330   -1.733040
 C   -1.728672   -2.480221   -0.585246
 O   -1.295504   -1.617289    0.465873
 H   -0.223704   -0.958441   -3.401261
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 C   -1.089544   -1.191204   -2.761739
 H   -1.896569   -1.564732   -3.410033
 H   -1.420470   -0.261620   -2.282477
 H   -3.480699   -2.692998   -1.858133
 C   -3.151903   -2.111553   -0.982870
 H   -3.844242   -2.329239   -0.155058
 H   -3.222981   -1.042608   -1.218567
 H    3.073834    3.432394    1.120755
 C    3.095595    3.493894    0.022203
 H    2.193451    4.031342   -0.305906
 H    3.990738    4.052076   -0.293219
 H    4.736915    1.037154    0.921073
 C    4.694130    1.124469   -0.174737
 P    3.070384    1.803289   -0.674895
 H    5.518167    1.770887   -0.515219
 H    4.823307    0.120668   -0.606383
 C    3.271177    2.077403   -2.471443
 H    4.160947    2.686342   -2.694837
 H    2.375105    2.582414   -2.861624
 H    3.361485    1.104827   -2.978490
70
Figure 3_prod / electronic energy: -3155.88950452 a.u. / lowest freq: 21.62 cm-1
 H   -1.158855   -0.853872    2.044678
 H   -2.081368    0.534440    1.412845
 O    0.476218    1.273606    2.005172
 C   -1.632766    0.101521    2.318332
 H   -2.432894   -0.100666    3.046635
 C   -0.605099    1.058362    2.919658
 H    0.524730   -0.514821    3.893677
 H   -1.708831    2.852240    2.370142
 C    0.037748    0.436514    4.155433
 C   -1.246887    2.403039    3.261372
 H    0.800788    1.111086    4.572434
 H   -0.716472    0.240474    4.932049
 H   -0.490899    3.101512    3.652262
 H   -2.026382    2.277814    4.028140
Cu   -1.162098   -1.530549   -0.469595
 H    3.580583    0.620775   -0.295027
 H    4.155902   -0.696748    1.828001
 H    2.467465   -0.158497    1.567577
 C    3.113119   -1.032974    1.727857
 H    5.013044   -0.445128   -0.480147
 H    2.813949   -1.499307    2.678963
 C    4.011688   -0.207170   -0.872112
 H    4.132527    0.132623   -1.911993
 C    3.106855   -1.430692   -0.824697
 C    2.945747   -2.057257    0.604145
 O    1.763095   -1.042039   -1.140811
 H    4.896752   -2.999208    0.793143
 B    0.857046   -1.733858   -0.337362
 H    3.652152   -3.642033    1.890565
 C    3.831372   -3.266557    0.871685
 O    1.571398   -2.467038    0.608300
 H    4.595766   -2.740742   -1.760293
 C    3.543447   -2.443828   -1.883977
 H    3.430968   -1.987531   -2.879035
 H    3.625644   -4.087120    0.171499
 H    2.917986   -3.348697   -1.857648
 H   -1.188959    4.543120   -0.961219
 H    0.838043    4.659257    0.115279
 H   -2.279828    3.395564   -1.769932
 C   -1.230561    3.715188   -1.680966
 O   -0.748295    2.177348    0.104616
 H    1.217478    4.989554   -1.597762
 C    1.435817    4.327569   -0.747385
 H   -0.904775    4.086148   -2.664441
 B    0.397248    1.808796    0.768095
 H    2.497981    4.443808   -0.486318
 C   -0.374050    2.539678   -1.237950
 C    1.163803    2.862937   -1.086359
 O    1.537557    2.088052    0.061507
 H   -1.693283    1.038056   -2.022193
 C   -0.638926    1.330245   -2.128884
 H   -0.452594    1.559433   -3.188203
 H   -0.013144    0.474822   -1.835748
 H    1.667555    2.926311   -3.195542
 C    2.005995    2.427305   -2.274763
 H    3.058190    2.701403   -2.107369
 H    1.953583    1.339765   -2.409554
 H   -3.849992   -3.526552   -1.811768
 C   -4.138767   -2.476486   -1.968429
 H   -3.730136   -2.151784   -2.937054
 H   -5.237257   -2.405102   -1.996484
 H   -3.969700   -3.065287    1.097540
 C   -4.312146   -2.048283    0.854783
 P   -3.430509   -1.445333   -0.632444
 H   -5.401729   -2.061155    0.696600
 H   -4.080638   -1.396766    1.709930
 C   -4.218331    0.182703   -0.927440
 H   -5.316094    0.104994   -0.887227
 H   -3.927434    0.563017   -1.917896
 H   -3.880941    0.905727   -0.169933
35
Figure 3_L-Cu-Bpin / electronic energy: -2512.09747879 a.u. / lowest freq: 23.70 cm-1
 H   -3.966569   -2.370555   -0.091079
 H   -3.807068   -0.481958   -2.357598
 C   -4.300635   -1.524404    0.527882
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 C   -4.141575    0.306361   -1.666690
 H   -5.393074   -1.419924    0.438009
 H   -4.044913   -1.745522    1.575060
 H   -5.242483    0.322371   -1.642579
 H   -3.774702    1.270837   -2.048864
 P   -3.438874    0.000252   -0.004071
 C   -4.231120    1.295459    1.018181
 H   -5.326265    1.285342    0.903062
 H   -3.978324    1.134755    2.076846
 H   -3.846004    2.282421    0.721008
 H    3.908707   -2.418790   -1.177398
 H    3.178529   -2.542187    1.157081
 C    3.960241   -1.319391   -1.165315
 H    3.658664   -0.959332   -2.157930
 H    5.009094   -1.032819   -0.991557
 C    3.381449   -1.465540    1.257698
 O    1.691138   -1.070941   -0.382227
 H    4.437392   -1.340205    1.540068
 C    3.058289   -0.772965   -0.067653
 H    2.751180   -1.078631    2.072035
 B    0.869426   -0.027376    0.045169
 H    2.597061    1.082407   -2.068948
 C    3.034990    0.788202    0.049573
 H    4.301435    1.400842   -1.634829
 O    1.677868    1.040108    0.438088
 C    3.260011    1.490169   -1.291420
 H    5.023511    1.114048    0.867358
 H    3.740760    0.997181    2.103774
 C    3.976365    1.366007    1.096660
 H    3.026918    2.559483   -1.177997
 H    3.888770    2.463056    1.112142
Cu   -1.167130   -0.038843    0.055765
59
Figure 3_para-NMe2_pc1 / electronic energy: -2955.28953194 a.u. / lowest freq: 19.21 cm-1
 H    1.479945    1.524019    2.416808
 H   -1.037372    0.078138    2.232063
 C    1.037927    2.401492    1.921216
 C   -1.464579    1.017236    1.849373
 H    0.630269    3.081742    2.685511
 H    1.837329    2.915703    1.366610
 H   -1.734189    1.664685    2.698543
 H   -2.371929    0.772811    1.277064
 P   -0.248151    1.831167    0.750060
 C   -1.096501    3.384165    0.279014
 H   -1.409974    3.961652    1.162876
 H   -0.421529    4.001504   -0.332996
 H   -1.984445    3.142302   -0.323958
 H   -3.394859   -2.638351    0.356341
 C   -4.569333   -0.846937   -0.044354
 C   -3.420857   -1.668054   -0.139260
 H   -5.355066    1.092653   -0.656446
 C   -4.509282    0.406404   -0.696065
 H    4.261498   -3.279540    1.638543
 C   -2.299837   -1.264325   -0.854550
 H    3.430978   -1.335262    2.889521
 H   -1.436323   -1.934741   -0.882265
 C   -3.378399    0.791731   -1.407625
 C   -2.242219   -0.023480   -1.509280
 C    4.754008   -2.656479    0.876641
 C    4.066112   -0.693426    2.260617
 H    4.655618   -3.168086   -0.089963
 O    2.762241   -1.384597    0.385961
 H   -3.379009    1.768564   -1.900518
 H    5.062930   -0.637704    2.722891
 H    5.823130   -2.590521    1.131955
 C    4.116457   -1.275485    0.846396
 C   -1.049060    0.455018   -2.236224
 B    2.428691   -0.249076   -0.353412
 H   -0.039005   -1.433981   -2.600099
 C   -0.008457   -0.343896   -2.689857
 C    4.738242   -0.285225   -0.194138
 H    4.541799   -1.691186   -1.854603
 O    3.594775    0.479409   -0.596766
 H    6.209829   -1.540389   -1.231647
 H    6.650529    0.086715    0.772743
 C    5.280425   -0.989167   -1.439808
 H    0.693637    0.047576   -3.431383
 C    5.797197    0.652823    0.368021
 H    5.495739   -0.234083   -2.210667
 H    6.175966    1.309209   -0.430153
Cu    0.564609    0.432684   -0.872031
 H   -1.120368    1.479864   -2.619018
 H    3.626123    0.315071    2.254665
 H    5.393711    1.293572    1.163244
 H   -6.448188    0.573165    1.462320
 H   -7.190130    0.054371   -0.075448
 C   -6.764255   -0.309956    0.874159
 H   -7.573229   -0.808609    1.421989
 N   -5.689222   -1.247912    0.652312
 H   -5.427562   -3.341983    0.802712
 H   -6.626579   -2.629767    1.896388
 C   -5.647095   -2.463086    1.431529
 H   -4.888662   -2.428297    2.236860
59
Figure 3_para-NMe2_ts(CuBadd) / electronic energy: -2955.27152489 a.u. / lowest freq: -202.76 cm-1
 H    1.379351    1.949989    2.490398
 H   -1.430913    1.366103    1.951738
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 C    1.269210    2.903932    1.953962
 C   -1.500094    2.335546    1.436778
 H    0.938852    3.682529    2.659076
 H    2.249679    3.181522    1.539116
 H   -1.741145    3.120951    2.169704
 H   -2.306245    2.267261    0.691241
 P    0.080343    2.678391    0.584653
 C   -0.132032    4.366707   -0.078181
 H   -0.407187    5.075884    0.717447
 H    0.805007    4.697384   -0.550409
 H   -0.919764    4.354976   -0.845710
 H   -2.759219   -2.008469    1.373097
 C   -4.181310   -1.002820    0.072752
 C   -2.894627   -1.419446    0.465141
 H   -5.223718    0.070485   -1.510734
 C   -4.258130   -0.266061   -1.130753
 H    2.833084   -3.125120    2.307532
 C   -1.759021   -1.094924   -0.277803
 H    2.868098   -0.760419    2.951793
 H   -0.790319   -1.440957    0.095428
 C   -3.120616    0.052249   -1.863647
 C   -1.822430   -0.337635   -1.468295
 C    3.431156   -2.953968    1.400040
 C    3.624715   -0.585327    2.172483
 H    3.059957   -3.629630    0.618429
 O    1.983740   -1.218517    0.555368
 H   -3.240964    0.629087   -2.786338
 H    4.615378   -0.786466    2.605647
 H    4.475124   -3.219020    1.627489
 C    3.327855   -1.496275    0.980761
 C   -0.634354    0.063738   -2.216926
 B    2.037706   -0.277016   -0.458753
 H    0.646096   -1.602550   -1.576141
 C    0.666330   -0.572442   -1.964712
 C    4.159085   -1.120214   -0.295261
 H    3.283978   -2.718875   -1.501182
 O    3.333815   -0.107193   -0.901567
 H    4.942696   -3.059733   -0.937003
 H    6.152686   -1.257500    0.550525
 C    4.267230   -2.269638   -1.296082
 H    1.384099   -0.479021   -2.788907
 C    5.535346   -0.540202   -0.011732
 H    4.667238   -1.881354   -2.244550
 H    6.050180   -0.319743   -0.958777
Cu    0.518516    1.042817   -0.827335
 H   -0.794300    0.534676   -3.191331
 H    3.576669    0.476207    1.886864
 H    5.471428    0.393037    0.563097
 H   -6.789045   -0.043063   -0.014960
 H   -6.765054   -1.688905   -0.702616
 C   -6.615141   -1.104170    0.227662
 H   -7.393636   -1.401322    0.942236
 N   -5.317031   -1.305182    0.824758
 H   -4.882604   -3.286425    1.501859
 H   -6.176820   -2.411618    2.366136
 C   -5.204098   -2.291273    1.871694
 H   -4.484983   -1.977088    2.645490
59
Figure 3_para-NMe2_L-Cu-alkyl_01 / electronic energy: -2955.32654850 a.u. / lowest freq: 24.87 cm-1
 H    1.025355    2.129053    2.738448
 H   -0.154850    4.214965    0.990474
 C    1.985960    2.412384    2.283806
 C    0.839478    4.373621    0.546637
 H    2.394254    3.286185    2.814829
 H    2.684432    1.570807    2.397805
 H    1.380425    5.132318    1.133205
 H    0.700335    4.741894   -0.480652
 P    1.743742    2.783581    0.508084
 C    3.420166    3.267906   -0.042717
 H    3.850765    4.037626    0.616413
 H    4.077217    2.385249   -0.045776
 H    3.367653    3.658059   -1.070132
 H   -3.474573   -2.137388    0.848134
 C   -4.255634   -0.229180    0.160886
 C   -3.282987   -1.242441    0.254724
 H   -4.632870    1.695863   -0.784424
 C   -3.922591    0.879338   -0.648354
 H    1.146242   -3.880569    2.138805
 C   -2.055448   -1.146414   -0.404920
 H    0.409925   -1.557355    2.186927
 H   -1.338177   -1.959663   -0.275899
 C   -2.695462    0.959543   -1.297789
 C   -1.709151   -0.043685   -1.206478
 C    2.072610   -3.641926    1.595426
 C    1.379547   -1.245932    1.771908
 H    2.293727   -4.479430    0.920928
 O    0.901021   -2.512557   -0.184005
 H   -2.492937    1.842950   -1.913462
 H    2.069690   -1.059882    2.607296
 H    2.885873   -3.559127    2.332388
 C    1.897800   -2.337298    0.835533
 C   -0.404681    0.097085   -1.923641
 B    1.246354   -1.718188   -1.252222
 H   -0.484090   -2.004186   -2.636649
 C    0.266385   -1.233359   -2.370339
 C    3.153323   -1.884405   -0.003125
 H    3.408909   -3.826395   -0.966924
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 O     2.552303   -1.298846   -1.167639
 H     4.557360   -3.518389    0.365464
 H     4.394153   -1.184900    1.643407
 C     4.015467   -3.054119   -0.471201
 H     0.857015   -1.037877   -3.280957
 C     4.014743   -0.829159    0.673633
 H     4.754623   -2.687091   -1.198488
 H     4.878831   -0.586511    0.037168
Cu     0.701465    1.259066   -0.749843
 H    -0.595387    0.709957   -2.823593
 H     1.221034   -0.302701    1.224252
 H     3.442334    0.094194    0.830348
 H    -6.276387    1.631683    0.573284
 H    -6.824370    0.454207   -0.650103
 C    -6.543940    0.574555    0.416193
 H    -7.436468    0.376867    1.024218
 N    -5.479972   -0.310741    0.827514
 H    -5.961427   -2.387723    0.643811
 H    -6.835802   -1.470281    1.901767
 C    -5.866554   -1.579152    1.397448
 H    -5.144178   -1.915863    2.157745
59
Figure 3_para-NMe2_L-Cu-alkyl_02 / electronic energy: -2955.32118714 a.u. / lowest freq: 17.17 cm-1
 H     6.279836    1.111865    1.565747
 H     6.896257    0.453534   -1.025047
 H     6.895033   -1.487176    0.935342
 C     5.201086    0.954773    1.411500
 H     4.737990    1.901681    1.096226
 H     4.739597    0.650845    2.362847
 C     5.845718    0.261344   -1.293054
 C     5.845057   -1.758078    0.744255
 H     5.396395    1.187440   -1.681480
 H     5.395646   -2.140256    1.672891
 H     5.809574   -0.496998   -2.089362
 H     5.810592   -2.559755   -0.008470
 P     4.879049   -0.324634    0.145448
Cu     2.717358   -0.689413   -0.249491
 C     0.790672   -0.947399   -0.583619
 H     0.450572   -2.093831    1.292207
 H    -0.247205    0.125546    1.756966
 C     0.128194    0.377017   -0.359194
 C    -0.353691    0.790119    0.895663
 H     0.268798    1.033422   -2.411235
 C    -0.070821    1.298276   -1.403996
 C    -0.996422    2.011775    1.094900
 C    -0.703252    2.525392   -1.225980
 H    -1.354874    2.245897    2.098035
 H    -0.830993    3.171628   -2.095345
 C    -1.185568    2.926162    0.039069
 H     0.664722   -1.189511   -1.654896
 C     0.146127   -2.105102    0.231110
 H     0.516780   -3.067767   -0.164172
 B    -1.423337   -2.057542    0.139669
 O    -2.260590   -1.904893    1.216053
 H    -2.837431    0.414279   -0.493044
 O    -2.115944   -2.094899   -1.045610
 H    -3.975157    0.079612    1.449045
 H    -3.213501   -0.027499   -2.171597
 C    -3.521546   -0.170051   -1.125512
 C    -3.619934   -1.952875    0.752260
 H    -4.495541   -1.193893    2.574089
 C    -3.461169   -1.660495   -0.788929
 C    -4.434248   -0.915796    1.511229
 H    -4.046601   -3.553882    2.126595
 H    -3.574067   -4.124104    0.510263
 H    -4.538718    0.231850   -1.008764
 C    -4.147730   -3.355381    1.049264
 H    -5.459551   -0.857125    1.115484
 C    -4.413774   -2.437566   -1.684192
 H    -4.225938   -2.180580   -2.737336
 H    -4.282227   -3.521924   -1.574244
 H    -5.209080   -3.458068    0.780443
 H    -5.460320   -2.185984   -1.454530
 N    -1.817115    4.152157    0.231919
 C    -2.218912    4.915673   -0.924445
 H    -2.692601    5.850363   -0.597330
 H    -2.938601    4.377191   -1.573998
 H    -1.352663    5.193440   -1.546988
 C    -2.518933    4.379665    1.471554
 H    -1.836435    4.337150    2.336078
 H    -3.332878    3.647980    1.652137
 H    -2.962872    5.383359    1.460354
59
Figure 3_para-NMe2_L-Cu-alkyl_03 / electronic energy: -2955.32513805 a.u. / lowest freq: 19.52 cm-1
 H     3.008334    3.362081   -0.231745
 H     1.574743    3.186573    2.322982
 C     2.102075    3.773477   -0.699135
 C     0.728485    3.671462    1.813827
 H     2.114623    4.869844   -0.597693
 H     2.114120    3.509798   -1.767199
 H     0.866228    4.763407    1.843133
 H    -0.192008    3.406020    2.354879
 P     0.616283    3.058621    0.094084
 C    -0.746809    4.052543   -0.614626
 H    -0.584790    5.130692   -0.461337
 H    -0.826484    3.847748   -1.692754
 H    -1.694576    3.755113   -0.141685
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 B    1.905018   -1.798342    0.313934
 O    2.731727   -1.205432    1.239464
 O    2.572279   -2.099570   -0.847240
 C    3.948740   -0.838511    0.569297
 C    3.970899   -1.836060   -0.646851
 C    5.116706   -0.977462    1.532054
 C    3.793354    0.619475    0.137974
 C    4.640175   -3.168402   -0.312940
 C    4.558092   -1.262106   -1.927266
 H    4.237714   -3.598616    0.616309
 H    5.729070   -3.060458   -0.204916
 H    4.444576   -3.881889   -1.126920
 H    3.988134   -0.393137   -2.281406
 H    4.538857   -2.024915   -2.719705
 H    5.604715   -0.958554   -1.773301
 H    2.955371    0.737185   -0.566862
 H    4.707781    1.010638   -0.331020
 H    3.572570    1.228429    1.027446
 H    6.071516   -0.801063    1.013880
 H    5.148176   -1.972925    1.993906
 H    5.026487   -0.233190    2.337431
 C   -2.667882   -0.399226   -1.225528
 C   -4.051493   -0.319400   -1.127819
 C   -1.856014   -0.978703   -0.227940
 C   -4.738745   -0.809566    0.006231
 C   -2.554081   -1.492904    0.876812
 C   -3.944650   -1.414427    0.997810
 C   -0.366742   -1.004546   -0.368971
 C    0.371801   -2.016207    0.529139
 H   -4.404879   -1.843308    1.888725
 H   -2.002866   -1.980427    1.684853
 H   -4.600779    0.138156   -1.951534
 H   -2.188047    0.009847   -2.121639
Cu    0.238652    0.871344   -0.128701
 H    0.064603   -3.064174    0.326465
 H    0.156858   -1.829527    1.595055
 H   -0.130993   -1.237510   -1.424729
 H   -6.615088    0.605983   -1.459406
 H   -6.801653   -1.125312   -1.851172
 C   -6.899515   -0.373094   -1.042083
 H   -7.961192   -0.307195   -0.769969
 N   -6.122967   -0.695888    0.131290
 H   -6.651109   -2.528553    1.099559
 H   -7.857720   -1.214696    1.162154
 C   -6.781468   -1.430365    1.184310
 H   -6.411377   -1.127266    2.177019
59
Figure 3_para-NMe2_ts(BHE) / electronic energy: -2955.27529180 a.u. / lowest freq: -965.54 cm-1
 H    0.891234   -4.295333    1.979147
 H    2.931756   -2.320334    1.177043
 C    0.705113   -4.477442    0.910384
 C    2.690426   -2.554243    0.129560
 H    1.403246   -5.247391    0.546537
 H   -0.326810   -4.842515    0.798744
 H    3.299972   -3.410442   -0.198976
 H    2.936340   -1.672862   -0.482393
 P    0.902710   -2.913196   -0.015411
 C    0.709021   -3.429490   -1.758689
 H    1.382591   -4.262220   -2.013712
 H   -0.332424   -3.735799   -1.937349
 H    0.928363   -2.568274   -2.407179
 B   -2.473215    0.904149    0.317067
 O   -3.402364    1.481001    1.137643
 O   -3.024796    0.363998   -0.812426
 C   -4.703719    1.090114    0.654197
 C   -4.408928    0.762442   -0.856144
 C   -5.686044    2.227747    0.875854
 C   -5.123593   -0.139159    1.458340
 C   -4.491780    1.989639   -1.761359
 C   -5.237796   -0.373628   -1.432441
 H   -3.916847    2.832665   -1.350372
 H   -5.531680    2.314660   -1.908995
 H   -4.067025    1.737639   -2.744043
 H   -5.054911   -1.318804   -0.904851
 H   -4.983579   -0.522624   -2.492365
 H   -6.311491   -0.139716   -1.371529
 H   -4.426553   -0.976515    1.302981
 H   -6.136874   -0.472026    1.191462
 H   -5.115129    0.112303    2.529104
 H   -6.659770    1.990822    0.421415
 H   -5.319596    3.170030    0.447765
 H   -5.843078    2.382786    1.953459
 C    2.273228    1.145272   -1.418655
 C    3.644974    1.340965   -1.307433
 C    1.424857    1.015575   -0.297253
 C    4.281542    1.418713   -0.048400
 C    2.067973    1.115650    0.954954
 C    3.443173    1.314567    1.078754
 C   -0.002623    0.750968   -0.452051
 C   -0.949106    0.828348    0.648100
 H    3.862083    1.384695    2.083402
 H    1.481300    1.027869    1.874063
 H    4.225192    1.435472   -2.226154
 H    1.835004    1.084740   -2.420046
Cu   -0.237320   -1.096393    0.462868
 H   -0.659516    1.432901    1.518824
 H   -1.189828   -0.376521    1.566431
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 H   -0.399870    0.722079   -1.470993
 H    6.347386    1.186073   -1.888102
 H    6.088632    2.918485   -1.550652
 C    6.415668    1.957756   -1.103647
 H    7.476812    2.053132   -0.839179
 N    5.660033    1.589770    0.068717
 H    5.815809    2.874549    1.771183
 H    7.299726    2.015026    1.278660
 C    6.209020    1.922346    1.360010
 H    6.005854    1.132809    2.102082
59
Figure 3_para-NMe2_pc2 / electronic energy: -2955.31547918 a.u. / lowest freq: 26.79 cm-1
 H    0.405099   -4.327440    1.537649
 H    2.703392   -2.449207    1.432521
 C    0.308557   -4.232430    0.445796
 C    2.564980   -2.467706    0.341240
 H    0.937700   -4.992717   -0.042657
 H   -0.745609   -4.408251    0.183818
 H    3.094041   -3.338571   -0.076391
 H    2.999243   -1.547397   -0.076560
 P    0.778518   -2.535450   -0.049426
 C    0.764547   -2.621663   -1.877589
 H    1.369819   -3.462954   -2.249643
 H   -0.271391   -2.739264   -2.229901
 H    1.164234   -1.683918   -2.291185
 B   -2.396279    1.005701    0.214685
 O   -3.374706    1.532315    1.015464
 O   -2.905922    0.369654   -0.891311
 C   -4.634892    1.004899    0.559248
 C   -4.318193    0.638392   -0.938446
 C   -5.713496    2.060715    0.738178
 C   -4.943655   -0.219621    1.418132
 C   -4.521719    1.809690   -1.898341
 C   -5.043649   -0.593540   -1.455240
 H   -4.026661    2.721634   -1.532886
 H   -5.588690    2.027847   -2.050575
 H   -4.081127    1.553144   -2.872974
 H   -4.775494   -1.491742   -0.883634
 H   -4.779446   -0.769513   -2.508709
 H   -6.133569   -0.452230   -1.399096
 H   -4.166502   -0.991115    1.310159
 H   -5.919145   -0.658855    1.165075
 H   -4.966298    0.081839    2.475738
 H   -6.666192    1.715984    0.308276
 H   -5.437581    3.010924    0.262460
 H   -5.874542    2.251681    1.809445
 C    2.358796    0.861640   -1.412297
 C    3.738253    1.013833   -1.335234
 C    1.537140    0.911887   -0.278216
 C    4.378756    1.225721   -0.090817
 C    2.173578    1.115353    0.957017
 C    3.549095    1.266048    1.057709
 C    0.081297    0.707809   -0.404475
 C   -0.880019    1.125988    0.505270
 H    3.983640    1.412517    2.046180
 H    1.580505    1.137672    1.875512
 H    4.317726    0.970819   -2.257218
 H    1.902656    0.701783   -2.393844
Cu   -0.493057   -0.879058    0.897437
 H   -0.562997    1.674850    1.399865
 H   -1.326090   -1.285159    2.199561
 H   -0.255440    0.378640   -1.395612
 H    6.477470    0.384200   -1.719695
 H    6.267480    2.145812   -1.909005
 C    6.550206    1.352799   -1.193768
 H    7.601959    1.507332   -0.925647
 N    5.739220    1.383111    0.000995
 H    5.982064    2.540799    1.764549
 H    7.439348    1.727468    1.153921
 C    6.356324    1.618306    1.285857
 H    6.187716    0.783050    1.988448
59
Figure 3_para-NMe2_ts(H>B) / electronic energy: -2955.30163554 a.u. / lowest freq: -466.10 cm-1
 H    0.354752    4.505612   -1.535751
 H    2.408665    2.324712   -1.728123
 C    0.445977    4.444191   -0.440990
 C    2.457691    2.412583   -0.632548
 H    1.245693    5.122696   -0.105713
 H   -0.510309    4.764923   -0.001364
 H    3.143638    3.231741   -0.366170
 H    2.851656    1.468095   -0.228685
 P    0.782735    2.712746    0.041083
 C    1.086240    2.827651    1.840544
 H    1.859695    3.576923    2.070050
 H    0.153807    3.101134    2.356454
 H    1.413597    1.846278    2.215217
 B   -2.377181   -0.589122   -0.406342
 O   -3.349495   -1.142288   -1.257030
 O   -2.916631   -0.412099    0.887348
 C   -4.616637   -0.960588   -0.629175
 C   -4.230998   -0.963108    0.896868
 C   -5.542344   -2.094558   -1.048291
 C   -5.205814    0.376494   -1.085873
 C   -4.132531   -2.377746    1.474312
 C   -5.132291   -0.108351    1.777286
 H   -3.506838   -3.022401    0.838899
 H   -5.119420   -2.850498    1.590620
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 H   -3.659340   -2.322394    2.466239
 H   -5.095325    0.949644    1.485199
 H   -4.806869   -0.179583    2.826557
 H   -6.176980   -0.452361    1.723471
 H   -4.574624    1.220783   -0.774935
 H   -6.220654    0.531187   -0.690207
 H   -5.260645    0.384722   -2.185072
 H   -6.493875   -2.051515   -0.495928
 H   -5.081203   -3.076714   -0.879224
 H   -5.769949   -2.010976   -2.122015
 C    2.384722   -0.964350    1.347285
 C    3.765292   -1.109959    1.271985
 C    1.561988   -1.014838    0.213580
 C    4.406566   -1.322718    0.028884
 C    2.200596   -1.216300   -1.019884
 C    3.576326   -1.366597   -1.119622
 C    0.108123   -0.812561    0.356134
 C   -0.855859   -0.970380   -0.601131
 H    4.011572   -1.517341   -2.107271
 H    1.610549   -1.243481   -1.939716
 H    4.343732   -1.063937    2.194505
 H    1.927210   -0.806565    2.328824
Cu   -0.746881    1.159372   -0.505836
 H   -0.539602   -1.257218   -1.614651
 H   -2.268724    1.048273   -1.040417
 H   -0.221163   -0.606293    1.383972
 H    6.292505   -2.250720    1.846150
 H    7.628671   -1.607793    0.867426
 C    6.576297   -1.454967    1.134146
 H    6.502337   -0.488523    1.663649
 N    5.767508   -1.480029   -0.062219
 H    7.466999   -1.840342   -1.210939
 H    6.008396   -2.657444   -1.813514
 C    6.384158   -1.730575   -1.344168
 H    6.217920   -0.902613   -2.055878
59
Figure 3_para-NMe2_int1 / electronic energy: -2955.30314274 a.u. / lowest freq: 19.51 cm-1
 H    0.394133    4.553647   -1.642897
 H    2.334127    2.252253   -1.771313
 C    0.547199    4.568904   -0.553445
 C    2.449973    2.421374   -0.690589
 H    1.397435    5.226700   -0.314712
 H   -0.364617    4.970220   -0.086627
 H    3.194489    3.215587   -0.525164
 H    2.810408    1.487286   -0.233438
 P    0.833863    2.864703    0.043141
 C    1.237191    3.093067    1.811884
 H    2.063770    3.807775    1.946519
 H    0.349270    3.459691    2.347847
 H    1.524508    2.122623    2.243431
 B   -2.408544   -0.307190   -0.353943
 O   -3.350460   -0.825480   -1.311028
 O   -2.992234   -0.460699    0.961401
 C   -4.606220   -0.904736   -0.663461
 C   -4.190062   -1.203153    0.823632
 C   -5.436841   -1.999193   -1.322088
 C   -5.332193    0.439364   -0.800631
 C   -3.869157   -2.686452    1.042464
 C   -5.197577   -0.738169    1.868423
 H   -3.178616   -3.056258    0.269773
 H   -4.771107   -3.317939    1.039653
 H   -3.373912   -2.802253    2.018603
 H   -5.343631    0.349887    1.829723
 H   -4.835902   -0.991395    2.877261
 H   -6.173842   -1.228728    1.727492
 H   -4.785895    1.245629   -0.289045
 H   -6.354229    0.400617   -0.394087
 H   -5.398333    0.700313   -1.868078
 H   -6.378942   -2.169048   -0.777389
 H   -4.883350   -2.946574   -1.372655
 H   -5.690885   -1.706772   -2.352976
 C    2.358748   -1.037972    1.348484
 C    3.734004   -1.219327    1.253403
 C    1.519178   -1.057777    0.226120
 C    4.352590   -1.439738    0.000350
 C    2.135923   -1.272153   -1.016436
 C    3.505551   -1.457424   -1.136388
 C    0.074735   -0.801333    0.387457
 C   -0.891589   -0.808490   -0.570896
 H    3.923129   -1.617738   -2.130231
 H    1.533099   -1.284893   -1.928222
 H    4.326495   -1.194313    2.167883
 H    1.919121   -0.872691    2.336998
Cu   -0.752930    1.328292   -0.296610
 H   -0.581212   -1.026874   -1.604702
 H   -2.372912    1.100632   -0.581703
 H   -0.238310   -0.633643    1.428224
 H    6.244471   -2.418747    1.784733
 H    7.579679   -1.803459    0.787747
 C    6.535540   -1.626724    1.071681
 H    6.493201   -0.661260    1.606544
 N    5.707850   -1.628280   -0.111893
 H    7.384055   -2.000114   -1.290911
 H    5.904012   -2.786252   -1.881770
 C    6.301248   -1.871674   -1.406195
 H    6.137183   -1.031937   -2.104555
59
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Figure 3_para-NMe2_ts(Cu>O) / electronic energy: -2955.29561577 a.u. / lowest freq: -37.84 cm-1
 H    -1.029215    4.835624   -1.303232
 H     1.219430    3.020538   -1.834503
 C    -0.850533    4.686205   -0.228053
 C     1.347714    2.903216   -0.748319
 H    -0.103239    5.415969    0.119802
 H    -1.798639    4.856338    0.303301
 H     2.019778    3.690844   -0.373964
 H     1.802991    1.918119   -0.563192
 P    -0.287706    2.972971    0.065369
 C     0.127812    2.960302    1.845301
 H     0.827982    3.770900    2.099670
 H    -0.792555    3.073271    2.437043
 H     0.585970    1.993358    2.101336
 B    -1.988916   -0.914376   -0.816358
 O    -2.949409   -1.899656   -1.208858
 O    -2.357125   -0.495792    0.550574
 C    -4.119576   -1.685444   -0.436313
 C    -3.535661   -1.188463    0.939663
 C    -4.900320   -2.990801   -0.345913
 C    -4.991411   -0.621106   -1.115570
 C    -3.103206   -2.349557    1.838531
 C    -4.448113   -0.246578    1.714270
 H    -2.458767   -3.049293    1.286640
 H    -3.961435   -2.903900    2.247586
 H    -2.522276   -1.949280    2.683286
 H    -4.641421    0.677744    1.152659
 H    -3.973822    0.033633    2.667489
 H    -5.412902   -0.725052    1.944521
 H    -4.490811    0.357026   -1.145639
 H    -5.960650   -0.499641   -0.609417
 H    -5.182812   -0.930727   -2.154257
 H    -5.734414   -2.904643    0.367911
 H    -4.254100   -3.821248   -0.031558
 H    -5.321083   -3.246022   -1.330510
 C     2.641910   -0.988802    1.205205
 C     4.031664   -0.967395    1.237951
 C     1.916841   -1.051380    0.005725
 C     4.787112   -1.003139    0.042642
 C     2.670859   -1.080670   -1.178998
 C     4.058886   -1.057491   -1.171737
 C     0.443855   -1.038986    0.037134
 C    -0.421334   -1.198471   -0.983558
 H     4.583585   -1.079343   -2.126800
 H     2.159233   -1.113103   -2.144569
 H     4.529254   -0.920085    2.206305
 H     2.096035   -0.955888    2.153364
Cu    -1.568217    1.292162   -0.574381
 H    -0.016498   -1.386536   -1.989079
 H    -2.207413    0.188195   -1.656781
 H     0.012041   -0.851350    1.029208
 H     6.674422   -0.154010   -1.832486
 H     7.972288   -1.012088   -0.972864
 C     6.896657   -1.022198   -1.186080
 H     6.681251   -1.936891   -1.766731
 H     6.622531   -0.007148    1.886070
 N     6.160990   -0.980814    0.055886
 H     7.949340   -0.905879    1.121113
 C     6.869666   -0.918582    1.312289
 H     6.652783   -1.789504    1.956642
59
Figure 3_para-NMe2_int2 / electronic energy: -2955.30214865 a.u. / lowest freq: 23.78 cm-1
 H     4.284078   -3.066870   -2.250525
 H     2.663405   -4.293477   -0.129878
 C     4.959166   -2.677467   -1.474152
 C     3.389322   -3.895132    0.594460
 H     5.733716   -3.428252   -1.253798
 H     5.437645   -1.765675   -1.861647
 H     4.218464   -4.610393    0.708501
 H     2.878004   -3.774897    1.561124
 P     3.989146   -2.267813    0.019481
 C     5.275677   -1.830951    1.244152
 H     6.022755   -2.633850    1.342494
 H     5.781697   -0.906588    0.927786
 H     4.805203   -1.651080    2.222136
 B     0.780740    0.869769   -0.856132
 O     1.237287    2.157874   -1.331484
 O     1.297807    0.773480    0.551766
 C     2.236785    2.657663   -0.470388
 C     1.840924    2.039166    0.921631
 C     2.202387    4.181801   -0.499289
 C     3.616773    2.184206   -0.949854
 C     0.733312    2.832598    1.617038
 C     3.005331    1.823080    1.877909
 H    -0.104411    3.024622    0.931272
 H     1.098552    3.794540    2.007096
 H     0.351203    2.245048    2.465229
 H     3.738287    1.115809    1.462754
 H     2.639263    1.405107    2.828307
 H     3.518083    2.771951    2.098025
 H     3.732131    1.089267   -0.877807
 H     4.435392    2.645936   -0.377539
 H     3.737246    2.456376   -2.008899
 H     2.883821    4.611492    0.251805
 H     1.188563    4.560798   -0.314376
 H     2.519313    4.543729   -1.489447
 C    -3.737418   -0.249673    1.174755
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 C   -5.105534   -0.496876    1.215393
 C   -3.055695    0.027500   -0.019377
 C   -5.882148   -0.480641    0.033981
 C   -3.831323    0.039856   -1.190369
 C   -5.198155   -0.204331   -1.175431
 C   -1.602447    0.285642    0.005885
 C   -0.792532    0.618628   -1.013506
 H   -5.739512   -0.181263   -2.121396
 H   -3.354193    0.244169   -2.152621
 H   -5.570104   -0.701734    2.179849
 H   -3.175289   -0.270372    2.113824
Cu    2.407772   -0.765086   -0.290416
 H   -1.232629    0.718891   -2.017494
 H    1.371810   -0.120877   -1.544512
 H   -1.145030    0.193622    1.000527
 H   -7.645478   -1.460290   -1.894295
 H   -9.048355   -0.905437   -0.955853
 C   -7.993585   -0.698778   -1.173168
 H   -7.942409    0.283978   -1.674884
 H   -7.494012   -1.930097    1.782685
 N   -7.236074   -0.721431    0.055712
 H   -8.964637   -1.183623    1.121779
 C   -7.895990   -1.018453    1.304517
 H   -7.806208   -0.192542    2.032922
59
Figure 3_para-NMe2_ts(C-Brot) / electronic energy: -2955.29669845 a.u. / lowest freq: -78.52 cm-1
 H    4.120289   -3.689341   -1.650676
 H    3.056738   -4.069270    1.075326
 C    4.912793   -3.071486   -1.203206
 C    3.863309   -3.418231    1.443588
 H    5.742108   -3.720666   -0.882257
 H    5.275566   -2.371401   -1.970478
 H    4.754946   -4.029058    1.653261
 H    3.522133   -2.942270    2.374853
 P    4.223751   -2.126633    0.201646
 C    5.690329   -1.279712    0.894647
 H    6.502734   -1.994921    1.097676
 H    6.049951   -0.522165    0.182351
 H    5.414159   -0.773024    1.831169
 B    0.722961    0.635462   -0.771885
 O    0.908199    1.943285   -1.348472
 O    1.379842    0.732439    0.584458
 C    1.990918    2.590390   -0.715613
 C    1.904962    2.046865    0.760981
 C    1.802935    4.099108   -0.833635
 C    3.303916    2.203604   -1.412239
 C    0.910992    2.834864    1.614587
 C    3.243017    1.958320    1.484242
 H   -0.047312    2.959712    1.091240
 H    1.295270    3.831189    1.879588
 H    0.719713    2.281798    2.546280
 H    3.939889    1.290033    0.958103
 H    3.095042    1.555349    2.498187
 H    3.713101    2.949582    1.577020
 H    3.525303    1.128238   -1.317806
 H    4.164223    2.762052   -1.014523
 H    3.211901    2.424930   -2.485956
 H    2.563819    4.644047   -0.253251
 H    0.807576    4.407993   -0.488074
 H    1.899306    4.402568   -1.887313
 C   -4.173133    0.995042    0.605257
 C   -5.514140    0.635744    0.687606
 C   -3.224502    0.218621   -0.076384
 C   -5.986697   -0.552714    0.084681
 C   -3.699254   -0.959913   -0.675030
 C   -5.032170   -1.340940   -0.604415
 C   -1.816840    0.659235   -0.137227
 C   -0.789597    0.077925   -0.779146
 H   -5.332795   -2.266558   -1.095128
 H   -3.007278   -1.606704   -1.220748
 H   -6.195710    1.289580    1.231561
 H   -3.850145    1.922682    1.087901
Cu    2.530641   -0.798620   -0.257003
 H   -1.004461   -0.845783   -1.337746
 H    1.424290   -0.281457   -1.473128
 H   -1.620373    1.582502    0.424372
 H   -7.239618   -3.013039   -0.194103
 H   -8.834550   -2.252445   -0.339510
 C   -7.765705   -2.105430   -0.536316
 H   -7.630012   -2.031187   -1.631463
 H   -8.046153    0.152640    1.830532
 N   -7.308762   -0.925258    0.159510
 H   -9.267485   -0.492634    0.717097
 C   -8.271455   -0.036597    0.766711
 H   -8.322885    0.942043    0.254478
59
Figure 3_para-NMe2_int3 / electronic energy: -2955.30153963 a.u. / lowest freq: 19.79 cm-1
 H    4.550200   -3.031514   -2.203556
 H    3.903556   -4.050734    0.483112
 C    5.278219   -2.349396   -1.740014
 C    4.667572   -3.361828    0.872892
 H    6.249562   -2.859947   -1.650760
 H    5.388819   -1.471261   -2.393330
 H    5.652134   -3.852490    0.829112
 H    4.422681   -3.133252    1.920813
 P    4.653856   -1.818320   -0.106056
 C    6.054411   -0.866803    0.585470
```

```
 H    6.989289   -1.447776    0.551780
 H    6.186850    0.062149    0.010920
 H    5.834721   -0.599693    1.629830
 B    0.655260    0.376145   -0.422724
 O    0.713706    1.665984   -1.068726
 O    1.470561    0.542443    0.839975
 C    1.683526    2.482411   -0.451091
 C    1.725949    1.932709    1.022993
 C    1.246366    3.939979   -0.552203
 C    3.025986    2.316740   -1.176610
 C    0.599992    2.500254    1.889576
 C    3.063942    2.107861    1.727616
 H   -0.371705    2.405002    1.384047
 H    0.767050    3.557930    2.141803
 H    0.549267    1.927165    2.827594
 H    3.865309    1.562804    1.207863
 H    3.002824    1.714487    2.754051
 H    3.343653    3.170915    1.787847
 H    3.432258    1.296411   -1.071053
 H    3.786751    3.023212   -0.812213
 H    2.870692    2.498313   -2.250392
 H    1.914103    4.598480    0.024998
 H    0.219048    4.074132   -0.187845
 H    1.274473    4.265426   -1.603433
 C   -4.381893    0.931180   -0.772669
 C   -5.727118    0.617435   -0.611888
 C   -3.351760    0.072125   -0.361546
 C   -6.122644   -0.602351   -0.016072
 C   -3.750149   -1.142188    0.221264
 C   -5.086549   -1.478031    0.392265
 C   -1.943612    0.474004   -0.545081
 C   -0.828261   -0.185376   -0.188907
 H   -5.325344   -2.437332    0.851554
 H   -2.993163   -1.856261    0.556378
 H   -6.473347    1.334509   -0.953966
 H   -4.120841    1.887531   -1.236393
Cu    2.724224   -0.769001   -0.148487
 H   -0.936903   -1.166435    0.299327
 H    1.287324   -0.561675   -1.139398
 H   -1.812010    1.450536   -1.030813
 H   -7.389397   -2.302356    1.771554
 H   -8.903716   -2.245707    0.847743
 C   -7.812315   -2.186356    0.758053
 H   -7.477639   -3.050353    0.154947
 H   -8.423807    0.960615    0.195160
 N   -7.447958   -0.923712    0.160705
 H   -9.461326   -0.453913   -0.087907
 C   -8.476280   -0.023327   -0.304021
 H   -8.418712    0.150505   -1.393878
44
Figure 3_para-NMe2-alkenylBpin / electronic energy: -853.456934437 a.u. / lowest freq: 23.23 cm-1
 B   -2.187170   -0.365211    0.009480
 O   -3.150062   -1.308190    0.256850
 O   -2.719971    0.871376   -0.253825
 C   -4.429772   -0.720739   -0.045141
 C   -4.122547    0.819094    0.064576
 C   -5.461729   -1.234491    0.945780
 C   -4.799537   -1.155667   -1.462554
 C   -4.280376    1.361085    1.484676
 C   -4.893795    1.689895   -0.914167
 H   -3.742396    0.739095    2.215571
 H   -5.337156    1.416990    1.783044
 H   -3.856508    2.375071    1.528609
 H   -4.661526    1.436198   -1.956775
 H   -4.636808    2.747934   -0.756642
 H   -5.977402    1.578257   -0.758380
 H   -4.071062   -0.786727   -2.199959
 H   -5.798937   -0.798203   -1.749417
 H   -4.801313   -2.254633   -1.510976
 H   -6.427272   -0.727499    0.798153
 H   -5.140704   -1.082014    1.984379
 H   -5.619453   -2.312545    0.794328
 C    2.524789    1.319156   -0.116960
 C    3.911059    1.255250   -0.091630
 C    1.719306    0.170822   -0.054482
 C    4.579018    0.009600   -0.003909
 C    2.385000   -1.064718    0.028476
 C    3.767329   -1.153399    0.052138
 C    0.259119    0.304712   -0.075142
 C   -0.668799   -0.668118    0.038170
 H    4.224495   -2.140270    0.117856
 H    1.807980   -1.991876    0.074166
 H    4.477072    2.184934   -0.144841
 H    2.045955    2.300298   -0.188373
 H   -0.341817   -1.706766    0.171089
 H   -0.096635    1.336458   -0.193713
 H    6.587387    1.699032   -0.957837
 H    6.513293    1.810645    0.822063
 C    6.741153    1.134989   -0.020836
 H    7.804145    0.873333    0.040392
 N    5.945699   -0.071055    0.023558
 H    6.334805   -1.911285    1.011367
 H    7.683963   -1.215909    0.088537
 C    6.597253   -1.359645    0.091378
 H    6.341286   -1.999507   -0.771386
59
Figure 3_para-NMe2_pc2_rev / electronic energy: -2955.31296303 a.u. / lowest freq: 21.29 cm-1
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 H   -0.783698    4.066132   -1.075681
 H    1.870100    3.574211   -2.230537
 C   -0.342588    3.934881   -0.076336
 C    2.248318    3.491723   -1.200670
 H    0.036425    4.903561    0.285749
 H   -1.135605    3.581582    0.600037
 H    2.489384    4.496460   -0.819951
 H    3.165753    2.885732   -1.220087
 P    0.982293    2.674483   -0.163804
 C    1.706941    2.728852    1.515391
 H    2.120011    3.721628    1.752315
 H    0.924409    2.482772    2.249346
 H    2.492039    1.963698    1.597529
 B    1.858086   -0.976205    0.479137
 O    2.852081   -0.462483    1.276217
 O    2.347444   -1.816214   -0.487549
 C    4.109751   -0.772323    0.643990
 C    3.742133   -2.039377   -0.209852
 C    5.164813   -1.003452    1.712340
 C    4.483544    0.430085   -0.221866
 C    3.842491   -3.341440    0.583216
 C    4.496223   -2.163938   -1.523349
 H    3.319257   -3.267528    1.548361
 H    4.889487   -3.617470    0.774202
 H    3.373408   -4.150670    0.004691
 H    4.295108   -1.314387   -2.188731
 H    4.185232   -3.081379   -2.044446
 H    5.580281   -2.225824   -1.344581
 H    3.725430    0.610570   -0.999468
 H    5.457803    0.290225   -0.711641
 H    4.547774    1.327521    0.411157
 H    6.110664   -1.332062    1.256087
 H    4.845753   -1.758101    2.442644
 H    5.356817   -0.065881    2.254835
 C   -2.947238   -1.767450   -0.814629
 C   -4.325510   -1.642926   -0.705981
 C   -2.065220   -0.989170   -0.051634
 C   -4.905403   -0.709133    0.186731
 C   -2.640273   -0.060543    0.830237
 C   -4.014903    0.082771    0.953572
 C   -0.607828   -1.141683   -0.217342
 C    0.357568   -0.631249    0.639947
 H   -4.398078    0.826375    1.652023
 H   -1.997660    0.587631    1.431961
 H   -4.955560   -2.277220   -1.328849
 H   -2.539463   -2.493064   -1.524378
Cu    0.108486    0.709906   -0.955726
 H    0.042635   -0.094870    1.542602
 H   -0.493394    0.820019   -2.438453
 H   -0.299213   -1.870662   -0.974409
 H   -7.004667   -2.455070   -0.347416
 H   -8.185060   -1.129603   -0.294539
 C   -7.141468   -1.373891   -0.525490
 H   -6.983019   -1.187397   -1.602816
 N   -6.266353   -0.574329    0.300451
 H   -6.527093    0.215843    2.252739
 H   -7.919818    0.354587    1.161267
 C   -6.825161    0.402407    1.205961
 H   -6.525245    1.434158    0.947957
59
Figure 3_para-NMe2_ts(CuHadd_rev) / electronic energy: -2955.28486892 a.u. / lowest freq: -860.20 cm-1
 H    0.069199    4.355812   -1.490584
 H    2.615737    3.132393   -2.278165
 C    0.426423    4.360776   -0.450260
 C    2.918488    3.178014   -1.221651
 H    0.987994    5.288581   -0.260340
 H   -0.451938    4.328277    0.211622
 H    3.365708    4.162372   -1.014714
 H    3.673149    2.397098   -1.046945
 P    1.459339    2.880075   -0.160961
 C    2.098543    3.144576    1.531195
 H    2.592056    4.123358    1.634452
 H    1.264080    3.080523    2.245489
 H    2.813851    2.345683    1.774622
 B    1.577937   -1.238966    0.435086
 O    2.476335   -1.380572    1.484755
 O    2.183233   -1.547462   -0.780985
 C    3.785123   -1.491770    0.915473
 C    3.479755   -2.087029   -0.506157
 C    4.651570   -2.371943    1.801898
 C    4.368436   -0.080048    0.838437
 C    3.353493   -3.610679   -0.493124
 C    4.445019   -1.651685   -1.598756
 H    2.677473   -3.948244    0.306676
 H    4.328286   -4.102230   -0.358288
 H    2.931868   -3.942365   -1.453606
 H    4.420282   -0.564028   -1.748864
 H    4.170998   -2.129061   -2.551504
 H    5.476420   -1.949288   -1.354737
 H    3.746498    0.559595    0.194083
 H    5.396849   -0.076304    0.449314
 H    4.381105    0.359850    1.846669
 H    5.634393   -2.545927    1.337607
 H    4.177375   -3.343370    1.994170
 H    4.817102   -1.879433    2.771929
 C   -3.104426   -1.532834   -1.027438
 C   -4.479411   -1.497480   -0.808304
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 C   -2.227831   -0.668707   -0.366887
 C   -5.050072   -0.574011    0.096833
 C   -2.792312    0.252543    0.523605
 C   -4.160429    0.308219    0.756864
 C   -0.750756   -0.742163   -0.592331
 C    0.136049   -0.792336    0.555451
 H   -4.538631    1.053185    1.456819
 H   -2.141099    0.960383    1.045812
 H   -5.110061   -2.201184   -1.351400
 H   -2.705518   -2.263613   -1.737288
Cu    0.395086    0.969944   -0.490844
 H   -0.289596   -0.550362    1.536131
 H   -0.666509    0.578832   -1.615521
 H   -0.477709   -1.394957   -1.428633
 H   -7.090801   -2.465753   -0.220881
 H   -8.327919   -1.193930   -0.133794
 C   -7.289076   -1.397173   -0.420187
 H   -7.207444   -1.239542   -1.510886
 N   -6.407021   -0.529295    0.322722
 H   -6.525140    0.297238    2.271287
 H   -8.035919    0.276236    1.341038
 C   -6.952027    0.422906    1.260565
 H   -6.776135    1.469779    0.951290
59
Figure 3_para-NMe2_L-Cu-alkyl_rev / electronic energy: -2955.33794627 a.u. / lowest freq: 25.95 cm-1
 H    2.037107    2.373024    1.544652
 H   -0.821333    2.875862    2.106699
 C    1.914582    2.885974    0.579498
 C   -0.842675    3.423713    1.152696
 H    2.099364    3.962679    0.717519
 H    2.653325    2.476142   -0.125170
 H   -0.514270    4.460859    1.322372
 H   -1.879985    3.431755    0.786054
 P    0.230408    2.575736   -0.063020
 C    0.132099    3.658399   -1.532754
 H    0.351564    4.707468   -1.280406
 H    0.851446    3.310057   -2.288940
 H   -0.876833    3.592250   -1.966765
 B   -2.145595   -1.248813   -0.377364
 O   -3.105541   -0.842229   -1.311215
 O   -2.713939   -1.288973    0.899523
 C   -4.175875   -0.237033   -0.588400
 C   -4.103992   -0.986010    0.792541
 C   -5.477570   -0.427663   -1.351392
 C   -3.857178    1.256141   -0.461471
 C   -4.873431   -2.307699    0.786137
 C   -4.525460   -0.144943    1.989906
 H   -4.603748   -2.921250   -0.086522
 H   -5.962352   -2.150632    0.780415
 H   -4.613507   -2.876633    1.691487
 H   -3.877038    0.733197    2.111126
 H   -4.456737   -0.742874    2.911390
 H   -5.566311    0.198611    1.885380
 H   -2.918303    1.408333    0.093380
 H   -4.660096    1.814668    0.041910
 H   -3.721482    1.679725   -1.468419
 H   -6.333484   -0.050276   -0.770972
 H   -5.654882   -1.484961   -1.588883
 H   -5.439614    0.128653   -2.300356
 C    2.543070   -2.420465   -0.703223
 C    3.859557   -1.966482   -0.761067
 C    1.635549   -1.959926    0.255072
 C    4.345896   -1.019831    0.167934
 C    2.119409   -1.019980    1.172654
 C    3.431668   -0.555170    1.141143
 C    0.178046   -2.368767    0.234247
 C   -0.685436   -1.504002   -0.690121
 H    3.745074    0.174962    1.887504
 H    1.443524   -0.629692    1.941100
 H    4.513476   -2.362601   -1.538272
 H    2.210389   -3.154120   -1.444573
Cu   -0.239372    0.427069   -0.416820
 H   -0.477155   -1.688256   -1.759564
 H   -0.219163   -2.309325    1.261221
 H    0.120196   -3.438079   -0.048486
 H    6.088902   -0.557469   -1.958194
 H    7.486105   -0.480676   -0.855503
 C    6.490998   -0.921987   -0.992922
 H    6.626737   -2.013150   -1.077860
 N    5.653455   -0.571724    0.129611
 H    5.515991    1.455673    0.785424
 H    7.130338    0.704754    0.852780
 C    6.059152    0.512376    0.991127
 H    5.907588    0.266162    2.055017
80
Figure 3_para-NMe2_pc3_01 / electronic energy: -3794.16568164 a.u. / lowest freq: 17.56 cm-1
 C   -0.013648   -1.135612   -1.049692
 C    0.215308   -1.906717    0.079903
 C    1.548480   -1.963161    0.761131
 O    2.419560   -2.940563    0.144736
 P    3.636826   -2.479819   -0.774461
 O    3.361741   -1.646398   -1.963195
 O    4.593530   -1.783397    0.319951
 O    4.319317   -3.869019   -1.156343
 C    5.736287   -1.046372   -0.099662
 H   -0.864586   -1.348730   -1.704314
 H    0.779417   -0.509864   -1.474939
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 H   -0.476221   -2.724085    0.316830
 H    2.040864   -0.981111    0.752130
 H    1.448350   -2.281967    1.806395
 B    0.288093    2.579913   -1.164736
 O    1.418844    2.135597   -1.804945
 O    0.589010    3.475825   -0.165257
 C    2.560203    2.576112   -1.050846
 C    1.982471    3.816957   -0.280207
 C    3.701705    2.884049   -2.005338
 C    2.943939    1.424694   -0.124302
 C    2.063301    5.111422   -1.088317
 C    2.571782    4.031017    1.104666
 H    1.656054    4.979030   -2.101881
 H    3.097797    5.474288   -1.173164
 H    1.467992    5.886584   -0.583624
 H    2.413035    3.163579    1.757697
 H    2.102078    4.904606    1.580846
 H    3.653522    4.222447    1.037088
 H    2.130779    1.208942    0.586444
 H    3.857568    1.642536    0.447954
 H    3.116309    0.527308   -0.735330
 H    4.563189    3.301563   -1.462348
 H    3.398979    3.596439   -2.783751
 H    4.027078    1.958028   -2.502186
 C   -4.082078    0.654234    0.486453
 C   -5.287722   -0.023324    0.325297
 C   -3.111766    0.755650   -0.531066
 C   -5.615008   -0.658218   -0.893335
 C   -3.460998    0.132898   -1.744999
 C   -4.661493   -0.552502   -1.927286
 C   -1.797248    1.418232   -0.292594
 C   -1.152138    2.081687   -1.518672
 H   -4.851752   -1.008385   -2.899898
 H   -2.767974    0.175842   -2.589154
 H   -5.985554   -0.047105    1.163555
 H   -3.885301    1.135870    1.448894
Cu   -0.766435   -0.120478    0.533552
 H   -1.773362    2.913917   -1.914734
 H   -1.042742    1.364167   -2.348718
 H   -1.923720    2.179472    0.497184
 H    6.113694   -0.504263    0.776389
 H    5.477445   -0.328906   -0.892022
 H    6.521757   -1.724244   -0.469335
 C    4.637475   -4.854088   -0.179302
 H    5.299464   -5.584157   -0.661527
 H    3.726622   -5.362147    0.169425
 H    5.159456   -4.408413    0.681268
 H    1.691176    0.578501    2.942724
 H    0.700501    2.044487    2.704040
 H    0.816431    1.296919    4.332029
 C    0.768560    1.092683    3.250968
 H    0.396529   -1.928933    3.694535
 P   -0.687919    0.071687    2.817199
 H   -0.507270   -1.078070    4.982688
 C   -0.527922   -1.379480    3.923813
 H   -2.197476    1.956871    3.071498
 H   -1.852076    1.195621    4.657763
 C   -2.059677    0.999083    3.594357
 H   -1.378191   -2.058504    3.759891
 H   -2.991748    0.420640    3.514159
 H   -6.313355   -2.795169   -2.534616
 H   -8.047166   -2.515299   -2.256165
 C   -7.069900   -2.019609   -2.309282
 H   -7.096611   -1.325449   -3.169290
 N   -6.809356   -1.338497   -1.066750
 H   -7.302095   -1.967179    0.904606
 H   -8.616643   -2.021320   -0.291428
 C   -7.737346   -1.448506    0.028998
 H   -8.095628   -0.461718    0.375557
80
Figure 3_para-NMe2_pc3_02 / electronic energy: -3794.16837386 a.u. / lowest freq: 22.64 cm-1
 C   -0.098724   -1.841118   -0.494157
 C    0.195694   -1.809351    0.864080
 C    1.582697   -1.508101    1.361985
 O    2.463462   -2.651475    1.263913
 P    3.164112   -2.992139   -0.131306
 O    3.428895   -1.860349   -1.044876
 O    4.435393   -3.784637    0.439112
 O    2.266293   -4.110528   -0.850686
 C    5.347456   -4.377694   -0.480096
 H   -0.995678   -2.348750   -0.861431
 H    0.678182   -1.658601   -1.242594
 H   -0.478849   -2.305108    1.571720
 H    2.038471   -0.674565    0.805777
 H    1.574012   -1.251815    2.428843
 B   -3.372385    0.748421   -1.149417
 O   -4.056350    0.805933    0.046223
 O   -3.703456   -0.371543   -1.869474
 C   -4.669573   -0.473574    0.267172
 C   -4.779907   -1.044898   -1.196404
 C   -5.999308   -0.278462    0.977402
 C   -3.713555   -1.275273    1.148676
 C   -6.074203   -0.640194   -1.900130
 C   -4.573050   -2.547333   -1.308266
 H   -6.248257    0.443710   -1.827745
 H   -6.946434   -1.162602   -1.481420
 H   -5.996809   -0.898384   -2.966496
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 H   -3.581823   -2.850245   -0.946124
 H   -4.656318   -2.855664   -2.360955
 H   -5.338521   -3.090768   -0.733715
 H   -2.737753   -1.396855    0.654522
 H   -4.113360   -2.269543    1.393480
 H   -3.549431   -0.730333    2.089928
 H   -6.523901   -1.239150    1.091720
 H   -6.653305    0.415663    0.433833
 H   -5.827958    0.135876    1.982240
 C    1.577828    1.452170   -1.431132
 C    2.725038    2.208521   -1.228001
 C    0.273787    1.993189   -1.360881
 C    2.656693    3.593596   -0.953493
 C    0.222466    3.374584   -1.109766
 C    1.366108    4.151276   -0.900713
 C   -0.925201    1.106503   -1.447381
 C   -2.292691    1.800076   -1.561535
 H    1.231328    5.214525   -0.698923
 H   -0.745454    3.878838   -1.057973
 H    3.688210    1.700148   -1.283874
 H    1.706776    0.382426   -1.623790
Cu   -0.623472   -0.019678    0.222605
 H   -2.468213    2.242586   -2.563438
 H   -2.372016    2.626945   -0.838012
 H   -0.800860    0.408320   -2.291855
 H    6.188270   -4.769508    0.105150
 H    5.723147   -3.634409   -1.199716
 H    4.872967   -5.206609   -1.028920
 C    1.718979   -5.205305   -0.129073
 H    1.360375   -5.933823   -0.867142
 H    0.873837   -4.877734    0.495354
 H    2.475515   -5.685674    0.511116
 H    1.727133    1.354203    2.596471
 H    1.247157    2.657826    1.480135
 H    0.901311    2.812878    3.233942
 C    0.954399    2.109113    2.388556
 H   -0.266425   -0.297607    3.907899
 P   -0.651720    1.282992    2.098305
 H   -0.983296    1.221590    4.532875
 C   -1.008202    0.490595    3.709779
 H   -1.544958    3.361947    1.250432
 H   -1.866631    3.214611    3.007693
 C   -1.840754    2.668968    2.051661
 H   -2.003154    0.022082    3.677384
 H   -2.840305    2.276424    1.813479
 H    5.035493    3.042959    0.404193
 H    5.337176    3.036521   -1.354347
 C    5.053299    3.678074   -0.505428
 H    5.852787    4.420767   -0.384163
 N    3.803825    4.359020   -0.749209
 H    3.046753    6.328748   -0.843832
 H    4.640555    6.152785   -0.098017
 C    3.653519    5.681168   -0.190958
 H    3.179506    5.679614    0.812234
80
Figure 3_para-NMe2_ts(AS)_01 / electronic energy: -3794.13369549 a.u. / lowest freq: -333.24 cm-1
 C   -0.185555   -1.002249   -1.094395
 C   -0.045900   -1.983247   -0.083214
 C    1.004439   -1.965111    0.838722
 O    2.487683   -3.265587    0.196268
 P    3.578805   -2.534904   -0.581240
 O    3.260468   -1.620817   -1.718547
 O    4.427125   -1.739169    0.582787
 O    4.660956   -3.640697   -1.101747
 C    5.557572   -0.988359    0.206053
 H   -0.983095   -1.112642   -1.832194
 H    0.693001   -0.431432   -1.417586
 H   -0.809412   -2.760930    0.020354
 H    1.721533   -1.144147    0.850197
 H    0.942660   -2.568527    1.742576
 B    0.282466    2.460085   -1.315549
 O    1.386796    1.845996   -1.843975
 O    0.619551    3.487920   -0.469800
 C    2.536798    2.312683   -1.112852
 C    2.040559    3.710480   -0.604903
 C    3.738955    2.336789   -2.040003
 C    2.767139    1.311577    0.015450
 C    2.227164    4.816307   -1.642472
 C    2.616419    4.146460    0.731369
 H    1.833052    4.515423   -2.624772
 H    3.287272    5.082696   -1.760922
 H    1.681027    5.713965   -1.317022
 H    2.399094    3.425538    1.528936
 H    2.189017    5.117395    1.023053
 H    3.708068    4.265003    0.657720
 H    1.886528    1.264301    0.674816
 H    3.645963    1.569598    0.623953
 H    2.928803    0.321091   -0.433678
 H    4.620219    2.748824   -1.525366
 H    3.547905    2.931920   -2.942687
 H    3.969312    1.306831   -2.350174
 C   -4.049740    0.574744    0.490960
 C   -5.264215   -0.094673    0.380287
 C   -3.116603    0.644652   -0.558545
 C   -5.631298   -0.750500   -0.816739
 C   -3.501272    0.006602   -1.751078
 C   -4.710025   -0.669692   -1.885213
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 C   -1.795496    1.318388   -0.374330
 C   -1.181449    1.981769   -1.610222
 H   -4.933924   -1.139350   -2.843364
 H   -2.835643    0.032585   -2.617365
 H   -5.935680   -0.096886    1.239389
 H   -3.822878    1.075648    1.435021
Cu   -0.722577   -0.096594    0.587447
 H   -1.814381    2.828732   -1.941043
 H   -1.131629    1.279248   -2.456478
 H   -1.883650    2.067512    0.429704
 H    5.908895   -0.433505    1.088181
 H    5.323202   -0.271554   -0.598049
 H    6.376408   -1.641248   -0.144103
 C    5.095318   -4.654388   -0.223645
 H    5.894826   -5.216426   -0.727602
 H    4.277193   -5.347888    0.030238
 H    5.499445   -4.237177    0.714965
 H    1.662265    1.358004    2.928618
 H    0.466047    2.588569    2.429941
 H    0.602380    2.114542    4.157669
 C    0.653954    1.752739    3.119368
 H    0.859195   -1.250774    3.788649
 P   -0.586318    0.446344    2.823245
 H   -0.128043   -0.451687    5.052062
 C   -0.137574   -0.852771    4.026944
 H   -2.398606    2.059844    2.975589
 H   -1.933301    1.443518    4.590552
 C   -2.104647    1.162950    3.540068
 H   -0.866453   -1.674851    3.968462
 H   -2.921294    0.427969    3.495532
 H   -6.393628   -2.896593   -2.408950
 H   -8.114202   -2.614928   -2.062882
 C   -7.140774   -2.119682   -2.163645
 H   -7.203534   -1.433190   -3.027295
 N   -6.826907   -1.426246   -0.937812
 H   -7.278544   -1.994622    1.060271
 H   -8.623529   -2.064590   -0.099698
 C   -7.730751   -1.493968    0.183991
 H   -8.067210   -0.493056    0.509530
80
Figure 3_para-NMe2_ts(AS)_02 / electronic energy: -3794.13722913 a.u. / lowest freq: -346.50 cm-1
 C    0.412377    1.709915   -0.577616
 C    0.308614    1.975481    0.819115
 C   -0.833094    1.607117    1.540142
 O   -2.225910    3.118845    1.494396
 P   -2.904945    3.143477    0.125287
 O   -2.902293    1.927972   -0.748712
 O   -4.419550    3.668550    0.436395
 O   -2.284242    4.374152   -0.754942
 C   -5.325299    3.794554   -0.638535
 H    1.299122    2.037896   -1.126010
 H   -0.514596    1.639298   -1.155058
 H    1.128342    2.468707    1.350759
 H   -1.585744    0.969662    1.073666
 H   -0.827552    1.652982    2.628849
 B    3.207998   -0.733382   -1.261112
 O    4.101863   -1.031309   -0.261116
 O    3.397466    0.525760   -1.764531
 C    4.765882    0.189798    0.113281
 C    4.591919    1.073549   -1.178100
 C    6.207969   -0.112785    0.484901
 C    4.013121    0.738396    1.323910
 C    5.717302    0.881729   -2.192513
 C    4.375381    2.553651   -0.906838
 H    5.891506   -0.184084   -2.402537
 H    6.659284    1.327399   -1.842456
 H    5.435081    1.371050   -3.136131
 H    3.483109    2.729532   -0.291729
 H    4.241729    3.089235   -1.858315
 H    5.246590    2.986358   -0.392302
 H    2.953657    0.921477    1.083436
 H    4.455964    1.672031    1.698712
 H    4.052652   -0.006290    2.132160
 H    6.757034    0.818771    0.689160
 H    6.728277   -0.658267   -0.313059
 H    6.238572   -0.730379    1.394898
 C   -1.790109   -1.237200   -1.215545
 C   -2.945360   -1.977149   -1.002654
 C   -0.517433   -1.836233   -1.331793
 C   -2.912505   -3.388642   -0.905478
 C   -0.493693   -3.235952   -1.239321
 C   -1.645219   -3.995296   -1.028864
 C    0.708901   -0.990491   -1.471494
 C    2.048635   -1.697292   -1.687024
 H   -1.541559   -5.078866   -0.967580
 H    0.454102   -3.769871   -1.337692
 H   -3.887602   -1.437004   -0.906696
 H   -1.898884   -0.148053   -1.262734
Cu    0.649100   -0.038137    0.304147
 H    2.156664   -2.034275   -2.736768
 H    2.132544   -2.598475   -1.061530
 H    0.559028   -0.236303   -2.254364
 H   -6.283575    4.146174   -0.230463
 H   -5.484084    2.828954   -1.145762
 H   -4.971604    4.526427   -1.385213
 C   -2.091957    5.629101   -0.143694
 H   -1.717494    6.324857   -0.908410
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 H   -1.356394    5.571835    0.675339
 H   -3.034626    6.033459    0.264477
 H   -1.585281   -1.484003    2.662186
 H   -1.253604   -2.772994    1.474805
 H   -0.811887   -3.012607    3.197569
 C   -0.876174   -2.276659    2.381273
 H    0.622067   -0.047103    3.934912
 P    0.752924   -1.536441    2.023930
 H    1.279254   -1.645421    4.414501
 C    1.291684   -0.866851    3.636495
 H    1.464274   -3.568214    0.926414
 H    1.910731   -3.595280    2.661548
 C    1.853352   -2.966183    1.760038
 H    2.311092   -0.463984    3.548112
 H    2.856740   -2.605071    1.489780
 H   -5.254263   -2.868060    0.543656
 H   -5.591845   -2.760077   -1.204131
 C   -5.299746   -3.451283   -0.396788
 H   -6.103502   -4.191594   -0.296360
 N   -4.060952   -4.129140   -0.698042
 H   -3.461507   -6.080658   -1.247922
 H   -4.953289   -5.969407   -0.301056
 C   -3.950502   -5.540575   -0.420124
 H   -3.378386   -5.754401    0.504133
80
Figure 3_para-NMe2_pi-allyl_01 / electronic energy: -3794.16230939 a.u. / lowest freq: 19.87 cm-1
 C    0.875811    1.817945   -1.438411
 C    1.425378    2.479938   -0.302808
 C    0.728435    2.545748    0.888128
 O   -2.384896    1.981952    1.100363
 P   -2.983033    2.394480   -0.219040
 O   -2.208153    2.347011   -1.506879
 O   -4.380522    1.535931   -0.375931
 O   -3.569510    3.926173   -0.102339
 C   -5.127143    1.678861   -1.560047
 H    1.520135    1.652668   -2.303974
 H   -0.209972    1.910548   -1.611485
 H    2.498696    2.697010   -0.293195
 H   -0.369075    2.435116    0.934617
 H    1.238893    2.894280    1.789965
 B    3.305820   -1.012957   -0.882701
 O    4.079943   -1.261494    0.221199
 O    3.801699    0.005687   -1.648580
 C    5.065894   -0.216161    0.320655
 C    5.118490    0.328819   -1.155699
 C    6.374456   -0.802058    0.825321
 C    4.526587    0.800674    1.324723
 C    6.114916   -0.424317   -2.034845
 C    5.346703    1.825944   -1.272374
 H    5.976308   -1.513120   -1.959315
 H    7.154290   -0.185111   -1.768450
 H    5.953951   -0.136095   -3.083861
 H    4.555576    2.400557   -0.774297
 H    5.363475    2.119616   -2.332227
 H    6.312787    2.104411   -0.825730
 H    3.564637    1.216970    0.993342
 H    5.230727    1.629259    1.485191
 H    4.366433    0.298918    2.290433
 H    7.164557   -0.036480    0.824041
 H    6.706206   -1.649915    0.212253
 H    6.249642   -1.159039    1.858221
 C   -1.782498   -0.922050   -1.206134
 C   -3.021297   -1.483780   -0.941780
 C   -0.583996   -1.648743   -1.079812
 C   -3.147979   -2.838082   -0.550977
 C   -0.712469   -2.991367   -0.697469
 C   -1.951121   -3.579269   -0.442423
 C    0.731775   -0.979037   -1.327376
 C    1.993356   -1.824809   -1.176346
 H   -1.974726   -4.631431   -0.157284
 H    0.174633   -3.621003   -0.602541
 H   -3.894489   -0.836228   -1.003082
 H   -1.755510    0.137987   -1.479357
Cu    0.815693    0.485012    0.062392
 H    2.140819   -2.428076   -2.093721
 H    1.888632   -2.544232   -0.352713
 H    0.719049   -0.492789   -2.308023
 H   -6.061737    1.110133   -1.443466
 H   -4.581985    1.294088   -2.438202
 H   -5.384265    2.735123   -1.754750
 C   -4.335603    4.270762    1.024711
 H   -4.551245    5.348564    0.976340
 H   -3.795560    4.057494    1.962494
 H   -5.294949    3.723375    1.050524
 H   -1.809682    0.104452    2.096655
 H   -1.613670   -1.613980    1.650614
 H   -1.465038   -1.138595    3.376306
 C   -1.269743   -0.827733    2.338482
 H    0.458089    1.353424    3.575442
 P    0.507341   -0.547513    2.075251
 H    0.871972   -0.150337    4.453923
 C    1.037872    0.420611    3.527681
 H    0.884325   -2.895617    1.624415
 H    1.144764   -2.515628    3.353037
 C    1.310546   -2.163211    2.323606
 H    2.106005    0.668858    3.443434
 H    2.389188   -2.072248    2.129154
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 H   -5.518948   -1.746982    0.429654
 H   -5.719394   -2.109959   -1.303884
 C   -5.560337   -2.566353   -0.311729
 H   -6.440447   -3.181054   -0.086552
 N   -4.377881   -3.395832   -0.285712
 H   -4.038631   -5.475427   -0.508067
 H   -5.513754   -5.014915    0.364251
 C   -4.461243   -4.748817    0.207765
 H   -3.933601   -4.881983    1.171122
80
Figure 3_para-NMe2_pi-allyl_02 / electronic energy: -3794.15615510 a.u. / lowest freq: 16.22 cm-1
 C   -0.513788   -0.907893   -1.666995
 C   -1.187002   -1.932278   -0.952543
 C   -0.612388   -2.491996    0.182255
 O    2.447310   -2.710480    0.777740
 P    3.200840   -2.491081   -0.508923
 O    2.581069   -1.823717   -1.701887
 O    4.590511   -1.716973   -0.076562
 O    3.795413   -3.928919   -1.044160
 C    5.519798   -1.386125   -1.076575
 H   -1.028439   -0.403389   -2.486609
 H    0.589167   -0.928925   -1.689268
 H   -2.259857   -2.075317   -1.132122
 H    0.480733   -2.540639    0.324376
 H   -1.229413   -3.118971    0.833054
 B    0.539353    2.698281   -0.995847
 O    1.635160    2.403835   -1.752302
 O    0.866230    3.294481    0.197357
 C    2.790476    2.543540   -0.894830
 C    2.279961    3.583013    0.162972
 C    3.980592    2.996694   -1.720775
 C    3.047630    1.166836   -0.293802
 C    2.436249    5.031143   -0.296327
 C    2.863494    3.406266    1.553928
 H    2.046276    5.175298   -1.315069
 H    3.489087    5.347464   -0.277877
 H    1.868245    5.687218    0.379577
 H    2.629282    2.418572    1.969751
 H    2.456898    4.168977    2.234788
 H    3.957529    3.521731    1.529876
 H    2.209414    0.851202    0.347015
 H    3.969317    1.139713    0.303917
 H    3.125038    0.420107   -1.094863
 H    4.845445    3.195661   -1.069964
 H    3.758763    3.904580   -2.297515
 H    4.263733    2.202803   -2.427412
 C   -3.634152    0.571377    0.742948
 C   -4.889121   -0.018997    0.671674
 C   -2.905684    0.943869   -0.403006
 C   -5.503041   -0.275485   -0.577587
 C   -3.530212    0.703763   -1.640762
 C   -4.784271    0.118842   -1.734692
 C   -1.532648    1.479262   -0.272115
 C   -0.939672    2.337024   -1.375175
 H   -5.213293   -0.030780   -2.725307
 H   -3.019445    0.983344   -2.565271
 H   -5.397723   -0.273048    1.601523
 H   -3.200111    0.757702    1.730608
Cu   -0.725837   -0.302436    0.263298
 H   -1.536977    3.266158   -1.461153
 H   -0.969201    1.847573   -2.358585
 H   -1.412969    1.985867    0.693656
 H    6.267313   -0.704438   -0.643018
 H    5.039408   -0.884462   -1.933699
 H    6.044060   -2.281084   -1.457314
 C    4.350955   -4.816339   -0.106639
 H    4.654918   -5.730756   -0.637928
 H    3.623281   -5.083244    0.677751
 H    5.242705   -4.388586    0.386216
 H    0.064809    2.328825    2.503103
 H   -1.541793    1.854628    3.126329
 H   -0.094640    1.666462    4.167592
 C   -0.470488    1.603567    3.134980
 H    2.156700    0.388988    2.563976
 P   -0.213302   -0.070613    2.463798
 H    1.637314   -0.636831    3.931507
 C    1.521945   -0.461506    2.850874
 H   -2.262257   -1.019984    3.355729
 H   -0.981526   -0.943589    4.611330
 C   -1.189026   -1.159650    3.552187
 H    1.855846   -1.341833    2.272789
 H   -0.928986   -2.206759    3.338835
 H   -6.744700   -1.717275   -2.611666
 H   -8.327636   -1.553344   -1.823859
 C   -7.353322   -1.068675   -1.957665
 H   -7.522048   -0.115199   -2.489775
 N   -6.735219   -0.871713   -0.666331
 H   -6.880777   -1.910922    1.174565
 H   -8.393941   -1.719174    0.267621
 C   -7.456271   -1.218374    0.536240
 H   -7.709206   -0.330770    1.144635
56
Figure 3_L-Cu-OtBu_dimer / electronic energy: -4668.27269506 a.u. / lowest freq: 20.28 cm-1
 H    1.454781    3.185323    2.121955
 H   -1.091667    3.295320    2.232897
 H    1.480610    4.376760    0.788877
 C    1.390257    3.304563    1.028715
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 H     2.248895    2.774926    0.584062
 H    -1.141168    4.483981    0.897486
 C    -1.116435    3.408141    1.137329
 C     0.084478    2.685555    0.510787
 O     0.044189    1.344738    0.873648
 H    -2.049560    2.947919    0.774353
 H     0.052315    3.874754   -1.357879
 C     0.025055    2.825701   -1.018825
 H     0.875658    2.290877   -1.472279
 H    -0.901160    2.361194   -1.396152
 H     2.958274    1.006115   -2.657041
 H     3.299551   -1.873435   -2.121429
 C     3.677359    1.175331   -1.841405
 C     3.978968   -1.600940   -1.299765
 H     4.699652    1.104301   -2.245503
 H     3.518839    2.190392   -1.447525
 H     4.999010   -1.491753   -1.701120
 H     3.968610   -2.417548   -0.562485
 P     3.392482   -0.052886   -0.509011
 C     4.751395    0.319901    0.663359
 H     5.728245    0.345249    0.155766
 H     4.568915    1.292893    1.143584
 H     4.770992   -0.448839    1.450266
Cu     1.387359   -0.047785    0.355891
 H     1.052783   -3.300511    2.261431
 H     2.049259   -2.926990    0.836004
 O    -0.048207   -1.342931    0.876207
 C     1.110810   -3.401807    1.166003
 H     1.154224   -4.474801    0.916365
 C    -0.077761   -2.683448    0.511400
 H    -1.486976   -3.182509    2.088692
 H     0.959296   -2.370999   -1.370977
 C    -1.393184   -3.307099    0.998157
 C     0.017837   -2.822386   -1.016552
 H    -2.243357   -2.784789    0.529205
 H    -1.470986   -4.380974    0.761611
 H    -0.814236   -2.274610   -1.489485
 H    -0.015593   -3.870539   -1.357852
 H    -2.864028   -0.603368   -2.784246
 H    -3.433166    2.132063   -1.768599
 C    -3.581006   -0.953346   -2.026339
 C    -4.101882    1.661026   -1.032388
 H    -4.600512   -0.883806   -2.437656
 H    -3.356876   -2.007230   -1.803518
 H    -5.099460    1.538334   -1.483310
 H    -4.181695    2.333019   -0.164790
 P    -3.397860    0.051973   -0.503299
 C    -4.732552   -0.612373    0.562621
 H    -5.709729   -0.575241    0.056317
 H    -4.504550   -1.654856    0.830705
 H    -4.786261   -0.026266    1.492473
Cu    -1.393433    0.048543    0.362283
28
Figure 3_L-Cu-OtBu / electronic energy: -2334.10735270 a.u. / lowest freq: -39.13 cm-1
 H    -4.105877   -1.332535    0.968255
 H    -4.149740   -1.387400   -0.808196
 O    -1.712519   -0.853226    0.000001
 C    -4.074557   -0.711355    0.058637
 H    -4.956088   -0.048773    0.060108
 C    -2.745372    0.062111    0.000906
 H    -2.638090    0.394148    2.149194
 H    -2.753281    0.265927   -2.166060
 C    -2.653965    0.994061    1.224813
 C    -2.718854    0.919727   -1.279501
 H    -1.712633    1.569392    1.184920
 H    -3.490501    1.710689    1.287963
 H    -1.776368    1.492537   -1.324725
 H    -3.557324    1.634317   -1.340220
 H     2.442116    1.017710   -2.209934
 H     3.078065   -1.733910   -1.400494
 C     2.702639    1.337847   -1.190198
 C     3.315084   -1.349708   -0.397345
 H     3.784909    1.532944   -1.136890
 H     2.155445    2.266931   -0.971809
 H     4.370113   -1.036408   -0.368346
 H     3.157970   -2.162063    0.327594
 P     2.201656    0.043634    0.000306
 C     2.853579    0.661225    1.592861
 H     3.931571    0.875098    1.526895
 H     2.317993    1.579995    1.874683
 H     2.679866   -0.091178    2.376412
Cu     0.062960   -0.408951   -0.003275
70
Figure 3_ed / electronic energy: -3155.87460188 a.u. / lowest freq: 11.42 cm-1
 H    -0.953281   -3.166097   -0.309839
 H    -2.577969   -2.483931   -0.153509
 O    -0.722801   -0.949157    1.165859
 C    -1.784111   -3.004943    0.394843
 H    -2.158222   -3.987377    0.724568
 C    -1.300935   -2.179344    1.589376
 H     0.648291   -3.149536    1.617528
 H    -3.221244   -1.298799    2.101803
 C    -0.183773   -2.938745    2.311306
 C    -2.439912   -1.904482    2.572798
 H     0.208864   -2.337581    3.146164
 H    -0.544498   -3.898139    2.713555
 H    -2.060320   -1.341525    3.439455
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 H   -2.878571   -2.846939    2.937460
Cu    1.139839   -0.920846    0.386293
 H    1.056430    4.912258    0.610864
 H    2.420469    3.941746    2.458899
 H    0.701370    3.458516    2.402659
 C    1.735449    3.084044    2.391288
 H    2.707250    4.756558   -0.052951
 H    1.879972    2.458170    3.283891
 C    1.657698    4.452166   -0.184163
 H    1.306082    4.849580   -1.147882
 C    1.534322    2.938372   -0.174971
 C    2.012113    2.248287    1.144500
 O    0.145692    2.568639   -0.221946
 H    4.143931    2.596400    0.951770
 B   -0.029916    1.375300    0.444402
 H    3.702501    1.320418    2.112925
 C    3.450475    1.762470    1.137384
 O    1.127301    1.108628    1.201500
 H    3.251675    2.634595   -1.503243
 C    2.195444    2.340356   -1.418544
 H    1.664689    2.695001   -2.313853
 H    3.609342    0.994382    0.369926
 H    2.135444    1.240689   -1.404032
 H   -3.741486   -1.478482   -2.045890
 H   -4.291404   -1.318464    0.099435
 H   -2.833922   -0.708588   -3.361743
 C   -3.485339   -0.510025   -2.496037
 O   -1.630269   -0.279491   -1.014975
 H   -5.500527   -0.242437   -0.645178
 C   -4.684450   -0.292834    0.091969
 H   -4.409992   -0.043182   -2.870615
 B   -1.338180    0.190930    0.348230
 H   -5.115024   -0.091914    1.085474
 C   -2.753803    0.399038   -1.508504
 C   -3.582938    0.736127   -0.195713
 O   -2.623638    0.690654    0.835872
 H   -1.601520    1.343872   -3.063483
 C   -2.292899    1.655469   -2.264419
 H   -3.130173    2.197298   -2.730793
 H   -1.740687    2.341103   -1.608781
 H   -4.940611    2.237160   -1.041325
 C   -4.225555    2.125176   -0.210655
 H   -4.773476    2.286728    0.730889
 H   -3.466517    2.914749   -0.291729
 H    4.749033   -1.452497   -0.129415
 C    4.256493   -1.368792   -1.109548
 H    4.274484   -0.314095   -1.421428
 H    4.817512   -1.966521   -1.844659
 H    3.139485   -3.910893    0.308949
 C    2.717087   -3.740696   -0.692506
 P    2.524841   -1.944693   -0.980227
 H    3.382198   -4.194279   -1.443776
 H    1.733374   -4.230143   -0.742993
 C    1.932965   -1.853706   -2.708395
 H    2.575860   -2.437454   -3.385113
 H    1.920774   -0.803126   -3.035062
 H    0.902696   -2.235271   -2.761689
70
Figure 3_ts(TB) / electronic energy: -3155.86594930 a.u. / lowest freq: -80.57 cm-1
 H    3.010276   -2.382916    0.118642
 H    1.683795   -3.550734    0.289052
 O    0.986480   -1.022586    1.231429
 C    2.428017   -2.966919    0.847086
 H    3.108602   -3.663642    1.360560
 C    1.764613   -2.038365    1.865178
 H    3.454412   -0.689234    1.957273
 H    0.067382   -3.345104    2.249766
 C    2.833443   -1.280682    2.648443
 C    0.860433   -2.829879    2.810029
 H    2.364821   -0.587587    3.363520
 H    3.486796   -1.968789    3.205755
 H    0.379103   -2.153513    3.532327
 H    1.437600   -3.583696    3.368135
Cu    1.191646    0.705211   -0.156501
 H   -4.427383    0.766248   -0.614487
 H   -4.518683    0.953062    1.818726
 H   -3.273614   -0.182983    1.196620
 C   -3.444824    0.713535    1.807889
 H   -4.940033    2.443526   -0.292598
 H   -3.136606    0.474696    2.836818
 C   -4.170605    1.821119   -0.775127
 H   -4.205093    2.017783   -1.857471
 C   -2.789480    2.154856   -0.232080
 C   -2.601465    1.882699    1.299916
 O   -1.819873    1.275125   -0.815333
 H   -3.824652    3.498708    2.084955
 B   -0.832690    0.986003    0.123485
 H   -2.656331    2.821205    3.244537
 C   -2.803566    3.100143    2.190308
 O   -1.228345    1.472481    1.363096
 H   -3.133588    4.320679   -0.285336
 C   -2.402291    3.578362   -0.637798
 H   -2.355518    3.636570   -1.735582
 H   -2.091022    3.901305    1.952964
 H   -1.410567    3.846106   -0.243686
 H    0.204209   -4.250825   -1.796312
 H   -0.675749   -4.205721    0.241701
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 H    0.503640   -3.256638   -3.237470
 C   -0.244142   -3.509492   -2.470797
 O    0.458693   -1.748160   -1.013589
 H   -2.092610   -4.638531   -0.753443
 C   -1.697902   -3.906637   -0.032981
 H   -1.103862   -3.973045   -2.978655
 B    0.018530   -1.182613    0.206285
 H   -2.317693   -3.950556    0.875196
 C   -0.662553   -2.241330   -1.733040
 C   -1.728672   -2.480221   -0.585246
 O   -1.295504   -1.617289    0.465873
 H   -0.223704   -0.958441   -3.401261
 C   -1.089544   -1.191204   -2.761739
 H   -1.896569   -1.564732   -3.410033
 H   -1.420470   -0.261620   -2.282477
 H   -3.480699   -2.692998   -1.858133
 C   -3.151903   -2.111553   -0.982870
 H   -3.844242   -2.329239   -0.155058
 H   -3.222981   -1.042608   -1.218567
 H    3.073834    3.432394    1.120755
 C    3.095595    3.493894    0.022203
 H    2.193451    4.031342   -0.305906
 H    3.990738    4.052076   -0.293219
 H    4.736915    1.037154    0.921073
 C    4.694130    1.124469   -0.174737
 P    3.070384    1.803289   -0.674895
 H    5.518167    1.770887   -0.515219
 H    4.823307    0.120668   -0.606383
 C    3.271177    2.077403   -2.471443
 H    4.160947    2.686342   -2.694837
 H    2.375105    2.582414   -2.861624
 H    3.361485    1.104827   -2.978490
70
Figure 3_prod / electronic energy: -3155.88950452 a.u. / lowest freq: 21.62 cm-1
 H   -1.158855   -0.853872    2.044678
 H   -2.081368    0.534440    1.412845
 O    0.476218    1.273606    2.005172
 C   -1.632766    0.101521    2.318332
 H   -2.432894   -0.100666    3.046635
 C   -0.605099    1.058362    2.919658
 H    0.524730   -0.514821    3.893677
 H   -1.708831    2.852240    2.370142
 C    0.037748    0.436514    4.155433
 C   -1.246887    2.403039    3.261372
 H    0.800788    1.111086    4.572434
 H   -0.716472    0.240474    4.932049
 H   -0.490899    3.101512    3.652262
 H   -2.026382    2.277814    4.028140
Cu   -1.162098   -1.530549   -0.469595
 H    3.580583    0.620775   -0.295027
 H    4.155902   -0.696748    1.828001
 H    2.467465   -0.158497    1.567577
 C    3.113119   -1.032974    1.727857
 H    5.013044   -0.445128   -0.480147
 H    2.813949   -1.499307    2.678963
 C    4.011688   -0.207170   -0.872112
 H    4.132527    0.132623   -1.911993
 C    3.106855   -1.430692   -0.824697
 C    2.945747   -2.057257    0.604145
 O    1.763095   -1.042039   -1.140811
 H    4.896752   -2.999208    0.793143
 B    0.857046   -1.733858   -0.337362
 H    3.652152   -3.642033    1.890565
 C    3.831372   -3.266557    0.871685
 O    1.571398   -2.467038    0.608300
 H    4.595766   -2.740742   -1.760293
 C    3.543447   -2.443828   -1.883977
 H    3.430968   -1.987531   -2.879035
 H    3.625644   -4.087120    0.171499
 H    2.917986   -3.348697   -1.857648
 H   -1.188959    4.543120   -0.961219
 H    0.838043    4.659257    0.115279
 H   -2.279828    3.395564   -1.769932
 C   -1.230561    3.715188   -1.680966
 O   -0.748295    2.177348    0.104616
 H    1.217478    4.989554   -1.597762
 C    1.435817    4.327569   -0.747385
 H   -0.904775    4.086148   -2.664441
 B    0.397248    1.808796    0.768095
 H    2.497981    4.443808   -0.486318
 C   -0.374050    2.539678   -1.237950
 C    1.163803    2.862937   -1.086359
 O    1.537557    2.088052    0.061507
 H   -1.693283    1.038056   -2.022193
 C   -0.638926    1.330245   -2.128884
 H   -0.452594    1.559433   -3.188203
 H   -0.013144    0.474822   -1.835748
 H    1.667555    2.926311   -3.195542
 C    2.005995    2.427305   -2.274763
 H    3.058190    2.701403   -2.107369
 H    1.953583    1.339765   -2.409554
 H   -3.849992   -3.526552   -1.811768
 C   -4.138767   -2.476486   -1.968429
 H   -3.730136   -2.151784   -2.937054
 H   -5.237257   -2.405102   -1.996484
 H   -3.969700   -3.065287    1.097540
 C   -4.312146   -2.048283    0.854783
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 P   -3.430509   -1.445333   -0.632444
 H   -5.401729   -2.061155    0.696600
 H   -4.080638   -1.396766    1.709930
 C   -4.218331    0.182703   -0.927440
 H   -5.316094    0.104994   -0.887227
 H   -3.927434    0.563017   -1.917896
 H   -3.880941    0.905727   -0.169933
35
Figure 3_L-Cu-Bpin / electronic energy: -2512.09747879 a.u. / lowest freq: 23.70 cm-1
 H   -3.966569   -2.370555   -0.091079
 H   -3.807068   -0.481958   -2.357598
 C   -4.300635   -1.524404    0.527882
 C   -4.141575    0.306361   -1.666690
 H   -5.393074   -1.419924    0.438009
 H   -4.044913   -1.745522    1.575060
 H   -5.242483    0.322371   -1.642579
 H   -3.774702    1.270837   -2.048864
 P   -3.438874    0.000252   -0.004071
 C   -4.231120    1.295459    1.018181
 H   -5.326265    1.285342    0.903062
 H   -3.978324    1.134755    2.076846
 H   -3.846004    2.282421    0.721008
 H    3.908707   -2.418790   -1.177398
 H    3.178529   -2.542187    1.157081
 C    3.960241   -1.319391   -1.165315
 H    3.658664   -0.959332   -2.157930
 H    5.009094   -1.032819   -0.991557
 C    3.381449   -1.465540    1.257698
 O    1.691138   -1.070941   -0.382227
 H    4.437392   -1.340205    1.540068
 C    3.058289   -0.772965   -0.067653
 H    2.751180   -1.078631    2.072035
 B    0.869426   -0.027376    0.045169
 H    2.597061    1.082407   -2.068948
 C    3.034990    0.788202    0.049573
 H    4.301435    1.400842   -1.634829
 O    1.677868    1.040108    0.438088
 C    3.260011    1.490169   -1.291420
 H    5.023511    1.114048    0.867358
 H    3.740760    0.997181    2.103774
 C    3.976365    1.366007    1.096660
 H    3.026918    2.559483   -1.177997
 H    3.888770    2.463056    1.112142
Cu   -1.167130   -0.038843    0.055765
51
Figure 3_para-H_pc1 / electronic energy: -2821.45221106 a.u. / lowest freq: 16.87 cm-1
 H    0.564165    2.801199    1.367690
 H   -1.590737    1.055295    2.367112
 C   -0.121268    3.208404    0.609283
 C   -2.237026    1.578675    1.646988
 H   -0.634099    4.092259    1.019570
 H    0.479762    3.508326   -0.262570
 H   -2.597662    2.516215    2.098075
 H   -3.098493    0.932050    1.422848
 P   -1.299326    1.901652    0.110146
 C   -2.505786    2.807144   -0.926482
 H   -2.906981    3.691071   -0.406638
 H   -2.017095    3.129159   -1.858424
 H   -3.337836    2.135926   -1.186586
 H   -5.558352   -1.682195    2.226864
 H   -3.266888   -2.642355    2.450043
 C   -4.821344   -1.539456    1.433214
 C   -3.538842   -2.077556    1.554708
 H   -6.153183   -0.394889    0.172086
 C   -5.152011   -0.818693    0.284574
 H    3.921807   -1.855544    2.666229
 C   -2.594671   -1.894621    0.546832
 H    3.229154    0.489726    2.890296
 H   -1.592351   -2.311697    0.672755
 C   -4.209149   -0.635427   -0.724386
 C   -2.911457   -1.164134   -0.613976
 C    4.268902   -1.717263    1.630939
 C    3.731678    0.700712    1.934521
 H    4.049362   -2.640633    1.078795
 O    2.173805   -0.778699    0.889763
 H   -4.479364   -0.071670   -1.621734
 H    4.788200    0.925255    2.144587
 H    5.360339   -1.574096    1.656380
 C    3.577837   -0.510789    1.012748
 C   -1.926922   -0.906108   -1.682674
 B    1.681596   -0.168636   -0.262242
 H   -0.510868   -2.507280   -1.274832
 C   -0.742745   -1.614390   -1.862876
 C    3.982318   -0.203577   -0.468371
 H    3.577471   -2.238090   -1.149898
 O    2.755695    0.302009   -1.014867
 H    5.315468   -1.879385   -0.939899
 H    6.007977    0.515280   -0.146626
 C    4.349008   -1.461108   -1.258337
 H   -0.202315   -1.525282   -2.809577
 C    5.074486    0.843815   -0.629415
 H    4.421469   -1.206659   -2.326313
 H    5.283620    1.003092   -1.698059
Cu   -0.293675    0.039165   -0.745781
 H   -2.270882   -0.247656   -2.487949
 H    3.263920    1.595594    1.497701
 H    4.778807    1.809319   -0.198164
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51
Figure 3_para-H_ts(CuBadd) / electronic energy: -2821.43913646 a.u. / lowest freq: -187.71 cm-1
 H    0.155279    2.399615    2.061692
 H   -2.444870    1.068999    1.944153
 C   -0.202834    3.120230    1.311597
 C   -2.758664    1.807242    1.191673
 H   -0.703978    3.958854    1.819815
 H    0.667735    3.499429    0.756036
 H   -3.179291    2.688640    1.699907
 H   -3.531297    1.342799    0.560851
 P   -1.323613    2.257979    0.154888
 C   -1.950167    3.592509   -0.922937
 H   -2.384783    4.412358   -0.330805
 H   -1.125164    3.985617   -1.535502
 H   -2.715700    3.183777   -1.598779
 H   -4.991156   -2.349056    2.164086
 H   -2.538163   -2.404700    2.642179
 C   -4.266041   -2.125115    1.378391
 C   -2.895769   -2.154762    1.638768
 H   -5.758879   -1.792541   -0.152482
 C   -4.689964   -1.811552    0.080399
 H    3.284658   -1.849375    2.735074
 C   -1.964860   -1.868915    0.640938
 H    2.661768    0.520530    2.804407
 H   -0.900302   -1.892105    0.890864
 C   -3.771122   -1.523632   -0.919786
 C   -2.372594   -1.524617   -0.675530
 C    3.725912   -1.765475    1.730661
 C    3.238631    0.681742    1.881788
 H    3.526791   -2.703838    1.196729
 O    1.736492   -0.801666    0.764990
 H   -4.128502   -1.274801   -1.923880
 H    4.280127    0.897138    2.161741
 H    4.814252   -1.650621    1.847495
 C    3.134173   -0.567389    1.006024
 C   -1.433479   -1.137104   -1.710445
 B    1.399376   -0.195959   -0.431172
 H    0.350880   -2.132995   -0.907213
 C    0.014942   -1.305288   -1.548576
 C    3.681332   -0.343397   -0.447361
 H    3.228588   -2.385182   -1.081991
 O    2.526223    0.196968   -1.120956
 H    4.956495   -2.097016   -0.741278
 H    5.692777    0.304191    0.039542
 C    4.042163   -1.647870   -1.155809
 H    0.581576   -1.277497   -2.487222
 C    4.829604    0.646772   -0.551447
 H    4.214697   -1.440937   -2.222306
 H    5.151938    0.737220   -1.599469
Cu   -0.486472    0.466506   -0.830603
 H   -1.831358   -0.979344   -2.716919
 H    2.822803    1.563721    1.372010
 H    4.538760    1.645849   -0.201081
51
Figure 3_para-H_L-Cu-alkyl_01 / electronic energy: -2821.49278031 a.u. / lowest freq: 25.43 cm-1
 H    0.532217    2.955099    1.794118
 H   -1.972094    1.499635    2.306578
 C   -0.019501    3.578683    1.075545
 C   -2.462297    2.172866    1.587342
 H   -0.481135    4.421552    1.613081
 H    0.691806    3.973721    0.335318
 H   -2.802042    3.079929    2.110962
 H   -3.332263    1.644697    1.169461
 P   -1.294390    2.570604    0.235458
 C   -2.209791    3.802612   -0.758448
 H   -2.566847    4.636826   -0.134920
 H   -1.554836    4.197924   -1.549196
 H   -3.070366    3.314313   -1.239415
 H   -4.117883   -3.359184    2.041856
 H   -1.656795   -3.785744    2.117141
 C   -3.454469   -2.924955    1.290052
 C   -2.080407   -3.158788    1.326609
 H   -5.040651   -1.932106    0.202116
 C   -3.965191   -2.123733    0.262060
 H    3.178829   -2.016399    2.588517
 C   -1.227876   -2.607138    0.368108
 H    1.076143   -0.787921    2.430364
 H   -0.154774   -2.791323    0.445215
 C   -3.119184   -1.572244   -0.692290
 C   -1.717356   -1.784760   -0.672122
 C    3.671887   -1.395724    1.825713
 C    1.565632   -0.050694    1.777403
 H    4.356849   -2.038136    1.257317
 O    1.942932   -1.778399    0.183941
 H   -3.542163   -0.945021   -1.484291
 H    2.002594    0.735111    2.410044
 H    4.261396   -0.624756    2.344674
 C    2.624672   -0.755810    0.929481
 C   -0.848656   -1.128152   -1.678755
 B    1.605860   -1.251351   -1.040490
 H    0.428631   -2.919401   -1.950717
 C    0.504012   -1.814955   -1.997277
 C    3.203085    0.157454   -0.216418
 H    4.614064   -1.356385   -0.914252
 O    2.285807   -0.085242   -1.294502
 H    5.360331   -0.060145    0.061115
 H    3.771338    1.861587    1.010655
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 C     4.587364   -0.279818   -0.689520
 H     0.785937   -1.560809   -3.032459
 C     3.194385    1.644637    0.099102
 H     4.839447    0.264448   -1.611614
 H     3.645564    2.206601   -0.732173
Cu    -0.782705    0.690760   -0.855766
 H    -1.431115   -1.001690   -2.607962
 H     0.787788    0.398248    1.138264
 H     2.167246    2.007194    0.232973
51
Figure 3_para-H_L-Cu-alkyl_02 / electronic energy: -2821.48741938 a.u. / lowest freq: 16.34 cm-1
 H     4.655816   -2.219648    1.835286
 H     4.611303    0.697791    2.171188
 C     5.173151   -2.070175    0.875864
 C     5.141355    0.777570    1.210565
 H     6.258281   -2.019331    1.055510
 H     4.952666   -2.932725    0.229407
 H     6.225835    0.705689    1.387228
 H     4.909889    1.759961    0.772885
 P     4.557339   -0.540214    0.083899
 C     5.648332   -0.359542   -1.372856
 H     6.710407   -0.389783   -1.084085
 H     5.443617   -1.171872   -2.086018
 H     5.438181    0.597194   -1.873727
 B    -1.949269   -1.175075    0.049555
 O    -2.786331   -1.164560    1.136547
 O    -2.611370   -0.859305   -1.110698
 C    -4.133223   -0.976628    0.667814
 C    -3.905709   -0.344635   -0.756373
 C    -4.881232   -0.083760    1.645231
 C    -4.786767   -2.356449    0.611264
 C    -3.788057    1.179197   -0.724832
 C    -4.919285   -0.768639   -1.807545
 H    -3.062286    1.512298    0.031641
 H    -4.757075    1.657619   -0.520708
 H    -3.431186    1.529629   -1.704438
 H    -4.907118   -1.854201   -1.971572
 H    -4.688871   -0.279046   -2.765463
 H    -5.936220   -0.469874   -1.510793
 H    -4.269155   -3.016770   -0.100350
 H    -5.846080   -2.293155    0.323295
 H    -4.728621   -2.822133    1.606215
 H    -5.886685    0.150560    1.263679
 H    -4.346166    0.857421    1.827204
 H    -4.996280   -0.599929    2.610168
 C     0.085937    2.101785   -1.125006
 C    -0.259966    3.401425   -0.771255
 C     0.039849    1.033661   -0.199441
 C    -0.670980    3.700449    0.532054
 C    -0.376461    1.362207    1.110159
 C    -0.723997    2.665724    1.465990
 C     0.412980   -0.347171   -0.598424
 C    -0.402643   -1.459067    0.108159
 H    -1.044212    2.872689    2.491484
 H    -0.435969    0.577383    1.868020
 H    -0.946655    4.720603    0.809892
 H    -0.218322    4.192877   -1.525294
 H     0.393298    1.890460   -2.154508
Cu     2.365400   -0.474012   -0.310661
 H    -0.096347   -1.612041    1.157569
 H    -0.196512   -2.424061   -0.389198
 H     0.246030   -0.437480   -1.686614
51
Figure 3_para-H_L-Cu-alkyl_03 / electronic energy: -2821.49162681 a.u. / lowest freq: 19.82 cm-1
 H    -0.620601    3.508722   -1.594911
 H     2.202611    2.855307   -2.185705
 C    -0.268108    3.845450   -0.608980
 C     2.461381    3.173932   -1.164868
 H     0.073631    4.889349   -0.687752
 H    -1.108766    3.797132    0.098812
 H     2.671833    4.254721   -1.165006
 H     3.363959    2.626678   -0.854488
 P     1.086718    2.760967   -0.031043
 C     1.596457    3.544697    1.541525
 H     1.815048    4.614612    1.401297
 H     0.795026    3.434111    2.287221
 H     2.494274    3.037107    1.924644
 B    -1.592338   -1.558278   -0.362782
 O    -2.256147   -0.773074   -1.274830
 O    -2.281580   -1.664509    0.819060
 C    -3.316977   -0.094601   -0.580957
 C    -3.564745   -1.039504    0.652681
 C    -4.507547    0.063673   -1.512518
 C    -2.773404    1.277134   -0.183547
 C    -4.575338   -2.148065    0.363963
 C    -3.936708   -0.316106    1.937495
 H    -4.336858   -2.677355   -0.570667
 H    -5.599449   -1.754487    0.289855
 H    -4.546922   -2.881388    1.183259
 H    -3.147776    0.377411    2.256810
 H    -4.090889   -1.047457    2.744849
 H    -4.872441    0.248545    1.808482
 H    -1.902914    1.179612    0.484710
 H    -3.534794    1.895310    0.313702
 H    -2.440988    1.801177   -1.091249
 H    -5.365267    0.498812   -0.977620
 H    -4.815906   -0.896536   -1.946105
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 H   -4.246364    0.739970   -2.340101
 C    3.162624   -1.442340    1.197011
 C    4.525376   -1.683445    1.076538
 C    2.248995   -1.741022    0.155808
 C    5.050184   -2.240641   -0.095638
 C    2.800850   -2.321151   -1.006209
 C    4.171705   -2.557956   -1.130070
 C    0.808530   -1.416587    0.306130
 C   -0.174250   -2.171926   -0.607030
 H    4.555897   -3.004837   -2.051880
 H    2.143711   -2.590005   -1.836626
 H    6.122018   -2.427918   -0.194602
 H    5.191869   -1.434777    1.907740
 H    2.775490   -0.998599    2.120523
Cu    0.747989    0.562531    0.113521
 H   -0.154759   -3.267597   -0.429785
 H    0.073925   -2.022971   -1.671218
 H    0.522314   -1.579746    1.361418
51
Figure 3_para-H_ts(BHE) / electronic energy: -2821.44270924 a.u. / lowest freq: -1002.20 cm-1
 H    2.587951   -3.646098    1.807074
 H    4.058409   -1.097904    1.423936
 C    2.553407   -3.752480    0.712646
 C    3.995576   -1.288881    0.342627
 H    3.461135   -4.271341    0.367716
 H    1.670194   -4.355868    0.454455
 H    4.846940   -1.915932    0.035015
 H    4.047286   -0.321725   -0.180851
 P    2.403173   -2.097410   -0.048240
 C    2.528515   -2.430909   -1.841302
 H    3.432714   -3.009155   -2.086773
 H    1.639138   -2.985471   -2.175810
 H    2.553819   -1.469384   -2.375644
 B   -1.980683    0.588970    0.321225
 O   -3.020238    0.863809    1.164796
 O   -2.383934   -0.002469   -0.844293
 C   -4.184688    0.190091    0.645261
 C   -3.824751    0.039432   -0.878914
 C   -5.418373    1.030572    0.927977
 C   -4.278973   -1.151830    1.369228
 C   -4.215553    1.259273   -1.710424
 C   -4.345885   -1.230680   -1.530688
 H   -3.858485    2.192050   -1.249065
 H   -5.304708    1.328081   -1.843206
 H   -3.752981    1.175280   -2.704736
 H   -3.930564   -2.130133   -1.057950
 H   -4.066523   -1.246804   -2.594706
 H   -5.443691   -1.275161   -1.468084
 H   -3.393965   -1.775839    1.172893
 H   -5.176161   -1.712643    1.070447
 H   -4.331275   -0.971074    2.452872
 H   -6.308132    0.577911    0.464828
 H   -5.309062    2.054967    0.548633
 H   -5.591299    1.086366    2.012822
 C    2.545151    2.137114   -1.328444
 C    3.815756    2.678147   -1.176330
 C    1.752484    1.765002   -0.212683
 C    4.362268    2.882414    0.096316
 C    2.322177    1.990728    1.066350
 C    3.597034    2.534534    1.210544
 C    0.451789    1.147547   -0.404923
 C   -0.489248    0.899032    0.668133
 H    4.000979    2.685144    2.215986
 H    1.761740    1.718020    1.964671
 H    5.360989    3.308863    0.214366
 H    4.392363    2.947520   -2.066237
 H    2.141083    1.982835   -2.333751
Cu    0.734034   -0.742791    0.450671
 H   -0.371899    1.493603    1.583245
 H   -0.417834   -0.421710    1.534906
 H    0.103929    1.027460   -1.435301
51
Figure 3_para-H_pc2 / electronic energy: -2821.47614749 a.u. / lowest freq: 16.86 cm-1
 H    1.842917   -3.888981    1.419815
 H    3.736870   -1.589359    1.605411
 C    1.847006   -3.763772    0.326775
 C    3.718384   -1.595053    0.505336
 H    2.661155   -4.364484   -0.107528
 H    0.882443   -4.127064   -0.058749
 H    4.448946   -2.330571    0.134243
 H    4.003461   -0.593217    0.150769
 P    2.028739   -1.989475   -0.073576
 C    2.200418   -1.994213   -1.894808
 H    2.980262   -2.696951   -2.226856
 H    1.240100   -2.279676   -2.350019
 H    2.460233   -0.982833   -2.239336
 B   -1.838132    0.845262    0.216132
 O   -2.894739    1.149042    1.030658
 O   -2.214235    0.144110   -0.901874
 C   -4.019505    0.369913    0.578321
 C   -3.653392    0.106027   -0.929977
 C   -5.297188    1.163928    0.792557
 C   -4.038398   -0.907746    1.415503
 C   -4.113727    1.224682   -1.862865
 C   -4.106619   -1.243159   -1.463797
 H   -3.814802    2.213691   -1.484549
 H   -5.204893    1.216782   -1.998258
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 H   -3.645111    1.084170   -2.848150
 H   -3.645562   -2.073228   -0.912766
 H   -3.825008   -1.341647   -2.522780
 H   -5.200621   -1.340070   -1.394252
 H   -3.111089   -1.484367    1.281235
 H   -4.896289   -1.547327    1.162810
 H   -4.111587   -0.638223    2.479256
 H   -6.161445    0.629176    0.370548
 H   -5.240015    2.158214    0.330854
 H   -5.474811    1.300814    1.869466
 C    2.858306    1.680153   -1.377626
 C    4.184116    2.095076   -1.262822
 C    2.041548    1.545982   -0.244300
 C    4.721870    2.384568   -0.008734
 C    2.594889    1.845421    1.012292
 C    3.918758    2.260834    1.127156
 C    0.654174    1.054532   -0.398902
 C   -0.372109    1.246900    0.517421
 H    4.331868    2.479979    2.114655
 H    1.989931    1.731731    1.915117
 H    5.762000    2.705138    0.084916
 H    4.800236    2.192872   -2.159952
 H    2.442476    1.457908   -2.364334
Cu    0.403038   -0.646099    0.815827
 H   -0.171690    1.816266    1.432387
 H   -0.363027   -1.256048    2.068206
 H    0.395138    0.710351   -1.407593
51
Figure 3_para-H_ts(H>B) / electronic energy: -2821.46264111 a.u. / lowest freq: -449.57 cm-1
 H    1.908537    4.001781   -1.462481
 H    3.587185    1.516416   -1.704817
 C    1.974904    3.891650   -0.369795
 C    3.631126    1.558697   -0.606368
 H    2.872279    4.415685   -0.006155
 H    1.079471    4.351815    0.073628
 H    4.441429    2.239367   -0.302442
 H    3.850502    0.548373   -0.229889
 P    2.020373    2.115891    0.059653
 C    2.305463    2.122306    1.864988
 H    3.180593    2.734507    2.132651
 H    1.415744    2.518368    2.376605
 H    2.470157    1.089872    2.207705
 B   -1.725644   -0.459298   -0.418668
 O   -2.813968   -0.808383   -1.237283
 O   -2.188760   -0.107272    0.869479
 C   -3.990226   -0.293363   -0.617389
 C   -3.597492   -0.321494    0.906727
 C   -5.170868   -1.182955   -0.981922
 C   -4.238318    1.125509   -1.136727
 C   -3.837561   -1.690794    1.547737
 C   -4.253839    0.764048    1.748615
 H   -3.404689   -2.495767    0.935377
 H   -4.907828   -1.898632    1.696460
 H   -3.344471   -1.713118    2.531128
 H   -3.973964    1.768221    1.403263
 H   -3.934397    0.667788    2.797643
 H   -5.351034    0.675261    1.720134
 H   -3.421456    1.806818   -0.859469
 H   -5.184127    1.540247   -0.757584
 H   -4.292681    1.096842   -2.235582
 H   -6.076137   -0.882392   -0.431973
 H   -4.962967   -2.239473   -0.766056
 H   -5.384030   -1.095602   -2.058213
 C    2.861922   -1.852598    1.295400
 C    4.191869   -2.254127    1.176268
 C    2.048009   -1.690876    0.163384
 C    4.737734   -2.504622   -0.082169
 C    2.611445   -1.949363   -1.097597
 C    3.937859   -2.353556   -1.217697
 C    0.662034   -1.205235    0.338881
 C   -0.331647   -1.184262   -0.605303
 H    4.357104   -2.541962   -2.209091
 H    2.013063   -1.811427   -2.001229
 H    4.804241   -2.371495    2.073659
 H    2.440477   -1.658143    2.285694
Cu    0.277598    0.828432   -0.534224
 H   -0.097670   -1.552831   -1.614368
 H   -1.224873    1.030217   -1.114772
 H    0.398571   -0.940785    1.371820
 H    5.780568   -2.814893   -0.180387
51
Figure 3_para-H_int1 / electronic energy: -2821.46389768 a.u. / lowest freq: 24.91 cm-1
 H    2.177289    4.048566   -1.424842
 H    3.625940    1.430141   -1.702736
 C    2.257418    3.931167   -0.333953
 C    3.697411    1.459631   -0.605384
 H    3.202298    4.378526    0.011393
 H    1.413556    4.463648    0.129621
 H    4.574655    2.059023   -0.315716
 H    3.829296    0.429622   -0.240613
 P    2.161308    2.158457    0.098955
 C    2.490613    2.140439    1.896798
 H    3.430512    2.661361    2.136156
 H    1.659889    2.626576    2.429545
 H    2.558486    1.097833    2.241696
 B   -1.714371   -0.128451   -0.460298
 O   -2.814246   -0.452570   -1.323973
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 O   -2.226113   -0.017643    0.886848
 C   -4.005994   -0.168278   -0.612144
 C   -3.575856   -0.448896    0.873853
 C   -5.120447   -1.069896   -1.127227
 C   -4.387913    1.299445   -0.837539
 C   -3.606574   -1.944208    1.210609
 C   -4.367180    0.328658    1.918061
 H   -3.081372   -2.531481    0.442492
 H   -4.631358   -2.333606    1.311156
 H   -3.086772   -2.100961    2.168100
 H   -4.231593    1.411892    1.797252
 H   -4.023790    0.058479    2.928791
 H   -5.442778    0.099797    1.854568
 H   -3.623603    1.980383   -0.434609
 H   -5.354945    1.551448   -0.376605
 H   -4.466519    1.483749   -1.919950
 H   -6.036237   -0.954794   -0.526331
 H   -4.820709   -2.126489   -1.111470
 H   -5.364086   -0.807412   -2.168490
 C    2.682694   -2.080728    1.239809
 C    3.978619   -2.583347    1.126234
 C    1.915160   -1.789088    0.101856
 C    4.535571   -2.804588   -0.132691
 C    2.489818   -2.018395   -1.159495
 C    3.782385   -2.521009   -1.274933
 C    0.566720   -1.204583    0.274671
 C   -0.378525   -0.998365   -0.684526
 H    4.211840   -2.685712   -2.266230
 H    1.925525   -1.783226   -2.065071
 H    4.555363   -2.803190    2.028038
 H    2.251687   -1.908738    2.230243
Cu    0.313301    1.013403   -0.435708
 H   -0.134390   -1.293231   -1.716796
 H   -1.302236    1.194160   -0.823802
 H    0.298769   -0.979468    1.316330
 H    5.551161   -3.196234   -0.226409
51
Figure 3_para-H_ts(Cu>O) / electronic energy: -2821.45732695 a.u. / lowest freq: -34.56 cm-1
 H    0.933174    4.432955   -1.801058
 H    2.906194    2.302193   -1.211083
 C    0.724513    4.482283   -0.721986
 C    2.644537    2.419108   -0.149077
 H    1.429772    5.182112   -0.247780
 H   -0.301845    4.854737   -0.587633
 H    3.267950    3.209622    0.296376
 H    2.850774    1.464132    0.357530
 P    0.865693    2.809744   -0.001458
 C    0.631703    3.083387    1.790574
 H    1.342726    3.825271    2.185770
 H   -0.396378    3.429369    1.974396
 H    0.768497    2.128273    2.319672
 B   -1.254056   -0.895288   -0.764619
 O   -2.355072   -1.742404   -1.096282
 O   -1.551994   -0.304208    0.545181
 C   -3.483903   -1.264822   -0.381190
 C   -2.843298   -0.734903    0.958178
 C   -4.468975   -2.411784   -0.192053
 C   -4.161223   -0.147097   -1.185267
 C   -2.642277   -1.848966    1.988295
 C   -3.584052    0.432601    1.598019
 H   -2.129706   -2.711498    1.537445
 H   -3.592621   -2.191438    2.425363
 H   -2.008152   -1.469042    2.803664
 H   -3.596381    1.309905    0.936618
 H   -3.082414    0.724792    2.533458
 H   -4.623869    0.163292    1.841116
 H   -3.509808    0.731585   -1.294066
 H   -5.104417    0.177023   -0.721081
 H   -4.386162   -0.524551   -2.194304
 H   -5.301241   -2.116273    0.465599
 H   -3.978531   -3.295187    0.238127
 H   -4.893151   -2.703766   -1.164890
 C    3.349998   -1.375184    1.236713
 C    4.716659   -1.649077    1.270877
 C    2.577966   -1.651576    0.095868
 C    5.344365   -2.211341    0.160003
 C    3.226963   -2.218995   -1.014442
 C    4.591084   -2.495770   -0.981672
 C    1.139394   -1.319626    0.111177
 C    0.241628   -1.455709   -0.883209
 H    5.072751   -2.938607   -1.857080
 H    2.657767   -2.448380   -1.918431
 H    5.292935   -1.423395    2.171708
 H    2.864010   -0.936035    2.112925
Cu   -0.429567    1.199210   -0.787037
 H    0.580435   -1.862551   -1.846950
 H   -1.289170    0.142828   -1.723507
 H    0.780188   -0.898407    1.059027
 H    6.415059   -2.428070    0.182083
51
Figure 3_para-H_int2 / electronic energy: -2821.46396376 a.u. / lowest freq: 9.86 cm-1
 H    3.685776   -2.794150   -2.165296
 H    2.570999   -4.122931    0.174321
 C    4.320752   -2.193988   -1.496725
 C    3.222599   -3.502408    0.807405
 H    5.257488   -2.738486   -1.300829
 H    4.553049   -1.246225   -2.004959
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 H     4.197230   -4.001103    0.922639
 H     2.748024   -3.400787    1.794568
 P     3.410042   -1.849991    0.050359
 C     4.669842   -1.045022    1.104238
 H     5.582540   -1.657623    1.171497
 H     4.929545   -0.062326    0.683167
 H     4.261275   -0.893396    2.114326
 B    -0.306351    0.638997   -0.852150
 O    -0.055484    1.964330   -1.372805
 O     0.224318    0.668159    0.552279
 C     0.865014    2.638464   -0.542477
 C     0.587496    2.009974    0.875089
 C     0.593166    4.137248   -0.613930
 C     2.294539    2.370478   -1.035826
 C    -0.608944    2.656016    1.574726
 C     1.790037    1.991094    1.808220
 H    -1.480337    2.700285    0.905698
 H    -0.381224    3.673346    1.926128
 H    -0.884076    2.047630    2.449612
 H     2.608808    1.386630    1.391852
 H     1.508871    1.551170    2.777301
 H     2.165628    3.009260    1.992461
 H     2.569570    1.305271   -0.955947
 H     3.042436    2.956154   -0.480577
 H     2.359351    2.644923   -2.099160
 H     1.213468    4.692185    0.107146
 H    -0.463395    4.359760   -0.414937
 H     0.829987    4.511020   -1.621725
 C    -4.679595   -0.848684    1.249484
 C    -6.015111   -1.248478    1.282903
 C    -4.011812   -0.632420    0.032761
 C    -6.716097   -1.447388    0.094050
 C    -4.732799   -0.843159   -1.155944
 C    -6.066096   -1.243002   -1.125414
 C    -2.598207   -0.199143    0.053757
 C    -1.830864    0.164684   -0.986579
 H    -6.603635   -1.399202   -2.064215
 H    -4.242988   -0.694308   -2.121217
 H    -6.510783   -1.405153    2.244356
 H    -4.138323   -0.693895    2.187405
Cu     1.548818   -0.715842   -0.233305
 H    -2.273597    0.140762   -1.993539
 H     0.415914   -0.277887   -1.508964
 H    -2.147601   -0.161732    1.054333
 H    -7.762797   -1.760396    0.115527
51
Figure 3_para-H_ts(C-Brot) / electronic energy: -2821.45857138 a.u. / lowest freq: -89.13 cm-1
 H     3.555473   -3.319837   -1.684444
 H     2.888926   -3.808986    1.148877
 C     4.279776   -2.571244   -1.330737
 C     3.609385   -3.023905    1.421728
 H     5.236787   -3.067619   -1.107413
 H     4.431542   -1.837625   -2.136587
 H     4.609179   -3.471674    1.531551
 H     3.297516   -2.590821    2.383612
 P     3.603656   -1.721702    0.139760
 C     4.972665   -0.620386    0.650310
 H     5.914578   -1.179845    0.761361
 H     5.112732    0.167699   -0.104650
 H     4.723347   -0.141527    1.608740
 B    -0.334792    0.428686   -0.712393
 O    -0.356134    1.734800   -1.319635
 O     0.310936    0.652099    0.632308
 C     0.613779    2.556627   -0.706586
 C     0.621086    2.037238    0.780616
 C     0.189413    4.014808   -0.847960
 C     1.969892    2.373226   -1.404998
 C    -0.481706    2.673034    1.627947
 C     1.959781    2.178994    1.493794
 H    -1.449281    2.640768    1.108001
 H    -0.256931    3.720741    1.877144
 H    -0.580852    2.109510    2.567745
 H     2.749834    1.608204    0.984043
 H     1.879767    1.794254    2.522335
 H     2.270839    3.233624    1.548823
 H     2.379815    1.357221   -1.282400
 H     2.721778    3.086399   -1.035431
 H     1.834007    2.543207   -2.483384
 H     0.843418    4.678978   -0.261825
 H    -0.847941    4.162601   -0.520156
 H     0.252818    4.320931   -1.903332
 C    -5.236269    0.115132    0.662101
 C    -6.504853   -0.456962    0.753835
 C    -4.188535   -0.534796   -0.010516
 C    -6.756197   -1.698283    0.170849
 C    -4.460765   -1.785543   -0.592546
 C    -5.725982   -2.358697   -0.503048
 C    -2.860888    0.114514   -0.079156
 C    -1.754266   -0.340717   -0.687362
 H    -5.910964   -3.331732   -0.965312
 H    -3.670504   -2.320978   -1.123889
 H    -7.301788    0.071104    1.283582
 H    -5.048781    1.089478    1.122605
Cu     1.681888   -0.696135   -0.184536
 H    -1.827117   -1.311092   -1.200350
 H     0.479473   -0.394233   -1.395934
 H    -2.811714    1.079302    0.441700
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 H   -7.747901   -2.151488    0.241085
51
Figure 3_para-H_int3 / electronic energy: -2821.46355865 a.u. / lowest freq: 19.13 cm-1
 H    3.791442   -2.752377   -2.171400
 H    3.335160   -3.828092    0.543063
 C    4.461911   -2.005412   -1.721024
 C    4.029168   -3.057438    0.909892
 H    5.477539   -2.424414   -1.649299
 H    4.478609   -1.122070   -2.376797
 H    5.060624   -3.436673    0.843593
 H    3.787172   -2.849709    1.962772
 P    3.820684   -1.533289   -0.075604
 C    5.123935   -0.429361    0.578451
 H    6.114671   -0.906138    0.519351
 H    5.142642    0.505791   -0.001026
 H    4.904054   -0.183592    1.627939
 B   -0.375005    0.236714   -0.393982
 O   -0.473468    1.493068   -1.093060
 O    0.433199    0.546903    0.844282
 C    0.451475    2.417373   -0.561674
 C    0.581078    1.962548    0.938734
 C   -0.099612    3.828022   -0.734934
 C    1.778846    2.304112   -1.324033
 C   -0.560926    2.489119    1.809547
 C    1.920579    2.282152    1.587364
 H   -1.536289    2.303899    1.337115
 H   -0.463527    3.566603    2.009502
 H   -0.546281    1.958350    2.773168
 H    2.745323    1.759430    1.080959
 H    1.916338    1.959751    2.639889
 H    2.123132    3.363985    1.563529
 H    2.248925    1.314058   -1.190968
 H    2.505936    3.068184   -1.011523
 H    1.582622    2.430588   -2.399000
 H    0.543353    4.571811   -0.238833
 H   -1.116125    3.914102   -0.328335
 H   -0.144855    4.079375   -1.805645
 C   -5.453498    0.120283   -0.620139
 C   -6.732657   -0.395700   -0.414820
 C   -4.307904   -0.584458   -0.214945
 C   -6.896942   -1.634554    0.203606
 C   -4.492925   -1.831991    0.406896
 C   -5.768662   -2.349591    0.613034
 C   -2.974610    0.010457   -0.450716
 C   -1.776904   -0.485479   -0.101367
 H   -5.885551   -3.321811    1.098632
 H   -3.624734   -2.408947    0.734107
 H   -7.606545    0.174209   -0.740684
 H   -5.333385    1.092462   -1.106719
Cu    1.792659   -0.689487   -0.095607
 H   -1.747405   -1.453118    0.422298
 H    0.341959   -0.657962   -1.085610
 H   -2.991996    0.976828   -0.971436
 H   -7.897109   -2.043894    0.364925
36
Figure 3_para-H-alkenylBpin / electronic energy: -719.616306926 a.u. / lowest freq: 11.87 cm-1
 B    0.922364   -0.365147   -0.028404
 O    1.894117   -1.316245   -0.173823
 O    1.433940    0.892512    0.148584
 C    3.161660   -0.695762    0.122071
 C    2.848301    0.828137   -0.120020
 C    4.227554   -1.277336   -0.792080
 C    3.487647   -1.014695    1.579963
 C    3.048728    1.254565   -1.573413
 C    3.579766    1.781941    0.809984
 H    2.542480    0.568799   -2.269063
 H    4.114997    1.296474   -1.838243
 H    2.618726    2.256986   -1.714756
 H    3.324723    1.603424    1.862628
 H    3.311513    2.820863    0.566919
 H    4.668438    1.676163    0.689783
 H    2.735025   -0.594781    2.263998
 H    4.475038   -0.625732    1.866988
 H    3.496130   -2.106186    1.715677
 H    5.185806   -0.755417   -0.649802
 H    3.942879   -1.205244   -1.849722
 H    4.382907   -2.340283   -0.555288
 C   -3.806743    1.248461    0.192092
 C   -5.197110    1.149758    0.183811
 C   -2.998838    0.113525    0.018524
 C   -5.806490   -0.090352   -0.001273
 C   -3.628094   -1.129019   -0.169041
 C   -5.016012   -1.228789   -0.178362
 C   -1.532965    0.275159    0.038943
 C   -0.597425   -0.686080   -0.066780
 H   -5.487864   -2.203239   -0.325431
 H   -3.028632   -2.030869   -0.311211
 H   -6.895940   -0.172912   -0.008967
 H   -5.805802    2.046357    0.322501
 H   -3.332001    2.222916    0.336640
 H   -0.908917   -1.730947   -0.184153
 H   -1.195659    1.312156    0.158923
51
Figure 3_para-H_pc2_rev / electronic energy: -2821.47379868 a.u. / lowest freq: 7.91 cm-1
 H   -1.891178    3.978014   -0.931188
 H    0.744047    3.624321   -2.162854
 C   -1.423624    3.847381    0.056070
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 C    1.151378    3.545628   -1.143938
 H   -1.079604    4.824743    0.429409
 H   -2.184530    3.446734    0.742937
 H    1.348260    4.555441   -0.751758
 H    2.097993    2.988858   -1.192969
 P   -0.044323    2.653433   -0.087134
 C    0.722927    2.708951    1.571856
 H    1.104996    3.713018    1.812745
 H   -0.030718    2.423580    2.321600
 H    1.536897    1.971636    1.621928
 B    1.102592   -0.917294    0.434901
 O    2.077244   -0.385678    1.240564
 O    1.619144   -1.663471   -0.591113
 C    3.341842   -0.590656    0.577678
 C    3.030149   -1.822737   -0.347978
 C    4.419115   -0.828932    1.621918
 C    3.642515    0.678496   -0.217408
 C    3.217667   -3.162541    0.361369
 C    3.768633   -1.824250   -1.676306
 H    2.700440   -3.180345    1.332312
 H    4.281459   -3.384639    0.527720
 H    2.792959   -3.961665   -0.263554
 H    3.510439   -0.949604   -2.287383
 H    3.503685   -2.725677   -2.248492
 H    4.856875   -1.832938   -1.513446
 H    2.868808    0.861297   -0.978421
 H    4.617661    0.617777   -0.720916
 H    3.665851    1.539695    0.466539
 H    5.375239   -1.082784    1.140221
 H    4.145585   -1.638707    2.310567
 H    4.570256    0.085147    2.214904
 C   -3.617294   -2.197209   -0.667879
 C   -4.991323   -2.269942   -0.448642
 C   -2.817753   -1.296165    0.051025
 C   -5.595783   -1.436609    0.492725
 C   -3.440203   -0.459363    0.992321
 C   -4.813321   -0.530049    1.210661
 C   -1.359240   -1.259465   -0.201703
 C   -0.416609   -0.694550    0.649415
 H   -5.278382    0.132255    1.945004
 H   -2.846450    0.266451    1.553338
 H   -6.673261   -1.490682    0.665071
 H   -5.594624   -2.980078   -1.019309
 H   -3.149664   -2.849674   -1.410087
Cu   -0.861513    0.660040   -0.871013
 H   -0.747026   -0.236954    1.588859
 H   -1.585117    0.803311   -2.288746
 H   -1.010698   -1.929456   -0.994853
51
Figure 3_para-H_ts(CuHadd_rev) / electronic energy: -2821.44750747 a.u. / lowest freq: -855.62 cm-1
 H   -1.330551    4.368876   -1.136190
 H    1.158195    3.399148   -2.330387
 C   -0.826994    4.346554   -0.158696
 C    1.606738    3.370838   -1.326658
 H   -0.300223    5.299961    0.002086
 H   -1.595927    4.224235    0.618919
 H    2.050826    4.351962   -1.099259
 H    2.398031    2.606747   -1.325252
 P    0.324426    2.927325   -0.103469
 C    1.167391    3.143064    1.503663
 H    1.603931    4.148955    1.603105
 H    0.441570    2.977998    2.313962
 H    1.960141    2.387561    1.601059
 B    0.867817   -1.151517    0.394912
 O    1.813088   -1.205805    1.408948
 O    1.446995   -1.423180   -0.840481
 C    3.105293   -1.255184    0.793770
 C    2.781319   -1.886734   -0.607765
 C    4.044685   -2.078555    1.660496
 C    3.613888    0.182142    0.678939
 C    2.738673   -3.414709   -0.569790
 C    3.681629   -1.417980   -1.740777
 H    2.112156   -3.776817    0.259174
 H    3.742881   -3.850929   -0.463899
 H    2.301443   -3.783682   -1.509424
 H    3.590980   -0.336286   -1.907499
 H    3.402524   -1.926871   -2.675572
 H    4.735587   -1.653775   -1.527860
 H    2.949901    0.782358    0.038053
 H    4.631742    0.228547    0.265422
 H    3.629132    0.639600    1.679355
 H    5.015547   -2.219918    1.161478
 H    3.620080   -3.065087    1.888164
 H    4.225179   -1.561132    2.614682
 C   -3.696575   -2.160240   -0.695928
 C   -5.037964   -2.373073   -0.373534
 C   -3.005899   -1.054783   -0.188479
 C   -5.708398   -1.480806    0.461591
 C   -3.690662   -0.160967    0.645970
 C   -5.028328   -0.371733    0.970540
 C   -1.554119   -0.870335   -0.505079
 C   -0.604145   -0.843195    0.588872
 H   -5.547974    0.337775    1.619359
 H   -3.165645    0.717370    1.033337
 H   -6.759343   -1.644468    0.711554
 H   -5.560324   -3.242599   -0.780094
 H   -3.175606   -2.864784   -1.349943
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Cu   -0.652452    0.961645   -0.409202
 H   -1.001567   -0.666295    1.595801
 H   -1.781161    0.504844   -1.439332
 H   -1.235758   -1.437226   -1.387004
51
Figure 3_para-H_L-Cu-alkyl_rev / electronic energy: -2821.50134039 a.u. / lowest freq: 25.16 cm-1
 H    3.749134    1.612199   -0.357362
 H    2.302766    1.652954    2.199722
 C    3.117850    2.461184   -0.661479
 C    1.662024    2.456293    1.806879
 H    3.568339    3.399532   -0.302631
 H    3.076063    2.476206   -1.760949
 H    2.125722    3.429969    2.028412
 H    0.686677    2.395086    2.312548
 P    1.434052    2.221375    0.007930
 C    0.543286    3.736150   -0.500092
 H    1.113208    4.642479   -0.242463
 H    0.368830    3.714629   -1.586087
 H   -0.433743    3.773554    0.004356
 B   -1.580959   -1.098638   -0.554028
 O   -2.515107   -0.428762   -1.354234
 O   -2.066660   -1.204020    0.754091
 C   -3.405971    0.256803   -0.475347
 C   -3.389440   -0.669889    0.792066
 C   -4.766674    0.406720   -1.137351
 C   -2.804476    1.639291   -0.197651
 C   -4.370094   -1.838573    0.677503
 C   -3.599878    0.057501    2.112669
 H   -4.260113   -2.354822   -0.287787
 H   -5.415581   -1.513036    0.784491
 H   -4.153060   -2.564703    1.475228
 H   -2.805575    0.792709    2.299499
 H   -3.590630   -0.665518    2.942252
 H   -4.570395    0.577259    2.126469
 H   -1.829739    1.547851    0.307219
 H   -3.463978    2.265985    0.420762
 H   -2.637546    2.152816   -1.156567
 H   -5.501428    0.823695   -0.431284
 H   -5.143607   -0.555932   -1.507873
 H   -4.694390    1.092827   -1.994881
 C    3.005321   -2.385335   -0.908308
 C    4.301228   -1.906269   -0.710803
 C    2.009907   -2.199475    0.059724
 C    4.632044   -1.236162    0.468100
 C    2.360149   -1.532348    1.243264
 C    3.654961   -1.056814    1.449306
 C    0.571751   -2.597904   -0.201968
 C   -0.207051   -1.545355   -1.002127
 H    3.904198   -0.544855    2.382675
 H    1.597069   -1.378805    2.012852
 H    5.646758   -0.861941    0.624414
 H    5.060175   -2.058525   -1.482869
 H    2.756682   -2.903958   -1.839126
Cu    0.521828    0.275183   -0.564290
 H   -0.069866   -1.635357   -2.093205
 H    0.076223   -2.756294    0.769299
 H    0.563335   -3.576370   -0.716694
72
Figure 3_para-H_pc3_01 / electronic energy: -3660.33447417 a.u. / lowest freq: 14.60 cm-1
 C    0.916980   -0.936335   -0.680959
 C    1.192007   -0.785498    0.670668
 C    2.307941    0.096830    1.153532
 O    3.573582   -0.598356    1.177527
 P    4.383558   -0.816841   -0.184189
 O    4.248086    0.226628   -1.221642
 O    5.836892   -1.033019    0.457107
 O    3.965376   -2.255928   -0.758277
 C    6.928571   -1.360565   -0.396663
 H    0.331528   -1.784672   -1.047871
 H    1.511536   -0.405558   -1.431718
 H    0.824154   -1.531213    1.385330
 H    2.410385    0.992672    0.521698
 H    2.145686    0.417487    2.190332
 B   -3.195507   -0.502407   -1.040797
 O   -3.802702   -0.822203    0.153771
 O   -2.806899   -1.623571   -1.728763
 C   -3.563938   -2.215298    0.412429
 C   -3.299495   -2.780724   -1.033226
 C   -4.768788   -2.813562    1.119792
 C   -2.334766   -2.286167    1.316957
 C   -4.576558   -3.222999   -1.744981
 C   -2.252674   -3.881750   -1.099243
 H   -5.349837   -2.441641   -1.702441
 H   -4.988209   -4.145273   -1.309955
 H   -4.348185   -3.414656   -2.803702
 H   -1.278351   -3.537964   -0.726937
 H   -2.120556   -4.208815   -2.141123
 H   -2.566391   -4.754332   -0.506158
 H   -1.466838   -1.812330    0.833926
 H   -2.074056   -3.320890    1.581163
 H   -2.544001   -1.738474    2.247459
 H   -4.638005   -3.897460    1.257388
 H   -5.698898   -2.639672    0.563398
 H   -4.881576   -2.357410    2.114700
 C    0.507164    2.787395   -1.809659
 C    1.071561    4.051871   -1.699897
 C   -0.859492    2.541968   -1.517122
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 C    0.296499    5.148622   -1.303020
 C   -1.624907    3.671349   -1.151266
 C   -1.056779    4.942584   -1.041280
 C   -1.384136    1.158617   -1.531262
 C   -2.908153    0.968330   -1.491809
 H   -1.689587    5.785959   -0.749018
 H   -2.691320    3.555047   -0.946639
 H    0.740949    6.142423   -1.211638
 H    2.132936    4.187107   -1.927110
 H    1.138112    1.947451   -2.117716
Cu   -0.397686    0.408786    0.087142
 H   -3.392644    1.221449   -2.457210
 H   -3.368392    1.623933   -0.735596
 H   -0.956800    0.606479   -2.383466
 H    7.833938   -1.367533    0.222827
 H    7.043147   -0.612049   -1.195455
 H    6.793573   -2.355738   -0.849566
 C    3.845319   -3.388929    0.090570
 H    3.873347   -4.281053   -0.548241
 H    2.888409   -3.364958    0.633840
 H    4.672147   -3.441716    0.815783
 H    0.990944    2.822909    2.378122
 H   -0.236855    3.681235    1.413184
 H   -0.431930    3.548286    3.193516
 C   -0.085925    3.028588    2.286483
 H    0.336172    0.319730    3.718503
 P   -0.991114    1.460857    2.026887
 H   -1.053700    1.165295    4.465862
 C   -0.730077    0.564760    3.601162
 H   -2.952918    2.702221    1.348057
 H   -2.991443    2.384596    3.110900
 C   -2.747009    1.954289    2.127488
 H   -1.299050   -0.377019    3.588987
 H   -3.378411    1.074483    1.933030
72
Figure 3_para-H_pc3_02 / electronic energy: -3660.33292348 a.u. / lowest freq: 26.47 cm-1
 C   -0.154708   -1.252905   -1.354020
 C    0.178896   -2.077433   -0.294226
 C    1.408472   -1.870612    0.537763
 O    2.570565   -2.473494   -0.075849
 P    3.692823   -1.556991   -0.741713
 O    3.307758   -0.650192   -1.842733
 O    4.283952   -0.813515    0.560888
 O    4.788510   -2.624706   -1.188181
 C    5.210865    0.255353    0.409755
 H   -0.854162   -1.592225   -2.124518
 H    0.462354   -0.382323   -1.605530
 H   -0.279398   -3.071592   -0.229545
 H    1.598785   -0.801528    0.704256
 H    1.310075   -2.354616    1.517721
 B   -0.859559    2.387265   -1.009868
 O    0.415964    2.352909   -1.516756
 O   -0.943816    3.190579    0.103017
 C    1.288938    2.990194   -0.568801
 C    0.294848    3.917124    0.217147
 C    2.396044    3.715592   -1.314815
 C    1.877873    1.880302    0.298383
 C    0.085548    5.272117   -0.457144
 C    0.636217    4.115643    1.684640
 H   -0.139911    5.157082   -1.527879
 H    0.970203    5.916910   -0.354821
 H   -0.767389    5.780589    0.015998
 H    0.674811    3.164750    2.230488
 H   -0.123750    4.752165    2.161759
 H    1.610997    4.615945    1.788685
 H    1.083415    1.363015    0.858584
 H    2.616591    2.264135    1.016931
 H    2.369280    1.150272   -0.359945
 H    3.033866    4.277038   -0.615373
 H    1.996607    4.414447   -2.061709
 H    3.026427    2.983825   -1.841504
 C   -4.622545   -0.894236   -0.207497
 C   -5.542502   -1.852202   -0.619920
 C   -3.655092   -0.348803   -1.087737
 C   -5.549547   -2.313024   -1.940364
 C   -3.698289   -0.817719   -2.421365
 C   -4.619730   -1.780254   -2.833763
 C   -2.642039    0.608602   -0.594480
 C   -2.048624    1.576948   -1.625606
 H   -4.612539   -2.113802   -3.875753
 H   -2.990563   -0.422290   -3.153551
 H   -6.272654   -3.064095   -2.266822
 H   -6.272291   -2.239335    0.097489
 H   -4.645444   -0.541426    0.827148
Cu   -1.312094   -0.702322    0.228025
 H   -2.817630    2.268541   -2.032720
 H   -1.640357    1.035273   -2.494274
 H   -3.059896    1.176550    0.253776
 H    5.328101    0.726330    1.393867
 H    4.844842    1.001231   -0.311176
 H    6.189226   -0.121994    0.072399
 C    5.314760   -3.594773   -0.288605
 H    6.215034   -4.012988   -0.755615
 H    4.585718   -4.400286   -0.117373
 H    5.587237   -3.137353    0.674648
 H    0.565130    0.434578    3.007558
 H   -0.794942    1.543950    2.683397
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 H   -0.662141    0.733565    4.279978
 C   -0.503393    0.615896    3.196779
 H    0.088050   -2.403308    3.356051
 P   -1.499503   -0.758144    2.511923
 H   -1.148926   -2.017719    4.591171
 C   -0.979976   -2.197795    3.518074
 H   -3.561181    0.511581    2.711028
 H   -3.126615   -0.255072    4.271717
 C   -3.163975   -0.400124    3.180865
 H   -1.550651   -3.086690    3.209071
 H   -3.843320   -1.235070    2.954397
72
Figure 3_para-H_ts(AS)_01 / electronic energy: -3660.29889725 a.u. / lowest freq: -278.04 cm-1
 C    0.009580   -1.218146    1.559352
 C   -0.156334   -2.287634    0.645735
 C   -0.834340   -2.122161   -0.565171
 O   -2.783091   -2.866887   -0.356910
 P   -3.710907   -1.688293   -0.079721
 O   -3.705953   -0.483287   -0.965700
 O   -5.194990   -2.356838    0.041364
 O   -3.438936   -1.153105    1.447266
 C   -6.301835   -1.502515    0.233828
 H    0.480985   -1.408760    2.526217
 H   -0.663837   -0.356169    1.509822
 H    0.307329   -3.256704    0.855069
 H   -1.229260   -1.142312   -0.847431
 H   -0.732489   -2.858755   -1.359301
 B    0.650489    2.521291    0.224810
 O    0.408568    3.839540   -0.053561
 O   -0.504726    1.797080    0.346516
 C   -1.005733    4.072120    0.108748
 C   -1.608142    2.630905   -0.071839
 C   -1.466828    5.086364   -0.924563
 C   -1.205845    4.630324    1.517012
 C   -1.909595    2.278477   -1.526398
 C   -2.819042    2.323561    0.793111
 H   -1.037750    2.458316   -2.174203
 H   -2.751613    2.872703   -1.910289
 H   -2.205572    1.220248   -1.579630
 H   -2.581414    2.389812    1.863452
 H   -3.177278    1.308526    0.569919
 H   -3.633005    3.031634    0.572160
 H   -0.885459    3.909547    2.284041
 H   -2.257760    4.890225    1.702655
 H   -0.600617    5.541435    1.633019
 H   -2.558076    5.219194   -0.874929
 H   -1.197811    4.781425   -1.944409
 H   -0.996777    6.061334   -0.726853
 C    3.738727   -1.051048    2.199080
 C    4.976487   -1.661551    2.367369
 C    3.545408   -0.006972    1.267857
 C    6.076845   -1.251748    1.607774
 C    4.669833    0.401068    0.527095
 C    5.912393   -0.214828    0.691347
 C    2.193322    0.593281    1.097602
 C    2.098471    1.924869    0.362198
 H    6.763860    0.129126    0.097618
 H    4.577217    1.218320   -0.190467
 H    7.049916   -1.731368    1.736762
 H    5.086897   -2.464258    3.101444
 H    2.887491   -1.386186    2.799489
Cu    1.237238   -0.823458    0.040873
 H    2.492645    1.851047   -0.668736
 H    2.737320    2.692813    0.844190
 H    1.714620    0.679970    2.082504
 H   -7.212794   -2.117377    0.206251
 H   -6.360482   -0.737714   -0.557313
 H   -6.253575   -0.989419    1.209855
 C   -3.312862   -2.081007    2.499472
 H   -2.939638   -1.544549    3.383769
 H   -2.606157   -2.887229    2.244958
 H   -4.284377   -2.540757    2.751545
 H   -0.303231   -0.749257   -3.177627
 H    0.493736    0.833348   -2.996619
 H    0.986728   -0.265764   -4.325242
 C    0.654305   -0.218068   -3.277027
 H    1.182274   -3.231751   -2.629941
 P    1.897747   -0.955839   -2.160558
 H    2.367718   -2.663453   -3.849433
 C    2.109969   -2.661403   -2.779199
 H    3.406589    0.929941   -2.473821
 H    3.629639   -0.313436   -3.743092
 C    3.454272   -0.150855   -2.668531
 H    2.914325   -3.155136   -2.213466
 H    4.293410   -0.573023   -2.098019
72
Figure 3_para-H_ts(AS)_02 / electronic energy: -3660.30030627 a.u. / lowest freq: -282.42 cm-1
 C    0.530275   -1.255921   -0.520077
 C    0.721628   -1.392169    0.884545
 C    1.605091   -0.556600    1.573315
 O    3.523918   -1.392439    1.543431
 P    4.130298   -1.158353    0.162594
 O    3.609721   -0.069345   -0.724757
 O    5.731798   -1.000227    0.440597
 O    4.061226   -2.549755   -0.695401
 C    6.586608   -0.730202   -0.649030
 H   -0.141229   -1.941745   -1.042953
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 H    1.352665   -0.837491   -1.108721
 H    0.167611   -2.149762    1.447274
 H    2.050511    0.300963    1.066945
 H    1.626007   -0.559549    2.662783
 B   -3.023207   -0.280186   -1.277507
 O   -3.952276   -0.290622   -0.267005
 O   -2.678206   -1.543076   -1.676952
 C   -4.038000   -1.634269    0.240466
 C   -3.505375   -2.487639   -0.973014
 C   -5.472566   -1.931687    0.644801
 C   -3.124722   -1.685938    1.463168
 C   -4.609216   -2.921756   -1.934000
 C   -2.656692   -3.684403   -0.572754
 H   -5.233861   -2.069482   -2.240329
 H   -5.258401   -3.688131   -1.487114
 H   -4.150036   -3.346164   -2.838778
 H   -1.772422   -3.382959    0.004490
 H   -2.309260   -4.212539   -1.472802
 H   -3.244064   -4.391113    0.032529
 H   -2.090871   -1.416968    1.193891
 H   -3.120155   -2.676842    1.938434
 H   -3.481598   -0.953478    2.202087
 H   -5.579207   -2.982584    0.952922
 H   -6.176218   -1.733868   -0.174114
 H   -5.758964   -1.298264    1.497509
 C    1.305708    2.272901   -1.435120
 C    2.031276    3.456546   -1.352615
 C   -0.103735    2.279734   -1.551051
 C    1.383880    4.695213   -1.388513
 C   -0.734521    3.536226   -1.598127
 C   -0.002969    4.723591   -1.518376
 C   -0.855678    0.988147   -1.573217
 C   -2.366159    1.037575   -1.814816
 H   -0.528458    5.681437   -1.563099
 H   -1.818550    3.596694   -1.712034
 H    1.954491    5.624489   -1.320741
 H    3.118919    3.406876   -1.253044
 H    1.854428    1.326711   -1.381924
Cu   -0.407425    0.290391    0.274529
 H   -2.586785    1.201044   -2.887658
 H   -2.832534    1.872170   -1.270790
 H   -0.388784    0.304468   -2.293065
 H    7.609741   -0.637866   -0.257736
 H    6.310372    0.209633   -1.154356
 H    6.566335   -1.543820   -1.394575
 C    4.399551   -3.764096   -0.065686
 H    4.355526   -4.560137   -0.822784
 H    3.698589   -4.005947    0.749958
 H    5.420859   -3.735773    0.352239
 H    1.015282    2.734443    2.404710
 H    0.169674    3.660907    1.136712
 H   -0.322721    3.842538    2.852541
 C    0.038283    3.132453    2.092687
 H   -0.379112    0.640692    3.887158
 P   -1.132876    1.751996    1.866415
 H   -1.647679    1.852791    4.257926
 C   -1.333095    1.071214    3.549532
 H   -2.632523    3.188808    0.632138
 H   -3.040818    3.192139    2.376334
 C   -2.731535    2.561053    1.529188
 H   -2.088762    0.272373    3.538159
 H   -3.495617    1.794122    1.333788
72
Figure 3_para-H_pi-allyl_01 / electronic energy: -3660.32333278 a.u. / lowest freq: 24.00 cm-1
 C   -0.120800   -1.531426   -1.506721
 C   -0.608322   -2.293013   -0.410657
 C    0.044011   -2.269962    0.810284
 O    2.972569   -1.189920    1.035550
 P    3.714950   -1.347226   -0.266303
 O    3.010066   -1.368631   -1.594862
 O    4.879370   -0.184617   -0.265166
 O    4.629618   -2.711639   -0.216973
 C    5.749634   -0.107727   -1.367942
 H   -0.744938   -1.449979   -2.398300
 H    0.970629   -1.414056   -1.629005
 H   -1.635753   -2.666218   -0.456958
 H    1.114480   -2.010201    0.891747
 H   -0.441341   -2.707662    1.686886
 B   -3.094251    0.655121   -0.812699
 O   -3.970758    0.781904    0.232733
 O   -3.297215   -0.495730   -1.525968
 C   -4.697089   -0.456735    0.354388
 C   -4.553921   -1.059779   -1.089966
 C   -6.125073   -0.162893    0.781822
 C   -3.982223   -1.281258    1.423794
 C   -5.623092   -0.553720   -2.056679
 C   -4.484020   -2.575602   -1.143525
 H   -5.711607    0.542621   -2.025464
 H   -6.607583   -0.989145   -1.834596
 H   -5.344373   -0.841450   -3.080906
 H   -3.670920   -2.978826   -0.527506
 H   -4.325350   -2.905726   -2.180502
 H   -5.429030   -3.012636   -0.787647
 H   -2.941594   -1.493551    1.134970
 H   -4.493267   -2.235668    1.613976
 H   -3.966970   -0.710864    2.364266
 H   -6.723071   -1.086563    0.790856
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 H   -6.607810    0.562881    0.114798
 H   -6.131349    0.255808    1.798994
 C    1.879495    1.729324   -1.285394
 C    2.958604    2.575259   -1.053044
 C    0.554588    2.168654   -1.096693
 C    2.751781    3.893525   -0.638825
 C    0.362953    3.500251   -0.693772
 C    1.447378    4.351629   -0.468337
 C   -0.580899    1.214620   -1.315735
 C   -1.997844    1.742327   -1.107501
 H    1.264548    5.383598   -0.157338
 H   -0.646375    3.893193   -0.559405
 H    3.600364    4.555330   -0.449781
 H    3.971647    2.186248   -1.173971
 H    2.079381    0.692401   -1.575388
Cu   -0.342507   -0.251955    0.040840
 H   -2.315360    2.320040   -1.998825
 H   -2.037795    2.445852   -0.264854
 H   -0.484117    0.771805   -2.312702
 H    6.427220    0.744257   -1.209394
 H    5.201996    0.041381   -2.313445
 H    6.359572   -1.023163   -1.468636
 C    5.375543   -2.982598    0.943882
 H    5.872800   -3.954972    0.811135
 H    4.732146   -3.030648    1.838565
 H    6.151206   -2.216020    1.121465
 H    2.234019    0.629095    2.009282
 H    1.685658    2.277588    1.580455
 H    1.682509    1.777342    3.305011
 C    1.527254    1.435917    2.270126
 H    0.340545   -1.085301    3.502646
 P   -0.158202    0.791301    2.059317
 H   -0.321567    0.289888    4.439344
 C   -0.415662   -0.287610    3.507068
 H   -1.057711    3.003603    1.656490
 H   -1.143626    2.571521    3.389536
 C   -1.279897    2.193682    2.364784
 H   -1.415563   -0.743073    3.464061
 H   -2.322483    1.873102    2.223434
72
Figure 3_para-H_pi-allyl_02 / electronic energy: -3660.31700817 a.u. / lowest freq: 17.23 cm-1
 C   -1.384643   -0.458336   -2.244618
 C   -0.972902   -1.799940   -2.043945
 C    0.166102   -2.059680   -1.296819
 O    3.093783   -2.792692   -0.137705
 P    3.671925   -1.473658   -0.563565
 O    2.858492   -0.446593   -1.308608
 O    4.303903   -0.788830    0.800014
 O    5.031074   -1.707143   -1.460068
 C    4.972930    0.441343    0.687246
 H   -2.356646   -0.256728   -2.698868
 H   -0.630887    0.335792   -2.312069
 H   -1.699724   -2.601525   -2.220999
 H    0.997922   -1.335232   -1.248955
 H    0.399926   -3.075124   -0.969182
 B   -1.150909    2.626541   -0.348907
 O   -0.002257    2.195445   -0.956108
 O   -0.922291    3.627869    0.551314
 C    1.108876    2.736064   -0.207095
 C    0.464907    4.017507    0.428985
 C    2.273629    2.977231   -1.150413
 C    1.488958    1.682600    0.828150
 C    0.512991    5.229199   -0.497920
 C    0.999003    4.381682    1.803887
 H    0.154861    4.978169   -1.507485
 H    1.533287    5.630331   -0.582051
 H   -0.135596    6.020112   -0.093451
 H    0.813085    3.584499    2.535724
 H    0.507852    5.296876    2.166468
 H    2.082009    4.571411    1.758894
 H    0.643743    1.465650    1.499927
 H    2.341054    2.006143    1.443561
 H    1.785428    0.768426    0.292545
 H    3.099085    3.479169   -0.622398
 H    1.982915    3.596541   -2.009872
 H    2.634240    2.003096   -1.515309
 C   -4.341920   -1.172810    0.682222
 C   -5.482028   -1.937338    0.449479
 C   -3.935025   -0.165348   -0.213844
 C   -6.258122   -1.714753   -0.689927
 C   -4.737283    0.052054   -1.347109
 C   -5.879647   -0.712317   -1.582197
 C   -2.686826    0.611017    0.049860
 C   -2.550069    1.971302   -0.631268
 H   -6.482340   -0.516359   -2.472768
 H   -4.470967    0.836893   -2.057829
 H   -7.154630   -2.310777   -0.875208
 H   -5.771488   -2.709094    1.167198
 H   -3.749422   -1.352164    1.583518
Cu   -1.211131   -0.729293   -0.249316
 H   -3.360308    2.637929   -0.283659
 H   -2.662468    1.883802   -1.723729
 H   -2.565133    0.733465    1.136289
 H    5.095618    0.864887    1.695915
 H    4.409154    1.158460    0.068157
 H    5.975933    0.319988    0.239659
 C    5.964401   -2.665905   -1.028416
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 H     6.767978   -2.721408   -1.777853
 H     5.503522   -3.662422   -0.923764
 H     6.413327   -2.394367   -0.055922
 H    -0.847975    0.601727    3.110208
 H    -2.320213   -0.409272    3.165181
 H    -0.896388   -0.849847    4.157491
 C    -1.221019   -0.430043    3.193418
 H     1.690751   -0.621712    2.161716
 P    -0.567551   -1.436236    1.821315
 H     1.332907   -2.052972    3.172230
 C     1.204093   -1.605302    2.174501
 H    -2.329820   -3.110388    1.953772
 H    -1.025917   -3.433167    3.143083
 C    -1.242288   -3.104857    2.115123
 H     1.702755   -2.231182    1.414857
 H    -0.782012   -3.809116    1.406914
56
Figure 3_L-Cu-OtBu_dimer / electronic energy: -4668.27269506 a.u. / lowest freq: 20.28 cm-1
 H     1.454781    3.185323    2.121955
 H    -1.091667    3.295320    2.232897
 H     1.480610    4.376760    0.788877
 C     1.390257    3.304563    1.028715
 H     2.248895    2.774926    0.584062
 H    -1.141168    4.483981    0.897486
 C    -1.116435    3.408141    1.137329
 C     0.084478    2.685555    0.510787
 O     0.044189    1.344738    0.873648
 H    -2.049560    2.947919    0.774353
 H     0.052315    3.874754   -1.357879
 C     0.025055    2.825701   -1.018825
 H     0.875658    2.290877   -1.472279
 H    -0.901160    2.361194   -1.396152
 H     2.958274    1.006115   -2.657041
 H     3.299551   -1.873435   -2.121429
 C     3.677359    1.175331   -1.841405
 C     3.978968   -1.600940   -1.299765
 H     4.699652    1.104301   -2.245503
 H     3.518839    2.190392   -1.447525
 H     4.999010   -1.491753   -1.701120
 H     3.968610   -2.417548   -0.562485
 P     3.392482   -0.052886   -0.509011
 C     4.751395    0.319901    0.663359
 H     5.728245    0.345249    0.155766
 H     4.568915    1.292893    1.143584
 H     4.770992   -0.448839    1.450266
Cu     1.387359   -0.047785    0.355891
 H     1.052783   -3.300511    2.261431
 H     2.049259   -2.926990    0.836004
 O    -0.048207   -1.342931    0.876207
 C     1.110810   -3.401807    1.166003
 H     1.154224   -4.474801    0.916365
 C    -0.077761   -2.683448    0.511400
 H    -1.486976   -3.182509    2.088692
 H     0.959296   -2.370999   -1.370977
 C    -1.393184   -3.307099    0.998157
 C     0.017837   -2.822386   -1.016552
 H    -2.243357   -2.784789    0.529205
 H    -1.470986   -4.380974    0.761611
 H    -0.814236   -2.274610   -1.489485
 H    -0.015593   -3.870539   -1.357852
 H    -2.864028   -0.603368   -2.784246
 H    -3.433166    2.132063   -1.768599
 C    -3.581006   -0.953346   -2.026339
 C    -4.101882    1.661026   -1.032388
 H    -4.600512   -0.883806   -2.437656
 H    -3.356876   -2.007230   -1.803518
 H    -5.099460    1.538334   -1.483310
 H    -4.181695    2.333019   -0.164790
 P    -3.397860    0.051973   -0.503299
 C    -4.732552   -0.612373    0.562621
 H    -5.709729   -0.575241    0.056317
 H    -4.504550   -1.654856    0.830705
 H    -4.786261   -0.026266    1.492473
Cu    -1.393433    0.048543    0.362283
28
Figure 3_L-Cu-OtBu / electronic energy: -2334.10735270 a.u. / lowest freq: -39.13 cm-1
 H    -4.105877   -1.332535    0.968255
 H    -4.149740   -1.387400   -0.808196
 O    -1.712519   -0.853226    0.000001
 C    -4.074557   -0.711355    0.058637
 H    -4.956088   -0.048773    0.060108
 C    -2.745372    0.062111    0.000906
 H    -2.638090    0.394148    2.149194
 H    -2.753281    0.265927   -2.166060
 C    -2.653965    0.994061    1.224813
 C    -2.718854    0.919727   -1.279501
 H    -1.712633    1.569392    1.184920
 H    -3.490501    1.710689    1.287963
 H    -1.776368    1.492537   -1.324725
 H    -3.557324    1.634317   -1.340220
 H     2.442116    1.017710   -2.209934
 H     3.078065   -1.733910   -1.400494
 C     2.702639    1.337847   -1.190198
 C     3.315084   -1.349708   -0.397345
 H     3.784909    1.532944   -1.136890
 H     2.155445    2.266931   -0.971809
 H     4.370113   -1.036408   -0.368346
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 H     3.157970   -2.162063    0.327594
 P     2.201656    0.043634    0.000306
 C     2.853579    0.661225    1.592861
 H     3.931571    0.875098    1.526895
 H     2.317993    1.579995    1.874683
 H     2.679866   -0.091178    2.376412
Cu     0.062960   -0.408951   -0.003275
70
Figure 3_ed / electronic energy: -3155.87460188 a.u. / lowest freq: 11.42 cm-1
 H    -0.953281   -3.166097   -0.309839
 H    -2.577969   -2.483931   -0.153509
 O    -0.722801   -0.949157    1.165859
 C    -1.784111   -3.004943    0.394843
 H    -2.158222   -3.987377    0.724568
 C    -1.300935   -2.179344    1.589376
 H     0.648291   -3.149536    1.617528
 H    -3.221244   -1.298799    2.101803
 C    -0.183773   -2.938745    2.311306
 C    -2.439912   -1.904482    2.572798
 H     0.208864   -2.337581    3.146164
 H    -0.544498   -3.898139    2.713555
 H    -2.060320   -1.341525    3.439455
 H    -2.878571   -2.846939    2.937460
Cu     1.139839   -0.920846    0.386293
 H     1.056430    4.912258    0.610864
 H     2.420469    3.941746    2.458899
 H     0.701370    3.458516    2.402659
 C     1.735449    3.084044    2.391288
 H     2.707250    4.756558   -0.052951
 H     1.879972    2.458170    3.283891
 C     1.657698    4.452166   -0.184163
 H     1.306082    4.849580   -1.147882
 C     1.534322    2.938372   -0.174971
 C     2.012113    2.248287    1.144500
 O     0.145692    2.568639   -0.221946
 H     4.143931    2.596400    0.951770
 B    -0.029916    1.375300    0.444402
 H     3.702501    1.320418    2.112925
 C     3.450475    1.762470    1.137384
 O     1.127301    1.108628    1.201500
 H     3.251675    2.634595   -1.503243
 C     2.195444    2.340356   -1.418544
 H     1.664689    2.695001   -2.313853
 H     3.609342    0.994382    0.369926
 H     2.135444    1.240689   -1.404032
 H    -3.741486   -1.478482   -2.045890
 H    -4.291404   -1.318464    0.099435
 H    -2.833922   -0.708588   -3.361743
 C    -3.485339   -0.510025   -2.496037
 O    -1.630269   -0.279491   -1.014975
 H    -5.500527   -0.242437   -0.645178
 C    -4.684450   -0.292834    0.091969
 H    -4.409992   -0.043182   -2.870615
 B    -1.338180    0.190930    0.348230
 H    -5.115024   -0.091914    1.085474
 C    -2.753803    0.399038   -1.508504
 C    -3.582938    0.736127   -0.195713
 O    -2.623638    0.690654    0.835872
 H    -1.601520    1.343872   -3.063483
 C    -2.292899    1.655469   -2.264419
 H    -3.130173    2.197298   -2.730793
 H    -1.740687    2.341103   -1.608781
 H    -4.940611    2.237160   -1.041325
 C    -4.225555    2.125176   -0.210655
 H    -4.773476    2.286728    0.730889
 H    -3.466517    2.914749   -0.291729
 H     4.749033   -1.452497   -0.129415
 C     4.256493   -1.368792   -1.109548
 H     4.274484   -0.314095   -1.421428
 H     4.817512   -1.966521   -1.844659
 H     3.139485   -3.910893    0.308949
 C     2.717087   -3.740696   -0.692506
 P     2.524841   -1.944693   -0.980227
 H     3.382198   -4.194279   -1.443776
 H     1.733374   -4.230143   -0.742993
 C     1.932965   -1.853706   -2.708395
 H     2.575860   -2.437454   -3.385113
 H     1.920774   -0.803126   -3.035062
 H     0.902696   -2.235271   -2.761689
70
Figure 3_ts(TB) / electronic energy: -3155.86594930 a.u. / lowest freq: -80.57 cm-1
 H     3.010276   -2.382916    0.118642
 H     1.683795   -3.550734    0.289052
 O     0.986480   -1.022586    1.231429
 C     2.428017   -2.966919    0.847086
 H     3.108602   -3.663642    1.360560
 C     1.764613   -2.038365    1.865178
 H     3.454412   -0.689234    1.957273
 H     0.067382   -3.345104    2.249766
 C     2.833443   -1.280682    2.648443
 C     0.860433   -2.829879    2.810029
 H     2.364821   -0.587587    3.363520
 H     3.486796   -1.968789    3.205755
 H     0.379103   -2.153513    3.532327
 H     1.437600   -3.583696    3.368135
Cu     1.191646    0.705211   -0.156501
 H    -4.427383    0.766248   -0.614487
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 H   -4.518683    0.953062    1.818726
 H   -3.273614   -0.182983    1.196620
 C   -3.444824    0.713535    1.807889
 H   -4.940033    2.443526   -0.292598
 H   -3.136606    0.474696    2.836818
 C   -4.170605    1.821119   -0.775127
 H   -4.205093    2.017783   -1.857471
 C   -2.789480    2.154856   -0.232080
 C   -2.601465    1.882699    1.299916
 O   -1.819873    1.275125   -0.815333
 H   -3.824652    3.498708    2.084955
 B   -0.832690    0.986003    0.123485
 H   -2.656331    2.821205    3.244537
 C   -2.803566    3.100143    2.190308
 O   -1.228345    1.472481    1.363096
 H   -3.133588    4.320679   -0.285336
 C   -2.402291    3.578362   -0.637798
 H   -2.355518    3.636570   -1.735582
 H   -2.091022    3.901305    1.952964
 H   -1.410567    3.846106   -0.243686
 H    0.204209   -4.250825   -1.796312
 H   -0.675749   -4.205721    0.241701
 H    0.503640   -3.256638   -3.237470
 C   -0.244142   -3.509492   -2.470797
 O    0.458693   -1.748160   -1.013589
 H   -2.092610   -4.638531   -0.753443
 C   -1.697902   -3.906637   -0.032981
 H   -1.103862   -3.973045   -2.978655
 B    0.018530   -1.182613    0.206285
 H   -2.317693   -3.950556    0.875196
 C   -0.662553   -2.241330   -1.733040
 C   -1.728672   -2.480221   -0.585246
 O   -1.295504   -1.617289    0.465873
 H   -0.223704   -0.958441   -3.401261
 C   -1.089544   -1.191204   -2.761739
 H   -1.896569   -1.564732   -3.410033
 H   -1.420470   -0.261620   -2.282477
 H   -3.480699   -2.692998   -1.858133
 C   -3.151903   -2.111553   -0.982870
 H   -3.844242   -2.329239   -0.155058
 H   -3.222981   -1.042608   -1.218567
 H    3.073834    3.432394    1.120755
 C    3.095595    3.493894    0.022203
 H    2.193451    4.031342   -0.305906
 H    3.990738    4.052076   -0.293219
 H    4.736915    1.037154    0.921073
 C    4.694130    1.124469   -0.174737
 P    3.070384    1.803289   -0.674895
 H    5.518167    1.770887   -0.515219
 H    4.823307    0.120668   -0.606383
 C    3.271177    2.077403   -2.471443
 H    4.160947    2.686342   -2.694837
 H    2.375105    2.582414   -2.861624
 H    3.361485    1.104827   -2.978490
70
Figure 3_prod / electronic energy: -3155.88950452 a.u. / lowest freq: 21.62 cm-1
 H   -1.158855   -0.853872    2.044678
 H   -2.081368    0.534440    1.412845
 O    0.476218    1.273606    2.005172
 C   -1.632766    0.101521    2.318332
 H   -2.432894   -0.100666    3.046635
 C   -0.605099    1.058362    2.919658
 H    0.524730   -0.514821    3.893677
 H   -1.708831    2.852240    2.370142
 C    0.037748    0.436514    4.155433
 C   -1.246887    2.403039    3.261372
 H    0.800788    1.111086    4.572434
 H   -0.716472    0.240474    4.932049
 H   -0.490899    3.101512    3.652262
 H   -2.026382    2.277814    4.028140
Cu   -1.162098   -1.530549   -0.469595
 H    3.580583    0.620775   -0.295027
 H    4.155902   -0.696748    1.828001
 H    2.467465   -0.158497    1.567577
 C    3.113119   -1.032974    1.727857
 H    5.013044   -0.445128   -0.480147
 H    2.813949   -1.499307    2.678963
 C    4.011688   -0.207170   -0.872112
 H    4.132527    0.132623   -1.911993
 C    3.106855   -1.430692   -0.824697
 C    2.945747   -2.057257    0.604145
 O    1.763095   -1.042039   -1.140811
 H    4.896752   -2.999208    0.793143
 B    0.857046   -1.733858   -0.337362
 H    3.652152   -3.642033    1.890565
 C    3.831372   -3.266557    0.871685
 O    1.571398   -2.467038    0.608300
 H    4.595766   -2.740742   -1.760293
 C    3.543447   -2.443828   -1.883977
 H    3.430968   -1.987531   -2.879035
 H    3.625644   -4.087120    0.171499
 H    2.917986   -3.348697   -1.857648
 H   -1.188959    4.543120   -0.961219
 H    0.838043    4.659257    0.115279
 H   -2.279828    3.395564   -1.769932
 C   -1.230561    3.715188   -1.680966
 O   -0.748295    2.177348    0.104616
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 H     1.217478    4.989554   -1.597762
 C     1.435817    4.327569   -0.747385
 H    -0.904775    4.086148   -2.664441
 B     0.397248    1.808796    0.768095
 H     2.497981    4.443808   -0.486318
 C    -0.374050    2.539678   -1.237950
 C     1.163803    2.862937   -1.086359
 O     1.537557    2.088052    0.061507
 H    -1.693283    1.038056   -2.022193
 C    -0.638926    1.330245   -2.128884
 H    -0.452594    1.559433   -3.188203
 H    -0.013144    0.474822   -1.835748
 H     1.667555    2.926311   -3.195542
 C     2.005995    2.427305   -2.274763
 H     3.058190    2.701403   -2.107369
 H     1.953583    1.339765   -2.409554
 H    -3.849992   -3.526552   -1.811768
 C    -4.138767   -2.476486   -1.968429
 H    -3.730136   -2.151784   -2.937054
 H    -5.237257   -2.405102   -1.996484
 H    -3.969700   -3.065287    1.097540
 C    -4.312146   -2.048283    0.854783
 P    -3.430509   -1.445333   -0.632444
 H    -5.401729   -2.061155    0.696600
 H    -4.080638   -1.396766    1.709930
 C    -4.218331    0.182703   -0.927440
 H    -5.316094    0.104994   -0.887227
 H    -3.927434    0.563017   -1.917896
 H    -3.880941    0.905727   -0.169933
35
Figure 3_L-Cu-Bpin / electronic energy: -2512.09747879 a.u. / lowest freq: 23.70 cm-1
 H    -3.966569   -2.370555   -0.091079
 H    -3.807068   -0.481958   -2.357598
 C    -4.300635   -1.524404    0.527882
 C    -4.141575    0.306361   -1.666690
 H    -5.393074   -1.419924    0.438009
 H    -4.044913   -1.745522    1.575060
 H    -5.242483    0.322371   -1.642579
 H    -3.774702    1.270837   -2.048864
 P    -3.438874    0.000252   -0.004071
 C    -4.231120    1.295459    1.018181
 H    -5.326265    1.285342    0.903062
 H    -3.978324    1.134755    2.076846
 H    -3.846004    2.282421    0.721008
 H     3.908707   -2.418790   -1.177398
 H     3.178529   -2.542187    1.157081
 C     3.960241   -1.319391   -1.165315
 H     3.658664   -0.959332   -2.157930
 H     5.009094   -1.032819   -0.991557
 C     3.381449   -1.465540    1.257698
 O     1.691138   -1.070941   -0.382227
 H     4.437392   -1.340205    1.540068
 C     3.058289   -0.772965   -0.067653
 H     2.751180   -1.078631    2.072035
 B     0.869426   -0.027376    0.045169
 H     2.597061    1.082407   -2.068948
 C     3.034990    0.788202    0.049573
 H     4.301435    1.400842   -1.634829
 O     1.677868    1.040108    0.438088
 C     3.260011    1.490169   -1.291420
 H     5.023511    1.114048    0.867358
 H     3.740760    0.997181    2.103774
 C     3.976365    1.366007    1.096660
 H     3.026918    2.559483   -1.177997
 H     3.888770    2.463056    1.112142
Cu    -1.167130   -0.038843    0.055765
57
Figure 3_para-CO2Me_pc1 / electronic energy: -3049.09919044 a.u. / lowest freq: 22.13 cm-1
 H     1.435319    1.421360    2.809595
 H    -1.178778    0.212172    2.245164
 C     1.099762    2.366926    2.357969
 C    -1.481218    1.208365    1.889386
 H     0.650685    3.002131    3.137322
 H     1.981934    2.872876    1.937825
 H    -1.806136    1.815463    2.748713
 H    -2.325623    1.085134    1.195517
 P    -0.080615    1.993325    1.013172
 C    -0.737438    3.638199    0.556932
 H    -1.133684    4.175227    1.432567
 H     0.065076    4.236474    0.099670
 H    -1.541130    3.516207   -0.184609
 H    -3.214769   -2.352863    0.025529
 C    -4.285678   -0.524565   -0.396961
 C    -3.161054   -1.360741   -0.424849
 H    -5.072016    1.399940   -0.960799
 C    -4.196578    0.747549   -0.977001
 H     4.060058   -3.789977    0.868466
 C    -1.979037   -0.935643   -1.016043
 H     3.524869   -2.154336    2.619487
 H    -1.115815   -1.605206   -1.012783
 C    -3.013616    1.173666   -1.563401
 C    -1.874768    0.345329   -1.595692
 C     4.611692   -3.053894    0.264414
 C     4.219638   -1.449550    2.138870
 H     4.426330   -3.280454   -0.793838
 O     2.788231   -1.476162    0.226202
 H    -2.960199    2.169792   -2.010384
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 H     5.227898   -1.636003    2.537763
 H     5.685668   -3.185258    0.468280
 C     4.157595   -1.646485    0.623339
 C    -0.625615    0.850596   -2.182545
 B     2.590820   -0.170866   -0.210132
 H     0.413925   -1.034331   -2.523501
 C     0.467910    0.058314   -2.539613
 C     4.873414   -0.501869   -0.170990
 H     4.452475   -1.397583   -2.116749
 O     3.823599    0.467313   -0.311069
 H     6.136912   -1.626780   -1.567881
 H     6.838739   -0.608766    0.749973
 C     5.289517   -0.925367   -1.580989
 H     1.233796    0.473449   -3.200847
 C     6.053889    0.136073    0.546226
 H     5.591897   -0.032209   -2.147850
 H     6.491421    0.923909   -0.085414
Cu     0.807570    0.713731   -0.648612
 H    -0.659049    1.886162   -2.537997
 H     3.915424   -0.430347    2.420396
 H     5.752452    0.595889    1.496599
 O    -6.571709   -0.253324    0.239839
 H    -7.522643   -2.702962    0.623374
 C    -5.573686   -0.935596    0.222935
 H    -7.030021   -2.001516    2.194715
 C    -6.709841   -2.644400    1.361810
 O    -5.517880   -2.153482    0.766889
 H    -6.476677   -3.647539    1.736859
57
Figure 3_para-CO2Me_ts(CuBadd) / electronic energy: -3049.09101988 a.u. / lowest freq: -166.47 cm-1
 H     0.993034    1.763959    2.875192
 H    -1.663765    1.036261    1.850063
 C     0.879846    2.747227    2.394686
 C    -1.722485    2.033716    1.390643
 H     0.374431    3.437716    3.087315
 H     1.884459    3.132161    2.164295
 H    -2.138179    2.746486    2.119649
 H    -2.390939    1.971854    0.518414
 P    -0.057613    2.544647    0.841389
 C    -0.292064    4.253500    0.242091
 H    -0.758331    4.887353    1.011790
 H     0.682111    4.681648   -0.037234
 H    -0.930433    4.238424   -0.653742
 H    -2.692339   -2.162761    0.680002
 C    -3.910851   -0.802126   -0.473207
 C    -2.697810   -1.408494   -0.109258
 H    -4.825138    0.627176   -1.806013
 C    -3.885659    0.157868   -1.504370
 H     3.018506   -3.518662    1.798303
 C    -1.507008   -1.062323   -0.727442
 H     2.951263   -1.355925    2.952124
 H    -0.585311   -1.549491   -0.399322
 C    -2.704694    0.508964   -2.125667
 C    -1.457462   -0.068081   -1.747695
 C     3.670934   -3.143738    0.995642
 C     3.750620   -1.003627    2.283607
 H     3.368339   -3.632407    0.060305
 O     2.234506   -1.281009    0.456340
 H    -2.715532    1.264068   -2.916798
 H     4.716837   -1.285217    2.726720
 H     4.704123   -3.441881    1.230390
 C     3.557746   -1.630640    0.903161
 C    -0.226363    0.379250   -2.337802
 B     2.330991   -0.151656   -0.330718
 H     1.058417   -1.322465   -1.834000
 C     1.061576   -0.247705   -2.059515
 C     4.458917   -0.970772   -0.199090
 H     3.714210   -2.272909   -1.789826
 O     3.642942    0.138934   -0.628582
 H     5.336761   -2.711871   -1.190248
 H     6.400321   -1.263797    0.718751
 C     4.667550   -1.869190   -1.416975
 H     1.858379    0.011142   -2.766007
 C     5.794848   -0.445843    0.299671
 H     5.122076   -1.277308   -2.225220
 H     6.356415   -0.001618   -0.535645
Cu     0.752405    1.095281   -0.636672
 H    -0.289031    1.115637   -3.143941
 H     3.692821    0.094149    2.236722
 H     5.668638    0.326227    1.070141
 O    -6.257922   -0.601775   -0.090453
 H    -7.013748   -2.839006    1.122025
 C    -5.195311   -1.120720    0.176701
 H    -6.707003   -1.555151    2.327650
 C    -6.265721   -2.421540    1.812699
 O    -5.079891   -2.062497    1.126247
 H    -5.978628   -3.181955    2.548691
57
Figure 3_para-CO2Me_L-Cu-alkyl_01 / electronic energy: -3049.14412054 a.u. / lowest freq: 25.48 cm-1
 H     2.426184    1.890357    2.400102
 H    -0.513718    1.984924    2.212853
 C     2.464442    2.837419    1.842637
 C    -0.396502    2.950539    1.698365
 H     2.395067    3.673705    2.555605
 H     3.427306    2.896737    1.314419
 H    -0.335782    3.755551    2.447094
 H    -1.283880    3.106340    1.066903
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 P    1.091582    2.894351    0.636224
 C    1.199633    4.590420   -0.035887
 H    1.187495    5.343008    0.767396
 H    2.128993    4.696473   -0.615186
 H    0.351557    4.769127   -0.713369
 H   -2.991258   -2.250264    0.476888
 C   -3.738984   -0.387285   -0.316740
 C   -2.766422   -1.384027   -0.148918
 H   -4.174499    1.489557   -1.286637
 C   -3.421830    0.711467   -1.137653
 H    1.576179   -3.655582    2.239554
 C   -1.527454   -1.292075   -0.767406
 H    0.622509   -1.417108    2.080737
 H   -0.790866   -2.077211   -0.592389
 C   -2.189767    0.806416   -1.754190
 C   -1.182467   -0.187330   -1.589332
 C    2.528003   -3.353999    1.777895
 C    1.602950   -1.032578    1.763808
 H    2.891617   -4.194869    1.173373
 O    1.463104   -2.410626   -0.172690
 H   -1.971848    1.672868   -2.386546
 H    2.172663   -0.757282    2.663141
 H    3.250853   -3.163055    2.585446
 C    2.319660   -2.103444    0.940467
 C    0.128969   -0.029498   -2.223301
 B    1.854017   -1.627237   -1.231816
 H    0.338802   -2.157063   -2.783562
 C    0.972605   -1.298915   -2.484815
 C    3.613892   -1.564829    0.221288
 H    4.133865   -3.508680   -0.628502
 O    3.090751   -1.070337   -1.022382
 H    5.112663   -3.049043    0.792470
 H    4.598767   -0.709199    1.961842
 C    4.617175   -2.666377   -0.111538
 H    1.646692   -1.094905   -3.332479
 C    4.303510   -0.418363    0.942487
 H    5.389432   -2.258129   -0.780134
 H    5.210773   -0.122750    0.394911
Cu    0.840471    1.289146   -0.894271
 H    0.022409    0.571455   -3.142136
 H    1.428172   -0.125179    1.163036
 H    3.644111    0.456593    0.999149
 O   -5.943565    0.381642    0.179433
 H   -7.312317   -1.762041    0.924641
 C   -5.073543   -0.451681    0.311267
 H   -6.727203   -0.887434    2.369997
 C   -6.510084   -1.713061    1.675890
 O   -5.243996   -1.550656    1.061240
 H   -6.465296   -2.658197    2.230205
57
Figure 3_para-CO2Me_L-Cu-alkyl_02 / electronic energy: -3049.13832151 a.u. / lowest freq: 19.41 cm-1
 O    2.244377    4.342312   -1.532769
 H    1.950561    6.699297   -0.399134
 C    1.773640    4.043598   -0.457102
 H    3.505733    5.999501    0.140941
 C    2.443738    6.125680    0.399602
 O    1.813340    4.872091    0.596365
 H    2.357970    6.665872    1.350085
 H   -5.182916   -1.892914   -2.006704
 H   -4.709281    0.983610   -2.145039
 C   -5.688604   -1.738486   -1.041903
 C   -5.228030    1.086956   -1.180457
 H   -6.752122   -1.518413   -1.222997
 H   -5.605779   -2.667838   -0.458947
 H   -6.308591    1.197689   -1.360612
 H   -4.848991    1.992306   -0.683677
 P   -4.870003   -0.373904   -0.140358
 C   -5.946120   -0.123398    1.316291
 H   -6.994536    0.029379    1.017014
 H   -5.882561   -0.999467    1.978554
 H   -5.598980    0.757172    1.877062
 B    1.312956   -2.335175   -0.097975
 O    2.140559   -2.296342   -1.189403
 O    2.014861   -2.369154    1.080412
 C    3.499107   -2.438465   -0.736731
 C    3.386642   -2.052418    0.786628
 C    4.389015   -1.520498   -1.560308
 C    3.896724   -3.896519   -0.960008
 C    3.562426   -0.555343    1.041644
 C    4.292644   -2.848141    1.712706
 H    2.915757    0.045207    0.384885
 H    4.604975   -0.237870    0.894967
 H    3.278898   -0.335613    2.081447
 H    4.084953   -3.924991    1.663504
 H    4.137929   -2.521507    2.751826
 H    5.350782   -2.681981    1.460195
 H    3.267847   -4.579660   -0.369906
 H    4.949597   -4.074997   -0.697675
 H    3.761100   -4.144619   -2.023075
 H    5.421895   -1.534348   -1.180612
 H    4.022453   -0.485588   -1.547656
 H    4.406954   -1.860907   -2.606543
 C   -0.021578    1.236180    1.361004
 C    0.584984    2.455603    1.120208
 C   -0.149399    0.242403    0.354949
 C    1.104181    2.762320   -0.151186
 C    0.377645    0.574743   -0.919420
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 C    0.986828    1.796516   -1.160994
 C   -0.789976   -1.047913    0.636928
 C   -0.256997   -2.259634   -0.166398
 H    1.393223    2.019100   -2.150536
 H    0.319308   -0.153047   -1.730953
 H    0.672091    3.187362    1.925659
 H   -0.407988    1.019723    2.361687
Cu   -2.712128   -0.705655    0.294110
 H   -0.580810   -2.245287   -1.221255
 H   -0.690588   -3.182494    0.256628
 H   -0.708208   -1.256581    1.717361
57
Figure 3_para-CO2Me_L-Cu-alkyl_03 / electronic energy: -3049.14208777 a.u. / lowest freq: 14.95 cm-1
 H   -1.946223    3.311733   -1.972582
 H    1.027524    3.267564   -1.957210
 C   -1.861440    3.764052   -0.973492
 C    1.005143    3.656256   -0.928106
 H   -1.711135    4.849368   -1.082054
 H   -2.801129    3.586382   -0.430209
 H    1.003790    4.756919   -0.955568
 H    1.911352    3.305053   -0.412564
 P   -0.468762    3.002120   -0.065797
 C   -0.464800    3.910132    1.521867
 H   -0.445538    4.998749    1.358359
 H   -1.363405    3.646793    2.099727
 H    0.418722    3.616384    2.108201
 B   -2.322275   -1.738928   -0.327198
 O   -3.123241   -1.116386   -1.254029
 O   -2.977109   -1.947878    0.859809
 C   -4.287533   -0.628691   -0.564308
 C   -4.357698   -1.586072    0.680505
 C   -5.490321   -0.695574   -1.490569
 C   -3.994445    0.823066   -0.186528
 C   -5.129479   -2.873660    0.397154
 C   -4.872485   -0.933117    1.953696
 H   -4.780836   -3.353647   -0.529310
 H   -6.209972   -2.689536    0.310304
 H   -4.966375   -3.579617    1.224703
 H   -4.224990   -0.106797    2.275768
 H   -4.903797   -1.673813    2.766387
 H   -5.891859   -0.544604    1.808046
 H   -3.125252    0.891004    0.487318
 H   -4.855623    1.306558    0.296862
 H   -3.753587    1.381425   -1.102687
 H   -6.411330   -0.427624   -0.951057
 H   -5.616238   -1.696531   -1.923763
 H   -5.363353    0.017782   -2.318507
 C    2.325838   -0.712257    1.231659
 C    3.698653   -0.634401    1.092690
 C    1.479964   -1.162885    0.180217
 C    4.321705   -1.008007   -0.113299
 C    2.132142   -1.561322   -1.013465
 C    3.509811   -1.476866   -1.155155
 C    0.022326   -1.162475    0.345687
 C   -0.812384   -2.077314   -0.564716
 H    3.983273   -1.783729   -2.090975
 H    1.539457   -1.936763   -1.850072
 H    4.309874   -0.280604    1.925293
 H    1.866258   -0.409090    2.177613
Cu   -0.376433    0.780126    0.123614
 H   -0.598284   -3.150713   -0.381693
 H   -0.593463   -1.892062   -1.629053
 H   -0.231306   -1.338333    1.405923
 O    6.354271   -1.235751   -1.345246
 H    8.124492    0.319268   -0.181364
 C    5.782229   -0.930516   -0.321859
 H    8.311881   -1.338994    0.461615
 C    7.845751   -0.358161    0.639355
 O    6.438086   -0.472135    0.754508
 H    8.202514    0.050728    1.592331
57
Figure 3_para-CO2Me_ts(BHE) / electronic energy: -3049.09404597 a.u. / lowest freq: -926.85 cm-1
 H    0.561445   -4.309756    1.907086
 H    2.671340   -2.354903    1.231925
 C    0.391807   -4.449601    0.829310
 C    2.454900   -2.557281    0.172620
 H    1.071819   -5.229607    0.453263
 H   -0.649194   -4.773647    0.683051
 H    3.050216   -3.421657   -0.160004
 H    2.742138   -1.669489   -0.411510
 P    0.665387   -2.864588   -0.036480
 C    0.503968   -3.303518   -1.803328
 H    1.162914   -4.142252   -2.075925
 H   -0.540182   -3.576342   -2.017626
 H    0.759616   -2.423577   -2.412449
 B   -2.708014    0.937387    0.304450
 O   -3.654760    1.474765    1.129653
 O   -3.232091    0.432718   -0.853479
 C   -4.943041    1.077068    0.615476
 C   -4.623306    0.810179   -0.901624
 C   -5.949467    2.187230    0.864854
 C   -5.347907   -0.187972    1.370227
 C   -4.714021    2.069233   -1.761040
 C   -5.424310   -0.317200   -1.531140
 H   -4.160027    2.905457   -1.309207
 H   -5.757299    2.382068   -1.910928
 H   -4.271386    1.863007   -2.746469
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 H   -5.237420   -1.277311   -1.032531
 H   -5.149465   -0.425789   -2.590818
 H   -6.502096   -0.100166   -1.481461
 H   -4.631808   -1.005444    1.196481
 H   -6.350194   -0.532172    1.077484
 H   -5.359226    0.026038    2.449004
 H   -6.914738    1.944529    0.395764
 H   -5.599556    3.149560    0.468830
 H   -6.116999    2.305540    1.945484
 C    2.087537    1.085282   -1.324010
 C    3.456262    1.200288   -1.169063
 C    1.208203    1.005437   -0.208712
 C    4.036888    1.249799    0.112544
 C    1.812656    1.071152    1.077550
 C    3.184691    1.186339    1.225701
 C   -0.209609    0.828847   -0.406026
 C   -1.188150    0.870399    0.657991
 H    3.624666    1.228461    2.224791
 H    1.190224    1.016186    1.973819
 H    4.098061    1.252822   -2.050596
 H    1.661743    1.042548   -2.330470
Cu   -0.492559   -1.047330    0.482087
 H   -0.915500    1.404234    1.576218
 H   -1.519606   -0.458356    1.559168
 H   -0.568128    0.783069   -1.438740
 O    6.026534    1.404619    1.420739
 H    8.027566    0.669986   -0.177933
 C    5.491989    1.366538    0.333930
 H    7.875670    2.450966   -0.132751
 C    7.597314    1.543836   -0.689621
 O    6.190174    1.426664   -0.809573
 H    7.991578    1.603985   -1.711070
57
Figure 3_para-CO2Me_pc2 / electronic energy: -3049.12196245 a.u. / lowest freq: 28.36 cm-1
 H   -0.171196   -4.364058    1.412220
 H    2.226929   -2.581782    1.638367
 C   -0.086395   -4.260804    0.320281
 C    2.229231   -2.580501    0.538142
 H    0.591812   -5.035917   -0.069062
 H   -1.087959   -4.403802   -0.112442
 H    2.779182   -3.462833    0.175977
 H    2.742702   -1.670075    0.195043
 P    0.507604   -2.579950   -0.078423
 C    0.717231   -2.632489   -1.894349
 H    1.315189   -3.503404   -2.205203
 H   -0.269972   -2.683223   -2.377611
 H    1.221846   -1.714865   -2.230398
 B   -2.610699    1.050522    0.239134
 O   -3.600017    1.563172    1.031702
 O   -3.093931    0.460869   -0.901502
 C   -4.855290    1.063457    0.528555
 C   -4.505911    0.732229   -0.971383
 C   -5.924794    2.128088    0.708340
 C   -5.199831   -0.178290    1.347895
 C   -4.687897    1.924980   -1.908162
 C   -5.218588   -0.487546   -1.532907
 H   -4.197115    2.827108   -1.513792
 H   -5.751376    2.149518   -2.074534
 H   -4.230787    1.688838   -2.880333
 H   -4.965714   -1.398380   -0.974627
 H   -4.927087   -0.640779   -2.582673
 H   -6.309487   -0.346409   -1.501778
 H   -4.425351   -0.953123    1.245401
 H   -6.170052   -0.602493    1.052700
 H   -5.254755    0.097647    2.411223
 H   -6.872902    1.802935    0.254023
 H   -5.629512    3.084256    0.256887
 H   -6.103315    2.299592    1.780078
 C    2.168412    0.842084   -1.290337
 C    3.549506    0.937969   -1.165786
 C    1.331899    0.879953   -0.162833
 C    4.132356    1.074444    0.099251
 C    1.928741    1.019828    1.102874
 C    3.307401    1.114263    1.230587
 C   -0.126723    0.728039   -0.340126
 C   -1.098133    1.117695    0.576405
 H    3.765219    1.215982    2.216314
 H    1.308004    1.033464    2.001548
 H    4.181552    0.907895   -2.054288
 H    1.722545    0.736355   -2.282644
Cu   -0.788673   -0.907610    0.795458
 H   -0.792396    1.596583    1.513605
 H   -1.722087   -1.360603    1.996686
 H   -0.442400    0.492431   -1.363528
 O    6.145961    1.263958    1.369952
 H    8.114902    0.401226   -0.232049
 C    5.606959    1.175779    0.292402
 H    7.998201    2.186671   -0.280868
 C    7.693164    1.255930   -0.780616
 O    6.277840    1.160403   -0.859868
 H    8.059500    1.250693   -1.813517
57
Figure 3_para-CO2Me_ts(H>B) / electronic energy: -3049.10879459 a.u. / lowest freq: -424.75 cm-1
 H   -0.051572    4.457596   -1.588343
 H    2.147325    2.438748   -1.636803
 C   -0.001644    4.442178   -0.489319
 C    2.156458    2.552059   -0.542544
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 H    0.732425    5.188421   -0.148323
 H   -0.996028    4.702771   -0.097469
 H    2.783101    3.417246   -0.275166
 H    2.595662    1.642517   -0.106217
 P    0.445019    2.760375    0.069866
 C    0.668732    2.950004    1.874417
 H    1.379518    3.757173    2.109421
 H   -0.301205    3.171121    2.344178
 H    1.045545    2.004821    2.293239
 B   -2.588893   -0.669968   -0.395839
 O   -3.564522   -1.231183   -1.234370
 O   -3.114640   -0.482559    0.899897
 C   -4.827863   -1.033658   -0.601020
 C   -4.433686   -1.025592    0.922696
 C   -5.764709   -2.163289   -1.005548
 C   -5.406554    0.304901   -1.066311
 C   -4.339794   -2.435218    1.511904
 C   -5.323719   -0.156838    1.800445
 H   -3.722003   -3.089275    0.878401
 H   -5.328930   -2.900501    1.637869
 H   -3.860848   -2.374093    2.500708
 H   -5.281259    0.898236    1.498723
 H   -4.993164   -0.221340    2.848495
 H   -6.370918   -0.494113    1.754980
 H   -4.766731    1.146546   -0.765230
 H   -6.417746    0.471866   -0.666584
 H   -5.467214    0.304480   -2.165170
 H   -6.713022   -2.106997   -0.449012
 H   -5.310921   -3.147656   -0.829817
 H   -5.996949   -2.087206   -2.078786
 C    2.215355   -0.938280    1.261607
 C    3.597005   -1.019078    1.129453
 C    1.372052   -0.966224    0.138455
 C    4.175415   -1.129805   -0.139831
 C    1.965845   -1.077657   -1.131543
 C    3.343881   -1.157501   -1.267578
 C   -0.084252   -0.831283    0.334456
 C   -1.062613   -1.018445   -0.609274
 H    3.797555   -1.240451   -2.257048
 H    1.342168   -1.084459   -2.028041
 H    4.232936   -0.996249    2.015466
 H    1.773371   -0.847980    2.257292
Cu   -0.937005    1.077099   -0.493025
 H   -0.758293   -1.286957   -1.630944
 H   -2.452547    0.935089   -1.048099
 H   -0.392817   -0.673048    1.376057
 O    6.183236   -1.284055   -1.424099
 H    8.159385   -0.454445    0.182172
 C    5.648818   -1.220158   -0.342294
 H    8.043313   -2.240505    0.198665
 C    7.740830   -1.319215    0.717258
 O    6.326107   -1.226063    0.806561
 H    8.113388   -1.333529    1.747856
57
Figure 3_para-CO2Me_int1 / electronic energy: -3049.10990203 a.u. / lowest freq: 12.40 cm-1
 H    0.059559    4.565253   -1.595214
 H    2.109742    2.371868   -1.737990
 C    0.203874    4.569912   -0.504565
 C    2.199806    2.511436   -0.650655
 H    1.024605    5.257717   -0.248766
 H   -0.726702    4.925821   -0.037803
 H    2.906776    3.330883   -0.448175
 H    2.594420    1.581224   -0.214900
 P    0.557063    2.871235    0.068898
 C    0.926825    3.084877    1.846210
 H    1.726643    3.825149    2.002698
 H    0.019962    3.412931    2.375445
 H    1.241700    2.118696    2.267978
 B   -2.638590   -0.370031   -0.360582
 O   -3.589888   -0.902195   -1.294981
 O   -3.199536   -0.494826    0.963626
 C   -4.838045   -0.968861   -0.628322
 C   -4.401205   -1.239815    0.857727
 C   -5.677097   -2.074696   -1.255808
 C   -5.563216    0.373522   -0.781001
 C   -4.076241   -2.718088    1.100545
 C   -5.392827   -0.753769    1.907478
 H   -3.398283   -3.104134    0.324550
 H   -4.978482   -3.348498    1.123952
 H   -3.566261   -2.814825    2.071090
 H   -5.539054    0.333390    1.849709
 H   -5.016872   -0.987968    2.915570
 H   -6.370854   -1.246457    1.788942
 H   -5.009146    1.188338   -0.291729
 H   -6.579392    0.343811   -0.359652
 H   -5.644146    0.614375   -1.852033
 H   -6.613036   -2.232133   -0.697194
 H   -5.125468   -3.023706   -1.294344
 H   -5.942286   -1.801827   -2.289201
 C    2.165593   -0.985264    1.261029
 C    3.544076   -1.099759    1.116180
 C    1.311238   -0.999815    0.146581
 C    4.106323   -1.234985   -0.157772
 C    1.888713   -1.144683   -1.127106
 C    3.262818   -1.259241   -1.276580
 C   -0.138946   -0.806410    0.352704
 C   -1.118972   -0.847870   -0.593065
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 H    3.704271   -1.365013   -2.269407
 H    1.255376   -1.151199   -2.016625
 H    4.189560   -1.082163    1.995358
 H    1.735808   -0.874520    2.260053
Cu   -0.967754    1.272917   -0.312479
 H   -0.818158   -1.052103   -1.631988
 H   -2.583498    1.034436   -0.622707
 H   -0.434858   -0.668164    1.401682
 O    6.096239   -1.432286   -1.463742
 H    8.098999   -0.597083    0.114539
 C    5.576306   -1.349427   -0.376263
 H    7.968624   -2.382082    0.139513
 C    7.680063   -1.456395    0.658065
 O    6.267279   -1.350609    0.764051
 H    8.065072   -1.469658    1.684039
57
Figure 3_para-CO2Me_ts(Cu>O) / electronic energy: -3049.10330689 a.u. / lowest freq: -56.48 cm-1
 H   -1.229580    4.830263   -1.294614
 H    1.026053    3.019048   -1.824270
 C   -1.052385    4.680565   -0.219261
 C    1.152800    2.905531   -0.737516
 H   -0.308031    5.412240    0.130732
 H   -2.001937    4.846590    0.310730
 H    1.819372    3.698339   -0.364469
 H    1.614559    1.924295   -0.548826
 P   -0.483843    2.969666    0.073819
 C   -0.073346    2.954985    1.854571
 H    0.625620    3.765881    2.111096
 H   -0.995562    3.067721    2.443456
 H    0.384282    1.988304    2.112496
 B   -2.262151   -0.899613   -0.799306
 O   -3.225254   -1.881748   -1.185078
 O   -2.593278   -0.500484    0.578447
 C   -4.376310   -1.683445   -0.378167
 C   -3.757612   -1.206468    0.989336
 C   -5.150473   -2.992400   -0.289010
 C   -5.265475   -0.610433   -1.019063
 C   -3.295997   -2.380139    1.856934
 C   -4.653449   -0.281879    1.802775
 H   -2.666999   -3.070062    1.275500
 H   -4.140656   -2.943013    2.281987
 H   -2.691062   -1.991682    2.690268
 H   -4.872440    0.647183    1.258831
 H   -4.152990   -0.009173    2.744725
 H   -5.606178   -0.772451    2.056420
 H   -4.767868    0.369515   -1.043759
 H   -6.223463   -0.499817   -0.489658
 H   -5.479358   -0.903045   -2.058242
 H   -5.965990   -2.920549    0.447414
 H   -4.493886   -3.825663   -0.005110
 H   -5.595782   -3.232488   -1.266542
 C    2.418470   -0.986242    1.081985
 C    3.807741   -0.941341    1.056710
 C    1.664811   -1.038028   -0.103465
 C    4.486857   -0.944365   -0.166832
 C    2.361483   -1.042050   -1.325729
 C    3.748197   -0.996822   -1.356393
 C    0.194164   -1.034430   -0.015352
 C   -0.697214   -1.181020   -1.014671
 H    4.280382   -0.993787   -2.309656
 H    1.809468   -1.066774   -2.267579
 H    4.369796   -0.899897    1.990650
 H    1.897066   -0.977412    2.042878
Cu   -1.774924    1.293536   -0.568233
 H   -0.323787   -1.358548   -2.033332
 H   -2.488736    0.210365   -1.621012
 H   -0.203300   -0.863771    0.992897
 O    6.594031   -0.887503   -1.292744
 H    8.329298    0.160073    0.417261
 C    5.972912   -0.879114   -0.256318
 H    8.422961   -1.625197    0.511234
 C    7.974021   -0.727466    0.960864
 O    6.556010   -0.802917    0.940901
 H    8.262700   -0.657391    2.015880
57
Figure 3_para-CO2Me_int2 / electronic energy: -3049.11054654 a.u. / lowest freq: 19.39 cm-1
 H   -4.297236    3.392366   -2.119303
 H   -2.912166    4.289964    0.331417
 C   -5.054227    2.928278   -1.470057
 C   -3.708221    3.797830    0.909685
 H   -5.828505    3.670768   -1.222941
 H   -5.514788    2.095196   -2.021670
 H   -4.543751    4.501413    1.046754
 H   -3.298092    3.525625    1.893418
 P   -4.248137    2.284996    0.038777
 C   -5.656801    1.697350    1.047325
 H   -6.416325    2.485401    1.168741
 H   -6.120943    0.825434    0.562428
 H   -5.294444    1.389855    2.039448
 B   -1.068204   -0.880424   -0.869942
 O   -1.541764   -2.174606   -1.304620
 O   -1.549067   -0.745388    0.545343
 C   -2.529496   -2.643405   -0.411267
 C   -2.100375   -1.995270    0.957391
 C   -2.510446   -4.167761   -0.402265
 C   -3.911511   -2.166489   -0.880086
 C   -0.989166   -2.783304    1.652844
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 C   -3.244270   -1.739707    1.928233
 H   -0.166701   -3.004550    0.957422
 H   -1.358258   -3.729611    2.075630
 H   -0.584198   -2.177451    2.477191
 H   -3.975297   -1.033611    1.507717
 H   -2.855753   -1.302483    2.860844
 H   -3.765123   -2.675672    2.181778
 H   -4.004615   -1.067478   -0.853467
 H   -4.725525   -2.589199   -0.272433
 H   -4.058749   -2.480781   -1.923950
 H   -3.181976   -4.570900    0.371991
 H   -1.497340   -4.552979   -0.226589
 H   -2.849475   -4.551337   -1.376764
 C    3.507503    0.177461    1.036479
 C    4.882297    0.384694    1.027849
 C    2.797089   -0.088091   -0.147056
 C    5.591139    0.336653   -0.177737
 C    3.523361   -0.129155   -1.351614
 C    4.895286    0.078461   -1.366338
 C    1.340232   -0.309489   -0.072608
 C    0.507299   -0.659371   -1.066882
 H    5.448558    0.042868   -2.306957
 H    3.006520   -0.324353   -2.293530
 H    5.411147    0.584367    1.960878
 H    2.964531    0.216728    1.984663
Cu   -2.661818    0.790342   -0.294269
 H    0.924609   -0.799142   -2.074986
 H   -1.648922    0.105383   -1.562181
 H    0.910225   -0.181373    0.929021
 O    7.709417    0.524247   -1.268902
 H    9.313735    1.817409    0.389522
 C    7.064534    0.544364   -0.247023
 H    9.546201    0.057348    0.621709
 C    9.016686    0.947023    0.992789
 O    7.610363    0.754214    0.952351
 H    9.271407    1.119869    2.044701
57
Figure 3_para-CO2Me_ts(C-Brot) / electronic energy: -3049.10479731 a.u. / lowest freq: -95.59 cm-1
 H    4.374967   -3.690214   -1.645321
 H    3.318720   -4.085761    1.083617
 C    5.172476   -3.082435   -1.193005
 C    4.127667   -3.439269    1.454663
 H    5.996370   -3.740728   -0.876796
 H    5.541154   -2.379353   -1.954736
 H    5.017492   -4.054094    1.660093
 H    3.789050   -2.967187    2.388827
 P    4.491482   -2.142630    0.219081
 C    5.963074   -1.305906    0.913192
 H    6.776506   -2.024415    1.099729
 H    6.317406   -0.537699    0.209715
 H    5.694519   -0.813625    1.859522
 B    1.019073    0.640288   -0.798995
 O    1.227990    1.953452   -1.351206
 O    1.623386    0.712851    0.579751
 C    2.283989    2.591186   -0.663152
 C    2.134161    2.027557    0.799729
 C    2.100483    4.101156   -0.767477
 C    3.626306    2.213332   -1.306806
 C    1.100440    2.800741    1.619009
 C    3.437681    1.933474    1.581887
 H    0.171188    2.946120    1.050954
 H    1.476123    3.787666    1.927878
 H    0.857789    2.226353    2.525609
 H    4.155343    1.263642    1.086920
 H    3.243376    1.529865    2.587562
 H    3.905290    2.923387    1.697410
 H    3.852396    1.139246   -1.206446
 H    4.465406    2.775635   -0.870995
 H    3.577764    2.438748   -2.382506
 H    2.830907    4.637072   -0.141641
 H    1.088783    4.403707   -0.466649
 H    2.248703    4.421415   -1.810048
 C   -3.891760    1.032046    0.484144
 C   -5.230888    0.662660    0.547443
 C   -2.950480    0.263780   -0.221781
 C   -5.669027   -0.497817   -0.099786
 C   -3.407138   -0.898345   -0.870242
 C   -4.741839   -1.272525   -0.809678
 C   -1.540608    0.702384   -0.244883
 C   -0.505174    0.103857   -0.855023
 H   -5.084813   -2.178076   -1.313870
 H   -2.707396   -1.521538   -1.430784
 H   -5.940670    1.275480    1.104634
 H   -3.560045    1.939840    0.995037
Cu    2.804332   -0.805472   -0.236025
 H   -0.714557   -0.821485   -1.411477
 H    1.725412   -0.275732   -1.482440
 H   -1.355615    1.624861    0.319105
 O   -7.499160   -1.954503   -0.589559
 H   -9.355789   -1.439924    1.276456
 C   -7.088243   -0.950017   -0.058034
 H   -9.712084   -0.559944   -0.239545
 C   -9.240772   -0.480467    0.750945
 O   -7.870814   -0.124047    0.638455
 H   -9.720212    0.319063    1.327290
57
Figure 3_para-CO2Me_int3 / electronic energy: -3049.10988776 a.u. / lowest freq: 14.53 cm-1
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 H     4.813035   -3.052863   -2.189324
 H     4.169529   -4.062733    0.500371
 C     5.541839   -2.368943   -1.729673
 C     4.934278   -3.373225    0.887605
 H     6.513370   -2.879123   -1.640652
 H     5.651099   -1.492996   -2.386136
 H     5.918436   -3.864706    0.844458
 H     4.690490   -3.141325    1.935053
 P     4.921636   -1.832951   -0.095971
 C     6.323385   -0.880097    0.590613
 H     7.257560   -1.462214    0.557942
 H     6.456191    0.046646    0.012613
 H     6.105046   -0.609129    1.634242
 B     0.934928    0.377401   -0.427825
 O     0.994971    1.661195   -1.082684
 O     1.741776    0.547981    0.835702
 C     1.966674    2.479528   -0.468222
 C     2.003797    1.939625    1.009680
 C     1.533702    3.937378   -0.580205
 C     3.309853    2.305230   -1.190105
 C     0.879458    2.517869    1.870873
 C     3.341550    2.112159    1.714913
 H    -0.092063    2.428259    1.363883
 H     1.053097    3.575545    2.118215
 H     0.823134    1.949813    2.811556
 H     4.140898    1.560172    1.199474
 H     3.277227    1.725933    2.743795
 H     3.626169    3.174226    1.768200
 H     3.714668    1.285112   -1.077553
 H     4.071065    3.012578   -0.828558
 H     3.157006    2.480792   -2.265196
 H     2.201733    4.597465   -0.005323
 H     0.505772    4.076955   -0.219802
 H     1.565973    4.255727   -1.633438
 C    -4.094329    0.931758   -0.796535
 C    -5.435029    0.609695   -0.617771
 C    -3.068622    0.073369   -0.364507
 C    -5.790684   -0.592896    0.003135
 C    -3.442333   -1.134630    0.253033
 C    -4.778716   -1.461013    0.434504
 C    -1.664176    0.479475   -0.564805
 C    -0.554027   -0.173754   -0.184414
 H    -5.057136   -2.399456    0.918015
 H    -2.674976   -1.830414    0.598797
 H    -6.210929    1.295568   -0.960421
 H    -3.828747    1.875063   -1.281116
Cu     2.993894   -0.778002   -0.136294
 H    -0.666420   -1.139868    0.330065
 H     1.550486   -0.570115   -1.134513
 H    -1.535411    1.442573   -1.074958
 O    -7.554688   -2.020604    0.752507
 H    -9.702266   -0.492772    1.012126
 C    -7.209362   -0.988904    0.226099
 H    -9.734523   -1.281177   -0.593931
 C    -9.454296   -0.366111   -0.051783
 O    -8.074469   -0.076608   -0.220394
 H   -10.000122    0.490991   -0.462329
42
Figure 3_para-CO2Me-alkenylBpin / electronic energy: -947.261050912 a.u. / lowest freq: 13.61 cm-1
 B     2.536731   -0.351136   -0.017816
 O     3.507318   -1.307017    0.091467
 O     3.044449    0.917279   -0.089343
 C     4.760349   -0.629615    0.319214
 C     4.471353    0.802509   -0.264709
 C     5.875327   -1.387204   -0.382583
 C     4.996326   -0.622611    1.828498
 C     4.745855    0.900135   -1.764214
 C     5.160646    1.939871    0.470457
 H     4.269808    0.075213   -2.315220
 H     5.823957    0.886700   -1.979228
 H     4.330817    1.845090   -2.144324
 H     4.841247    2.001481    1.518889
 H     4.920642    2.897749   -0.014329
 H     6.253003    1.810310    0.441985
 H     4.207048   -0.068094    2.357891
 H     5.967553   -0.174767    2.082696
 H     4.987792   -1.658529    2.197849
 H     6.823693   -0.833725   -0.309558
 H     5.649454   -1.557045   -1.443307
 H     6.018218   -2.368010    0.094703
 C    -2.207218    1.219150    0.141935
 C    -3.592625    1.099338    0.165560
 C    -1.385376    0.103371   -0.083437
 C    -4.189417   -0.146927   -0.050480
 C    -1.997705   -1.142169   -0.304573
 C    -3.380002   -1.264785   -0.289389
 C     0.078353    0.284197   -0.078553
 C     1.016202   -0.679307   -0.047860
 H    -3.852270   -2.233203   -0.464204
 H    -1.388084   -2.026100   -0.502335
 H    -4.214799    1.975709    0.350685
 H    -1.746933    2.196518    0.307586
 H     0.706356   -1.730832   -0.015627
 H     0.406700    1.330741   -0.083277
 O    -6.220518   -1.390859   -0.242301
 H    -8.075832    0.017569    1.049167
 C    -5.670406   -0.334915   -0.040108
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 H   -8.154100    0.388896   -0.700309
 C   -7.745844    0.716413    0.266859
 O   -6.327659    0.794119    0.220526
 H   -8.101542    1.727137    0.496846
57
Figure 3_para-CO2Me_pc2_rev / electronic energy: -3049.11948820 a.u. / lowest freq: 23.81 cm-1
 H    0.525731   -4.098132   -1.127027
 H   -2.133548   -3.569521   -2.217176
 C    0.106754   -3.962919   -0.118894
 C   -2.501294   -3.455270   -1.186660
 H   -0.287410   -4.924075    0.246390
 H    0.919260   -3.629819    0.544320
 H   -2.784680   -4.441679   -0.788146
 H   -3.389805   -2.807777   -1.210333
 P   -1.193631   -2.677857   -0.174212
 C   -1.874439   -2.705835    1.522698
 H   -2.286306   -3.693433    1.781824
 H   -1.071454   -2.455663    2.232627
 H   -2.655076   -1.937903    1.617639
 B   -2.086799    0.946607    0.454982
 O   -3.015879    0.549158    1.381007
 O   -2.642996    1.648814   -0.581118
 C   -4.321657    0.818147    0.830839
 C   -4.010131    1.938674   -0.229766
 C   -5.255730    1.243912    1.951122
 C   -4.817339   -0.477061    0.191685
 C   -4.032306    3.345113    0.365718
 C   -4.866222    1.886699   -1.484609
 H   -3.426170    3.405551    1.282014
 H   -5.056587    3.666007    0.603435
 H   -3.612276    4.050977   -0.365663
 H   -4.743544    0.937781   -2.022523
 H   -4.576095    2.700761   -2.165077
 H   -5.929956    2.016317   -1.234832
 H   -4.147676   -0.799455   -0.619435
 H   -5.830358   -0.362731   -0.219386
 H   -4.845736   -1.271729    0.951427
 H   -6.234083    1.541531    1.544872
 H   -4.844610    2.082943    2.527120
 H   -5.416770    0.403993    2.642976
 C    2.652956    1.839546   -0.980996
 C    4.035313    1.751233   -0.877990
 C    1.817632    1.018498   -0.207197
 C    4.621345    0.832842   -0.000030
 C    2.416611    0.101774    0.674110
 C    3.797981    0.007692    0.776618
 C    0.349699    1.127380   -0.351099
 C   -0.572861    0.625489    0.562342
 H    4.245860   -0.714739    1.460100
 H    1.793809   -0.562492    1.277049
 H    4.678736    2.392036   -1.483903
 H    2.206159    2.552859   -1.677819
Cu   -0.319241   -0.730500   -0.992539
 H   -0.212133    0.142698    1.477524
 H    0.294599   -0.914557   -2.452985
 H    0.007174    1.837453   -1.110925
 O    6.852420    1.466518   -0.574995
 H    8.415247    0.605578    1.395473
 C    6.108877    0.762807    0.066365
 O    6.540804   -0.171200    0.914868
 C    7.947214   -0.323718    1.039659
 H    8.105359   -1.123093    1.772746
 H    8.399546   -0.606680    0.077996
57
Figure 3_para-CO2Me_ts(CuHadd_rev) / electronic energy: -3049.09338527 a.u. / lowest freq: -781.57 cm-1
 H   -0.378765   -4.449445   -1.451089
 H   -2.924169   -3.220043   -2.177435
 C   -0.680286   -4.402830   -0.394333
 C   -3.184590   -3.212375   -1.108839
 H   -1.242851   -5.312713   -0.133562
 H    0.232203   -4.354767    0.218620
 H   -3.637403   -4.178644   -0.838782
 H   -3.919749   -2.412029   -0.940529
 P   -1.680821   -2.898081   -0.118697
 C   -2.253362   -3.089253    1.606376
 H   -2.755447   -4.056337    1.763575
 H   -1.389325   -3.012604    2.283220
 H   -2.946500   -2.271034    1.849691
 B   -1.803858    1.216010    0.423557
 O   -2.666203    1.370909    1.497654
 O   -2.441614    1.510670   -0.776644
 C   -3.992444    1.492190    0.968379
 C   -3.725846    2.065052   -0.470462
 C   -4.819546    2.394799    1.869413
 C   -4.594599    0.087255    0.930401
 C   -3.586110    3.587256   -0.484810
 C   -4.726941    1.622272   -1.526968
 H   -2.883832    3.931654    0.288964
 H   -4.552452    4.089007   -0.329321
 H   -3.190888    3.900019   -1.462692
 H   -4.718248    0.532342   -1.660830
 H   -4.476547    2.082272   -2.494645
 H   -5.747237    1.935468   -1.257459
 H   -4.003940   -0.567558    0.272474
 H   -5.635971    0.092148    0.577744
 H   -4.576340   -0.340199    1.943875
 H   -5.813622    2.574277    1.432070
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 H   -4.328903    3.363041    2.034659
 H   -4.961891    1.916405    2.850110
 C    2.745481    1.760647   -0.955098
 C    4.121353    1.770507   -0.746626
 C    1.962324    0.695775   -0.495358
 C    4.742902    0.711745   -0.077552
 C    2.591831   -0.360773    0.177353
 C    3.964914   -0.358265    0.385242
 C    0.478473    0.717334   -0.683344
 C   -0.356211    0.767676    0.499919
 H    4.442146   -1.192889    0.900597
 H    1.989353   -1.204339    0.526108
 H    4.731387    2.601486   -1.106217
 H    2.270005    2.593212   -1.479488
Cu   -0.608855   -1.006455   -0.535073
 H    0.111107    0.529016    1.462329
 H    0.437894   -0.643675   -1.682520
 H    0.158025    1.353628   -1.515231
 O    6.921794    1.679260   -0.248373
 H    8.444220    0.422883    1.562573
 C    6.221585    0.760793    0.106061
 O    6.700804   -0.331430    0.703000
 C    8.105753   -0.389657    0.903268
 H    8.308174   -1.358384    1.374230
 H    8.641625   -0.319976   -0.054469
57
Figure 3_para-CO2Me_L-Cu-alkyl_rev / electronic energy: -3049.14832622 a.u. / lowest freq: 12.50 cm-1
 H   -1.736057    2.195766   -1.783283
 H    1.054623    3.167151   -1.779205
 C   -1.856525    2.643400   -0.785653
 C    0.841487    3.608232   -0.794120
 H   -2.160993    3.695538   -0.898652
 H   -2.646481    2.093993   -0.252271
 H    0.395797    4.605236   -0.935151
 H    1.791280    3.712470   -0.249065
 P   -0.283624    2.507410    0.138057
 C   -0.615538    3.452358    1.667388
 H   -0.978265    4.467141    1.441789
 H   -1.370499    2.923359    2.267773
 H    0.307982    3.521751    2.261213
 B    2.445886   -1.144019    0.410001
 O    3.415216   -0.591429    1.252665
 O    2.955788   -1.274327   -0.883487
 C    4.416675   -0.006019    0.420460
 C    4.333340   -0.898353   -0.869775
 C    5.758912   -0.040056    1.134625
 C    4.000461    1.443850    0.152328
 C    5.166318   -2.176412   -0.758636
 C    4.668191   -0.171741   -2.165050
 H    4.974422   -2.697457    0.191259
 H    6.244926   -1.972879   -0.833510
 H    4.887954   -2.855526   -1.578331
 H    3.964492    0.648760   -2.359078
 H    4.609521   -0.872202   -3.011886
 H    5.689202    0.238883   -2.134209
 H    3.042173    1.481843   -0.388564
 H    4.753624    1.994603   -0.429872
 H    3.863168    1.958878    1.115182
 H    6.564682    0.308785    0.470482
 H    6.004919   -1.051462    1.484361
 H    5.734296    0.622393    2.013286
 C   -2.153216   -2.535738    0.930649
 C   -3.476917   -2.107093    0.955495
 C   -1.269764   -2.095110   -0.063349
 C   -3.954065   -1.227076   -0.022109
 C   -1.766770   -1.231733   -1.052479
 C   -3.087621   -0.800960   -1.038130
 C    0.197008   -2.454588   -0.022812
 C    1.019594   -1.464916    0.811362
 H   -3.453138   -0.128344   -1.815249
 H   -1.095206   -0.888241   -1.844915
 H   -4.158288   -2.447257    1.738175
 H   -1.791147   -3.217659    1.705056
Cu    0.427520    0.418361    0.477322
 H    0.866245   -1.596506    1.897075
 H    0.583978   -2.470296   -1.054301
 H    0.295651   -3.486842    0.362170
 O   -6.170170   -1.168444    0.872840
 H   -7.239614    1.113929    0.091339
 C   -5.370195   -0.773995    0.057662
 O   -5.668735    0.138628   -0.870216
 C   -6.995972    0.642972   -0.872038
 H   -7.038370    1.390690   -1.672307
 H   -7.723250   -0.157567   -1.071839
78
Figure 3_para-CO2Me_pc3_01 / electronic energy: -3887.98535988 a.u. / lowest freq: 10.79 cm-1
 C   -0.427545   -1.696973   -0.715003
 C   -0.193242   -1.827592    0.642400
 C    1.201943   -1.832333    1.204650
 O    1.777747   -3.154389    1.191300
 P    2.363153   -3.751896   -0.173317
 O    2.939388   -2.790908   -1.136681
 O    3.354615   -4.834806    0.468179
 O    1.184030   -4.608465   -0.846262
 C    4.139391   -5.654041   -0.393448
 H   -1.387082   -1.986785   -1.152980
 H    0.405514   -1.586387   -1.416442
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 H   -0.978177   -2.231199    1.293247
 H    1.860437   -1.153361    0.641084
 H    1.209636   -1.532495    2.260305
 B   -3.325403    1.450205   -1.064514
 O   -4.038898    1.492227    0.112095
 O   -3.774524    0.461609   -1.900672
 C   -4.818532    0.285728    0.190825
 C   -4.955807   -0.119337   -1.323187
 C   -6.132914    0.578661    0.894780
 C   -3.992582   -0.711384    1.002304
 C   -6.158942    0.526153   -2.008358
 C   -4.948540   -1.617971   -1.580637
 H   -6.189920    1.611225   -1.829428
 H   -7.105979    0.087394   -1.662635
 H   -6.080888    0.364311   -3.093414
 H   -4.017312   -2.085679   -1.234922
 H   -5.043762   -1.810484   -2.659468
 H   -5.795210   -2.104540   -1.072875
 H   -3.015972   -0.889284    0.524419
 H   -4.507815   -1.674197    1.127207
 H   -3.809483   -0.289449    2.001129
 H   -6.785922   -0.307239    0.884334
 H   -6.667870    1.414327    0.425156
 H   -5.942525    0.845657    1.944898
 C    1.652500    1.356138   -1.596251
 C    2.918710    1.853649   -1.350680
 C    0.472278    2.071293   -1.242695
 C    3.093566    3.115332   -0.750667
 C    0.676088    3.357420   -0.677688
 C    1.946715    3.857081   -0.434665
 C   -0.844126    1.456179   -1.397785
 C   -2.085876    2.356397   -1.359025
 H    2.069536    4.847398    0.010834
 H   -0.186608    3.974736   -0.420285
 H    3.793983    1.261693   -1.625477
 H    1.550643    0.372831   -2.064174
Cu   -0.682340    0.132272    0.173298
 H   -2.204343    2.938955   -2.294925
 H   -2.021087    3.090719   -0.541345
 H   -0.864845    0.789185   -2.272971
 H    4.764500   -6.288560    0.246921
 H    4.785775   -5.038876   -1.037594
 H    3.501554   -6.294370   -1.023354
 C    0.366874   -5.476348   -0.073067
 H   -0.215028   -6.088164   -0.773904
 H   -0.322786   -4.898482    0.560830
 H    0.973913   -6.138686    0.563862
 H    1.780562    0.790510    2.697931
 H    1.499833    2.351870    1.889158
 H    1.138847    2.176820    3.637938
 C    1.117908    1.668107    2.661730
 H   -0.493720   -0.762437    3.727983
 P   -0.577074    1.143910    2.217564
 H   -0.970823    0.723448    4.605832
 C   -1.094608    0.157790    3.669370
 H   -1.171127    3.426313    1.684945
 H   -1.510038    3.076400    3.409668
 C   -1.559788    2.673581    2.386169
 H   -2.151131   -0.129369    3.564508
 H   -2.605016    2.460575    2.116459
 O    4.607720    4.768265    0.068391
 H    6.909881    3.520985    0.509028
 C    4.420990    3.689825   -0.451835
 H    6.933096    4.302550   -1.098315
 C    6.742414    3.358669   -0.566328
 O    5.430239    2.885778   -0.815367
 H    7.426674    2.584375   -0.933274
78
Figure 3_para-CO2Me_pc3_02 / electronic energy: -3887.98357896 a.u. / lowest freq: 18.65 cm-1
 C   -0.167061   -1.111222   -0.821260
 C   -0.002520   -1.750535    0.391213
 C    1.340678   -1.976739    1.020642
 O    1.983991   -3.148863    0.475555
 P    3.201199   -3.002283   -0.545371
 O    2.984965   -2.265778   -1.807863
 O    4.324184   -2.361655    0.416345
 O    3.619655   -4.519468   -0.791190
 C    5.529510   -1.842824   -0.135026
 H   -1.091786   -1.233235   -1.393638
 H    0.693265   -0.696973   -1.359873
 H   -0.820102   -2.370159    0.778816
 H    1.997946   -1.105755    0.888880
 H    1.240345   -2.168361    2.096065
 B    0.736042    2.489464   -1.417781
 O    1.727913    1.779550   -2.046756
 O    1.249543    3.426747   -0.551819
 C    2.975224    2.102064   -1.408298
 C    2.668353    3.514372   -0.797087
 C    4.090243    2.073730   -2.439556
 C    3.209362    1.031821   -0.344616
 C    2.881142    4.652453   -1.794521
 C    3.399227    3.818200    0.499602
 H    2.384227    4.446900   -2.754441
 H    3.949366    4.829282   -1.985691
 H    2.448874    5.575495   -1.380873
 H    3.178611    3.081027    1.280384
 H    3.101319    4.809056    0.873808
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 H    4.486640    3.832181    0.330597
 H    2.413897    1.061403    0.416374
 H    4.178589    1.155800    0.159840
 H    3.188018    0.046534   -0.831464
 H    5.040882    2.401660   -1.992495
 H    3.865433    2.718474   -3.299328
 H    4.222526    1.047456   -2.813089
 C   -3.699168    1.153502    0.639855
 C   -4.900762    0.470891    0.612811
 C   -2.813310    1.173439   -0.475895
 C   -5.310964   -0.231243   -0.534534
 C   -3.270763    0.493404   -1.637449
 C   -4.474781   -0.193610   -1.661433
 C   -1.498361    1.798308   -0.375135
 C   -0.785741    2.212688   -1.664567
 H   -4.779570   -0.710833   -2.573345
 H   -2.656892    0.499536   -2.540039
 H   -5.554065    0.471231    1.488855
 H   -3.415111    1.696884    1.543927
Cu   -0.610228    0.240836    0.644505
 H   -1.269514    3.094304   -2.135630
 H   -0.829949    1.408004   -2.415489
 H   -1.506834    2.617849    0.360807
 H    5.992202   -1.207260    0.630450
 H    5.328940   -1.244968   -1.036170
 H    6.222251   -2.659756   -0.390741
 C    3.841875   -5.432307    0.278715
 H    4.269740   -6.342396   -0.159461
 H    2.895353   -5.680194    0.780638
 H    4.549545   -5.019722    1.014202
 H    2.081022    1.462217    2.658119
 H    1.013379    2.790439    2.134275
 H    1.260676    2.472162    3.887750
 C    1.155536    2.008119    2.894651
 H    1.091339   -0.864347    3.905431
 P   -0.261407    0.852754    2.832509
 H    0.239946    0.127981    5.124436
 C    0.142439   -0.361400    4.142905
 H   -1.832903    2.698480    2.965460
 H   -1.298902    2.192551    4.597733
 C   -1.600770    1.832052    3.602110
 H   -0.648858   -1.124203    4.195612
 H   -2.507310    1.217327    3.702806
 O   -7.335555   -1.022520    0.450188
 H   -8.940235   -1.714449   -1.531001
 C   -6.591340   -0.965398   -0.504677
 H   -8.046434   -3.153320   -0.960059
 C   -8.058098   -2.347403   -1.708927
 O   -6.862696   -1.588241   -1.661084
 H   -8.112047   -2.779250   -2.715395
78
Figure 3_para-CO2Me_ts(AS)_01 / electronic energy: -3887.94585044 a.u. / lowest freq: -275.06 cm-1
 C   -0.237810   -1.039093   -0.868720
 C   -0.077884   -1.884157    0.250857
 C    1.034448   -1.794730    1.089113
 O    2.395414   -3.366193    0.558327
 P    3.432250   -2.857152   -0.433162
 O    3.050611   -2.047912   -1.630491
 O    4.509960   -2.030787    0.498946
 O    4.326246   -4.125030   -0.946811
 C    5.629952   -1.441325   -0.116409
 H   -1.113474   -1.162156   -1.510033
 H    0.647034   -0.583549   -1.330317
 H   -0.885333   -2.567131    0.532624
 H    1.825087   -1.069829    0.895518
 H    1.021781   -2.262126    2.071280
 B    0.549762    2.388425   -1.444083
 O    1.542229    1.637894   -2.013130
 O    1.046626    3.431542   -0.703880
 C    2.794875    2.057777   -1.437322
 C    2.462206    3.522149   -0.984202
 C    3.889986    1.931361   -2.481775
 C    3.072758    1.116824   -0.269460
 C    2.633210    4.546804   -2.103932
 C    3.204006    3.983788    0.258228
 H    2.134433    4.222377   -3.029323
 H    3.695302    4.725842   -2.324936
 H    2.182401    5.499940   -1.790613
 H    2.998016    3.343290    1.123852
 H    2.906472    5.011823    0.513419
 H    4.289143    3.981503    0.075251
 H    2.280391    1.198192    0.491413
 H    4.037105    1.331651    0.212923
 H    3.092444    0.085263   -0.651773
 H    4.844739    2.314399   -2.090473
 H    3.642743    2.476883   -3.402054
 H    4.023971    0.870397   -2.738321
 C   -3.739903    0.788151    0.744300
 C   -4.974119    0.158777    0.713421
 C   -2.911802    0.861173   -0.398659
 C   -5.447442   -0.427085   -0.468886
 C   -3.413629    0.281051   -1.582754
 C   -4.649670   -0.353267   -1.617279
 C   -1.575507    1.498721   -0.314016
 C   -0.966348    2.024275   -1.613580
 H   -5.007077   -0.791561   -2.550546
 H   -2.827242    0.328142   -2.501861
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 H   -5.597598    0.120439    1.609331
 H   -3.399813    1.247243    1.674137
Cu   -0.495683    0.134414    0.727716
 H   -1.542661    2.896658   -1.978148
 H   -1.013773    1.263326   -2.407192
 H   -1.600458    2.297954    0.443205
 H    6.133144   -0.804322    0.625947
 H    5.343607   -0.820674   -0.981828
 H    6.349369   -2.203082   -0.465323
 C    4.790756   -5.069106   -0.009554
 H    5.397977   -5.810087   -0.549144
 H    3.955687   -5.587124    0.489984
 H    5.419328   -4.599018    0.766797
 H    2.116467    1.751066    2.694605
 H    0.939610    2.968450    2.118813
 H    1.181433    2.710191    3.881070
 C    1.142409    2.218722    2.897175
 H    1.301250   -0.679120    3.917752
 P   -0.161853    0.942942    2.859917
 H    0.420901    0.287560    5.142024
 C    0.332298   -0.225965    4.172464
 H   -1.952597    2.588613    2.905842
 H   -1.326225    2.251174    4.549093
 C   -1.601828    1.797859    3.584824
 H   -0.417148   -1.026802    4.254713
 H   -2.418553    1.080308    3.750111
 O   -7.508804   -1.136315    0.506279
 H   -9.177351   -1.524625   -1.551676
 C   -6.778728   -1.085328   -0.456808
 H   -8.460780   -3.071893   -1.008702
 C   -8.368825   -2.248514   -1.731908
 O   -7.097955   -1.624220   -1.636788
 H   -8.444781   -2.641569   -2.752440
78
Figure 3_para-CO2Me_ts(AS)_02 / electronic energy: -3887.94832102 a.u. / lowest freq: -271.05 cm-1
 C   -0.843389   -1.663203   -0.704559
 C   -0.911702   -2.011216    0.670226
 C    0.201900   -1.856262    1.503156
 O    1.364985   -3.615098    1.455695
 P    2.147792   -3.631248    0.146146
 O    2.369791   -2.363665   -0.622396
 O    3.556848   -4.369630    0.516414
 O    1.455012   -4.698010   -0.882097
 C    4.508517   -4.561143   -0.507806
 H   -1.725690   -1.782394   -1.338237
 H    0.131102   -1.717639   -1.200588
 H   -1.849170   -2.369225    1.106262
 H    1.098690   -1.363285    1.125168
 H    0.101439   -1.961632    2.582667
 B   -3.159088    1.291339   -1.257956
 O   -4.020794    1.706036   -0.272923
 O   -3.531191    0.092488   -1.802200
 C   -4.875729    0.593926    0.055426
 C   -4.810532   -0.277077   -1.254365
 C   -6.260494    1.107201    0.411223
 C   -4.241315   -0.093787    1.262422
 C   -5.870071    0.108305   -2.283610
 C   -4.830187   -1.778520   -1.015605
 H   -5.873630    1.192492   -2.470640
 H   -6.876736   -0.193983   -1.961036
 H   -5.647820   -0.398212   -3.234212
 H   -3.988870   -2.103712   -0.389443
 H   -4.760716   -2.308391   -1.976999
 H   -5.767740   -2.081600   -0.525804
 H   -3.219667   -0.432853    1.028434
 H   -4.829205   -0.957019    1.604836
 H   -4.180386    0.628051    2.089712
 H   -6.954779    0.268809    0.572049
 H   -6.669299    1.755804   -0.374259
 H   -6.214337    1.690728    1.342587
 C    1.848661    0.906976   -1.153115
 C    3.109573    1.438832   -0.933015
 C    0.699504    1.731445   -1.224571
 C    3.285574    2.822800   -0.775964
 C    0.896343    3.117989   -1.065757
 C    2.161353    3.651372   -0.845803
 C   -0.641785    1.122590   -1.421131
 C   -1.839280    2.054162   -1.620963
 H    2.293122    4.729747   -0.733205
 H    0.046673    3.799214   -1.130225
 H    3.970984    0.771046   -0.879590
 H    1.759673   -0.180089   -1.245182
Cu   -0.802434    0.058889    0.288652
 H   -1.866420    2.447406   -2.655842
 H   -1.784097    2.929642   -0.957696
 H   -0.595955    0.382785   -2.229949
 H    5.425798   -4.955431   -0.048031
 H    4.744157   -3.614115   -1.020227
 H    4.153110   -5.285793   -1.260836
 C    1.046408   -5.957153   -0.399205
 H    0.638458   -6.527178   -1.246109
 H    0.267677   -5.860653    0.375238
 H    1.891011   -6.523353    0.030401
 H    1.611983    0.960054    2.719660
 H    1.505762    2.366797    1.628658
 H    1.095203    2.551887    3.365681
 C    1.044107    1.875991    2.498277
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 H   -0.800210   -0.151962    3.934304
 P   -0.682742    1.438083    2.103432
 H   -1.210215    1.503354    4.489226
 C   -1.334072    0.773567    3.674294
 H   -1.025821    3.628142    1.141853
 H   -1.521636    3.602751    2.863328
 C   -1.534430    3.038781    1.918360
 H   -2.402481    0.538263    3.565309
 H   -2.572117    2.863129    1.598746
 O    4.799345    4.632087   -0.404016
 H    7.024422    3.556331    0.614338
 C    4.615230    3.445736   -0.553236
 H    7.183587    3.770119   -1.154702
 C    6.921861    3.056224   -0.360070
 O    5.607829    2.551887   -0.540307
 H    7.593577    2.190987   -0.403444
78
Figure 3_para-CO2Me_pi-allyl_01 / electronic energy: -3887.97108875 a.u. / lowest freq: 20.87 cm-1
 C   -1.064258   -1.683443   -1.652510
 C   -1.790985   -2.328145   -0.618258
 C   -1.201528   -2.562325    0.613419
 O    1.865716   -2.334262    1.014445
 P    2.602297   -2.632938   -0.266627
 O    1.976543   -2.416663   -1.617612
 O    4.027307   -1.818125   -0.169654
 O    3.119260   -4.191714   -0.249317
 C    4.919924   -1.891501   -1.254959
 H   -1.598619   -1.379796   -2.554312
 H    0.021090   -1.872640   -1.734551
 H   -2.879947   -2.384971   -0.706906
 H   -0.105580   -2.623700    0.735424
 H   -1.824300   -2.884259    1.452529
 B   -3.361817    1.245888   -0.776445
 O   -4.165404    1.542048    0.293534
 O   -3.879536    0.244734   -1.553816
 C   -5.194780    0.535116    0.361667
 C   -5.240562    0.021719   -1.121411
 C   -6.485628    1.162626    0.858509
 C   -4.705420   -0.524665    1.348110
 C   -6.135222    0.874832   -2.018755
 C   -5.598137   -1.445657   -1.277120
 H   -5.916635    1.947184   -1.905592
 H   -7.199986    0.712155   -1.799945
 H   -5.954683    0.601481   -3.068550
 H   -4.932199   -2.102997   -0.704772
 H   -5.539012   -1.733518   -2.336930
 H   -6.628163   -1.622854   -0.933410
 H   -3.779036   -1.002938    0.995474
 H   -5.459347   -1.307570    1.513187
 H   -4.498793   -0.043157    2.315214
 H   -7.306520    0.430969    0.823006
 H   -6.769462    2.039193    0.261647
 H   -6.365681    1.487683    1.902471
 C    1.707111    0.847708   -1.246996
 C    2.982524    1.315821   -0.970669
 C    0.567786    1.643533   -1.011305
 C    3.171782    2.605835   -0.455884
 C    0.773239    2.941736   -0.511363
 C    2.053181    3.413969   -0.236007
 C   -0.791948    1.084932   -1.279262
 C   -1.996639    1.987196   -1.022250
 H    2.195818    4.423119    0.156424
 H   -0.075970    3.604201   -0.338549
 H    3.839925    0.663441   -1.131402
 H    1.599425   -0.179855   -1.607723
Cu   -0.975460   -0.479741   -0.028238
 H   -2.127523    2.684048   -1.873960
 H   -1.835222    2.620568   -0.139792
 H   -0.819801    0.694965   -2.302391
 H    5.743032   -1.185803   -1.069558
 H    4.427003   -1.626767   -2.205150
 H    5.347976   -2.904126   -1.363804
 C    3.674785   -4.705570    0.936837
 H    3.915840   -5.765506    0.768053
 H    2.967325   -4.629833    1.779298
 H    4.602638   -4.176463    1.218539
 H    1.688448   -0.420316    2.053965
 H    1.588042    1.329343    1.683760
 H    1.408415    0.783145    3.384615
 C    1.202559    0.530407    2.333149
 H   -0.599038   -1.702094    3.373217
 P   -0.584327    0.336571    2.067347
 H   -0.902569   -0.268528    4.403033
 C   -1.127518   -0.740586    3.434495
 H   -0.863715    2.730674    1.850485
 H   -1.158397    2.188277    3.528214
 C   -1.328805    1.949561    2.467459
 H   -2.209925   -0.921645    3.366024
 H   -2.408730    1.926982    2.259041
 O    4.719347    4.221355    0.384955
 H    6.948792    2.864850    0.946862
 C    4.518877    3.141742   -0.121154
 H    7.086484    3.630418   -0.664575
 C    6.825092    2.703065   -0.134020
 O    5.500800    2.296168   -0.440694
 H    7.481632    1.889421   -0.463348
78
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Figure 3_para-CO2Me_pi-allyl_02 / electronic energy: -3887.96383511 a.u. / lowest freq: 21.15 cm-1
 C   -0.807470   -0.074775   -2.058156
 C   -0.674831   -1.461347   -1.806138
 C    0.452974   -1.923744   -1.142044
 O    3.228041   -3.287554   -0.195673
 P    4.042106   -2.132989   -0.705417
 O    3.412958   -0.979918   -1.443868
 O    4.889107   -1.559302    0.589986
 O    5.262770   -2.673634   -1.666256
 C    5.798655   -0.506980    0.392949
 H   -1.752589    0.316837   -2.439338
 H    0.088693    0.533836   -2.229522
 H   -1.566778   -2.095535   -1.870333
 H    1.420092   -1.394079   -1.211936
 H    0.500421   -2.948932   -0.767960
 B    0.265167    2.922515   -0.299151
 O    1.221623    2.164922   -0.919788
 O    0.801169    3.910678    0.474781
 C    2.494865    2.492742   -0.322239
 C    2.225300    3.940582    0.222319
 C    3.582298    2.377084   -1.375768
 C    2.725638    1.466790    0.783165
 C    2.470697    5.025172   -0.823767
 C    2.951500    4.274935    1.513843
 H    1.968612    4.789480   -1.773982
 H    3.544043    5.157470   -1.021499
 H    2.068926    5.980231   -0.454224
 H    2.651954    3.606040    2.331252
 H    2.723738    5.307686    1.816745
 H    4.039990    4.192754    1.375062
 H    1.922641    1.511030    1.536001
 H    3.686244    1.624383    1.294279
 H    2.748340    0.470967    0.317810
 H    4.545275    2.726861   -0.972413
 H    3.345244    2.969059   -2.270165
 H    3.683030    1.318078   -1.660015
 C   -3.563905   -0.037852    1.149707
 C   -4.836151   -0.576112    1.035094
 C   -3.036110    0.828330    0.170300
 C   -5.643080   -0.260343   -0.065693
 C   -3.868847    1.154809   -0.915946
 C   -5.146880    0.618702   -1.035210
 C   -1.641212    1.331383    0.302248
 C   -1.267316    2.608796   -0.444924
 H   -5.769155    0.887133   -1.890540
 H   -3.514362    1.843509   -1.685060
 H   -5.223807   -1.250143    1.801639
 H   -2.953225   -0.291801    2.019251
Cu   -0.509166   -0.300250   -0.068219
 H   -1.872264    3.452190   -0.065927
 H   -1.485121    2.523368   -1.521928
 H   -1.406851    1.448054    1.370546
 H    6.107241   -0.127193    1.378932
 H    5.349708    0.321313   -0.179178
 H    6.702466   -0.843462   -0.145877
 C    5.992994   -3.800366   -1.248905
 H    6.723190   -4.046755   -2.033951
 H    5.335725   -4.670752   -1.085442
 H    6.542843   -3.609151   -0.309540
 H    0.354412    0.891861    3.253124
 H   -1.296340    0.233449    3.425622
 H    0.061481   -0.518759    4.317854
 C   -0.230645   -0.031574    3.375463
 H    2.483939   -0.844330    2.206652
 P    0.091155   -1.147880    1.970971
 H    1.874976   -2.195739    3.205706
 C    1.799604   -1.702569    2.224050
 H   -1.983380   -2.411098    2.180766
 H   -0.737550   -2.989449    3.335558
 C   -0.914105   -2.631669    2.309879
 H    2.115832   -2.401228    1.430770
 H   -0.632528   -3.423263    1.600493
 O   -7.452061   -1.629838    0.675088
 H   -9.622339   -0.762794   -0.568032
 C   -6.997024   -0.872138   -0.149603
 H   -8.933515   -2.135789   -1.486989
 C   -8.969279   -1.039304   -1.408612
 O   -7.666351   -0.498802   -1.241341
 H   -9.362258   -0.613336   -2.338897
39
Figure 4_para-NMe2_L-Cu-OtBu / electronic energy: -2316.39314463 a.u. / lowest freq: 15.08 cm-1
 C   -0.498289   -1.681031   -0.152427
 C   -1.237584   -1.347445   -1.296960
 C   -0.972772   -1.195660    1.077755
 C   -2.117048   -0.420108    1.164329
 C   -2.866748   -0.083896    0.006808
 C   -2.387165   -0.574274   -1.233136
 H   -0.433126   -1.421984    2.000711
 H   -2.433199   -0.070901    2.146691
 H   -2.914625   -0.347791   -2.159106
 H   -0.893051   -1.698055   -2.274189
 C    0.753302   -2.444880   -0.295478
 C    1.630903   -2.802337    0.703754
 H    0.930584   -2.850613   -1.299387
 H    1.426444   -2.608632    1.761807
 H    2.439541   -3.506045    0.485823
 H    4.298713    2.871785    0.015425
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 H     3.509208    2.904737   -1.577772
 C     3.326495    2.970794   -0.493313
 O     2.994493    0.630073   -0.377034
 H     2.916786    3.969814   -0.270799
 C     2.389030    1.833825   -0.053365
 H     3.101309    1.791959    2.002391
 H     1.185507    1.850956   -1.864681
 C     2.150477    1.936142    1.464495
 C     1.038819    1.982646   -0.780483
 H     1.722253    2.906564    1.767228
 H     0.565379    2.964444   -0.610641
 H     1.455039    1.143091    1.789784
 H     0.332986    1.204281   -0.442150
Cu     2.180374   -0.979899   -0.070442
 H    -3.715353    1.862691    1.825944
 H    -5.384116    1.738855    1.224422
 C    -4.451297    1.180414    1.364695
 H    -4.655702    0.366484    2.081475
 H    -4.116738    1.611727   -1.816209
 N    -4.001101    0.675892    0.086451
 H    -5.608480    1.615344   -0.849938
 C    -4.728955    1.017009   -1.115351
 H    -5.083448    0.119332   -1.650825
81
Figure 4_para-NMe2_ed / electronic energy: -3138.15747466 a.u. / lowest freq: 11.30 cm-1
 H     4.204122   -2.473274   -1.322121
 H     4.869496   -1.220495   -0.256980
 O     2.575860   -0.360423   -1.543458
 C     4.718839   -1.500848   -1.307941
 H     5.707407   -1.623681   -1.778208
 C     3.894428   -0.448334   -2.056020
 H     3.213778   -1.847023   -3.573003
 H     4.725237    1.242237   -0.955942
 C     3.727242   -0.874611   -3.515756
 C     4.585723    0.918059   -1.995265
 H     3.117702   -0.136792   -4.059537
 H     4.700270   -0.965702   -4.022722
 H     3.968341    1.674862   -2.503299
 H     5.568541    0.880918   -2.491556
Cu     0.484364   -1.494231   -0.171853
 H     0.053852    3.682072    1.605925
 H     0.408602    4.663620   -0.642665
 H     1.461989    3.287071   -0.174371
 C     0.738814    3.651343   -0.918904
 H    -1.512230    4.335165    1.050586
 H     1.257408    3.711193   -1.887357
 C    -0.990230    3.425468    1.385049
 H    -1.462527    3.089452    2.320561
 C    -1.091758    2.328946    0.335072
 C    -0.436088    2.681463   -1.047479
 O    -0.308662    1.203183    0.758760
 H    -1.911994    4.092972   -1.782999
 B     0.339330    0.651268   -0.337602
 H    -0.871054    3.383663   -3.040820
 C    -1.411988    3.167558   -2.107379
 O     0.115686    1.420097   -1.457376
 H    -3.219659    2.667540   -0.059796
 C    -2.536005    1.850374    0.214319
 H    -2.859951    1.440988    1.182259
 H    -2.178900    2.413450   -2.329004
 H    -2.626037    1.050049   -0.533307
 H     4.527594   -1.720908    2.211271
 H     5.105012    0.210458    1.295198
 H     3.176300   -2.681617    2.847966
 C     3.579665   -1.661267    2.761322
 O     2.412552   -1.258334    0.719012
 H     4.915830    0.741558    2.987754
 C     4.563054    0.899008    1.957656
 H     3.785779   -1.292445    3.777551
 B     2.203261   -0.119295   -0.201627
 H     4.827637    1.925871    1.663411
 C     2.563926   -0.772973    2.050999
 C     3.046491    0.728557    1.835564
 O     2.696036    1.028660    0.493849
 H     0.894180   -1.939992    2.751545
 C     1.220276   -0.887936    2.779148
 H     1.305724   -0.595116    3.835999
 H     0.445685   -0.264713    2.312057
 H     2.567530    1.498699    3.822379
 C     2.361858    1.728110    2.765388
 H     2.746600    2.739212    2.561324
 H     1.277785    1.738281    2.601325
 H    -0.870315   -2.609096   -2.025216
 H    -2.879863   -1.563980   -2.649096
 H     0.519423   -3.980540   -0.579614
 C    -1.101005   -2.628051   -0.952876
 C    -3.215039   -1.503768   -1.609667
 C    -0.291797   -3.391745   -0.140590
 H    -5.039144   -0.546093   -2.170250
 C    -2.390627   -2.010391   -0.595848
 C    -4.446391   -0.923689   -1.337868
 H    -0.565185   -3.629841    0.892540
 C    -2.859005   -1.901423    0.723029
 C    -4.919896   -0.813034   -0.008560
 H    -2.242273   -2.259312    1.551737
 C    -4.084561   -1.326090    1.016550
 H    -4.386869   -1.256257    2.060869
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 H   -7.200782   -0.328076   -1.545018
 H   -7.792631    0.850694   -0.357603
 C   -6.885786    0.402621   -0.780441
 H   -6.319907    1.203342   -1.290347
 H   -6.634912   -1.041893    2.160383
 N   -6.120783   -0.217873    0.277142
 H   -7.533665    0.407593    1.674105
 C   -6.546114   -0.067800    1.650187
 H   -5.853898    0.561081    2.239554
81
Figure 4_para-NMe2_ts(TB) / electronic energy: -3138.15700613 a.u. / lowest freq: -44.46 cm-1
 H    4.417597   -2.241907   -1.596214
 H    5.020680   -1.053167   -0.418788
 O    2.632610   -0.255388   -1.516362
 C    4.855490   -1.238012   -1.490115
 H    5.834890   -1.230791   -1.992960
 C    3.930462   -0.181259   -2.098787
 H    3.278768   -1.464964   -3.725064
 H    4.700610    1.434633   -0.851599
 C    3.717252   -0.464957   -3.584574
 C    4.519934    1.219684   -1.913441
 H    3.025128    0.274312   -4.015646
 H    4.667341   -0.419601   -4.138201
 H    3.821245    1.977859   -2.298262
 H    5.472582    1.313785   -2.457729
Cu    0.476209   -1.436993   -0.292358
 H    0.107788    3.608624    1.762222
 H    0.430173    4.636838   -0.474018
 H    1.415086    3.188866   -0.081537
 C    0.686693    3.614008   -0.788097
 H   -1.443559    4.358829    1.296103
 H    1.170024    3.669797   -1.774935
 C   -0.957013    3.412982    1.580497
 H   -1.405552    3.074049    2.526733
 C   -1.160805    2.356237    0.504661
 C   -0.548886    2.719593   -0.893394
 O   -0.425245    1.176905    0.854326
 H   -1.977972    4.237619   -1.507878
 B    0.106704    0.600153   -0.297058
 H   -1.030940    3.526007   -2.837108
 C   -1.541560    3.301224   -1.888633
 O   -0.098232    1.443879   -1.371912
 H   -3.287425    2.820174    0.228496
 C   -2.634866    1.957918    0.432277
 H   -2.932926    1.518664    1.395827
 H   -2.355877    2.596459   -2.103975
 H   -2.800483    1.198564   -0.344922
 H    4.514148   -1.881689    2.205318
 H    5.083014    0.116849    1.448091
 H    3.155038   -2.912848    2.699525
 C    3.541672   -1.882731    2.714063
 O    2.468858   -1.341919    0.650076
 H    4.826211    0.528329    3.165438
 C    4.506962    0.750730    2.136688
 H    3.693294   -1.593648    3.764852
 B    2.352890   -0.158709   -0.159478
 H    4.761125    1.799177    1.921062
 C    2.542366   -0.957739    2.030856
 C    3.000241    0.563086    1.953128
 O    2.692813    0.951418    0.617070
 H    0.857554   -2.199502    2.537416
 C    1.166549   -1.151060    2.672389
 H    1.200099   -0.951232    3.753282
 H    0.407012   -0.495795    2.224920
 H    2.407742    1.170165    3.960362
 C    2.254419    1.480542    2.915535
 H    2.636925    2.507361    2.810407
 H    1.181150    1.492358    2.690966
 H   -0.796972   -2.492390   -2.254887
 H   -2.775166   -1.347780   -2.763368
 H    0.657329   -3.920590   -0.938162
 C   -1.021749   -2.614406   -1.188347
 C   -3.123864   -1.410614   -1.728664
 C   -0.174373   -3.406422   -0.447536
 H   -4.913740   -0.341308   -2.186335
 C   -2.322333   -2.054070   -0.776148
 C   -4.342978   -0.833982   -1.399947
 H   -0.425299   -3.735824    0.565907
 C   -2.803629   -2.091457    0.541813
 C   -4.826216   -0.865441   -0.070235
 H   -2.208796   -2.564081    1.328037
 C   -4.015806   -1.518625    0.892634
 H   -4.329277   -1.566417    1.935037
 H   -6.543546   -1.257822    2.076392
 H   -7.404097    0.254733    1.735358
 C   -6.429851   -0.242630    1.659660
 H   -5.719123    0.309027    2.301973
 N   -6.012309   -0.271352    0.276416
 H   -7.672797    0.870218   -0.254111
 C   -6.760583    0.470461   -0.712471
 H   -7.066463   -0.166598   -1.559895
 H   -6.186029    1.322169   -1.120435
81
Figure 4_para-NMe2_prod / electronic energy: -3138.17640839 a.u. / lowest freq: 16.18 cm-1
 H    6.224452   -0.802365   -1.263057
 H    5.767131   -0.093661    0.310918
 O    3.566993   -0.595087   -1.218047
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 C    5.845342    0.104476   -0.767333
 H    6.578210    0.911249   -0.919026
 C    4.489559    0.502500   -1.347181
 H    4.959130   -0.144553   -3.363909
 H    3.839549    1.546984    0.448392
 C    4.596696    0.756590   -2.846479
 C    3.909615    1.723671   -0.635094
 H    3.613409    1.023374   -3.262107
 H    5.297209    1.579490   -3.052021
 H    2.900692    1.946605   -1.013587
 H    4.549543    2.603891   -0.797800
Cu    0.324225   -0.636409   -1.182082
 H    0.131419    2.647383    2.992026
 H    1.247250    4.509135    1.718618
 H    1.771926    2.832401    1.392899
 C    1.361739    3.744578    0.935463
 H   -1.022480    4.002704    2.839846
 H    2.095910    4.113444    0.203783
 C   -0.855757    2.939023    2.609000
 H   -1.612050    2.352976    3.153073
 C   -0.981666    2.679038    1.114395
 C    0.040209    3.459765    0.219287
 O   -0.634692    1.317700    0.842905
 H   -0.803402    5.455381    0.393513
 B    0.023232    1.221392   -0.389734
 H    0.278709    5.226132   -1.000753
 C   -0.500718    4.744609   -0.391073
 O    0.311365    2.515481   -0.827144
 H   -2.808705    3.877617    0.913161
 C   -2.434265    2.870643    0.675084
 H   -3.062895    2.134170    1.197475
 H   -1.364158    4.552249   -1.041463
 H   -2.548095    2.698699   -0.405058
 H    3.199330   -3.833982    1.013727
 H    3.963147   -2.865567    2.943115
 H    1.560341   -4.293812    0.496574
 C    2.131023   -3.747654    1.261864
 O    1.887357   -1.778203   -0.057419
 H    2.570723   -2.485681    3.996650
 C    3.305717   -2.060690    3.296820
 H    1.958967   -4.235113    2.231927
 B    3.068631   -1.057184   -0.057617
 H    3.922281   -1.338599    3.852110
 C    1.675643   -2.291981    1.278744
 C    2.603612   -1.355178    2.148260
 O    3.594363   -0.920557    1.195485
 H   -0.379791   -2.878306    0.972850
 C    0.196336   -2.197478    1.616997
 H    0.024365   -2.497745    2.661542
 H   -0.192144   -1.178914    1.475347
 H    1.165995   -0.349398    3.444638
 C    1.887528   -0.105262    2.651919
 H    2.632522    0.588109    3.069699
 H    1.343280    0.403677    1.844650
 H   -1.041754   -0.760079   -3.373408
 H   -2.839605    0.650207   -2.645006
 H    0.631610   -2.496796   -3.012373
 C   -1.150559   -1.423244   -2.507770
 C   -3.189885   -0.116594   -1.947888
 C   -0.193178   -2.382404   -2.303091
 H   -4.904898    1.037099   -1.417990
 C   -2.425199   -1.279496   -1.775976
 C   -4.364013    0.107224   -1.245036
 H   -0.310744   -3.174571   -1.557878
 C   -2.912457   -2.231423   -0.870021
 C   -4.845039   -0.843182   -0.311472
 H   -2.367580   -3.166220   -0.714496
 C   -4.086433   -2.028894   -0.155641
 H   -4.414072   -2.805990    0.534227
 H   -5.750918   -1.833387    2.134370
 H   -7.405049   -1.281480    1.790537
 C   -6.475332   -1.629994    1.325575
 H   -6.691810   -2.587947    0.820137
 H   -6.108842    1.491212    0.471150
 N   -5.995040   -0.625907    0.404674
 H   -7.587449    0.615607    0.917526
 C   -6.728001    0.607439    0.236536
 H   -7.113425    0.729380   -0.791691
46
Figure 4_para-NMe2_L-Cu-Bpin / electronic energy: -2494.38389228 a.u. / lowest freq: 19.78 cm-1
 H    4.799727   -1.415644   -2.552250
 H    5.475356   -0.107818   -1.560557
 C    5.040299   -1.115093   -1.521252
 H    2.808444   -2.662696   -1.862332
 O    2.855620   -0.165281   -1.134220
 H    5.800872   -1.811273   -1.134869
 C    3.782342   -1.156385   -0.665646
 C    3.103125   -2.519542   -0.811947
 B    2.158354    0.368157   -0.053667
 H    3.774257   -3.344235   -0.529284
 H    4.982641    1.136059    0.299253
 H    2.193385   -2.579750   -0.196068
 H    6.097709   -0.137237    0.872268
 C    5.098489    0.302797    1.008129
 C    3.987366   -0.733797    0.827789
 O    2.745653   -0.079343    1.126549
 H    5.039673    0.715904    2.026139
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 H    5.096116   -2.462449    1.541583
 C    4.194100   -1.885951    1.800027
 H    3.334398   -2.568865    1.811330
 H    4.324421   -1.492596    2.819570
Cu    0.554196    1.615224   -0.133750
 C   -2.255257    1.543002    0.142642
 C   -2.964751    1.138133    1.283683
 C   -2.494206    0.827379   -1.044055
 C   -3.397369   -0.220707   -1.095716
 C   -4.127242   -0.619417    0.054472
 C   -3.877648    0.093813    1.252799
 H   -1.954131    1.087886   -1.957878
 H   -3.536961   -0.738011   -2.044257
 H   -4.400243   -0.168001    2.172324
 H   -2.799242    1.662495    2.229260
 C   -1.304797    2.660731    0.233473
 C   -0.647700    3.271861   -0.794387
 H   -1.175502    3.076775    1.240265
 H   -0.830772    3.019930   -1.843789
 H   -0.039482    4.159905   -0.602622
 H   -4.358148   -2.813226   -1.638393
 H   -6.015393   -3.126180   -1.083342
 C   -5.271698   -2.336794   -1.243075
 H   -5.663729   -1.657769   -2.020930
 H   -5.118539   -2.335573    2.010711
 N   -5.026737   -1.649141    0.005068
 H   -6.443952   -2.851465    0.946803
 C   -5.777570   -2.014295    1.185551
 H   -6.402275   -1.181875    1.555097
70
Figure 4_para-NMe2_pc1 / electronic energy: -2937.58317342 a.u. / lowest freq: -6.61 cm-1
 H   -1.371180    3.037561   -0.097667
 C   -2.950545    1.837672    0.804587
 C   -1.606225    2.189138    0.544298
 H   -4.181872    0.424900    1.915077
 C   -3.168357    0.737398    1.664231
 H    4.336200    3.243287   -1.706808
 C   -0.554190    1.450291    1.070858
 H    3.782918    1.310772   -3.119092
 H    0.465532    1.745226    0.808677
 C   -2.105348    0.006997    2.175280
 C   -0.770590    0.334148    1.896304
 C    4.992771    2.653095   -1.049642
 C    4.577876    0.746609   -2.608877
 H    4.875684    3.036540   -0.027288
 O    3.320561    0.975162   -0.590498
 H   -2.321071   -0.854098    2.813882
 H    5.526789    0.942737   -3.129980
 H    6.032415    2.822237   -1.369970
 C    4.631306    1.178416   -1.142756
 C    0.328320   -0.483202    2.435713
 B    3.279900   -0.258386    0.045452
 H    1.915755    0.988289    2.331725
 C    1.642716   -0.052027    2.525073
 C    5.508463    0.229394   -0.256646
 H    5.174893    1.392867    1.561608
 O    4.561163   -0.782266    0.127687
 H    6.782812    1.645982    0.826245
 H    7.371941    0.336855   -1.367016
 C    6.000378    0.899314    1.026881
 H    2.357767   -0.624867    3.123355
 C    6.676150   -0.423643   -0.979844
 H    6.421566    0.132068    1.693408
 H    7.234414   -1.066888   -0.283082
Cu    1.569465   -1.097849    0.758229
 H    0.034285   -1.401941    2.953388
 H    4.343406   -0.324245   -2.702513
 H    6.339283   -1.049460   -1.816766
 H   -2.143209   -3.635660    0.845726
 H    0.262131   -3.431218    0.836454
 H   -4.374579   -2.870709    0.240550
 C   -2.239700   -2.786663    0.162258
 C   -3.515143   -2.351459   -0.183000
 C    0.250952   -2.677671    0.041034
 H    1.375316   -2.014567   -1.688587
 C   -1.082039   -2.179334   -0.340536
 C    1.405310   -2.502443   -0.709910
 C   -3.697681   -1.241087   -1.036008
 C   -1.266809   -1.094596   -1.212625
 H    2.272124   -3.144672   -0.532834
 C   -2.530114   -0.635945   -1.556406
 H   -0.397088   -0.574429   -1.623165
 H   -2.604586    0.222789   -2.222589
 H   -5.554660    2.428652    1.694840
 H   -6.052455    2.806586    0.024811
 C   -5.355418    2.212000    0.627974
 H   -5.584212    1.149697    0.446176
 H   -3.275987    4.526328    0.111491
 N   -4.000603    2.525964    0.237706
 H   -4.690166    4.130536   -0.897698
 C   -3.743878    3.736665   -0.506600
 H   -3.082895    3.551571   -1.369934
 H   -6.144101   -1.609787    0.189220
 H   -7.023841   -0.923277   -1.186206
 C   -6.123066   -1.483630   -0.906030
 H   -6.192813   -2.490054   -1.361437
 H   -4.736777   -0.009156   -3.320588
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 N   -4.953449   -0.753022   -1.333886
 H   -4.551635    1.204051   -2.019951
 C   -5.097469    0.294084   -2.319328
 H   -6.157537    0.560157   -2.411306
70
Figure 4_para-NMe2_ts(CuBadd)_01 / electronic energy: -2937.57583746 a.u. / lowest freq: -173.04 cm-1
 H    1.267216    2.947995    0.443482
 C    2.750572    1.874417   -0.730806
 C    1.440029    2.179614   -0.310238
 H    3.862961    0.600775   -2.103040
 C    2.879257    0.877198   -1.723342
 H   -3.876822    2.861787    2.271666
 C    0.337100    1.495522   -0.814271
 H   -3.553994    0.603232    3.173528
 H   -0.648677    1.756084   -0.418425
 C    1.770744    0.205259   -2.219094
 C    0.460261    0.483640   -1.785908
 C   -4.569231    2.517486    1.489120
 C   -4.371206    0.250807    2.527058
 H   -4.393187    3.125689    0.592423
 O   -3.042271    0.857618    0.635050
 H    1.925475   -0.573149   -2.972282
 H   -5.319779    0.389141    3.065776
 H   -5.596222    2.697648    1.841372
 C   -4.346638    1.038653    1.217809
 C   -0.682718   -0.286159   -2.284884
 B   -3.119493   -0.191936   -0.257164
 H   -2.242230    1.151281   -1.751342
 C   -2.050449    0.097770   -1.995975
 C   -5.283139    0.424001    0.117530
 H   -4.772452    1.942837   -1.369012
 O   -4.422149   -0.561038   -0.491870
 H   -6.368603    2.179580   -0.606505
 H   -7.156343    0.446511    1.209181
 C   -5.658986    1.424219   -0.974057
 H   -2.805188   -0.304104   -2.681352
 C   -6.527455   -0.264777    0.652578
 H   -6.134128    0.884669   -1.806672
 H   -7.122562   -0.662394   -0.182852
Cu   -1.456624   -1.300846   -0.695884
 H   -0.501502   -0.940275   -3.142487
 H   -4.222150   -0.824867    2.350432
 H   -6.274151   -1.101778    1.316197
 H    2.083153   -3.579348   -1.030674
 H   -0.284905   -3.594108   -0.734069
 H    4.318345   -2.740264   -0.559548
 C    2.198694   -2.777310   -0.295481
 C    3.475680   -2.297575   -0.028963
 C   -0.276349   -2.796191    0.017337
 H   -1.390483   -2.115441    1.767807
 C    1.060451   -2.268446    0.345511
 C   -1.436722   -2.616668    0.795874
 C    3.681903   -1.246044    0.892244
 C    1.270933   -1.238336    1.277437
 H   -2.277005   -3.304989    0.664212
 C    2.537113   -0.741505    1.551831
 H    0.418502   -0.791389    1.795971
 H    2.628549    0.068223    2.275007
 H    6.020974   -1.359565   -0.576679
 H    6.990875   -0.777025    0.788755
 C    6.091622   -1.347291    0.524236
 H    6.240721   -2.390908    0.861270
 H    4.502307    1.152031    1.985346
 N    4.936194   -0.725483    1.125341
 H    6.169880    0.583468    2.173665
 C    5.121983    0.259174    2.165530
 H    4.880491   -0.132792    3.171904
 H    5.249937    2.638310   -1.800969
 H    5.918969    2.794444   -0.155356
 C    5.161239    2.276423   -0.757431
 H    5.414109    1.204291   -0.746561
 H    3.161303    4.498223    0.147939
 N    3.856910    2.507440   -0.185712
 H    4.637742    4.014072    1.021601
 C    3.663600    3.656539    0.664481
 H    3.062321    3.407476    1.555153
70
Figure 4_para-NMe2_ts(CuBadd)_02 / electronic energy: -2937.56458202 a.u. / lowest freq: -194.19 cm-1
 H   -3.563543    3.487368    0.078929
 C   -1.708859    4.562316   -0.295700
 C   -2.525692    3.413075   -0.246954
 H    0.320819    5.206876   -0.757740
 C   -0.371724    4.365898   -0.710924
 H   -5.637367   -2.257196    0.625067
 C   -2.041389    2.158411   -0.611383
 H   -3.992106   -2.464117    2.427626
 H   -2.725993    1.307987   -0.541481
 C    0.097195    3.108941   -1.072519
 C   -0.715180    1.958907   -1.039367
 C   -5.072047   -2.913985   -0.052703
 C   -3.500425   -3.267595    1.859704
 H   -5.190645   -2.527266   -1.073345
 O   -3.020521   -1.660591    0.158679
 H    1.141666    3.009142   -1.383807
 H   -3.990116   -4.218305    2.115131
 H   -5.520691   -3.917672   -0.001496
 C   -3.612068   -2.957305    0.367400
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 C   -0.168327    0.642584   -1.385774
 B   -1.703677   -1.853393   -0.197326
 H   -2.074616   -0.351332   -1.789053
 C   -1.012848   -0.529500   -1.570538
 C   -2.701226   -3.877359   -0.521061
 H   -3.306429   -2.924392   -2.392418
 O   -1.443440   -3.170440   -0.492935
 H   -4.080385   -4.505742   -2.097897
 H   -3.462080   -5.803132    0.119311
 C   -3.149319   -3.932704   -1.980289
 H   -0.588295   -1.305448   -2.217241
 C   -2.497719   -5.281648    0.022746
 H   -2.365695   -4.422938   -2.576672
 H   -1.865010   -5.863370   -0.663952
Cu   -0.233373   -0.502868    0.274602
 H    0.822653    0.631843   -1.848908
 H   -2.449468   -3.315203    2.182663
 H   -2.006697   -5.268566    1.004437
 H    3.023176    1.850603    1.299032
 H    0.899771    1.020922    1.981290
 H    5.273760    1.582051    0.413082
 C    3.356366    0.850997    1.004502
 C    4.640826    0.698762    0.496988
 C    1.118855   -0.012680    1.689095
 H   -0.582984   -0.752222    2.795481
 C    2.475852   -0.231222    1.149029
 C    0.247622   -1.022895    2.136578
 C    5.121280   -0.569373    0.093817
 C    2.951383   -1.488922    0.743591
 H    0.569263   -2.067464    2.194441
 C    4.229665   -1.661287    0.229189
 H    2.302688   -2.366393    0.816733
 H    4.536288   -2.663965   -0.068600
 H   -0.717132    7.116253   -0.741652
 H   -1.805426    7.821885    0.461652
 C   -1.256690    6.909049    0.197349
 H   -0.499975    6.726745    0.985966
 H   -4.283988    5.547605   -0.009507
 N   -2.188935    5.818128    0.044929
 H   -3.712945    6.990702    0.842955
 C   -3.491978    5.932498    0.654241
 H   -3.570010    5.391228    1.618058
 H    6.195941   -2.447290   -1.642964
 H    7.854762   -1.963954   -1.231610
 C    6.833609   -2.038438   -0.838977
 H    6.843860   -2.773238   -0.013800
 H    6.901764    1.175393   -1.187598
 N    6.391159   -0.734125   -0.405988
 H    8.254554    0.064005   -0.883137
 C    7.282437    0.397828   -0.500679
 H    7.455385    0.872831    0.481479
70
Figure 4_para-NMe2_L-Cu-alkyl_01 / electronic energy: -2937.61855973 a.u. / lowest freq: 28.24 cm-1
 H    1.007223    3.304130    0.305896
 C    2.370554    1.951600   -0.707919
 C    1.101542    2.451490   -0.367942
 H    3.338709    0.440813   -1.942959
 C    2.391612    0.868449   -1.612910
 H   -3.430490    2.886824    2.553021
 C   -0.072126    1.876395   -0.863261
 H   -1.636700    1.274401    2.066088
 H   -1.024446    2.298081   -0.536180
 C    1.215673    0.304319   -2.091079
 C   -0.064938    0.770911   -1.730704
 C   -4.220924    2.196801    2.222493
 C   -2.402808    0.507541    1.880579
 H   -5.010655    2.791426    1.745159
 O   -3.204980    1.815084    0.062663
 H    1.292898   -0.549491   -2.773080
 H   -2.627394    0.003573    2.831606
 H   -4.639409    1.707396    3.114883
 C   -3.640760    1.166304    1.270309
 C   -1.296672    0.074848   -2.219934
 B   -3.338857    0.906081   -0.960704
 H   -2.347633    1.983605   -2.648953
 C   -2.576812    0.949109   -2.325373
 C   -4.671290    0.118704    0.716232
 H   -6.046888    1.658735    0.002128
 O   -4.146110   -0.146985   -0.595811
 H   -6.571383    0.853018    1.507473
 H   -4.996898   -0.994721    2.550344
 C   -6.072951    0.698989    0.539344
 H   -3.232577    0.511590   -3.096786
 C   -4.732122   -1.182473    1.498862
 H   -6.679951   -0.003187   -0.050919
 H   -5.496203   -1.846450    1.067795
Cu   -1.421244   -1.486869   -0.977192
 H   -1.068323   -0.340799   -3.217565
 H   -1.975052   -0.230267    1.181854
 H   -3.770537   -1.709737    1.465016
 H    2.167774   -3.679584   -1.183204
 H   -0.195004   -3.770569   -1.076940
 H    4.323505   -2.719607   -0.589068
 C    2.202981   -2.898333   -0.418576
 C    3.433019   -2.350566   -0.081590
 C   -0.263513   -3.098466   -0.212406
 H   -1.552811   -2.546241    1.425333
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 C    1.012184   -2.485792    0.193572
 C   -1.461402   -3.033929    0.450046
 C    3.530039   -1.323094    0.886721
 C    1.108188   -1.464431    1.155546
 H   -2.298035   -3.662146    0.130792
 C    2.322208   -0.896063    1.496752
 H    0.205401   -1.079691    1.637433
 H    2.330525   -0.092839    2.232184
 H    4.892439    2.453086   -1.833554
 H    5.626180    2.581951   -0.211035
 C    4.804170    2.124325   -0.777820
 H    4.960446    1.035799   -0.746981
 H    3.143163    4.584910   -0.201003
 N    3.545884    2.484456   -0.169564
 H    4.470874    4.039954    0.862235
 C    3.477729    3.773238    0.477019
 H    2.792297    3.754933    1.338741
 H    5.965600   -1.166468   -0.465976
 H    6.807712   -0.711603    1.029108
 C    5.952583   -1.271757    0.633172
 H    6.108570   -2.339334    0.870639
 H    4.171347    1.150943    1.924737
 N    4.733085   -0.756917    1.212612
 H    5.830993    0.642061    2.299441
 C    4.796723    0.288723    2.210752
 H    4.473721   -0.064332    3.206929
70
Figure 4_para-NMe2_L-Cu-alkyl_02 / electronic energy: -2937.61545910 a.u. / lowest freq: 21.88 cm-1
 C   -2.999364   -2.133815   -0.536684
 C   -2.986210   -1.097159   -1.482874
 C   -3.565156   -1.848965    0.716164
 C   -4.070781   -0.594899    1.017778
 C   -4.026459    0.461440    0.073326
 C   -3.490356    0.162343   -1.201893
 H   -3.614535   -2.626184    1.482857
 H   -4.503301   -0.433424    2.004443
 H   -3.438650    0.929245   -1.973440
 H   -2.548261   -1.279740   -2.468297
 C   -2.362122   -3.418959   -0.867168
 C   -2.113950   -4.468010   -0.022275
 H   -2.123151   -3.552720   -1.929538
 H   -2.450192   -4.473423    1.019763
 H   -1.745767   -5.416110   -0.424074
 B    3.410343   -1.049985   -0.086124
 O    3.977735   -0.334260   -1.110115
 O    3.782042   -0.565854    1.144198
 C    4.895638    0.617798   -0.545531
 C    4.397909    0.717373    0.944809
 C    4.805203    1.917154   -1.330864
 C    6.296674    0.021803   -0.673024
 C    3.309502    1.773960    1.142298
 C    5.502135    0.909124    1.972289
 H    2.499547    1.661001    0.406286
 H    3.716231    2.793118    1.067393
 H    2.868682    1.649937    2.142415
 H    6.224991    0.082985    1.956963
 H    5.065244    0.959054    2.980726
 H    6.041804    1.851172    1.791137
 H    6.387206   -0.916726   -0.105912
 H    7.069117    0.720693   -0.320601
 H    6.494485   -0.202261   -1.731852
 H    5.413911    2.702571   -0.857791
 H    3.768781    2.271981   -1.404930
 H    5.184604    1.764077   -2.352328
 C   -0.233320    0.073798    1.213879
 C   -0.782352    1.335191    1.020931
 C    0.493709   -0.606633    0.218346
 C   -0.651254    2.010593   -0.210912
 C    0.626377    0.080982   -0.999400
 C    0.084530    1.350030   -1.211455
 C    1.064107   -1.972587    0.460490
 C    2.398948   -2.238775   -0.279531
 H    0.241159    1.820155   -2.182976
 H    1.186365   -0.375764   -1.819157
 H   -1.329454    1.792946    1.845656
 H   -0.369818   -0.408332    2.187790
Cu   -0.476928   -3.134107    0.037298
 H    2.252976   -2.423901   -1.357833
 H    2.845317   -3.169723    0.113412
 H    1.257764   -2.053599    1.544971
 H   -4.439375    1.674633    2.493395
 H   -5.307953    3.036094    1.767436
 C   -5.103601    1.963546    1.663448
 H   -6.059598    1.420521    1.787601
 H   -3.644801    2.920571   -1.136672
 N   -4.482633    1.717495    0.381484
 H   -4.985687    3.645267   -0.228223
 C   -4.617007    2.708915   -0.664297
 H   -5.329531    2.395258   -1.449656
 H   -0.904965    4.249063    1.440192
 H   -2.156175    4.947107    0.374588
 C   -1.708213    4.004553    0.715799
 H   -2.492249    3.450726    1.255772
 H    0.237441    4.250345   -1.615837
 N   -1.237482    3.259087   -0.426576
 H   -1.403835    4.954325   -1.624690
 C   -0.845238    4.009478   -1.594561
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 H   -1.082640    3.463247   -2.521563
70
Figure 4_para-NMe2_L-Cu-alkyl_03 / electronic energy: -2937.61764213 a.u. / lowest freq: 21.08 cm-1
 B    3.591087    1.251832   -0.135976
 O    4.249845    0.587186   -1.143675
 O    4.276068    1.186668    1.051584
 C    5.290927   -0.200165   -0.540674
 C    5.552298    0.573273    0.803681
 C    6.483023   -0.264992   -1.481083
 C    4.716982   -1.599297   -0.321070
 C    6.575360    1.698125    0.652190
 C    5.918931   -0.311684    1.984812
 H    6.334238    2.347244   -0.202850
 H    7.593102    1.304353    0.516668
 H    6.564623    2.317925    1.561038
 H    5.124167   -1.033325    2.214643
 H    6.080537    0.308631    2.878901
 H    6.848920   -0.864709    1.783199
 H    3.857187   -1.573283    0.366609
 H    5.468905   -2.293308    0.081616
 H    4.366772   -1.993840   -1.286388
 H    7.330407   -0.777102   -1.000460
 H    6.809264    0.735960   -1.792406
 H    6.214697   -0.829960   -2.386396
 C   -1.232092    1.033972    1.258578
 C   -2.584009    1.329187    1.148270
 C   -0.271811    1.458067    0.316596
 C   -3.085059    2.074263    0.057957
 C   -0.776895    2.231361   -0.739854
 C   -2.135801    2.532598   -0.871969
 C    1.162929    1.047405    0.446823
 C    2.186918    1.921465   -0.303106
 H   -2.445611    3.139125   -1.723896
 H   -0.092762    2.617991   -1.499756
 H   -3.259571    0.957836    1.919210
 H   -0.901433    0.431975    2.112074
Cu    1.142414   -0.854725   -0.121258
 H    2.181499    2.971697    0.057504
 H    1.961644    1.961258   -1.382253
 H    1.423960    1.043563    1.521044
 H   -3.564200   -0.818998   -1.977758
 C   -3.127510   -1.369928   -1.146091
 H   -1.236605   -1.456793   -2.119652
 C   -1.796565   -1.735836   -1.223580
 C   -3.907406   -1.675189   -0.000228
 H    0.845287   -2.288686   -2.230091
 C   -3.264839   -2.375940    1.048324
 C   -1.156289   -2.428497   -0.180168
 C    1.153489   -2.643990   -1.241306
 H   -3.809863   -2.641972    1.953300
 C   -1.926210   -2.729152    0.952294
 C    0.268718   -2.795325   -0.207360
 H   -1.460251   -3.256903    1.789520
 H    0.623030   -3.317752    0.690045
 H    2.153267   -3.078991   -1.166463
 H   -5.079586    2.739754    1.911258
 H   -6.358753    2.307877    0.742840
 C   -5.321160    2.101413    1.037031
 H   -5.281304    1.051808    1.364671
 H   -4.460117    4.325853   -0.854548
 N   -4.450328    2.327379   -0.091485
 H   -5.961299    3.381707   -1.061031
 C   -4.865423    3.313966   -1.059055
 H   -4.557404    3.032421   -2.078881
 H   -5.558681   -1.278573    2.177753
 H   -7.007658   -1.242376    1.155338
 C   -6.001450   -1.668668    1.245672
 H   -6.104095   -2.763943    1.353758
 H   -5.386699    0.298596   -1.287385
 N   -5.220696   -1.299795    0.086720
 H   -6.914179   -0.451981   -0.782035
 C   -5.868930   -0.661116   -1.038799
 H   -5.865749   -1.301035   -1.939576
70
Figure 4_para-NMe2_ts(BHE) / electronic energy: -2937.57872574 a.u. / lowest freq: -844.05 cm-1
 B   -3.572840    0.691576    0.047383
 O   -4.595866    1.346271    0.670996
 O   -4.000206   -0.175344   -0.918664
 C   -5.821823    0.694021    0.280073
 C   -5.418833    0.029728   -1.088783
 C   -6.930838    1.727571    0.183171
 C   -6.141398   -0.328344    1.368947
 C   -5.595220    0.967227   -2.280770
 C   -6.086160   -1.307017   -1.365038
 H   -5.122173    1.943657   -2.098453
 H   -6.657683    1.131490   -2.510631
 H   -5.116750    0.519415   -3.164021
 H   -5.840089   -2.051523   -0.596906
 H   -5.749904   -1.698052   -2.336763
 H   -7.179639   -1.190575   -1.405827
 H   -5.348387   -1.086692    1.454113
 H   -7.096053   -0.839579    1.179810
 H   -6.215671    0.190808    2.335631
 H   -7.852863    1.268489   -0.203978
 H   -6.653099    2.563793   -0.471795
 H   -7.147460    2.136275    1.181191
 C    1.294688    1.018287   -1.356926
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 C    2.605204    1.454649   -1.222030
 C    0.348920    1.130970   -0.320360
 C    3.072311    2.022177   -0.015833
 C    0.814913    1.718923    0.870323
 C    2.127218    2.162018    1.020136
 C   -1.015586    0.616187   -0.485972
 C   -2.074125    0.898602    0.443146
 H    2.412643    2.606958    1.973586
 H    0.137549    1.837321    1.720523
 H    3.281638    1.325975   -2.067004
 H    0.989206    0.566400   -2.305245
Cu   -1.211443   -0.942474    0.855985
 H   -1.919369    1.721022    1.152479
 H   -2.260593   -0.081587    1.691345
 H   -1.284624    0.241019   -1.478119
 H    3.976393   -0.812520    1.833958
 C    3.426693   -1.288169    1.022197
 H    1.669294   -1.432045    2.222913
 C    2.103929   -1.642855    1.242179
 C    4.044907   -1.499054   -0.233315
 H   -0.252619   -2.600744    2.603819
 C    3.266065   -2.128268   -1.230469
 C    1.318853   -2.240160    0.242748
 C   -0.773833   -2.725812    1.649129
 H    3.688675   -2.336733   -2.212933
 C    1.940230   -2.469084   -0.992523
 C   -0.099191   -2.600773    0.428382
 H    1.366709   -2.934352   -1.799641
 H   -0.573978   -3.040408   -0.457272
 H   -1.703583   -3.300859    1.690259
 H    5.396688   -1.011632   -2.588620
 H    6.966309   -0.965871   -1.767624
 C    5.966176   -1.414958   -1.734435
 H    6.078741   -2.504523   -1.891934
 H    5.674212    0.305159    1.069289
 N    5.337875   -1.093383   -0.475172
 H    7.118812   -0.263863    0.214902
 C    6.143936   -0.578142    0.607627
 H    6.322983   -1.330067    1.399427
 H    4.934264    3.169905   -1.778479
 H    6.277430    2.713782   -0.696212
 C    5.262226    2.440436   -1.011542
 H    5.327976    1.451246   -1.490991
 H    4.251088    4.147166    1.371172
 N    4.396786    2.405384    0.142783
 H    5.852133    3.366293    1.279628
 C    4.772292    3.171403    1.306194
 H    4.564469    2.620514    2.238452
70
Figure 4_para-NMe2_pc2 / electronic energy: -2937.60609935 a.u. / lowest freq: 21.56 cm-1
 B    3.399923    0.892410    0.227561
 O    4.509456    1.497390   -0.293715
 O    3.700867   -0.205496    0.992774
 C    5.611159    0.584072   -0.112312
 C    5.134777   -0.265547    1.123258
 C    6.889645    1.372484    0.114917
 C    5.716898   -0.240878   -1.393926
 C    5.492845    0.375484    2.462249
 C    5.570649   -1.721411    1.100565
 H    5.199826    1.435473    2.493049
 H    6.570929    0.305742    2.666977
 H    4.955925   -0.148784    3.266634
 H    5.170544   -2.248116    0.224431
 H    5.203589   -2.233345    2.002481
 H    6.668257   -1.799385    1.088195
 H    4.793620   -0.809182   -1.581415
 H    6.564104   -0.940653   -1.358625
 H    5.864973    0.439613   -2.245072
 H    7.721117    0.693620    0.357479
 H    6.782716    2.102328    0.928173
 H    7.156659    1.921357   -0.800315
 C   -1.471271    0.912569    1.465071
 C   -2.805822    1.272359    1.363065
 C   -0.532994    1.244039    0.477498
 C   -3.288068    1.961580    0.225802
 C   -1.002902    1.966087   -0.631878
 C   -2.337712    2.320924   -0.760940
 C    0.862693    0.807717    0.611739
 C    1.944246    1.368594   -0.032539
 H   -2.646429    2.864978   -1.653139
 H   -0.310747    2.237949   -1.433522
 H   -3.487154    0.981025    2.161425
 H   -1.144349    0.350358    2.344040
Cu    1.486306   -0.280227   -1.271478
 H    1.788790    2.257885   -0.652722
 H    2.242398    0.169909   -2.594571
 H    1.048942    0.060756    1.392074
 H   -3.761106   -0.817228   -1.880892
 C   -3.156731   -1.296193   -1.111233
 H   -1.381889   -1.058098   -2.272789
 C   -1.796489   -1.438306   -1.334919
 C   -3.748476   -1.726365    0.100654
 H    0.565209   -2.250175   -2.751542
 C   -2.897578   -2.340352    1.046915
 C   -0.944342   -2.015038   -0.380857
 C    1.128124   -2.264475   -1.813611
 H   -3.296082   -2.707480    1.992479
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 C   -1.532634   -2.458351    0.809654
 C    0.505853   -2.173566   -0.593031
 H   -0.903523   -2.916401    1.578646
 H    1.086294   -2.431641    0.300419
 H    2.161325   -2.616162   -1.876666
 H   -5.193910   -1.667122    2.463056
 H   -6.736238   -1.798795    1.597489
 C   -5.674662   -2.071228    1.556011
 H   -5.606604   -3.174413    1.602975
 H   -5.600310   -0.008769   -1.023192
 N   -5.086661   -1.528606    0.353570
 H   -6.959301   -0.876296   -0.284594
 C   -5.944569   -0.999480   -0.682565
 H   -6.003377   -1.662929   -1.565667
 H   -5.334955    2.557183    2.064361
 H   -6.565915    2.192155    0.828360
 C   -5.543919    1.963887    1.154508
 H   -5.513506    0.897361    1.429907
 H   -4.618380    4.063930   -1.041100
 N   -4.622583    2.252792    0.078985
 H   -6.155534    3.167609   -0.993655
 C   -5.065923    3.053005   -1.039807
 H   -4.823044    2.576150   -2.004212
44
Figure 4_para-NMe2-alkenylBpin / electronic energy: -853.456934437 a.u. / lowest freq: 23.23 cm-1
 B   -2.187170   -0.365211    0.009480
 O   -3.150062   -1.308190    0.256850
 O   -2.719971    0.871376   -0.253825
 C   -4.429772   -0.720739   -0.045141
 C   -4.122547    0.819094    0.064576
 C   -5.461729   -1.234491    0.945780
 C   -4.799537   -1.155667   -1.462554
 C   -4.280376    1.361085    1.484676
 C   -4.893795    1.689895   -0.914167
 H   -3.742396    0.739095    2.215571
 H   -5.337156    1.416990    1.783044
 H   -3.856508    2.375071    1.528609
 H   -4.661526    1.436198   -1.956775
 H   -4.636808    2.747934   -0.756642
 H   -5.977402    1.578257   -0.758380
 H   -4.071062   -0.786727   -2.199959
 H   -5.798937   -0.798203   -1.749417
 H   -4.801313   -2.254633   -1.510976
 H   -6.427272   -0.727499    0.798153
 H   -5.140704   -1.082014    1.984379
 H   -5.619453   -2.312545    0.794328
 C    2.524789    1.319156   -0.116960
 C    3.911059    1.255250   -0.091630
 C    1.719306    0.170822   -0.054482
 C    4.579018    0.009600   -0.003909
 C    2.385000   -1.064718    0.028476
 C    3.767329   -1.153399    0.052138
 C    0.259119    0.304712   -0.075142
 C   -0.668799   -0.668118    0.038170
 H    4.224495   -2.140270    0.117856
 H    1.807980   -1.991876    0.074166
 H    4.477072    2.184934   -0.144841
 H    2.045955    2.300298   -0.188373
 H   -0.341817   -1.706766    0.171089
 H   -0.096635    1.336458   -0.193713
 H    6.587387    1.699032   -0.957837
 H    6.513293    1.810645    0.822063
 C    6.741153    1.134989   -0.020836
 H    7.804145    0.873333    0.040392
 N    5.945699   -0.071055    0.023558
 H    6.334805   -1.911285    1.011367
 H    7.683963   -1.215909    0.088537
 C    6.597253   -1.359645    0.091378
 H    6.341286   -1.999507   -0.771386
91
Figure 4_para-NMe2_pc3_01 / electronic energy: -3776.45374198 a.u. / lowest freq: 10.37 cm-1
 C   -0.175567   -1.502915   -0.659644
 C   -0.775804   -1.431034    0.578250
 C   -0.627727   -2.523397    1.595808
 O   -1.678133   -3.501917    1.456009
 P   -1.686819   -4.501593    0.205834
 O   -0.379719   -5.000628   -0.267975
 O   -2.712095   -5.578110    0.805034
 O   -2.488713   -3.773074   -0.979771
 C   -3.053239   -6.719095    0.024418
 H   -0.518154   -0.909724   -1.510426
 H    0.491273   -2.337799   -0.901248
 H   -1.615263   -0.745014    0.737510
 H    0.349171   -3.023814    1.506218
 H   -0.738677   -2.147456    2.620092
 B    0.148375    1.784831   -2.109446
 O   -0.887228    2.592722   -1.717111
 O   -0.244123    0.885515   -3.070988
 C   -2.103307    2.102743   -2.310191
 C   -1.565285    1.243783   -3.516197
 C   -2.971990    3.286683   -2.705661
 C   -2.821143    1.266247   -1.253427
 C   -1.400078    2.052378   -4.801685
 C   -2.356847   -0.024485   -3.799271
 H   -0.834008    2.979006   -4.624649
 H   -2.372073    2.316707   -5.242468
 H   -0.841946    1.450502   -5.533667
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 H   -2.366473   -0.709193   -2.940437
 H   -1.907667   -0.558718   -4.649432
 H   -3.397299    0.218889   -4.062485
 H   -2.217077    0.400455   -0.951901
 H   -3.792649    0.901314   -1.616714
 H   -2.990720    1.882145   -0.359733
 H   -3.872981    2.946671   -3.238035
 H   -2.431472    3.996036   -3.345510
 H   -3.294753    3.823898   -1.801102
 C    4.258457   -0.768608   -0.621219
 C    5.574357   -0.874365   -0.187173
 C    3.554157    0.451758   -0.647121
 C    6.289641    0.256052    0.270964
 C    4.284232    1.571952   -0.219644
 C    5.606366    1.485933    0.225591
 C    2.127351    0.496274   -1.070556
 C    1.606199    1.865907   -1.533599
 H    6.104213    2.405213    0.536282
 H    3.815343    2.559221   -0.234740
 H    6.048907   -1.855996   -0.208880
 H    3.749020   -1.677729   -0.959740
Cu    0.918296   -0.149394    0.427460
 H    2.261857    2.298836   -2.322215
 H    1.611324    2.608214   -0.716082
 H    1.989050   -0.228523   -1.889625
 H   -3.688929   -7.358285    0.649521
 H   -2.152270   -7.279038   -0.268788
 H   -3.611125   -6.429802   -0.880395
 C   -3.705746   -3.078260   -0.746402
 H   -4.196160   -2.945871   -1.719219
 H   -3.511944   -2.089866   -0.301898
 H   -4.375067   -3.649105   -0.084059
 H   -2.006674    4.286585    1.114485
 C   -2.003044    3.346884    1.665126
 H    0.058023    3.041061    1.225331
 C   -3.188682    2.865216    2.270667
 C   -0.818476    2.629394    1.730127
 C   -3.105440    1.621712    2.941770
 C   -0.732096    1.401251    2.403232
 H   -3.984173    1.190270    3.420292
 C   -1.906634    0.922805    3.001864
 C    0.508319    0.606246    2.473268
 H   -1.884944   -0.035441    3.529405
 H    0.461042   -0.282153    3.111038
 H    2.627987    0.411541    2.234595
 C    1.731607    0.981899    1.974559
 H    1.905853    1.966626    1.532811
 H    9.344264    1.108889    1.349644
 H    9.332841   -0.976701    0.938612
 H    8.481826    1.973063    0.048550
 C    8.348095    1.364486    0.965781
 H    8.461238   -1.283984   -0.587420
 C    8.333987   -1.061805    0.491234
 N    7.596886    0.153996    0.738918
 H    7.864452    2.003777    1.722182
 H    7.846972   -1.933660    0.957107
 H   -5.451789    5.183116    1.454311
 H   -6.388885    3.740103    2.659943
 H   -3.737016    5.537121    1.736145
 C   -4.441223    4.762824    1.387636
 H   -5.453380    2.807381    3.842652
 C   -5.573293    3.014692    2.766002
 N   -4.367209    3.565525    2.193123
 H   -4.225304    4.566514    0.321067
 H   -5.886505    2.075262    2.273550
91
Figure 4_para-NMe2_pc3_02 / electronic energy: -3776.46237503 a.u. / lowest freq: 23.42 cm-1
 C   -1.514921   -1.753517   -0.851369
 C   -0.991846   -2.137027    0.362962
 C    0.489359   -2.337495    0.555718
 O    1.008296   -3.316590   -0.363581
 P    2.060646   -2.848849   -1.474707
 O    1.599888   -1.884899   -2.496143
 O    3.293950   -2.345146   -0.575602
 O    2.507915   -4.242178   -2.100933
 C    4.060339   -1.195017   -0.922956
 H   -2.578356   -1.881227   -1.073888
 H   -0.856301   -1.589912   -1.710538
 H   -1.652813   -2.569881    1.120900
 H    1.042579   -1.393763    0.432995
 H    0.704410   -2.706949    1.565806
 B   -4.340635    1.246255   -0.428050
 O   -4.863187    1.216411    0.845680
 O   -4.882983    0.268108   -1.221950
 C   -5.575944   -0.022642    1.000992
 C   -5.928259   -0.390606   -0.489201
 C   -6.777654    0.194917    1.905422
 C   -4.604904   -1.010442    1.648526
 C   -7.254561    0.206299   -0.956075
 C   -5.886875   -1.878715   -0.799969
 H   -7.310088    1.283450   -0.739080
 H   -8.113193   -0.290597   -0.481718
 H   -7.341617    0.075750   -2.044760
 H   -4.892373   -2.305592   -0.614403
 H   -6.131558   -2.044359   -1.859557
 H   -6.621946   -2.426241   -0.190915
 H   -3.700838   -1.133277    1.031920
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 H   -5.063694   -1.996506    1.807452
 H   -4.292101   -0.618727    2.628047
 H   -7.379856   -0.723627    1.976107
 H   -7.420598    1.008012    1.544224
 H   -6.438288    0.456187    2.918777
 C    0.399675    1.226884   -2.006674
 C    1.698260    1.707705   -2.064654
 C   -0.658571    1.945192   -1.408616
 C    2.043373    2.961930   -1.513861
 C   -0.326046    3.235692   -0.965393
 C    0.980604    3.736205   -1.016208
 C   -1.980080    1.291742   -1.194390
 C   -3.180829    2.195786   -0.881125
 H    1.160776    4.739447   -0.628530
 H   -1.101640    3.879146   -0.541794
 H    2.453136    1.070620   -2.525227
 H    0.219516    0.226626   -2.408477
Cu   -1.502519   -0.042777    0.276440
 H   -3.463057    2.832593   -1.744865
 H   -2.959968    2.884384   -0.048919
 H   -2.221530    0.665747   -2.068079
 H    4.843740   -1.101601   -0.160856
 H    3.433980   -0.291954   -0.908201
 H    4.526656   -1.307421   -1.913629
 C    3.030156   -5.304165   -1.310166
 H    3.292949   -6.116145   -1.999218
 H    2.278810   -5.665186   -0.592458
 H    3.932094   -4.983483   -0.767351
 H    3.250382    1.942129    0.797832
 C    2.771781    1.236903    1.478492
 H    0.846744    1.928656    0.901147
 C    3.541224    0.327985    2.242904
 C    1.387731    1.230802    1.542274
 C    2.834394   -0.547391    3.100987
 C    0.681453    0.345518    2.372064
 H    3.371603   -1.255709    3.731453
 C    1.445301   -0.530729    3.154430
 C   -0.792885    0.297550    2.399556
 H    0.938247   -1.233745    3.822153
 H   -1.231275   -0.511016    2.994627
 H   -1.215499    2.213699    1.513272
 C   -1.618657    1.274424    1.902632
 H   -2.693752    1.254082    2.099723
 H    3.210268    4.996516   -0.095053
 H    4.729445    4.899750   -0.998127
 C    3.644307    4.751277   -1.076822
 H    3.251590    5.481746   -1.812940
 H    4.399476    1.631277   -2.029237
 N    3.374159    3.379182   -1.434065
 H    5.351969    3.122054   -2.033686
 C    4.358465    2.708610   -2.251874
 H    4.172810    2.819038   -3.339244
 H    5.432285    2.334163    1.814913
 H    6.674369    1.125516    1.399935
 C    5.596178    1.326034    1.391012
 H    5.272687    1.352294    0.337040
 H    5.555170   -0.387473    4.050745
 N    4.911489    0.294640    2.137675
 H    6.739020   -0.512999    2.727229
 C    5.674033   -0.603892    2.972676
 H    5.384010   -1.654816    2.805770
91
Figure 4_para-NMe2_ts(AS)_01 / electronic energy: -3776.41596452 a.u. / lowest freq: -320.16 cm-1
 C   -0.549349   -1.544162    0.360646
 C   -0.473757   -1.613072   -1.063316
 C   -1.552141   -1.210639   -1.854343
 O   -2.882969   -2.786378   -2.112357
 P   -3.678425   -2.970530   -0.821620
 O   -3.831765   -1.840525    0.149418
 O   -5.123250   -3.551851   -1.311867
 O   -3.057976   -4.235477    0.011433
 C   -6.112771   -3.806421   -0.338539
 H    0.256176   -1.954269    0.974609
 H   -1.544929   -1.562553    0.815419
 H    0.425566   -2.007744   -1.546668
 H   -2.385774   -0.671249   -1.403585
 H   -1.436799   -1.131418   -2.934918
 B    1.840759    0.338315    2.429524
 O    3.087657    0.444243    1.876382
 O    1.633797   -0.885579    3.010406
 C    3.676086   -0.869304    1.858907
 C    2.886130   -1.598138    3.007058
 C    5.173474   -0.749105    2.088000
 C    3.407318   -1.460253    0.476313
 C    3.517659   -1.404291    4.383968
 C    2.621224   -3.073385    2.755222
 H    3.725308   -0.342713    4.585619
 H    4.456444   -1.968245    4.481802
 H    2.817765   -1.764300    5.152310
 H    2.034155   -3.233837    1.841587
 H    2.061128   -3.502143    3.599202
 H    3.569402   -3.623899    2.660855
 H    2.329509   -1.563424    0.284267
 H    3.878762   -2.446086    0.354870
 H    3.819205   -0.781902   -0.282801
 H    5.633039   -1.744620    2.181684
 H    5.403179   -0.171301    2.992752
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 H     5.638763   -0.239337    1.230933
 C    -2.890921    1.329956    1.003579
 C    -3.929572    2.153819    0.592648
 C    -1.629548    1.838837    1.381020
 C    -3.781718    3.561001    0.546191
 C    -1.488222    3.235161    1.332203
 C    -2.521685    4.075829    0.924953
 C    -0.514801    0.908729    1.709317
 C     0.748597    1.463952    2.355151
 H    -2.338891    5.150520    0.913510
 H    -0.539269    3.693837    1.621575
 H    -4.869574    1.684324    0.302400
 H    -3.068475    0.248283    0.992915
Cu    -0.247857    0.317469   -0.206759
 H     0.521653    1.840300    3.373475
 H     1.160056    2.319091    1.796401
 H    -0.888352    0.058147    2.290572
 H    -7.002625   -4.192437   -0.855623
 H    -6.386391   -2.889050    0.207925
 H    -5.777194   -4.560796    0.394051
 C    -2.743316   -5.425268   -0.674310
 H    -2.366783   -6.150048    0.061922
 H    -1.967392   -5.258929   -1.439643
 H    -3.629634   -5.858306   -1.169525
 H     3.717639   -0.416650   -3.672850
 C     3.584765    0.323548   -2.884641
 H     1.465827    0.278273   -3.113183
 C     4.709753    0.852179   -2.197999
 C     2.298648    0.722296   -2.561896
 C     4.455995    1.802098   -1.178662
 C     2.048369    1.660130   -1.544598
 H     5.277064    2.238732   -0.611743
 C     3.160035    2.177506   -0.863762
 C     0.700412    2.111675   -1.176549
 H     3.003280    2.899093   -0.058296
 H     0.654598    2.813526   -0.337129
 H    -1.394202    2.308514   -1.519091
 C    -0.460875    1.832033   -1.833517
 H    -0.475448    1.287997   -2.780504
 H    -5.502598    6.290938   -0.330411
 H    -6.750736    4.609566   -0.583144
 H    -4.228733    6.276982    0.901345
 C    -4.570716    5.796097   -0.030530
 H    -6.504917    3.129279    0.357850
 C    -6.031490    3.809250   -0.369380
 N    -4.815686    4.385896    0.154333
 H    -3.812131    5.999995   -0.810831
 H    -5.868284    3.239877   -1.304633
 H     8.019452    0.452207   -2.060277
 H     7.282261   -0.720308   -3.631005
 H     7.222928    2.017529   -1.795952
 C     7.095671    0.924813   -1.707012
 H     5.821744   -0.213123   -4.501364
 C     6.205378   -0.547019   -3.522330
 N     5.981200    0.442628   -2.492138
 H     6.981017    0.684327   -0.635252
 H     5.729297   -1.515123   -3.284178
91
Figure 4_para-NMe2_ts(AS)_02 / electronic energy: -3776.41562681 a.u. / lowest freq: -278.62 cm-1
 C     0.476224   -1.314942   -0.767141
 C     0.073041   -1.759053    0.528738
 C     0.967640   -1.760253    1.596070
 O     2.114392   -3.524065    1.574401
 P     3.156732   -3.413495    0.465130
 O     3.596279   -2.073736   -0.041211
 O     4.418425   -4.303554    0.996919
 O     2.647372   -4.269244   -0.834037
 C     5.584763   -4.358713    0.205243
 H    -0.207567   -1.417359   -1.614251
 H     1.542597   -1.362846   -1.008157
 H    -0.942920   -2.133217    0.689439
 H     1.920310   -1.235632    1.508762
 H     0.623366   -2.001738    2.601338
 B    -1.526938    1.233101   -2.354799
 O    -2.763148    1.321047   -1.774134
 O    -1.447420    0.202364   -3.253545
 C    -3.513684    0.145327   -2.138661
 C    -2.771696   -0.330744   -3.443818
 C    -4.972156    0.526100   -2.332373
 C    -3.385159   -0.845378   -0.984865
 C    -3.332811    0.299925   -4.716611
 C    -2.679158   -1.839374   -3.607354
 H    -3.417024    1.392912   -4.622957
 H    -4.323605   -0.106910   -4.964558
 H    -2.653018    0.083764   -5.553861
 H    -2.153858   -2.313448   -2.767931
 H    -2.129952   -2.079817   -4.529597
 H    -3.683110   -2.283164   -3.685719
 H    -2.336546   -1.126167   -0.818665
 H    -3.965843   -1.760521   -1.167856
 H    -3.759031   -0.375092   -0.065847
 H    -5.552596   -0.337008   -2.691454
 H    -5.090191    1.350437   -3.047630
 H    -5.398869    0.846546   -1.370137
 C     3.202006    1.274048   -0.597295
 C     4.338947    1.875576   -0.075133
 C     2.053485    2.012042   -0.946359
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 C    4.404602    3.275110    0.129695
 C    2.125412    3.398117   -0.747994
 C    3.260222    4.020116   -0.229231
 C    0.832948    1.314024   -1.450073
 C   -0.314449    2.162073   -1.994075
 H    3.246302    5.103594   -0.107371
 H    1.270171    4.027656   -1.005840
 H    5.186078    1.237924    0.179231
 H    3.209137    0.183089   -0.701683
Cu    0.213794    0.367419    0.230297
 H    0.016732    2.715098   -2.896443
 H   -0.647881    2.922034   -1.269686
 H    1.123080    0.573686   -2.204932
 H    6.309849   -5.005574    0.719323
 H    6.029813   -3.359150    0.071560
 H    5.381530   -4.784806   -0.792503
 C    2.097218   -5.552279   -0.643537
 H    1.698989   -5.898693   -1.608177
 H    1.280969   -5.532590    0.096628
 H    2.858660   -6.273985   -0.299242
 H   -5.031453    2.251117    1.355225
 C   -4.356136    1.504806    1.771775
 H   -2.649917    2.685575    1.283354
 C   -4.869905    0.308570    2.335383
 C   -2.993672    1.750101    1.729702
 C   -3.929447   -0.611067    2.865510
 C   -2.063391    0.840212    2.257580
 H   -4.261808   -1.545549    3.315785
 C   -2.571121   -0.338908    2.825477
 C   -0.614220    1.085400    2.260055
 H   -1.874774   -1.070360    3.246015
 H   -0.039517    0.476564    2.965750
 H    1.109884    2.243578    1.777194
 C    0.052912    2.056567    1.571009
 H   -0.467556    2.799428    0.960539
 H    6.542003    5.602857    1.227253
 H    7.473040    3.727270    1.384257
 H    5.453344    5.839129   -0.158245
 C    5.572930    5.310131    0.805272
 H    7.105305    2.565412    0.088998
 C    6.688503    3.079403    0.974514
 N    5.528849    3.876372    0.653122
 H    4.788010    5.681345    1.488799
 H    6.464863    2.307991    1.732755
 H   -8.165687    0.622934    1.914875
 H   -7.797876   -1.204650    2.860408
 H   -7.099024    1.981189    2.336561
 C   -7.145644    1.010997    1.812008
 H   -6.450129   -1.255032    4.017556
 C   -6.705594   -1.174907    2.946441
 N   -6.212403    0.051245    2.359446
 H   -6.963769    1.197467    0.739260
 H   -6.304826   -2.067494    2.435461
91
Figure 4_para-NMe2_ts(AS)_03 / electronic energy: -3776.42214536 a.u. / lowest freq: -265.50 cm-1
 C   -1.710847   -1.464956   -1.002066
 C   -1.408677   -2.157776    0.208212
 C   -0.112651   -2.205202    0.706091
 O    0.955541   -3.766410   -0.289737
 P    1.866901   -3.050169   -1.280109
 O    1.340292   -2.009323   -2.217965
 O    3.066846   -2.433177   -0.343235
 O    2.654718   -4.169140   -2.169138
 C    3.954330   -1.479558   -0.878060
 H   -2.726204   -1.511360   -1.403600
 H   -0.900860   -1.374569   -1.734053
 H   -2.200431   -2.688463    0.746284
 H    0.647318   -1.519002    0.332080
 H    0.093206   -2.666373    1.671002
 B   -4.267295    1.196461   -0.487168
 O   -4.909836    1.325989    0.717961
 O   -4.704677    0.108073   -1.193177
 C   -5.618706    0.097044    0.967409
 C   -5.814635   -0.475639   -0.485922
 C   -6.907707    0.395736    1.713507
 C   -4.695082   -0.765999    1.825410
 C   -7.091120    0.021309   -1.160085
 C   -5.722627   -1.989717   -0.586548
 H   -7.186256    1.115006   -1.088659
 H   -7.987326   -0.437201   -0.718220
 H   -7.059089   -0.245760   -2.226543
 H   -4.748904   -2.364227   -0.243512
 H   -5.857019   -2.301903   -1.632638
 H   -6.511584   -2.466990    0.014089
 H   -3.738415   -0.940788    1.308865
 H   -5.146727   -1.736973    2.071962
 H   -4.478751   -0.241246    2.767840
 H   -7.497002   -0.524054    1.846079
 H   -7.523651    1.133778    1.183760
 H   -6.677521    0.798891    2.710670
 C    0.573855    1.222011   -1.906429
 C    1.843157    1.774849   -1.969521
 C   -0.531983    1.930263   -1.394386
 C    2.103811    3.078833   -1.491411
 C   -0.284140    3.253801   -1.000361
 C    0.989966    3.821560   -1.048934
 C   -1.859680    1.257944   -1.260450
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 C   -3.083176    2.119026   -0.944995
 H    1.108023    4.854425   -0.720663
 H   -1.105400    3.876349   -0.637625
 H    2.647733    1.159806   -2.371054
 H    0.470307    0.182205   -2.229307
Cu   -1.472909    0.001674    0.297287
 H   -3.365231    2.717863   -1.833750
 H   -2.883637    2.839271   -0.137064
 H   -2.061753    0.660707   -2.156713
 H    4.779903   -1.353853   -0.163051
 H    3.458990   -0.505498   -1.019144
 H    4.376629   -1.802170   -1.845551
 C    3.249976   -5.272581   -1.524831
 H    3.738143   -5.889065   -2.293211
 H    2.500756   -5.885680   -0.997904
 H    4.012165   -4.950844   -0.794577
 H    3.369015    2.015038    0.861237
 C    2.862502    1.298907    1.508903
 H    0.970298    2.143594    1.035345
 C    3.593190    0.296469    2.195041
 C    1.484048    1.371474    1.610610
 C    2.854514   -0.598966    3.008118
 C    0.748751    0.468821    2.395468
 H    3.360496   -1.387676    3.563547
 C    1.474464   -0.507639    3.094550
 C   -0.719507    0.474555    2.452680
 H    0.937860   -1.230335    3.716232
 H   -1.167552   -0.325429    3.053557
 H   -1.160785    2.329660    1.460971
 C   -1.551936    1.418370    1.920727
 H   -2.625381    1.392075    2.126813
 H    3.147870    5.188888   -0.097613
 H    4.679270    5.155054   -0.984950
 C    3.602640    4.961172   -1.074653
 H    3.187809    5.671819   -1.816188
 H    4.549549    1.847406   -1.807068
 N    3.394370    3.578239   -1.433652
 H    5.404467    3.390835   -1.950413
 C    4.447422    2.890796   -2.145930
 H    4.286789    2.872888   -3.241267
 H    5.556251    2.180112    1.626372
 H    6.741152    0.903706    1.266756
 C    5.672458    1.147589    1.252444
 H    5.338151    1.132210    0.200665
 H    5.566032   -0.793555    3.841031
 N    4.950814    0.193670    2.064373
 H    6.732155   -0.796715    2.500522
 C    5.665236   -0.864047    2.743443
 H    5.310022   -1.862334    2.433899
91
Figure 4_para-NMe2_ts(AS)_04 / electronic energy: -3776.41714465 a.u. / lowest freq: -193.45 cm-1
 C   -1.123253    1.674619    0.892002
 C   -0.806745    2.469511   -0.246917
 C    0.409798    2.360780   -0.900030
 O    1.772165    3.863565   -0.141894
 P    3.013888    3.268779    0.502224
 O    2.962421    2.453459    1.752820
 O    3.728781    2.410766   -0.711810
 O    4.095185    4.473168    0.745567
 C    4.895115    1.680174   -0.416887
 H   -2.044954    1.888767    1.437947
 H   -0.311242    1.235043    1.482650
 H   -1.549236    3.176015   -0.631382
 H    1.126718    1.590487   -0.612894
 H    0.568426    2.843504   -1.862261
 B   -0.482394   -1.398412    2.258449
 O    0.497212   -0.499244    2.584824
 O    0.015135   -2.658983    2.064196
 C    1.772545   -1.131922    2.349085
 C    1.400146   -2.651292    2.475443
 C    2.780529   -0.612554    3.359719
 C    2.209230   -0.744337    0.939532
 C    1.444827   -3.158832    3.914794
 C    2.196364   -3.568813    1.563900
 H    0.893265   -2.492072    4.594347
 H    2.478774   -3.247817    4.278087
 H    0.976917   -4.153194    3.962031
 H    2.020411   -3.326248    0.508877
 H    1.902773   -4.616321    1.729295
 H    3.273765   -3.480022    1.769660
 H    1.472638   -1.066806    0.188080
 H    3.175453   -1.201015    0.682185
 H    2.326877    0.347967    0.901304
 H    3.734116   -1.154756    3.265099
 H    2.417465   -0.718971    4.390857
 H    2.966423    0.452488    3.154180
 C   -4.567420   -1.080012   -0.669333
 C   -5.892016   -0.753669   -0.937805
 C   -3.839694   -0.499853    0.383602
 C   -6.585370    0.195142   -0.151610
 C   -4.546320    0.417190    1.179793
 C   -5.872109    0.758070    0.931486
 C   -2.406555   -0.846657    0.623433
 C   -1.994539   -1.004549    2.090577
 H   -6.353836    1.473520    1.598137
 H   -4.050685    0.885254    2.034475
 H   -6.391264   -1.254948   -1.767227
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 H   -4.083017   -1.829687   -1.301397
Cu   -1.394635    0.406927   -0.591619
 H   -2.630849   -1.781439    2.556650
 H   -2.173390   -0.079267    2.660573
 H   -2.161144   -1.774598    0.080351
 H    5.340734    1.349742   -1.366833
 H    4.678050    0.796700    0.206039
 H    5.641311    2.298002    0.111994
 C    4.295681    5.436424   -0.261902
 H    5.034003    6.163571    0.106511
 H    3.361266    5.968294   -0.504329
 H    4.686193    4.981395   -1.189074
 H    1.775988   -3.991462   -1.888017
 C    1.847450   -2.921114   -2.075727
 H   -0.263758   -2.760316   -2.293682
 C    3.106804   -2.267997   -2.050532
 C    0.682029   -2.213614   -2.309324
 C    3.124694   -0.889274   -2.374184
 C    0.695459   -0.832123   -2.572473
 H    4.065086   -0.343077   -2.410593
 C    1.949374   -0.201953   -2.625310
 C   -0.527144   -0.049802   -2.769387
 H    2.010674    0.866333   -2.846785
 H   -0.383275    0.957998   -3.171938
 H   -2.025762   -1.517423   -2.304728
 C   -1.803470   -0.478892   -2.559216
 H   -2.649496    0.152460   -2.846713
 H    5.497161   -1.336772   -1.118492
 H    6.297472   -2.906341   -1.324433
 C    5.522490   -2.248782   -1.735987
 H    5.826532   -1.959531   -2.758838
 H    3.517933   -4.694841   -0.780280
 N    4.249532   -2.936732   -1.709245
 H    5.225350   -4.720195   -1.250190
 C    4.230648   -4.376373   -1.557070
 H    3.966205   -4.894144   -2.496677
 H   -8.109280    2.387529    0.600754
 H   -9.612317    1.597206    0.092365
 C   -8.606362    1.409171    0.487071
 H   -8.715676    0.969122    1.496535
 H   -8.109945   -0.027767   -2.447454
 N   -7.890631    0.546637   -0.422850
 H   -9.612029    0.306277   -1.570060
 C   -8.612371   -0.134364   -1.470888
 H   -8.737126   -1.216135   -1.273435
91
Figure 4_para-NMe2_pi-allyl_01 / electronic energy: -3776.42561792 a.u. / lowest freq: 19.65 cm-1
 C    0.275898    1.464053    0.193334
 C   -0.211004    1.680924   -1.153069
 C    0.595222    1.506597   -2.237910
 O    3.202992    3.516694   -2.359087
 P    3.483172    3.197718   -0.925377
 O    3.385168    1.798675   -0.372235
 O    4.967941    3.823185   -0.575972
 O    2.523176    4.111313    0.066559
 C    5.496360    3.627389    0.710258
 H   -0.406401    1.644485    1.025470
 H    1.337320    1.688203    0.364848
 H   -1.285999    1.835848   -1.304666
 H    1.679025    1.403528   -2.115922
 H    0.194253    1.580063   -3.251533
 B   -1.824004   -0.525274    2.126868
 O   -3.150032   -0.734353    1.873528
 O   -1.590784    0.676701    2.737323
 C   -3.849866    0.504014    2.121015
 C   -2.860231    1.263334    3.083196
 C   -5.210529    0.200002    2.725716
 C   -4.023895    1.193932    0.769773
 C   -3.103313    0.961571    4.559961
 C   -2.783070    2.764910    2.860243
 H   -3.161077   -0.121041    4.747239
 H   -4.030661    1.428907    4.920571
 H   -2.265698    1.362628    5.148990
 H   -2.462278    3.010192    1.839238
 H   -2.057504    3.206110    3.559283
 H   -3.761141    3.235283    3.041602
 H   -3.053872    1.371790    0.280793
 H   -4.545890    2.155795    0.871843
 H   -4.623811    0.551049    0.111320
 H   -5.726784    1.132537    2.998858
 H   -5.131470   -0.431454    3.619852
 H   -5.834287   -0.328846    1.990109
 C    3.053097   -1.119152    0.767843
 C    4.188968   -1.875162    0.520112
 C    1.821596   -1.716930    1.101945
 C    4.168547   -3.289569    0.606629
 C    1.799183   -3.118449    1.178813
 C    2.931589   -3.889295    0.943592
 C    0.616914   -0.871694    1.332143
 C   -0.669206   -1.538414    1.791602
 H    2.847453   -4.972441    1.030585
 H    0.871159   -3.635518    1.433177
 H    5.105623   -1.351003    0.249113
 H    3.121895   -0.032358    0.638669
Cu    0.361617   -0.345726   -0.604400
 H   -0.460776   -2.086071    2.734827
 H   -1.024476   -2.303234    1.083081
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 H    0.866761   -0.018739    1.969457
 H    6.450013    4.173008    0.776836
 H    5.685309    2.560110    0.917725
 H    4.820430    4.013191    1.494475
 C    2.348645    5.469774   -0.239703
 H    1.638257    5.897599    0.484472
 H    1.946438    5.609690   -1.257519
 H    3.297644    6.031600   -0.167403
 H   -4.521988   -2.645350   -0.723444
 C   -3.965835   -1.986020   -1.387652
 H   -2.150456   -3.034783   -1.011085
 C   -4.618599   -0.915603   -2.050255
 C   -2.609895   -2.201465   -1.548167
 C   -3.838226   -0.124735   -2.930002
 C   -1.825762   -1.388521   -2.384343
 H   -4.292564    0.692385   -3.488988
 C   -2.481767   -0.364073   -3.084224
 C   -0.372885   -1.546875   -2.511579
 H   -1.904181    0.276738   -3.756280
 H    0.090732   -1.020285   -3.351949
 H    1.490347   -2.415713   -1.937631
 C    0.427832   -2.298301   -1.708094
 H    0.017501   -2.942704   -0.926966
 H    6.208574   -5.904543    0.199411
 H    7.308139   -4.151451   -0.143518
 H    4.891532   -5.857194    1.387549
 C    5.216902   -5.482381    0.401423
 H    6.870969   -2.673310    0.736905
 C    6.523978   -3.394414   -0.022940
 N    5.292621   -4.040729    0.369333
 H    4.518770   -5.882881   -0.356559
 H    6.427195   -2.852455   -0.981284
 H   -7.726150   -1.073810   -0.844491
 H   -7.623353    0.529271   -2.188342
 H   -6.830508   -2.521005   -1.366502
 C   -6.722549   -1.499029   -0.961054
 H   -6.611403    0.266089   -3.627880
 C   -6.588145    0.436603   -2.536869
 N   -5.939968   -0.643929   -1.826751
 H   -6.275749   -1.578824    0.043878
 H   -6.087312    1.402316   -2.353741
91
Figure 4_para-NMe2_pi-allyl_02 / electronic energy: -3776.43298427 a.u. / lowest freq: 24.82 cm-1
 C   -1.845792   -1.634381   -0.752155
 C   -1.773057   -2.092163    0.614921
 C   -0.608153   -2.020612    1.322910
 O    1.011214   -4.607009   -0.418548
 P    1.702478   -3.446427   -1.056022
 O    0.976968   -2.366839   -1.816776
 O    2.617348   -2.741177    0.133650
 O    2.893400   -3.964585   -2.076477
 C    3.379622   -1.605382   -0.186991
 H   -2.819300   -1.657173   -1.245919
 H   -0.952990   -1.832715   -1.366555
 H   -2.698948   -2.343923    1.144008
 H    0.348238   -1.824534    0.825764
 H   -0.580110   -2.267091    2.386494
 B   -4.197969    1.058653   -0.673050
 O   -4.796944    1.493627    0.477672
 O   -4.735526   -0.106827   -1.137171
 C   -5.662350    0.446261    0.958287
 C   -5.889457   -0.429418   -0.335901
 C   -6.926110    1.064709    1.533694
 C   -4.890784   -0.282285    2.056116
 C   -7.118044   -0.013332   -1.140644
 C   -5.908716   -1.929404   -0.089050
 H   -7.120796    1.067799   -1.344125
 H   -8.050327   -0.274356   -0.620064
 H   -7.105885   -0.539394   -2.106309
 H   -4.966938   -2.284334    0.349963
 H   -6.057536   -2.459211   -1.041232
 H   -6.734070   -2.202335    0.585271
 H   -3.948029   -0.694258    1.669068
 H   -5.476869   -1.102287    2.493946
 H   -4.645757    0.429689    2.858001
 H   -7.635848    0.280872    1.837362
 H   -7.422332    1.726683    0.812448
 H   -6.676390    1.659583    2.424712
 C    0.697105    0.749350   -1.982952
 C    1.967722    1.289787   -2.100654
 C   -0.424361    1.543337   -1.669319
 C    2.209978    2.665777   -1.885687
 C   -0.192102    2.921551   -1.522768
 C    1.078365    3.476301   -1.636674
 C   -1.763776    0.912489   -1.503971
 C   -2.983276    1.805988   -1.332760
 H    1.184686    4.553861   -1.513736
 H   -1.024560    3.598531   -1.319115
 H    2.787520    0.611559   -2.333482
 H    0.604600   -0.336951   -2.096300
Cu   -1.366939    0.003349    0.275164
 H   -3.281023    2.193161   -2.326383
 H   -2.759541    2.684403   -0.710655
 H   -1.936255    0.170033   -2.287083
 H    4.168238   -1.492883    0.573087
 H    2.768541   -0.687730   -0.190259
 H    3.868643   -1.703034   -1.172398
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 C     3.756758   -4.976874   -1.630174
 H     4.306713   -5.373220   -2.497489
 H     3.200533   -5.802768   -1.155413
 H     4.493013   -4.596091   -0.898147
 H     3.520737    2.311201    0.770368
 C     2.981735    1.667688    1.466030
 H     1.114421    2.446244    0.813635
 C     3.678506    0.748462    2.292819
 C     1.601008    1.739865    1.488836
 C     2.900415   -0.073863    3.146170
 C     0.828576    0.914348    2.322839
 H     3.377944   -0.801309    3.801227
 C     1.518434    0.013125    3.148896
 C    -0.635866    0.936958    2.331561
 H     0.951366   -0.648850    3.809394
 H    -1.107220    0.267283    3.059481
 H    -1.046184    2.540840    0.962883
 C    -1.450399    1.746747    1.594008
 H    -2.528609    1.760151    1.777482
 H     3.220601    5.012373   -0.876933
 H     4.758609    4.822547   -1.736859
 C     3.684182    4.607832   -1.791030
 H     3.268371    5.158965   -2.655740
 H     4.648983    1.415911   -1.801017
 N     3.487903    3.179936   -1.890943
 H     5.528218    2.897460   -2.213430
 C     4.582655    2.361258   -2.362365
 H     4.495325    2.109295   -3.436200
 H     5.628878    2.538436    1.510051
 H     6.870401    1.270455    1.478378
 C     5.801211    1.463401    1.333635
 H     5.555581    1.249044    0.278660
 H     5.551748   -0.206050    4.123084
 N     5.039058    0.641418    2.247613
 H     6.793261   -0.304208    2.855982
 C     5.714713   -0.360775    3.042826
 H     5.381412   -1.383150    2.791709
31
Figure 4_para-H_L-Cu-OtBu / electronic energy: -2182.55158904 a.u. / lowest freq: 27.42 cm-1
 C    -1.928903    0.522589    0.151598
 C    -2.367593   -0.225683    1.253706
 C    -2.102115   -0.011349   -1.135516
 C    -2.688512   -1.261082   -1.309804
 C    -3.114996   -1.999957   -0.203840
 C    -2.955887   -1.476382    1.078595
 H    -1.771969    0.551062   -2.011760
 H    -2.813794   -1.663778   -2.317510
 H    -3.574222   -2.981095   -0.344130
 H    -3.288621   -2.045895    1.949330
 H    -2.235906    0.177972    2.261012
 C    -1.259656    1.821554    0.396510
 C    -0.717088    2.656046   -0.552234
 H    -1.320811    2.184359    1.429681
 H    -0.795346    2.453802   -1.625268
 H    -0.394506    3.662142   -0.268341
 H     4.530550   -0.752582   -0.259174
 H     4.027421   -1.250156    1.372998
 C     3.815244   -1.377041    0.299445
 O     2.253156    0.399694    0.393393
 H     3.992832   -2.431959    0.032888
 C     2.377225   -0.924049   -0.002265
 H     2.762220   -0.403423   -2.080931
 H     1.541412   -1.679023    1.858641
 C     2.104007   -1.077496   -1.509356
 C     1.391935   -1.816035    0.775636
 H     2.263369   -2.107308   -1.870669
 H     1.509123   -2.887576    0.542110
 H     1.058778   -0.800471   -1.732575
 H     0.351559   -1.530222    0.541548
Cu     0.717611    1.355859    0.135178
73
Figure 4_para-H_ed / electronic energy: -3004.31675967 a.u. / lowest freq: 18.65 cm-1
 H     3.619191   -2.264669   -1.749936
 H     4.266501   -1.175749   -0.505774
 O     1.949337   -0.170082   -1.609307
 C     4.111933   -1.294478   -1.586572
 H     5.098836   -1.319410   -2.074826
 C     3.259546   -0.155654   -2.153842
 H     2.578672   -1.323182   -3.854781
 H     4.092980    1.357629   -0.822653
 C     3.068593   -0.356994   -3.657714
 C     3.930529    1.197632   -1.896566
 H     2.429252    0.439557   -4.067961
 H     4.032070   -0.340764   -4.189999
 H     3.287115    2.011562   -2.264231
 H     4.899863    1.258362   -2.416090
Cu    -0.160418   -1.427890   -0.362048
 H    -0.411425    3.489115    2.064807
 H    -0.007268    4.717351   -0.037120
 H     0.983004    3.246351    0.240167
 C     0.274489    3.735377   -0.444532
 H    -1.960254    4.254603    1.616556
 H     0.792081    3.895542   -1.402045
 C    -1.464625    3.293986    1.825295
 H    -1.939289    2.855115    2.715937
 C    -1.609640    2.344579    0.645320
 C    -0.944654    2.845473   -0.685761
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 O   -0.869698    1.144563    0.915905
 H   -2.363477    4.400287   -1.216594
 B   -0.261796    0.708405   -0.252137
 H   -1.352053    3.825117   -2.564025
 C   -1.900826    3.507594   -1.664783
 O   -0.453083    1.623046   -1.261128
 H   -3.720451    2.814612    0.302784
 C   -3.072589    1.942536    0.474264
 H   -3.413052    1.436418    1.389023
 H   -2.697637    2.821254   -1.980626
 H   -3.196720    1.240754   -0.362796
 H    3.863313   -2.185662    1.867486
 H    4.511960   -0.154138    1.280872
 H    2.478421   -3.191367    2.340032
 C    2.917343   -2.185591    2.423964
 O    1.769845   -1.417455    0.478043
 H    4.332384    0.096385    3.037314
 C    3.991648    0.435628    2.047753
 H    3.133605   -1.997570    3.486385
 B    1.610529   -0.135498   -0.242723
 H    4.295027    1.486059    1.925271
 C    1.935704   -1.157563    1.873593
 C    2.471126    0.341396    1.900857
 O    2.137628    0.863859    0.623254
 H    0.223867   -2.360932    2.391686
 C    0.586647   -1.337631    2.577852
 H    0.680646   -1.213786    3.666458
 H   -0.163776   -0.620148    2.217851
 H    1.996609    0.796453    3.982743
 C    1.815564    1.204764    2.976558
 H    2.245120    2.217650    2.941658
 H    0.735250    1.289146    2.807762
 H   -1.679063   -2.140085   -2.282828
 H   -3.795277   -1.158184   -2.565882
 H   -0.234830   -3.794901   -1.229143
 C   -1.821183   -2.352731   -1.216690
 C   -4.012623   -1.222335   -1.496547
 C   -0.992472   -3.282823   -0.627991
 H   -5.942423   -0.281258   -1.689780
 C   -3.071117   -1.806086   -0.637709
 C   -5.219612   -0.728445   -1.003444
 H   -1.208932   -3.712609    0.355140
 C   -3.358995   -1.863327    0.734910
 C   -5.500426   -0.803365    0.359634
 H   -2.629670   -2.285905    1.430590
 C   -4.562943   -1.369220    1.226793
 H   -6.443219   -0.413157    0.749851
 H   -4.769201   -1.419351    2.298430
73
Figure 4_para-H_ts(TB) / electronic energy: -3004.31639795 a.u. / lowest freq: -60.21 cm-1
 H    3.753405   -2.066390   -1.981357
 H    4.355791   -1.151636   -0.581042
 O    2.047132   -0.048275   -1.582915
 C    4.226136   -1.122048   -1.672131
 H    5.224538   -1.065114   -2.132966
 C    3.368353    0.072327   -2.097909
 H    2.731371   -0.855836   -3.955148
 H    4.145556    1.398779   -0.549457
 C    3.204579    0.078829   -3.617103
 C    4.007124    1.385977   -1.638478
 H    2.561383    0.917221   -3.924934
 H    4.176848    0.180201   -4.123072
 H    3.359527    2.234761   -1.905676
 H    4.986632    1.530516   -2.120781
Cu   -0.177828   -1.366305   -0.515400
 H   -0.437976    3.287028    2.315428
 H    0.135878    4.643976    0.367946
 H    1.015860    3.084750    0.516224
 C    0.362919    3.689711   -0.129907
 H   -1.945709    4.150273    1.907863
 H    0.917571    3.909068   -1.054470
 C   -1.490916    3.155477    2.034653
 H   -2.005004    2.653183    2.868214
 C   -1.638492    2.329465    0.765945
 C   -0.905397    2.915690   -0.489854
 O   -0.967298    1.073894    0.939435
 H   -2.189523    4.620313   -0.887230
 B   -0.380310    0.697860   -0.263629
 H   -1.193441    4.101722   -2.268547
 C   -1.785699    3.741989   -1.413795
 O   -0.483546    1.725278   -1.177001
 H   -3.716696    2.931510    0.416390
 C   -3.112323    2.017144    0.510018
 H   -3.504154    1.429042    1.352547
 H   -2.624723    3.153948   -1.808781
 H   -3.237129    1.416629   -0.402478
 H    3.799730   -2.389363    1.764902
 H    4.462200   -0.303322    1.398672
 H    2.399983   -3.432726    2.096956
 C    2.832329   -2.437690    2.280884
 O    1.774267   -1.493761    0.357369
 H    4.206646   -0.216460    3.161747
 C    3.905939    0.211302    2.194246
 H    3.005604   -2.338606    3.362891
 B    1.704522   -0.169315   -0.237932
 H    4.205251    1.269933    2.182383
 C    1.871092   -1.365464    1.783794
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 C    2.394177    0.124472    1.975850
 O    2.112417    0.758996    0.733855
 H    0.141833   -2.611209    2.103242
 C    0.491658   -1.610272    2.400485
 H    0.534997   -1.588003    3.499015
 H   -0.242874   -0.861090    2.073468
 H    1.814991    0.385514    4.061818
 C    1.682013    0.885160    3.090197
 H    2.109374    1.896146    3.173027
 H    0.611183    0.984764    2.874992
 H   -1.694646   -2.053582   -2.448698
 H   -3.772377   -0.994495   -2.659564
 H   -0.216185   -3.722688   -1.473581
 C   -1.822442   -2.306831   -1.389836
 C   -3.995925   -1.128691   -1.597945
 C   -0.972531   -3.242976   -0.845049
 H   -5.903353   -0.132828   -1.730292
 C   -3.069135   -1.788308   -0.779139
 C   -5.193958   -0.643867   -1.075243
 H   -1.166024   -3.706625    0.127402
 C   -3.365801   -1.937610    0.584788
 C   -5.481553   -0.806285    0.278601
 H   -2.649808   -2.425363    1.250904
 C   -4.561069   -1.453258    1.106443
 H   -6.416981   -0.422724    0.692461
 H   -4.773833   -1.575610    2.170974
73
Figure 4_para-H_prod / electronic energy: -3004.33626287 a.u. / lowest freq: 26.41 cm-1
 H    5.348395   -0.107970   -2.225416
 H    5.117517    0.760311   -0.681798
 O    2.783294   -0.349937   -1.549881
 C    4.912337    0.789933   -1.761382
 H    5.413372    1.673575   -2.184425
 C    3.410476    0.855386   -2.028923
 H    3.546140   -0.012461   -4.014137
 H    2.976805    2.052510   -0.261823
 C    3.125514    0.879796   -3.526290
 C    2.768758    2.060409   -1.341845
 H    2.040165    0.895217   -3.707387
 H    3.568904    1.772352   -3.991818
 H    1.677574    2.050509   -1.483770
 H    3.169444    2.996342   -1.759513
Cu   -0.252587   -0.944169   -0.805791
 H   -0.584937    2.826738    2.924124
 H    0.022704    4.624356    1.307468
 H    0.800502    3.029547    1.103381
 C    0.180907    3.790687    0.607235
 H   -1.986905    3.924575    2.781423
 H    0.743991    4.172788   -0.257092
 C   -1.648548    2.884302    2.655934
 H   -2.209778    2.258682    3.366392
 C   -1.895847    2.395054    1.236341
 C   -1.142570    3.196630    0.121105
 O   -1.336373    1.084750    1.089372
 H   -2.306789    5.031007    0.170640
 B   -0.818252    0.924432   -0.199879
 H   -1.367380    4.788319   -1.322227
 C   -1.972099    4.276602   -0.558279
 O   -0.829235    2.169640   -0.831340
 H   -3.922509    3.230412    1.137455
 C   -3.398861    2.275833    0.978004
 H   -3.820990    1.529394    1.667479
 H   -2.855591    3.855543   -1.055860
 H   -3.597470    1.930954   -0.047466
 H    3.567732   -3.149568    1.089485
 H    4.435183   -1.754803    2.711103
 H    2.004209   -3.996206    1.014509
 C    2.576627   -3.231850    1.560056
 O    1.647699   -1.593316    0.099990
 H    3.204015   -1.446054    3.966869
 C    3.697252   -1.028838    3.076381
 H    2.708880   -3.575609    2.595570
 B    2.636468   -0.689614   -0.258016
 H    4.235901   -0.119608    3.381228
 C    1.820025   -1.908812    1.503615
 C    2.669239   -0.681414    2.013357
 O    3.357559   -0.259305    0.818041
 H   -0.071495   -2.917387    1.736709
 C    0.451781   -2.042663    2.151277
 H    0.557164   -2.197325    3.235469
 H   -0.170338   -1.152860    1.979979
 H    1.309999    0.278060    3.427347
 C    1.806258    0.491527    2.469828
 H    2.449159    1.373362    2.607235
 H    1.029835    0.731452    1.730750
 H   -1.631548   -1.522018   -2.903178
 H   -3.640445   -0.363064   -2.529774
 H    0.206159   -3.016242   -2.347001
 C   -1.652194   -2.039114   -1.937497
 C   -3.869883   -0.965068   -1.646248
 C   -0.604890   -2.869901   -1.628193
 H   -5.785459   -0.029249   -1.332053
 C   -2.931515   -1.907302   -1.199446
 C   -5.071548   -0.772853   -0.969779
 H   -0.628845   -3.554340   -0.774914
 C   -3.237067   -2.662925   -0.057625
 C   -5.359504   -1.522574    0.171121
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 H   -2.528234   -3.406992    0.312675
 C   -4.437738   -2.469073    0.621515
 H   -6.299968   -1.371920    0.706202
 H   -4.656159   -3.062817    1.512554
38
Figure 4_para-H_L-Cu-Bpin / electronic energy: -2360.54260251 a.u. / lowest freq: 16.87 cm-1
 H   -4.091233    0.951489   -2.601318
 H   -4.474831   -0.589276   -1.804192
 C   -4.312667    0.482689   -1.630677
 H   -2.485387    2.532506   -1.628704
 O   -1.994779    0.038800   -1.122535
 H   -5.247872    0.921665   -1.249798
 C   -3.165826    0.730417   -0.661765
 C   -2.826614    2.221949   -0.629896
 B   -1.265895   -0.418220   -0.029211
 H   -3.698100    2.836281   -0.358263
 H   -3.843594   -1.869068   -0.005503
 H   -2.015247    2.430792    0.083109
 H   -5.268076   -0.956097    0.567650
 C   -4.203781   -1.161250    0.755890
 C   -3.366456    0.119280    0.765633
 O   -2.026203   -0.250883    1.123944
 H   -4.116979   -1.650997    1.737263
 H   -4.902270    1.471978    1.496214
 C   -3.916678    1.088154    1.802297
 H   -3.242177    1.940318    1.958342
 H   -4.038345    0.575203    2.768359
Cu    0.617594   -1.188792   -0.089272
 C    3.335949   -0.334136    0.137067
 C    3.899437    0.230213    1.291086
 C    3.364986    0.407046   -1.056377
 C    3.954613    1.666580   -1.092640
 C    4.521611    2.212902    0.061038
 C    4.491147    1.491358    1.253563
 H    2.917198    0.000270   -1.965905
 H    3.968714    2.229312   -2.028862
 H    4.983618    3.202227    0.029110
 H    4.928173    1.913318    2.161469
 H    3.873106   -0.330505    2.229192
 C    2.713956   -1.672138    0.230877
 C    2.243089   -2.427340   -0.799011
 H    2.714739   -2.113383    1.234622
 H    2.333012   -2.119724   -1.845467
 H    1.896044   -3.447942   -0.616150
54
Figure 4_para-H_pc1 / electronic energy: -2669.90144009 a.u. / lowest freq: -6.95 cm-1
 H    4.526083    2.947197    1.659768
 H    2.068393    3.174821    2.028713
 C    3.819489    2.544541    0.930260
 C    2.445267    2.672319    1.134486
 H    5.356328    1.770110   -0.376468
 C    4.282817    1.887440   -0.210104
 H   -3.947999    1.733054    2.785530
 C    1.543482    2.152475    0.209237
 H   -3.319846   -0.614468    3.082854
 H    0.472072    2.251264    0.399178
 C    3.382644    1.367060   -1.135569
 C    1.996742    1.495252   -0.949486
 C   -4.404692    1.551252    1.801019
 C   -3.915735   -0.866126    2.192824
 H   -4.213283    2.431577    1.173519
 O   -2.428888    0.491826    0.905983
 H    3.756427    0.850725   -2.023436
 H   -4.951964   -1.047302    2.513996
 H   -5.491389    1.451882    1.945890
 C   -3.824364    0.284842    1.190920
 C    1.069168    0.931420   -1.947648
 B   -2.100026   -0.201619   -0.246566
 H   -0.694566    2.092778   -1.440965
 C   -0.276373    1.271049   -2.027464
 C   -4.392350   -0.087185   -0.221924
 H   -3.981950    1.889969   -1.054108
 O   -3.245235   -0.677518   -0.859224
 H   -5.701533    1.612244   -0.661365
 H   -6.393875   -0.700531    0.352913
 C   -4.786025    1.139061   -1.045854
 H   -0.849001    0.992102   -2.916984
 C   -5.532771   -1.093187   -0.209284
 H   -4.970151    0.829800   -2.085381
 H   -5.864543   -1.293327   -1.239186
Cu   -0.198712   -0.440422   -0.916913
 H    1.529055    0.381036   -2.774026
 H   -3.512045   -1.798378    1.769856
 H   -5.227758   -2.048326    0.237689
 H    3.759391   -2.409637   -1.489341
 H    1.396353   -2.360114   -1.810821
 H    5.792782   -1.937419   -0.157151
 C    3.663364   -1.986432   -0.485543
 C    4.807816   -1.723576    0.265292
 C    1.194985   -2.068212   -0.774492
 H   -0.220943   -2.394329    0.837905
 C    2.383712   -1.732012    0.031589
 C   -0.058656   -2.355040   -0.243441
 C    4.697654   -1.183016    1.545771
 H    5.593575   -0.968742    2.133083
 C    2.288147   -1.174935    1.318762
 H   -0.789236   -2.900516   -0.846500
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 C    3.431545   -0.904993    2.064998
 H    1.306979   -0.938647    1.738522
 H    3.333189   -0.462930    3.059452
54
Figure 4_para-H_ts(CuBadd)_01 / electronic energy: -2669.89657616 a.u. / lowest freq: -163.08 cm-1
 H    4.199534    3.205904    1.384609
 H    1.773082    3.122498    1.970892
 C    3.483312    2.729406    0.711297
 C    2.128051    2.682351    1.035082
 H    4.972460    2.166586   -0.750344
 C    3.911886    2.148562   -0.485507
 H   -3.526846    1.576486    2.896930
 C    1.213463    2.068777    0.181365
 H   -2.907297   -0.800261    2.935062
 H    0.161351    2.031215    0.476035
 C    3.002963    1.538376   -1.342288
 C    1.625967    1.486476   -1.037405
 C   -4.049447    1.490242    1.932754
 C   -3.583337   -0.961992    2.082720
 H   -3.876773    2.417399    1.370900
 O   -2.165707    0.480556    0.808943
 H    3.357551    1.085355   -2.272367
 H   -4.593475   -1.146465    2.475899
 H   -5.126851    1.398454    2.137876
 C   -3.544527    0.270780    1.180549
 C    0.689627    0.814593   -1.938149
 B   -1.959124   -0.158495   -0.393005
 H   -1.141750    1.764171   -1.209255
 C   -0.741822    0.909888   -1.770058
 C   -4.220268    0.029394   -0.214414
 H   -3.781388    2.050446   -0.920736
 O   -3.137346   -0.554197   -0.972734
 H   -5.482171    1.799527   -0.445371
 H   -6.189679   -0.561690    0.466016
 C   -4.610072    1.326545   -0.919626
 H   -1.344060    0.675016   -2.654186
 C   -5.393073   -0.935786   -0.194736
 H   -4.866430    1.103522   -1.965721
 H   -5.811919   -1.038549   -1.206823
Cu   -0.082664   -0.763650   -0.902801
 H    1.079444    0.496069   -2.908981
 H   -3.245768   -1.862527    1.548148
 H   -5.092033   -1.933909    0.149541
 H    3.739948   -2.385964   -1.407450
 H    1.411330   -2.773580   -1.467189
 H    5.794144   -1.555922   -0.303641
 C    3.670035   -1.891039   -0.434808
 C    4.826244   -1.424273    0.186441
 C    1.214712   -2.274214   -0.511712
 H   -0.186027   -2.320860    1.163100
 C    2.411078   -1.744876    0.170329
 C   -0.038251   -2.485973    0.091490
 C    4.749415   -0.789150    1.425774
 H    5.653363   -0.416455    1.912821
 C    2.347848   -1.090916    1.413469
 H   -0.743342   -3.179687   -0.375703
 C    3.502969   -0.620754    2.030792
 H    1.382871   -0.938168    1.902817
 H    3.427415   -0.109660    2.993561
54
Figure 4_para-H_ts(CuBadd)_02 / electronic energy: -2669.89201608 a.u. / lowest freq: -175.57 cm-1
 H    4.113744    4.842078    0.775262
 H    1.633192    4.891830    1.062011
 C    3.491905    4.048226    0.355260
 C    2.105120    4.072059    0.513283
 H    5.153775    2.955244   -0.493602
 C    4.069809    2.991503   -0.353813
 H   -4.963344    2.301923    1.010987
 C    1.307094    3.062800   -0.021405
 H   -3.930727    0.745940    2.600670
 H    0.225218    3.109589    0.129748
 C    3.277914    1.982123   -0.891254
 C    1.873068    1.984641   -0.738200
 C   -4.994772    1.552402    0.206506
 C   -4.095654   -0.070777    1.882659
 H   -4.820447    2.070217   -0.745779
 O   -2.636733    1.057783    0.361999
 H    3.746653    1.162470   -1.443471
 H   -5.098583   -0.485386    2.058337
 H   -6.004724    1.115742    0.187936
 C   -3.953214    0.476099    0.463098
 C    1.082808    0.883509   -1.283114
 B   -1.796939    0.100684   -0.150844
 H   -0.867504    1.873615   -1.301522
 C   -0.368537    0.900842   -1.389624
 C   -3.893070   -0.654263   -0.625534
 H   -3.697966    0.762284   -2.279017
 O   -2.486660   -0.981542   -0.639383
 H   -5.324792    0.045349   -2.122765
 H   -5.756177   -1.658547   -0.156236
 C   -4.248344   -0.156077   -2.024681
 H   -0.775710    0.302393   -2.212504
 C   -4.691347   -1.902544   -0.289072
 H   -3.976023   -0.928782   -2.758444
 H   -4.610778   -2.632484   -1.108203
Cu    0.203702   -0.063774    0.264220
 H    1.625611    0.166942   -1.907074
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 H   -3.351399   -0.855113    2.087025
 H   -4.324667   -2.381989    0.627856
 H    4.097695   -0.752970    0.967879
 H    2.064803   -0.124450    1.989214
 H    5.495849   -2.311950   -0.357480
 C    3.652455   -1.658288    0.546472
 C    4.437201   -2.533273   -0.200931
 C    1.488680   -0.940412    1.537944
 H   -0.229579   -0.488974    2.762559
 C    2.287954   -1.914365    0.763415
 C    0.161673   -1.121423    1.960476
 C    3.876266   -3.688199   -0.747516
 H    4.489598   -4.374307   -1.336139
 C    1.737118   -3.085157    0.213422
 H   -0.363827   -2.069468    1.811658
 C    2.523069   -3.958210   -0.534217
 H    0.678394   -3.312310    0.359620
 H    2.073019   -4.860094   -0.956641
54
Figure 4_para-H_L-Cu-alkyl_01 / electronic energy: -2669.93751624 a.u. / lowest freq: 16.81 cm-1
 H    3.517841    3.568113    1.129892
 H    1.063163    3.763756    1.549427
 C    2.803033    3.017369    0.513774
 C    1.432574    3.121011    0.744663
 H    4.312473    2.096614   -0.733267
 C    3.242632    2.194139   -0.528322
 H   -3.542082    1.888232    2.719067
 C    0.515455    2.419239   -0.040784
 H   -1.347668    0.853575    2.372493
 H   -0.550092    2.514754    0.176109
 C    2.332087    1.492532   -1.308171
 C    0.936352    1.573218   -1.089094
 C   -4.060916    1.134910    2.107946
 C   -1.840311    0.003042    1.879398
 H   -4.888037    1.633621    1.586088
 O   -2.627453    1.487184    0.193466
 H    2.700751    0.847640   -2.112575
 H   -2.091488   -0.743772    2.645815
 H   -4.478617    0.376417    2.787157
 C   -3.081787    0.499897    1.136619
 C    0.001911    0.767294   -1.919079
 B   -2.361058    0.835786   -0.986586
 H   -1.408062    2.457606   -2.194526
 C   -1.422299    1.352653   -2.125066
 C   -3.700663   -0.589394    0.188661
 H   -5.291435    0.734437   -0.511915
 O   -2.918964   -0.422700   -1.007909
 H   -5.828740   -0.487401    0.675039
 H   -4.040098   -2.144108    1.663333
 C   -5.156046   -0.304058   -0.175152
 H   -1.813850    0.978143   -3.085524
 C   -3.551957   -2.017811    0.685236
 H   -5.456153   -0.969374   -0.998091
 H   -4.024833   -2.713002   -0.024233
Cu    0.053660   -1.014159   -1.010155
 H    0.476463    0.606057   -2.902371
 H   -1.116564   -0.440850    1.175752
 H   -2.495649   -2.299092    0.779499
 H    3.975118   -2.319889   -1.249849
 H    1.714086   -2.916845   -1.414654
 H    5.858847   -1.135806   -0.154524
 C    3.806889   -1.776506   -0.316345
 C    4.865289   -1.109937    0.298651
 C    1.436642   -2.490514   -0.443263
 H   -0.052825   -2.592979    1.114311
 C    2.524249   -1.761269    0.248210
 C    0.215150   -2.819362    0.077894
 C    4.652486   -0.407836    1.483158
 H    5.478469    0.121646    1.963530
 C    2.319654   -1.039990    1.436224
 H   -0.443498   -3.503026   -0.465542
 C    3.374969   -0.370536    2.046184
 H    1.322902   -0.980767    1.880063
 H    3.197719    0.193569    2.964409
54
Figure 4_para-H_L-Cu-alkyl_02 / electronic energy: -2669.93402914 a.u. / lowest freq: 18.78 cm-1
 C    4.003046   -0.290454    0.383196
 C    3.660617    0.751408    1.257768
 C    4.608967    0.028967   -0.841623
 C    4.857277    1.355899   -1.180902
 C    4.507698    2.384692   -0.304312
 C    3.909839    2.078255    0.917414
 H    4.895202   -0.764073   -1.535985
 H    5.331783    1.588692   -2.136995
 H    4.701270    3.425334   -0.574273
 H    3.626708    2.876329    1.606839
 H    3.179011    0.516492    2.210479
 C    3.680551   -1.681488    0.776702
 C    3.737473   -2.790862   -0.020035
 H    3.465905   -1.821110    1.843070
 H    4.080390   -2.750488   -1.058835
 H    3.610507   -3.784897    0.418215
 B   -2.524955   -1.119973    0.130981
 O   -3.274618   -0.631770    1.170502
 O   -3.044085   -0.763130   -1.088427
 C   -4.457626   -0.018473    0.627138
 C   -4.037724    0.251341   -0.866115
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 C   -4.780754    1.233149    1.427888
 C   -5.591670   -1.033885    0.757727
 C   -3.348646    1.602598   -1.059590
 C   -5.156911    0.086034   -1.881863
 H   -2.539507    1.752113   -0.329139
 H   -4.061029    2.435837   -0.972564
 H   -2.901159    1.634561   -2.063727
 H   -5.573555   -0.929639   -1.868716
 H   -4.770857    0.280890   -2.893486
 H   -5.969415    0.801741   -1.684567
 H   -5.379156   -1.949687    0.186036
 H   -6.549230   -0.619289    0.410266
 H   -5.703258   -1.312900    1.815912
 H   -5.631839    1.769681    0.981817
 H   -3.921783    1.915161    1.476873
 H   -5.054013    0.958383    2.457733
 C    0.635333    1.105687   -1.136356
 C    0.787687    2.463585   -0.883528
 C    0.133767    0.212668   -0.161731
 C    0.445963    2.999006    0.363036
 C   -0.194820    0.774867    1.090362
 C   -0.042712    2.138638    1.345025
 C   -0.017867   -1.239231   -0.456055
 C   -1.186771   -1.932866    0.285825
 H   -0.316554    2.533083    2.328043
 H   -0.591910    0.133282    1.880326
 H    0.563646    4.066766    0.562202
 H    1.175470    3.117488   -1.669833
 H    0.907852    0.708960   -2.119790
Cu    1.798799   -1.941933   -0.099842
 H   -0.971815   -2.097921    1.355515
 H   -1.325226   -2.942999   -0.138747
 H   -0.184525   -1.343874   -1.542595
54
Figure 4_para-H_L-Cu-alkyl_03 / electronic energy: -2669.93662784 a.u. / lowest freq: 14.18 cm-1
 B   -2.514191    1.122633    0.242061
 O   -3.085841    0.287674    1.173100
 O   -3.183898    1.091187   -0.954207
 C   -4.018364   -0.560412    0.479802
 C   -4.377794    0.308010   -0.780258
 C   -5.192695   -0.876063    1.391553
 C   -3.267174   -1.843623    0.122977
 C   -5.524258    1.284861   -0.523959
 C   -4.640877   -0.489347   -2.047812
 H   -5.364630    1.856994    0.402101
 H   -6.491516    0.766884   -0.452285
 H   -5.576950    1.999943   -1.358018
 H   -3.758875   -1.068093   -2.352508
 H   -4.896931    0.194008   -2.871063
 H   -5.484526   -1.181485   -1.904867
 H   -2.413257   -1.634160   -0.540862
 H   -3.921121   -2.578569   -0.367811
 H   -2.875859   -2.295003    1.046711
 H   -5.969011   -1.433082    0.845422
 H   -5.642220    0.035525    1.806553
 H   -4.856804   -1.500074    2.233052
 C    2.268286    1.596178   -1.177729
 C    3.567653    2.072867   -1.059342
 C    1.294475    1.808955   -0.172863
 C    3.962613    2.790031    0.075553
 C    1.712098    2.548359    0.952383
 C    3.020566    3.021328    1.075856
 C   -0.072134    1.233880   -0.313544
 C   -1.195046    1.929341    0.481131
 H    3.301879    3.586182    1.969638
 H    1.000352    2.755837    1.754947
 H    4.985289    3.162105    0.173440
 H    4.286738    1.879502   -1.860282
 H    1.986483    1.026155   -2.069348
Cu    0.182332   -0.675705    0.187992
 H   -1.307722    2.994233    0.190639
 H   -0.985292    1.920875    1.563752
 H   -0.338678    1.227187   -1.385653
 H    5.079036   -0.262103    1.688234
 C    4.592708   -0.802645    0.873397
 H    2.789344   -1.112448    1.993158
 H    6.273696   -0.604035   -0.471069
 C    3.301179   -1.286711    1.044235
 C    5.261881   -0.993750   -0.337783
 H    0.851208   -2.131752    2.215429
 C    4.629499   -1.672256   -1.377499
 C    2.652751   -1.973526    0.004143
 C    0.486189   -2.480435    1.244247
 H    5.144064   -1.822097   -2.329363
 C    3.333404   -2.156148   -1.207638
 C    1.267260   -2.482664    0.123066
 H    2.836113   -2.680973   -2.027688
 H    0.888749   -3.000068   -0.766740
 H   -0.471620   -3.007506    1.241771
54
Figure 4_para-H_ts(BHE) / electronic energy: -2669.89885582 a.u. / lowest freq: -839.76 cm-1
 B   -2.395824    0.575511    0.228088
 O   -3.486182    1.027255    0.910411
 O   -2.715702   -0.208423   -0.843130
 C   -4.632978    0.305873    0.409253
 C   -4.146652   -0.134619   -1.021245
 C   -5.842371    1.224928    0.414907
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 C   -4.856785   -0.872453    1.354714
 C   -4.406101    0.921920   -2.092706
 C   -4.661034   -1.489009   -1.479200
 H   -4.043395    1.911675   -1.777389
 H   -5.476469    1.001718   -2.330184
 H   -3.869780    0.641484   -3.011061
 H   -4.341393   -2.294200   -0.805106
 H   -4.273294   -1.712631   -2.483963
 H   -5.760150   -1.488238   -1.531425
 H   -3.994013   -1.555702    1.359567
 H   -5.755351   -1.445170    1.084071
 H   -4.989718   -0.488405    2.376713
 H   -6.707028    0.728347   -0.050427
 H   -5.645142    2.162165   -0.121417
 H   -6.112302    1.476733    1.451101
 C    2.286497    1.702596   -1.264341
 C    3.525429    2.316487   -1.121884
 C    1.407128    1.554945   -0.170925
 C    3.939543    2.803886    0.120677
 C    1.848626    2.040503    1.078481
 C    3.090291    2.658401    1.217119
 C    0.113451    0.893554   -0.352389
 C   -0.923478    0.909571    0.640052
 H    3.398810    3.026542    2.199366
 H    1.212145    1.933654    1.960543
 H    4.913530    3.285799    0.232108
 H    4.182064    2.410073   -1.990957
 H    1.980447    1.322985   -2.243273
Cu    0.150735   -0.847959    0.757424
 H   -0.837563    1.634122    1.458179
 H   -0.940687   -0.280274    1.755326
 H   -0.156031    0.614322   -1.375536
 H    5.317195   -0.247444    1.536877
 C    4.768553   -0.674365    0.694082
 H    3.046556   -1.134120    1.893772
 H    6.354485   -0.305710   -0.729685
 C    3.486537   -1.176109    0.894394
 C    5.348654   -0.703112   -0.575535
 H    1.384777   -2.660685    2.138785
 C    4.626418   -1.228180   -1.646124
 C    2.751114   -1.717407   -0.173566
 C    0.818933   -2.684844    1.201834
 H    5.066876   -1.250042   -2.645867
 C    3.338828   -1.723552   -1.447625
 C    1.389304   -2.267947   -0.004945
 H    2.777518   -2.130160   -2.293223
 H    0.911987   -2.599712   -0.934507
 H   -0.040639   -3.360931    1.183443
54
Figure 4_para-H_pc2 / electronic energy: -2669.92145947 a.u. / lowest freq: -9.23 cm-1
 B   -2.201411    0.864498   -0.130727
 O   -3.342660    1.385239    0.405356
 O   -2.424382   -0.250276   -0.894245
 C   -4.383207    0.401751    0.221566
 C   -3.852307   -0.416893   -1.013768
 C   -5.706946    1.109946   -0.008430
 C   -4.436313   -0.425819    1.504244
 C   -4.264540    0.185566   -2.354632
 C   -4.179972   -1.900245   -0.977708
 H   -4.045112    1.262640   -2.398634
 H   -5.336945    0.039399   -2.547795
 H   -3.700864   -0.309507   -3.159108
 H   -3.740419   -2.389954   -0.098912
 H   -3.781464   -2.392013   -1.877400
 H   -5.269032   -2.056209   -0.959105
 H   -3.480299   -0.938266    1.689052
 H   -5.240346   -1.174654    1.470961
 H   -4.623863    0.246195    2.354325
 H   -6.494832    0.382447   -0.254611
 H   -5.641180    1.845991   -0.820470
 H   -6.009085    1.640943    0.906284
 C    2.614476    1.376987   -1.471369
 C    3.910333    1.872287   -1.352397
 C    1.688736    1.533169   -0.429756
 C    4.308075    2.521637   -0.183345
 C    2.102550    2.182756    0.745211
 C    3.400032    2.672586    0.865758
 C    0.323939    0.990151   -0.575663
 C   -0.776699    1.443005    0.117137
 H    3.706822    3.170012    1.788769
 H    1.405822    2.288489    1.580643
 H    5.326960    2.903921   -0.086502
 H    4.619233    1.740433   -2.173100
 H    2.310883    0.859792   -2.384795
Cu   -0.139344   -0.231732    1.240663
 H   -0.671002    2.311311    0.775555
 H   -0.854839    0.102580    2.603680
 H    0.180232    0.282806   -1.399541
 H    5.187420   -0.699180    1.418489
 C    4.501524   -1.103098    0.670202
 H    2.794624   -0.958420    1.971353
 H    6.035726   -1.338137   -0.835435
 C    3.154171   -1.254790    0.982383
 C    4.976965   -1.457644   -0.594418
 H    0.958818   -2.282238    2.475016
 C    4.088703   -1.948890   -1.549420
 C    2.251824   -1.762374    0.033515
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 C    0.315764   -2.230516    1.591369
 H    4.448226   -2.220671   -2.544886
 C    2.736434   -2.090834   -1.240009
 C    0.821399   -1.983154    0.337498
 H    2.043108   -2.474287   -1.993685
 H    0.179626   -2.184082   -0.527118
 H   -0.693517   -2.634807    1.704690
36
Figure 4_para-H-alkenylBpin / electronic energy: -719.616306926 a.u. / lowest freq: 11.87 cm-1
 B    0.922364   -0.365147   -0.028404
 O    1.894117   -1.316245   -0.173823
 O    1.433940    0.892512    0.148584
 C    3.161660   -0.695762    0.122071
 C    2.848301    0.828137   -0.120020
 C    4.227554   -1.277336   -0.792080
 C    3.487647   -1.014695    1.579963
 C    3.048728    1.254565   -1.573413
 C    3.579766    1.781941    0.809984
 H    2.542480    0.568799   -2.269063
 H    4.114997    1.296474   -1.838243
 H    2.618726    2.256986   -1.714756
 H    3.324723    1.603424    1.862628
 H    3.311513    2.820863    0.566919
 H    4.668438    1.676163    0.689783
 H    2.735025   -0.594781    2.263998
 H    4.475038   -0.625732    1.866988
 H    3.496130   -2.106186    1.715677
 H    5.185806   -0.755417   -0.649802
 H    3.942879   -1.205244   -1.849722
 H    4.382907   -2.340283   -0.555288
 C   -3.806743    1.248461    0.192092
 C   -5.197110    1.149758    0.183811
 C   -2.998838    0.113525    0.018524
 C   -5.806490   -0.090352   -0.001273
 C   -3.628094   -1.129019   -0.169041
 C   -5.016012   -1.228789   -0.178362
 C   -1.532965    0.275159    0.038943
 C   -0.597425   -0.686080   -0.066780
 H   -5.487864   -2.203239   -0.325431
 H   -3.028632   -2.030869   -0.311211
 H   -6.895940   -0.172912   -0.008967
 H   -5.805802    2.046357    0.322501
 H   -3.332001    2.222916    0.336640
 H   -0.908917   -1.730947   -0.184153
 H   -1.195659    1.312156    0.158923
75
Figure 4_para-H_pc3_01 / electronic energy: -3508.77967897 a.u. / lowest freq: -6.16 cm-1
 C    0.950693    0.488510   -0.713090
 C    1.316633    0.225649    0.587395
 C    2.240967    1.127317    1.354419
 O    3.615187    0.758138    1.131462
 P    4.324780    1.108053   -0.261181
 O    3.955381    2.388604   -0.897168
 O    5.841255    0.933215    0.223443
 O    4.053131   -0.123551   -1.253915
 C    6.893601    1.117437   -0.718938
 H    0.553798   -0.286579   -1.374373
 H    1.274818    1.414210   -1.201031
 H    1.197430   -0.785845    0.992296
 H    2.096032    2.182950    1.076809
 H    2.099394    1.025874    2.437175
 B   -2.241842   -1.175948   -1.401357
 O   -2.363727   -2.310977   -0.643875
 O   -1.393736   -1.359104   -2.465930
 C   -1.407330   -3.279069   -1.115047
 C   -1.102363   -2.765070   -2.572339
 C   -2.028611   -4.664525   -1.039880
 C   -0.190835   -3.205856   -0.195917
 C   -2.052016   -3.340049   -3.621388
 C    0.340300   -2.942214   -3.020678
 H   -3.103883   -3.220127   -3.321962
 H   -1.859726   -4.407609   -3.800445
 H   -1.907763   -2.801722   -4.569593
 H    1.043312   -2.409577   -2.366314
 H    0.463948   -2.546607   -4.039592
 H    0.613248   -4.008243   -3.033200
 H    0.280109   -2.215423   -0.242153
 H    0.562400   -3.959477   -0.466044
 H   -0.504443   -3.384284    0.841673
 H   -1.350648   -5.417833   -1.468691
 H   -2.988317   -4.712876   -1.570425
 H   -2.209050   -4.930077    0.012375
 C   -1.861212    3.862824   -1.212240
 C   -2.363323    5.142461   -1.006446
 C   -2.596948    2.705512   -0.865869
 C   -3.630966    5.327331   -0.442397
 C   -3.876778    2.916984   -0.315107
 C   -4.380098    4.202702   -0.102639
 C   -2.000892    1.361555   -1.048482
 C   -2.975016    0.177273   -1.097444
 H   -5.376692    4.322939    0.332140
 H   -4.495955    2.058510   -0.044607
 H   -4.027414    6.332320   -0.279257
 H   -1.761274    6.010255   -1.291265
 H   -0.866209    3.740115   -1.653104
Cu   -0.677468    0.975118    0.445897
 H   -3.755710    0.326903   -1.875932
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 H   -3.529322    0.060969   -0.150213
 H   -1.388616    1.369634   -1.964294
 H    7.837665    1.063392   -0.163137
 H    6.815894    2.099802   -1.208570
 H    6.880965    0.327651   -1.486321
 C    4.169528   -1.474761   -0.829963
 H    4.180742   -2.097820   -1.733344
 H    3.312084   -1.762952   -0.202729
 H    5.100998   -1.641769   -0.266983
 H   -2.943174   -3.387328    2.720989
 H   -1.011538   -4.412360    3.920564
 C   -2.076358   -2.778123    2.987191
 H   -2.907323   -1.010039    2.102523
 C   -0.994181   -3.352842    3.654763
 C   -2.055750   -1.430248    2.640058
 C    0.113127   -2.565234    3.972916
 C   -0.955656   -0.622272    2.967878
 H    0.968709   -3.004908    4.490929
 C    0.129332   -1.213793    3.634299
 C   -0.898860    0.818680    2.634179
 H    0.997013   -0.599874    3.891644
 H   -0.046955    1.363356    3.052221
 H   -1.848486    2.628516    2.002471
 C   -1.905242    1.536966    2.039493
 H   -2.882361    1.102975    1.812763
75
Figure 4_para-H_pc3_02 / electronic energy: -3508.78340558 a.u. / lowest freq: 29.76 cm-1
 C   -0.368967   -1.608150   -0.595580
 C    0.117772   -1.719012    0.681946
 C    1.593992   -1.631504    0.986136
 O    2.357216   -2.537753    0.171852
 P    3.272302   -1.962266   -1.007030
 O    2.601629   -1.286533   -2.138813
 O    4.305900   -1.042454   -0.190722
 O    4.076173   -3.256642   -1.462838
 C    4.884552    0.120124   -0.776446
 H   -1.392031   -1.906905   -0.842358
 H    0.313897   -1.454368   -1.437742
 H   -0.525120   -2.116540    1.473636
 H    1.980610   -0.610117    0.846847
 H    1.789189   -1.906853    2.029859
 B   -3.682361    0.511674   -0.834521
 O   -4.361838    0.640202    0.354873
 O   -3.797662   -0.754227   -1.351969
 C   -4.728686   -0.677448    0.798905
 C   -4.739477   -1.488637   -0.549105
 C   -6.067158   -0.615323    1.515555
 C   -3.634387   -1.135738    1.762865
 C   -6.084685   -1.432937   -1.270346
 C   -4.272606   -2.929945   -0.423850
 H   -6.444512   -0.398247   -1.371682
 H   -6.852411   -2.019915   -0.745983
 H   -5.965031   -1.850179   -2.281110
 H   -3.251098   -2.998741   -0.027325
 H   -4.286765   -3.413229   -1.411818
 H   -4.941287   -3.497516    0.240936
 H   -2.653147   -1.153885    1.263554
 H   -3.839161   -2.133182    2.176752
 H   -3.572436   -0.424739    2.600173
 H   -6.412716   -1.626623    1.778582
 H   -6.835926   -0.131346    0.899357
 H   -5.966130   -0.039241    2.447227
 C    1.002503    1.732104   -2.174009
 C    2.055393    2.626250   -2.324997
 C   -0.272891    2.150821   -1.720760
 C    1.891861    3.984711   -2.027517
 C   -0.420114    3.527126   -1.449904
 C    0.643074    4.422856   -1.592071
 C   -1.342390    1.150876   -1.487577
 C   -2.794752    1.649120   -1.445731
 H    0.484433    5.481130   -1.365637
 H   -1.386636    3.911939   -1.116747
 H    2.720392    4.687379   -2.144258
 H    3.020787    2.257200   -2.683722
 H    1.181053    0.672890   -2.383141
Cu   -0.745883    0.246093    0.242754
 H   -3.150327    1.969099   -2.446343
 H   -2.900066    2.526793   -0.787600
 H   -1.254800    0.349948   -2.237014
 H    5.574819    0.539135   -0.033893
 H    4.111874    0.863060   -1.019018
 H    5.449779   -0.130008   -1.687453
 C    4.822866   -4.055677   -0.550173
 H    5.453065   -4.722622   -1.151361
 H    4.151019   -4.657452    0.079234
 H    5.464925   -3.431229    0.089090
 H    3.659146    2.801665    1.011561
 H    4.847819    1.703412    2.911736
 C    3.105225    2.185738    1.723887
 H    1.239105    2.488402    0.705070
 C    3.770867    1.570466    2.785918
 C    1.733522    2.014132    1.557182
 C    3.049788    0.783964    3.684300
 C    0.996348    1.220762    2.454389
 H    3.559484    0.298440    4.519983
 C    1.677420    0.610533    3.517754
 C   -0.453282    0.978989    2.289114
```

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 H     1.120001   -0.016425    4.219063
 H    -0.886802    0.231447    2.961669
 H    -0.946110    2.682743    1.057570
 C    -1.294827    1.762845    1.535875
 H    -2.378106    1.630583    1.606854
75
Figure 4_para-H_ts(AS)_01 / electronic energy: -3508.73604808 a.u. / lowest freq: -180.59 cm-1
 C     0.717243   -0.773795   -0.570214
 C     0.701234   -1.231357    0.781221
 C     1.620391   -0.751237    1.704458
 O     3.478301   -1.915355    1.549176
 P     4.134614   -1.468246    0.252179
 O     3.889255   -0.094400   -0.298946
 O     5.730437   -1.751910    0.459807
 O     3.744389   -2.522773   -0.941799
 C     6.623170   -1.358621   -0.559100
 H     0.026991   -1.207288   -1.299166
 H     1.665665   -0.398983   -0.967704
 H    -0.041514   -1.966886    1.104354
 H     2.279651    0.079319    1.447158
 H     1.551101   -1.034222    2.754501
 B    -2.382885    0.533561   -1.804899
 O    -3.424120    0.159961   -1.000660
 O    -2.034311   -0.445708   -2.696452
 C    -3.682386   -1.241518   -1.222194
 C    -3.039499   -1.477714   -2.640696
 C    -5.180287   -1.487956   -1.148674
 C    -2.973840   -2.008707   -0.109088
 C    -4.012130   -1.217745   -3.789281
 C    -2.372361   -2.832190   -2.816676
 H    -4.513061   -0.244095   -3.681462
 H    -4.780803   -2.001005   -3.853076
 H    -3.453300   -1.206790   -4.736481
 H    -1.560635   -2.987775   -2.093915
 H    -1.944001   -2.908934   -3.826943
 H    -3.107016   -3.642646   -2.696773
 H    -1.888081   -1.849592   -0.145771
 H    -3.167204   -3.088809   -0.174185
 H    -3.339013   -1.650439    0.863010
 H    -5.412170   -2.533676   -1.400228
 H    -5.738881   -0.830562   -1.827493
 H    -5.535203   -1.299751   -0.124596
 C     2.075834    2.726166   -0.876565
 C     2.887881    3.818175   -0.585243
 C     0.686359    2.884425   -1.065751
 C     2.344208    5.101729   -0.476822
 C     0.157430    4.181705   -0.961601
 C     0.975273    5.275177   -0.670841
 C    -0.168861    1.687887   -1.329852
 C    -1.635782    1.909749   -1.686749
 H     0.533322    6.272348   -0.596194
 H    -0.912001    4.345544   -1.108481
 H     2.983722    5.956645   -0.244358
 H     3.959487    3.662169   -0.435870
 H     2.532306    1.731240   -0.925348
Cu    -0.065749    0.733555    0.455293
 H    -1.711368    2.452869   -2.650194
 H    -2.153456    2.531824   -0.939850
 H     0.307195    1.076298   -2.105081
 H     7.643567   -1.590341   -0.221834
 H     6.549675   -0.278037   -0.763211
 H     6.433865   -1.903023   -1.500637
 C     3.779993   -3.905106   -0.675009
 H     3.477892   -4.434665   -1.590239
 H     3.089297   -4.176899    0.140216
 H     4.793715   -4.241493   -0.395465
 H    -5.303500    0.363368    2.543311
 H    -4.964840   -1.801921    3.726447
 C    -4.295777    0.037562    2.810440
 H    -3.374561    1.789017    1.974818
 C    -4.106277   -1.175604    3.473519
 C    -3.204702    0.839370    2.485269
 C    -2.815934   -1.584651    3.812853
 C    -1.904047    0.444374    2.832015
 H    -2.658306   -2.533568    4.330140
 C    -1.725626   -0.778574    3.496809
 C    -0.718270    1.286111    2.553013
 H    -0.715706   -1.096396    3.769350
 H     0.164129    1.060795    3.160161
 H     0.215216    3.010950    1.727172
 C    -0.674025    2.375828    1.737110
 H    -1.557089    2.758795    1.219099
75
Figure 4_para-H_ts(AS)_02 / electronic energy: -3508.73603238 a.u. / lowest freq: -178.40 cm-1
 C    -0.682013   -1.444171   -1.355671
 C    -0.324901   -2.497474   -0.464381
 C     0.639454   -2.318536    0.507844
 O     2.629359   -3.105650   -0.271734
 P     3.440379   -1.928030   -0.773046
 O     2.919933   -0.981243   -1.808455
 O     3.851421   -1.098722    0.594843
 O     4.900153   -2.463417   -1.287864
 C     4.687142    0.027459    0.484988
 H    -1.412728   -1.650857   -2.140344
 H     0.047180   -0.656063   -1.577715
 H    -0.864271   -3.448806   -0.505450
 H     1.149465   -1.361643    0.632093
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 H    0.797671   -3.064441    1.284888
 B   -1.049319    1.934329   -1.683393
 O    0.181936    1.477206   -2.064025
 O   -0.980937    3.152111   -1.061900
 C    1.170845    2.296100   -1.407090
 C    0.377379    3.632214   -1.201483
 C    2.403852    2.377449   -2.289107
 C    1.517417    1.599800   -0.092552
 C    0.412388    4.537053   -2.430766
 C    0.762385    4.413391    0.041664
 H    0.168676    3.981265   -3.348614
 H    1.400971    5.001519   -2.558729
 H   -0.331430    5.338726   -2.310952
 H    0.582340    3.831794    0.953935
 H    0.172330    5.340144    0.103039
 H    1.827203    4.689544    0.006791
 H    0.634875    1.513396    0.560388
 H    2.296086    2.144764    0.459546
 H    1.902409    0.598680   -0.331734
 H    3.154677    3.049666   -1.845766
 H    2.160978    2.741370   -3.296696
 H    2.833520    1.367093   -2.372205
 C   -4.832780   -0.577898    0.457938
 C   -5.953882   -1.404505    0.451549
 C   -3.963834   -0.504489   -0.648591
 C   -6.249142   -2.181564   -0.669520
 C   -4.287168   -1.286666   -1.773556
 C   -5.409626   -2.112456   -1.782410
 C   -2.746304    0.355729   -0.597505
 C   -2.366919    1.099847   -1.878819
 H   -5.633020   -2.706106   -2.672650
 H   -3.649078   -1.249800   -2.659756
 H   -7.128795   -2.829436   -0.678662
 H   -6.608990   -1.433181    1.326182
 H   -4.626716    0.037329    1.338418
Cu   -1.484306   -0.893406    0.367035
 H   -3.202311    1.767282   -2.162641
 H   -2.219551    0.408633   -2.722817
 H   -2.850962    1.085637    0.220875
 H    4.642915    0.583115    1.433595
 H    4.369440    0.696010   -0.332092
 H    5.736640   -0.262916    0.300210
 C    5.579733   -3.438663   -0.533939
 H    6.562089   -3.603051   -1.000676
 H    5.029684   -4.393926   -0.514994
 H    5.739867   -3.114489    0.509529
 H    2.659745    0.205676    3.684732
 H    2.448481    2.684128    3.865540
 C    1.698334    0.689928    3.501839
 H    0.702164   -1.169201    3.110834
 C    1.578962    2.077866    3.601456
 C    0.591800   -0.085038    3.171154
 C    0.347103    2.686154    3.364924
 C   -0.650029    0.517757    2.913155
 H    0.244639    3.769945    3.449422
 C   -0.756658    1.912615    3.011794
 C   -1.847854   -0.256654    2.531189
 H   -1.717098    2.394166    2.810607
 H   -2.754433    0.338865    2.387988
 H   -2.921234   -2.070531    2.241071
 C   -1.951589   -1.608577    2.449611
 H   -1.137160   -2.279027    2.732232
75
Figure 4_para-H_ts(AS)_03 / electronic energy: -3508.73783576 a.u. / lowest freq: -216.07 cm-1
 C   -0.548225   -1.487136   -0.812942
 C   -0.230365   -1.885670    0.517694
 C    0.975594   -1.531499    1.102433
 O    2.498311   -2.965804    0.421521
 P    3.232484   -2.220860   -0.682667
 O    2.499961   -1.544196   -1.801768
 O    4.167076   -1.130512    0.117151
 O    4.341441   -3.216268   -1.348779
 C    4.817030   -0.116385   -0.611930
 H   -1.494451   -1.812253   -1.252239
 H    0.296227   -1.336780   -1.496330
 H   -0.940383   -2.483411    1.096891
 H    1.623114   -0.782999    0.646165
 H    1.184070   -1.775065    2.143919
 B   -3.663118    0.478440   -0.777567
 O   -4.357037    0.683412    0.386762
 O   -3.821359   -0.791545   -1.259952
 C   -4.832027   -0.594934    0.851848
 C   -4.829576   -1.452605   -0.469494
 C   -6.196927   -0.419310    1.495821
 C   -3.820352   -1.087101    1.884534
 C   -6.140582   -1.359216   -1.246726
 C   -4.433659   -2.907839   -0.279358
 H   -6.446414   -0.313112   -1.396519
 H   -6.954699   -1.891060   -0.733851
 H   -6.002679   -1.816852   -2.237271
 H   -3.423159   -3.007065    0.138719
 H   -4.451996   -3.428101   -1.248220
 H   -5.140613   -3.416188    0.393328
 H   -2.823138   -1.203211    1.434751
 H   -4.118059   -2.049711    2.323250
 H   -3.745077   -0.349650    2.697480
 H   -6.622279   -1.395041    1.774460
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 H   -6.900067    0.091642    0.825669
 H   -6.101615    0.181958    2.411934
 C    1.097088    1.553068   -2.139383
 C    2.145349    2.443481   -2.348214
 C   -0.188084    2.010570   -1.774866
 C    1.955774    3.819334   -2.191426
 C   -0.362377    3.398314   -1.631153
 C    0.694226    4.288939   -1.832190
 C   -1.289902    1.028315   -1.536910
 C   -2.717756    1.560403   -1.410258
 H    0.522643    5.361679   -1.711407
 H   -1.342347    3.800043   -1.367154
 H    2.781587    4.516213   -2.352655
 H    3.126211    2.055221   -2.634638
 H    1.299178    0.481185   -2.232369
Cu   -0.708318    0.196411    0.229137
 H   -3.093326    1.872594   -2.404431
 H   -2.767286    2.452302   -0.768127
 H   -1.256872    0.262321   -2.319027
 H    5.523069    0.387920    0.063784
 H    4.100562    0.627481   -0.996246
 H    5.386757   -0.523611   -1.465198
 C    5.155507   -4.003672   -0.508718
 H    5.798795   -4.624978   -1.148394
 H    4.550285   -4.660914    0.136596
 H    5.797373   -3.377371    0.134825
 H    3.551077    3.277792    0.675555
 H    4.958099    2.213090    2.440025
 C    3.097200    2.615262    1.416028
 H    1.136230    2.831836    0.571933
 C    3.883793    2.018872    2.402899
 C    1.729257    2.365287    1.361509
 C    3.293892    1.167542    3.336668
 C    1.125954    1.505941    2.293380
 H    3.903078    0.693380    4.109250
 C    1.926140    0.912038    3.279621
 C   -0.317213    1.179430    2.254425
 H    1.469444    0.233720    4.005315
 H   -0.645067    0.418479    2.970867
 H   -1.021721    2.718018    0.930415
 C   -1.264544    1.830734    1.521023
 H   -2.325456    1.601603    1.656409
75
Figure 4_para-H_ts(AS)_04 / electronic energy: -3508.73372533 a.u. / lowest freq: -167.66 cm-1
 C   -0.926706   -1.592200   -1.257863
 C   -0.414296   -2.522846   -0.316061
 C    0.672441   -2.215002    0.481842
 O    2.524444   -3.079300   -0.442179
 P    3.399560   -1.926894   -0.897031
 O    2.903908   -0.867693   -1.829413
 O    3.939296   -1.247017    0.505816
 O    4.786680   -2.524105   -1.529270
 C    4.779058   -0.120643    0.431690
 H   -1.751707   -1.895057   -1.905177
 H   -0.270421   -0.802622   -1.646260
 H   -0.931712   -3.474949   -0.163215
 H    1.157538   -1.240453    0.413479
 H    0.949598   -2.850382    1.320390
 B   -1.341310    1.832285   -1.678962
 O   -0.116891    1.412279   -2.120315
 O   -1.289526    3.068933   -1.096471
 C    0.877022    2.304469   -1.573151
 C    0.032873    3.605294   -1.323089
 C    2.020732    2.438850   -2.563096
 C    1.386763    1.666648   -0.285228
 C   -0.046640    4.505541   -2.553364
 C    0.453417    4.411661   -0.106634
 H   -0.332460    3.937775   -3.451526
 H    0.915128    5.001840   -2.747290
 H   -0.807306    5.282628   -2.386164
 H    0.364031    3.825933    0.816919
 H   -0.183699    5.303501   -0.010602
 H    1.496427    4.748067   -0.206722
 H    0.573342    1.525932    0.443776
 H    2.159254    2.287513    0.189823
 H    1.834128    0.694444   -0.540357
 H    2.749829    3.184612   -2.210570
 H    1.666651    2.738635   -3.558533
 H    2.528090    1.465657   -2.644161
 C   -4.949496   -0.664776    0.762896
 C   -6.057023   -1.506366    0.835563
 C   -4.129157   -0.621140   -0.381729
 C   -6.390056   -2.329090   -0.241688
 C   -4.495864   -1.443350   -1.463709
 C   -5.604247   -2.285724   -1.393689
 C   -2.928788    0.266033   -0.423714
 C   -2.635636    0.947320   -1.763837
 H   -5.858918   -2.911718   -2.252960
 H   -3.908112   -1.423517   -2.384242
 H   -7.258326   -2.989955   -0.187827
 H   -6.671549   -1.512280    1.739724
 H   -4.716549   -0.013305    1.609244
Cu   -1.477824   -0.812908    0.478792
 H   -3.504089    1.572249   -2.046362
 H   -2.504688    0.213468   -2.573731
 H   -3.024042    1.039010    0.355702
 H    5.237800    0.030584    1.420265
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 H     4.222412    0.790116    0.155062
 H     5.591023   -0.264136   -0.302336
 C     5.449952   -3.575778   -0.869234
 H     6.416345   -3.733522   -1.370344
 H     4.870416   -4.512840   -0.912657
 H     5.642922   -3.337799    0.191466
 H     0.467919    3.757761    3.448279
 H     2.892734    3.191039    3.394262
 C     0.784445    2.722841    3.302120
 H    -1.230364    1.993907    3.172044
 C     2.143856    2.404430    3.277273
 C    -0.172192    1.725365    3.144019
 C     2.541764    1.079501    3.105900
 C     0.217267    0.387223    2.969614
 H     3.602447    0.822510    3.084094
 C     1.585532    0.077642    2.960084
 C    -0.764602   -0.702232    2.802692
 H     1.908446   -0.956640    2.824349
 H    -0.371913   -1.712648    2.949735
 H    -2.579837    0.423574    2.571644
 C    -2.097266   -0.556233    2.584950
 H    -2.752947   -1.432000    2.605400
75
Figure 4_para-H_pi-allyl_01 / electronic energy: -3508.74217018 a.u. / lowest freq: 25.81 cm-1
 C     0.584876   -0.947588    0.034822
 C     0.359625   -0.992681    1.463346
 C     1.169295   -0.309208    2.322865
 O     4.169687   -1.706519    2.319008
 P     4.220324   -1.403243    0.856574
 O     3.644349   -0.136425    0.271491
 O     5.788811   -1.556938    0.379425
 O     3.509223   -2.622576   -0.007567
 C     6.120359   -1.249057   -0.950704
 H    -0.085972   -1.512481   -0.616083
 H     1.629224   -0.860693   -0.289129
 H    -0.562268   -1.446640    1.844418
 H     2.119549    0.107393    1.966421
 H     0.941503   -0.261611    3.390269
 B    -2.271881   -0.161249   -1.744424
 O    -3.436227   -0.289242   -1.044238
 O    -1.866101   -1.338517   -2.311404
 C    -3.744906   -1.696054   -0.950349
 C    -2.937419   -2.294865   -2.161639
 C    -5.250458   -1.881789   -1.030700
 C    -3.225721   -2.177506    0.401151
 C    -3.728064   -2.290651   -3.467735
 C    -2.341819   -3.670682   -1.912422
 H    -4.184186   -1.308286   -3.661131
 H    -4.523438   -3.049343   -3.457304
 H    -3.046005   -2.518663   -4.299775
 H    -1.626203   -3.662207   -1.079872
 H    -1.810027   -4.014474   -2.811690
 H    -3.133861   -4.399968   -1.685996
 H    -2.132101   -2.091199    0.458093
 H    -3.497276   -3.225744    0.589823
 H    -3.659071   -1.555385    1.196966
 H    -5.504903   -2.951900   -1.059958
 H    -5.675135   -1.396415   -1.918992
 H    -5.726944   -1.443481   -0.141219
 C     2.255017    2.148523   -1.393828
 C     3.093061    3.252436   -1.528070
 C     0.878191    2.254839   -1.674139
 C     2.586386    4.483948   -1.949734
 C     0.380642    3.499119   -2.095560
 C     1.226370    4.599422   -2.234737
 C    -0.006328    1.056909   -1.514275
 C    -1.472470    1.182930   -1.896444
 H     0.816240    5.554986   -2.571487
 H    -0.680836    3.615502   -2.322416
 H     3.247832    5.347301   -2.054322
 H     4.155956    3.146641   -1.296125
 H     2.676415    1.207313   -1.019676
Cu     0.113765    0.921924    0.508013
 H    -1.529241    1.469126   -2.966520
 H    -1.982946    1.985597   -1.342041
 H     0.450162    0.204095   -2.025810
 H     7.189337   -1.465211   -1.097976
 H     5.940279   -0.185095   -1.179856
 H     5.541153   -1.856481   -1.668949
 C     3.786199   -3.950423    0.355550
 H     3.155875   -4.613176   -0.256775
 H     3.569315   -4.132904    1.421543
 H     4.844273   -4.211724    0.172567
 H    -5.299594    1.508563    1.338146
 H    -5.459885   -0.137080    3.200231
 C    -4.419691    1.277078    1.941749
 H    -3.159768    2.629403    0.848110
 C    -4.508766    0.355337    2.985302
 C    -3.209230    1.903138    1.661793
 C    -3.379233    0.060507    3.750242
 C    -2.066992    1.617096    2.424286
 H    -3.441511   -0.662933    4.566071
 C    -2.168535    0.689333    3.472480
 C    -0.761310    2.262404    2.166108
 H    -1.282266    0.457497    4.068643
 H    -0.022917    2.175100    2.969528
 H     0.520780    3.522124    1.025546
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 C   -0.440099    3.003140    1.073960
 H   -1.167986    3.239364    0.294250
75
Figure 4_para-H_pi-allyl_02 / electronic energy: -3508.74606185 a.u. / lowest freq: 24.74 cm-1
 C   -0.700038   -1.696972   -0.407138
 C   -0.645462   -1.797394    1.027550
 C    0.427347   -1.315448    1.724674
 O    2.720884   -3.891467    0.470763
 P    3.095124   -2.698358   -0.344702
 O    2.160691   -2.052696   -1.336825
 O    3.606187   -1.543443    0.732714
 O    4.490494   -2.965083   -1.180914
 C    4.050855   -0.303254    0.242765
 H   -1.623951   -2.001368   -0.901883
 H    0.253700   -1.841269   -0.943835
 H   -1.547221   -2.086788    1.577844
 H    1.376856   -1.088639    1.224551
 H    0.416339   -1.279804    2.816373
 B   -3.552105    0.333731   -0.905505
 O   -4.323760    0.880403    0.084139
 O   -3.777364   -1.002727   -1.068470
 C   -4.969597   -0.195857    0.793807
 C   -4.906345   -1.375230   -0.251642
 C   -6.376136    0.226535    1.184140
 C   -4.131788   -0.449265    2.043968
 C   -6.121820   -1.427117   -1.174011
 C   -4.645845   -2.744303    0.354668
 H   -6.323337   -0.446734   -1.630607
 H   -7.023000   -1.755985   -0.637465
 H   -5.924129   -2.143448   -1.984730
 H   -3.685968   -2.778997    0.887047
 H   -4.620307   -3.504946   -0.439237
 H   -5.446721   -3.014699    1.058920
 H   -3.094506   -0.696386    1.777393
 H   -4.540832   -1.264235    2.656983
 H   -4.113703    0.463610    2.657692
 H   -6.912953   -0.613734    1.649476
 H   -6.953478    0.575858    0.318708
 H   -6.330346    1.045445    1.916907
 C    1.359415    0.922342   -2.117663
 C    2.449380    1.728621   -2.437599
 C    0.060349    1.464535   -2.042057
 C    2.278811    3.089493   -2.695301
 C   -0.096551    2.837255   -2.305038
 C    0.998257    3.637698   -2.631031
 C   -1.094776    0.577990   -1.691075
 C   -2.497611    1.170146   -1.716844
 H    0.844622    4.699725   -2.838009
 H   -1.087771    3.292365   -2.271853
 H    3.136804    3.717483   -2.946868
 H    3.446035    1.282701   -2.480243
 H    1.538442   -0.139756   -1.905543
Cu   -0.543297    0.198677    0.227798
 H   -2.831810    1.250968   -2.769463
 H   -2.514593    2.190732   -1.309316
 H   -1.052136   -0.330699   -2.298271
 H    4.769581    0.116903    0.962965
 H    3.219854    0.414423    0.128657
 H    4.560001   -0.402560   -0.730784
 C    5.568789   -3.562342   -0.506900
 H    6.333996   -3.832533   -1.250005
 H    5.254981   -4.473187    0.029985
 H    6.024587   -2.872026    0.226490
 H    3.539620    3.929244    0.239880
 H    4.985135    3.107840    2.099804
 C    3.122212    3.285735    1.017461
 H    1.166703    3.290718    0.134018
 C    3.930820    2.825143    2.058040
 C    1.779280    2.926917    0.961340
 C    3.391606    1.991803    3.037500
 C    1.222795    2.098537    1.947939
 H    4.020926    1.618590    3.848275
 C    2.048234    1.629069    2.980167
 C   -0.204729    1.714881    1.950414
 H    1.628808    0.974008    3.748053
 H   -0.525306    1.125066    2.815388
 H   -0.929881    2.850933    0.279177
 C   -1.155953    2.134186    1.072017
 H   -2.211835    1.904141    1.243265
37
Figure 4_para-CO2Me_L-Cu-OtBu / electronic energy: -2410.19525632 a.u. / lowest freq: 22.92 cm-1
 O    4.336955    0.759818    1.270722
 C    3.813648    0.295280    0.286819
 H    6.377229    0.525856   -0.503619
 H    5.509179    2.083275   -0.668008
 O    4.342290    0.376550   -0.932416
 C    5.585015    1.055967   -1.052360
 H    5.822111    1.073396   -2.122151
 C    0.010075   -1.714613    0.394777
 C    0.582229   -1.171455    1.554508
 C    0.718612   -1.618072   -0.813666
 C    1.948488   -0.976825   -0.864820
 C    2.504190   -0.423182    0.295604
 C    1.815193   -0.531701    1.506735
 H    0.301415   -2.034699   -1.732230
 H    2.481274   -0.897947   -1.812852
 H    2.252815   -0.101531    2.409225
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 H    0.045094   -1.242163    2.503364
 C   -1.342937   -2.314111    0.481494
 C   -2.079671   -2.809549   -0.567100
 H   -1.717994   -2.466818    1.500272
 H   -1.687861   -2.868343   -1.587441
 H   -2.998795   -3.367964   -0.366085
 H   -2.944270    1.978775    2.074160
 H   -1.417812    2.872316    1.807937
 C   -2.008539    1.995866    1.492595
 H   -1.435711    1.088443    1.750046
 H   -4.066576    3.290377    0.191900
 C   -3.113534    3.274596   -0.360508
 H   -2.555499    4.193638   -0.116482
Cu   -2.537132   -0.824824   -0.280275
 O   -3.124385    0.907277   -0.332852
 C   -2.331382    1.997552   -0.012765
 H   -3.349866    3.287741   -1.436568
 C   -1.010162    1.982770   -0.803870
 H   -0.408892    1.098739   -0.528849
 H   -0.393737    2.878382   -0.618903
 H   -1.221520    1.924120   -1.884025
79
Figure 4_para-CO2Me_ed / electronic energy: -3231.96398916 a.u. / lowest freq: 15.21 cm-1
 H    0.420682   -3.251735   -2.320503
 H   -0.175830   -3.471261   -0.650799
 O    1.955117   -1.819943   -0.653003
 C    0.630249   -3.729857   -1.350328
 H    0.640391   -4.819753   -1.505728
 C    1.975125   -3.245229   -0.807090
 H    2.877977   -2.986213   -2.760945
 H    1.449595   -3.770970    1.228008
 C    3.084590   -3.519002   -1.818846
 C    2.284444   -3.911866    0.529255
 H    4.053468   -3.167625   -1.432714
 H    3.165145   -4.594057   -2.040137
 H    3.191858   -3.483655    0.978429
 H    2.438577   -4.992884    0.390597
Cu    0.959252   -0.450176   -1.751397
 H    1.688894    3.331223    2.550758
 H    4.062624    3.209383    2.003339
 H    3.211415    1.635152    2.125613
 C    3.811369    2.281009    1.469953
 H    2.017490    4.823225    1.631737
 H    4.747827    1.749614    1.245316
 C    1.414832    3.902195    1.654494
 H    0.357324    4.191254    1.748279
 C    1.614663    3.096669    0.379835
 C    3.074105    2.560251    0.161475
 O    0.852524    1.881477    0.464377
 H    4.072080    4.421708   -0.335553
 B    1.567401    0.853709   -0.118499
 H    4.930401    2.954623   -0.863795
 C    3.936242    3.413343   -0.755669
 O    2.836693    1.286292   -0.461300
 H    1.573778    4.852979   -0.927776
 C    1.074600    3.879490   -0.816498
 H    0.000704    4.063223   -0.665995
 H    3.498791    3.508262   -1.758384
 H    1.197716    3.315218   -1.752992
 H   -0.546745   -3.306409    2.554131
 H    1.531925   -2.994349    3.125422
 H   -2.069415   -2.529581    2.071316
 C   -1.129676   -2.378206    2.624370
 O   -0.033393   -1.504611    0.698049
 H    0.892351   -2.118771    4.540081
 C    1.515113   -2.025026    3.637865
 H   -1.384286   -2.206040    3.681228
 B    1.275630   -1.018536    0.389143
 H    2.544255   -1.799802    3.956289
 C   -0.380969   -1.186436    2.030491
 C    1.026437   -0.896428    2.726834
 O    1.943970   -0.794526    1.641596
 H   -2.219308   -0.249259    1.421576
 C   -1.328214    0.019000    2.009226
 H   -1.662159    0.300392    3.019356
 H   -0.859327    0.888196    1.531404
 H    0.309578    0.379686    4.344007
 C    1.047937    0.404716    3.528356
 H    2.041818    0.545378    3.980875
 H    0.836211    1.267423    2.886840
 H   -1.480762    2.670109   -1.934889
 H   -3.551039    2.762847   -0.560174
 H    0.138588    1.498410   -3.193718
 C   -2.050555    1.758400   -1.744805
 C   -3.204757    1.814283   -0.974125
 C   -0.317129    0.516744   -3.021337
 O   -5.577960    1.782225    0.600505
 C   -1.593258    0.539761   -2.265238
 H    1.066895   -0.445687   -4.344669
 C    0.218282   -0.579980   -3.667465
 C   -3.926334    0.648284   -0.702746
 C   -5.128814    0.745085    0.174689
 C   -2.335732   -0.622660   -2.005270
 H   -0.317333   -1.530799   -3.743457
 C   -3.485958   -0.571457   -1.231013
 H   -7.650876    0.053593    0.784382
 O   -5.655991   -0.447498    0.450667
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 H   -1.999666   -1.587784   -2.388893
 H   -6.615238    0.012629    2.244759
 C   -6.813372   -0.464599    1.274230
 H   -4.040598   -1.486635   -1.021383
 H   -7.066224   -1.520237    1.425069
79
Figure 4_para-CO2Me_ts(TB) / electronic energy: -3231.96311685 a.u. / lowest freq: -92.45 cm-1
 H    0.681867   -3.477638   -2.006275
 H    0.314635   -3.758978   -0.284690
 O    2.142023   -1.749222   -0.570850
 C    1.077837   -3.885811   -1.063540
 H    1.266205   -4.960079   -1.211862
 C    2.369347   -3.166580   -0.678741
 H    3.025695   -2.863016   -2.718795
 H    2.134294   -3.637772    1.425287
 C    3.406443   -3.312169   -1.787565
 C    2.907424   -3.694108    0.647028
 H    4.340690   -2.798861   -1.515027
 H    3.630431   -4.371895   -1.980955
 H    3.779441   -3.110250    0.975641
 H    3.209731   -4.747226    0.544617
Cu    0.944775   -0.512861   -1.670883
 H    1.496334    3.496852    2.382626
 H    3.856397    3.475277    1.805579
 H    3.078669    1.862048    1.923997
 C    3.640409    2.540339    1.267918
 H    1.717127    5.000228    1.451955
 H    4.596853    2.053530    1.026785
 C    1.169794    4.045842    1.490642
 H    0.099215    4.272306    1.606039
 C    1.392252    3.250116    0.213801
 C    2.873984    2.795867   -0.028734
 O    0.700748    1.993018    0.305099
 H    3.777875    4.710292   -0.509125
 B    1.449253    1.015968   -0.327470
 H    4.693636    3.291987   -1.072350
 C    3.681263    3.703491   -0.943824
 O    2.693627    1.520954   -0.667637
 H    1.236721    5.001699   -1.091829
 C    0.791898    4.002715   -0.973928
 H   -0.288281    4.129403   -0.808974
 H    3.226461    3.794247   -1.939156
 H    0.932342    3.446080   -1.912535
 H   -0.245652   -3.207022    2.888422
 H    1.870978   -2.683044    3.229542
 H   -1.818881   -2.607023    2.321886
 C   -0.892543   -2.320662    2.842620
 O    0.169437   -1.639457    0.817034
 H    1.188244   -1.799549    4.619847
 C    1.770198   -1.693079    3.692486
 H   -1.158959   -2.029204    3.869912
 B    1.400199   -1.052499    0.458779
 H    2.779642   -1.346975    3.960796
 C   -0.229681   -1.167580    2.095407
 C    1.139850   -0.677277    2.739360
 O    2.021726   -0.545932    1.619643
 H   -2.093542   -0.460878    1.299338
 C   -1.260356   -0.053664    1.890867
 H   -1.667556    0.308513    2.846852
 H   -0.835759    0.795432    1.340916
 H    0.295700    0.610569    4.275144
 C    1.024679    0.665429    3.452381
 H    1.997789    0.947143    3.883058
 H    0.713225    1.451280    2.755529
 H   -1.568998    2.343117   -1.972658
 H   -3.641409    2.517060   -0.609794
 H   -0.067348    1.118155   -3.333434
 C   -2.150426    1.447079   -1.746723
 C   -3.304215    1.547849   -0.981512
 C   -0.446591    0.145623   -3.000167
 O   -5.671812    1.612125    0.595276
 C   -1.704371    0.203014   -2.216356
 H    0.941981   -0.912662   -4.246694
 C    0.136704   -0.998731   -3.511096
 C   -4.044299    0.403097   -0.669066
 C   -5.263348    0.555506    0.176126
 C   -2.452126   -0.940992   -1.897683
 H   -0.338762   -1.979736   -3.426340
 C   -3.609016   -0.843177   -1.135584
 H   -7.819468    0.028777    0.745412
 O   -5.861366   -0.609076    0.427537
 H   -2.127437   -1.925590   -2.239372
 H   -6.818497   -0.138801    2.219573
 C   -7.032837   -0.567873    1.230070
 H   -4.177608   -1.741572   -0.892898
 H   -7.368459   -1.605465    1.339170
79
Figure 4_para-CO2Me_prod / electronic energy: -3231.97269053 a.u. / lowest freq: 15.93 cm-1
 H    1.125135   -3.822630   -1.711189
 H    1.302296   -4.295693   -0.004487
 O    2.239310   -1.760014   -0.422705
 C    1.851128   -4.108577   -0.938227
 H    2.338886   -5.044377   -1.248944
 C    2.893212   -3.009915   -0.751149
 H    2.953705   -2.458520   -2.844885
 H    3.312062   -3.526263    1.328060
 C    3.651123   -2.742909   -2.043481
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 C    3.853750   -3.354101    0.384346
 H    4.375059   -1.926080   -1.905410
 H    4.196184   -3.642771   -2.363600
 H    4.576005   -2.540079    0.543671
 H    4.410244   -4.273186    0.147969
Cu    1.157484   -0.289500   -1.652307
 H    1.043123    3.332437    2.540237
 H    3.318792    3.881415    1.978201
 H    2.868544    2.167855    1.715244
 C    3.261678    3.074760    1.232198
 H    0.856766    5.000439    1.944522
 H    4.282567    2.855255    0.885707
 C    0.548730    3.955385    1.784743
 H   -0.537189    3.893288    1.952871
 C    0.876715    3.510467    0.367392
 C    2.401945    3.465291    0.028261
 O    0.498405    2.140047    0.185688
 H    2.819332    5.597561    0.040926
 B    1.384072    1.519692   -0.701737
 H    4.027992    4.609892   -0.814736
 C    2.951069    4.727015   -0.620414
 O    2.464374    2.380036   -0.907407
 H    0.245728    5.418516   -0.513411
 C    0.063357    4.339783   -0.629242
 H   -1.007376    4.155230   -0.455448
 H    2.458498    4.938080   -1.578979
 H    0.293617    4.055750   -1.667095
 H   -0.403632   -3.360182    3.204542
 H    1.801493   -2.842743    3.435850
 H   -1.891770   -2.825894    2.389729
 C   -1.015769   -2.482213    2.959719
 O    0.306448   -2.108502    0.979397
 H    1.024659   -1.935546    4.762849
 C    1.653667   -1.840862    3.866147
 H   -1.377717   -2.033338    3.896803
 B    1.530260   -1.549805    0.744353
 H    2.636867   -1.457072    4.175780
 C   -0.247474   -1.457353    2.140981
 C    1.042338   -0.879945    2.849954
 O    1.983077   -0.769664    1.763388
 H   -1.951960   -0.849068    0.988230
 C   -1.197033   -0.376155    1.631772
 H   -1.719934    0.120335    2.462446
 H   -0.670532    0.388805    1.042979
 H    0.054903    0.468933    4.229794
 C    0.842725    0.494895    3.462046
 H    1.773609    0.831965    3.942144
 H    0.567207    1.221381    2.688443
 H   -1.462582    1.981108   -2.110429
 H   -3.561124    2.209626   -0.797569
 H   -0.093555    0.609375   -3.666640
 C   -2.057826    1.097138   -1.873794
 C   -3.224408    1.227378   -1.134294
 C   -0.348233   -0.273012   -3.070254
 O   -5.612344    1.351664    0.413160
 C   -1.608512   -0.165270   -2.291608
 H    1.138489   -1.482708   -4.025255
 C    0.352982   -1.440019   -3.265379
 C   -3.980404    0.097108   -0.801189
 C   -5.212896    0.282857    0.016463
 C   -2.375234   -1.291700   -1.959471
 H    0.009184   -2.393589   -2.857257
 C   -3.548104   -1.164370   -1.224110
 H   -7.784847   -0.196258    0.568787
 O   -5.833940   -0.868620    0.275335
 H   -2.058997   -2.284279   -2.285616
 H   -6.798485   -0.360999    2.052801
 C   -7.011196   -0.798889    1.066721
 H   -4.132102   -2.050609   -0.973139
 H   -7.364444   -1.829593    1.185704
44
Figure 4_para-CO2Me_L-Cu-Bpin / electronic energy: -2588.18751234 a.u. / lowest freq: 14.46 cm-1
 O   -5.558121   -1.400456    1.413493
 C   -4.969777   -1.172026    0.384072
 H   -7.163184   -2.439305   -0.423265
 H   -5.906142   -3.642941   -0.001942
 O   -5.196452   -1.831828   -0.750376
 C   -6.185835   -2.851673   -0.712461
 H   -6.241573   -3.264395   -1.726124
 H    4.596257   -1.951192   -2.559203
 H    5.484395   -0.617074   -1.792449
 C    4.972644   -1.568700   -1.598251
 H    2.556436   -2.877138   -1.552758
 O    2.943343   -0.362946   -1.100888
 H    5.708685   -2.291062   -1.212281
 C    3.816702   -1.397656   -0.623669
 C    2.995315   -2.686828   -0.562093
 B    2.418217    0.336598   -0.019858
 H    3.612027   -3.555217   -0.286175
 H    5.340083    0.832942   -0.014573
 H    2.170961   -2.598449    0.160892
 H    6.371485   -0.503922    0.567895
 C    5.443585    0.055939    0.757457
 C    4.219527   -0.860717    0.791137
 O    3.087406   -0.046909    1.137136
 H    5.540628    0.559310    1.730999
 H    5.204109   -2.638584    1.561175
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 C     4.408484   -1.935449    1.851979
 H     3.484232   -2.503069    2.022068
 H     4.698517   -1.471045    2.806504
Cu     0.892565    1.683854   -0.131888
 C    -1.933435    1.861067    0.053621
 C    -2.606066    1.627684    1.262643
 C    -2.265714    1.075501   -1.063093
 C    -3.245727    0.096270   -0.973930
 C    -3.914350   -0.125684    0.236957
 C    -3.586356    0.647025    1.354776
 H    -1.749925    1.223553   -2.013889
 H    -3.494314   -0.505676   -1.848632
 H    -4.106732    0.469324    2.297533
 H    -2.351340    2.224215    2.142147
 C    -0.880322    2.897095    0.016024
 C    -0.164441    3.288343   -1.075469
 H    -0.732491    3.439754    0.956894
 H    -0.352253    2.892878   -2.078434
 H     0.519865    4.138290   -1.005459
66
Figure 4_para-CO2Me_pc1 / electronic energy: -3125.20059961 a.u. / lowest freq: 10.22 cm-1
 H     2.243341   -0.139889    2.297012
 C     3.206258    1.319070    1.043262
 C     2.089418    0.698100    1.614480
 H     3.875048    2.867748   -0.304432
 C     3.012456    2.380059    0.151621
 H    -4.521605   -2.965262    2.337865
 C     0.806937    1.116469    1.294933
 H    -4.333543   -3.285536   -0.093182
 H    -0.046594    0.598008    1.737798
 C     1.727126    2.793723   -0.173120
 C     0.597223    2.171710    0.386352
 C    -5.127863   -2.052593    2.237162
 C    -5.100898   -2.507649   -0.221491
 H    -4.831865   -1.359853    3.035793
 O    -3.565553   -0.958573    0.754721
 H     1.588441    3.612482   -0.883727
 H    -6.088770   -2.986985   -0.159855
 H    -6.183084   -2.328778    2.385284
 C    -4.919729   -1.443418    0.860348
 C    -0.747417    2.625805    0.003202
 B    -3.571522    0.171362   -0.033962
 H    -1.860182    1.871742    1.714418
 C    -1.909290    2.365948    0.739746
 C    -5.750657   -0.143838    0.580146
 H    -5.048179    0.860769    2.387045
 O    -4.857216    0.604372   -0.270051
 H    -6.710825    0.220753    2.513375
 H    -7.727730   -1.021081    0.442466
 C    -5.985793    0.694747    1.835820
 H    -2.792922    2.989751    0.580833
 C    -7.064700   -0.371371   -0.148984
 H    -6.383795    1.677049    1.541307
 H    -7.578982    0.589470   -0.300160
Cu    -1.884880    1.022785   -0.758559
 H    -0.781304    3.411170   -0.759324
 H    -4.982640   -2.078937   -1.228121
 H    -6.911180   -0.831179   -1.133966
 H     1.641155    1.094762   -3.080120
 H    -0.738741    1.172498   -3.133150
 H     3.781449    0.126528   -2.279884
 C     1.631266    0.231620   -2.409905
 C     2.829664   -0.309117   -1.970152
 C    -0.850606    0.320824   -2.454875
 H    -2.231808   -1.289888   -1.965089
 C     0.397033   -0.302500   -1.996640
 C    -2.117112   -0.257249   -2.305076
 C     2.837183   -1.397994   -1.091687
 C     0.417364   -1.412488   -1.128296
 H    -2.946097    0.124379   -2.908155
 C     1.617080   -1.948944   -0.681075
 H    -0.518665   -1.848978   -0.773165
 H     1.610665   -2.792021    0.011101
 C     4.147420   -1.885499   -0.582949
 O     5.218831   -1.458567   -0.951633
 O     4.020964   -2.838755    0.336890
 H     5.913709   -3.708927    0.214219
 C     5.216545   -3.292341    0.955789
 H     4.917238   -4.072931    1.664633
 H     5.701531   -2.464810    1.492623
 C     4.554758    0.777202    1.361604
 O     4.753261   -0.139186    2.127715
 O     5.529156    1.400091    0.703195
 H     7.155072    0.904851    1.912215
 C     6.841578    0.878761    0.858531
 H     7.497529    1.520148    0.258459
 H     6.885452   -0.153892    0.484718
66
Figure 4_para-CO2Me_ts(CuBadd)_01 / electronic energy: -3125.19811105 a.u. / lowest freq: -136.24 cm-1
 H     2.044335    0.071331    2.289177
 C     2.984159    1.451023    0.932932
 C     1.875707    0.823783    1.515815
 H     3.615964    2.900494   -0.540645
 C     2.764595    2.403458   -0.073282
 H    -4.248609   -2.146151    3.121078
 C     0.586642    1.125726    1.105321
 H    -4.009569   -3.122415    0.884275
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 H   -0.252339    0.601896    1.569800
 C    1.477772    2.702324   -0.489469
 C    0.348848    2.072248    0.081853
 C   -4.908676   -1.339719    2.768880
 C   -4.807416   -2.452283    0.531660
 H   -4.674805   -0.435520    3.345733
 O   -3.382698   -0.603546    1.049115
 H    1.327218    3.440793   -1.281492
 H   -5.773208   -2.947264    0.708572
 H   -5.947804   -1.632986    2.981563
 C   -4.710147   -1.123162    1.278208
 C   -0.982699    2.386373   -0.413824
 B   -3.451666    0.256166   -0.018159
 H   -2.139681    1.700803    1.308112
 C   -2.205193    2.019476    0.261315
 C   -5.611769   -0.000401    0.650589
 H   -5.012196    1.502817    2.120663
 O   -4.743725    0.546591   -0.368169
 H   -6.633662    0.812253    2.402240
 H   -7.527807   -1.007845    0.738269
 C   -5.922945    1.132022    1.626778
 H   -3.071230    2.659862    0.064648
 C   -6.889487   -0.501234   -0.001210
 H   -6.373461    1.969226    1.073525
 H   -7.454803    0.347424   -0.413762
Cu   -1.828807    0.678168   -1.164988
 H   -1.038875    3.182446   -1.162884
 H   -4.680393   -2.314436   -0.552460
 H   -6.680757   -1.200157   -0.821549
 H    1.574026    0.551635   -3.354096
 H   -0.802219    0.337397   -3.512204
 H    3.761749   -0.064942   -2.359239
 C    1.617941   -0.190904   -2.553487
 C    2.843216   -0.533700   -2.001779
 C   -0.864693   -0.336280   -2.651235
 H   -2.171967   -1.837378   -1.751670
 C    0.424088   -0.768211   -2.084609
 C   -2.105131   -0.917277   -2.338662
 C    2.917296   -1.462195   -0.957799
 C    0.512659   -1.715025   -1.046052
 H   -2.960802   -0.717313   -2.990300
 C    1.738374   -2.056257   -0.491623
 H   -0.391873   -2.179272   -0.647624
 H    1.781409   -2.778960    0.324025
 C    4.249052   -1.748535   -0.356757
 O    5.285000   -1.252167   -0.738721
 O    4.183522   -2.612930    0.652652
 H    6.157419   -3.284871    0.672540
 C    5.393507   -2.875441    1.349478
 H    5.146993   -3.613170    2.121682
 H    5.767670   -1.954269    1.817227
 C    4.341538    1.048733    1.372422
 O    4.564131    0.228324    2.236744
 O    5.310477    1.683598    0.712032
 H    6.876013    1.470803    2.071049
 C    6.643457    1.298653    1.009811
 H    7.290064    1.923586    0.382470
 H    6.799122    0.238364    0.765882
66
Figure 4_para-CO2Me_ts(CuBadd)_02 / electronic energy: -3125.18742203 a.u. / lowest freq: -164.30 cm-1
 H    0.411987    4.818150    0.085534
 C    2.284394    3.849907   -0.354687
 C    0.885020    3.900687   -0.271218
 H    3.971019    2.609553   -0.898453
 C    2.884263    2.667410   -0.817054
 H   -6.170348    2.447904    0.193487
 C    0.106910    2.811745   -0.629857
 H   -5.245908    1.385293    2.200500
 H   -0.979622    2.889329   -0.541316
 C    2.110492    1.574414   -1.172258
 C    0.697572    1.605075   -1.081933
 C   -6.179171    1.506445   -0.375409
 C   -5.403181    0.403694    1.729729
 H   -5.944889    1.740547   -1.422030
 O   -3.844090    1.049324    0.036446
 H    2.596387    0.663171   -1.530024
 H   -6.426732    0.074132    1.959277
 H   -7.197101    1.090994   -0.327747
 C   -5.179353    0.532206    0.224261
 C   -0.072989    0.418875   -1.406285
 B   -3.006979   -0.021998   -0.149176
 H   -2.015556    1.362179   -1.735111
 C   -1.515562    0.403255   -1.554613
 C   -5.094591   -0.856919   -0.504116
 H   -4.775451    0.037837   -2.472453
 O   -3.696320   -1.189631   -0.349622
 H   -6.430087   -0.576588   -2.210719
 H   -7.005362   -1.689073    0.089386
 C   -5.366558   -0.763298   -2.003856
 H   -1.907096   -0.400077   -2.187793
 C   -5.938103   -1.956336    0.117814
 H   -5.086284   -1.714423   -2.479885
 H   -5.807867   -2.891099   -0.447278
Cu   -1.013844   -0.065781    0.325960
 H    0.489308   -0.440661   -1.782603
 H   -4.695427   -0.307025    2.182443
 H   -5.653297   -2.150200    1.160084
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 H     2.890492   -0.220479    1.299919
 H     0.781240    0.482994    2.029890
 H     4.448961   -1.942200    0.415014
 C     2.526763   -1.229238    1.090719
 C     3.400180   -2.186953    0.593927
 C     0.282243   -0.469620    1.817993
 H    -1.496568    0.170486    2.852231
 C     1.174031   -1.535082    1.323761
 C    -1.038861   -0.624752    2.257644
 C     2.947473   -3.481455    0.315479
 C     0.730486   -2.842389    1.051296
 H    -1.504707   -1.610895    2.349319
 C     1.602862   -3.799768    0.551811
 H    -0.314721   -3.111765    1.218392
 H     1.240051   -4.806879    0.341928
 C     3.064690    5.043841    0.047011
 O     2.582391    6.069229    0.472735
 O     4.383580    4.877628   -0.105805
 H     4.970980    6.865781   -0.330920
 C     5.208872    5.970808    0.262981
 H     6.241321    5.660080    0.064782
 H     5.091645    6.210981    1.330051
 C     3.923061   -4.471015   -0.220376
 O     5.095277   -4.239769   -0.401321
 O     3.364941   -5.652970   -0.486662
 H     5.006554   -6.919074   -0.272694
 C     4.222374   -6.662630   -0.999849
 H     4.697397   -6.337362   -1.936726
 H     3.589931   -7.537904   -1.187116
66
Figure 4_para-CO2Me_L-Cu-alkyl_01 / electronic energy: -3125.23833982 a.u. / lowest freq: 20.99 cm-1
 H     1.454609   -1.179568    2.169217
 C     2.362794    0.704943    1.669023
 C     1.266607   -0.138387    1.896288
 H     2.944355    2.723736    1.154156
 C     2.108356    2.042128    1.321954
 H    -2.853561   -3.696920    1.627569
 C    -0.035301    0.322897    1.770961
 H    -1.431291   -2.307955    0.181944
 H    -0.861955   -0.367335    1.947174
 C     0.809628    2.498828    1.178691
 C    -0.313466    1.654002    1.372365
 C    -3.779687   -3.237440    1.252111
 C    -2.333223   -1.917094   -0.310703
 H    -4.499027   -3.197030    2.080299
 O    -3.038564   -0.993605    1.762580
 H     0.638876    3.542118    0.895735
 H    -2.569565   -2.566667   -1.165725
 H    -4.187130   -3.889516    0.464711
 C    -3.479630   -1.856918    0.697818
 C    -1.677981    2.153034    1.123700
 B    -3.425191    0.284115    1.437096
 H    -2.461793    1.453925    3.068109
 C    -2.811523    1.597544    2.027652
 C    -4.723659   -1.074262    0.146675
 H    -5.852343   -1.298688    2.003932
 O    -4.361791    0.289769    0.430962
 H    -6.385857   -2.383510    0.689551
 H    -5.106129   -2.282730   -1.612270
 C    -6.006608   -1.376978    0.917478
 H    -3.613867    2.352581    2.065682
 C    -4.958561   -1.225248   -1.346827
 H    -6.777218   -0.646834    0.630297
 H    -5.861101   -0.670606   -1.643457
Cu    -1.851562    1.686633   -0.821700
 H    -1.666254    3.254556    1.173432
 H    -2.098315   -0.907177   -0.685346
 H    -4.114903   -0.828694   -1.925157
 H     1.652672    2.570670   -2.275882
 H    -0.627574    2.671611   -2.827220
 H     3.717298    1.317019   -1.685542
 C     1.621292    1.482714   -2.180216
 C     2.777603    0.787552   -1.849666
 C    -0.807335    1.603205   -2.658532
 H    -2.287593    0.049644   -2.867884
 C     0.407386    0.808147   -2.368882
 C    -2.069473    1.121246   -2.860691
 C     2.739408   -0.598078   -1.681598
 C     0.389085   -0.590719   -2.243441
 H    -2.860967    1.788513   -3.213818
 C     1.537130   -1.285233   -1.888328
 H    -0.535277   -1.146283   -2.408654
 H     1.501501   -2.368071   -1.764328
 C     3.991068   -1.286875   -1.248551
 O     5.073186   -0.748646   -1.209809
 O     3.786026   -2.551302   -0.900206
 H     5.721820   -3.308892   -1.078499
 C     4.897443   -3.250193   -0.353286
 H     4.537379   -4.257762   -0.116329
 H     5.240683   -2.747836    0.561714
 C     3.727700    0.146440    1.774768
 O     3.978284   -1.016823    2.012825
 O     4.682614    1.061731    1.583065
 H     6.246530    0.158591    2.622213
 C     6.025296    0.606128    1.642007
 H     6.655476    1.490091    1.488082
 H     6.217635   -0.131192    0.850144
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66
Figure 4_para-CO2Me_L-Cu-alkyl_02 / electronic energy: -3125.23509021 a.u. / lowest freq: 10.91 cm-1
 C    2.262491    2.712946   -0.674996
 C    2.352996    1.760144   -1.699748
 C    2.963084    2.485711    0.520612
 C    3.709360    1.327772    0.692632
 C    3.783325    0.377472   -0.332993
 C    3.105772    0.605131   -1.532693
 H    2.916599    3.212831    1.333846
 H    4.234348    1.152534    1.632130
 H    3.157302   -0.145698   -2.322553
 H    1.808151    1.921345   -2.632957
 C    1.386415    3.888545   -0.885004
 C    1.096108    4.868796    0.023224
 H    1.017208    4.007488   -1.910512
 H    1.550238    4.901184    1.018645
 H    0.542023    5.757188   -0.293140
 B   -3.761779    0.616004   -0.156748
 O   -4.067849   -0.201151   -1.213305
 O   -4.191835    0.098308    1.038175
 C   -4.872292   -1.291230   -0.727567
 C   -4.560643   -1.274796    0.816906
 C   -4.455699   -2.566855   -1.443319
 C   -6.326738   -0.954633   -1.050581
 C   -3.349504   -2.127607    1.195227
 C   -5.743280   -1.626040    1.705767
 H   -2.478383   -1.894292    0.565453
 H   -3.567223   -3.202204    1.111880
 H   -3.074301   -1.911563    2.237966
 H   -6.574461   -0.920688    1.576191
 H   -5.436408   -1.595807    2.761865
 H   -6.105534   -2.641974    1.487460
 H   -6.650672   -0.037761   -0.535873
 H   -7.005837   -1.771900   -0.767809
 H   -6.424865   -0.786164   -2.133286
 H   -4.984196   -3.438032   -1.027786
 H   -3.374670   -2.740119   -1.360815
 H   -4.706260   -2.494532   -2.512223
 C   -0.049108    0.245792    1.570888
 C    0.775267   -0.858629    1.465145
 C   -0.835180    0.703450    0.482247
 C    0.858607   -1.583561    0.264239
 C   -0.743629   -0.047021   -0.715726
 C    0.080291   -1.158818   -0.820745
 C   -1.667100    1.914393    0.601281
 C   -2.938457    1.952512   -0.277890
 H    0.130366   -1.705626   -1.764140
 H   -1.332418    0.251605   -1.585132
 H    1.379286   -1.182642    2.315825
 H   -0.095334    0.792235    2.517850
Cu   -0.323892    3.328845    0.195967
 H   -2.711914    2.145852   -1.340488
 H   -3.565690    2.802740    0.042334
 H   -1.942673    2.051660    1.660912
 C    4.537356   -0.902659   -0.185862
 O    4.669474   -1.707756   -1.078765
 O    5.046451   -1.063229    1.029662
 H    6.077770   -2.234656    2.317049
 C    5.691891   -2.303231    1.293481
 H    6.520929   -2.472823    0.591468
 H    4.964136   -3.123109    1.217858
 C    1.784049   -2.733047    0.188672
 O    2.485876   -3.109979    1.104383
 O    1.780905   -3.329836   -1.006697
 H    3.737006   -4.018162   -1.069586
 C    2.708920   -4.386634   -1.192863
 H    2.562568   -4.747018   -2.218191
 H    2.524654   -5.206696   -0.483165
66
Figure 4_para-CO2Me_L-Cu-alkyl_03 / electronic energy: -3125.23447326 a.u. / lowest freq: 15.81 cm-1
 B   -4.075815   -0.978398   -0.081646
 O   -5.146829   -1.739202   -0.477284
 O   -4.468720    0.222097    0.452355
 C   -6.325796   -0.916294   -0.410310
 C   -5.897440    0.184266    0.627527
 C   -7.510023   -1.768695    0.015400
 C   -6.560778   -0.352353   -1.811123
 C   -6.158866   -0.228023    2.075221
 C   -6.472844    1.566245    0.364934
 H   -5.760976   -1.232398    2.283326
 H   -7.232661   -0.221286    2.311149
 H   -5.654265    0.481309    2.747515
 H   -6.159887    1.959463   -0.611242
 H   -6.128612    2.268215    1.139031
 H   -7.572577    1.540356    0.396222
 H   -5.726983    0.290496   -2.131248
 H   -7.491206    0.231315   -1.863714
 H   -6.637020   -1.185835   -2.524884
 H   -8.403764   -1.143978    0.163827
 H   -7.306286   -2.315786    0.945160
 H   -7.738454   -2.506535   -0.767964
 C    0.756677   -0.729217    1.525048
 C    2.093978   -1.066368    1.468718
 C   -0.163737   -1.120969    0.514744
 C    2.602134   -1.829312    0.401620
 C    0.360832   -1.922350   -0.528922
 C    1.708291   -2.255975   -0.588801
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 C   -1.557258   -0.657008    0.552364
 C   -2.588714   -1.445674   -0.253275
 H    2.078386   -2.858767   -1.420557
 H   -0.304319   -2.275689   -1.319801
 H    2.781356   -0.732875    2.249299
 H    0.392699   -0.117341    2.356383
Cu   -1.316846    1.204697   -0.124656
 H   -2.557655   -2.533901   -0.029799
 H   -2.388605   -1.395963   -1.341676
 H   -1.883053   -0.527358    1.598916
 H    3.355647    0.516407   -2.143454
 C    2.998645    1.167329   -1.343714
 H    1.026326    1.346280   -2.161344
 C    1.694572    1.638489   -1.348466
 C    3.868173    1.497265   -0.297498
 H   -0.843819    2.583187   -2.262452
 C    3.413136    2.305911    0.746754
 C    1.228857    2.457789   -0.306610
 C   -1.081020    2.953375   -1.259906
 H    4.081831    2.556492    1.570835
 C    2.105430    2.780269    0.738399
 C   -0.161131    2.967918   -0.248703
 H    1.753537    3.408278    1.560533
 H   -0.411194    3.513905    0.668704
 H   -2.027098    3.490036   -1.143040
 H    7.637693    0.950294    1.843007
 C    7.216280    0.593543    0.896208
 H    7.877030    0.876052    0.063939
 H    7.099550   -0.498870    0.924596
 O    5.941712    1.209638    0.770638
 C    5.248016    0.927393   -0.325160
 O    5.686616    0.281481   -1.248776
 H    5.904137   -3.645497   -1.806318
 C    5.803901   -3.051190   -0.890165
 H    6.216478   -3.611318   -0.038222
 H    6.345108   -2.101286   -1.001836
 O    4.415575   -2.809976   -0.724035
 C    4.051433   -2.110665    0.355069
 O    4.847865   -1.747265    1.196131
66
Figure 4_para-CO2Me_ts(BHE) / electronic energy: -3125.19981935 a.u. / lowest freq: -841.51 cm-1
 B   -3.879519    0.747206    0.113332
 O   -4.873836    1.321118    0.848835
 O   -4.341177    0.018839   -0.945096
 C   -6.117884    0.730549    0.411848
 C   -5.762556    0.254736   -1.044861
 C   -7.220949    1.771749    0.489349
 C   -6.410293   -0.428229    1.362741
 C   -5.961860    1.343601   -2.096464
 C   -6.451077   -1.028783   -1.477523
 H   -5.484826    2.288046   -1.795284
 H   -7.028734    1.534027   -2.281446
 H   -5.502615    1.017128   -3.040990
 H   -6.176604   -1.875050   -0.834209
 H   -6.163468   -1.277400   -2.509744
 H   -7.544289   -0.906502   -1.450850
 H   -5.620303   -1.193212    1.319230
 H   -7.373677   -0.906814    1.136382
 H   -6.451647   -0.043472    2.392265
 H   -8.155823    1.373364    0.067308
 H   -6.954364    2.688686   -0.052159
 H   -7.409138    2.037804    1.539892
 C    0.902776    0.985837   -1.498849
 C    2.236953    1.338491   -1.401221
 C    0.031581    1.082376   -0.390049
 C    2.767544    1.806991   -0.190867
 C    0.578374    1.566261    0.820424
 C    1.916517    1.921779    0.915688
 C   -1.355262    0.653111   -0.521713
 C   -2.361291    0.882590    0.469624
 H    2.315446    2.279435    1.866315
 H   -0.051872    1.651171    1.708743
 H    2.902044    1.235066   -2.261064
 H    0.511871    0.606483   -2.446730
Cu   -1.573063   -1.013150    0.695826
 H   -2.140370    1.595062    1.272299
 H   -2.601059   -0.293349    1.645662
 H   -1.678557    0.348291   -1.521946
 H    3.454821   -1.036212    2.075487
 C    2.944647   -1.444413    1.201326
 H    1.080277   -1.690749    2.223954
 C    1.609566   -1.811527    1.276286
 C    3.649536   -1.561501   -0.001820
 H   -0.803784   -2.873908    2.316084
 C    2.993238   -2.062351   -1.130710
 C    0.934879   -2.303991    0.144721
 C   -1.252816   -2.896442    1.318645
 H    3.530601   -2.153647   -2.075366
 C    1.652860   -2.421615   -1.056153
 C   -0.493755   -2.673359    0.168987
 H    1.145386   -2.798170   -1.947710
 H   -0.902623   -3.007082   -0.791485
 H   -2.204752   -3.428437    1.236369
 H    7.210759   -0.894156   -2.441191
 C    6.928938   -0.697263   -1.400373
 H    7.632790   -1.199981   -0.721531
 H    6.936567    0.384631   -1.208328
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 O    5.613164   -1.210874   -1.243556
 C    5.064844   -1.096998   -0.037771
 O    5.655261   -0.657763    0.923168
 H    6.133630    3.040878    2.306331
 C    6.007257    2.686850    1.276410
 H    6.398823    3.437849    0.575025
 H    6.545649    1.738588    1.138562
 O    4.613686    2.488905    1.091593
 C    4.218484    2.105262   -0.122623
 O    4.978495    2.007862   -1.061918
66
Figure 4_para-CO2Me_pc2 / electronic energy: -3125.21803273 a.u. / lowest freq: 26.75 cm-1
 B   -3.788137    0.842095   -0.054901
 O   -4.828444    1.448047    0.585792
 O   -4.189089   -0.070851   -0.992828
 C   -6.022209    0.709454    0.250896
 C   -5.622950    0.036174   -1.115829
 C   -7.195589    1.670373    0.167381
 C   -6.243954   -0.305443    1.370304
 C   -5.904277    0.924466   -2.325467
 C   -6.206922   -1.349730   -1.333673
 H   -5.491252    1.935011   -2.188816
 H   -6.982925    1.011351   -2.519347
 H   -5.430004    0.482265   -3.213910
 H   -5.878774   -2.056308   -0.560276
 H   -5.884079   -1.741043   -2.309889
 H   -7.306579   -1.310489   -1.330651
 H   -5.402458   -1.010219    1.447294
 H   -7.171676   -0.875432    1.219276
 H   -6.320558    0.229046    2.328309
 H   -8.100643    1.146337   -0.174442
 H   -6.992130    2.503771   -0.517769
 H   -7.401548    2.092319    1.162078
 C    1.019022    0.831811   -1.506423
 C    2.364172    1.165183   -1.437198
 C    0.149502    1.118591   -0.443539
 C    2.878255    1.784678   -0.294994
 C    0.669397    1.769605    0.688518
 C    2.017244    2.095784    0.764418
 C   -1.260819    0.700814   -0.545595
 C   -2.292277    1.165263    0.245345
 H    2.412295    2.573821    1.661515
 H    0.019699    1.998472    1.536044
 H    3.042681    0.915152   -2.254520
 H    0.631804    0.323445   -2.392525
Cu   -1.802212   -0.669444    1.106851
 H   -2.082230    1.927280    1.003545
 H   -2.651539   -0.506867    2.418313
 H   -1.508209    0.116217   -1.438751
 H    3.350221   -0.862425    2.048387
 C    2.820401   -1.329139    1.216236
 H    0.918281   -1.293058    2.207002
 C    1.457760   -1.572898    1.298854
 C    3.527649   -1.637252    0.048750
 H   -0.883634   -2.772002    2.379310
 C    2.849991   -2.212420   -1.030554
 C    0.762976   -2.129403    0.212606
 C   -1.384148   -2.682875    1.410853
 H    3.391009   -2.452597   -1.946515
 C    1.481977   -2.448324   -0.948551
 C   -0.690354   -2.384507    0.261777
 H    0.957037   -2.880821   -1.803902
 H   -1.176893   -2.559147   -0.703903
 H   -2.391458   -3.102334    1.347097
 H    7.105331   -1.306021   -2.433668
 C    6.856532   -1.076161   -1.391224
 H    7.530947   -1.624488   -0.717657
 H    6.951215    0.003716   -1.212735
 O    5.508747   -1.489362   -1.207739
 C    4.970041   -1.264253   -0.013569
 O    5.584197   -0.791277    0.915675
 H    6.286159    3.001701    2.156260
 C    6.150750    2.617916    1.138627
 H    6.577994    3.325984    0.413731
 H    6.644013    1.641095    1.035358
 O    4.748660    2.478667    0.949837
 C    4.349095    2.021185   -0.232213
 O    5.105321    1.801817   -1.151091
42
Figure 4_para-CO2Me-alkenylBpin / electronic energy: -947.261050912 a.u. / lowest freq: 13.61 cm-1
 B    2.536731   -0.351136   -0.017816
 O    3.507318   -1.307017    0.091467
 O    3.044449    0.917279   -0.089343
 C    4.760349   -0.629615    0.319214
 C    4.471353    0.802509   -0.264709
 C    5.875327   -1.387204   -0.382583
 C    4.996326   -0.622611    1.828498
 C    4.745855    0.900135   -1.764214
 C    5.160646    1.939871    0.470457
 H    4.269808    0.075213   -2.315220
 H    5.823957    0.886700   -1.979228
 H    4.330817    1.845090   -2.144324
 H    4.841247    2.001481    1.518889
 H    4.920642    2.897749   -0.014329
 H    6.253003    1.810310    0.441985
 H    4.207048   -0.068094    2.357891
 H    5.967553   -0.174767    2.082696
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 H     4.987792   -1.658529    2.197849
 H     6.823693   -0.833725   -0.309558
 H     5.649454   -1.557045   -1.443307
 H     6.018218   -2.368010    0.094703
 C    -2.207218    1.219150    0.141935
 C    -3.592625    1.099338    0.165560
 C    -1.385376    0.103371   -0.083437
 C    -4.189417   -0.146927   -0.050480
 C    -1.997705   -1.142169   -0.304573
 C    -3.380002   -1.264785   -0.289389
 C     0.078353    0.284197   -0.078553
 C     1.016202   -0.679307   -0.047860
 H    -3.852270   -2.233203   -0.464204
 H    -1.388084   -2.026100   -0.502335
 H    -4.214799    1.975709    0.350685
 H    -1.746933    2.196518    0.307586
 H     0.706356   -1.730832   -0.015627
 H     0.406700    1.330741   -0.083277
 O    -6.220518   -1.390859   -0.242301
 H    -8.075832    0.017569    1.049167
 C    -5.670406   -0.334915   -0.040108
 H    -8.154100    0.388896   -0.700309
 C    -7.745844    0.716413    0.266859
 O    -6.327659    0.794119    0.220526
 H    -8.101542    1.727137    0.496846
87
Figure 4_para-CO2Me_pc3_01 / electronic energy: -3964.07601958 a.u. / lowest freq: 7.26 cm-1
 C     0.117077    1.571292    0.782291
 C    -0.392408    1.691214   -0.487956
 C     0.179204    2.660615   -1.483812
 O    -0.495493    3.928253   -1.404864
 P    -0.186750    4.925795   -0.188915
 O     1.200219    4.952120    0.317930
 O    -0.755568    6.261736   -0.862774
 O    -1.221466    4.566870    0.983901
 C    -0.687339    7.489418   -0.142679
 H    -0.445079    1.106901    1.597140
 H     0.999426    2.147537    1.080825
 H    -1.393095    1.306030   -0.712736
 H     1.257895    2.809874   -1.320770
 H     0.023942    2.324816   -2.516143
 B    -0.531144   -1.761991    2.109368
 O    -1.672026   -2.188102    1.483509
 O    -0.806826   -0.921509    3.159073
 C    -2.796772   -1.483215    2.042608
 C    -2.222231   -0.986702    3.422476
 C    -3.976292   -2.438224    2.139993
 C    -3.146392   -0.337592    1.096341
 C    -2.420713   -2.000260    4.548315
 C    -2.708660    0.384991    3.862521
 H    -2.072080   -3.001777    4.254728
 H    -3.476368   -2.072834    4.846623
 H    -1.836868   -1.683410    5.424967
 H    -2.448993    1.166327    3.136138
 H    -2.244192    0.650472    4.823514
 H    -3.800261    0.384425    4.001094
 H    -2.337182    0.400042    1.037923
 H    -4.060131    0.182082    1.418270
 H    -3.316148   -0.742267    0.090043
 H    -4.819033   -1.962741    2.664135
 H    -3.711287   -3.363442    2.667885
 H    -4.315833   -2.708295    1.128728
 C     4.109231   -0.169967    0.864059
 C     5.407401   -0.347334    0.420725
 C     3.163392   -1.227446    0.868257
 C     5.839862   -1.603223   -0.043433
 C     3.625936   -2.486572    0.421740
 C     4.928269   -2.665635   -0.027592
 C     1.775287   -0.973826    1.275604
 C     0.919908   -2.182059    1.677712
 H     5.260124   -3.647798   -0.372645
 H     2.948069   -3.342416    0.426292
 H     6.107198    0.490412    0.431542
 H     3.794257    0.816861    1.217504
Cu     0.827759   -0.052826   -0.281519
 H     1.387473   -2.740042    2.517144
 H     0.831891   -2.908492    0.851941
 H     1.762614   -0.213569    2.071234
 H    -1.104721    8.266821   -0.794064
 H     0.355232    7.741292    0.103077
 H    -1.277810    7.440768    0.785741
 C    -2.598261    4.326554    0.723916
 H    -3.125052    4.385908    1.684697
 H    -2.743291    3.323782    0.293436
 H    -3.016900    5.079083    0.037704
 H    -3.080316   -3.692817   -1.229254
 C    -2.800443   -2.747866   -1.695015
 H    -0.719834   -3.022456   -1.282538
 C    -3.787810   -1.914924   -2.231937
 C    -1.466585   -2.363826   -1.727170
 C    -3.414817   -0.701963   -2.823133
 C    -1.081953   -1.144810   -2.304669
 H    -4.186018   -0.054034   -3.243600
 C    -2.078786   -0.325821   -2.861642
 C     0.325846   -0.692837   -2.334404
 H    -1.797493    0.623153   -3.325358
 H     0.527615    0.176203   -2.967382
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 H     2.410327   -1.062122   -2.026780
 C     1.387807   -1.378908   -1.802554
 H     1.282204   -2.369428   -1.352493
 H    -6.805737   -4.755030   -0.841670
 H    -7.295435   -3.945490   -2.369075
 C    -6.821325   -3.804648   -1.386955
 O    -5.464811   -3.406112   -1.530122
 H    -7.392173   -3.057105   -0.817225
 C    -5.238169   -2.251786   -2.158893
 O    -6.120644   -1.555579   -2.600817
 H     9.795293    0.091295   -0.798463
 H     9.373369   -1.198179   -1.974417
 C     9.326191   -0.892430   -0.918689
 O     7.984031   -0.751437   -0.484714
 H     9.864762   -1.634879   -0.311347
 C     7.215866   -1.847600   -0.531356
 O     7.627292   -2.912256   -0.935299
87
Figure 4_para-CO2Me_pc3_02 / electronic energy: -3964.08215085 a.u. / lowest freq: 18.88 cm-1
 C     1.751368    1.642526   -0.949525
 C     1.168041    2.091841    0.204683
 C    -0.321330    2.321792    0.311317
 O    -0.794789    3.179455   -0.737015
 P    -1.761643    2.593447   -1.870636
 O    -1.208909    1.571337   -2.784706
 O    -3.025417    2.122772   -1.000259
 O    -2.204239    3.917302   -2.635728
 C    -3.880586    1.063022   -1.425885
 H     2.832535    1.706924   -1.103492
 H     1.142228    1.437131   -1.836065
 H     1.791757    2.520437    0.995561
 H    -0.880502    1.374417    0.284863
 H    -0.565981    2.815397    1.259618
 B     4.568308   -1.187133   -0.329184
 O     5.061113   -1.137542    0.954215
 O     5.054497   -0.163827   -1.102194
 C     5.701072    0.139599    1.129961
 C     6.065088    0.530757   -0.349713
 C     6.890540   -0.015447    2.062206
 C     4.661421    1.072004    1.752128
 C     7.418883   -0.017623   -0.796979
 C     5.978445    2.018062   -0.653288
 H     7.509333   -1.092942   -0.582556
 H     8.251323    0.506912   -0.306080
 H     7.519999    0.120573   -1.883438
 H     4.970753    2.416092   -0.476179
 H     6.230299    2.197297   -1.708916
 H     6.689726    2.583789   -0.032825
 H     3.779224    1.166096    1.099241
 H     5.070301    2.074669    1.940247
 H     4.329077    0.652097    2.713364
 H     7.440254    0.933944    2.148931
 H     7.584299   -0.791669    1.714111
 H     6.541891   -0.298260    3.066561
 C    -0.130583   -1.439342   -1.983175
 C    -1.413287   -1.948867   -1.966339
 C     0.948256   -2.097503   -1.332329
 C    -1.692973   -3.173507   -1.331525
 C     0.664359   -3.369583   -0.779867
 C    -0.625707   -3.888754   -0.775843
 C     2.233261   -1.407707   -1.173958
 C     3.485347   -2.213009   -0.810865
 H    -0.825324   -4.855544   -0.307387
 H     1.465549   -3.948284   -0.315802
 H    -2.218028   -1.386015   -2.441284
 H     0.030476   -0.468139   -2.456906
Cu     1.679751   -0.045535    0.268596
 H     3.839804   -2.828269   -1.661824
 H     3.288836   -2.911339    0.018300
 H     2.430282   -0.761294   -2.041205
 H    -4.838670    1.194174   -0.908864
 H    -3.452635    0.089732   -1.150364
 H    -4.053269    1.091117   -2.511910
 C    -2.798391    5.022988   -1.962900
 H    -3.086502    5.749734   -2.732020
 H    -2.081628    5.489276   -1.271055
 H    -3.694678    4.709972   -1.406335
 H    -3.169371   -1.528142    0.768137
 C    -2.585485   -0.894306    1.438596
 H    -0.722695   -1.785251    0.885203
 C    -3.241122    0.078027    2.202092
 C    -1.207380   -1.034175    1.510179
 C    -2.491661    0.895331    3.056179
 C    -0.440708   -0.199890    2.341765
 H    -2.991770    1.652284    3.661634
 C    -1.109538    0.755624    3.121649
 C     1.035422   -0.265487    2.367312
 H    -0.531160    1.413295    3.775519
 H     1.536060    0.523527    2.938068
 H     1.301718   -2.248267    1.556908
 C     1.775758   -1.326441    1.905825
 H     2.850649   -1.375396    2.101691
 O    -5.391520   -0.483123    1.326114
 C    -4.718753    0.207866    2.054986
 H    -7.174294    0.464668    3.048871
 O    -5.229055    1.176095    2.814774
 C    -6.634668    1.372573    2.742747
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 H   -6.941336    1.644378    1.722074
 H   -6.865946    2.192822    3.431734
 O   -3.356931   -4.792801   -0.760920
 C   -3.068362   -3.689494   -1.166158
 H   -5.543526   -3.380981   -0.222027
 O   -3.995951   -2.769840   -1.474266
 C   -5.352107   -3.132805   -1.275576
 H   -5.949628   -2.259593   -1.561590
 H   -5.627220   -3.993948   -1.902685
87
Figure 4_para-CO2Me_ts(AS)_01 / electronic energy: -3964.02907638 a.u. / lowest freq: -190.00 cm-1
 C    0.333117    1.436836    0.703143
 C   -0.082487    1.779294   -0.617388
 C    0.832968    1.788864   -1.660883
 O    1.908730    3.732297   -1.694403
 P    2.829368    3.693453   -0.486130
 O    3.330743    2.384990    0.054342
 O    4.063651    4.700306   -0.847288
 O    2.106106    4.463453    0.769458
 C    5.115066    4.837750    0.083268
 H   -0.382559    1.481145    1.527870
 H    1.383405    1.606443    0.962844
 H   -1.130819    2.018484   -0.820677
 H    1.846595    1.414614   -1.507829
 H    0.508656    1.969857   -2.685201
 B   -1.583828   -1.144209    2.248981
 O   -2.736769   -1.226934    1.518611
 O   -1.664420   -0.209866    3.246098
 C   -3.611547   -0.156442    1.930994
 C   -3.041898    0.205722    3.353692
 C   -5.046943   -0.657124    1.923571
 C   -3.453939    0.976312    0.920783
 C   -3.670824   -0.618407    4.474812
 C   -3.088722    1.684497    3.700976
 H   -3.644025   -1.694857    4.248098
 H   -4.715591   -0.327034    4.653737
 H   -3.105149   -0.454442    5.403550
 H   -2.504612    2.290331    2.995879
 H   -2.672369    1.842593    4.706723
 H   -4.126464    2.050152    3.700744
 H   -2.443357    1.402287    0.948455
 H   -4.171823    1.786698    1.111312
 H   -3.637056    0.583919   -0.088449
 H   -5.721670    0.096746    2.356296
 H   -5.155112   -1.591916    2.488954
 H   -5.371563   -0.844283    0.889383
 C    3.250652   -0.947633    0.767462
 C    4.441793   -1.508885    0.332220
 C    2.136065   -1.755065    1.090470
 C    4.570626   -2.900965    0.206625
 C    2.284745   -3.149237    0.974139
 C    3.479838   -3.710634    0.538761
 C    0.852107   -1.115013    1.485285
 C   -0.296056   -1.999476    1.960319
 H    3.580864   -4.794329    0.449225
 H    1.452321   -3.809001    1.225450
 H    5.281314   -0.860418    0.076470
 H    3.175320    0.144036    0.818481
Cu    0.339935   -0.285884   -0.288329
 H   -0.002228   -2.530066    2.887911
 H   -0.542264   -2.779215    1.222468
 H    1.055304   -0.330251    2.223251
 H    5.837753    5.557435   -0.327546
 H    5.626459    3.877081    0.257845
 H    4.752625    5.220475    1.053213
 C    1.463501    5.695112    0.536760
 H    0.999583    6.020415    1.479169
 H    0.681217    5.603222   -0.234738
 H    2.177420    6.472112    0.212179
 H   -4.604095   -2.429799   -1.098866
 C   -3.965623   -1.721346   -1.626473
 H   -2.170208   -2.771750   -1.123492
 C   -4.531358   -0.616701   -2.270537
 C   -2.589665   -1.906298   -1.637519
 C   -3.704703    0.287639   -2.946729
 C   -1.751186   -0.995463   -2.294680
 H   -4.152307    1.146202   -3.450018
 C   -2.329272    0.098092   -2.958441
 C   -0.279887   -1.148161   -2.306794
 H   -1.687159    0.811463   -3.480672
 H    0.251719   -0.545402   -3.049237
 H    1.506977   -2.160576   -1.743729
 C    0.434409   -2.043247   -1.569087
 H   -0.043493   -2.788629   -0.928333
 H   -8.411157   -1.786727   -0.635144
 H   -8.567112   -1.108397   -2.291548
 C   -8.059121   -1.008639   -1.321663
 O   -6.657959   -1.206675   -1.461575
 H   -8.273206   -0.015311   -0.902007
 C   -5.997728   -0.338300   -2.227258
 O   -6.530293    0.581104   -2.799599
 H    8.688330   -2.346799   -1.151368
 H    7.877496   -3.725848   -1.968261
 C    8.018774   -3.203115   -1.010740
 O    6.790311   -2.674938   -0.533985
 H    8.456285   -3.903197   -0.284042
 C    5.819147   -3.552341   -0.271520
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 O    5.955546   -4.745404   -0.414308
87
Figure 4_para-CO2Me_ts(AS)_02 / electronic energy: -3964.02804325 a.u. / lowest freq: -184.57 cm-1
 C   -0.648260   -1.773198    0.177986
 C   -0.578165   -1.919115   -1.238419
 C   -1.634700   -1.496786   -2.037912
 O   -3.138030   -3.108695   -2.164844
 P   -3.819770   -3.160545   -0.807086
 O   -3.837506   -1.955146    0.088794
 O   -5.330715   -3.704058   -1.106069
 O   -3.176323   -4.383347    0.075066
 C   -6.231611   -3.830131   -0.027898
 H    0.158408   -2.153477    0.809981
 H   -1.645011   -1.745397    0.630946
 H    0.311496   -2.352848   -1.705510
 H   -2.477200   -0.962124   -1.598930
 H   -1.550305   -1.506068   -3.124195
 B    1.956357   -0.007794    1.939008
 O    3.092243   -0.022108    1.179186
 O    1.823059   -1.139685    2.698867
 C    3.698403   -1.323301    1.295032
 C    3.063945   -1.869780    2.629261
 C    5.210689   -1.165523    1.326472
 C    3.292153   -2.130568    0.064831
 C    3.871923   -1.495667    3.870270
 C    2.763979   -3.359775    2.629595
 H    4.102398   -0.420041    3.891898
 H    4.816418   -2.055872    3.922565
 H    3.281597   -1.732794    4.767562
 H    2.055831   -3.636094    1.837325
 H    2.320490   -3.648633    3.593744
 H    3.688539   -3.940266    2.492134
 H    2.201044   -2.246162   -0.004604
 H    3.747299   -3.130906    0.073128
 H    3.635069   -1.605260   -0.836198
 H    5.695402   -2.128768    1.545580
 H    5.528587   -0.431949    2.078468
 H    5.569226   -0.826545    0.343583
 C   -2.861227    1.143322    0.954920
 C   -3.910094    2.020801    0.721321
 C   -1.562198    1.618074    1.251143
 C   -3.708368    3.407765    0.785245
 C   -1.379119    3.012625    1.326831
 C   -2.433285    3.889822    1.098924
 C   -0.449228    0.649794    1.427696
 C    0.895560    1.152187    1.934621
 H   -2.277585    4.968662    1.165241
 H   -0.397039    3.419102    1.576055
 H   -4.898889    1.624822    0.484749
 H   -3.054501    0.067552    0.875284
Cu   -0.342911    0.064291   -0.516866
 H    0.783908    1.541126    2.966569
 H    1.279924    1.984455    1.328148
 H   -0.794522   -0.192513    2.037449
 H   -7.187062   -4.196924   -0.429574
 H   -6.400330   -2.861884    0.471050
 H   -5.868042   -4.550616    0.725351
 C   -2.994121   -5.640957   -0.533494
 H   -2.382486   -6.261129    0.137932
 H   -2.476953   -5.545909   -1.502257
 H   -3.957508   -6.153110   -0.702998
 H    4.445642   -0.150406   -2.711194
 C    3.946621    0.657398   -2.174682
 H    1.991101    0.049435   -2.808301
 C    4.701830    1.559313   -1.416593
 C    2.564584    0.776881   -2.229181
 C    4.059774    2.600303   -0.742641
 C    1.909941    1.798557   -1.526482
 H    4.654258    3.304909   -0.158976
 C    2.677802    2.716395   -0.797227
 C    0.439387    1.936316   -1.509016
 H    2.180065    3.526936   -0.259732
 H    0.045488    2.684285   -0.813850
 H   -1.489210    1.604351   -2.349362
 C   -0.428633    1.336922   -2.369470
 H   -0.088239    0.723915   -3.207296
 H   -7.891376    4.013652   -0.323838
 H   -6.827609    5.347345   -0.888987
 C   -7.051233    4.664762   -0.055988
 O   -5.951536    3.806892    0.209153
 H   -7.310665    5.259430    0.832349
 C   -4.796466    4.390658    0.534817
 O   -4.664103    5.590201    0.609718
 H    8.237194   -0.902089   -2.154738
 H    8.337686    0.029167   -0.620579
 C    8.047444    0.067334   -1.680425
 O    6.652813    0.308350   -1.814277
 H    8.630882    0.851108   -2.184880
 C    6.180645    1.428897   -1.265986
 O    6.878586    2.230133   -0.693350
87
Figure 4_para-CO2Me_ts(AS)_03 / electronic energy: -3964.03280404 a.u. / lowest freq: -217.46 cm-1
 C    2.034752    1.374398   -1.011573
 C    1.771916    2.130468    0.166557
 C    0.489282    2.217454    0.680661
 O   -0.584812    3.847258   -0.383551
 P   -1.507491    3.107602   -1.337330
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 O   -1.053818    1.869738   -2.053407
 O   -2.855112    2.791762   -0.454092
 O   -2.066850    4.149785   -2.464009
 C   -3.848092    1.943228   -0.979120
 H    3.052077    1.332268   -1.407592
 H    1.215264    1.289646   -1.734494
 H    2.588685    2.637748    0.688301
 H   -0.304060    1.588031    0.278266
 H    0.298063    2.718539    1.628351
 B    4.476848   -1.237075   -0.337851
 O    5.071051   -1.271686    0.895717
 O    4.980059   -0.243707   -1.132167
 C    5.885315   -0.089678    1.033274
 C    6.117658    0.338121   -0.466080
 C    7.152541   -0.438492    1.796348
 C    5.056412    0.918977    1.824453
 C    7.365006   -0.287481   -1.085536
 C    6.111997    1.839979   -0.703681
 H    7.392107   -1.375946   -0.928391
 H    8.284899    0.149081   -0.671339
 H    7.355415   -0.102294   -2.169523
 H    5.161124    2.299641   -0.403202
 H    6.265294    2.046176   -1.773099
 H    6.926100    2.324485   -0.143973
 H    4.121128    1.161132    1.299324
 H    5.605901    1.854260    2.000760
 H    4.796357    0.485454    2.801428
 H    7.833368    0.425337    1.829704
 H    7.682266   -1.284832    1.340414
 H    6.901761   -0.712706    2.831672
 C   -0.371880   -1.314522   -1.741441
 C   -1.626088   -1.902295   -1.792838
 C    0.751410   -2.027111   -1.266077
 C   -1.810420   -3.230768   -1.383593
 C    0.558354   -3.371653   -0.895959
 C   -0.699664   -3.963288   -0.955748
 C    2.068561   -1.341011   -1.136563
 C    3.289492   -2.175425   -0.755402
 H   -0.835447   -5.003102   -0.650836
 H    1.403752   -3.968715   -0.550383
 H   -2.481238   -1.314616   -2.129110
 H   -0.293385   -0.259252   -2.019541
Cu    1.649512   -0.017689    0.360163
 H    3.588230   -2.818987   -1.606009
 H    3.075670   -2.851372    0.086312
 H    2.273429   -0.782481   -2.056578
 H   -4.760356    2.083035   -0.380872
 H   -3.548384    0.883417   -0.927537
 H   -4.087734    2.184041   -2.029048
 C   -2.493533    5.432007   -2.062507
 H   -2.883176    5.950533   -2.950198
 H   -1.662478    6.019870   -1.639950
 H   -3.296784    5.375894   -1.307631
 H   -3.355856   -1.902562    0.811990
 C   -2.794246   -1.185539    1.412292
 H   -0.918468   -2.173227    1.114884
 C   -3.469779   -0.097034    1.971919
 C   -1.424340   -1.328151    1.583806
 C   -2.760437    0.841103    2.728347
 C   -0.699405   -0.379458    2.319673
 H   -3.278286    1.694530    3.166224
 C   -1.390167    0.692337    2.904234
 C    0.774038   -0.436018    2.457550
 H   -0.838027    1.435897    3.483954
 H    1.218686    0.363313    3.060224
 H    1.188444   -2.338397    1.541626
 C    1.585948   -1.431205    2.003469
 H    2.651321   -1.430449    2.254488
 O   -5.587424   -0.790693    1.108523
 C   -4.935358    0.026387    1.713024
 H   -7.438052    0.581504    2.493210
 O   -5.450467    1.145365    2.217951
 C   -6.838827    1.365334    2.007482
 H   -7.074814    1.383165    0.933726
 H   -7.065469    2.338975    2.455974
 O   -3.352978   -5.024956   -1.036364
 C   -3.153940   -3.865659   -1.315912
 H   -5.654429   -3.823953   -0.402068
 O   -4.136581   -2.995932   -1.559614
 C   -5.467650   -3.469474   -1.425624
 H   -6.120877   -2.618725   -1.647606
 H   -5.667385   -4.288681   -2.131891
87
Figure 4_para-CO2Me_ts(AS)_04 / electronic energy: -3964.02741833 a.u. / lowest freq: -157.56 cm-1
 C   -1.195792    1.524242    1.057283
 C   -0.946814    2.351096   -0.070091
 C    0.222997    2.240497   -0.796044
 O    1.744777    3.807541   -0.125902
 P    2.800476    3.174204    0.757907
 O    2.459341    2.459156    2.026814
 O    3.640448    2.167181   -0.249419
 O    3.940746    4.294463    1.118253
 C    4.756058    1.478755    0.263708
 H   -2.115659    1.676007    1.624693
 H   -0.350433    1.094716    1.609541
 H   -1.726537    3.034556   -0.420087
 H    0.991833    1.516508   -0.523994
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 H    0.340448    2.753180   -1.748305
 B   -0.476414   -1.574774    2.322493
 O    0.477703   -0.652300    2.650369
 O    0.055324   -2.807950    2.065720
 C    1.766115   -1.226556    2.345400
 C    1.455582   -2.763104    2.426909
 C    2.787320   -0.696960    3.336176
 C    2.127948   -0.766664    0.936715
 C    1.572919   -3.320272    3.843140
 C    2.247121   -3.619173    1.453577
 H    1.024063   -2.699571    4.567034
 H    2.622764   -3.383125    4.163709
 H    1.144009   -4.332777    3.869509
 H    2.022743   -3.354975    0.412600
 H    2.001347   -4.681794    1.597727
 H    3.328092   -3.495330    1.616891
 H    1.379656   -1.102934    0.203205
 H    3.106418   -1.155004    0.621512
 H    2.177636    0.330166    0.939074
 H    3.768580   -1.167297    3.168271
 H    2.484724   -0.883628    4.375300
 H    2.882698    0.389334    3.183178
 C   -4.535062   -1.176637   -0.614193
 C   -5.850501   -0.822795   -0.882033
 C   -3.832398   -0.645580    0.486941
 C   -6.523643    0.077318   -0.045687
 C   -4.536107    0.234587    1.332998
 C   -5.851766    0.592185    1.069086
 C   -2.411156   -1.015682    0.726170
 C   -1.998856   -1.211781    2.187591
 H   -6.380086    1.279341    1.733221
 H   -4.048009    0.646517    2.218508
 H   -6.366042   -1.253835   -1.741544
 H   -4.036279   -1.897266   -1.266525
Cu   -1.377723    0.257811   -0.464963
 H   -2.617552   -2.017557    2.625105
 H   -2.191760   -0.310533    2.789445
 H   -2.173823   -1.929121    0.158087
 H    5.032608    0.683999   -0.444788
 H    4.538633    1.021721    1.243076
 H    5.622550    2.152712    0.385459
 C    4.403162    5.152004    0.102639
 H    5.246709    5.730850    0.506452
 H    3.617626    5.851446   -0.228082
 H    4.756453    4.590528   -0.780189
 H    2.542129   -3.532008   -1.982754
 C    2.353682   -2.479196   -2.198266
 H    0.227834   -2.721100   -2.273287
 C    3.436035   -1.595846   -2.282951
 C    1.056275   -2.015573   -2.360450
 C    3.209197   -0.251920   -2.588273
 C    0.815624   -0.656507   -2.620918
 H    4.044649    0.443110   -2.666184
 C    1.909639    0.207348   -2.763920
 C   -0.547576   -0.096083   -2.716218
 H    1.743512    1.261826   -2.989469
 H   -0.612794    0.918000   -3.122376
 H   -1.723722   -1.808652   -2.155952
 C   -1.702344   -0.751546   -2.432067
 H   -2.662898   -0.275575   -2.649879
 O    5.028979   -3.245239   -1.611657
 C    4.802557   -2.120330   -1.986323
 H    7.401971   -2.440076   -2.413709
 O    5.747399   -1.197741   -2.156857
 C    7.080729   -1.566136   -1.829441
 H    7.169739   -1.795523   -0.757595
 H    7.706666   -0.701275   -2.076442
 O   -8.540532    1.269976    0.416008
 C   -7.929692    0.499619   -0.287066
 H   -9.901116    1.359248   -1.864013
 O   -8.456285   -0.063590   -1.376627
 C   -9.798349    0.278206   -1.689770
 H  -10.050268   -0.269659   -2.605121
 H  -10.480831   -0.017926   -0.879755
87
Figure 4_para-CO2Me_pi-allyl_01 / electronic energy: -3964.04377838 a.u. / lowest freq: 17.67 cm-1
 C    0.046643    1.811794    0.879397
 C   -0.562366    2.336395   -0.317465
 C    0.156098    2.468144   -1.474901
 O    3.230647    2.104601   -1.393240
 P    3.820705    2.571567   -0.090882
 O    3.046470    2.534985    1.200431
 O    5.235107    1.746549    0.089892
 O    4.370518    4.113046   -0.240538
 C    5.979716    1.933615    1.269101
 H   -0.587232    1.674686    1.758785
 H    1.112261    2.042839    1.062664
 H   -1.651087    2.456296   -0.351411
 H    1.260037    2.395663   -1.487011
 H   -0.352928    2.752120   -2.399690
 B   -2.052615   -0.796363    1.906709
 O   -3.297010   -0.898175    1.355797
 O   -2.020925    0.056587    2.976888
 C   -4.144417    0.089480    1.979139
 C   -3.387413    0.365943    3.329964
 C   -5.542489   -0.487458    2.125686
 C   -4.170826    1.307797    1.061642
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 C   -3.788331   -0.595578    4.445852
 C   -3.462235    1.800887    3.823801
 H   -3.748094   -1.643053    4.111177
 H   -4.803212   -0.385899    4.812545
 H   -3.087695   -0.481521    5.285792
 H   -3.032849    2.508400    3.102612
 H   -2.905412    1.898391    4.767254
 H   -4.507072    2.087510    4.015628
 H   -3.173816    1.762071    0.972915
 H   -4.868060    2.073935    1.428863
 H   -4.494331    0.999286    0.058230
 H   -6.192158    0.204613    2.682034
 H   -5.531381   -1.453876    2.646392
 H   -5.981439   -0.644478    1.128922
 C    2.939510   -0.757246    0.893464
 C    4.133828   -1.364823    0.532949
 C    1.727521   -1.471467    0.879131
 C    4.157740   -2.719762    0.176224
 C    1.764854   -2.832946    0.529768
 C    2.963431   -3.448222    0.188890
 C    0.459177   -0.767382    1.230354
 C   -0.800391   -1.601784    1.404268
 H    2.985869   -4.507221   -0.076358
 H    0.846409   -3.422646    0.525098
 H    5.048260   -0.771546    0.510590
 H    2.935655    0.303663    1.164014
Cu    0.183599    0.334176   -0.453991
 H   -0.605126   -2.371976    2.179252
 H   -1.062442   -2.160161    0.492796
 H    0.636482   -0.143968    2.112292
 H    6.928948    1.387910    1.161746
 H    5.447572    1.551325    2.156327
 H    6.208817    2.999816    1.442799
 C    5.126632    4.451576   -1.376754
 H    5.329429    5.532404   -1.343729
 H    4.584271    4.219082   -2.308588
 H    6.092148    3.915372   -1.399947
 H   -4.512185   -2.244083   -1.326707
 C   -3.983964   -1.416823   -1.799506
 H   -2.067423   -2.337417   -1.558036
 C   -4.695230   -0.305157   -2.259774
 C   -2.601694   -1.459621   -1.924779
 C   -4.010004    0.753016   -2.866630
 C   -1.901871   -0.391142   -2.502424
 H   -4.572839    1.614722   -3.229369
 C   -2.627274    0.709110   -2.986315
 C   -0.425491   -0.374611   -2.598883
 H   -2.096095    1.542827   -3.450905
 H   -0.002519    0.386780   -3.260953
 H    1.493496   -1.211911   -2.208508
 C    0.419939   -1.256901   -2.004922
 H    0.056803   -2.125531   -1.451766
 H   -8.324026   -2.046413   -0.554656
 H   -8.663428   -1.203588   -2.104455
 C   -8.095552   -1.164451   -1.163498
 O   -6.697251   -1.207434   -1.417632
 H   -8.367998   -0.249636   -0.618143
 C   -6.173931   -0.181410   -2.087143
 O   -6.825370    0.752357   -2.487631
 H    8.462224   -2.393685   -0.515791
 H    7.677710   -3.605335   -1.584331
 C    7.720309   -3.199028   -0.563305
 O    6.477456   -2.620871   -0.193562
 H    8.001647   -4.004687    0.130661
 C    5.410779   -3.421092   -0.218092
 O    5.469704   -4.587770   -0.529785
87
Figure 4_para-CO2Me_pi-allyl_02 / electronic energy: -3964.03936221 a.u. / lowest freq: 10.51 cm-1
 C    2.144889    1.521265   -0.881065
 C    2.096421    2.092430    0.439418
 C    0.925334    2.116453    1.143178
 O   -0.391163    4.579275   -0.630740
 P   -1.209473    3.489475   -1.243105
 O   -0.599890    2.307202   -1.954375
 O   -2.202850    2.928489   -0.041483
 O   -2.319889    4.102457   -2.294022
 C   -3.089447    1.876933   -0.330295
 H    3.118913    1.442287   -1.366957
 H    1.258048    1.700774   -1.510106
 H    3.031038    2.353403    0.947152
 H   -0.033547    1.913575    0.653659
 H    0.899825    2.453385    2.181607
 B    4.379033   -1.215294   -0.549335
 O    4.966950   -1.614109    0.619450
 O    4.946167   -0.084914   -1.064045
 C    5.859299   -0.568691    1.053460
 C    6.115091    0.234329   -0.280530
 C    7.102870   -1.193626    1.664063
 C    5.101984    0.231872    2.111033
 C    7.323887   -0.267185   -1.066150
 C    6.192352    1.742014   -0.105370
 H    7.284846   -1.356409   -1.215751
 H    8.267226   -0.016984   -0.560670
 H    7.327923    0.210706   -2.056438
 H    5.267550    2.153172    0.320169
 H    6.357129    2.221769   -1.081208
 H    7.030926    2.013316    0.553136
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 H     4.172946    0.654253    1.700791
 H     5.709036    1.053544    2.515916
 H     4.832531   -0.435634    2.943035
 H     7.834014   -0.416585    1.932183
 H     7.580803   -1.904006    0.977370
 H     6.833739   -1.737303    2.581485
 C    -0.515379   -0.836459   -1.857703
 C    -1.791028   -1.374143   -1.965441
 C     0.589908   -1.653315   -1.541058
 C    -2.008842   -2.743235   -1.772695
 C     0.362310   -3.032430   -1.377613
 C    -0.915507   -3.568859   -1.495568
 C     1.947029   -1.041071   -1.394696
 C     3.140850   -1.958687   -1.169716
 H    -1.079565   -4.639458   -1.357396
 H     1.193164   -3.704414   -1.157672
 H    -2.632136   -0.716371   -2.187679
 H    -0.402574    0.247088   -1.986822
Cu     1.585880    0.014449    0.316613
 H     3.429269   -2.415529   -2.135693
 H     2.892471   -2.790251   -0.495384
 H     2.132098   -0.376088   -2.242532
 H    -3.873133    1.866881    0.442057
 H    -2.581237    0.897766   -0.321042
 H    -3.575955    2.004921   -1.312913
 C    -3.061284    5.228695   -1.897929
 H    -3.594814    5.618522   -2.777781
 H    -2.407343    6.021177   -1.497078
 H    -3.806734    4.973751   -1.122782
 H    -3.423832   -2.304206    0.952042
 C    -2.836936   -1.573614    1.510111
 H    -0.963202   -2.500110    1.045405
 C    -3.494665   -0.517973    2.148009
 C    -1.454372   -1.677944    1.568301
 C    -2.753989    0.423914    2.868537
 C    -0.700764   -0.728626    2.273733
 H    -3.259428    1.252382    3.365249
 C    -1.370427    0.312875    2.932560
 C     0.776303   -0.779804    2.340926
 H    -0.796119    1.055473    3.491075
 H     1.236824   -0.070688    3.036691
 H     1.169398   -2.510722    1.131522
 C     1.578919   -1.685123    1.717985
 H     2.651883   -1.713139    1.929942
 O    -5.656624   -1.249113    1.438975
 C    -4.977552   -0.420000    1.995010
 H    -7.428657    0.091872    2.913307
 O    -5.471663    0.696160    2.526120
 C    -6.874929    0.897141    2.409406
 H    -7.176158    0.936058    1.352782
 H    -7.087210    1.856997    2.893121
 O    -3.602624   -4.522022   -1.665585
 C    -3.373252   -3.342029   -1.792121
 H    -5.866977   -3.388163   -0.918829
 O    -4.326674   -2.422296   -1.932448
 C    -5.672628   -2.870194   -1.868047
 H    -6.296939   -1.972120   -1.933341
 H    -5.902203   -3.548064   -2.703325
28
Figure 5_L-Cu-OtBu / electronic energy: -2105.43166785 a.u. / lowest freq: -23.37 cm-1
 H    -2.704480   -2.048822    0.818816
 H    -4.301582   -1.101667   -0.940475
 C    -2.658666   -1.043988    1.268837
 C    -4.196671   -0.108356   -0.475492
 H    -3.439797   -0.974757    2.045007
 H    -5.015485    0.023598    0.251074
 H    -1.676412   -0.941768    1.762027
 H    -4.312650    0.645511   -1.270500
 C    -2.805351    0.023588    0.167675
 C    -2.678464    1.420447    0.804762
 H    -3.458897    1.625661    1.557187
 H    -1.695054    1.520794    1.296165
 H    -2.738503    2.192609    0.020881
 O    -1.860689   -0.155323   -0.825869
 C     3.997368    0.783125    0.130748
 C     3.914366   -0.658005    0.635704
 C     2.535325    1.194497    0.096251
 H     4.429490    0.814026   -0.881402
 H     4.594999    1.436575    0.780124
 C     2.666910   -1.177468   -0.061207
 H     3.776910   -0.674927    1.727899
 H     4.802507   -1.255885    0.391071
 O     1.827463   -0.017513   -0.220858
 H     2.297263    1.943006   -0.671740
 H     2.184472    1.562885    1.074344
 H     2.115269   -1.930463    0.518555
 H     2.884068   -1.587009   -1.060647
Cu    -0.073283   -0.085163   -0.498215
70
Figure 5_ed / electronic energy: -2927.19598297 a.u. / lowest freq: 14.28 cm-1
 H    -1.175057   -3.260504   -0.875513
 H    -2.758073   -2.528487   -0.577961
 O    -0.831969   -1.279630    0.898288
 C    -1.983838   -3.164248   -0.134233
 H    -2.403083   -4.164716    0.057389
 C    -1.439752   -2.546730    1.154625
 H     0.474500   -3.570309    0.976696
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 H   -3.308769   -1.688114    1.852845
 C   -0.334327   -3.443678    1.718263
 C   -2.540690   -2.385060    2.203933
 H    0.098924   -2.999031    2.627896
 H   -0.722533   -4.442337    1.971545
 H   -2.117476   -1.970960    3.132259
 H   -3.003887   -3.357017    2.435674
Cu    0.984487   -1.242903    0.168791
 H    0.669959    4.643374    1.521621
 H    2.425783    3.393077    2.809754
 H    0.749046    2.781327    2.894655
 C    1.783144    2.519610    2.626715
 H    2.207553    4.848748    0.637258
 H    2.109677    1.707154    3.292461
 C    1.174695    4.475441    0.561298
 H    0.653825    5.070708   -0.203343
 C    1.157667    3.007406    0.169061
 C    1.875496    2.047240    1.178177
 O   -0.192783    2.521686    0.196703
 H    3.932554    2.610774    0.773896
 B   -0.189178    1.185777    0.545746
 H    3.740918    1.042499    1.591803
 C    3.312724    1.702744    0.822677
 O    1.068487    0.860624    1.067205
 H    2.675063    3.244254   -1.394788
 C    1.662300    2.835556   -1.264361
 H    0.986290    3.367235   -1.949610
 H    3.371050    1.183711   -0.142557
 H    1.670432    1.773932   -1.555875
 H   -3.864946   -1.340641   -2.304587
 H   -4.450843   -1.469203   -0.163670
 H   -2.974818   -0.387599   -3.506701
 C   -3.619981   -0.316489   -2.616867
 O   -1.747189   -0.261794   -1.137911
 H   -5.643664   -0.279988   -0.744294
 C   -4.827002   -0.446941   -0.025039
 H   -4.551587    0.188565   -2.917037
 B   -1.458479   -0.008497    0.282035
 H   -5.253886   -0.381373    0.988040
 C   -2.888981    0.458159   -1.520188
 C   -3.710563    0.596533   -0.164003
 O   -2.749982    0.379990    0.844040
 H   -1.776071    1.623721   -2.949543
 C   -2.454537    1.813189   -2.102190
 H   -3.305205    2.404818   -2.474172
 H   -1.898632    2.405668   -1.364497
 H   -5.055815    2.224942   -0.756934
 C   -4.333737    1.980105    0.038349
 H   -4.869958    2.004137    0.999953
 H   -3.565105    2.763531    0.067734
 H    3.925937   -2.905807    0.289671
 H    5.988558   -1.948788   -0.572086
 H    3.859037   -1.294296    1.066346
 C    3.914546   -1.819371    0.102686
 C    5.073285   -1.376870   -0.774980
 H    4.581688   -2.664903   -2.455034
 H    5.288929   -0.309454   -0.610680
 O    2.738029   -1.499689   -0.658096
 C    4.515218   -1.600641   -2.181044
 H    5.030876   -1.013749   -2.952708
 C    3.061263   -1.183915   -2.022280
 H    2.921481   -0.101380   -2.177043
 H    2.367160   -1.727464   -2.678136
70
Figure 5_ts(TB) / electronic energy: -2927.19056412 a.u. / lowest freq: -26.17 cm-1
 H   -1.569892   -3.716781   -0.629179
 H   -3.010279   -2.804981   -0.142745
 O   -0.692215   -1.651377    0.849583
 C   -2.214090   -3.463995    0.225980
 H   -2.671935   -4.390854    0.606459
 C   -1.398901   -2.787145    1.328881
 H    0.355236   -4.022784    1.006152
 H   -3.045730   -1.622707    2.136656
 C   -0.317582   -3.743014    1.833042
 C   -2.303874   -2.353977    2.483612
 H    0.286871   -3.255178    2.613450
 H   -0.753242   -4.662344    2.253464
 H   -1.705834   -1.874761    3.273698
 H   -2.831570   -3.216795    2.920158
Cu    1.007254   -1.058612   -0.206431
 H   -0.671057    4.362707   -0.319158
 H   -0.406165    4.317703    2.144214
 H   -1.310203    2.944934    1.427031
 C   -0.441556    3.223242    2.039293
 H    0.884488    5.169378    0.023585
 H   -0.587365    2.785506    3.038010
 C    0.409833    4.331379   -0.509824
 H    0.568529    4.483828   -1.588010
 C    1.015403    3.004514   -0.080340
 C    0.849303    2.665990    1.440897
 O    0.298743    1.932493   -0.708371
 H    2.226273    4.128932    2.262897
 B    0.236938    0.858200    0.166747
 H    1.831106    2.785331    3.359777
 C    2.037958    3.045331    2.310818
 O    0.718108    1.237236    1.412237
 H    3.080359    3.737077   -0.173842
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 C     2.466657    2.907484   -0.554382
 H     2.487645    2.940600   -1.653884
 H     2.951808    2.517470    2.007212
 H     2.922310    1.958284   -0.234434
 H    -4.165840   -1.611863   -1.763487
 H    -4.344466   -1.073229    0.341867
 H    -3.334671   -1.262479   -3.291899
 C    -3.763270   -0.803589   -2.387761
 O    -1.663105   -0.887847   -1.252578
 H    -5.327152    0.238935   -0.360964
 C    -4.444217    0.017883    0.257717
 H    -4.598209   -0.157456   -2.700795
 B    -1.144385   -0.509690    0.039023
 H    -4.626537    0.417683    1.266928
 C    -2.680210   -0.002905   -1.664529
 C    -3.170249    0.657267   -0.302370
 O    -2.120673    0.390964    0.613361
 H    -1.669707    0.448664   -3.510396
 C    -2.087006    1.005727   -2.656853
 H    -2.845647    1.701268   -3.047132
 H    -1.271798    1.579597   -2.199064
 H    -4.144851    2.427079   -1.136669
 C    -3.376074    2.168241   -0.392270
 H    -3.708614    2.557123    0.582629
 H    -2.440329    2.675800   -0.660373
 H     3.885242   -2.856640    0.678618
 H     6.009881   -1.750590    0.290632
 H     3.492020   -1.236229    1.331115
 C     3.830334   -1.782680    0.439190
 C     5.131956   -1.253926   -0.143437
 H     5.161946   -2.583722   -1.864733
 H     5.223231   -0.172190    0.040682
 O     2.856037   -1.605969   -0.607928
 C     4.956200   -1.526078   -1.637518
 H     5.601067   -0.903892   -2.272341
 C     3.483515   -1.217127   -1.843418
 H     3.306016   -0.141402   -2.009870
 H     3.013986   -1.783541   -2.659399
70
Figure 5_prod / electronic energy: -2927.22806183 a.u. / lowest freq: 30.94 cm-1
 H     3.276020    1.755768    2.085458
 H     4.029585    0.342406    2.870323
 O     2.186270   -0.435275    1.195410
 C     3.123653    0.966737    2.837008
 H     2.996757    1.447150    3.818481
 C     1.900274    0.124848    2.486768
 H     0.785061    1.788148    1.647191
 H     2.606840   -1.652978    3.520826
 C     0.653062    1.000085    2.404111
 C     1.720913   -0.998914    3.508200
 H    -0.229847    0.414028    2.115866
 H     0.455099    1.479355    3.374955
 H     0.838651   -1.609358    3.270249
 H     1.588934   -0.579495    4.516801
Cu     0.228770    1.485133   -1.025090
 H    -4.112538   -1.553581   -0.051977
 H    -4.181854   -0.522862    2.151820
 H    -2.539314   -0.725474    1.467049
 C    -3.261673    0.005224    1.860192
 H    -5.640312   -0.636108   -0.088647
 H    -2.826043    0.454346    2.765227
 C    -4.659559   -0.758976   -0.574180
 H    -4.833675   -1.092503   -1.608478
 C    -3.896862    0.557419   -0.578139
 C    -3.533059    1.111883    0.838971
 O    -2.600100    0.368422   -1.163982
 H    -5.520232    1.650713    1.532227
 B    -1.677503    1.204260   -0.531009
 H    -4.188232    2.454088    2.397674
 C    -4.528130    2.112138    1.408299
 O    -2.284734    1.770599    0.588081
 H    -5.673565    1.731530   -1.102658
 C    -4.639451    1.576641   -1.444563
 H    -4.671868    1.207454   -2.480550
 H    -4.630508    2.996419    0.765511
 H    -4.121387    2.547036   -1.449024
 H     1.991771   -4.512916   -1.086183
 H     1.305285   -4.178282    1.089125
 H     2.028714   -3.696802   -2.664482
 C     1.386498   -3.947929   -1.807071
 O     1.897198   -1.916146   -0.619569
 H    -0.018969   -5.074783    0.295167
 C     0.233316   -4.154066    0.840600
 H     0.575396   -4.596962   -2.170296
 B     1.419007   -1.323079    0.525768
 H    -0.333300   -4.149529    1.783495
 C     0.821401   -2.673747   -1.199492
 C    -0.127613   -2.905924    0.038000
 O     0.170295   -1.771803    0.874043
 H     0.952484   -1.547462   -3.030190
 C     0.185587   -1.811182   -2.286381
 H    -0.624374   -2.342022   -2.806942
 H    -0.222943   -0.877171   -1.869541
 H    -1.839210   -3.682865   -1.037073
 C    -1.606657   -2.896469   -0.302760
 H    -2.198501   -3.097093    0.603125
 H    -1.911048   -1.923653   -0.710116
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 H    2.432321    2.911576    0.379233
 H    4.814424    3.067535    0.084388
 H    2.435795    3.905435   -1.105554
 C    2.767246    2.951850   -0.669479
 C    4.265867    2.709663   -0.797740
 H    4.227949    0.676294   -0.021505
 H    4.667130    3.227209   -1.682811
 O    2.142047    1.874717   -1.388189
 C    4.340110    1.194319   -0.985670
 H    5.270678    0.859635   -1.463903
 C    3.119281    0.922303   -1.844566
 H    3.316376    1.107600   -2.914364
 H    2.707584   -0.086112   -1.715087
35
Figure 5_L-Cu-Bpin / electronic energy: -2283.43209458 a.u. / lowest freq: 22.76 cm-1
 C   -5.260784   -0.804958   -0.048387
 C   -5.293281    0.702827    0.202688
 C   -3.822883   -1.154296    0.300503
 H   -5.461222   -1.022839   -1.109055
 H   -5.982006   -1.365265    0.561542
 C   -3.925652    1.140762   -0.298992
 H   -5.392254    0.910763    1.279464
 H   -6.110637    1.215215   -0.322449
 O   -3.066752    0.016018   -0.050192
 H   -3.423178   -2.009824   -0.261794
 H   -3.693767   -1.347943    1.378172
 H   -3.518349    2.015708    0.226810
 H   -3.929468    1.348028   -1.381708
 H    3.918074   -2.331036   -1.370471
 H    3.044653   -2.685215    0.885989
 C    4.011633   -1.243679   -1.229084
 H    3.785437   -0.761043   -2.188880
 H    5.058224   -1.025183   -0.965812
 C    3.274935   -1.635891    1.123478
 O    1.710196   -0.981460   -0.555812
 H    4.311859   -1.585818    1.487812
 C    3.065519   -0.783276   -0.129730
 H    2.602602   -1.319803    1.934937
 B    0.909509    0.040051   -0.050711
 H    2.827539    1.308033   -1.930157
 C    3.096366    0.755253    0.165928
 H    4.505090    1.493845   -1.342722
 O    1.726318    1.027058    0.493965
 C    3.445075    1.593414   -1.065373
 H    5.032596    0.892059    1.143877
 H    3.662520    0.691999    2.272102
 C    3.982616    1.163690    1.333844
 H    3.245725    2.652993   -0.845764
 H    3.936580    2.254328    1.473712
Cu   -1.081618    0.054302   -0.065690
51
Figure 5_pc1 / electronic energy: -2592.77992931 a.u. / lowest freq: 19.80 cm-1
 C   -2.256774    3.463345   -0.431192
 C   -0.964310    3.621498    0.368889
 C   -2.359336    1.951731   -0.555883
 H   -2.151603    3.925033   -1.425849
 H   -3.136331    3.900786    0.060559
 C   -0.089935    2.524336   -0.218867
 H   -1.149978    3.432389    1.437780
 H   -0.505645    4.614827    0.270123
 O   -1.004772    1.492393   -0.625737
 H   -2.888892    1.615033   -1.458130
 H   -2.849043    1.503292    0.324836
 H    0.629047    2.091111    0.488878
 H    0.460418    2.871923   -1.109582
 H   -5.676984   -0.746311    2.588672
 H   -3.383318   -1.555224    3.137693
 C   -4.945900   -0.909489    1.793391
 C   -3.662044   -1.364723    2.098281
 H   -6.288335   -0.309451    0.209274
 C   -5.286130   -0.664744    0.461928
 H    3.806883    0.851812    2.963475
 C   -2.726767   -1.573405    1.086880
 H    3.339323    2.426131    1.149221
 H   -1.721630   -1.914598    1.348521
 C   -4.350837   -0.869699   -0.549184
 C   -3.055314   -1.328491   -0.258813
 C    4.148244    0.065562    2.273197
 C    3.821373    1.732685    0.443703
 H    3.843114   -0.902595    2.691533
 O    2.129854    0.123352    0.949122
 H   -4.622902   -0.668400   -1.589065
 H    4.897060    1.962555    0.422108
 H    5.248244    0.100820    2.237239
 C    3.553077    0.294290    0.891767
 C   -2.081819   -1.500124   -1.354858
 B    1.675215   -0.432739   -0.250510
 H   -0.770223   -2.976838   -0.455773
 C   -0.964611   -2.314877   -1.305308
 C    3.963814   -0.765570   -0.184787
 H    3.380132   -2.454174    1.070867
 O    2.778964   -0.848681   -0.990382
 H    5.146910   -2.200649    0.978994
 H    6.045763   -0.202919   -0.452861
 C    4.206571   -2.154236    0.409567
 H   -0.430332   -2.563326   -2.226796
 C    5.142126   -0.365884   -1.060517
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 H    4.263842   -2.887605   -0.408580
 H    5.360789   -1.167524   -1.782183
Cu   -0.308706   -0.453469   -0.786896
 H   -2.387415   -1.092374   -2.325327
 H    3.402583    1.921309   -0.556069
 H    4.933966    0.549522   -1.630194
51
Figure 5_ts(CuBadd) / electronic energy: -2592.76023309 a.u. / lowest freq: -243.36 cm-1
 C   -3.274010    3.045404    0.166244
 C   -2.040626    3.418120    0.989909
 C   -2.852817    1.722993   -0.447858
 H   -3.457199    3.796108   -0.618400
 H   -4.186385    2.945347    0.769088
 C   -0.900267    2.974330    0.087388
 H   -2.024686    2.848931    1.932116
 H   -1.982754    4.488080    1.230706
 O   -1.431755    1.860471   -0.659073
 H   -3.320255    1.501649   -1.416693
 H   -3.029723    0.876766    0.236361
 H   -0.009072    2.634720    0.632701
 H   -0.605406    3.756413   -0.630012
 H   -4.677471   -2.053880    2.563563
 H   -2.244858   -1.677970    3.015210
 C   -3.960773   -1.989858    1.741637
 C   -2.602910   -1.780001    1.986088
 H   -5.438382   -2.299468    0.191032
 C   -4.380809   -2.124196    0.410705
 H    3.073614   -0.542635    3.184159
 C   -1.683329   -1.696108    0.941683
 H    2.496810    1.693014    2.329624
 H   -0.630683   -1.518346    1.179820
 C   -3.475928   -2.038968   -0.637669
 C   -2.089739   -1.805165   -0.418609
 C    3.592133   -0.829062    2.257111
 C    3.164306    1.506960    1.475318
 H    3.405780   -1.896593    2.082082
 O    1.711723   -0.284882    0.848383
 H   -3.834811   -2.139509   -1.666815
 H    4.182561    1.805460    1.764393
 H    4.671445   -0.680754    2.413140
 C    3.094098    0.026094    1.103154
 C   -1.178530   -1.628587   -1.522195
 B    1.490323   -0.180556   -0.511399
 H    0.697845   -2.170276   -0.515632
 C    0.285688   -1.555114   -1.333531
 C    3.758001   -0.288004   -0.283097
 H    3.302515   -2.423883   -0.163683
 O    2.672694   -0.032332   -1.200036
 H    5.008609   -2.024968    0.170871
 H    5.738004    0.501314    0.107704
 C    4.134920   -1.760064   -0.442124
 H    0.856298   -1.719718   -2.255331
 C    4.938805    0.597797   -0.642850
 H    4.382334   -1.953380   -1.496296
 H    5.350222    0.294050   -1.616858
Cu   -0.410252    0.267390   -1.129870
 H   -1.556408   -1.818636   -2.530618
 H    2.837081    2.146469    0.641887
 H    4.650096    1.654684   -0.712889
51
Figure 5_L-Cu-alkyl_01 / electronic energy: -2592.82066847 a.u. / lowest freq: 22.24 cm-1
 C   -2.086400    4.567242    0.310620
 C   -0.710788    4.578244    0.977216
 C   -2.386083    3.080683    0.226005
 H   -2.029335    5.004660   -0.698252
 H   -2.851141    5.111855    0.880344
 C   -0.030041    3.374599    0.341804
 H   -0.810543    4.432148    2.063754
 H   -0.151555    5.507389    0.804409
 O   -1.099935    2.461592    0.044109
 H   -3.028278    2.801796   -0.621167
 H   -2.835733    2.692867    1.154802
 H    0.681788    2.872597    1.011943
 H    0.482957    3.632441   -0.598489
 H   -4.135789   -3.813998    2.045288
 H   -1.654787   -4.103883    2.059166
 C   -3.509681   -3.279270    1.326940
 C   -2.124760   -3.437725    1.329359
 H   -5.165587   -2.285867    0.349438
 C   -4.080640   -2.423249    0.378696
 H    3.063619   -2.153180    2.587720
 C   -1.320355   -2.758757    0.411312
 H    1.119330   -0.673749    2.457172
 H   -0.237739   -2.888715    0.457819
 C   -3.280681   -1.745765   -0.533847
 C   -1.872486   -1.884047   -0.547794
 C    3.600155   -1.625550    1.785117
 C    1.688214   -0.014029    1.785780
 H    4.161300   -2.371206    1.206747
 O    1.777160   -1.799085    0.211694
 H   -3.748891   -1.077373   -1.264287
 H    2.248416    0.706151    2.399193
 H    4.316023   -0.933152    2.253737
 C    2.612727   -0.865305    0.915582
 C   -1.057791   -1.114487   -1.529748
 B    1.462136   -1.245745   -1.006853
 H    0.248606   -2.842498   -1.971171
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 C    0.303189   -1.735723   -1.939986
 C    3.261558   -0.057103   -0.266362
 H    4.381112   -1.777189   -1.014845
 O    2.259986   -0.163658   -1.291773
 H    5.372330   -0.603854   -0.103625
 H    4.188373    1.526095    0.894144
 C    4.533719   -0.707681   -0.807267
 H    0.538008   -1.406460   -2.965725
 C    3.512085    1.411761    0.033590
 H    4.812878   -0.215491   -1.750429
 H    3.982689    1.895972   -0.835022
Cu   -0.962947    0.673168   -0.746352
 H   -1.675969   -0.980232   -2.435433
 H    0.958235    0.534608    1.169686
 H    2.575117    1.941306    0.247211
51
Figure 5_L-Cu-alkyl_02 / electronic energy: -2592.81753394 a.u. / lowest freq: 23.37 cm-1
 C    6.449872    0.193421    0.318570
 C    6.318965   -1.295661    0.640087
 C    4.999307    0.649659    0.311017
 H    6.903289    0.334212   -0.674896
 H    7.051821    0.746214    1.052083
 C    5.072005   -1.683517   -0.138505
 H    6.157325   -1.444298    1.719036
 H    7.195271   -1.885326    0.338925
 O    4.256756   -0.499727   -0.132541
 H    4.795739    1.480985   -0.378391
 H    4.647454    0.928711    1.317603
 H    4.500707   -2.504098    0.317377
 H    5.300736   -1.946690   -1.184340
 B   -1.947471   -1.189567    0.048124
 O   -2.756359   -1.202361    1.155649
 O   -2.639331   -0.856333   -1.089321
 C   -4.115885   -1.010812    0.725185
 C   -3.927061   -0.355084   -0.694141
 C   -4.838939   -0.136320    1.737309
 C   -4.767190   -2.391372    0.663782
 C   -3.817670    1.168690   -0.641705
 C   -4.964035   -0.768510   -1.726369
 H   -3.073322    1.494762    0.099431
 H   -4.783588    1.637140   -0.403014
 H   -3.491328    1.536548   -1.625481
 H   -4.951072   -1.851408   -1.906917
 H   -4.759284   -0.263866   -2.682338
 H   -5.974542   -0.478963   -1.400034
 H   -4.266851   -3.039112   -0.071329
 H   -5.833774   -2.326303    0.404560
 H   -4.682211   -2.872112    1.649636
 H   -5.854647    0.103310    1.387433
 H   -4.300150    0.802243    1.921725
 H   -4.927623   -0.669815    2.695590
 C   -0.034756    2.095508   -1.154509
 C   -0.410591    3.382903   -0.784162
 C    0.003439    1.031396   -0.227348
 C   -0.768112    3.667217    0.537445
 C   -0.359420    1.343532    1.100052
 C   -0.736662    2.633589    1.473667
 C    0.395414   -0.344508   -0.647878
 C   -0.398529   -1.468602    0.065483
 H   -1.012453    2.830879    2.513726
 H   -0.350402    0.557480    1.858944
 H   -1.067360    4.676839    0.829119
 H   -0.434385    4.174508   -1.538624
 H    0.229124    1.892831   -2.197565
Cu    2.320687   -0.458151   -0.414786
 H   -0.067783   -1.629751    1.105619
 H   -0.199531   -2.427191   -0.446589
 H    0.196842   -0.425313   -1.731281
51
Figure 5_L-Cu-alkyl_03 / electronic energy: -2592.82107598 a.u. / lowest freq: 22.07 cm-1
 B   -1.498250   -1.589961   -0.373127
 O   -2.215679   -0.836160   -1.270258
 O   -2.157618   -1.730740    0.821537
 C   -3.296782   -0.211465   -0.556690
 C   -3.470892   -1.164253    0.684724
 C   -4.512035   -0.119960   -1.465375
 C   -2.820312    1.189088   -0.174712
 C   -4.437817   -2.317118    0.421626
 C   -3.843659   -0.455235    1.977522
 H   -4.196945   -2.839922   -0.515999
 H   -5.479575   -1.968900    0.368551
 H   -4.361120   -3.045494    1.242362
 H   -3.075827    0.269197    2.279146
 H   -3.950460   -1.191461    2.788014
 H   -4.803590    0.071988    1.869464
 H   -1.931433    1.143129    0.474053
 H   -3.603280    1.764514    0.339759
 H   -2.541345    1.728604   -1.091343
 H   -5.380795    0.272714   -0.915752
 H   -4.777882   -1.096964   -1.889305
 H   -4.301617    0.564954   -2.300357
 C    3.291182   -1.480709    1.134380
 C    4.649643   -1.737304    0.996299
 C    2.367023   -1.742361    0.095433
 C    5.155071   -2.272383   -0.194241
 C    2.897604   -2.298540   -1.085447
 C    4.264202   -2.550806   -1.228698
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 C    0.923405   -1.418039    0.275227
 C   -0.064266   -2.153382   -0.650712
 H    4.634214   -2.978849   -2.165035
 H    2.229405   -2.537401   -1.915958
 H    6.223349   -2.471418   -0.307859
 H    5.327213   -1.517898    1.826592
 H    2.917477   -1.052179    2.070441
Cu    0.762839    0.525407    0.166891
 H   -0.020868   -3.253209   -0.507750
 H    0.166981   -1.967479   -1.712675
 H    0.654233   -1.635842    1.325438
 H   -0.141567    2.783176   -1.691571
 H    1.611632    4.451738   -1.684511
 C    0.014282    3.327288   -0.749852
 C    0.854649    4.585298   -0.896031
 H    2.785780    2.899705    0.366269
 H    0.244923    5.463281   -1.148494
 O    0.765703    2.489674    0.145898
 H   -0.965641    3.538078   -0.292273
 C    1.822003    3.226865    0.789225
 C    1.523735    4.684022    0.474833
 H    2.433157    5.299627    0.473997
 H    1.806985    2.989797    1.862379
 H    0.824058    5.101281    1.215752
51
Figure 5_ts(BHE) / electronic energy: -2592.76459029 a.u. / lowest freq: -958.21 cm-1
 B   -2.077416   -0.379925   -0.354524
 O   -3.123566   -0.568053   -1.212795
 O   -2.464956    0.130751    0.853344
 C   -4.282788    0.060622   -0.627881
 C   -3.905255    0.094828    0.899664
 C   -5.516793   -0.761969   -0.959838
 C   -4.393319    1.452745   -1.246411
 C   -4.295090   -1.181317    1.642529
 C   -4.410421    1.315605    1.651075
 H   -3.947491   -2.079446    1.110555
 H   -5.383475   -1.255305    1.778903
 H   -3.823721   -1.173674    2.636076
 H   -4.002356    2.246050    1.235131
 H   -4.109016    1.253879    2.707287
 H   -5.509149    1.365868    1.614329
 H   -3.507890    2.065492   -1.018740
 H   -5.287825    1.983460   -0.890602
 H   -4.464456    1.353645   -2.339477
 H   -6.402090   -0.355461   -0.448129
 H   -5.395562   -1.814031   -0.670624
 H   -5.705441   -0.728266   -2.043007
 C    2.266054   -2.444108    1.180248
 C    3.498499   -3.055113    0.991103
 C    1.552025   -1.846090    0.107775
 C    4.088452   -3.110235   -0.277928
 C    2.165586   -1.922826   -1.171142
 C    3.403365   -2.537456   -1.351095
 C    0.293809   -1.170876    0.345262
 C   -0.594319   -0.713384   -0.720023
 H    3.840997   -2.568392   -2.353405
 H    1.667691   -1.476894   -2.036713
 H    5.057784   -3.592097   -0.424362
 H    4.010553   -3.500927    1.849118
 H    1.828877   -2.410822    2.182936
Cu    0.722468    0.764553   -0.298971
 H   -0.495236   -1.215975   -1.691723
 H   -0.423190    0.670195   -1.419134
 H   -0.093126   -1.174174    1.368654
 H    2.423927    2.892235   -1.605990
 H    4.705549    2.235747   -1.174680
 C    2.768919    2.983738   -0.567197
 C    4.278122    2.901337   -0.408722
 H    3.593661    0.307025    0.519494
 H    4.758604    3.884797   -0.498589
 O    2.259357    1.864349    0.183524
 H    2.353569    3.907748   -0.133654
 C    3.295510    1.260208    0.986503
 C    4.425243    2.274837    0.978358
 H    5.403172    1.801893    1.139175
 H    2.876227    1.053268    1.980501
 H    4.272645    3.032125    1.763185
51
Figure 5_pc2 / electronic energy: -2592.80440429 a.u. / lowest freq: -3.31 cm-1
 B   -1.960789   -0.666730   -0.256467
 O   -3.026608   -0.819707   -1.097813
 O   -2.301034   -0.087692    0.936967
 C   -4.125880   -0.071859   -0.538573
 C   -3.738184   -0.003791    0.986037
 C   -5.424885   -0.804074   -0.829999
 C   -4.122282    1.295784   -1.218007
 C   -4.227480   -1.210763    1.784292
 C   -4.137623    1.285464    1.684499
 H   -3.961049   -2.156488    1.289301
 H   -5.317172   -1.186399    1.929118
 H   -3.749333   -1.200025    2.774686
 H   -3.657031    2.159970    1.226987
 H   -3.835820    1.245182    2.741714
 H   -5.228685    1.424474    1.648245
 H   -3.183285    1.836446   -1.027181
 H   -4.964831    1.917778   -0.883244
 H   -4.210779    1.153676   -2.304999
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 H   -6.270976   -0.302734   -0.336198
 H   -5.389590   -1.847947   -0.491472
 H   -5.615846   -0.804869   -1.913297
 C    2.583005   -2.119498    1.272440
 C    3.850635   -2.682162    1.141216
 C    1.840403   -1.740497    0.143643
 C    4.405954   -2.870496   -0.124891
 C    2.410552   -1.936247   -1.125105
 C    3.679580   -2.494533   -1.256640
 C    0.510176   -1.121502    0.325512
 C   -0.518771   -1.131565   -0.604707
 H    4.108912   -2.632270   -2.251978
 H    1.862624   -1.632149   -2.020633
 H    5.401330   -3.308168   -0.230881
 H    4.409839   -2.972805    2.033959
 H    2.155236   -1.968089    2.267301
Cu    0.413747    0.678868   -0.756709
 H   -0.361437   -1.636152   -1.565842
 H   -0.251780    1.602415   -1.870120
 H    0.272386   -0.830401    1.356796
 H    2.287397    2.931346   -1.679662
 H    4.516154    2.885251   -0.758308
 C    2.359273    2.996969   -0.585446
 C    3.759714    3.306284   -0.077680
 H    3.660505    0.536702    0.489568
 H    3.939336    4.386316    0.009409
 O    2.031549    1.714024   -0.026419
 H    1.617762    3.731784   -0.231484
 C    3.010692    1.307290    0.937304
 C    3.784433    2.573900    1.263168
 H    4.798051    2.360108    1.628423
 H    2.490791    0.869359    1.800421
 H    3.255466    3.158909    2.031992
72
Figure 5_pc3 / electronic energy: -3431.66328451 a.u. / lowest freq: 14.43 cm-1
 C    1.010408   -1.143332   -0.590910
 C    1.263723   -0.932946    0.753021
 C    2.339120    0.005257    1.224145
 O    3.630457   -0.636774    1.283409
 P    4.446061   -0.892539   -0.069041
 O    4.256453    0.083785   -1.161983
 O    5.910541   -1.007292    0.570115
 O    4.083142   -2.377481   -0.557906
 C    7.018324   -1.277274   -0.284121
 H    0.451738   -2.021463   -0.929205
 H    1.594996   -0.624049   -1.358184
 H    0.886351   -1.649188    1.492322
 H    2.414123    0.888098    0.569856
 H    2.146537    0.345955    2.248578
 B   -3.333918   -0.481167   -0.853760
 O   -3.776878   -0.811543    0.408715
 O   -3.183692   -1.589659   -1.645283
 C   -3.618829   -2.232543    0.566885
 C   -3.673320   -2.733457   -0.923223
 C   -4.720646   -2.768025    1.465107
 C   -2.251766   -2.449272    1.214132
 C   -5.095886   -3.001936   -1.410122
 C   -2.780807   -3.927203   -1.224402
 H   -5.763263   -2.155663   -1.188883
 H   -5.517431   -3.908512   -0.952351
 H   -5.079318   -3.144443   -2.500664
 H   -1.723328   -3.701391   -1.033331
 H   -2.880462   -4.207914   -2.283332
 H   -3.070719   -4.795571   -0.613428
 H   -1.451222   -2.061708    0.565712
 H   -2.055538   -3.511394    1.418863
 H   -2.210336   -1.901234    2.167388
 H   -4.665193   -3.864893    1.534037
 H   -5.717181   -2.489398    1.098450
 H   -4.605964   -2.357918    2.479579
 C    0.572241    2.457739   -1.972140
 C    1.234884    3.678304   -1.985346
 C   -0.782037    2.338646   -1.567770
 C    0.573180    4.853992   -1.609147
 C   -1.437181    3.544757   -1.239964
 C   -0.770847    4.772372   -1.250364
 C   -1.411937    1.003045   -1.438937
 C   -2.939829    0.972990   -1.269875
 H   -1.318042    5.679652   -0.977160
 H   -2.492997    3.525021   -0.962431
 H    1.094880    5.813895   -1.612003
 H    2.284795    3.715197   -2.290160
 H    1.117132    1.552758   -2.259013
Cu   -0.329400    0.209213    0.090635
 H   -3.474264    1.317732   -2.179051
 H   -3.257098    1.642232   -0.452802
 H   -1.119678    0.376533   -2.298549
 H    7.915961   -1.294685    0.346179
 H    7.125636   -0.491751   -1.047399
 H    6.908177   -2.253606   -0.782046
 C    4.054495   -3.473897    0.345087
 H    3.901834   -4.381997   -0.251310
 H    3.227994   -3.370647    1.064737
 H    5.002806   -3.562818    0.897939
 H   -1.971063    1.044062    3.417643
 H   -0.828862    3.603090    3.684226
 H   -3.138933    3.158320    3.050836
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 C   -2.004209    1.413845    2.377317
 H    0.906218    2.473615    2.511381
 C   -1.013412    3.552308    2.600186
 O   -0.687974    1.341524    1.815774
 C   -2.362867    2.887231    2.322242
 H   -2.665133    0.761111    1.790627
 C   -0.017144    2.608364    1.928172
 H   -0.942518    4.570685    2.194113
 H   -2.722585    3.147810    1.315939
 H    0.252891    2.946939    0.916357
72
Figure 5_ts(AS)_01 / electronic energy: -3431.62747806 a.u. / lowest freq: -242.03 cm-1
 C    0.541084   -1.330169   -0.220517
 C    0.818266   -1.254836    1.185889
 C    1.724124   -0.325065    1.684133
 O    3.697270   -1.092990    1.648406
 P    4.231484   -1.060583    0.221125
 O    3.562569   -0.228468   -0.830974
 O    5.810459   -0.670492    0.382995
 O    4.310949   -2.590518   -0.355469
 C    6.611918   -0.584709   -0.773310
 H   -0.135396   -2.102533   -0.596644
 H    1.331601   -1.010120   -0.908009
 H    0.322240   -1.938996    1.881165
 H    2.112517    0.459746    1.033761
 H    1.818760   -0.171755    2.758837
 B   -3.032939   -0.580232   -1.187052
 O   -3.960129   -0.588495   -0.174376
 O   -2.644412   -1.840998   -1.546772
 C   -3.981496   -1.917754    0.381628
 C   -3.452535   -2.786767   -0.819654
 C   -5.390939   -2.253734    0.837389
 C   -3.026094   -1.894389    1.573498
 C   -4.561872   -3.248432   -1.761694
 C   -2.587787   -3.968252   -0.410551
 H   -5.208190   -2.411721   -2.066123
 H   -5.188893   -4.023701   -1.298786
 H   -4.106962   -3.671746   -2.669162
 H   -1.703337   -3.652243    0.158132
 H   -2.241218   -4.503526   -1.306713
 H   -3.164967   -4.673208    0.206432
 H   -2.016243   -1.585568    1.258499
 H   -2.956654   -2.871445    2.071772
 H   -3.385429   -1.159525    2.308751
 H   -5.444974   -3.294036    1.191934
 H   -6.123566   -2.120201    0.030870
 H   -5.680179   -1.596356    1.670559
 C    1.234268    2.072605   -1.565761
 C    1.932508    3.275481   -1.526580
 C   -0.178813    2.044641   -1.606196
 C    1.251751    4.496235   -1.534332
 C   -0.843660    3.284242   -1.636063
 C   -0.140614    4.489337   -1.598753
 C   -0.900646    0.739064   -1.546364
 C   -2.414705    0.744233   -1.754653
 H   -0.691689    5.433451   -1.621464
 H   -1.933023    3.315253   -1.693769
 H    1.801107    5.439881   -1.496885
 H    3.024632    3.254608   -1.480633
 H    1.807278    1.139977   -1.526605
Cu   -0.406670    0.264857    0.339037
 H   -2.659076    0.884070   -2.825753
 H   -2.890491    1.580329   -1.218761
 H   -0.425147    0.008884   -2.212220
 H    7.614809   -0.255036   -0.465853
 H    6.204751    0.142308   -1.495478
 H    6.704509   -1.561326   -1.279474
 C    4.824617   -3.607767    0.473681
 H    4.728343   -4.563104   -0.062068
 H    4.268865   -3.672068    1.423323
 H    5.891111   -3.443209    0.706668
 H   -2.735224    1.640026    2.846228
 H   -1.407095    4.057291    3.309304
 H   -3.520520    3.846576    2.127268
 C   -2.494379    1.943682    1.812671
 H    0.382943    2.626855    2.676616
 C   -1.317860    3.957505    2.217107
 O   -1.101648    1.692604    1.570257
 C   -2.632094    3.441623    1.624434
 H   -3.082774    1.329000    1.118689
 C   -0.312171    2.864112    1.857213
 H   -1.017367    4.932079    1.809881
 H   -2.698139    3.681263    0.552690
 H    0.271266    3.108404    0.957509
72
Figure 5_ts(AS)_02 / electronic energy: -3431.62868825 a.u. / lowest freq: -257.55 cm-1
 C   -0.323165   -1.633665   -1.016951
 C    0.073933   -2.343584    0.155606
 C    1.034564   -1.854972    1.031573
 O    2.929969   -2.677866    0.538975
 P    3.695617   -1.659967   -0.297182
 O    3.073067   -0.983633   -1.475690
 O    4.204054   -0.543159    0.800836
 O    5.101219   -2.334440   -0.780391
 C    4.971240    0.550085    0.355742
 H   -1.010172   -2.114330   -1.717884
 H    0.371456   -0.899258   -1.447074
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 H   -0.416829   -3.292032    0.395510
 H    1.457231   -0.859324    0.901008
 H    1.156967   -2.307864    2.014111
 B   -1.040652    1.803776   -1.668028
 O    0.267763    1.665823   -2.036000
 O   -1.235185    2.877292   -0.832841
 C    1.050877    2.544555   -1.202745
 C   -0.005423    3.633778   -0.800985
 C    2.242087    3.048961   -1.997504
 C    1.525063    1.712653   -0.014341
 C   -0.136534    4.750070   -1.834035
 C    0.188147    4.221509    0.586562
 H   -0.258988    4.345250   -2.849763
 H    0.741331    5.412201   -1.826002
 H   -1.025032    5.354858   -1.600010
 H    0.155151    3.449858    1.366091
 H   -0.604161    4.954706    0.798649
 H    1.157025    4.738938    0.652479
 H    0.669245    1.372318    0.591989
 H    2.202170    2.282424    0.638276
 H    2.060568    0.833645   -0.402471
 H    2.830974    3.764921   -1.404496
 H    1.933787    3.535104   -2.932446
 H    2.890280    2.198301   -2.254252
 C   -4.317591   -1.470735    0.220127
 C   -5.206164   -2.539278    0.159499
 C   -3.581809   -1.056336   -0.910703
 C   -5.395106   -3.232528   -1.039381
 C   -3.791371   -1.762500   -2.108735
 C   -4.682694   -2.834800   -2.169698
 C   -2.612886    0.065603   -0.787714
 C   -2.164787    0.783210   -2.057912
 H   -4.824684   -3.360627   -3.117585
 H   -3.254017   -1.468238   -3.012914
 H   -6.095554   -4.069327   -1.090528
 H   -5.762033   -2.831724    1.054360
 H   -4.181207   -0.936510    1.166063
Cu   -1.176706   -0.644045    0.421359
 H   -3.022558    1.288759   -2.542317
 H   -1.752370    0.078351   -2.796430
 H   -3.010360    0.799919   -0.067909
 H    5.041774    1.277283    1.178063
 H    4.511763    1.043348   -0.516813
 H    5.993817    0.240416    0.076279
 C    5.861018   -3.083193    0.141309
 H    6.787600   -3.395275   -0.361452
 H    5.317997   -3.981304    0.477942
 H    6.128427   -2.486691    1.030952
 H    0.367684    0.030462    3.240637
 H   -0.567766    2.670075    3.425821
 H   -0.534362    1.029546    5.256564
 C   -0.717169   -0.088955    3.393099
 H   -1.835487    2.163722    1.423726
 C   -1.510714    2.131667    3.610320
 O   -1.392201    0.282848    2.174013
 C   -1.250839    0.874120    4.439129
 H   -0.937249   -1.144929    3.601228
 C   -2.055591    1.558708    2.314153
 H   -2.217938    2.827930    4.080157
 H   -2.189657    0.492351    4.869176
 H   -3.141338    1.379525    2.370014
72
Figure 5_pi-allyl / electronic energy: -3431.66797676 a.u. / lowest freq: 24.27 cm-1
 C   -0.083301    0.083360   -2.274188
 C   -1.102079   -0.975871   -2.340474
 C   -0.846681   -2.293377   -2.388363
 O    1.698408   -1.408121   -0.457922
 P    3.083634   -1.149194   -1.062056
 O    3.235243   -0.579295   -2.430007
 O    3.822358   -0.218808    0.066165
 O    3.913407   -2.544187   -0.984039
 C    5.052448    0.402731   -0.242338
 H   -0.410995    1.028277   -2.712242
 H    0.920706   -0.200847   -2.620546
 H   -2.141691   -0.632990   -2.319019
 H    0.180825   -2.669817   -2.375260
 H   -1.656668   -3.027101   -2.435922
 B   -2.880348    0.960051    0.359457
 O   -3.569767    0.181028    1.248511
 O   -3.450777    0.966609   -0.883414
 C   -4.575043   -0.549282    0.514811
 C   -4.745418    0.336432   -0.774996
 C   -5.823816   -0.672833    1.371633
 C   -3.997470   -1.932017    0.221546
 C   -5.768856    1.456457   -0.596910
 C   -5.039338   -0.441969   -2.046262
 H   -5.583391    2.028430    0.324618
 H   -6.795053    1.064004   -0.561290
 H   -5.695476    2.150814   -1.446706
 H   -4.259500   -1.180379   -2.271796
 H   -5.110143    0.250742   -2.897628
 H   -6.000506   -0.969899   -1.956224
 H   -3.085254   -1.867483   -0.389752
 H   -4.724838   -2.568770   -0.302150
 H   -3.736489   -2.423299    1.170507
 H   -6.639673   -1.141701    0.801383
 H   -6.167327    0.303412    1.737504
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 H   -5.612537   -1.307281    2.245142
 C    1.632475    2.950667   -0.973521
 C    2.855394    3.548653   -0.695892
 C    0.773535    2.531608    0.063016
 C    3.256927    3.746885    0.628356
 C    1.190472    2.743563    1.387564
 C    2.418434    3.343640    1.665627
 C   -0.505139    1.840187   -0.277661
 C   -1.607618    1.787580    0.763983
 H    2.718964    3.497602    2.704915
 H    0.547662    2.434565    2.213288
 H    4.219770    4.214672    0.846541
 H    3.505032    3.859849   -1.517380
 H    1.334795    2.784802   -2.012199
Cu    0.363940    0.064422   -0.362543
 H   -1.960527    2.826875    0.929199
 H   -1.243296    1.429523    1.735313
 H   -0.894866    2.201200   -1.231602
 H    5.283275    1.110795    0.565483
 H    4.994564    0.948245   -1.196814
 H    5.867788   -0.338135   -0.308317
 C    3.885405   -3.324831    0.190611
 H    4.634118   -4.122250    0.081012
 H    2.897066   -3.788314    0.342179
 H    4.142465   -2.728243    1.082000
 H   -0.547311   -2.156135    1.055771
 H    1.915598   -2.556493    2.281969
 H   -0.267171   -3.225076    3.204434
 C   -0.589263   -1.482132    1.928434
 H    2.336225   -0.228898    1.832325
 C    1.471289   -1.873072    3.020540
 O    0.275478   -0.357064    1.684717
 C   -0.023752   -2.154366    3.168494
 H   -1.615223   -1.105989    2.042905
 C    1.475298   -0.455456    2.474098
 H    2.029206   -1.959283    3.963102
 H   -0.420452   -1.679251    4.079621
 H    1.415067    0.292625    3.282203
98
Figure 8_L3a-Cu-OtBu / electronic energy: -4500.61984018 a.u. / lowest freq: -20.29 cm-1
 P   -1.580542    0.896725    0.507317
 C   -2.908207    3.157185   -0.383641
 C   -4.006725    3.985801   -0.616704
 C   -3.065934    1.952882    0.310453
 C   -5.267815    3.615698   -0.152099
 C   -4.334988    1.587341    0.777167
 C   -5.430677    2.415956    0.544998
 C   -2.523549   -1.468960    3.766793
 C   -2.433956   -0.995007    2.458931
 C   -1.750721    0.195213    2.185586
 C   -1.940215   -0.754291    4.813269
 C   -1.270557    0.441252    4.550950
 C   -1.173132    0.911691    3.242472
 C   -2.488216   -0.166613   -2.032914
 C   -1.872393   -0.448550   -0.671022
 C   -1.299140   -1.669779   -0.734533
 C   -1.272709    0.069693   -2.972172
 C   -0.635837   -1.334154   -3.044849
 C   -1.568682   -2.215154   -2.148736
 C   -1.395589   -3.700880   -2.383493
 C   -2.968758   -1.580997   -2.446504
 C   -3.416732   -1.695439   -3.906676
 C   -4.117793   -2.103832   -1.580032
 C   -0.402948   -2.359373    0.224528
 C   -0.776860   -3.505808    0.883773
 C    0.975407   -1.984659    0.502411
 S    0.536953   -4.140203    1.811096
 C    1.617684   -2.882805    1.327412
 C   -2.109087   -4.184545    0.927504
 C    3.027464   -2.915300    1.833201
 P    1.678909   -0.407382   -0.087965
 C    3.102106    0.859929    3.522479
 C    2.302495    0.358977    2.498979
 C    4.452175    1.127830    3.286856
 C    2.843742    0.105397    1.231146
 C    4.993844    0.884481    2.025620
 C    4.195075    0.374971    1.000685
 C    3.810868    0.068843   -3.514968
 C    3.023741    0.281283   -2.383591
 C    4.288299   -1.209367   -3.809490
 C    2.730665   -0.792862   -1.528752
 C    3.979451   -2.281011   -2.970507
 C    3.204103   -2.074442   -1.829949
 H   -1.915778    3.440512   -0.746059
 H   -3.873260    4.924573   -1.159108
 H   -6.129053    4.263617   -0.331942
 H   -4.472168    0.649243    1.321329
 H   -6.418530    2.124936    0.910059
 H   -3.052633   -2.403325    3.968939
 H   -2.893523   -1.557737    1.644298
 H   -2.009117   -1.130195    5.836777
 H   -0.813928    1.005846    5.367081
 H   -0.634680    1.841763    3.037295
 H   -3.246522    0.627518   -2.056758
 H   -0.589719    0.827995   -2.558260
 H   -1.599587    0.429651   -3.958197
 H    0.397965   -1.358219   -2.675070
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 H   -0.612264   -1.725800   -4.072823
 H   -1.570304   -3.939191   -3.444195
 H   -2.092416   -4.304994   -1.785566
 H   -0.372211   -4.024525   -2.136174
 H   -4.283813   -1.039932   -4.086553
 H   -3.735264   -2.726536   -4.127997
 H   -2.643849   -1.427048   -4.637860
 H   -5.049987   -1.574746   -1.833824
 H   -3.945257   -1.962235   -0.505502
 H   -4.291685   -3.176350   -1.763069
 H   -2.830286   -3.652783    0.295310
 H   -2.511139   -4.201379    1.953149
 H   -2.051970   -5.227314    0.578596
 H    3.133815   -2.345375    2.769850
 H    3.720647   -2.481976    1.101170
 H    3.345945   -3.948938    2.031729
 H    2.665823    1.045999    4.506885
 H    1.245355    0.156678    2.688849
 H    5.080940    1.527152    4.086046
 H    6.049214    1.091790    1.833772
 H    4.633959    0.190791    0.017398
 H    4.040865    0.905396   -4.179302
 H    2.611508    1.276687   -2.160485
 H    4.894279   -1.374226   -4.703735
 H    4.343260   -3.284201   -3.205138
 H    2.955927   -2.917868   -1.180520
Cu    0.417430    1.531952   -0.315265
 H    1.533422    5.234717   -2.570756
 H    2.752520    5.897866   -1.444814
 H    3.117535    4.440494   -2.410028
 C    2.325100    4.966405   -1.852792
 H   -0.149226    5.110504   -0.667688
 C    1.752337    4.045194   -0.761300
 H    1.046191    5.717534    0.511698
 O    1.233972    2.914790   -1.363084
 C    0.662151    4.810177    0.015323
 H    3.662168    3.098170   -0.312532
 H    3.360480    4.550221    0.683303
 C    2.883951    3.670816    0.217078
 H    0.224040    4.154997    0.787863
 H    2.491679    3.029307    1.024769
39
Figure 8_para-NMe2-styrene-Cu-OtBu / electronic energy: -2316.39314463 a.u. / lowest freq: 15.08 cm-1
 C   -0.498289   -1.681031   -0.152427
 C   -1.237584   -1.347445   -1.296960
 C   -0.972772   -1.195660    1.077755
 C   -2.117048   -0.420108    1.164329
 C   -2.866748   -0.083896    0.006808
 C   -2.387165   -0.574274   -1.233136
 H   -0.433126   -1.421984    2.000711
 H   -2.433199   -0.070901    2.146691
 H   -2.914625   -0.347791   -2.159106
 H   -0.893051   -1.698055   -2.274189
 C    0.753302   -2.444880   -0.295478
 C    1.630903   -2.802337    0.703754
 H    0.930584   -2.850613   -1.299387
 H    1.426444   -2.608632    1.761807
 H    2.439541   -3.506045    0.485823
 H    4.298713    2.871785    0.015425
 H    3.509208    2.904737   -1.577772
 C    3.326495    2.970794   -0.493313
 O    2.994493    0.630073   -0.377034
 H    2.916786    3.969814   -0.270799
 C    2.389030    1.833825   -0.053365
 H    3.101309    1.791959    2.002391
 H    1.185507    1.850956   -1.864681
 C    2.150477    1.936142    1.464495
 C    1.038819    1.982646   -0.780483
 H    1.722253    2.906564    1.767228
 H    0.565379    2.964444   -0.610641
 H    1.455039    1.143091    1.789784
 H    0.332986    1.204281   -0.442150
Cu    2.180374   -0.979899   -0.070442
 H   -3.715353    1.862691    1.825944
 H   -5.384116    1.738855    1.224422
 C   -4.451297    1.180414    1.364695
 H   -4.655702    0.366484    2.081475
 H   -4.116738    1.611727   -1.816209
 N   -4.001101    0.675892    0.086451
 H   -5.608480    1.615344   -0.849938
 C   -4.728955    1.017009   -1.115351
 H   -5.083448    0.119332   -1.650825
78
Figure 8_para-NMe2-styrene-Cu-OtBu_dimer_01 / electronic energy: -4632.85611567 a.u. / lowest freq: 17.08 cm-1
 H   -7.925765    0.715391   -1.021346
 C   -8.200771   -0.269158   -0.603696
 H   -9.148271   -0.146730   -0.065705
 H   -6.965867   -0.469431    2.390185
 N   -7.195446   -0.774753    0.301890
 H   -8.382134   -0.955525   -1.450269
 H   -8.606424   -0.865389    1.833140
 C   -7.542999   -1.077656    1.671169
 H   -7.373502   -2.141109    1.916337
 H    3.101569    2.577516    1.852593
 H    5.030045    1.194239    2.090300
 H    2.311170    3.291857   -1.065131
 C    2.992298    2.373069    0.780948
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 C    2.229779    3.250818    0.026174
 C    4.926034    0.823930    1.066353
 H    6.548540   -0.542506    1.318698
 C    3.924139    1.356436    0.245248
 C    5.793314   -0.169291    0.627467
 H    1.777121    4.123165    0.505654
 C    3.830945    0.840543   -1.057331
 C    5.696113   -0.692791   -0.682893
 H    3.051431    1.203636   -1.733016
 C    4.683176   -0.153860   -1.514796
 H    4.549682   -0.525307   -2.530559
 H   -0.600718   -1.328084    3.214859
 H   -0.373603   -2.505842    1.898846
 C    0.148838   -1.932304    2.679455
 O    0.560934   -0.095044    1.215512
 H    0.590356   -2.649436    3.390269
 C    1.204924   -1.014539    2.048538
 H    1.232546    0.386606    3.708373
 H    1.684192   -2.398945    0.442334
 C    1.939281   -0.257266    3.160816
 C    2.207564   -1.849490    1.240958
 H    2.413798   -0.942127    3.881927
 H    2.745718   -2.579814    1.867074
 H    2.724262    0.382016    2.732081
 H    2.949082   -1.189097    0.766765
Cu    1.094136    1.651625    0.477976
 C   -3.232227   -1.395466   -1.059907
 C   -4.233045   -0.909952   -1.911227
 C   -3.607986   -1.678584    0.262767
 C   -4.903382   -1.480066    0.716894
 C   -5.914276   -0.983029   -0.143449
 C   -5.538581   -0.709213   -1.479991
 H   -2.861410   -2.039600    0.975448
 H   -5.125906   -1.704170    1.759744
 H   -6.269239   -0.331807   -2.194995
 H   -3.985348   -0.680286   -2.951486
 C   -1.845400   -1.548248   -1.549366
 C   -0.881445   -2.350470   -0.957519
 H   -1.663580   -1.169046   -2.561822
 H   -1.123885   -3.010466   -0.119141
 H    0.033467   -2.591340   -1.507949
 H   -0.702228    3.924383    0.608569
 H   -0.421759    4.102345   -1.142508
 C   -1.172374    3.831282   -0.383836
 O   -0.573692    1.518935   -0.600778
 H   -1.997462    4.559787   -0.438256
 C   -1.661657    2.395580   -0.609037
 H   -2.106702    1.976081    1.470005
 H   -1.661254    2.592964   -2.773445
 C   -2.644788    2.017690    0.509172
 C   -2.359672    2.305439   -1.971504
 H   -3.475155    2.736785    0.602597
 H   -3.247554    2.956012   -2.031660
 H   -3.078854    1.022843    0.321590
 H   -2.682680    1.270706   -2.155200
Cu   -0.635509   -0.450783   -0.313313
 H    5.376993   -2.732987   -2.568593
 C    6.360834   -2.243199   -2.446865
 H    7.135420   -2.998020   -2.628039
 H    7.012046   -2.753007    0.647538
 N    6.538763   -1.681583   -1.127925
 H    6.454057   -1.476843   -3.235361
 H    8.072833   -3.039408   -0.751101
 C    7.496464   -2.271252   -0.221696
 H    8.213028   -1.524947    0.162718
78
Figure 8_para-NMe2-styrene-Cu-OtBu_dimer_02 / electronic energy: -4632.85757242 a.u. / lowest freq: 25.42 cm-1
 H   -6.462330    0.112008    1.967236
 C   -6.947082   -0.011280    0.982018
 H   -7.920423   -0.488731    1.145750
 H   -6.071633   -2.939237   -0.088349
 N   -6.160173   -0.823652    0.084131
 H   -7.133561    0.996501    0.570660
 H   -7.696349   -2.226467    0.001442
 C   -6.687633   -2.077355   -0.401824
 H   -6.761252   -2.098819   -1.503685
 H    3.188918    0.310793    3.059058
 H    1.430575    1.942259    3.080155
 H    4.910621   -1.055380    1.986414
 C    3.393554    0.460794    1.992983
 C    4.356314   -0.328617    1.384945
 C    1.648060    2.235788    2.049922
 H    0.032691    3.630801    2.024705
 C    2.698143    1.605521    1.368131
 C    0.846682    3.193769    1.447293
 H    4.807571   -0.062531    0.424618
 C    2.927383    2.009672    0.043617
 C    1.050419    3.568628    0.098262
 H    3.734500    1.554299   -0.534569
 C    2.133734    2.961024   -0.581328
 H    2.351262    3.220533   -1.617111
 H    1.338319   -3.748788   -2.453139
 H    1.103798   -2.178380   -3.258273
 C    1.864153   -2.887820   -2.894963
 O    1.937472   -1.843844   -0.757848
 H    2.445594   -3.241466   -3.761790
 C    2.745875   -2.215070   -1.835405
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 H     3.315117   -4.089673   -0.890726
 H     2.695647   -0.253842   -2.777094
 C     3.802555   -3.207188   -1.334412
 C     3.442657   -0.989239   -2.441179
 H     4.471599   -3.548556   -2.140899
 H     4.079030   -1.252189   -3.301839
 H     4.419384   -2.733355   -0.553142
 H     4.076985   -0.504668   -1.682720
Cu     2.461619   -1.008065    0.958918
 C    -2.267941    0.415777   -1.031195
 C    -3.064715    1.184407   -0.173657
 C    -2.818342   -0.784611   -1.505407
 C    -4.091852   -1.199584   -1.143545
 C    -4.899844   -0.419405   -0.278836
 C    -4.345022    0.792574    0.195989
 H    -2.228725   -1.432984   -2.159629
 H    -4.459321   -2.147209   -1.536747
 H    -4.913660    1.434492    0.868226
 H    -2.661853    2.117561    0.230968
 C    -0.899830    0.865761   -1.354920
 C    -0.110320    0.411409   -2.400393
 H    -0.592035    1.785792   -0.844493
 H    -0.483215   -0.314617   -3.130669
 H     0.764871    0.992528   -2.705914
 H     1.458715   -2.384436    3.166273
 H     0.609176   -0.992257    3.888075
 C     0.464276   -1.940679    3.346866
 O     0.494470   -0.750855    1.283641
 H    -0.100230   -2.627559    3.998238
 C    -0.251878   -1.679112    2.013783
 H     0.597243   -3.382467    0.959788
 H    -1.558315   -0.123076    2.789105
 C    -0.395345   -3.001431    1.243551
 C    -1.645830   -1.098322    2.284569
 H    -0.924872   -3.770475    1.829847
 H    -2.259197   -1.764061    2.914148
 H    -0.960601   -2.837725    0.310480
 H    -2.178961   -0.940939    1.335543
Cu     0.428662   -0.539132   -0.699699
 H     1.341665    5.146277   -2.195034
 C     0.364083    4.695768   -1.951611
 H    -0.413337    5.392739   -2.285949
 H    -0.607129    5.572819    1.067597
 N     0.216057    4.457122   -0.534422
 H     0.261588    3.766442   -2.541499
 H    -1.452510    5.703368   -0.487171
 C    -0.916914    5.009190    0.171096
 H    -1.632285    4.230462    0.494367
98
Figure 8_L3a-Cu-OtBu / electronic energy: -4500.61984018 a.u. / lowest freq: -20.29 cm-1
 P    -1.580542    0.896725    0.507317
 C    -2.908207    3.157185   -0.383641
 C    -4.006725    3.985801   -0.616704
 C    -3.065934    1.952882    0.310453
 C    -5.267815    3.615698   -0.152099
 C    -4.334988    1.587341    0.777167
 C    -5.430677    2.415956    0.544998
 C    -2.523549   -1.468960    3.766793
 C    -2.433956   -0.995007    2.458931
 C    -1.750721    0.195213    2.185586
 C    -1.940215   -0.754291    4.813269
 C    -1.270557    0.441252    4.550950
 C    -1.173132    0.911691    3.242472
 C    -2.488216   -0.166613   -2.032914
 C    -1.872393   -0.448550   -0.671022
 C    -1.299140   -1.669779   -0.734533
 C    -1.272709    0.069693   -2.972172
 C    -0.635837   -1.334154   -3.044849
 C    -1.568682   -2.215154   -2.148736
 C    -1.395589   -3.700880   -2.383493
 C    -2.968758   -1.580997   -2.446504
 C    -3.416732   -1.695439   -3.906676
 C    -4.117793   -2.103832   -1.580032
 C    -0.402948   -2.359373    0.224528
 C    -0.776860   -3.505808    0.883773
 C     0.975407   -1.984659    0.502411
 S     0.536953   -4.140203    1.811096
 C     1.617684   -2.882805    1.327412
 C    -2.109087   -4.184545    0.927504
 C     3.027464   -2.915300    1.833201
 P     1.678909   -0.407382   -0.087965
 C     3.102106    0.859929    3.522479
 C     2.302495    0.358977    2.498979
 C     4.452175    1.127830    3.286856
 C     2.843742    0.105397    1.231146
 C     4.993844    0.884481    2.025620
 C     4.195075    0.374971    1.000685
 C     3.810868    0.068843   -3.514968
 C     3.023741    0.281283   -2.383591
 C     4.288299   -1.209367   -3.809490
 C     2.730665   -0.792862   -1.528752
 C     3.979451   -2.281011   -2.970507
 C     3.204103   -2.074442   -1.829949
 H    -1.915778    3.440512   -0.746059
 H    -3.873260    4.924573   -1.159108
 H    -6.129053    4.263617   -0.331942
 H    -4.472168    0.649243    1.321329
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 H   -6.418530    2.124936    0.910059
 H   -3.052633   -2.403325    3.968939
 H   -2.893523   -1.557737    1.644298
 H   -2.009117   -1.130195    5.836777
 H   -0.813928    1.005846    5.367081
 H   -0.634680    1.841763    3.037295
 H   -3.246522    0.627518   -2.056758
 H   -0.589719    0.827995   -2.558260
 H   -1.599587    0.429651   -3.958197
 H    0.397965   -1.358219   -2.675070
 H   -0.612264   -1.725800   -4.072823
 H   -1.570304   -3.939191   -3.444195
 H   -2.092416   -4.304994   -1.785566
 H   -0.372211   -4.024525   -2.136174
 H   -4.283813   -1.039932   -4.086553
 H   -3.735264   -2.726536   -4.127997
 H   -2.643849   -1.427048   -4.637860
 H   -5.049987   -1.574746   -1.833824
 H   -3.945257   -1.962235   -0.505502
 H   -4.291685   -3.176350   -1.763069
 H   -2.830286   -3.652783    0.295310
 H   -2.511139   -4.201379    1.953149
 H   -2.051970   -5.227314    0.578596
 H    3.133815   -2.345375    2.769850
 H    3.720647   -2.481976    1.101170
 H    3.345945   -3.948938    2.031729
 H    2.665823    1.045999    4.506885
 H    1.245355    0.156678    2.688849
 H    5.080940    1.527152    4.086046
 H    6.049214    1.091790    1.833772
 H    4.633959    0.190791    0.017398
 H    4.040865    0.905396   -4.179302
 H    2.611508    1.276687   -2.160485
 H    4.894279   -1.374226   -4.703735
 H    4.343260   -3.284201   -3.205138
 H    2.955927   -2.917868   -1.180520
Cu    0.417430    1.531952   -0.315265
 H    1.533422    5.234717   -2.570756
 H    2.752520    5.897866   -1.444814
 H    3.117535    4.440494   -2.410028
 C    2.325100    4.966405   -1.852792
 H   -0.149226    5.110504   -0.667688
 C    1.752337    4.045194   -0.761300
 H    1.046191    5.717534    0.511698
 O    1.233972    2.914790   -1.363084
 C    0.662151    4.810177    0.015323
 H    3.662168    3.098170   -0.312532
 H    3.360480    4.550221    0.683303
 C    2.883951    3.670816    0.217078
 H    0.224040    4.154997    0.787863
 H    2.491679    3.029307    1.024769
31
Figure 8_para-H-styrene-Cu-OtBu / electronic energy: -2182.55158904 a.u. / lowest freq: 27.42 cm-1
 C   -1.928903    0.522589    0.151598
 C   -2.367593   -0.225683    1.253706
 C   -2.102115   -0.011349   -1.135516
 C   -2.688512   -1.261082   -1.309804
 C   -3.114996   -1.999957   -0.203840
 C   -2.955887   -1.476382    1.078595
 H   -1.771969    0.551062   -2.011760
 H   -2.813794   -1.663778   -2.317510
 H   -3.574222   -2.981095   -0.344130
 H   -3.288621   -2.045895    1.949330
 H   -2.235906    0.177972    2.261012
 C   -1.259656    1.821554    0.396510
 C   -0.717088    2.656046   -0.552234
 H   -1.320811    2.184359    1.429681
 H   -0.795346    2.453802   -1.625268
 H   -0.394506    3.662142   -0.268341
 H    4.530550   -0.752582   -0.259174
 H    4.027421   -1.250156    1.372998
 C    3.815244   -1.377041    0.299445
 O    2.253156    0.399694    0.393393
 H    3.992832   -2.431959    0.032888
 C    2.377225   -0.924049   -0.002265
 H    2.762220   -0.403423   -2.080931
 H    1.541412   -1.679023    1.858641
 C    2.104007   -1.077496   -1.509356
 C    1.391935   -1.816035    0.775636
 H    2.263369   -2.107308   -1.870669
 H    1.509123   -2.887576    0.542110
 H    1.058778   -0.800471   -1.732575
 H    0.351559   -1.530222    0.541548
Cu    0.717611    1.355859    0.135178
62
Figure 8_para-H-styrene-Cu-OtBu_dimer_01 / electronic energy: -4365.17726958 a.u. / lowest freq: 25.56 cm-1
 H    3.514741    1.263553    1.925814
 H    5.285243   -0.183045    1.255991
 H    2.378842    3.063934   -0.336596
 C    3.205909    1.480231    0.897132
 C    2.459566    2.624335    0.662653
 C    4.965692   -0.143930    0.211265
 H    6.441398   -1.576387   -0.435288
 C    3.899793    0.691762   -0.149860
 C    5.615781   -0.928861   -0.739990
 H    2.202239    3.282115    1.497710
 C    3.504478    0.722838   -1.497777
```

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 C    5.210664   -0.892490   -2.073396
 H    2.661500    1.347589   -1.804722
 C    4.153265   -0.060209   -2.447728
 H    5.713910   -1.511945   -2.819337
 H    3.824774   -0.027722   -3.489360
 H   -0.303018   -2.577066    2.643930
 H   -0.540015   -3.224369    1.002910
 C    0.215723   -3.006743    1.772313
 O    0.603227   -0.820814    0.894786
 H    0.676314   -3.960194    2.076988
 C    1.254122   -2.010759    1.239259
 H    1.786857   -1.237377    3.199080
 H    1.230603   -2.821042   -0.777899
 C    2.278679   -1.728301    2.344034
 C    1.964689   -2.595471    0.011531
 H    2.757558   -2.652523    2.704881
 H    2.513218   -3.522433    0.245501
 H    3.069543   -1.061905    1.973065
 H    2.680949   -1.863001   -0.392188
Cu    1.221328    1.039117    0.721374
 C   -3.649322   -0.943566   -0.943916
 C   -4.639697   -0.102034   -1.469518
 C   -3.900003   -1.582538    0.282378
 C   -5.099235   -1.378329    0.958293
 C   -6.073426   -0.530064    0.427465
 C   -5.839997    0.104731   -0.791649
 H   -3.139290   -2.227831    0.728896
 H   -5.270698   -1.877633    1.914922
 H   -7.010927   -0.365274    0.963517
 H   -6.595215    0.769819   -1.217233
 H   -4.463056    0.402042   -2.423223
 C   -2.366288   -1.098817   -1.670615
 C   -1.479229   -2.146842   -1.483265
 H   -2.254738   -0.468990   -2.560381
 H   -1.714312   -2.987277   -0.823933
 H   -0.692514   -2.326082   -2.222587
 H   -0.323920    3.415865    1.673142
 H   -0.055639    3.992546    0.006587
 C   -0.819492    3.633154    0.713362
 O   -0.559833    1.370900   -0.052384
 H   -1.541977    4.448150    0.880529
 C   -1.506546    2.375613    0.169166
 H   -2.029840    1.583854    2.119040
 H   -1.446474    3.059835   -1.890748
 C   -2.542373    1.886588    1.191607
 C   -2.193658    2.710779   -1.160256
 H   -3.287585    2.659559    1.440242
 H   -2.964437    3.490963   -1.050652
 H   -3.080335    1.009257    0.801930
 H   -2.674578    1.811787   -1.571714
Cu   -0.856185   -0.556907   -0.400441
62
Figure 8_para-H-styrene-Cu-OtBu_dimer_02 / electronic energy: -4365.17671872 a.u. / lowest freq: 25.56 cm-1
 H    2.308649    2.256767    2.184766
 H    0.388875    3.520111    1.583267
 H    4.231863    0.808153    1.740181
 C    2.510166    1.944596    1.154310
 C    3.592141    1.115489    0.907320
 C    0.575064    3.370053    0.517117
 H   -1.147256    4.515144   -0.086180
 C    1.676425    2.599809    0.116974
 C   -0.292894    3.922167   -0.421370
 H    4.022470    0.996924   -0.090895
 C    1.883514    2.397597   -1.258240
 C   -0.079761    3.710153   -1.784036
 H    2.725960    1.795163   -1.604666
 C    1.013582    2.946606   -2.197095
 H   -0.764436    4.135257   -2.521684
 H    1.189908    2.773467   -3.261429
 H    1.263227   -4.123931   -0.715768
 H    0.810620   -3.150201   -2.136145
 C    1.660823   -3.488719   -1.522934
 O    1.504485   -1.584471   -0.100993
 H    2.318293   -4.104281   -2.157685
 C    2.393555   -2.281054   -0.927854
 H    3.218871   -3.401331    0.742156
 H    2.055729   -0.988989   -2.644029
 C    3.576381   -2.757652   -0.077038
 C    2.903085   -1.375389   -2.056720
 H    4.312237   -3.326082   -0.668228
 H    3.584635   -1.905524   -2.741084
 H    4.089866   -1.891441    0.371707
 H    3.443573   -0.514093   -1.634780
Cu    1.833829    0.065211    0.932770
 C   -2.991697   -0.173798   -1.096967
 C   -3.755992    0.925929   -0.682557
 C   -3.494085   -1.463692   -0.860570
 C   -4.721398   -1.642558   -0.228588
 C   -5.474157   -0.538318    0.177912
 C   -4.986870    0.747285   -0.053895
 H   -2.914080   -2.340749   -1.158905
 H   -5.093255   -2.653959   -0.047940
 H   -6.435690   -0.682045    0.676041
 H   -5.565146    1.618648    0.262656
 H   -3.369181    1.935130   -0.847020
 C   -1.682586    0.072238   -1.742572
 C   -0.940773   -0.848805   -2.465565
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 H   -1.411153    1.131538   -1.829631
 H   -1.300494   -1.868064   -2.639986
 H   -0.151372   -0.497972   -3.136403
 H    1.147002   -0.412360    3.482448
 H    0.184375    1.079902    3.662452
 C    0.121089   -0.016978    3.583525
 O   -0.144638    0.153703    1.217187
 H   -0.300164   -0.406608    4.524417
 C   -0.720450   -0.412601    2.361607
 H    0.238308   -2.339349    2.045700
 H   -2.129386    1.231868    2.553725
 C   -0.767988   -1.944772    2.251591
 C   -2.145262    0.130968    2.523228
 H   -1.162028   -2.415898    3.166915
 H   -2.626069   -0.238104    3.443989
 H   -1.420208   -2.243842    1.412795
 H   -2.767239   -0.174237    1.669091
Cu   -0.212020   -0.696389   -0.582250
98
Figure 8_L3a-Cu-OtBu / electronic energy: -4500.61984018 a.u. / lowest freq: -20.29 cm-1
 P   -1.580542    0.896725    0.507317
 C   -2.908207    3.157185   -0.383641
 C   -4.006725    3.985801   -0.616704
 C   -3.065934    1.952882    0.310453
 C   -5.267815    3.615698   -0.152099
 C   -4.334988    1.587341    0.777167
 C   -5.430677    2.415956    0.544998
 C   -2.523549   -1.468960    3.766793
 C   -2.433956   -0.995007    2.458931
 C   -1.750721    0.195213    2.185586
 C   -1.940215   -0.754291    4.813269
 C   -1.270557    0.441252    4.550950
 C   -1.173132    0.911691    3.242472
 C   -2.488216   -0.166613   -2.032914
 C   -1.872393   -0.448550   -0.671022
 C   -1.299140   -1.669779   -0.734533
 C   -1.272709    0.069693   -2.972172
 C   -0.635837   -1.334154   -3.044849
 C   -1.568682   -2.215154   -2.148736
 C   -1.395589   -3.700880   -2.383493
 C   -2.968758   -1.580997   -2.446504
 C   -3.416732   -1.695439   -3.906676
 C   -4.117793   -2.103832   -1.580032
 C   -0.402948   -2.359373    0.224528
 C   -0.776860   -3.505808    0.883773
 C    0.975407   -1.984659    0.502411
 S    0.536953   -4.140203    1.811096
 C    1.617684   -2.882805    1.327412
 C   -2.109087   -4.184545    0.927504
 C    3.027464   -2.915300    1.833201
 P    1.678909   -0.407382   -0.087965
 C    3.102106    0.859929    3.522479
 C    2.302495    0.358977    2.498979
 C    4.452175    1.127830    3.286856
 C    2.843742    0.105397    1.231146
 C    4.993844    0.884481    2.025620
 C    4.195075    0.374971    1.000685
 C    3.810868    0.068843   -3.514968
 C    3.023741    0.281283   -2.383591
 C    4.288299   -1.209367   -3.809490
 C    2.730665   -0.792862   -1.528752
 C    3.979451   -2.281011   -2.970507
 C    3.204103   -2.074442   -1.829949
 H   -1.915778    3.440512   -0.746059
 H   -3.873260    4.924573   -1.159108
 H   -6.129053    4.263617   -0.331942
 H   -4.472168    0.649243    1.321329
 H   -6.418530    2.124936    0.910059
 H   -3.052633   -2.403325    3.968939
 H   -2.893523   -1.557737    1.644298
 H   -2.009117   -1.130195    5.836777
 H   -0.813928    1.005846    5.367081
 H   -0.634680    1.841763    3.037295
 H   -3.246522    0.627518   -2.056758
 H   -0.589719    0.827995   -2.558260
 H   -1.599587    0.429651   -3.958197
 H    0.397965   -1.358219   -2.675070
 H   -0.612264   -1.725800   -4.072823
 H   -1.570304   -3.939191   -3.444195
 H   -2.092416   -4.304994   -1.785566
 H   -0.372211   -4.024525   -2.136174
 H   -4.283813   -1.039932   -4.086553
 H   -3.735264   -2.726536   -4.127997
 H   -2.643849   -1.427048   -4.637860
 H   -5.049987   -1.574746   -1.833824
 H   -3.945257   -1.962235   -0.505502
 H   -4.291685   -3.176350   -1.763069
 H   -2.830286   -3.652783    0.295310
 H   -2.511139   -4.201379    1.953149
 H   -2.051970   -5.227314    0.578596
 H    3.133815   -2.345375    2.769850
 H    3.720647   -2.481976    1.101170
 H    3.345945   -3.948938    2.031729
 H    2.665823    1.045999    4.506885
 H    1.245355    0.156678    2.688849
 H    5.080940    1.527152    4.086046
 H    6.049214    1.091790    1.833772
```

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 H     4.633959    0.190791    0.017398
 H     4.040865    0.905396   -4.179302
 H     2.611508    1.276687   -2.160485
 H     4.894279   -1.374226   -4.703735
 H     4.343260   -3.284201   -3.205138
 H     2.955927   -2.917868   -1.180520
Cu     0.417430    1.531952   -0.315265
 H     1.533422    5.234717   -2.570756
 H     2.752520    5.897866   -1.444814
 H     3.117535    4.440494   -2.410028
 C     2.325100    4.966405   -1.852792
 H    -0.149226    5.110504   -0.667688
 C     1.752337    4.045194   -0.761300
 H     1.046191    5.717534    0.511698
 O     1.233972    2.914790   -1.363084
 C     0.662151    4.810177    0.015323
 H     3.662168    3.098170   -0.312532
 H     3.360480    4.550221    0.683303
 C     2.883951    3.670816    0.217078
 H     0.224040    4.154997    0.787863
 H     2.491679    3.029307    1.024769
37
Figure 8_para-CO2Me-styrene-Cu-OtBu / electronic energy: -2410.19525632 a.u. / lowest freq: 22.92 cm-1
 O     4.336955    0.759818    1.270722
 C     3.813648    0.295280    0.286819
 H     6.377229    0.525856   -0.503619
 H     5.509179    2.083275   -0.668008
 O     4.342290    0.376550   -0.932416
 C     5.585015    1.055967   -1.052360
 H     5.822111    1.073396   -2.122151
 C     0.010075   -1.714613    0.394777
 C     0.582229   -1.171455    1.554508
 C     0.718612   -1.618072   -0.813666
 C     1.948488   -0.976825   -0.864820
 C     2.504190   -0.423182    0.295604
 C     1.815193   -0.531701    1.506735
 H     0.301415   -2.034699   -1.732230
 H     2.481274   -0.897947   -1.812852
 H     2.252815   -0.101531    2.409225
 H     0.045094   -1.242163    2.503364
 C    -1.342937   -2.314111    0.481494
 C    -2.079671   -2.809549   -0.567100
 H    -1.717994   -2.466818    1.500272
 H    -1.687861   -2.868343   -1.587441
 H    -2.998795   -3.367964   -0.366085
 H    -2.944270    1.978775    2.074160
 H    -1.417812    2.872316    1.807937
 C    -2.008539    1.995866    1.492595
 H    -1.435711    1.088443    1.750046
 H    -4.066576    3.290377    0.191900
 C    -3.113534    3.274596   -0.360508
 H    -2.555499    4.193638   -0.116482
Cu    -2.537132   -0.824824   -0.280275
 O    -3.124385    0.907277   -0.332852
 C    -2.331382    1.997552   -0.012765
 H    -3.349866    3.287741   -1.436568
 C    -1.010162    1.982770   -0.803870
 H    -0.408892    1.098739   -0.528849
 H    -0.393737    2.878382   -0.618903
 H    -1.221520    1.924120   -1.884025
74
Figure 8_para-CO2Me-styrene-Cu-OtBu_dimer_01 / electronic energy: -4820.46849056 a.u. / lowest freq: 9.94 cm-1
 H     8.207656   -3.073852   -2.206264
 H     6.791426   -3.872773   -2.971309
 C     7.177623   -3.425166   -2.048494
 O     7.528837   -1.893880    0.083288
 O     6.313860   -2.340173   -1.739697
 C     6.596392   -1.640021   -0.641189
 H     7.174299   -4.173172   -1.242481
 H     3.029102    3.112524    1.456027
 H     5.040726    1.907923    1.897441
 H     2.204195    3.165499   -1.537744
 C     2.905806    2.680005    0.456970
 C     2.120184    3.356994   -0.463192
 C     4.912895    1.307793    0.993455
 H     6.611886    0.045339    1.421087
 C     3.854951    1.594026    0.118494
 C     5.794364    0.265560    0.732178
 H     1.645334    4.300304   -0.179134
 C     3.712049    0.803993   -1.035393
 C     5.637159   -0.521284   -0.412425
 H     2.883631    0.986637   -1.724143
 C     4.588414   -0.239849   -1.297761
 H     4.455031   -0.850326   -2.191652
 H    -0.488721   -0.383560    3.772220
 H    -0.281710   -1.841067    2.770552
 C     0.253998   -1.093361    3.374652
 O     0.605045    0.312803    1.480027
 H     0.726094   -1.614518    4.222927
 C     1.280494   -0.347074    2.513143
 H     1.278319    1.439825    3.746910
 H     1.785883   -2.104920    1.336183
 C     1.998680    0.689260    3.384453
 C     2.299531   -1.337817    1.936386
 H     2.485122    0.225804    4.257506
 H     2.875299   -1.849098    2.724685
 H     2.773720    1.208475    2.803436
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 H    3.007518   -0.811606    1.278522
Cu    1.043118    1.862872    0.351970
 C   -3.055830   -1.632233   -0.703274
 C   -3.893850   -1.418929   -1.808088
 C   -3.620658   -1.580705    0.582384
 C   -4.971514   -1.312487    0.756345
 C   -5.795534   -1.085075   -0.353709
 C   -5.245055   -1.145225   -1.637338
 H   -2.991580   -1.725453    1.463575
 H   -5.392309   -1.264134    1.761307
 H   -5.889326   -0.967285   -2.500356
 H   -3.473192   -1.456577   -2.815614
 C   -1.610261   -1.858824   -0.926552
 C   -0.743417   -2.431558   -0.008167
 H   -1.284771   -1.781761   -1.969723
 H   -1.097868   -2.828513    0.947904
 H    0.229786   -2.799353   -0.346792
 H   -1.057723    4.057696   -0.551737
 H   -0.124095    3.639973   -2.013077
 C   -1.113513    3.568849   -1.537358
 O   -0.690986    1.458245   -0.471207
 H   -1.827736    4.130893   -2.159894
 C   -1.537813    2.104993   -1.377442
 H   -3.026655    2.597835    0.127282
 H   -0.418893    1.371006   -3.083949
 C   -2.971280    2.057177   -0.830784
 C   -1.465565    1.406191   -2.740727
 H   -3.698224    2.506697   -1.526565
 H   -2.066395    1.921117   -3.507682
 H   -3.273063    1.015793   -0.647988
 H   -1.832273    0.372377   -2.660071
Cu   -0.587779   -0.423172    0.106000
 H   -9.242075    0.553178    1.021017
 H   -9.205667   -0.656851    2.348441
 C   -9.032291   -0.495590    1.278350
 O   -7.969001   -0.494953   -1.148000
 O   -7.666015   -0.808816    1.044898
 C   -7.245856   -0.765195   -0.219101
 H   -9.692129   -1.147860    0.688645
74
Figure 8_para-CO2Me-styrene-Cu-OtBu_dimer_02 / electronic energy: -4820.47029487 a.u. / lowest freq: 18.80 cm-1
 H   -3.170699    0.139976   -3.213871
 H   -1.193383    1.447568   -3.334783
 H   -5.089447   -0.847681   -2.052155
 C   -3.388709    0.450599   -2.186507
 C   -4.464149   -0.120434   -1.526078
 C   -1.405916    1.929328   -2.378396
 H    0.407266    3.098395   -2.394125
 C   -2.562890    1.567775   -1.672219
 C   -0.505997    2.844410   -1.852768
 H   -4.904781    0.327194   -0.631216
 C   -2.813754    2.188507   -0.436443
 C   -0.740773    3.424426   -0.601517
 H   -3.709539    1.937045    0.135202
 C   -1.912671    3.102484    0.094750
 H   -2.107621    3.559008    1.065995
 H   -2.127368   -3.667020    2.628875
 H   -1.814156   -2.093659    3.403617
 C   -2.602695   -2.741224    2.989108
 O   -2.381778   -1.799356    0.811081
 H   -3.296878   -3.000154    3.804324
 C   -3.314496   -2.034370    1.829848
 H   -3.989714   -3.881380    0.905291
 H   -3.128771   -0.036235    2.670618
 C   -4.421696   -2.938595    1.276404
 C   -3.922181   -0.713633    2.318864
 H   -5.180273   -3.180211    2.037992
 H   -4.639126   -0.862554    3.142078
 H   -4.928219   -2.442349    0.432210
 H   -4.451387   -0.212287    1.493692
Cu   -2.686203   -0.954373   -0.930102
 C    1.964927    0.256658    1.181923
 C    2.674598    1.079042    0.294326
 C    2.569670   -0.931482    1.624285
 C    3.837498   -1.289239    1.185705
 C    4.536281   -0.463482    0.294815
 C    3.944798    0.725419   -0.143072
 H    2.036168   -1.598883    2.304695
 H    4.290579   -2.219487    1.530568
 H    4.490189    1.367220   -0.837195
 H    2.216285    2.003591   -0.065884
 C    0.600887    0.660547    1.582697
 C   -0.149090    0.121484    2.616113
 H    0.265064    1.608231    1.147953
 H    0.245593   -0.663606    3.269193
 H   -1.007934    0.677038    3.002455
 H   -1.745726   -2.515230   -2.963219
 H   -0.789226   -1.214364   -3.722578
 C   -0.720179   -2.149664   -3.144922
 O   -0.692402   -0.888179   -1.121343
 H   -0.198182   -2.898831   -3.761621
 C   -0.003559   -1.893050   -1.811980
 H   -0.993019   -3.491025   -0.719444
 H    1.416060   -0.460817   -2.625936
 C    0.030415   -3.191247   -0.991524
 C    1.429101   -1.418837   -2.083136
 H    0.516324   -4.017400   -1.535909
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 H     2.001799   -2.149259   -2.677616
 H     0.588197   -3.032362   -0.052648
 H     1.961389   -1.261274   -1.133949
Cu    -0.715474   -0.704379    0.859807
 H     1.917573    5.076522    1.928604
 H     0.541280    5.781670    2.844206
 C     0.944436    5.581615    1.845026
 O     1.317039    4.639410   -0.604178
 O    -0.005038    4.746899    1.195703
 C     0.296462    4.330730   -0.033886
 H     1.074957    6.527671    1.300012
 H     7.634086   -2.544406   -1.277507
 H     7.823014   -3.347636    0.317298
 C     7.621566   -2.396071   -0.187738
 O     6.525735   -0.120929   -0.982584
 O     6.337987   -1.974999    0.252252
 C     5.892140   -0.810506   -0.219616
 H     8.391747   -1.659139    0.081515
29
Figure 9_Cu-(OtBu)2_anion / electronic energy: -2106.15712863 a.u. / lowest freq: 16.07 cm-1
Cu    0.000000   -0.539536    0.000001
 O    1.743050   -0.619185   -0.567556
 C    2.750285    0.136326   -0.016010
 C    4.059753   -0.198057   -0.756660
 C    2.935008   -0.180735    1.482953
 C    2.464302    1.644928   -0.168920
 H    4.275008   -1.274381   -0.657174
 H    4.928514    0.366911   -0.378124
 H    3.943890    0.018695   -1.831004
 H    3.109171   -1.261228    1.614436
 H    2.013628    0.074766    2.033469
 H    3.776349    0.366015    1.943917
 H    1.545088    1.906102    0.382524
 H    2.290043    1.879226   -1.231876
 H    3.283509    2.285879    0.201447
 H   -2.290020    1.879251    1.231830
 H   -1.545079    1.906086   -0.382578
 H   -3.283496    2.285878   -0.201492
 C   -2.464290    1.644930    0.168881
 C   -2.750284    0.136326    0.016010
 H   -3.943869    0.018743    1.831020
 O   -1.743050   -0.619179    0.567561
 H   -2.013652    0.074711   -2.033477
 H   -4.928508    0.366936    0.378144
 H   -3.776369    0.365976   -1.943911
 C   -4.059747   -0.198030    0.756682
 C   -2.935027   -0.180769   -1.482943
 H   -4.275010   -1.274355    0.657222
 H   -3.109200   -1.261264   -1.614398
53
Figure 9_para-NMe2-styrene-Cu-(OtBu)2_anion_01 / electronic energy: -2549.33388221 a.u. / lowest freq: 17.24 cm-1
 H     3.160642   -0.812668    2.186115
 C     3.915360   -0.483155    0.167792
 C     2.943236   -0.871970    1.119739
 H     4.236086   -0.259957   -1.974989
 C     3.540694   -0.561908   -1.191966
 C     1.689509   -1.322972    0.726927
 H     0.969994   -1.590523    1.505471
 C     2.278223   -1.013545   -1.562946
 C     1.317894   -1.409674   -0.623601
 H     2.026460   -1.045711   -2.627099
 C    -0.024508   -1.840004   -1.067572
 H    -1.780758   -3.056011   -0.784427
 C    -0.947334   -2.541079   -0.297617
 H    -0.718803   -2.873717    0.720297
Cu    -1.417526   -0.586535   -0.252156
 H    -0.180490   -1.797553   -2.151965
 H     6.298032   -0.273942   -1.219753
 H     5.687146    1.379962   -0.946577
 C     6.075690    0.475015   -0.441150
 H     7.026228    0.738384    0.039061
 N     5.165662   -0.044103    0.551579
 H     4.785822    0.937153    2.404243
 H     6.482705    0.512798    2.066467
 C     5.445924    0.173510    1.950827
 H     5.336782   -0.754941    2.536487
 H    -4.229794    1.875619    0.750935
 H    -3.494862    1.321664   -0.768129
 H    -5.290825    1.307456   -0.567073
 C    -4.322013    1.136840   -0.063917
 C    -4.172411   -0.293129    0.504616
 H    -4.983494    0.203601    2.458872
 H    -6.245550   -0.320185    1.305379
 H    -3.798586   -1.147907   -1.473066
 O    -2.914213   -0.497329    1.011745
 H    -5.523025   -1.201590   -1.017310
 C    -5.205238   -0.492142    1.633125
 C    -4.493842   -1.297405   -0.628401
 H    -5.132187   -1.516547    2.035080
 H    -4.358538   -2.328224   -0.260870
 O    -1.062158    1.161865   -1.033945
 C    -0.540063    2.200215   -0.302804
 C    -0.629895    1.945968    1.218534
 C    -1.313739    3.497715   -0.626238
 C     0.946539    2.415468   -0.667732
 H    -1.649426    1.619327    1.475367
 H    -0.353592    2.829257    1.821824
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 H     0.051198    1.123386    1.501301
 H    -2.359751    3.408267   -0.292441
 H    -1.323562    3.654919   -1.717424
 H    -0.877934    4.393992   -0.150389
 H     1.045562    2.588196   -1.752501
 H     1.525409    1.510888   -0.421818
 H     1.404547    3.270065   -0.137684
53
Figure 9_para-NMe2-styrene-Cu-(OtBu)2_anion_02 / electronic energy: -2549.33285744 a.u. / lowest freq: 28.21 cm-1
 H     3.655175   -2.335738    0.268832
 C     3.838769   -0.190331   -0.065215
 C     3.213522   -1.353718    0.438453
 H     3.622319    1.975820   -0.173381
 C     3.198129    1.043124    0.198717
 C     2.027534   -1.277901    1.162724
 H     1.590112   -2.207926    1.535461
 C     2.013976    1.095519    0.921753
 C     1.393992   -0.056014    1.427576
 H     1.538589    2.065248    1.085165
 C     0.114404    0.059664    2.160012
 H    -0.468588   -2.037843    2.275303
 C    -0.724561   -0.997394    2.497634
 H    -1.497680   -0.857456    3.259721
Cu    -1.387829   -0.133732    0.803745
 H    -0.058841    1.033097    2.633600
 H     4.903781    1.427021   -2.076044
 H     5.815319    1.701003   -0.568140
 C     5.579752    0.949742   -1.342317
 H     6.516073    0.706972   -1.859667
 N     5.018808   -0.252528   -0.775087
 H     5.847433   -2.104933   -0.166357
 H     6.547133   -1.381521   -1.626494
 C     5.608050   -1.533439   -1.080366
 H     4.951413   -2.164946   -1.707847
 H    -3.919180   -0.462674   -2.141797
 H    -2.162672   -0.215110   -1.998320
 H    -2.815620   -1.523304   -3.060904
 C    -2.946208   -0.982741   -2.105982
 C    -2.893529   -1.906438   -0.867215
 H    -5.030122   -2.305668   -0.819202
 H    -4.138559   -3.464181   -1.847676
 H    -0.714483   -2.069327   -0.954907
 O    -2.953118   -1.180729    0.294982
 H    -1.535566   -3.386512   -1.834881
 C    -4.092163   -2.877031   -0.913491
 C    -1.591682   -2.739898   -0.941132
 H    -4.044955   -3.580815   -0.065519
 H    -1.509726   -3.380125   -0.046746
 O    -1.072333    1.289490   -0.493735
 C    -1.815747    2.441724   -0.466561
 C    -3.166152    2.242388    0.259407
 C    -2.103105    2.899272   -1.913239
 C    -1.037300    3.566554    0.255304
 H    -3.661305    1.340997   -0.133073
 H    -3.843636    3.109851    0.167638
 H    -2.993688    2.065170    1.336521
 H    -2.726920    2.151579   -2.429521
 H    -1.152772    2.979878   -2.466087
 H    -2.620291    3.873523   -1.967872
 H    -0.076577    3.745189   -0.255412
 H    -0.814245    3.257218    1.290258
 H    -1.589024    4.522861    0.297994
29
Figure 9_Cu-(OtBu)2_anion / electronic energy: -2106.15712863 a.u. / lowest freq: 16.07 cm-1
Cu     0.000000   -0.539536    0.000001
 O     1.743050   -0.619185   -0.567556
 C     2.750285    0.136326   -0.016010
 C     4.059753   -0.198057   -0.756660
 C     2.935008   -0.180735    1.482953
 C     2.464302    1.644928   -0.168920
 H     4.275008   -1.274381   -0.657174
 H     4.928514    0.366911   -0.378124
 H     3.943890    0.018695   -1.831004
 H     3.109171   -1.261228    1.614436
 H     2.013628    0.074766    2.033469
 H     3.776349    0.366015    1.943917
 H     1.545088    1.906102    0.382524
 H     2.290043    1.879226   -1.231876
 H     3.283509    2.285879    0.201447
 H    -2.290020    1.879251    1.231830
 H    -1.545079    1.906086   -0.382578
 H    -3.283496    2.285878   -0.201492
 C    -2.464290    1.644930    0.168881
 C    -2.750284    0.136326    0.016010
 H    -3.943869    0.018743    1.831020
 O    -1.743050   -0.619179    0.567561
 H    -2.013652    0.074711   -2.033477
 H    -4.928508    0.366936    0.378144
 H    -3.776369    0.365976   -1.943911
 C    -4.059747   -0.198030    0.756682
 C    -2.935027   -0.180769   -1.482943
 H    -4.275010   -1.274355    0.657222
 H    -3.109200   -1.261264   -1.614398
45
Figure 9_para-H-styrene-Cu-(OtBu)2_anion_01 / electronic energy: -2415.49693836 a.u. / lowest freq: 30.61 cm-1
 H     3.783420   -0.545963    2.673200
 C     4.652875   -0.193333    0.726185
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 C    3.644748   -0.623847    1.591881
 H    5.230920    0.047135   -1.342025
 C    4.454145   -0.289482   -0.650752
 C    2.454379   -1.140870    1.088434
 H    1.671339   -1.450034    1.785201
 C    3.261361   -0.806275   -1.153571
 C    2.238070   -1.241913   -0.297281
 H    3.110744   -0.866664   -2.234791
 C    0.977469   -1.752910   -0.874801
 H   -0.724957   -3.068054   -0.765674
 C    0.016665   -2.499222   -0.197542
 H    0.151523   -2.811624    0.843117
Cu   -0.555804   -0.580748   -0.216432
 H    0.936053   -1.727979   -1.969811
 H    5.582994    0.219040    1.124433
 H   -3.575350    1.708622    0.559463
 H   -2.659772    1.261537   -0.895395
 H   -4.463936    1.162839   -0.889732
 C   -3.547115    1.008629   -0.293078
 C   -3.390848   -0.439932    0.221271
 H   -4.419071   -0.087931    2.103242
 H   -5.530556   -0.590230    0.794865
 H   -2.764735   -1.175833   -1.739664
 O   -2.184609   -0.614347    0.852400
 H   -4.523153   -1.324750   -1.479347
 C   -4.523960   -0.742206    1.222517
 C   -3.538876   -1.398210   -0.984292
 H   -4.449833   -1.784874    1.573941
 H   -3.395997   -2.440232   -0.653247
 O   -0.194895    1.195461   -0.914309
 C    0.194629    2.245336   -0.117672
 C   -0.014252    1.946370    1.383323
 C   -0.623626    3.503861   -0.483920
 C    1.691273    2.557841   -0.344868
 H   -1.035562    1.566719    1.543077
 H    0.162747    2.825653    2.027842
 H    0.680969    1.151491    1.707095
 H   -1.688037    3.348955   -0.247100
 H   -0.545778    3.686283   -1.568395
 H   -0.283442    4.411401    0.045438
 H    1.872948    2.759445   -1.413820
 H    2.303365    1.686923   -0.061727
 H    2.045859    3.427861    0.236612
45
Figure 9_para-H-styrene-Cu-(OtBu)2_anion_02 / electronic energy: -2415.49618477 a.u. / lowest freq: 24.43 cm-1
 H   -3.821039   -2.889254    1.259373
 C   -4.241037   -0.778254    1.448990
 C   -3.600215   -1.884352    0.890176
 H   -4.439064    1.373695    1.394024
 C   -3.948404    0.497502    0.962367
 C   -2.677390   -1.718731   -0.141741
 H   -2.192115   -2.599644   -0.568498
 C   -3.024005    0.662431   -0.064833
 C   -2.371249   -0.441152   -0.638535
 H   -2.783785    1.664372   -0.426288
 C   -1.370495   -0.212153   -1.703334
 H   -0.561138   -2.226126   -1.926121
 C   -0.512574   -1.175377   -2.226939
 H    0.010262   -0.981246   -3.168566
Cu    0.423678   -0.146417   -0.774194
 H   -1.464420    0.746713   -2.225195
 H   -4.965270   -0.908556    2.256774
 H    3.581235    0.062622    1.451859
 H    1.825245    0.053080    1.738227
 H    2.903805   -1.070748    2.654105
 C    2.719086   -0.588486    1.677262
 C    2.514515   -1.598736    0.525863
 H    4.616163   -1.696153   -0.016427
 H    4.170298   -2.901175    1.226724
 H    0.464279   -2.052576    1.136667
 O    2.188781   -0.956407   -0.643797
 H    1.655875   -3.169313    1.854270
 C    3.823081   -2.386791    0.313550
 C    1.407044   -2.594597    0.944564
 H    3.689300   -3.141654   -0.479155
 H    1.219722   -3.310477    0.126725
 O    0.221566    1.310031    0.506808
 C    0.786431    2.534357    0.244484
 C    1.889514    2.443050   -0.833537
 C    1.413802    3.099972    1.536836
 C   -0.294385    3.523101   -0.249638
 H    2.592619    1.637811   -0.571379
 H    2.441810    3.389732   -0.969167
 H    1.443509    2.173698   -1.808248
 H    2.241084    2.452471    1.868671
 H    0.656053    3.109119    2.336889
 H    1.807091    4.124964    1.417086
 H   -1.085341    3.624832    0.511691
 H   -0.761528    3.130834   -1.168268
 H    0.103594    4.529368   -0.471433
29
Figure 9_Cu-(OtBu)2_anion / electronic energy: -2106.15712863 a.u. / lowest freq: 16.07 cm-1
Cu    0.000000   -0.539536    0.000001
 O    1.743050   -0.619185   -0.567556
 C    2.750285    0.136326   -0.016010
 C    4.059753   -0.198057   -0.756660
 C    2.935008   -0.180735    1.482953
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 C     2.464302    1.644928   -0.168920
 H     4.275008   -1.274381   -0.657174
 H     4.928514    0.366911   -0.378124
 H     3.943890    0.018695   -1.831004
 H     3.109171   -1.261228    1.614436
 H     2.013628    0.074766    2.033469
 H     3.776349    0.366015    1.943917
 H     1.545088    1.906102    0.382524
 H     2.290043    1.879226   -1.231876
 H     3.283509    2.285879    0.201447
 H    -2.290020    1.879251    1.231830
 H    -1.545079    1.906086   -0.382578
 H    -3.283496    2.285878   -0.201492
 C    -2.464290    1.644930    0.168881
 C    -2.750284    0.136326    0.016010
 H    -3.943869    0.018743    1.831020
 O    -1.743050   -0.619179    0.567561
 H    -2.013652    0.074711   -2.033477
 H    -4.928508    0.366936    0.378144
 H    -3.776369    0.365976   -1.943911
 C    -4.059747   -0.198030    0.756682
 C    -2.935027   -0.180769   -1.482943
 H    -4.275010   -1.274355    0.657222
 H    -3.109200   -1.261264   -1.614398
51
Figure 9_para-CO2Me-styrene-Cu-(OtBu)2_anion_01 / electronic energy: -2643.14335830 a.u. / lowest freq: 8.97 cm-1
 H     3.193351   -2.501304    0.308090
 C     3.510815   -0.375753    0.189639
 C     2.785691   -1.517859    0.550170
 H     3.537888    1.786325    0.220021
 C     2.987892    0.886969    0.501153
 C     1.572612   -1.404789    1.215799
 H     1.033476   -2.313153    1.492107
 C     1.772893    0.996522    1.162993
 C     1.041525   -0.143489    1.540162
 H     1.364567    1.984095    1.386038
 C    -0.252989    0.025560    2.225719
 H    -0.928790   -2.050112    2.304519
 C    -1.153688   -0.999376    2.507354
 H    -1.964887   -0.823519    3.220379
Cu    -1.655284   -0.114785    0.772991
 H    -0.405514    1.004376    2.693060
 H    -4.027532   -0.343343   -2.293586
 H    -2.273820   -0.134393   -2.067172
 H    -2.903703   -1.413421   -3.175855
 C    -3.067708   -0.882940   -2.220729
 C    -3.089594   -1.825371   -0.996597
 H    -5.229663   -2.196612   -1.056892
 H    -4.302878   -3.352011   -2.057767
 H    -0.909942   -2.015376   -0.973009
 O    -3.203609   -1.114262    0.173632
 H    -1.702127   -3.303416   -1.917506
 C    -4.295571   -2.778939   -1.114088
 C    -1.795900   -2.673530   -1.015518
 H    -4.297641   -3.494453   -0.274914
 H    -1.767666   -3.332584   -0.131573
 O    -1.206167    1.302430   -0.480460
 C    -1.915094    2.479181   -0.483900
 C    -3.291687    2.327604    0.202441
 C    -2.145401    2.934639   -1.940787
 C    -1.121146    3.581663    0.253326
 H    -3.810690    1.448435   -0.209503
 H    -3.931288    3.220858    0.092628
 H    -3.157673    2.142899    1.283780
 H    -2.773616    2.200945   -2.471145
 H    -1.177671    2.988179   -2.465800
 H    -2.634861    3.921699   -2.014790
 H    -0.142057    3.727100   -0.232184
 H    -0.936186    3.272360    1.295668
 H    -1.644127    4.554381    0.275353
 H     7.044407    1.550088   -1.525073
 H     6.597542    0.048012   -2.402266
 C     6.688054    0.519488   -1.412538
 O     5.425160    0.600048   -0.770457
 H     7.402201   -0.057727   -0.807167
 C     4.815585   -0.557479   -0.500137
 O     5.293915   -1.630990   -0.785085
51
Figure 9_para-CO2Me-styrene-Cu-(OtBu)2_anion_02 / electronic energy: -2643.14401653 a.u. / lowest freq: -0.92 cm-1
 H     2.945242   -0.961419    2.203217
 C     3.597816   -0.593670    0.183750
 C     2.664184   -0.995285    1.148686
 H     3.946245   -0.312483   -1.929752
 C     3.232266   -0.626650   -1.167264
 C     1.398658   -1.422049    0.774955
 H     0.685854   -1.711800    1.549930
 C     1.963612   -1.054139   -1.537734
 C     1.019301   -1.461343   -0.580264
 H     1.688096   -1.066138   -2.595211
 C    -0.322708   -1.878343   -1.023523
 H    -2.111385   -3.037393   -0.715181
 C    -1.273416   -2.523934   -0.235597
 H    -1.066529   -2.827126    0.795544
Cu    -1.666316   -0.560614   -0.239267
 H    -0.469867   -1.865270   -2.109220
 H    -4.449144    1.944204    0.666978
 H    -3.712498    1.365644   -0.841071
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 H   -5.507956    1.380770   -0.655233
 C   -4.547139    1.199430   -0.141323
 C   -4.428945   -0.226257    0.441902
 H   -5.266519    0.303534    2.375994
 H   -6.513057   -0.223406    1.207107
 H   -4.029097   -1.105905   -1.518649
 O   -3.182047   -0.442724    0.976462
 H   -5.761690   -1.129944   -1.094951
 C   -5.480652   -0.400673    1.555638
 C   -4.741893   -1.237474   -0.685660
 H   -5.423395   -1.420604    1.970794
 H   -4.629352   -2.266248   -0.305327
 O   -1.220048    1.168498   -0.990820
 C   -0.711046    2.197653   -0.235003
 C   -0.850820    1.933932    1.280107
 C   -1.461023    3.503335   -0.576467
 C    0.787933    2.396290   -0.553032
 H   -1.883894    1.627451    1.506071
 H   -0.574386    2.807313    1.897036
 H   -0.194738    1.096032    1.577405
 H   -2.519485    3.421063   -0.282307
 H   -1.429203    3.667935   -1.666138
 H   -1.034308    4.392043   -0.079091
 H    0.923219    2.571735   -1.633363
 H    1.347986    1.483987   -0.291819
 H    1.238847    3.243252   -0.005491
 H    7.525474    0.938724   -0.974402
 H    7.606154   -0.157147    0.446675
 C    7.040462    0.655319   -0.033138
 O    5.729367    0.230912   -0.371237
 H    7.014326    1.519412    0.646781
 C    4.940844   -0.146494    0.638979
 O    5.299432   -0.123973    1.793389
30
Figure 9_Cu-(OtBu)2_Na / electronic energy: -2268.34902130 a.u. / lowest freq: 24.55 cm-1
Cu   -0.145500    0.143878   -0.384317
Na    1.729878    2.552487    0.142140
 O    1.650416    0.461646   -0.010248
 C    2.575778   -0.582942    0.082575
 C    3.916715    0.012518    0.534562
 C    2.745245   -1.254875   -1.287017
 C    2.099517   -1.619806    1.109510
 H    4.267069    0.762279   -0.195412
 H    4.704175   -0.751652    0.632016
 H    3.803052    0.507767    1.513437
 H    3.064162   -0.512510   -2.036090
 H    1.782458   -1.676061   -1.620322
 H    3.489836   -2.067182   -1.265784
 H    1.144077   -2.062045    0.781932
 H    1.929619   -1.135991    2.084658
 H    2.827300   -2.435942    1.248346
 H   -2.475911   -2.204990    0.598228
 H   -1.726390   -1.012535    1.685966
 H   -3.468077   -1.379250    1.836005
 C   -2.642197   -1.246438    1.116123
 C   -2.915941   -0.136800    0.081686
 H   -4.111386   -1.424861   -1.198315
 O   -1.898530   -0.052830   -0.847731
 H   -2.161792    1.445449    1.371383
 H   -5.091247   -0.539194    0.005527
 H   -3.921198    1.192201    1.549921
 C   -4.220012   -0.465994   -0.666483
 C   -3.089490    1.202891    0.824926
 H   -4.426646    0.311360   -1.419553
 H   -3.271028    2.011482    0.098261
54
Figure 9_para-NMe2-styrene-Cu-(OtBu)2_Na_01 / electronic energy: -2711.56379480 a.u. / lowest freq: 25.95 cm-1
 H    0.090234    0.449078   -2.776777
 H    2.435531    0.907145   -2.501549
 H   -0.815485   -2.294763   -1.648334
 C    0.094490   -0.365685   -2.043749
 C   -0.925638   -1.305161   -2.102655
 C    2.500531    0.199453   -1.670159
 H    4.547520    0.698682   -1.313575
 C    1.370379   -0.548743   -1.317571
 C    3.708235    0.082518   -0.991538
 H   -1.698347   -1.217391   -2.872482
 C    1.509477   -1.432715   -0.236007
 C    3.847997   -0.809225    0.097157
 H    0.650898   -2.022040    0.097612
 C    2.704658   -1.565019    0.455971
 H    2.744600   -2.264701    1.290574
 H   -1.714289    4.413542    0.471485
 H   -1.242314    3.687363    2.034507
 C   -0.870950    3.984682    1.037891
 O   -1.311574    1.823320    0.163676
 H   -0.121865    4.779752    1.188186
 C   -0.301361    2.761215    0.296103
 H   -0.627785    3.589393   -1.686837
 H    0.503603    1.875299    2.113136
 C    0.211705    3.212050   -1.080770
 C    0.863664    2.181234    1.116758
 H    0.974062    4.005729   -1.010250
 H    1.686517    2.902537    1.255306
 H    0.658979    2.360985   -1.613725
 H    1.270461    1.288216    0.619029
Cu   -1.393573    0.060269   -0.696256
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 H   -1.811404   -2.829446    0.289756
 H   -2.122970   -2.282572    1.954471
 C   -2.602238   -2.662880    1.037814
 O   -3.010175   -0.405400    0.317999
 H   -3.063915   -3.637855    1.266021
 C   -3.619067   -1.632846    0.516147
 H   -3.470774   -2.287263   -1.556666
 H   -4.297014   -1.097394    2.518990
 C   -4.247359   -2.147722   -0.789309
 C   -4.729150   -1.456538    1.568978
 H   -4.772842   -3.107974   -0.655810
 H   -5.271582   -2.393109    1.779145
 H   -4.969347   -1.409271   -1.174233
 H   -5.463287   -0.709967    1.221947
Na   -3.092616    1.486896    1.310066
 H    4.390456   -1.482080    2.727997
 C    5.109114   -1.784537    1.944969
 H    6.115528   -1.721554    2.375679
 H    5.987410    0.952338    0.549876
 N    5.034266   -0.936396    0.778386
 H    4.915359   -2.844570    1.703300
 H    7.034865   -0.408557    1.018827
 C    6.170827   -0.128308    0.404097
 H    6.451849   -0.282442   -0.651778
54
Figure 9_para-NMe2-styrene-Cu-(OtBu)2_Na_02 / electronic energy: -2711.56379480 a.u. / lowest freq: 25.96 cm-1
 H   -5.987399    0.952340    0.549866
 C   -6.170821   -0.128306    0.404098
 H   -7.034856   -0.408545    1.018838
 H   -4.390448   -1.482091    2.727996
 N   -5.034260   -0.936393    0.778389
 H   -6.451851   -0.282451   -0.651773
 H   -6.115522   -1.721548    2.375684
 C   -5.109111   -1.784539    1.944968
 H   -4.915365   -2.844573    1.703295
 H    2.123004   -2.282553    1.954498
 H    1.811400   -2.829415    0.289788
 C    2.602251   -2.662860    1.037830
 O    3.010183   -0.405386    0.318007
 H    3.063923   -3.637841    1.266022
 C    3.619077   -1.632832    0.516147
 H    4.297052   -1.097370    2.518977
 H    3.470756   -2.287259   -1.556663
 C    4.729174   -1.456526    1.568963
 C    4.247350   -2.147713   -0.789316
 H    5.271597   -2.393102    1.779130
 H    4.772835   -3.107964   -0.655819
 H    5.463315   -0.709965    1.221918
 H    4.969333   -1.409264   -1.174253
Na    3.092598    1.486915    1.310080
 C   -1.370374   -0.548758   -1.317573
 C   -2.500525    0.199437   -1.670166
 C   -1.509473   -1.432725   -0.236006
 C   -2.704654   -1.565024    0.455973
 C   -3.847993   -0.809229    0.097156
 C   -3.708230    0.082505   -0.991545
 H   -0.650896   -2.022050    0.097616
 H   -2.744597   -2.264703    1.290579
 H   -4.547515    0.698668   -1.313586
 H   -2.435525    0.907125   -2.501559
 C   -0.094481   -0.365701   -2.043746
 C    0.925652   -1.305173   -2.102636
 H   -0.090224    0.449056   -2.776782
 H    0.815503   -2.294772   -1.648307
 H    1.698362   -1.217405   -2.872462
 H    1.242270    3.687373    2.034503
 H    1.714268    4.413539    0.471481
 C    0.870920    3.984684    1.037879
 O    1.311557    1.823314    0.163689
 H    0.121833    4.779755    1.188155
 C    0.301342    2.761211    0.296093
 H   -0.503653    1.875313    2.113122
 H    0.627796    3.589371   -1.686849
 C   -0.863697    2.181237    1.116735
 C   -0.211704    3.212034   -1.080791
 H   -1.686551    2.902543    1.255262
 H   -0.974060    4.005715   -1.010288
 H   -1.270485    1.288215    0.619009
 H   -0.658972    2.360966   -1.613746
Cu    1.393578    0.060270   -0.696249
30
Figure 9_Cu-(OtBu)2_Na / electronic energy: -2268.34902130 a.u. / lowest freq: 24.55 cm-1
Cu   -0.145500    0.143878   -0.384317
Na    1.729878    2.552487    0.142140
 O    1.650416    0.461646   -0.010248
 C    2.575778   -0.582942    0.082575
 C    3.916715    0.012518    0.534562
 C    2.745245   -1.254875   -1.287017
 C    2.099517   -1.619806    1.109510
 H    4.267069    0.762279   -0.195412
 H    4.704175   -0.751652    0.632016
 H    3.803052    0.507767    1.513437
 H    3.064162   -0.512510   -2.036090
 H    1.782458   -1.676061   -1.620322
 H    3.489836   -2.067182   -1.265784
 H    1.144077   -2.062045    0.781932
 H    1.929619   -1.135991    2.084658
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 H    2.827300   -2.435942    1.248346
 H   -2.475911   -2.204990    0.598228
 H   -1.726390   -1.012535    1.685966
 H   -3.468077   -1.379250    1.836005
 C   -2.642197   -1.246438    1.116123
 C   -2.915941   -0.136800    0.081686
 H   -4.111386   -1.424861   -1.198315
 O   -1.898530   -0.052830   -0.847731
 H   -2.161792    1.445449    1.371383
 H   -5.091247   -0.539194    0.005527
 H   -3.921198    1.192201    1.549921
 C   -4.220012   -0.465994   -0.666483
 C   -3.089490    1.202891    0.824926
 H   -4.426646    0.311360   -1.419553
 H   -3.271028    2.011482    0.098261
46
Figure 9_para-H-styrene-Cu-(OtBu)2_Na_01 / electronic energy: -2577.72481829 a.u. / lowest freq: 26.15 cm-1
 H    2.404371   -1.426215    2.217877
 H    1.857272   -2.445880    0.866553
 C    2.736710   -1.950285    1.306905
 O    2.403369    0.046996    0.011008
 H    3.457828   -2.731148    1.600153
 C    3.328443   -0.940216    0.309087
 H    4.266077    0.252579    1.878347
 H    2.919446   -2.195054   -1.427316
 C    4.557640   -0.270541    0.951114
 C    3.773609   -1.678367   -0.964356
 H    5.349603   -0.992186    1.210428
 H    4.557020   -2.428091   -0.764936
 H    4.988273    0.471392    0.257908
 H    4.166518   -0.955494   -1.697541
Na    2.202969    2.094209    0.616971
 C   -2.097327   -1.333228   -0.526504
 C   -3.392540   -0.903884   -0.850133
 C   -1.893822   -1.948323    0.719704
 C   -2.948853   -2.120068    1.610750
 C   -4.232541   -1.680761    1.278652
 C   -4.449850   -1.074471    0.042218
 H   -0.891133   -2.274560    1.007638
 H   -2.767077   -2.594439    2.578181
 H   -5.057220   -1.809619    1.983485
 H   -5.449698   -0.727791   -0.230313
 H   -3.570112   -0.421724   -1.815083
 C   -0.994833   -1.105150   -1.489262
 C    0.188291   -1.831012   -1.528447
 H   -1.268337   -0.515036   -2.371226
 H    0.368094   -2.672033   -0.851493
 H    0.801632   -1.808969   -2.434391
 H   -0.050540    3.950151    1.418870
 H    0.125594    4.359474   -0.311931
 C   -0.565228    3.945887    0.442237
 O    0.184030    1.742217   -0.013682
 H   -1.429421    4.626243    0.518694
 C   -0.967589    2.509008    0.060692
 H   -1.405605    1.950980    2.117188
 H   -0.998591    2.887011   -2.078082
 C   -1.913344    1.953864    1.138836
 C   -1.690982    2.538559   -1.294670
 H   -2.842125    2.541030    1.233361
 H   -2.573058    3.200159   -1.290919
 H   -2.187717    0.915307    0.902073
 H   -2.027511    1.527283   -1.565912
Cu    0.541305   -0.093084   -0.584753
46
Figure 9_para-H-styrene-Cu-(OtBu)2_Na_02 / electronic energy: -2577.72480787 a.u. / lowest freq: 31.39 cm-1
 H    1.255243   -0.534268   -2.361628
 H    3.564379   -0.438844   -1.827357
 H   -0.357796   -2.690752   -0.817788
 C    0.991276   -1.119957   -1.473854
 C   -0.189018   -1.851089   -1.499224
 C    3.394569   -0.911641   -0.856403
 H    5.456356   -0.728340   -0.254390
 C    2.102104   -1.338053   -0.518148
 C    4.458844   -1.072671    0.029443
 H   -0.809282   -1.837322   -2.400531
 C    1.908506   -1.940402    0.735863
 C    4.251303   -1.666057    1.273796
 H    0.908233   -2.264220    1.034659
 C    2.970450   -2.102449    1.620463
 H    5.081414   -1.787060    1.973643
 H    2.796383   -2.566899    2.594115
 H   -0.135480    4.339437   -0.344370
 H    0.075250    3.962099    1.389846
 C    0.571960    3.943805    0.404052
 O   -0.170166    1.727663    0.000197
 H    1.432256    4.631686    0.452681
 C    0.977153    2.503253    0.039453
 H    0.966933    2.850417   -2.104988
 H    1.456034    1.981864    2.095997
 C    1.674729    2.515168   -1.329609
 C    1.946295    1.972258    1.108832
 H    2.554936    3.178911   -1.351783
 H    2.872284    2.567520    1.177486
 H    2.008804    1.500997   -1.592428
 H    2.223879    0.931971    0.883707
Cu   -0.538573   -0.109309   -0.559328
 H   -1.969083   -2.538101    0.750861
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 H   -2.477241   -1.590149    2.167903
 C   -2.826254   -2.030443    1.219623
 O   -2.383548    0.039419    0.079152
 H   -3.588710   -2.792393    1.451908
 C   -3.356506   -0.922864    0.294216
 H   -2.974686   -2.048606   -1.530915
 H   -4.253437    0.198188    1.936076
 C   -3.816052   -1.539514   -1.036668
 C   -4.560874   -0.244163    0.972866
 H   -4.628518   -2.273545   -0.906411
 H   -5.387729   -0.944939    1.174518
 H   -4.171865   -0.746370   -1.714071
 H   -4.950795    0.564024    0.331313
Na   -2.171847    2.085175    0.679041
30
Figure 9_Cu-(OtBu)2_Na / electronic energy: -2268.34902130 a.u. / lowest freq: 24.55 cm-1
Cu   -0.145500    0.143878   -0.384317
Na    1.729878    2.552487    0.142140
 O    1.650416    0.461646   -0.010248
 C    2.575778   -0.582942    0.082575
 C    3.916715    0.012518    0.534562
 C    2.745245   -1.254875   -1.287017
 C    2.099517   -1.619806    1.109510
 H    4.267069    0.762279   -0.195412
 H    4.704175   -0.751652    0.632016
 H    3.803052    0.507767    1.513437
 H    3.064162   -0.512510   -2.036090
 H    1.782458   -1.676061   -1.620322
 H    3.489836   -2.067182   -1.265784
 H    1.144077   -2.062045    0.781932
 H    1.929619   -1.135991    2.084658
 H    2.827300   -2.435942    1.248346
 H   -2.475911   -2.204990    0.598228
 H   -1.726390   -1.012535    1.685966
 H   -3.468077   -1.379250    1.836005
 C   -2.642197   -1.246438    1.116123
 C   -2.915941   -0.136800    0.081686
 H   -4.111386   -1.424861   -1.198315
 O   -1.898530   -0.052830   -0.847731
 H   -2.161792    1.445449    1.371383
 H   -5.091247   -0.539194    0.005527
 H   -3.921198    1.192201    1.549921
 C   -4.220012   -0.465994   -0.666483
 C   -3.089490    1.202891    0.824926
 H   -4.426646    0.311360   -1.419553
 H   -3.271028    2.011482    0.098261
52
Figure 9_para-CO2Me-styrene-Cu-(OtBu)2_Na_01 / electronic energy: -2805.37090024 a.u. / lowest freq: 24.12 cm-1
 H   -2.227102   -2.408675   -1.975181
 H   -1.886356   -2.896267   -0.298449
 C   -2.686866   -2.785149   -1.047001
 O   -3.188787   -0.533149   -0.370212
 H   -3.105656   -3.785121   -1.247685
 C   -3.747080   -1.789086   -0.547986
 H   -4.434432   -1.316028   -2.564332
 H   -3.587772   -2.427372    1.531618
 C   -4.857063   -1.671333   -1.608564
 C   -4.364327   -2.306432    0.761425
 H   -5.365212   -2.630188   -1.802509
 H   -4.870154   -3.277683    0.633058
 H   -5.618402   -0.945094   -1.277776
 H   -5.101424   -1.579770    1.139701
Na   -3.349387    1.311841   -1.449362
 C    1.129747   -0.365687    1.469872
 C    2.154946    0.496068    1.888844
 C    1.412750   -1.287057    0.446763
 C    2.669923   -1.339151   -0.139416
 C    3.684009   -0.469023    0.282966
 C    3.414097    0.447581    1.303880
 H    0.631110   -1.959144    0.085493
 H    2.868867   -2.056016   -0.936939
 H    4.204568    1.124672    1.632894
 H    1.956149    1.220694    2.682030
 C   -0.206631   -0.261506    2.094867
 C   -1.156777   -1.274929    2.091868
 H   -0.315987    0.553206    2.818841
 H   -0.949759   -2.254405    1.650351
 H   -1.977345   -1.242312    2.814766
 H   -1.489586    3.489394   -2.279328
 H   -2.131199    4.291406   -0.815763
 C   -1.220767    3.878761   -1.281644
 O   -1.603615    1.760509   -0.283302
 H   -0.509506    4.707680   -1.431132
 C   -0.640617    2.749157   -0.410983
 H    0.348937    1.783854   -2.090144
 H   -1.164100    3.716304    1.464053
 C    0.614870    2.189804   -1.100332
 C   -0.265168    3.320417    0.964615
 H    1.399214    2.952417   -1.239612
 H    0.481761    4.128859    0.899829
 H    1.040396    1.368658   -0.505861
 H    0.150235    2.525019    1.600709
Cu   -1.629130    0.044011    0.652777
 H    6.735858   -0.565528   -2.380992
 H    6.380810   -2.308209   -2.627530
 C    6.460546   -1.507056   -1.883834
 O    5.947561    0.250155    0.027687
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 O    5.184469   -1.403854   -1.268634
 C    5.049891   -0.483111   -0.313265
 H    7.234198   -1.759818   -1.144420
52
Figure 9_para-CO2Me-styrene-Cu-(OtBu)2_Na_02 / electronic energy: -2805.37090023 a.u. / lowest freq: 24.12 cm-1
 H    2.227088   -2.408698    1.975162
 H    1.886344   -2.896274    0.298426
 C    2.686853   -2.785165    1.046980
 O    3.188780   -0.533160    0.370212
 H    3.105640   -3.785140    1.247655
 C    3.747070   -1.789100    0.547975
 H    4.434422   -1.316064    2.564327
 H    3.587762   -2.427371   -1.531635
 C    4.857053   -1.671360    1.608555
 C    4.364317   -2.306437   -0.761440
 H    5.365199   -2.630217    1.802490
 H    4.870142   -3.277689   -0.633080
 H    5.618393   -0.945119    1.277775
 H    5.101415   -1.579773   -1.139710
Na    3.349382    1.311819    1.449383
 C   -1.129746   -0.365669   -1.469873
 C   -2.154953    0.496072   -1.888855
 C   -1.412738   -1.287029   -0.446753
 C   -2.669910   -1.339130    0.139427
 C   -3.684007   -0.469018   -0.282966
 C   -3.414105    0.447576   -1.303891
 H   -0.631091   -1.959102   -0.085475
 H   -2.868847   -2.055987    0.936960
 H   -4.204583    1.124655   -1.632914
 H   -1.956164    1.220690   -2.682049
 C    0.206631   -0.261483   -2.094870
 C    1.156774   -1.274910   -2.091878
 H    0.315987    0.553232   -2.818839
 H    0.949752   -2.254388   -1.650367
 H    1.977343   -1.242290   -2.814776
 H    1.489590    3.489394    2.279340
 H    2.131216    4.291401    0.815780
 C    1.220779    3.878763    1.281656
 O    1.603617    1.760506    0.283319
 H    0.509522    4.707687    1.431139
 C    0.640626    2.749162    0.410992
 H   -0.348950    1.783865    2.090145
 H    1.164127    3.716301   -1.464044
 C   -0.614871    2.189819    1.100332
 C    0.265189    3.320423   -0.964609
 H   -1.399209    2.952440    1.239608
 H   -0.481732    4.128874   -0.899826
 H   -1.040400    1.368678    0.505856
 H   -0.150222    2.525030   -1.600704
Cu    1.629128    0.044017   -0.652775
 H   -6.735860   -0.565544    2.380988
 H   -6.380792   -2.308219    2.627535
 C   -6.460535   -1.507071    1.883835
 O   -5.947568    0.250135   -0.027695
 O   -5.184458   -1.403857    1.268637
 C   -5.049890   -0.483117    0.313263
 H   -7.234183   -1.759846    1.144421
20
Figure 10_NaOtBu-Cu-Me / electronic energy: -2075.35042459 a.u. / lowest freq: -32.54 cm-1
 C    3.221953   -0.519783    0.005284
Cu    1.340621   -0.098414   -0.003574
 H   -1.478034   -0.703054    2.162038
 H   -2.872543    1.024179    0.909696
 C   -1.474379   -1.325291    1.252498
 H   -2.320455   -2.029699    1.309466
 H   -0.538976   -1.908847    1.249832
 C   -2.835665    0.380576    0.014006
 H   -3.735891   -0.255014    0.021840
 O   -0.460359    0.451662   -0.010641
 C   -1.535470   -0.437480    0.000568
 H   -2.889157    1.026293   -0.879249
 C   -1.499572   -1.324249   -1.252987
 H   -2.344961   -2.030679   -1.292138
 H   -0.562929   -1.905455   -1.270822
 H   -1.524495   -0.701430   -2.161767
Na   -0.283095    2.541783    0.000274
 H    3.773445   -0.116646   -0.868202
 H    3.392415   -1.615852   -0.011246
 H    3.759300   -0.145330    0.900091
20
Figure 10_NaOtBu-Cu-Me_(145 deg) / electronic energy: -2075.34278322 a.u. / lowest freq: -11.41 cm-1
 C    3.195215   -0.262666   -0.051898
Cu    1.263689   -0.487463    0.029147
 H   -1.831025   -0.333351    2.159192
 H   -2.689612    1.599521    0.724063
 C   -1.906132   -0.992334    1.279333
 H   -2.890815   -1.487800    1.299861
 H   -1.127516   -1.767434    1.373859
 C   -2.748329    0.906532   -0.132060
 H   -3.769710    0.493818   -0.163307
 O   -0.423371    0.421053    0.035304
 C   -1.675416   -0.185382   -0.007261
 H   -2.590393    1.488072   -1.055644
 C   -1.757456   -1.125594   -1.219805
 H   -2.738037   -1.621777   -1.308863
 H   -0.981938   -1.905746   -1.138783
 H   -1.569365   -0.562837   -2.148283
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Na     0.490811    2.309283    0.012562
 H     3.502156    0.307366   -0.952765
 H     3.795164   -1.195700   -0.080440
 H     3.584856    0.308403    0.815381
20
Figure 10_NaOtBu-Cu-Me_(130 deg) / electronic energy: -2075.33621269 a.u. / lowest freq: 39.95 cm-1
 C     3.078089   -0.114627    0.061990
Cu     1.187825   -0.646941   -0.031046
 H    -1.756989    0.004668    2.184804
 H    -2.562606    1.862453    0.644384
 C    -1.931260   -0.719798    1.372819
 H    -2.945101   -1.137046    1.491874
 H    -1.203813   -1.539946    1.495099
 C    -2.716296    1.113910   -0.150771
 H    -3.764415    0.776105   -0.099299
 O    -0.423511    0.451462   -0.071281
 C    -1.718673   -0.043176    0.008539
 H    -2.566563    1.613147   -1.122152
 C    -1.947595   -1.074677   -1.107720
 H    -2.961210   -1.508135   -1.089814
 H    -1.217984   -1.896228   -1.004647
 H    -1.786391   -0.607058   -2.092349
Na     0.964399    2.049368   -0.027059
 H     3.377518    0.537870   -0.786355
 H     3.826453   -0.932510    0.055377
 H     3.308296    0.463444    0.982176
20
Figure 10_NaOtBu-Cu-Me_(115 deg) / electronic energy: -2075.32884553 a.u. / lowest freq: -9.37 cm-1
 C     2.967293    0.132829   -0.000767
Cu     1.192350   -0.780537    0.000271
 H    -1.778825   -0.255234    2.162147
 H    -2.475729    1.835265    0.891198
 C    -1.963858   -0.849723    1.252903
 H    -2.991152   -1.247818    1.301812
 H    -1.262066   -1.701570    1.264195
 C    -2.656724    1.212470   -0.000374
 H    -3.719583    0.918651    0.000204
 O    -0.394071    0.448667   -0.001628
 C    -1.706469    0.004698   -0.000128
 H    -2.476368    1.834309   -0.892732
 C    -1.965784   -0.851662   -1.251428
 H    -2.993071   -1.250048   -1.298076
 H    -1.263826   -1.703369   -1.262586
 H    -1.782306   -0.258466   -2.161825
Na     1.015181    1.993192    0.000270
 H     3.116662    0.783457   -0.891541
 H     3.869331   -0.510426   -0.000766
 H     3.117603    0.784698    0.888933
41
Figure 10_NaOtBu_ts(SN2')_01 / electronic energy: -2914.15039392 a.u. / lowest freq: -228.67 cm-1
 C    -0.133094    1.641930    0.888602
 C    -0.109601    0.311855    1.410961
 C    -0.394483   -0.775481    0.594068
 O    -2.474046   -1.200585    0.654651
 P    -3.206729   -0.242235   -0.276157
 O    -2.458145    0.566270   -1.290113
 O    -4.375642   -1.068664   -1.070636
 O    -4.092757    0.717543    0.715289
 C    -5.205559   -1.951004   -0.351809
 H    -0.038295    2.483054    1.580733
 H    -0.742875    1.824144   -0.004812
 H     0.123875    0.139860    2.465948
 H    -0.529283   -0.628906   -0.478302
 H    -0.219160   -1.791042    0.946132
 C     2.067390    2.723518   -0.431623
Cu     1.553396    0.927315    0.244784
 H    -5.948589   -2.361446   -1.051201
 H    -5.740163   -1.435195    0.465012
 H    -4.630018   -2.783875    0.084911
 C    -4.867026    1.745031    0.142700
 H    -5.396342    2.263655    0.955414
 H    -5.615969    1.348019   -0.565108
 H    -4.239205    2.473617   -0.396528
 H     2.726718   -2.093093   -1.960110
 H     5.078024   -1.450532   -1.360188
 C     2.523054   -2.331177   -0.903870
 H     2.714929   -3.404980   -0.748498
 H     1.454263   -2.146269   -0.720404
 C     4.865737   -1.688200   -0.302923
 H     5.166514   -2.734591   -0.136851
 O     3.105578   -0.099001   -0.224531
 C     3.380036   -1.449696    0.012823
 H     5.501491   -1.053057    0.337842
 C     3.116431   -1.805802    1.481502
 H     3.362172   -2.856439    1.704432
 H     2.056270   -1.645041    1.728422
 H     3.719942   -1.161031    2.140476
Na     4.415903    1.335318   -1.064931
 H     2.967944    3.070536    0.111648
 H     1.324567    3.529154   -0.348381
 H     2.283518    2.616014   -1.512574
41
Figure 10_NaOtBu_ts(SN2')_02 / electronic energy: -2914.15050466 a.u. / lowest freq: -245.56 cm-1
 C     0.204603    1.632068   -0.753728
 C     0.153844    0.335556   -1.351030
 C     0.395826   -0.805753   -0.594310
 O     2.456431   -1.277184   -0.638687
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 P     3.188157   -0.303001    0.279269
 O     2.461707    0.407061    1.379004
 O     4.465421   -1.153260    0.847306
 O     3.921145    0.842875   -0.634660
 C     5.328178   -0.532068    1.772580
 H     0.156540    2.513698   -1.398536
 H     0.787815    1.746173    0.168156
 H    -0.059717    0.230092   -2.419017
 H     0.508840   -0.727398    0.487711
 H     0.201258   -1.793813   -1.008910
 C    -2.020936    2.715909    0.531567
Cu    -1.521390    0.934825   -0.195478
 H     6.099247   -1.261901    2.057900
 H     4.786606   -0.211756    2.677980
 H     5.826000    0.352219    1.337417
 C     4.638695    0.450886   -1.781178
 H     4.942285    1.359954   -2.320543
 H     4.020361   -0.172501   -2.447800
 H     5.547170   -0.119646   -1.518758
 H    -2.762672   -2.085972    1.923447
 H    -5.099953   -1.420456    1.303610
 C    -2.551009   -2.320267    0.867888
 H    -2.753836   -3.390795    0.704098
 H    -1.478264   -2.147410    0.696988
 C    -4.879210   -1.648619    0.245898
 H    -5.188901   -2.690110    0.065918
 O    -3.102308   -0.076676    0.200321
 C    -3.387841   -1.422337   -0.051586
 H    -5.502186   -1.000349   -0.394224
 C    -3.111027   -1.768561   -1.520064
 H    -3.356285   -2.817217   -1.752729
 H    -2.048195   -1.607477   -1.754776
 H    -3.706730   -1.118101   -2.180431
Na    -4.403268    1.349697    1.068951
 H    -2.900733    3.095935   -0.023507
 H    -1.263051    3.510702    0.492083
 H    -2.267585    2.581144    1.602816
41
Figure 10_NaOtBu_ts(SN2')_03 / electronic energy: -2914.14886171 a.u. / lowest freq: -234.18 cm-1
 C     0.175881   -1.769436    0.698062
 C     0.107876   -0.550200    1.440967
 C     0.401262    0.661994    0.831975
 O     2.486465    1.098685    1.046471
 P     3.271593    0.299934    0.015376
 O     2.546715   -0.286730   -1.165408
 O     4.546092    1.198761   -0.494744
 O     4.095696   -0.832859    0.843511
 C     4.313658    2.188905   -1.466982
 H     0.064313   -2.720239    1.226122
 H     0.825741   -1.785684   -0.185677
 H    -0.177014   -0.564146    2.497387
 H     0.595034    0.699296   -0.240810
 H     0.197164    1.602411    1.341970
 C    -1.959255   -2.639854   -0.846824
Cu    -1.491186   -0.964070    0.109377
 H     5.268450    2.693479   -1.674618
 H     3.592040    2.946328   -1.112205
 H     3.928238    1.754997   -2.405206
 C     4.909552   -1.743015    0.139714
 H     5.145576   -2.580049    0.812888
 H     5.854333   -1.271880   -0.180497
 H     4.395116   -2.137035   -0.752051
 H    -2.601264    2.232369   -1.734660
 H    -4.984597    1.541560   -1.284699
 C    -2.441880    2.374937   -0.653976
 H    -2.644458    3.430401   -0.410854
 H    -1.380548    2.174757   -0.444795
 C    -4.806393    1.690779   -0.205261
 H    -5.105172    2.722912    0.036494
 O    -3.054568    0.090557   -0.223998
 C    -3.333714    1.412118    0.139299
 H    -5.468759    1.013098    0.360855
 C    -3.125909    1.614695    1.645236
 H    -3.374076    2.639554    1.964544
 H    -2.077983    1.418428    1.917118
 H    -3.758367    0.913273    2.212849
Na    -4.391408   -1.269594   -1.142919
 H    -2.820684   -3.119210   -0.342128
 H    -1.181445   -3.412008   -0.927302
 H    -2.225324   -2.360904   -1.885114
41
Figure 10_NaOtBu_ts(SN2')_04 / electronic energy: -2914.14810523 a.u. / lowest freq: -261.78 cm-1
 C     0.157622    1.766949   -0.675694
 C     0.189061    0.493544   -1.321172
 C     0.477803   -0.660162   -0.598361
 O     2.556118   -0.983744   -0.570752
 P     3.173712   -0.052668    0.478806
 O     2.323589    0.513579    1.568787
 O     4.465981   -0.832276    1.111936
 O     3.885390    1.207581   -0.281050
 C     4.914832   -2.071372    0.614054
 H     0.068330    2.670269   -1.285162
 H     0.714190    1.877471    0.262826
 H     0.007557    0.416835   -2.397484
 H     0.547394   -0.617080    0.489410
 H     0.351765   -1.640602   -1.056177
 C    -2.131353    2.666629    0.632167
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Cu   -1.533623    0.951766   -0.178454
 H    5.711096   -2.427090    1.284483
 H    5.332441   -1.987028   -0.403738
 H    4.111112   -2.824103    0.592217
 C    4.817564    0.963450   -1.305615
 H    5.016654    1.914827   -1.820240
 H    4.430687    0.239887   -2.043312
 H    5.772061    0.582299   -0.901595
 H   -2.644439   -2.174810    1.813851
 H   -5.015189   -1.614605    1.166558
 C   -2.416210   -2.384572    0.756635
 H   -2.578900   -3.458966    0.574211
 H   -1.349029   -2.170705    0.597380
 C   -4.763740   -1.812334    0.109486
 H   -5.015905   -2.864864   -0.094861
 O   -3.068405   -0.153405    0.136605
 C   -3.280304   -1.504107   -0.154818
 H   -5.406849   -1.184784   -0.531379
 C   -2.961260   -1.797363   -1.626110
 H   -3.157499   -2.848574   -1.891478
 H   -1.902048   -1.584801   -1.836006
 H   -3.572186   -1.154674   -2.280217
Na   -4.460361    1.187792    1.001849
 H   -3.013878    3.046188    0.080699
 H   -1.405631    3.491504    0.656964
 H   -2.393844    2.458666    1.688153
41
Figure 10_NaOtBu_ts(SN2)_01 / electronic energy: -2914.14526307 a.u. / lowest freq: -335.11 cm-1
 C   -0.732684   -1.213624   -0.880529
 C   -0.264324   -0.058796   -1.562968
 C    0.190900    1.043628   -0.854185
 O   -2.832123   -0.973348   -0.865731
 P   -3.198401   -0.057021    0.298439
 O   -2.229970    0.172855    1.416603
 O   -3.625247    1.410034   -0.290956
 O   -4.630434   -0.633961    0.840038
 C   -4.450852    1.477387   -1.429892
 H   -0.878866   -2.150013   -1.411944
 H   -0.799534   -1.215580    0.207863
 H   -0.188981   -0.093928   -2.654183
 H   -0.119027    1.175111    0.188498
 H    0.564670    1.923021   -1.383340
 C    1.795388   -2.603076   -0.645151
Cu    1.448961   -0.619260   -0.589894
 H   -4.638809    2.538500   -1.649056
 H   -5.421696    0.979031   -1.261944
 H   -3.970968    1.010210   -2.305453
 C   -5.236378   -0.005429    1.946438
 H   -6.194265   -0.509747    2.139062
 H   -5.437254    1.062136    1.749816
 H   -4.606864   -0.077816    2.848823
 H    2.683468    1.915352    2.151859
 H    4.897334    0.672365    2.074589
 C    2.865125    2.252651    1.118798
 H    3.396203    3.217343    1.160468
 H    1.887953    2.423751    0.644942
 C    5.029559    0.998131    1.028129
 H    5.624512    1.925208    1.044825
 O    3.005170   -0.041606    0.379657
 C    3.662370    1.190441    0.350484
 H    5.614910    0.230512    0.494618
 C    3.879460    1.643872   -1.099228
 H    4.437544    2.592001   -1.162000
 H    2.909531    1.785771   -1.601557
 H    4.438954    0.874354   -1.654923
Na    3.467846   -1.841269    1.395093
 H    1.291848   -3.149399   -1.458682
 H    1.509394   -3.135643    0.284258
 H    2.879222   -2.747612   -0.830491
41
Figure 10_NaOtBu_ts(SN2)_02 / electronic energy: -2914.14552014 a.u. / lowest freq: -358.84 cm-1
 C   -0.757372   -1.334434   -0.646208
 C   -0.288972   -0.305406   -1.507229
 C    0.173805    0.892643   -0.984462
 O   -2.844563   -1.086815   -0.642155
 P   -3.205192    0.041156    0.320711
 O   -2.216331    0.511992    1.340559
 O   -3.710440    1.268807   -0.638576
 O   -4.579915   -0.360720    1.109013
 C   -4.044002    2.498247   -0.036990
 H   -0.913423   -2.341325   -1.022726
 H   -0.802319   -1.167762    0.430250
 H   -0.224626   -0.512710   -2.579697
 H   -0.131401    1.186625    0.025850
 H    0.549072    1.673346   -1.649953
 C    1.764032   -2.703551   -0.266289
Cu    1.431881   -0.727215   -0.475289
 H   -4.383736    3.182790   -0.827728
 H   -3.176659    2.947584    0.474190
 H   -4.858226    2.386884    0.700412
 C   -5.672410   -0.874819    0.382329
 H   -6.476039   -1.102759    1.097238
 H   -5.401497   -1.798132   -0.155780
 H   -6.053075   -0.144271   -0.352605
 H    2.678474    2.083731    1.891189
 H    4.922115    0.904300    1.915997
 C    2.845901    2.322028    0.828626
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 H     3.356804    3.296587    0.770106
 H     1.862170    2.427829    0.349544
 C     5.037577    1.118075    0.839075
 H     5.609445    2.055221    0.749267
 O     3.035640   -0.031814    0.320326
 C     3.660076    1.207056    0.160077
 H     5.637467    0.313007    0.381809
 C     3.854150    1.515730   -1.329963
 H     4.379449    2.470390   -1.493954
 H     2.877977    1.573048   -1.836478
 H     4.436229    0.712083   -1.808759
Na     3.652147   -1.705538    1.460193
 H     1.178247   -3.368259   -0.920446
 H     1.578848   -3.074415    0.762544
 H     2.822576   -2.896011   -0.536808
41
Figure 10_NaOtBu_ts(SN2)_03 / electronic energy: -2914.14400540 a.u. / lowest freq: -344.79 cm-1
 C    -0.834209   -1.009869   -0.954730
 C    -0.349902    0.239919   -1.423615
 C     0.140810    1.181885   -0.533632
 O    -2.943841   -0.709672   -0.831634
 P    -3.220430    0.130474    0.419753
 O    -2.257679    0.055714    1.563798
 O    -3.407053    1.690129   -0.000598
 O    -4.759985   -0.180375    0.885176
 C    -4.184879    2.029576   -1.125056
 H    -1.027094   -1.824778   -1.646859
 H    -0.895084   -1.207036    0.116202
 H    -0.292763    0.406352   -2.503692
 H    -0.142333    1.120117    0.522756
 H     0.526854    2.135754   -0.899573
 C     1.656995   -2.490366   -1.024534
Cu     1.368091   -0.541914   -0.610415
 H    -4.016789    3.094108   -1.343305
 H    -5.260156    1.875122   -0.932482
 H    -3.899424    1.433453   -2.007425
 C    -5.092086   -1.495154    1.263144
 H    -6.170352   -1.527133    1.476302
 H    -4.546285   -1.805320    2.171354
 H    -4.869663   -2.216472    0.458248
 H     2.826799    1.464703    2.425043
 H     5.001629    0.251992    1.994107
 C     2.936720    1.973164    1.453918
 H     3.470374    2.922753    1.620179
 H     1.929055    2.211922    1.085673
 C     5.077147    0.756821    1.015377
 H     5.678192    1.668573    1.159879
 O     3.006891   -0.154989    0.316031
 C     3.674696    1.063395    0.463633
 H     5.627374    0.098893    0.321245
 C     3.813447    1.761980   -0.895390
 H     4.363938    2.713671   -0.822148
 H     2.819186    1.975575   -1.318020
 H     4.347002    1.107273   -1.602911
Na     3.616672   -2.104170    0.870856
 H     1.036711   -2.927797   -1.822173
 H     1.500276   -3.144431   -0.142719
 H     2.701881   -2.597584   -1.380211
41
Figure 10_NaOtBu_ts(SN2)_04 / electronic energy: -2914.14390216 a.u. / lowest freq: -336.71 cm-1
 C    -0.777866   -1.131968   -1.018650
 C    -0.228421   -0.013683   -1.701733
 C     0.229140    1.086673   -0.992859
 O    -2.865703   -0.800589   -1.098259
 P    -3.264471    0.102769    0.064300
 O    -2.286508    0.305988    1.188959
 O    -3.742359    1.509906   -0.591801
 O    -4.711571   -0.397830    0.648190
 C    -4.128317    2.567570    0.257242
 H    -0.935849   -2.073700   -1.537315
 H    -0.904263   -1.101206    0.063991
 H    -0.092111   -0.079105   -2.785505
 H    -0.132843    1.251291    0.028298
 H     0.671034    1.937089   -1.516792
 C     1.660920   -2.625846   -0.579323
Cu     1.396451   -0.628747   -0.603822
 H    -4.172166    3.487956   -0.342882
 H    -3.403251    2.710369    1.075231
 H    -5.123413    2.387139    0.698210
 C    -4.734208   -1.546309    1.461890
 H    -5.783266   -1.772482    1.701570
 H    -4.181387   -1.389554    2.403645
 H    -4.301472   -2.420564    0.944129
 H     2.659510    1.955818    2.115723
 H     4.797900    0.602836    2.155066
 C     2.877635    2.238449    1.073282
 H     3.443915    3.183902    1.085352
 H     1.917992    2.423272    0.569314
 C     4.980813    0.878360    1.101756
 H     5.625193    1.772093    1.102402
 O     2.929938   -0.083849    0.420623
 C     3.648063    1.112828    0.370902
 H     5.540186    0.060111    0.617613
 C     3.935455    1.501203   -1.085623
 H     4.536491    2.421637   -1.162813
 H     2.990604    1.664759   -1.627227
 H     4.478762    0.687615   -1.592634
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Na     3.294391   -1.870562    1.494277
 H     1.157222   -3.186797   -1.382583
 H     1.330428   -3.108494    0.362722
 H     2.742813   -2.818324   -0.729218
41
Figure 10_NaOtBu_ts(SN2')_chelate_01 / electronic energy: -2914.16942813 a.u. / lowest freq: -376.99 cm-1
 C    -0.898843    2.812291   -0.598162
 C    -0.256736    1.756285   -1.294793
 C     0.422121    0.729934   -0.614745
 O     2.335256    0.832044   -0.608703
 P     2.965349   -0.370449    0.121676
 O     2.026676   -1.238263    0.920216
 O     3.752169   -1.311234   -0.917243
 O     4.199991    0.180356    1.007598
 C     4.672743   -0.752335   -1.840011
 H    -1.436400    3.577319   -1.164848
 H    -0.506538    3.148650    0.368795
 H    -0.423454    1.642656   -2.370170
 H     0.412287    0.759975    0.476055
 H     0.442314   -0.247572   -1.094318
 C    -3.389316    2.200912    0.783950
Cu    -1.921811    1.205036   -0.081306
 H     4.230920    0.105398   -2.370765
 H     4.926027   -1.533789   -2.568262
 H     5.592766   -0.425880   -1.330219
 C     3.975177    1.207315    1.957023
 H     4.931013    1.408283    2.458466
 H     3.237802    0.896471    2.715103
 H     3.622789    2.130039    1.469563
 H    -2.681735   -1.266533   -2.205633
 H    -1.732599   -3.144875   -0.736916
 C    -3.511323   -1.163832   -1.487412
 H    -4.343077   -1.803956   -1.823790
 H    -3.857609   -0.116792   -1.515509
 C    -2.579787   -2.988730   -0.046670
 H    -3.382352   -3.680252   -0.347499
 O    -1.939095   -0.718296    0.276297
 C    -3.029723   -1.517162   -0.072138
 H    -2.271552   -3.284590    0.972500
 C    -4.180872   -1.329933    0.927566
 H    -5.030706   -1.998252    0.712202
 H    -4.546834   -0.293127    0.902380
 H    -3.828784   -1.538599    1.950720
Na    -0.121379   -1.681379    1.038767
 H    -3.255233    3.287707    0.909917
 H    -3.537442    1.756291    1.784030
 H    -4.314773    2.041960    0.201509
41
Figure 10_NaOtBu_ts(SN2')_chelate_02 / electronic energy: -2914.16958209 a.u. / lowest freq: -387.04 cm-1
 C    -0.896930    2.729544   -0.745099
 C    -0.325434    1.612074   -1.406465
 C     0.365147    0.613514   -0.695716
 O     2.272996    0.676378   -0.780429
 P     2.928135   -0.370722    0.142671
 O     1.997635   -1.175611    1.013297
 O     3.824797   -1.394279   -0.711766
 O     4.077611    0.378848    0.999609
 C     4.774361   -0.909900   -1.647035
 H    -1.447650    3.473044   -1.327700
 H    -0.436910    3.114441    0.172661
 H    -0.555005    1.435159   -2.461435
 H     0.405690    0.717527    0.388890
 H     0.344670   -0.397161   -1.100611
 C    -3.357151    2.261319    0.780168
Cu    -1.927033    1.194240   -0.055309
 H     4.312356   -0.205324   -2.356306
 H     5.160603   -1.775440   -2.200925
 H     5.611897   -0.408959   -1.136406
 C     3.766397    1.576557    1.688375
 H     4.687590    1.931509    2.168888
 H     3.006396    1.405760    2.469132
 H     3.400244    2.349214    0.994193
 H    -2.125569   -1.432111   -2.103515
 H    -1.558582   -3.205321   -0.372493
 C    -3.093375   -1.286467   -1.596799
 H    -3.833565   -1.954802   -2.065960
 H    -3.416867   -0.246191   -1.775300
 C    -2.515459   -2.997797    0.139147
 H    -3.252018   -3.719962   -0.246771
 O    -1.965677   -0.700134    0.446575
 C    -2.945659   -1.537936   -0.087578
 H    -2.395051   -3.200962    1.217960
 C    -4.295145   -1.298154    0.605086
 H    -5.077437   -1.984331    0.241413
 H    -4.635713   -0.266638    0.429405
 H    -4.190140   -1.437850    1.692730
Na    -0.141505   -1.586318    1.279189
 H    -3.118207    3.308654    1.029267
 H    -3.668772    1.745449    1.705116
 H    -4.218879    2.273541    0.087787
41
Figure 10_NaOtBu_ts(SN2')_chelate_03 / electronic energy: -2914.17005408 a.u. / lowest freq: -394.05 cm-1
 C    -1.057672    2.830908   -0.366436
 C    -0.480719    1.833566   -1.193824
 C     0.276337    0.777518   -0.648620
 O     2.157996    0.931923   -0.786648
 P     2.873155   -0.176807   -0.000220
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 O    2.031556   -1.261276    0.622313
 O    3.966544   -0.892802   -0.950160
 O    3.760497    0.596254    1.109371
 C    4.849524   -0.100882   -1.728498
 H   -1.666310    3.617669   -0.820714
 H   -0.566448    3.113778    0.571557
 H   -0.744316    1.789299   -2.254699
 H    0.336872    0.728228    0.439818
 H    0.274594   -0.167512   -1.189532
 C   -3.375359    2.041347    1.256238
Cu   -1.997305    1.173123    0.146612
 H    4.290815    0.547487   -2.421005
 H    5.483801   -0.784910   -2.307474
 H    5.491601    0.528819   -1.090968
 C    4.548063   -0.153215    2.019371
 H    5.116797    0.559883    2.630637
 H    5.257132   -0.811108    1.490786
 H    3.917135   -0.769298    2.679261
 H   -2.283270   -1.035261   -2.272701
 H   -1.559599   -3.068571   -0.937719
 C   -3.218352   -1.012919   -1.690008
 H   -3.976212   -1.602859   -2.230770
 H   -3.571243    0.032742   -1.650212
 C   -2.490243   -2.996648   -0.346862
 H   -3.230244   -3.657193   -0.825408
 O   -1.974830   -0.779245    0.357210
 C   -2.967728   -1.536376   -0.266432
 H   -2.303718   -3.398871    0.664504
 C   -4.273281   -1.476280    0.540552
 H   -5.065953   -2.102862    0.099882
 H   -4.643108   -0.440753    0.590185
 H   -4.094390   -1.818961    1.572225
Na   -0.092201   -1.743267    0.938092
 H   -3.138719    3.044943    1.647175
 H   -3.578426    1.375090    2.113044
 H   -4.305593    2.126769    0.665088
41
Figure 10_NaOtBu_ts(SN2')_chelate_04 / electronic energy: -2914.17005409 a.u. / lowest freq: -394.05 cm-1
 C   -1.057675   -2.830911    0.366431
 C   -0.480721   -1.833570    1.193819
 C    0.276336   -0.777523    0.648617
 O    2.157997   -0.931925    0.786648
 P    2.873155    0.176808    0.000222
 O    2.031555    1.261281   -0.622303
 O    3.966548    0.892798    0.950162
 O    3.760491   -0.596251   -1.109375
 C    4.849530    0.100874    1.728494
 H   -1.666314   -3.617671    0.820708
 H   -0.566453   -3.113779   -0.571563
 H   -0.744317   -1.789305    2.254695
 H    0.336873   -0.728232   -0.439821
 H    0.274594    0.167507    1.189530
 C   -3.375365   -2.041341   -1.256238
Cu   -1.997306   -1.173122   -0.146613
 H    4.290822   -0.547499    2.420999
 H    5.483808    0.784898    2.307472
 H    5.491605   -0.528825    1.090960
 C    4.548057    0.153219   -2.019373
 H    5.116792   -0.559876   -2.630640
 H    5.257126    0.811112   -1.490788
 H    3.917129    0.769304   -2.679262
 H   -2.283264    1.035260    2.272703
 H   -1.559593    3.068571    0.937721
 C   -3.218347    1.012921    1.690012
 H   -3.976204    1.602863    2.230775
 H   -3.571242   -0.032739    1.650216
 C   -2.490238    2.996649    0.346866
 H   -3.230239    3.657195    0.825410
 O   -1.974828    0.779246   -0.357207
 C   -2.967724    1.536378    0.266436
 H   -2.303713    3.398871   -0.664501
 C   -4.273277    1.476282   -0.540548
 H   -5.065950    2.102864   -0.099876
 H   -4.643105    0.440756   -0.590182
 H   -4.094387    1.818965   -1.572221
Na   -0.092201    1.743266   -0.938098
 H   -3.138725   -3.044936   -1.647180
 H   -3.578435   -1.375080   -2.113041
 H   -4.305596   -2.126766   -0.665084
41
Figure 10_NaOtBu_ts(SN2')_chelate_05 / electronic energy: -2914.16875021 a.u. / lowest freq: -369.05 cm-1
 C   -1.172153   -2.808136    0.653399
 C   -0.526574   -1.766145    1.367148
 C    0.281014   -0.820744    0.710962
 O    2.174151   -1.037026    0.914188
 P    2.962265   -0.076282    0.014741
 O    2.157933    0.976321   -0.718639
 O    4.155618    0.608310    0.865329
 O    3.818509   -0.991000   -0.991535
 C    3.845629    1.602876    1.823469
 H   -1.810893   -3.512087    1.193639
 H   -0.719356   -3.206679   -0.261929
 H   -0.779201   -1.594915    2.417844
 H    0.365412   -0.915896   -0.372910
 H    0.334095    0.179562    1.136708
 C   -3.513974   -2.072034   -0.946303
Cu   -2.037438   -1.162312   -0.009685
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 H    3.455056    2.514690    1.343871
 H    4.773301    1.851171    2.356048
 H    3.107397    1.236865    2.556287
 C    4.706454   -0.399240   -1.925155
 H    4.998200   -1.177638   -2.642290
 H    5.609601   -0.018650   -1.423067
 H    4.222807    0.426414   -2.470890
 H   -2.188636    1.436537    2.081539
 H   -1.320408    3.176553    0.449654
 C   -3.121334    1.386321    1.496765
 H   -3.836806    2.108450    1.923005
 H   -3.547705    0.375912    1.621383
 C   -2.250002    3.071577   -0.137716
 H   -2.946272    3.848854    0.214154
 O   -1.883523    0.740380   -0.460347
 C   -2.827086    1.652952    0.012260
 H   -2.030553    3.288570   -1.198132
 C   -4.128108    1.550867   -0.797492
 H   -4.878402    2.291466   -0.475719
 H   -4.567910    0.548108   -0.687199
 H   -3.920214    1.711227   -1.867447
Na    0.061288    1.469883   -1.167598
 H   -3.390455   -3.149277   -1.145680
 H   -3.660344   -1.556299   -1.911694
 H   -4.435877   -1.946016   -0.349857
41
Figure 10_NaOtBu_ts(SN2')_chelate_06 / electronic energy: -2914.16875021 a.u. / lowest freq: -369.05 cm-1
 C   -1.172156    2.808137   -0.653399
 C   -0.526577    1.766146   -1.367147
 C    0.281012    0.820746   -0.710962
 O    2.174150    1.037028   -0.914189
 P    2.962264    0.076283   -0.014742
 O    2.157932   -0.976326    0.718631
 O    4.155623   -0.608302   -0.865327
 O    3.818501    0.991000    0.991541
 C    3.845642   -1.602869   -1.823470
 H   -1.810898    3.512087   -1.193638
 H   -0.719360    3.206680    0.261929
 H   -0.779204    1.594916   -2.417843
 H    0.365410    0.915899    0.372911
 H    0.334094   -0.179561   -1.136707
 C   -3.513977    2.072029    0.946304
Cu   -2.037439    1.162311    0.009685
 H    3.455074   -2.514686   -1.343874
 H    4.773317   -1.851157   -2.356047
 H    3.107409   -1.236862   -2.556289
 C    4.706445    0.399239    1.925161
 H    4.998179    1.177633    2.642306
 H    5.609598    0.018661    1.423077
 H    4.222801   -0.426425    2.470885
 H   -2.188614   -1.436554   -2.081537
 H   -1.320406   -3.176562   -0.449637
 C   -3.121316   -1.386330   -1.496771
 H   -3.836789   -2.108459   -1.923013
 H   -3.547682   -0.375921   -1.621399
 C   -2.250004   -3.071578    0.137728
 H   -2.946273   -3.848857   -0.214141
 O   -1.883522   -0.740381    0.460348
 C   -2.827083   -1.652954   -0.012263
 H   -2.030560   -3.288564    1.198146
 C   -4.128112   -1.550861    0.797477
 H   -4.878406   -2.291459    0.475701
 H   -4.567910   -0.548100    0.687178
 H   -3.920228   -1.711218    1.867435
Na    0.061289   -1.469882    1.167600
 H   -3.390454    3.149270    1.145691
 H   -3.660355    1.556287    1.911690
 H   -4.435877    1.946022    0.349852
41
Figure 10_NaOtBu_ts(SN2)_chelate_01 / electronic energy: -2914.16222070 a.u. / lowest freq: -483.33 cm-1
 C    0.046666    1.813381    2.480662
 C   -0.009687    1.011423    1.408180
 C    0.222636    1.492657    0.053696
 O    2.227549    1.250165   -0.051063
 P    2.716352   -0.181094   -0.244801
 O    1.764508   -1.216225   -0.787407
 O    4.013897   -0.183335   -1.213228
 O    3.311954   -0.639053    1.192657
 C    5.063890    0.739305   -0.984731
 H   -0.098836    1.416887    3.488545
 H    0.237812    2.886269    2.380943
 H   -0.204763   -0.057714    1.526682
 H    0.162569    0.843032   -0.815021
 H    0.371953    2.553908   -0.127469
 C   -2.143516    3.124776   -0.572567
Cu   -2.022836    1.205096   -0.419704
 H    4.707126    1.777508   -1.071488
 H    5.833868    0.559095   -1.746867
 H    5.513301    0.599670    0.012624
 C    3.837889   -1.943005    1.349686
 H    4.343226   -1.984041    2.324037
 H    4.571819   -2.182780    0.562730
 H    3.040402   -2.703109    1.331384
 H   -4.220002   -1.148783   -1.820027
 H   -2.776811   -3.135403   -1.105123
 C   -4.398745   -0.928589   -0.755528
 H   -5.323378   -1.440696   -0.443739
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 H   -4.563337    0.158493   -0.660359
 C   -2.973300   -2.866868   -0.052595
 H   -3.853108   -3.442645    0.274521
 O   -2.032299   -0.699689   -0.378755
 C   -3.182209   -1.350184    0.082619
 H   -2.121118   -3.198828    0.566647
 C   -3.427276   -1.000814    1.557935
 H   -4.315057   -1.509609    1.967333
 H   -3.575144    0.086441    1.670315
 H   -2.554572   -1.285194    2.167541
Na   -0.284341   -1.840653   -0.937175
 H   -1.887616    3.667084    0.355626
 H   -3.205986    3.348348   -0.798167
 H   -1.540581    3.560493   -1.390088
41
Figure 10_NaOtBu_ts(SN2)_chelate_02 / electronic energy: -2914.16232564 a.u. / lowest freq: -494.81 cm-1
 C    0.111537    1.774155    2.433287
 C    0.020953    0.960961    1.371463
 C    0.339325    1.390947    0.017320
 O    2.328379    1.002285    0.034889
 P    2.766746   -0.430896   -0.278881
 O    1.700810   -1.406755   -0.706400
 O    3.913674   -0.433504   -1.407756
 O    3.613704   -0.991627    0.987124
 C    5.014382    0.453362   -1.311013
 H   -0.103027    1.410461    3.441300
 H    0.397449    2.824892    2.324988
 H   -0.272728   -0.084509    1.496977
 H    0.276412    0.719789   -0.834308
 H    0.572669    2.433420   -0.182350
 C   -1.863836    3.148311   -0.720292
Cu   -1.899376    1.230582   -0.518970
 H    4.676948    1.494474   -1.188195
 H    5.586560    0.369785   -2.244554
 H    5.667882    0.185990   -0.465113
 C    3.085250   -0.861773    2.292241
 H    3.836298   -1.246442    2.995679
 H    2.160319   -1.450338    2.414478
 H    2.870572    0.191762    2.533785
 H   -4.254426   -1.110586   -1.802645
 H   -2.912548   -3.114076   -0.950780
 C   -4.419036   -0.811520   -0.755256
 H   -5.363765   -1.260794   -0.408680
 H   -4.535469    0.285630   -0.733871
 C   -3.079331   -2.758968    0.081059
 H   -3.977952   -3.268987    0.461589
 O   -2.043372   -0.665734   -0.399729
 C   -3.219249   -1.228625    0.108387
 H   -2.231804   -3.082920    0.710904
 C   -3.441880   -0.765908    1.556073
 H   -4.353923   -1.198361    1.998590
 H   -3.533056    0.332726    1.592879
 H   -2.584613   -1.053051    2.185964
Na   -0.366010   -1.917891   -0.937687
 H   -1.587993    3.689643    0.202520
 H   -2.904045    3.439502   -0.971439
 H   -1.217179    3.522371   -1.534452
41
Figure 10_NaOtBu_ts(SN2)_chelate_03 / electronic energy: -2914.16068298 a.u. / lowest freq: -481.78 cm-1
 C   -0.072475    1.980003    2.489954
 C   -0.068055    1.123402    1.459210
 C    0.202727    1.544144    0.091685
 O    2.226701    1.377201    0.089244
 P    2.786853   -0.034706   -0.034395
 O    1.903256   -1.088505   -0.668147
 O    4.217009    0.021185   -0.794888
 O    3.270066   -0.484427    1.435541
 C    4.246000    0.200992   -2.197833
 H   -0.247201    1.633053    3.511356
 H    0.098962    3.050506    2.341497
 H   -0.243492    0.056786    1.623419
 H    0.213831    0.848247   -0.742703
 H    0.330056    2.599288   -0.134996
 C   -2.186919    3.064120   -0.641660
Cu   -1.995289    1.154536   -0.449995
 H    3.798311   -0.658793   -2.721983
 H    5.298053    0.293954   -2.498995
 H    3.712731    1.119016   -2.496104
 C    3.791375   -1.783697    1.644419
 H    4.187029   -1.820741    2.668366
 H    4.610022   -2.007017    0.941779
 H    3.009389   -2.553054    1.538935
 H   -4.024812   -1.248769   -1.909489
 H   -2.566755   -3.199200   -1.143236
 C   -4.259789   -1.039345   -0.853699
 H   -5.187291   -1.573544   -0.591162
 H   -4.452719    0.043368   -0.760508
 C   -2.820583   -2.947672   -0.098817
 H   -3.698793   -3.550866    0.180102
 O   -1.923015   -0.751890   -0.352275
 C   -3.077000   -1.438866    0.041290
 H   -1.990470   -3.263975    0.557594
 C   -3.406117   -1.112436    1.505370
 H   -4.305109   -1.641811    1.860590
 H   -3.578623   -0.029362    1.621624
 H   -2.562507   -1.389750    2.157605
Na   -0.107122   -1.834853   -0.790194
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 H   -1.966066    3.629459    0.281628
 H   -3.253731    3.243409   -0.885339
 H   -1.588983    3.509835   -1.457376
41
Figure 10_NaOtBu_ts(SN2)_chelate_04 / electronic energy: -2914.16231279 a.u. / lowest freq: -469.13 cm-1
 C   -0.007558   -2.229703    2.308588
 C    0.098439   -2.566992    1.016047
 C    0.008269   -1.582873   -0.047139
 O   -2.049968   -1.445741   -0.229074
 P   -2.456067    0.004462   -0.450443
 O   -1.851631    0.794685   -1.582505
 O   -4.063021    0.096282   -0.598294
 O   -2.146820    0.752666    0.967044
 C   -4.890052   -0.628828    0.295568
 H    0.030077   -2.986291    3.096474
 H   -0.152348   -1.188676    2.612302
 H    0.220208   -3.612649    0.722425
 H    0.055561   -0.524953    0.202954
 H    0.002637   -1.888518   -1.089046
 C    2.761345   -2.835110   -0.716559
Cu    2.209692   -0.995419   -0.531182
 H   -4.751797   -1.713874    0.171386
 H   -5.932273   -0.369912    0.065788
 H   -4.680173   -0.363322    1.344759
 C   -2.336841    2.148411    1.079563
 H   -2.097021    2.436131    2.112065
 H   -3.382143    2.429794    0.868622
 H   -1.680451    2.707133    0.392215
 H    4.144359    1.988657   -0.449395
 H    2.062676    3.449862   -0.803624
 C    3.739826    1.688573    0.530347
 H    4.147794    2.367321    1.296631
 H    4.102147    0.669514    0.747211
 C    1.710107    3.123055    0.189479
 H    2.066108    3.857866    0.928579
 O    1.745183    0.847525   -0.516377
 C    2.205917    1.701227    0.492973
 H    0.606635    3.159127    0.203351
 C    1.646627    1.250164    1.850500
 H    1.965310    1.908370    2.674852
 H    1.987036    0.226257    2.078244
 H    0.544696    1.243764    1.818386
Na    0.189370    1.443491   -1.897944
 H    2.918475   -3.320911    0.264093
 H    3.735977   -2.844776   -1.244589
 H    2.076945   -3.478958   -1.297952
41
Figure 10_NaOtBu_ts(SN2)_chelate_05 / electronic energy: -2914.16125846 a.u. / lowest freq: -469.63 cm-1
 C   -0.118222    1.944440    2.408962
 C    0.067334    2.325416    1.137419
 C    0.147299    1.374031    0.043174
 O    2.186343    1.047702    0.083898
 P    2.658023   -0.344623   -0.336185
 O    1.732447   -1.184786   -1.177374
 O    4.066310   -0.252491   -1.110863
 O    3.119426   -1.147013    1.002964
 C    5.149077    0.468347   -0.551816
 H   -0.144469    2.675431    3.221050
 H   -0.256774    0.891441    2.671566
 H    0.199109    3.381782    0.889608
 H   -0.037926    0.319173    0.235675
 H    0.307652    1.709688   -0.976203
 C   -2.295600    3.023429   -0.889789
Cu   -2.052671    1.127812   -0.635708
 H    4.863848    1.506643   -0.319266
 H    5.955652    0.478809   -1.296999
 H    5.516855   -0.016823    0.366369
 C    2.309929   -1.087934    2.158586
 H    2.847614   -1.596026    2.970966
 H    1.346634   -1.605960    2.006637
 H    2.114138   -0.044615    2.455281
 H   -4.398729   -1.436211   -1.020053
 H   -2.616661   -3.271425   -0.911020
 C   -4.184382   -1.205987    0.035739
 H   -4.869322   -1.794700    0.667028
 H   -4.401547   -0.136710    0.199394
 C   -2.420706   -2.987749    0.137056
 H   -3.045106   -3.630171    0.777812
 O   -1.884300   -0.761038   -0.513362
 C   -2.709311   -1.494123    0.347502
 H   -1.366156   -3.214021    0.373053
 C   -2.405465   -1.117373    1.804815
 H   -3.020517   -1.685696    2.520956
 H   -2.595399   -0.043232    1.966524
 H   -1.344839   -1.313994    2.030924
Na   -0.296364   -1.640663   -1.689386
 H   -2.489169    3.538686    0.069151
 H   -3.190491    3.173263   -1.526471
 H   -1.458813    3.550777   -1.382434
41
Figure 10_NaOtBu_ts(SN2)_chelate_06 / electronic energy: -2914.16058712 a.u. / lowest freq: -465.65 cm-1
 C   -0.393806    2.273412    2.458188
 C   -0.327149    2.592776    1.158680
 C   -0.084286    1.597641    0.130543
 O    1.988562    1.519317    0.218909
 P    2.475849    0.102318   -0.049635
 O    2.013789   -0.588778   -1.314768
```

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 O    4.090572    0.051230    0.057603
 O    2.069960   -0.772035    1.252316
 C    4.874887    0.528881   -1.019275
 H   -0.545994    3.039243    3.223187
 H   -0.283840    1.238449    2.795924
 H   -0.421462    3.633065    0.837170
 H   -0.127405    0.541826    0.389834
 H    0.043136    1.889549   -0.907863
 C   -2.784376    2.770638   -0.835996
Cu   -2.184603    0.950097   -0.621201
 H    4.659970   -0.022801   -1.948668
 H    5.930216    0.380168   -0.754259
 H    4.702414    1.603603   -1.194431
 C    2.322482   -2.162443    1.294804
 H    1.765565   -2.578930    2.144792
 H    3.396000   -2.363194    1.442229
 H    1.993728   -2.664235    0.370208
 H   -3.931073   -2.216595   -0.880874
 H   -1.706856   -3.480613   -1.004224
 C   -3.680216   -1.915650    0.148789
 H   -4.118282   -2.650601    0.843318
 H   -4.155429   -0.938386    0.338040
 C   -1.502679   -3.157632    0.030870
 H   -1.873362   -3.944978    0.705789
 O   -1.654683   -0.871955   -0.615807
 C   -2.158641   -1.796018    0.305873
 H   -0.409888   -3.093503    0.173943
 C   -1.814386   -1.352087    1.735561
 H   -2.170414   -2.069048    2.492876
 H   -2.273745   -0.372467    1.949043
 H   -0.722348   -1.248529    1.844397
Na    0.047209   -1.289646   -1.879095
 H   -3.162758    3.187489    0.115958
 H   -3.631731    2.767774   -1.550919
 H   -2.036571    3.481910   -1.230308
18
Figure 10_PMe3-Cu-Me / electronic energy: -2141.10632939 a.u. / lowest freq: 48.24 cm-1
 C   -3.174210   -0.000111    0.003034
Cu   -1.218128   -0.000017   -0.004377
 H    1.485695    1.864495   -1.486105
 H    1.472200    2.375435    0.220479
 H    2.900550    1.513940   -0.440413
 C    1.802113    1.585071   -0.470122
 H    1.484538   -1.003352   -2.163699
 P    1.016556    0.000356   -0.001208
 H    2.904425   -1.146053   -1.076522
 C    1.806153   -1.203373   -1.130683
 H    1.460582    0.354164    2.360314
 H    2.889868   -0.362876    1.546358
 C    1.790846   -0.381789    1.612029
 H    1.483705   -2.220634   -0.863119
 H    1.465084   -1.378167    1.945957
 H   -3.603801    0.847389    0.574237
 H   -3.603301   -0.916753    0.455292
 H   -3.611599    0.068762   -1.013271
18
Figure 10_PMe3-Cu-Me_(145 deg) / electronic energy: -2141.09872349 a.u. / lowest freq: 70.67 cm-1
 C    2.986403    0.429986    0.001317
Cu    1.209233   -0.403967   -0.002538
 H   -2.134640   -1.649554   -1.405264
 H   -2.266471   -2.064939    0.321256
 H   -3.305403   -0.775455   -0.367257
 C   -2.305420   -1.235190   -0.400235
 H   -1.132841    0.985699   -2.206823
 P   -0.993945   -0.020999   -0.000828
 H   -2.376578    1.680456   -1.116316
 C   -1.333018    1.334833   -1.183242
 H   -1.529418   -0.096182    2.370291
 H   -2.600021    1.060874    1.514468
 C   -1.569682    0.679821    1.590594
 H   -0.656624    2.176598   -0.972123
 H   -0.901078    1.500563    1.889487
 H    3.173312    0.957950    0.958111
 H    3.028690    1.211355   -0.784702
 H    3.872806   -0.214028   -0.165717
18
Figure 10_PMe3-Cu-Me_(130 deg) / electronic energy: -2141.09184945 a.u. / lowest freq: 64.28 cm-1
 C   -2.793067    0.634795    0.003198
Cu   -1.209852   -0.548529   -0.000796
 H    2.491441   -1.854450    0.548946
 H    2.364824   -1.620937   -1.211470
 H    3.382906   -0.510902   -0.237068
 C    2.449785   -1.096300   -0.247739
 H    1.416395    0.166783    2.383349
 P    0.974752   -0.035139    0.000431
 H    2.379267    1.363576    1.455654
 C    1.398590    0.868943    1.536305
 H    1.077859    0.788383   -2.284234
 H    2.176859    1.731554   -1.223537
 C    1.189601    1.247965   -1.290435
 H    0.627057    1.627213    1.737473
 H    0.403187    2.009430   -1.178877
 H   -2.698455    1.374689   -0.817631
 H   -2.819705    1.229379    0.939308
 H   -3.806671    0.197286   -0.103270
18
Figure 10_PMe3-Cu-Me_(115 deg) / electronic energy: -2141.08375606 a.u. / lowest freq: 53.84 cm-1
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 C   -2.523187    0.860312    0.018122
Cu   -1.240498   -0.655287   -0.018743
 H    2.637532   -1.753029    0.461357
 H    2.489760   -1.447281   -1.285540
 H    3.396412   -0.294798   -0.253736
 C    2.521929   -0.963755   -0.297257
 H    1.362090    0.063118    2.387118
 P    0.948757   -0.059198   -0.007318
 H    2.243148    1.366834    1.527303
 C    1.298745    0.801914    1.573915
 H    0.945775    0.903025   -2.244070
 H    2.035189    1.826601   -1.157993
 C    1.067047    1.305864   -1.227140
 H    0.475018    1.493639    1.804268
 H    0.255507    2.026002   -1.045499
 H   -2.485771    1.405727   -0.947115
 H   -2.198057    1.591325    0.786240
 H   -3.600725    0.684099    0.215153
39
Figure 10_PMe3_ts(SN2')_01 / electronic energy: -2979.90366207 a.u. / lowest freq: -311.45 cm-1
 C    0.127563    2.071313    0.221292
 C    0.103908    1.076812    1.228954
 C   -0.143248   -0.269568    0.937382
 O   -2.172044   -0.670485    1.292540
 P   -2.876243   -0.576753   -0.059972
 O   -2.316636   -1.263607   -1.261928
 O   -4.417030   -1.016380    0.257215
 O   -3.040548    1.009149   -0.455363
 C   -5.325802   -1.107936   -0.817611
 H    0.286269    3.116117    0.498956
 H   -0.424360    1.906662   -0.710472
 H    0.354453    1.346761    2.259571
 H   -0.288794   -0.608708   -0.091654
 H    0.083403   -1.034963    1.677734
 C    2.610225    2.197270   -1.324632
Cu    1.755649    0.963446   -0.048576
 H   -6.292702   -1.439558   -0.412833
 H   -4.985685   -1.834960   -1.573030
 H   -5.468829   -0.132587   -1.314667
 C   -3.496380    1.925100    0.511597
 H   -3.330144    2.940976    0.123959
 H   -2.954881    1.812279    1.465029
 H   -4.575193    1.799120    0.710584
 H    1.543670   -2.735327    0.256537
 H    1.863694   -2.357054   -1.455308
 H    3.077299   -3.272287   -0.501758
 C    2.328939   -2.466223   -0.464387
 H    3.046497   -1.439472    2.382309
 P    3.101891   -0.886756    0.023114
 H    4.535508   -2.081214    1.610927
 C    3.843916   -1.226062    1.655375
 H    4.177458   -0.637363   -2.131385
 H    5.184729   -1.623928   -1.024142
 C    4.533654   -0.739401   -1.095724
 H    4.392945   -0.336072    1.997270
 H    5.113496    0.159349   -0.839632
 H    2.706084    1.665063   -2.286928
 H    3.625814    2.405679   -0.944526
 H    2.104170    3.156945   -1.508170
39
Figure 10_PMe3_ts(SN2')_02 / electronic energy: -2979.90320903 a.u. / lowest freq: -287.91 cm-1
 C    0.003084    1.938674   -0.029517
 C   -0.018094    0.984289    1.017301
 C   -0.159841   -0.380593    0.745408
 O   -2.215703   -0.882820    0.889535
 P   -2.928366   -0.187386   -0.275418
 O   -2.213610   -0.053459   -1.583297
 O   -4.395028   -0.897948   -0.439048
 O   -3.422085    1.289115    0.195833
 C   -4.439637   -2.260435   -0.791177
 H    0.089837    3.001175    0.210328
 H   -0.495726    1.691069   -0.973345
 H    0.147933    1.299293    2.052129
 H   -0.232038   -0.732037   -0.285609
 H    0.035154   -1.119509    1.521476
 C    2.569047    2.111031   -1.449660
Cu    1.701534    0.910364   -0.153020
 H   -5.495179   -2.560784   -0.858306
 H   -3.940460   -2.891190   -0.035650
 H   -3.961297   -2.441217   -1.769504
 C   -4.011418    1.469293    1.462468
 H   -4.020297    2.546790    1.682570
 H   -3.443652    0.947523    2.249993
 H   -5.050990    1.099677    1.478321
 H    1.709026   -2.730466   -0.115553
 H    2.435052   -2.200428   -1.655690
 H    3.412778   -3.149427   -0.489610
 C    2.636239   -2.375578   -0.588347
 H    2.583114   -1.565326    2.417781
 P    3.163211   -0.809619    0.186695
 H    4.251900   -2.063661    1.984144
 C    3.513207   -1.249973    1.922634
 H    4.710160   -0.299173   -1.606710
 H    5.478219   -1.355159   -0.376201
 C    4.809885   -0.494119   -0.528911
 H    3.903567   -0.367005    2.450043
 H    5.253170    0.394532   -0.056012
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 H    2.779999    1.516433   -2.355924
 H    3.532358    2.430868   -1.015274
 H    2.006773    3.007882   -1.750348
39
Figure 10_PMe3_ts(SN2')_03 / electronic energy: -2979.90323285 a.u. / lowest freq: -289.25 cm-1
 C    0.061900    2.006077    0.342722
 C    0.096930    0.960089    1.295536
 C   -0.093769   -0.371568    0.911403
 O   -2.129041   -0.853469    1.207613
 P   -2.938491   -0.270664    0.053558
 O   -2.234291    0.045069   -1.236744
 O   -4.233945   -1.236636   -0.217354
 O   -3.722548    1.022237    0.649166
 C   -4.014864   -2.478650   -0.842608
 H    0.182497    3.041743    0.669339
 H   -0.500608    1.847163   -0.585005
 H    0.349150    1.177420    2.337967
 H   -0.261709   -0.619505   -0.138137
 H    0.157177   -1.180541    1.595940
 C    2.540147    2.336480   -1.184563
Cu    1.728351    0.974924   -0.015452
 H   -4.988511   -2.973754   -0.968818
 H   -3.368559   -3.130833   -0.228984
 H   -3.547870   -2.356718   -1.834972
 C   -4.541980    1.789124   -0.204400
 H   -4.698697    2.771439    0.264606
 H   -5.524182    1.309101   -0.352883
 H   -4.070377    1.937155   -1.189767
 H    1.669099   -2.735454    0.255093
 H    1.941843   -2.352111   -1.464699
 H    3.207759   -3.214879   -0.529640
 C    2.428969   -2.438680   -0.482126
 H    3.182963   -1.371985    2.345673
 P    3.145187   -0.825715   -0.016568
 H    4.671586   -1.957987    1.530118
 C    3.948296   -1.130668    1.593500
 H    4.151612   -0.537347   -2.200136
 H    5.234192   -1.468278   -1.116006
 C    4.538355   -0.617326   -1.173518
 H    4.472237   -0.218456    1.915713
 H    5.080092    0.309582   -0.934802
 H    2.859603    1.840514   -2.117234
 H    3.442246    2.710148   -0.667925
 H    1.910529    3.199608   -1.449317
39
Figure 10_PMe3_ts(SN2')_04 / electronic energy: -2979.90323285 a.u. / lowest freq: -289.26 cm-1
 C    0.061897    2.006075    0.342717
 C    0.096926    0.960090    1.295533
 C   -0.093770   -0.371569    0.911403
 O   -2.129039   -0.853471    1.207611
 P   -2.938490   -0.270665    0.053557
 O   -2.234292    0.045064   -1.236747
 O   -4.233948   -1.236634   -0.217349
 O   -3.722541    1.022240    0.649165
 C   -4.014871   -2.478648   -0.842605
 H    0.182490    3.041743    0.669330
 H   -0.500608    1.847156   -0.585013
 H    0.349143    1.177424    2.337964
 H   -0.261708   -0.619509   -0.138137
 H    0.157178   -1.180539    1.595942
 C    2.540152    2.336481   -1.184556
Cu    1.728351    0.974924   -0.015449
 H   -4.988520   -2.973747   -0.968817
 H   -3.368570   -3.130835   -0.228981
 H   -3.547876   -2.356717   -1.834968
 C   -4.541970    1.789131   -0.204401
 H   -4.698683    2.771446    0.264606
 H   -5.524173    1.309112   -0.352885
 H   -4.070365    1.937160   -1.189767
 H    1.669100   -2.735457    0.255096
 H    1.941837   -2.352112   -1.464696
 H    3.207757   -3.214880   -0.529643
 C    2.428967   -2.438682   -0.482125
 H    3.182969   -1.371983    2.345673
 P    3.145185   -0.825716   -0.016568
 H    4.671587   -1.957991    1.530113
 C    3.948300   -1.130670    1.593496
 H    4.151603   -0.537350   -2.200140
 H    5.234189   -1.468278   -1.116011
 C    4.538349   -0.617327   -1.173523
 H    4.472245   -0.218459    1.915707
 H    5.080086    0.309582   -0.934809
 H    2.859631    1.840515   -2.117219
 H    3.442237    2.710164   -0.667904
 H    1.910528    3.199601   -1.449327
39
Figure 10_PMe3_ts(SN2)_01 / electronic energy: -2979.90175960 a.u. / lowest freq: -328.91 cm-1
 C   -0.587825   -1.223973   -0.734058
 C   -0.083496   -0.182075   -1.544717
 C    0.430553    0.981582   -0.963620
 O   -2.674085   -0.892840   -0.660659
 P   -3.004909    0.112743    0.447403
 O   -1.912357    0.548083    1.374183
 O   -3.757899    1.391249   -0.253456
 O   -4.251212   -0.443323    1.326376
 C   -3.076632    2.100866   -1.258116
 H   -0.767092   -2.212690   -1.151431
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 H   -0.615750   -1.104462    0.349166
 H   -0.012191   -0.345248   -2.624415
 H    0.094052    1.256224    0.043552
 H    0.835918    1.777459   -1.593745
 C    2.084845   -2.551452   -0.227979
Cu    1.629771   -0.645861   -0.507719
 H   -3.765740    2.851498   -1.672343
 H   -2.750047    1.435256   -2.075921
 H   -2.191378    2.626381   -0.858517
 C   -5.375670   -0.999401    0.682036
 H   -6.007400   -1.468783    1.449716
 H   -5.078848   -1.763762   -0.054163
 H   -5.966560   -0.224348    0.165291
 H    2.503299    0.572287    2.656473
 H    3.431109   -0.920492    2.356585
 H    4.297379    0.625582    2.651955
 C    3.411658    0.166233    2.187150
 H    2.523906    2.749542    0.670289
 P    3.360947    0.491001    0.394757
 H    4.312582    2.707401    0.795952
 C    3.441291    2.307214    0.255131
 H    5.070250   -1.162470   -0.059763
 H    5.800287    0.436583    0.297056
 C    4.978235   -0.079016   -0.222487
 H    3.515867    2.589777   -0.805372
 H    5.051960    0.118403   -1.302134
 H    3.170609   -2.676830   -0.071769
 H    1.795910   -3.195456   -1.076546
 H    1.574617   -2.943270    0.669947
39
Figure 10_PMe3_ts(SN2)_02 / electronic energy: -2979.90254477 a.u. / lowest freq: -358.42 cm-1
 C    0.503120    1.408040   -0.473593
 C   -0.016433    0.575394   -1.492168
 C   -0.497039   -0.701994   -1.193734
 O    2.578614    1.163855   -0.571750
 P    2.976610   -0.052709    0.259082
 O    1.992790   -0.680693    1.197235
 O    3.548731   -1.138571   -0.825918
 O    4.321514    0.308178    1.115161
 C    4.032024   -2.372670   -0.345523
 H    0.637922    2.473468   -0.647084
 H    0.569123    1.039000    0.550656
 H   -0.123514    0.988339   -2.499848
 H   -0.133452   -1.204217   -0.289042
 H   -0.902274   -1.336073   -1.986301
 C   -2.174355    2.498571    0.438690
Cu   -1.708085    0.735208   -0.331615
 H    4.163436   -3.046526   -1.204411
 H    3.324023   -2.831698    0.364176
 H    5.006038   -2.257028    0.161426
 C    5.394445    0.961220    0.475211
 H    6.234778    0.999858    1.183215
 H    5.126500    1.990829    0.185543
 H    5.721480    0.420975   -0.430005
 H   -2.598665   -1.303815    2.402672
 H   -3.560426    0.194983    2.506686
 H   -4.390785   -1.388791    2.347842
 C   -3.509983   -0.801964    2.044978
 H   -2.577943   -2.874877   -0.085256
 P   -3.428365   -0.625710    0.232296
 H   -4.367968   -2.869677    0.022261
 C   -3.491934   -2.340900   -0.383771
 H   -5.169809    1.059812    0.223166
 H   -5.865277   -0.589301    0.097534
 C   -5.047564    0.067979   -0.235434
 H   -3.551761   -2.337377   -1.482127
 H   -5.097170    0.183158   -1.328325
 H   -3.262657    2.575978    0.609921
 H   -1.879987    3.350284   -0.198723
 H   -1.677707    2.633750    1.416423
39
Figure 10_PMe3_ts(SN2)_03 / electronic energy: -2979.90254477 a.u. / lowest freq: -358.42 cm-1
 C   -0.503120   -1.408036   -0.473599
 C    0.016439   -0.575389   -1.492170
 C    0.497048    0.701997   -1.193732
 O   -2.578615   -1.163843   -0.571769
 P   -2.976613    0.052710    0.259077
 O   -1.992793    0.680689    1.197234
 O   -3.548743    1.138580   -0.825910
 O   -4.321513   -0.308190    1.115157
 C   -4.032044    2.372670   -0.345500
 H   -0.637924   -2.473463   -0.647090
 H   -0.569129   -1.038996    0.550651
 H    0.123525   -0.988334   -2.499850
 H    0.133458    1.204219   -0.289041
 H    0.902288    1.336076   -1.986296
 C    2.174350   -2.498570    0.438703
Cu    1.708086   -0.735208   -0.331608
 H   -4.163459    3.046536   -1.204380
 H   -3.324047    2.831694    0.364205
 H   -5.006058    2.257017    0.161446
 C   -5.394444   -0.961231    0.475203
 H   -6.234774   -0.999881    1.183210
 H   -5.126495   -1.990835    0.185523
 H   -5.721484   -0.420977   -0.430005
 H    2.598676    1.303833    2.402667
 H    3.560434   -0.194965    2.506691
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 H     4.390796    1.388806    2.347832
 C     3.509992    0.801978    2.044974
 H     2.577959    2.874878   -0.085264
 P     3.428370    0.625709    0.232294
 H     4.367986    2.869669    0.022227
 C     3.491942    2.340893   -0.383788
 H     5.169808   -1.059819    0.223174
 H     5.865282    0.589291    0.097526
 C     5.047566   -0.067989   -0.235434
 H     3.551752    2.337361   -1.482145
 H     5.097169   -0.183178   -1.328324
 H     3.262649   -2.575975    0.609952
 H     1.879993   -3.350283   -0.198716
 H     1.677686   -2.633751    1.416428
39
Figure 10_PMe3_ts(SN2)_04 / electronic energy: -2979.90029845 a.u. / lowest freq: -334.51 cm-1
 C     0.430987    1.599527   -0.411687
 C    -0.033680    0.799351   -1.480885
 C    -0.410615   -0.528812   -1.263434
 O     2.531839    1.508811   -0.520866
 P     2.989521    0.173326    0.046390
 O     2.085873   -0.611606    0.957418
 O     3.413289   -0.713764   -1.260213
 O     4.432789    0.435830    0.771096
 C     3.996830   -1.979986   -1.067752
 H     0.497049    2.680095   -0.517025
 H     0.534308    1.171210    0.585878
 H    -0.177834    1.268172   -2.458981
 H     0.005877   -1.058673   -0.398529
 H    -0.778637   -1.136962   -2.093737
 C    -2.304967    2.454843    0.536796
Cu    -1.719884    0.762605   -0.311048
 H     3.890992   -2.552533   -2.001050
 H     3.499806   -2.537534   -0.255675
 H     5.073115   -1.896765   -0.835494
 C     4.814374   -0.262446    1.935109
 H     5.454314    0.397084    2.541032
 H     5.392923   -1.169493    1.687192
 H     3.938313   -0.559694    2.531502
 H    -2.234728   -1.491141    2.311552
 H    -3.317892   -0.099244    2.584814
 H    -4.009457   -1.745065    2.383465
 C    -3.213556   -1.058594    2.056644
 H    -2.292547   -2.898459   -0.292271
 P    -3.295901   -0.761429    0.259944
 H    -4.063877   -3.060748   -0.062968
 C    -3.267647   -2.426684   -0.482351
 H    -5.146495    0.779810    0.503555
 H    -5.731916   -0.908591    0.341249
 C    -4.997670   -0.173875   -0.022861
 H    -3.408807   -2.344112   -1.570226
 H    -5.157386   -0.004568   -1.098048
 H    -3.396839    2.444495    0.701920
 H    -2.068900    3.350803   -0.062733
 H    -1.823706    2.583793    1.522983
22
Figure 10_NHCMe2-Cu-Me / electronic energy: -1985.96094373 a.u. / lowest freq: 47.08 cm-1
 C     3.475391    0.002063    0.004430
Cu     1.521142    0.004375   -0.001634
 H    -1.135412    2.981141   -0.894012
 H    -3.137350    1.184719   -0.886358
 C    -0.769814    2.447027   -0.001471
 H     0.328227    2.458734   -0.004855
 H    -1.129885    2.980832    0.893515
 C    -2.645394    0.759300    0.002746
 N    -1.219353    1.079660   -0.000493
 H    -3.133239    1.184460    0.894244
 H    -3.126534   -1.205033   -0.886897
 C    -0.427861    0.001650   -0.001913
 C    -2.638619   -0.775607    0.002525
 N    -1.209960   -1.083240   -0.000302
 H    -3.123109   -1.205275    0.893693
 H    -1.107482   -2.983726   -0.894321
 C    -0.747529   -2.446288   -0.001472
 H     0.350624   -2.446961   -0.004459
 H    -1.102596   -2.983800    0.893295
 H     3.915586   -0.379653   -0.939434
 H     3.905569   -0.628204    0.809484
 H     3.910649    1.012075    0.149980
22
Figure 10_NHCMe2-Cu-Me_(145 deg) / electronic energy: -1985.95101987 a.u. / lowest freq: 65.14 cm-1
 C     3.192263    0.005839    0.763728
Cu     1.540502   -0.008810   -0.304097
 H    -1.261123    2.994500   -0.926348
 H    -3.258612    1.205091   -0.417059
 C    -0.725052    2.446519   -0.133506
 H     0.349264    2.449318   -0.360556
 H    -0.884226    2.975166    0.821115
 C    -2.558978    0.775877    0.317869
 N    -1.177782    1.083721   -0.045634
 H    -2.800938    1.204853    1.303510
 H    -3.267548   -1.182467   -0.417547
 C    -0.415497   -0.000999   -0.231950
 C    -2.565769   -0.758802    0.318610
 N    -1.186529   -1.078864   -0.041885
 H    -2.813668   -1.184740    1.304055
 H    -1.283941   -2.990151   -0.920397
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 C   -0.744891   -2.445394   -0.127327
 H    0.329753   -2.457080   -0.352608
 H   -0.909797   -2.971594    0.827657
 H    4.174743   -0.125412    0.265113
 H    3.139353   -0.792369    1.532272
 H    3.269899    0.958134    1.327698
22
Figure 10_NHCMe2-Cu-Me_(130 deg) / electronic energy: -1985.94203020 a.u. / lowest freq: 66.01 cm-1
 C    2.916804    0.083913    1.041177
Cu    1.560875   -0.165784   -0.382593
 H   -1.100020    3.080858   -0.903190
 H   -3.145116    1.504103   -0.169386
 C   -0.475067    2.434808   -0.265830
 H    0.519310    2.338318   -0.721144
 H   -0.364827    2.921445    0.718846
 C   -2.396185    0.956202    0.422162
 N   -1.058425    1.125576   -0.140292
 H   -2.427575    1.346944    1.453721
 H   -3.304045   -0.874436   -0.408646
 C   -0.396924   -0.030616   -0.299326
 C   -2.581140   -0.564038    0.364992
 N   -1.240045   -1.024008    0.014247
 H   -2.908275   -0.993768    1.323978
 H   -1.580590   -2.897149   -0.886411
 C   -0.952050   -2.427644   -0.110303
 H    0.103871   -2.550887   -0.385027
 H   -1.131651   -2.951636    0.842617
 H    4.005959   -0.021257    0.857926
 H    2.683544   -0.619927    1.866630
 H    2.780717    1.098398    1.470369
22
Figure 10_NHCMe2-Cu-Me_(115 deg) / electronic energy: -1985.93143678 a.u. / lowest freq: 49.29 cm-1
 C    2.478775   -0.091399    1.352414
Cu    1.608051    0.094442   -0.433366
 H   -1.537768    3.049061   -0.706323
 H   -3.289362    1.148637    0.069215
 C   -0.776413    2.437272   -0.196420
 H    0.169537    2.515997   -0.747986
 H   -0.625973    2.848507    0.817603
 C   -2.412817    0.667866    0.528173
 N   -1.178270    1.056842   -0.149620
 H   -2.374461    0.970828    1.589537
 H   -3.123948   -1.197031   -0.405492
 C   -0.367622    0.017056   -0.411851
 C   -2.404340   -0.853599    0.358155
 N   -1.036498   -1.100774   -0.088609
 H   -2.620024   -1.391946    1.293236
 H   -1.098327   -2.949076   -1.108221
 C   -0.555410   -2.440596   -0.292299
 H    0.512301   -2.399753   -0.545729
 H   -0.674382   -3.036973    0.626520
 H    3.574606   -0.068260    1.526464
 H    2.126534   -1.045913    1.796057
 H    2.058137    0.705032    2.001302
43
Figure 10_NHCMe2_ts(SN2')_01 / electronic energy: -2824.75801259 a.u. / lowest freq: -332.64 cm-1
 C    0.347635    1.989740   -0.106498
 C    0.246850    0.984148   -1.102161
 C    0.335188   -0.374155   -0.769588
 O    2.279104   -1.022377   -1.014600
 P    3.145405   -0.434619    0.098203
 O    2.543889   -0.069348    1.418038
 O    4.389749   -1.455385    0.377614
 O    3.898057    0.846345   -0.592058
 C    5.093834   -2.008917   -0.710569
 H    0.322083    3.042557   -0.399244
 H    0.898902    1.755833    0.811526
 H    0.041420    1.255547   -2.142199
 H    0.419730   -0.673858    0.275696
 H    0.016049   -1.132133   -1.483293
 C   -2.054671    2.452741    1.458220
Cu   -1.401508    1.107645    0.169195
 H    5.917017   -2.615302   -0.306195
 H    5.521837   -1.227267   -1.361779
 H    4.444989   -2.653343   -1.326395
 C    4.748954    1.639242    0.203466
 H    5.052822    2.514196   -0.389536
 H    5.657231    1.087109    0.503234
 H    4.239094    1.986426    1.117110
 H   -4.029718    0.269215   -2.887232
 H   -4.881871   -1.977450   -1.583513
 C   -4.042538    0.708315   -1.876872
 H   -3.257758    1.473465   -1.810943
 H   -5.020179    1.193009   -1.720559
 C   -4.738911   -1.399638   -0.658510
 N   -3.801834   -0.297237   -0.875356
 H   -5.719880   -1.004403   -0.347332
 H   -3.659247   -3.171653    0.093334
 C   -2.809476   -0.276428    0.013585
 C   -4.046347   -2.203154    0.450816
 N   -2.935964   -1.327374    0.823480
 H   -4.699727   -2.394831    1.314796
 H   -1.443302   -2.602748    1.591587
 C   -2.007503   -1.694413    1.861463
 H   -1.298626   -0.871089    2.019867
 H   -2.539757   -1.883256    2.806644
 H   -1.321857    3.185371    1.829575
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 H   -2.480181    1.914120    2.322455
 H   -2.876303    3.001571    0.963759
43
Figure 10_NHCMe2_ts(SN2')_02 / electronic energy: -2824.75692951 a.u. / lowest freq: -329.61 cm-1
 C    0.283321    2.135092    0.374609
 C    0.274001    1.402786   -0.839856
 C    0.431017    0.010974   -0.852735
 O    2.417126   -0.452685   -1.170397
 P    3.190172   -0.279043    0.144860
 O    2.435382   -0.361352    1.433776
 O    4.455113   -1.317223    0.091417
 O    4.019254    1.117033    0.113991
 C    4.192147   -2.683408   -0.125733
 H    0.205075    3.224788    0.347355
 H    0.809796    1.709640    1.237026
 H    0.078246    1.916912   -1.786052
 H    0.515010   -0.532412    0.088807
 H    0.174170   -0.557614   -1.745463
 C   -2.202755    2.111811    1.866871
Cu   -1.409323    1.113038    0.356908
 H    5.145749   -3.226994   -0.062406
 H    3.748446   -2.856292   -1.120785
 H    3.507676   -3.092801    0.637972
 C    4.778236    1.461888   -1.022559
 H    5.031143    2.529463   -0.949711
 H    4.210210    1.293852   -1.952099
 H    5.713751    0.879549   -1.072492
 H   -4.222145    0.721839   -2.724478
 H   -4.764591   -1.798333   -1.898961
 C   -4.116645    0.951166   -1.652385
 H   -3.337769    1.714636   -1.528343
 H   -5.073402    1.361814   -1.288765
 C   -4.601406   -1.409629   -0.882942
 N   -3.743968   -0.224921   -0.910880
 H   -5.583451   -1.154265   -0.451934
 H   -3.378906   -3.218713   -0.560824
 C   -2.705814   -0.315462   -0.079886
 C   -3.800501   -2.371524    0.004647
 N   -2.724725   -1.514644    0.501796
 H   -4.390643   -2.778946    0.838538
 H   -1.085867   -2.776878    0.917430
 C   -1.721502   -2.018545    1.404567
 H   -1.087935   -1.188502    1.744372
 H   -2.196254   -2.477305    2.285488
 H   -1.586830    2.901226    2.323795
 H   -2.472327    1.383953    2.651549
 H   -3.136106    2.568799    1.492447
43
Figure 10_NHCMe2_ts(SN2')_03 / electronic energy: -2824.75750602 a.u. / lowest freq: -318.36 cm-1
 C    0.299536    2.059787    0.304744
 C    0.227757    1.334570   -0.913709
 C    0.393992   -0.054861   -0.960835
 O    2.350016   -0.502323   -1.443443
 P    3.136604   -0.590563   -0.134792
 O    2.576732   -1.318870    1.042723
 O    4.598997   -1.158786   -0.587598
 O    3.489879    0.929706    0.369246
 C    5.565058   -1.390306    0.413351
 H    0.222045    3.149749    0.282499
 H    0.875678    1.647144    1.139891
 H   -0.023760    1.859369   -1.840663
 H    0.526515   -0.628229   -0.041276
 H    0.082261   -0.609228   -1.844776
 C   -2.062777    2.051232    1.945445
Cu   -1.396948    1.054423    0.374191
 H    6.464510   -1.795134   -0.072013
 H    5.205322   -2.115858    1.161325
 H    5.839714   -0.458696    0.938170
 C    3.942842    1.890269   -0.555517
 H    3.809604    2.886025   -0.107173
 H    3.373767    1.844973   -1.498085
 H    5.013337    1.752431   -0.788363
 H   -4.529644    0.936319   -2.394738
 H   -4.989704   -1.648563   -1.758612
 C   -4.300397    1.068784   -1.325750
 H   -3.503256    1.817108   -1.225970
 H   -5.204828    1.444324   -0.818696
 C   -4.722489   -1.352163   -0.733636
 N   -3.858625   -0.171777   -0.743749
 H   -5.654730   -1.131925   -0.187528
 H   -3.485952   -3.178493   -0.696853
 C   -2.750416   -0.334309   -0.020952
 C   -3.849217   -2.390038   -0.017183
 N   -2.727159   -1.579149    0.454902
 H   -4.360934   -2.875638    0.826772
 H   -1.041534   -2.844404    0.589835
 C   -1.648156   -2.163581    1.210156
 H   -1.000098   -1.365732    1.596487
 H   -2.047071   -2.731218    2.064375
 H   -1.397997    2.813436    2.379074
 H   -2.306911    1.314362    2.730014
 H   -3.002806    2.540423    1.634474
43
Figure 10_NHCMe2_ts(SN2')_04 / electronic energy: -2824.75669355 a.u. / lowest freq: -334.18 cm-1
 C    0.406872    1.945905    0.167794
 C    0.269392    1.141918   -0.993265
 C    0.348521   -0.253671   -0.926999
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 O    2.298302   -0.846276   -1.364389
 P    3.198233   -0.364838   -0.229175
 O    2.662963   -0.354048    1.174373
 O    4.611805   -1.188231   -0.304206
 O    3.741564    1.099827   -0.683997
 C    4.673287   -2.467075    0.281753
 H    0.404836    3.034397    0.070796
 H    0.960743    1.537143    1.020968
 H    0.046018    1.608490   -1.957576
 H    0.477072   -0.750225    0.035015
 H    0.005896   -0.861606   -1.763150
 C   -1.997724    2.196521    1.791082
Cu   -1.354638    1.057089    0.310957
 H    5.690370   -2.859016    0.136566
 H    3.962120   -3.167654   -0.190746
 H    4.457814   -2.428000    1.362723
 C    4.510541    1.860901    0.218664
 H    4.648272    2.861847   -0.215207
 H    5.504361    1.409082    0.380406
 H    4.009685    1.959938    1.195505
 H   -4.323972    0.779708   -2.607376
 H   -4.997008   -1.688174   -1.683032
 C   -4.178461    1.023345   -1.543139
 H   -3.363311    1.753241   -1.453893
 H   -5.105436    1.482621   -1.161436
 C   -4.761258   -1.285755   -0.686990
 N   -3.839419   -0.154128   -0.787622
 H   -5.704240   -0.962199   -0.216152
 H   -3.616783   -3.147268   -0.381180
 C   -2.774716   -0.281673    0.003285
 C   -3.973663   -2.271615    0.185867
 N   -2.837978   -1.460593    0.622173
 H   -4.548645   -2.636304    1.049567
 H   -1.242418   -2.789194    1.000017
 C   -1.823250   -1.992853    1.495062
 H   -1.141716   -1.183689    1.790328
 H   -2.282240   -2.411371    2.403792
 H   -1.301107    2.951590    2.185878
 H   -2.297733    1.530854    2.619002
 H   -2.904091    2.709960    1.424254
43
Figure 10_NHCMe2_ts(SN2)_01 / electronic energy: -2824.75588695 a.u. / lowest freq: -385.60 cm-1
 C    0.874804    1.594069    0.198186
 C    0.354569    1.244316   -1.070588
 C   -0.150865   -0.038489   -1.311656
 O    2.918276    1.310401    0.093500
 P    3.220058   -0.183412    0.197560
 O    2.219629   -1.118425    0.802118
 O    3.620032   -0.636243   -1.324485
 O    4.633626   -0.377159    0.992930
 C    3.941273   -1.987126   -1.561755
 H    1.037649    2.638480    0.455408
 H    0.879791    0.864192    1.007278
 H    0.281525    2.024870   -1.833952
 H    0.198133   -0.871381   -0.691389
 H   -0.558375   -0.288188   -2.294731
 C   -1.778477    2.427081    1.310919
Cu   -1.363405    0.974056    0.015731
 H    4.125734   -2.109503   -2.638774
 H    3.118856   -2.657980   -1.262715
 H    4.851028   -2.291794   -1.015069
 C    5.743822    0.413294    0.631018
 H    6.595313    0.105327    1.254778
 H    5.547398    1.484786    0.799635
 H    6.015062    0.272114   -0.429426
 H   -4.661334    0.866907   -2.289587
 H   -5.362077   -1.551797   -1.227821
 C   -4.413917    1.119658   -1.245527
 H   -3.568107    1.820308   -1.240568
 H   -5.285912    1.617396   -0.791681
 C   -5.013714   -1.136425   -0.269287
 N   -4.054508   -0.057303   -0.498860
 H   -5.892022   -0.756861    0.275788
 H   -4.072287   -3.111124    0.045087
 C   -2.863895   -0.291586    0.050895
 C   -4.191076   -2.140624    0.552010
 N   -2.896409   -1.469657    0.670682
 H   -4.619356   -2.327575    1.548879
 H   -1.494005   -3.026865    0.851510
 C   -1.794119   -2.093978    1.356186
 H   -0.935812   -1.410689    1.368124
 H   -2.067533   -2.332320    2.396324
 H   -1.492399    3.428533    0.944430
 H   -1.266197    2.273497    2.277597
 H   -2.863706    2.442218    1.513607
43
Figure 10_NHCMe2_ts(SN2)_02 / electronic energy: -2824.75588696 a.u. / lowest freq: -385.60 cm-1
 C    0.874813   -1.594057   -0.198211
 C    0.354587   -1.244287    1.070563
 C   -0.150844    0.038521    1.311618
 O    2.918289   -1.310401   -0.093544
 P    3.220073    0.183413   -0.197583
 O    2.219667    1.118428   -0.802177
 O    3.619984    0.636236    1.324482
 O    4.633675    0.377164   -0.992891
 C    3.941198    1.987122    1.561773
 H    1.037653   -2.638472   -0.455421
```
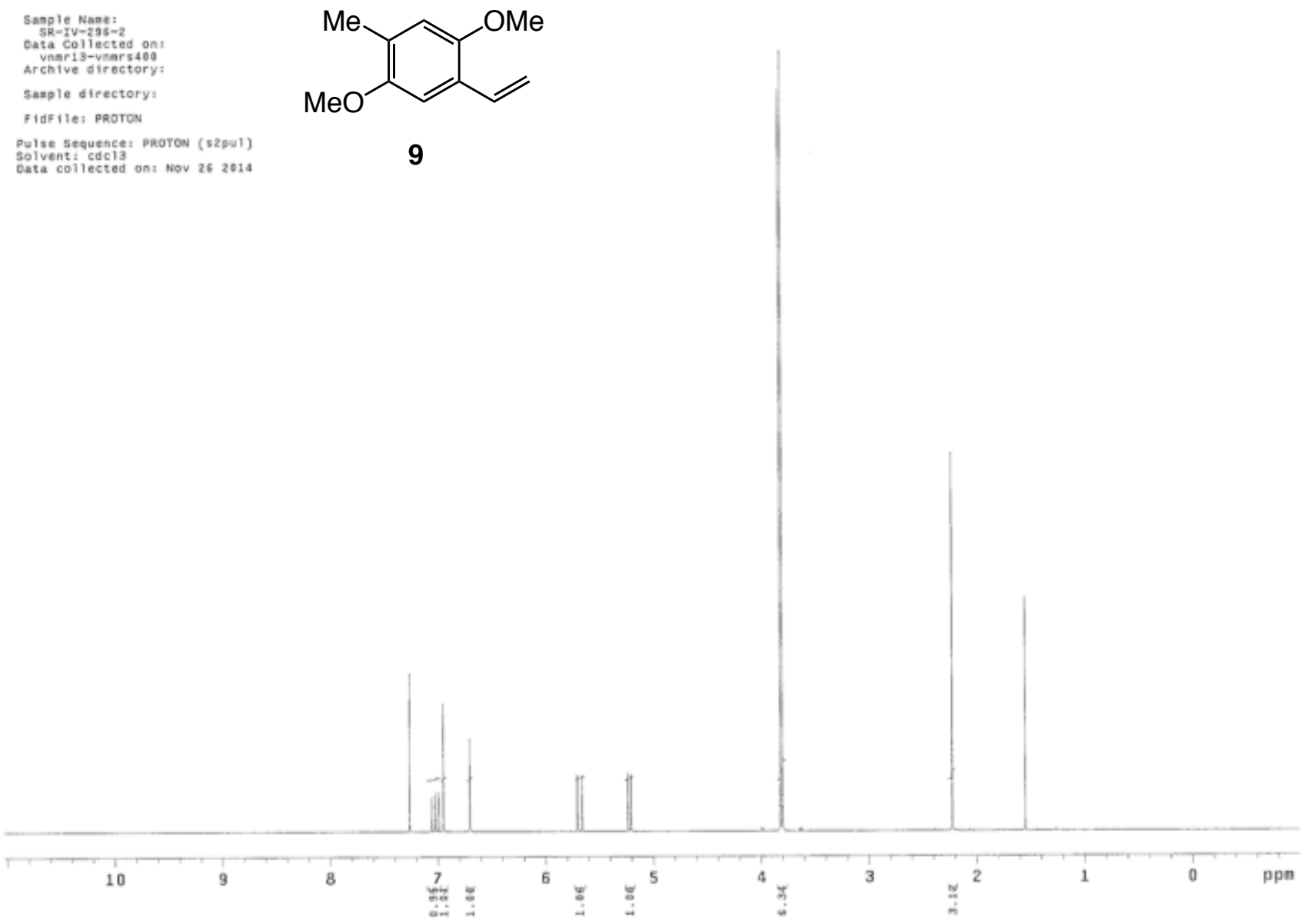

```
 H    0.879799   -0.864190   -1.007312
 H    0.281548   -2.024832    1.833937
 H    0.198147    0.871404    0.691334
 H   -0.558345    0.288235    2.294694
 C   -1.778480   -2.427088   -1.310904
Cu   -1.363394   -0.974041   -0.015746
 H    4.125690    2.109478    2.638789
 H    3.118754    2.657962    1.262775
 H    4.850929    2.291826    1.015065
 C    5.743862   -0.413273   -0.630915
 H    6.595386   -0.105290   -1.254622
 H    5.547464   -1.484767   -0.799547
 H    6.015033   -0.272091    0.429547
 H   -4.661352   -0.866931    2.289628
 H   -5.362228    1.551711    1.227782
 C   -4.413870   -1.119674    1.245582
 H   -3.568021   -1.820277    1.240666
 H   -5.285816   -1.617461    0.791695
 C   -5.013744    1.136364    0.269283
 N   -4.054486    0.057305    0.498932
 H   -5.891974    0.756736   -0.275876
 H   -4.072257    3.111061   -0.044918
 C   -2.863904    0.291580   -0.050893
 C   -4.191105    2.140620   -0.551944
 N   -2.896464    1.469624   -0.670730
 H   -4.619419    2.327699   -1.548772
 H   -1.494033    3.026815   -0.851531
 C   -1.794187    2.093959   -1.356241
 H   -0.935897    1.410649   -1.368244
 H   -2.067634    2.332356   -2.396357
 H   -1.492342   -3.428529   -0.944435
 H   -1.266259   -2.273480   -2.277610
 H   -2.863719   -2.442267   -1.513533
43
Figure 10_NHCMe2_ts(SN2)_03 / electronic energy: -2824.75502346 a.u. / lowest freq: -384.84 cm-1
 C    0.913335    1.557356    0.297525
 C    0.381459    1.518172   -1.013364
 C   -0.157416    0.332586   -1.529992
 O    2.931221    1.114186    0.111826
 P    3.145745   -0.402671    0.190623
 O    1.967032   -1.276497    0.495111
 O    3.915731   -0.864258   -1.178781
 O    4.327217   -0.728007    1.252447
 C    3.317792   -0.578839   -2.420380
 H    1.136882    2.512149    0.770074
 H    0.868301    0.672069    0.931269
 H    0.329691    2.451633   -1.582114
 H    0.186225   -0.624408   -1.124492
 H   -0.586897    0.321293   -2.535348
 C   -1.693667    2.188269    1.606639
Cu   -1.317603    1.037165    0.025530
 H    4.040459   -0.829451   -3.210368
 H    3.056795    0.489646   -2.508667
 H    2.406071   -1.179618   -2.582581
 C    5.510372    0.040662    1.246850
 H    6.155553   -0.330620    2.055633
 H    5.298097    1.108196    1.419777
 H    6.050786   -0.060526    0.290865
 H   -5.098509    1.135721   -1.619877
 H   -5.466803   -1.484064   -0.932010
 C   -4.583037    1.198599   -0.648261
 H   -3.777838    1.941549   -0.719741
 H   -5.308371    1.538933    0.108889
 C   -4.880308   -1.234659   -0.034947
 N   -4.022457   -0.076110   -0.282167
 H   -5.585273   -1.013012    0.782823
 H   -3.798037   -3.118329   -0.423698
 C   -2.741312   -0.309588    0.004053
 C   -3.864480   -2.322619    0.336028
 N   -2.606832   -1.577136    0.391176
 H   -4.075516   -2.796250    1.306439
 H   -1.134222   -3.026616   -0.000620
 C   -1.376308   -2.244345    0.737741
 H   -0.541465   -1.532413    0.769091
 H   -1.468184   -2.720564    1.726508
 H   -1.485013    3.255081    1.411643
 H   -1.101568    1.892204    2.490446
 H   -2.760016    2.095461    1.877122
43
Figure 10_NHCMe2_ts(SN2)_04 / electronic energy: -2824.75341246 a.u. / lowest freq: -372.56 cm-1
 C    0.792916    1.819029    0.349203
 C    0.251131    1.665370   -0.948072
 C   -0.171782    0.409629   -1.404414
 O    2.843365    1.605477    0.167173
 P    3.160766    0.120469    0.044347
 O    2.180626   -0.902583    0.551753
 O    3.475273   -0.110124   -1.542147
 O    4.625836   -0.108035    0.729696
 C    3.878933   -1.384940   -1.982598
 H    0.919016    2.812864    0.774973
 H    0.843527    0.969489    1.030012
 H    0.102373    2.561692   -1.557449
 H    0.267234   -0.491646   -0.964262
 H   -0.604975    0.312109   -2.403555
 C   -1.936219    2.249901    1.613322
Cu   -1.394198    1.058603    0.116152
 H    3.716268   -1.441303   -3.068919
```

H	3.294131	-2.185942	-1.499697
H	4.951201	-1.559622	-1.785434
C	4.934925	-1.285003	1.443800
H	5.706371	-1.038644	2.188430
H	5.337318	-2.066448	0.775962
H	4.051000	-1.689429	1.959404
H	-4.916692	0.736809	-1.980701
H	-5.163588	-1.865404	-1.200305
C	-4.541427	0.888929	-0.956302
H	-3.794896	1.693757	-0.965718
H	-5.385689	1.199701	-0.318914
C	-4.705628	-1.537562	-0.255556
N	-3.931242	-0.312452	-0.449079
H	-5.513942	-1.361019	0.473281
H	-3.385701	-3.293209	-0.470066
C	-2.690056	-0.406743	0.026828
C	-3.645006	-2.515367	0.267165
N	-2.494556	-1.639833	0.491718
H	-3.943909	-3.015433	1.199930
H	-0.851785	-2.945013	0.353937
C	-1.256537	-2.160659	1.014871
H	-0.510423	-1.359167	1.090384
H	-1.412571	-2.596171	2.014352
H	-1.759314	3.318676	1.399532
H	-1.398102	2.009628	2.547813
H	-3.014307	2.119835	1.813627

21. NMR Spectra

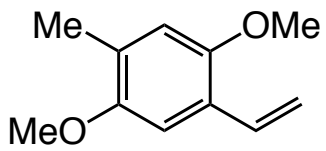


Sample Name:
SR-IV-236-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:

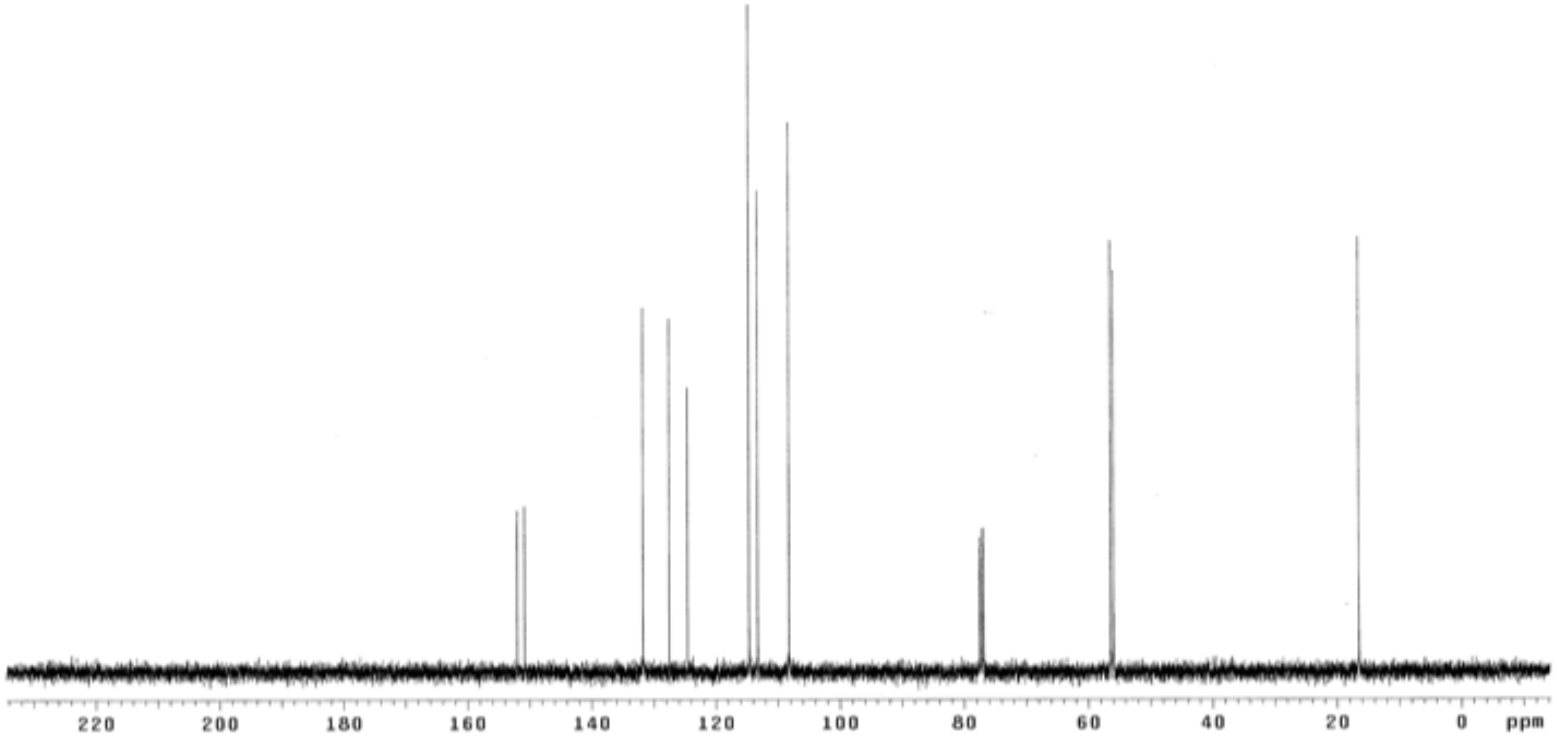
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 5 2014



9

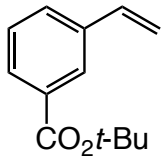


Sample Name:
SR-V-158
Data Collected on:
vnmr13-vnmrs400
Archive directory:

Sample directory:

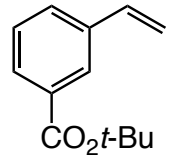
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 5 2015

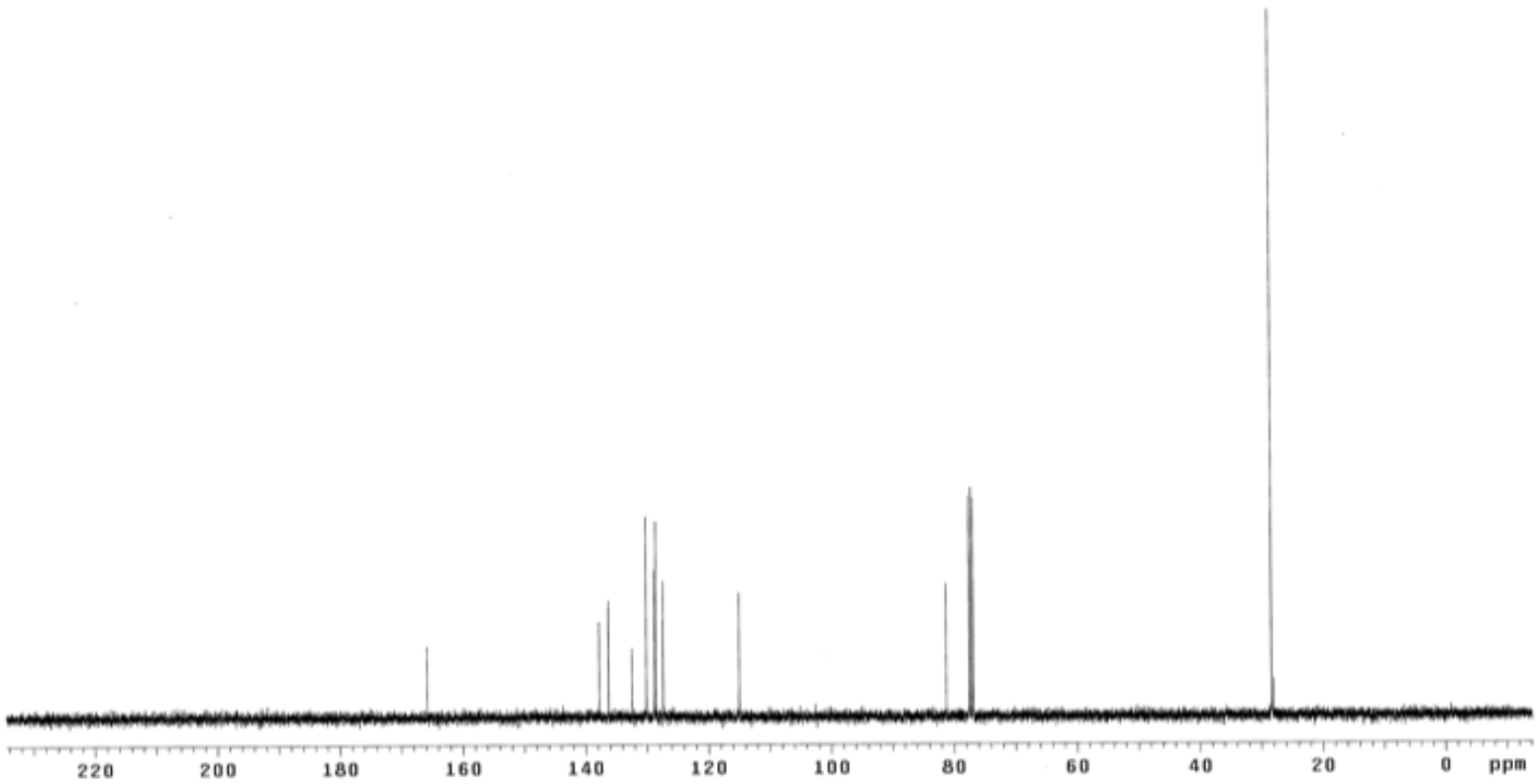


substrate for 2g

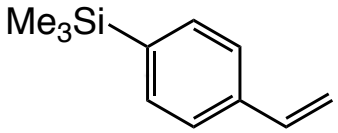
```
Sample Name:
  SR-V-158-carbon
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug  5 2015
```



substrate for 2g



```
Sample Name:
  SR-V-106
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 17 2015
```



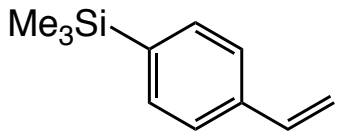
substrate for 2ad

Sample Name:
SR-V-106-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:

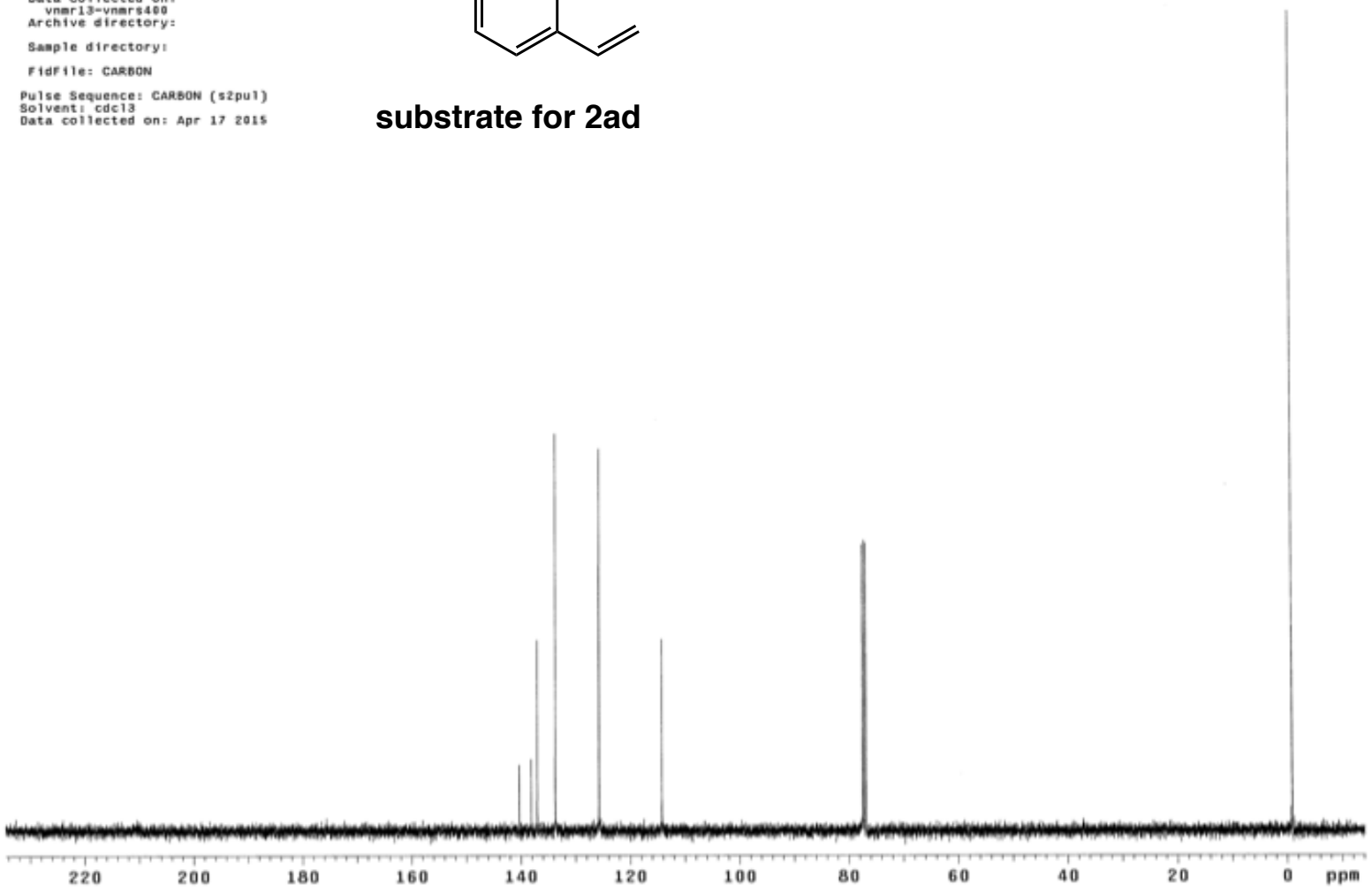
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 17 2015



substrate for 2ad

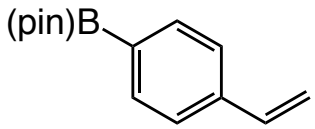


Data Collected on:
nmr14-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 6 2015



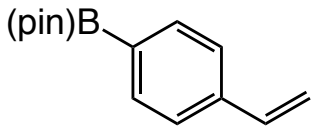
substrate for 2j

Sample Name:
SR-V-98-carbon
Data Collected on:
nmr14-vnmrs400
Archive directory:

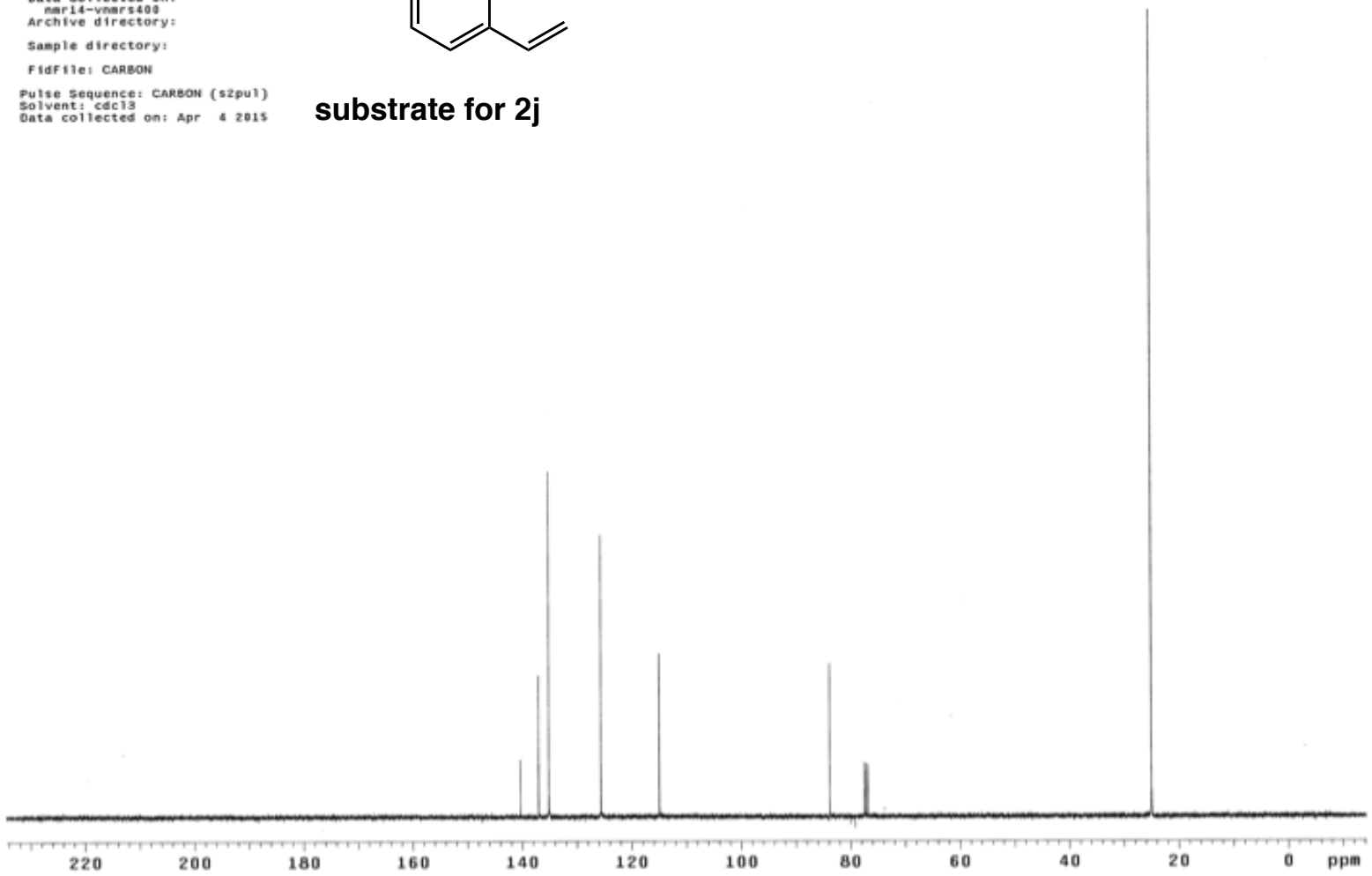
Sample directory:

FidFile: CARBON

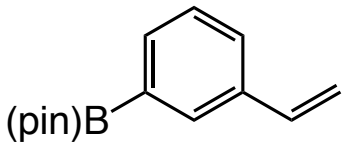
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 4 2015



substrate for 2j



```
Sample Name:
  SR-V-105
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 22 2015
```



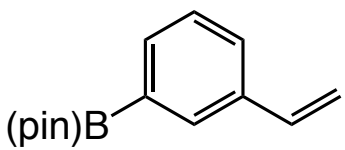
substrate for 2f

Sample Name:
SR-V-105-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:

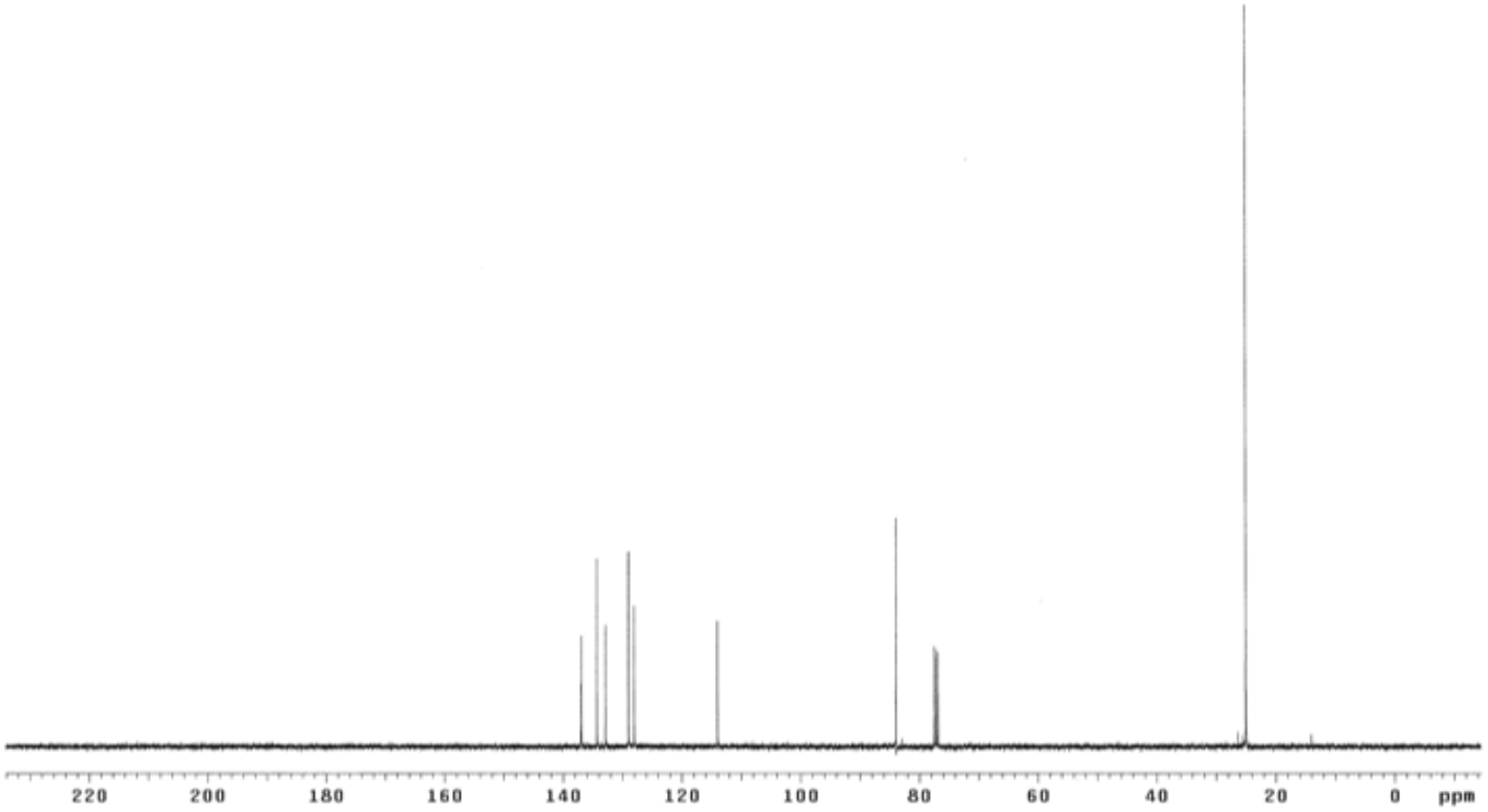
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 22 2015



substrate for 2f



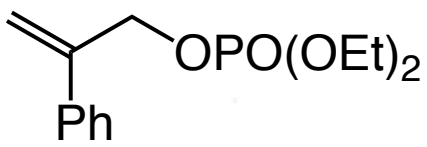
Sample Name:

Data Collected on:
vnmr13-vnmrs400
Archive directory:

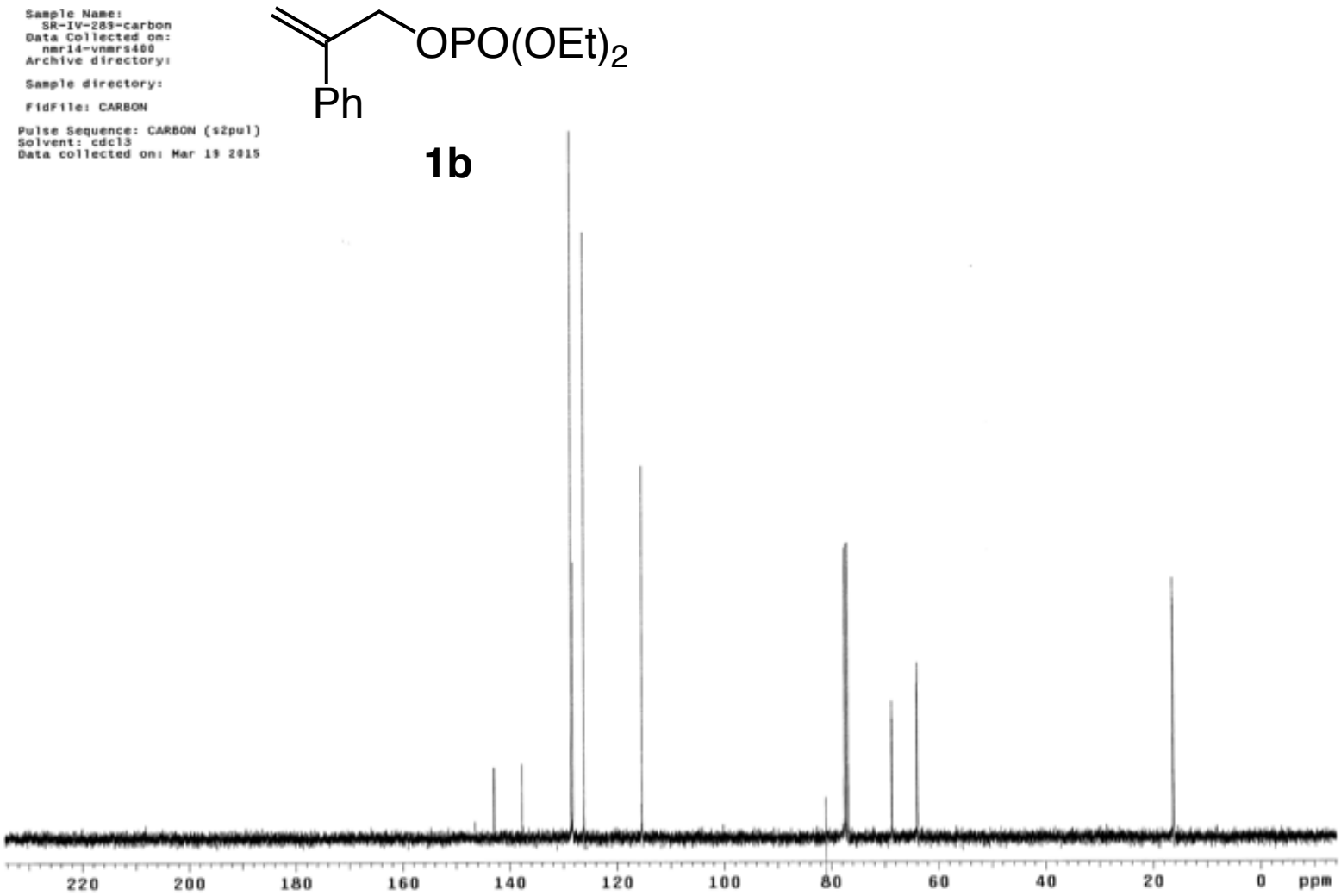
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 27 2014



1b

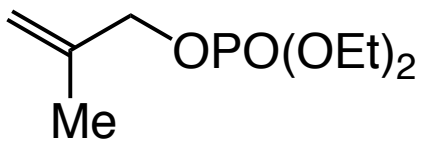

Sample Name:
SR-IV-283-carbon
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 19 2015
OPO(OEt)2
Ph
1b
220
200
180
160
140
120
100
80
60
40
20
0
ppm

Sample Name:
SR-IV-274-A
Data Collected on:
vnmr13-vnmrs400
Archive directory:

Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 7 2014



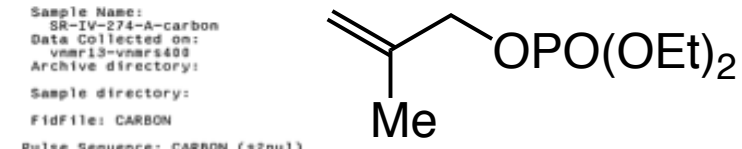
1c

Sample Name:
SR-IV-274-A-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:

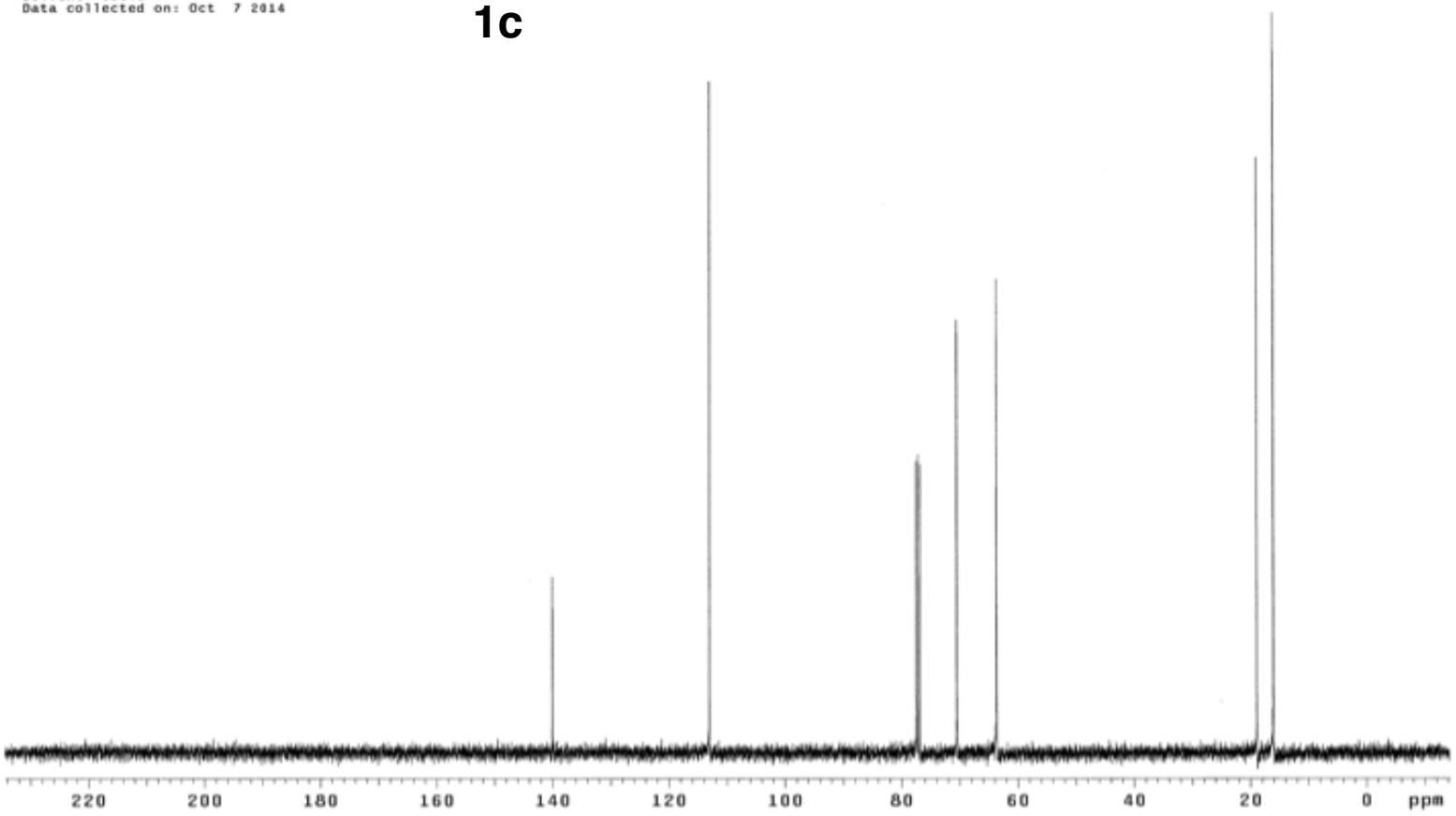
Sample directory:

FidFile: CARBON

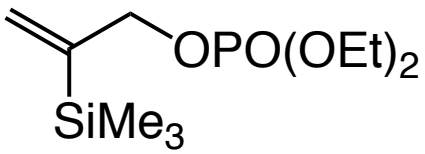
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 7 2014



1c



```
Sample Name:
  SR-V-39-phos
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 14 2015
```



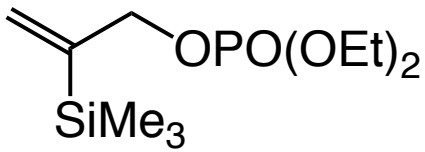
1d

Sample Name:
SR-IV-297-phos-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:

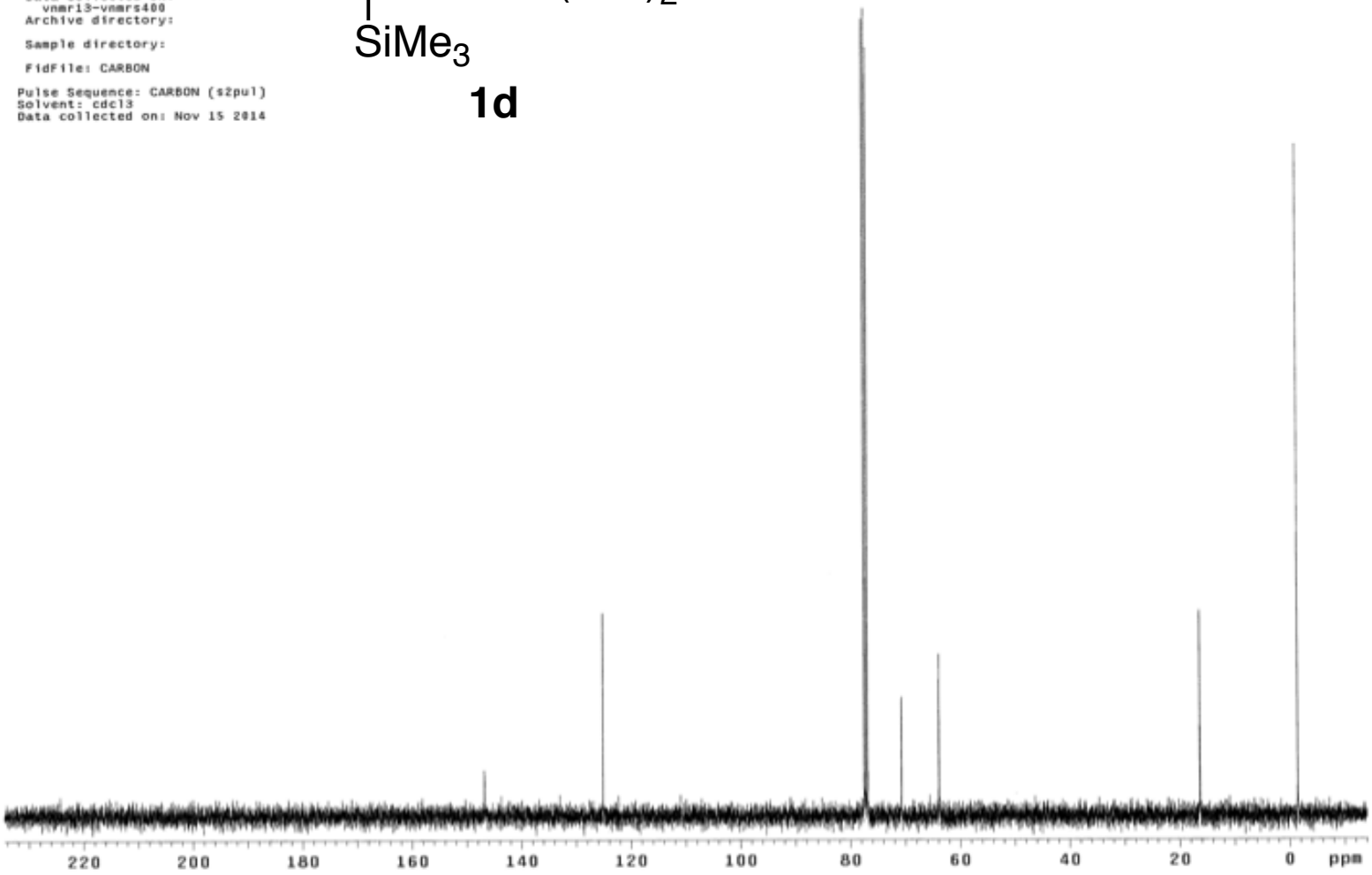
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 15 2014



1d

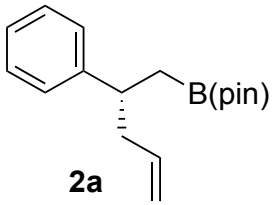


Sample Name:
SR-IV-264-A
Data Collected on:
vnmr13-vnmrs400
Archive directory:

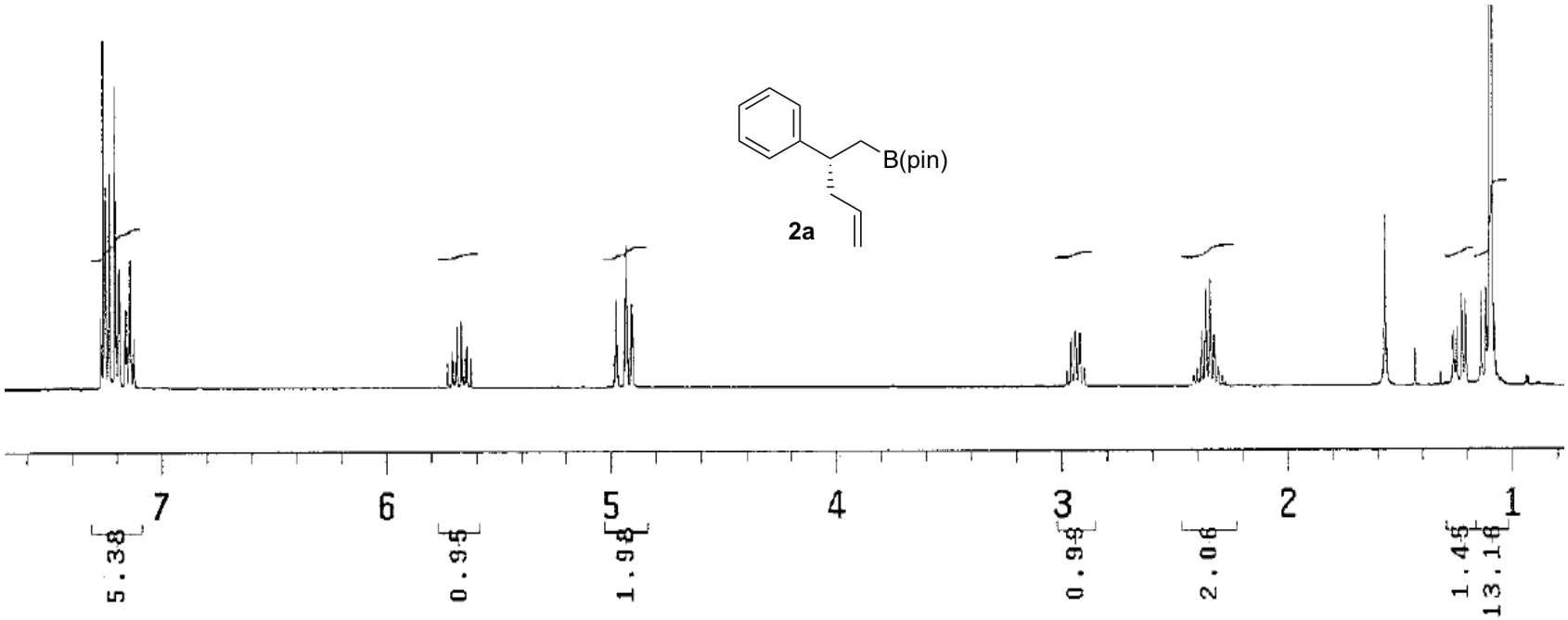
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 28 2014



2a

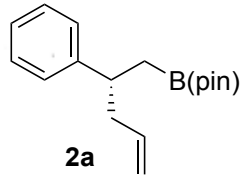

B(pin)
2a
7
6
5
4
3
2
1
5.38
0.95
1.98
0.99
2.06
1.45
13.16

Sample Name:
SR-IV-264-A-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:

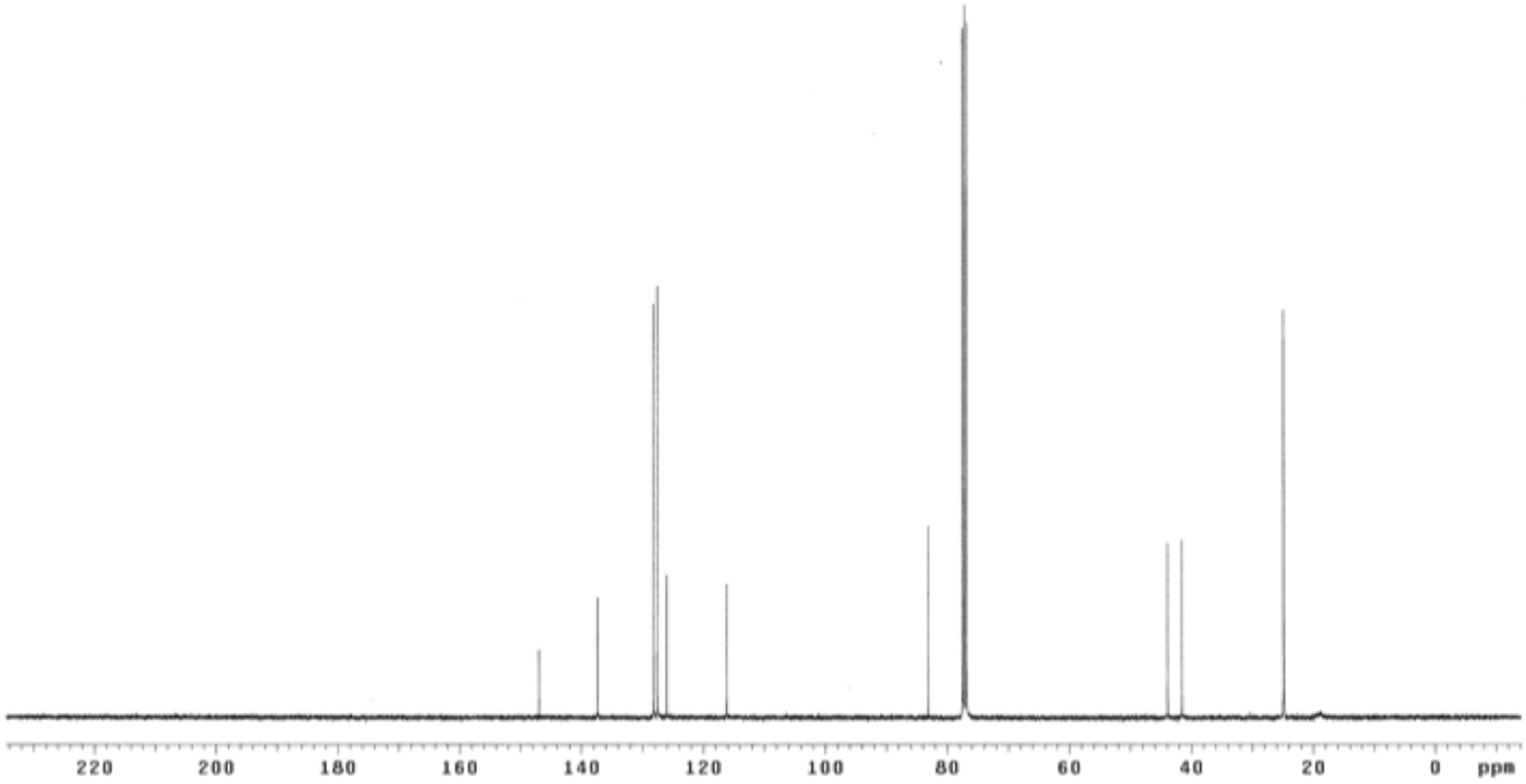
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 28 2014



2a

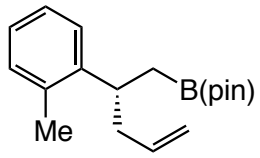


Sample Name:
SR-IV-263-2
Data Collected on:
vnmr13-vnmrs400
Archive directory:

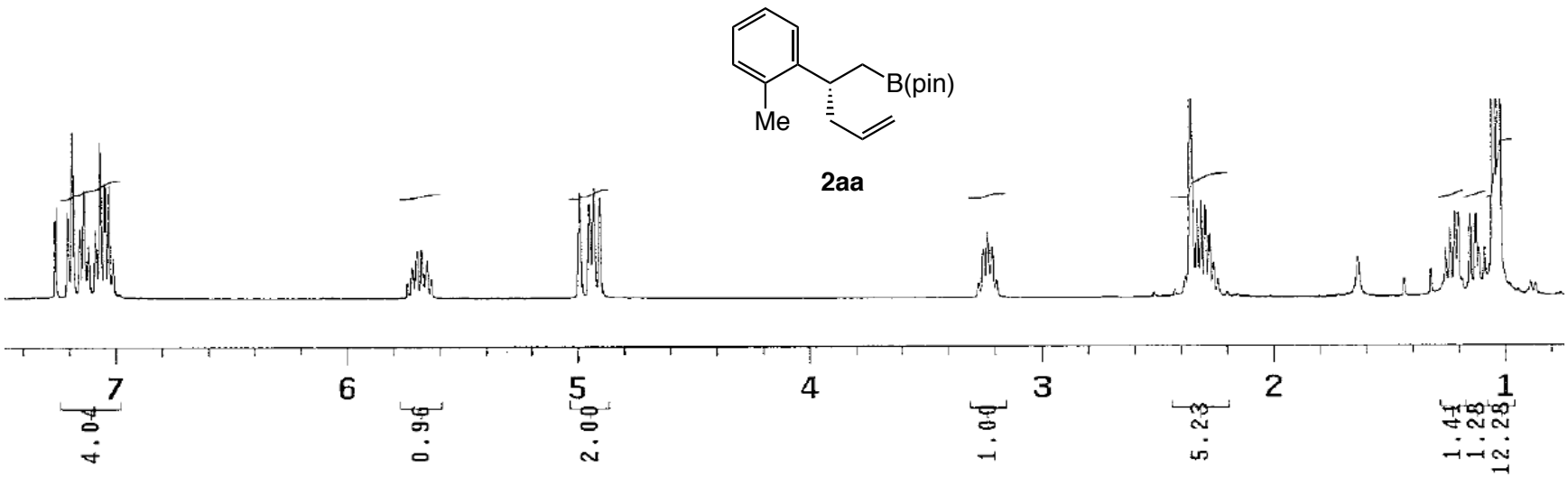
Sample directory:

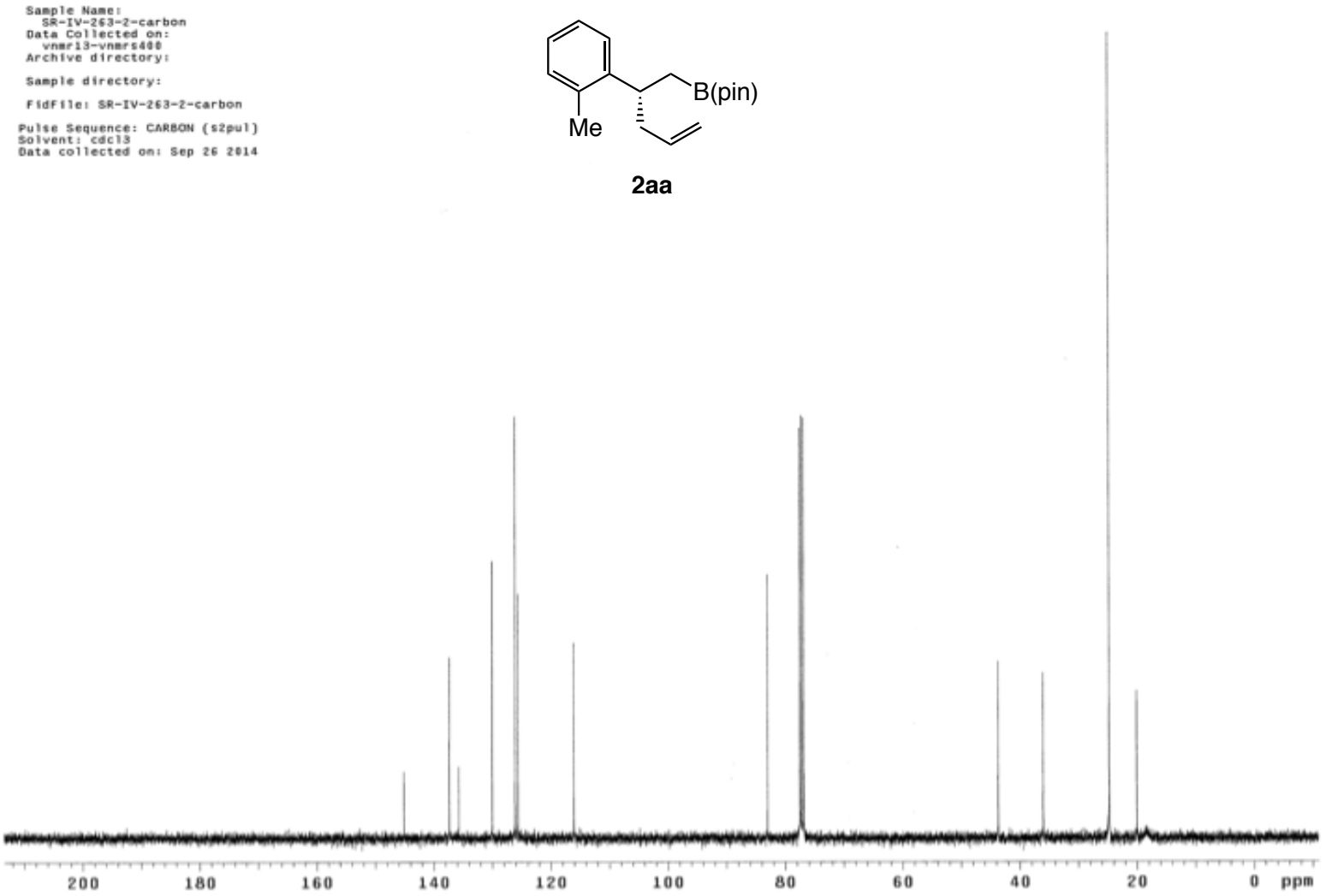
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 25 2014



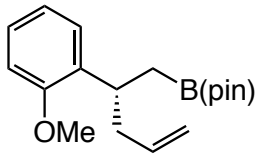
2aa


B(pin)
Me
2aa
7
6
5
4
3
2
1
4.04
0.96
2.00
1.00
5.23
1.44
1.28
12.28

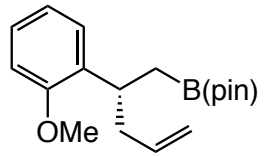

Sample Name:
SR-IV-263-2-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: SR-IV-263-2-carbon
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 26 2014
B(pin)
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

2aa

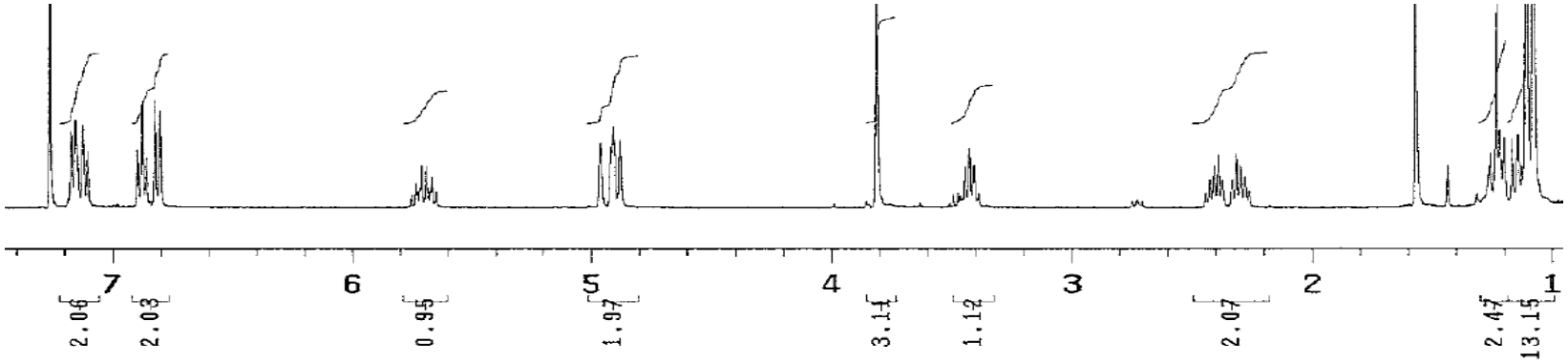
```
Sample Name:
  SR-IV-251-B
Data Collected on:
  vnmri3-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 23 2014
```

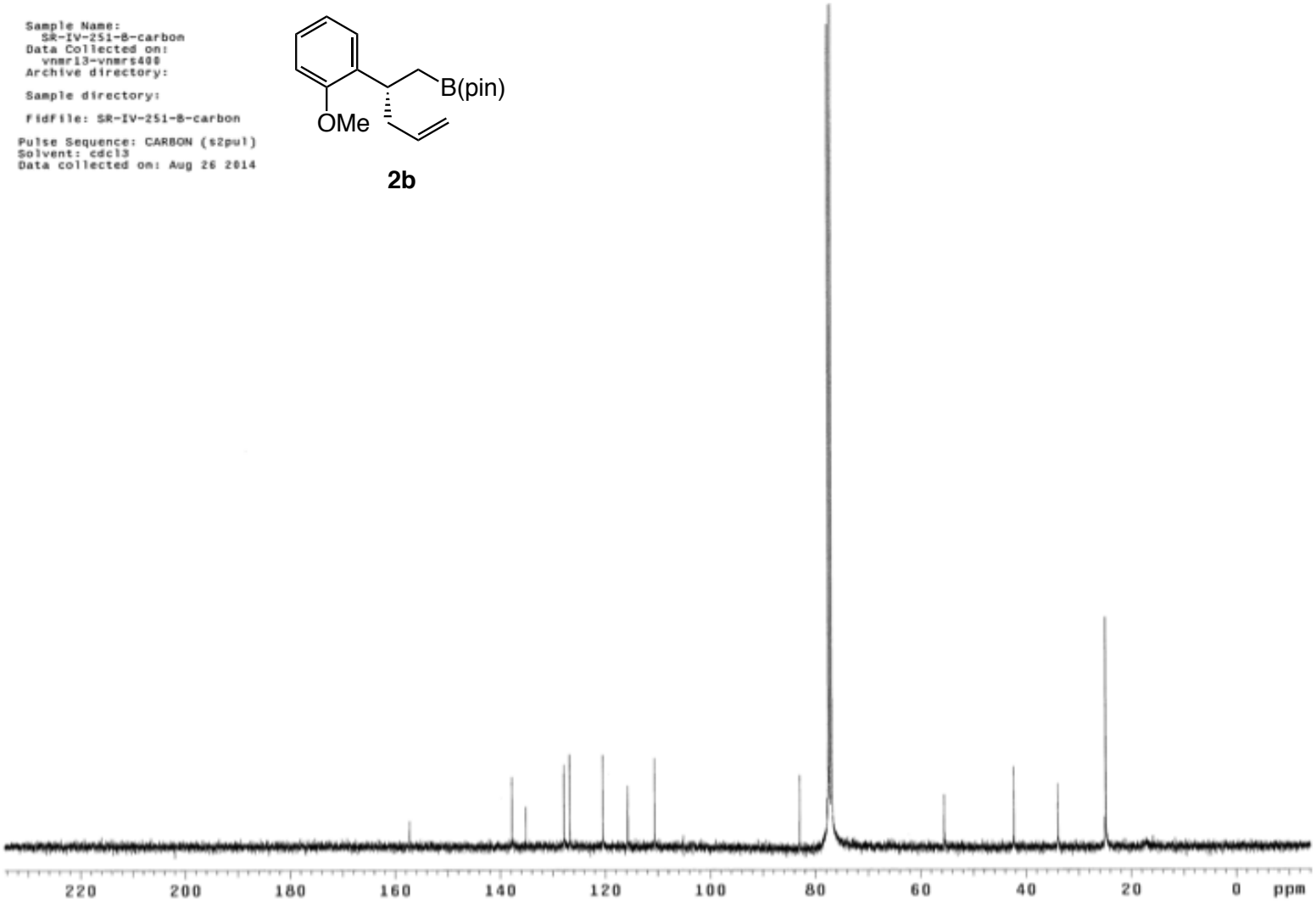


2b



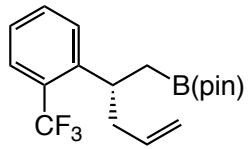
2b



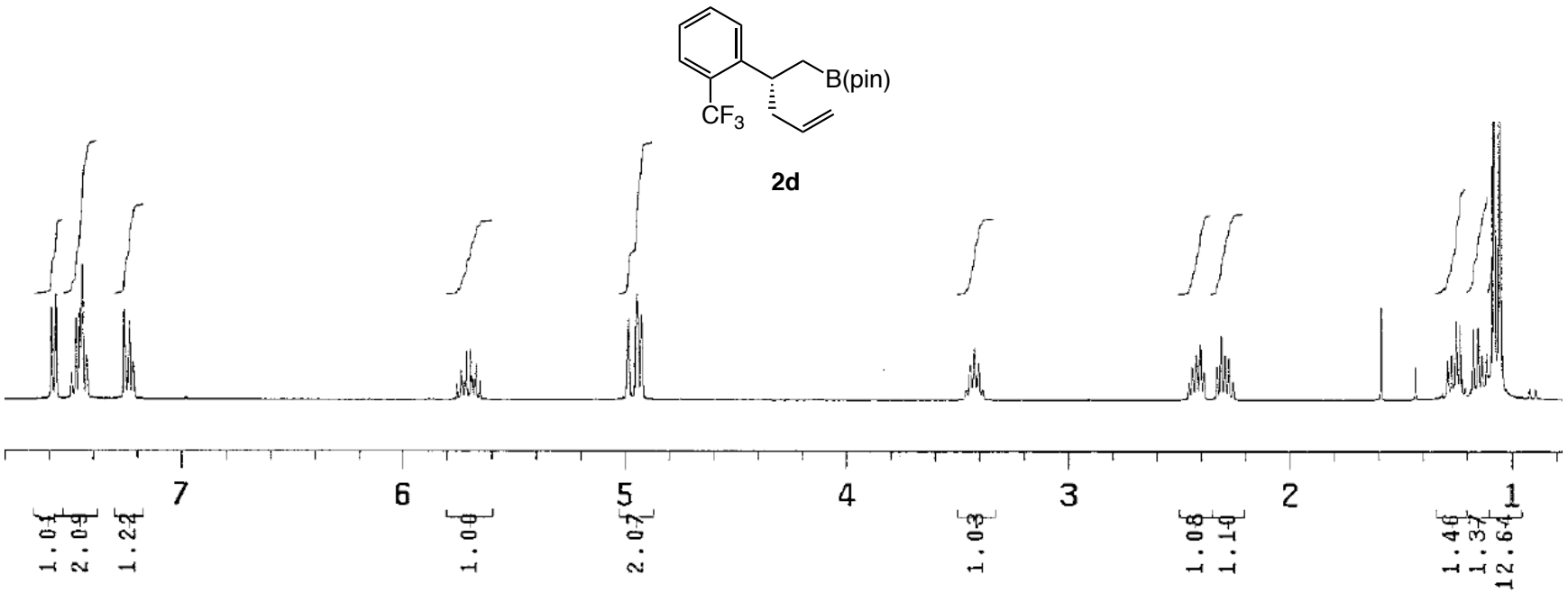

Sample Name:
SR-IV-251-B-carbon
Data Collected on:
vnmr13-vnmrs40$
Archive directory:
Sample directory:
FidFile: SR-IV-251-B-carbon
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 26 2014
B(pin)
OMe
220
200
180
160
140
120
100
80
60
40
20
0
ppm

2b

```
Sample Name:
  SR-V-128
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: SR-V-128

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 12 2015
```



2d



2d

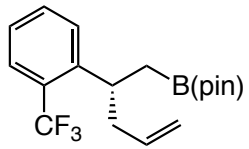
Sample Name:

Data Collected on:
vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 12 2015



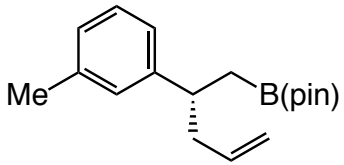
2d

Sample Name:
SR-V-33
Data Collected on:
vnmr13-vnmrs400
Archive directory:

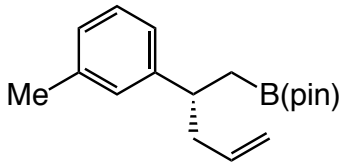
Sample directory:

FidFile: PROTON

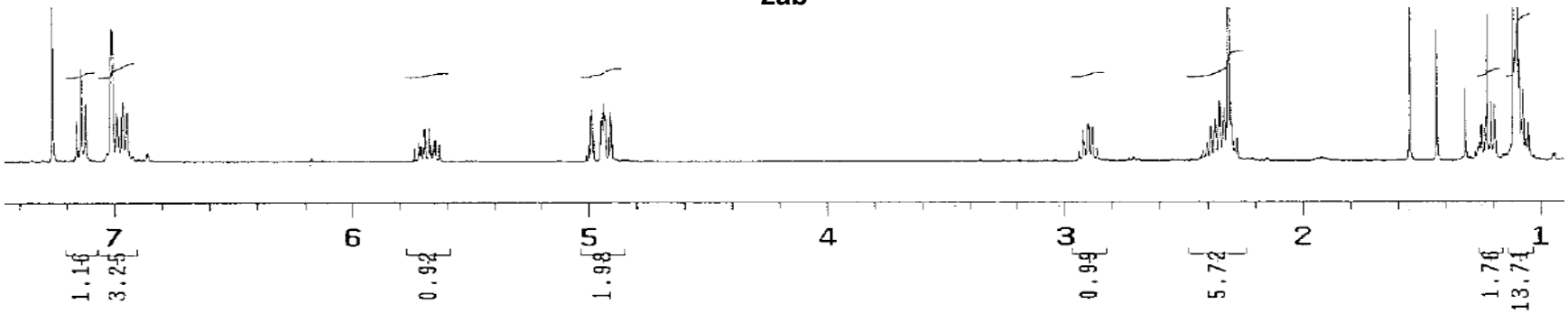
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 4 2015



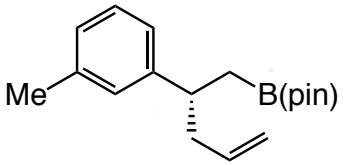
2ab



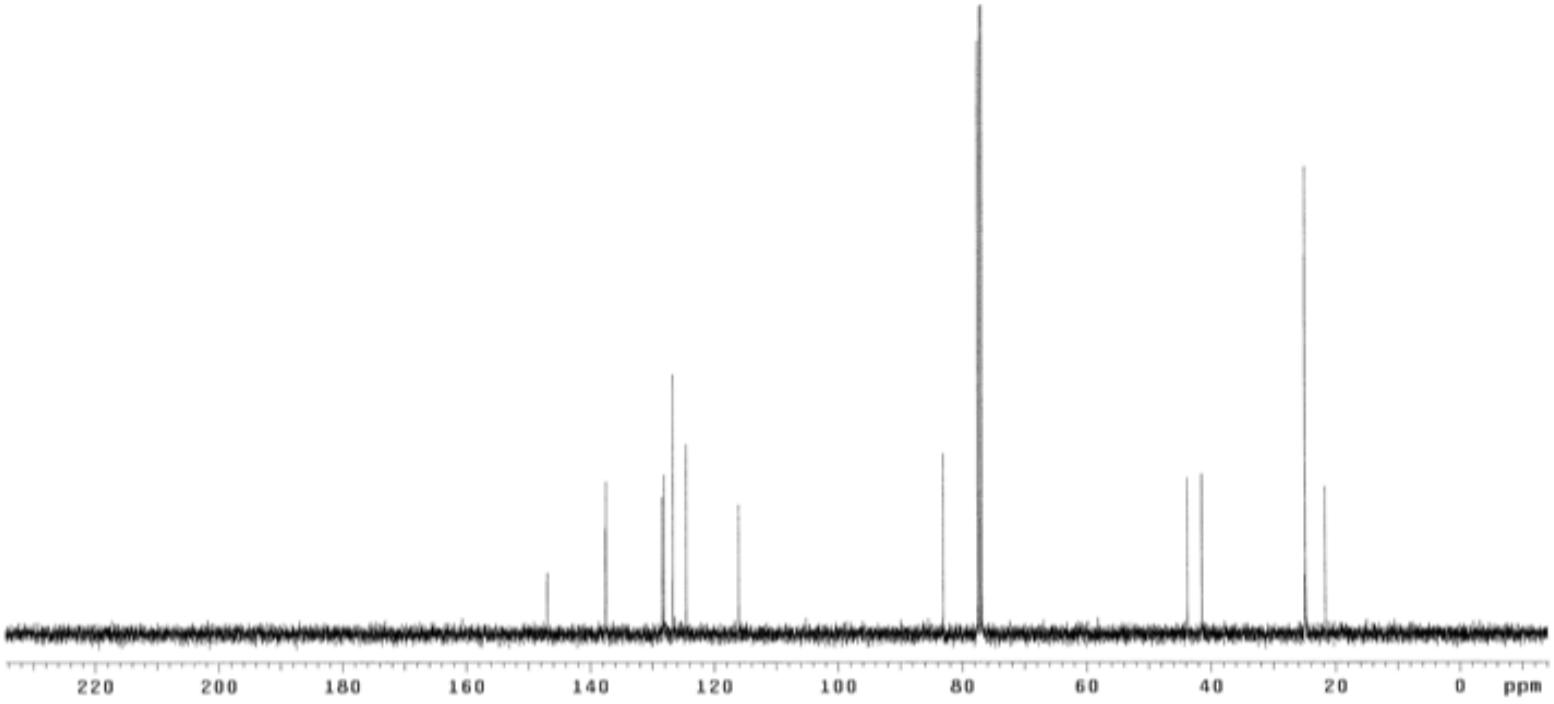
2ab



```
Sample Name:
  SR-V-33-carbon
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 23 2014
```



2ab

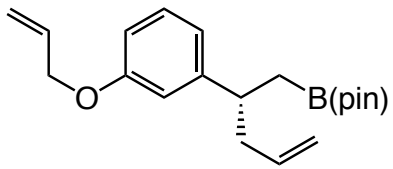


Sample Name:
JL-II-259PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

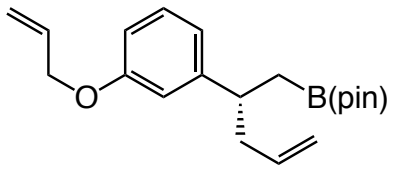
Sample directory:

FidFile: PROTON

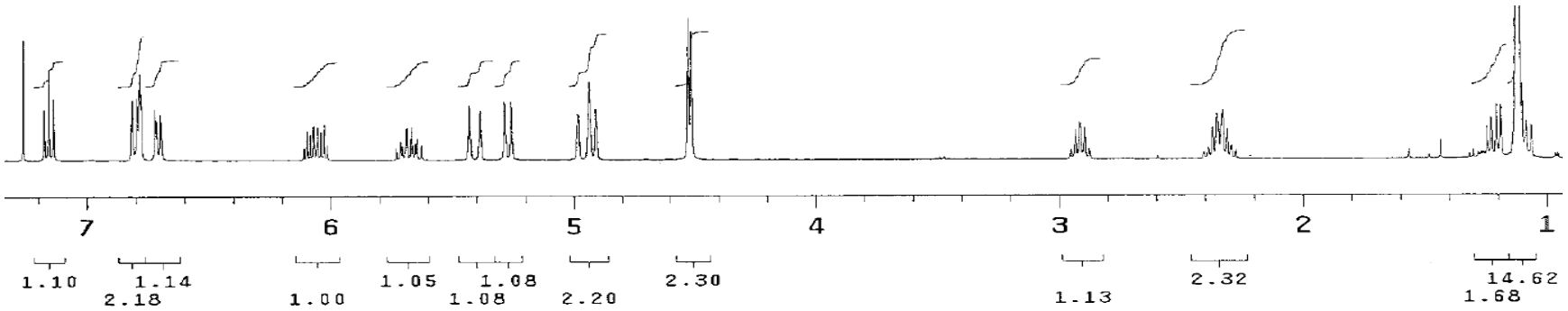
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 14 2014



2aj


O
B(pin)

2aj


7
6
5
4
3
2
1
1.10
1.14
2.18
1.00
1.05
1.08
1.08
2.20
2.30
1.13
2.32
14.62
1.68

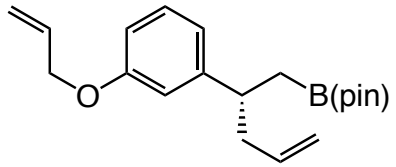
JL-II-298-C-PD

Sample Name:
JL-II-298-C-PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: JL-II-298-C-PD

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 14 2014



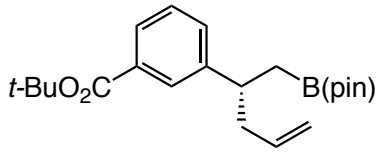
2aj

Sample Name:
SR-V-161
Data Collected on:
vnmr13-vnmrs400
Archive directory:

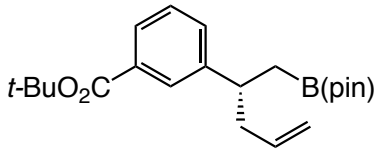
Sample directory:

FidFile: PROTON

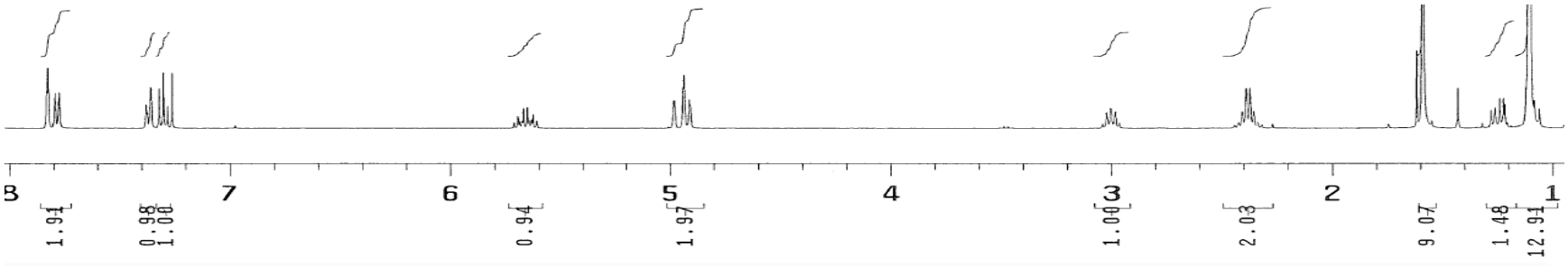
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 11 2015



2g



2g

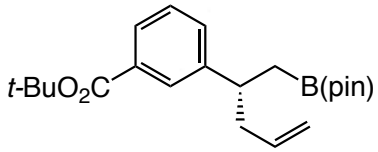


Sample Name:
SR-V-161-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:

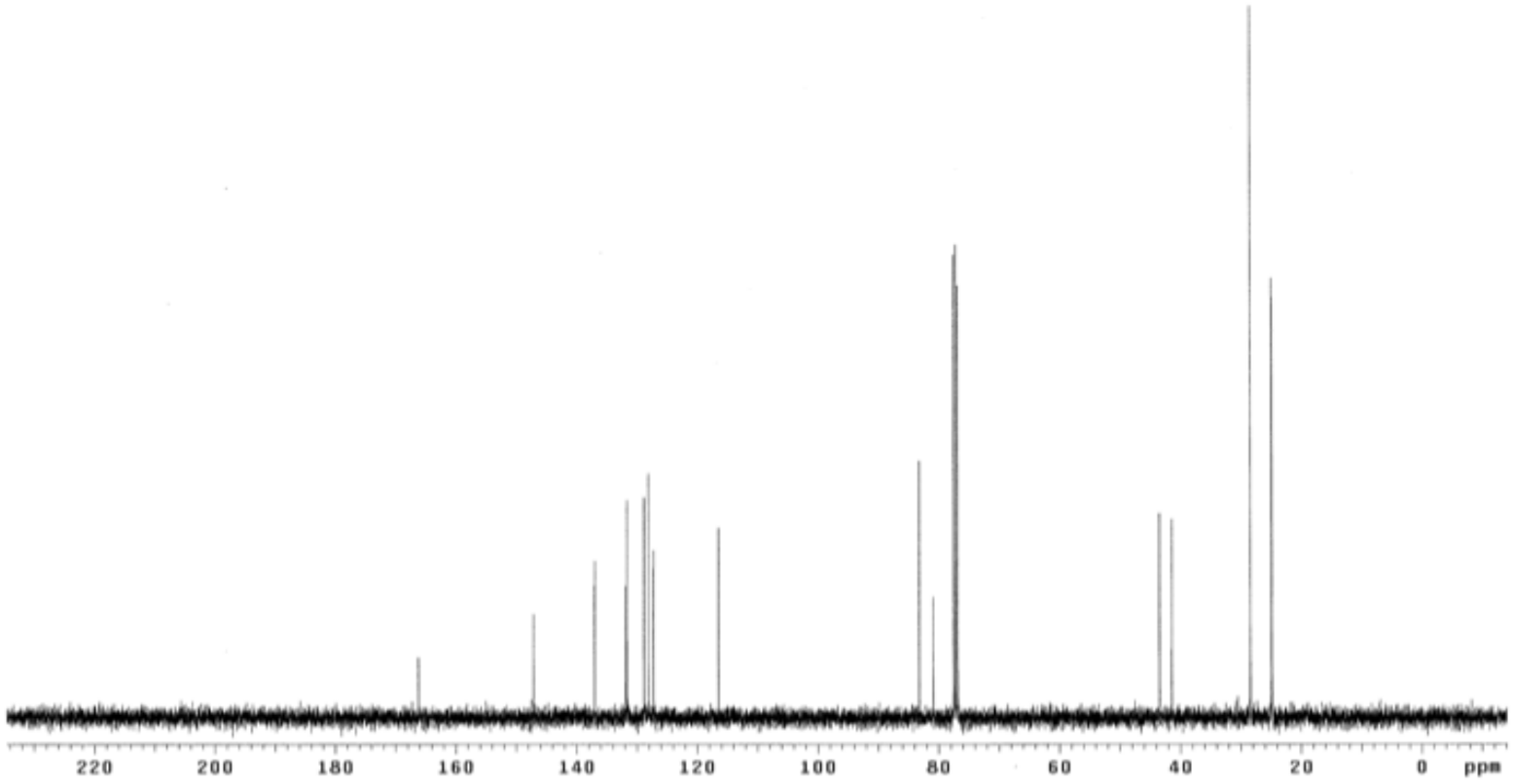
Sample directory:

FidFile: CARBON

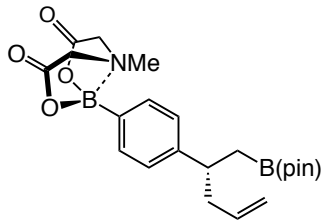
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 11 2015



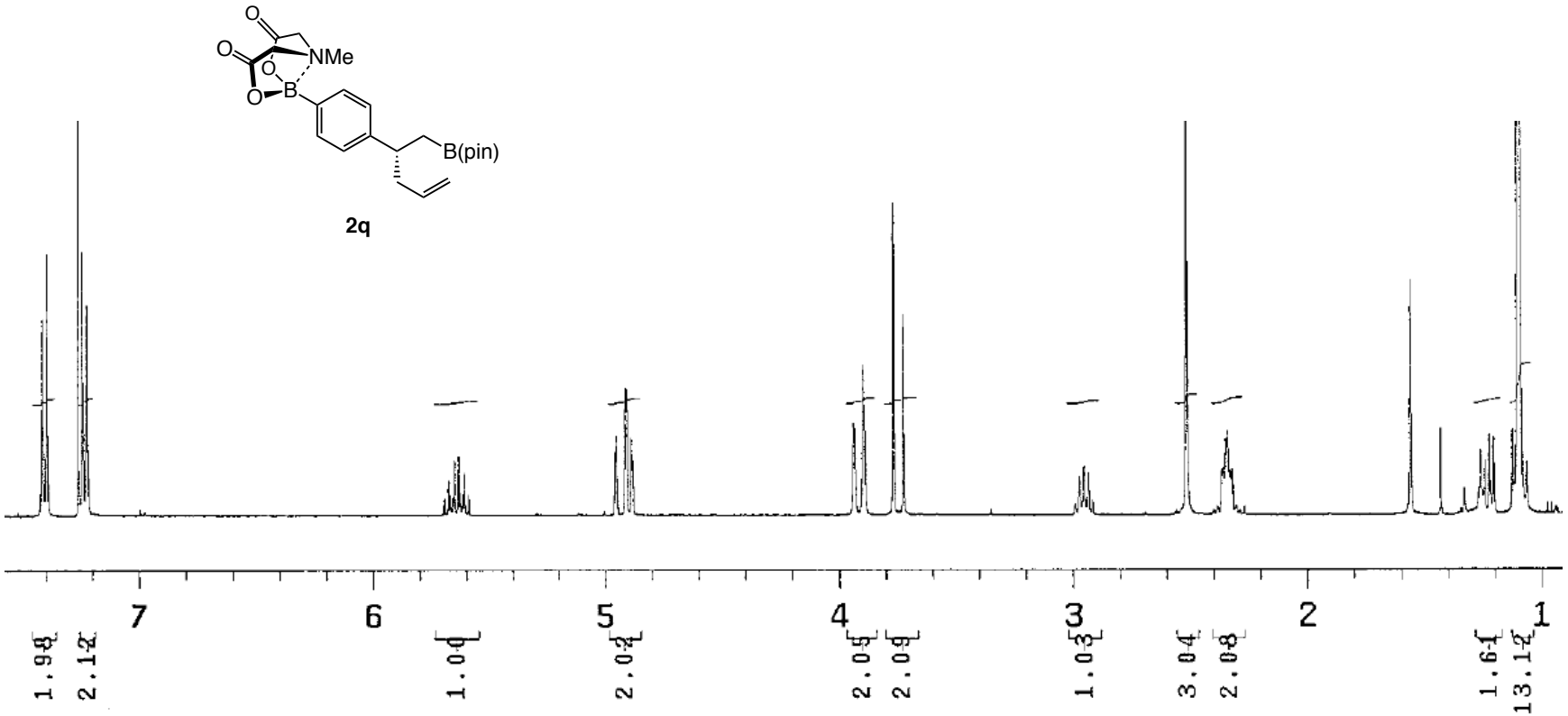
2g



```
Sample Name:
  SR-V-114
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May  4 2015
```



2q


O
O
NMe
O
B
O
B(pin)
7
6
5
4
3
2
1
1.98
2.12
1.00
2.02
2.05
2.09
1.03
3.04
2.08
1.64
13.12

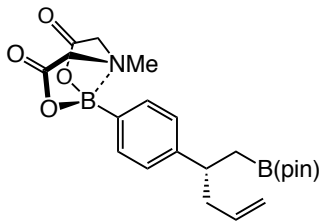
2q

Sample Name:
SR-V-114-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:

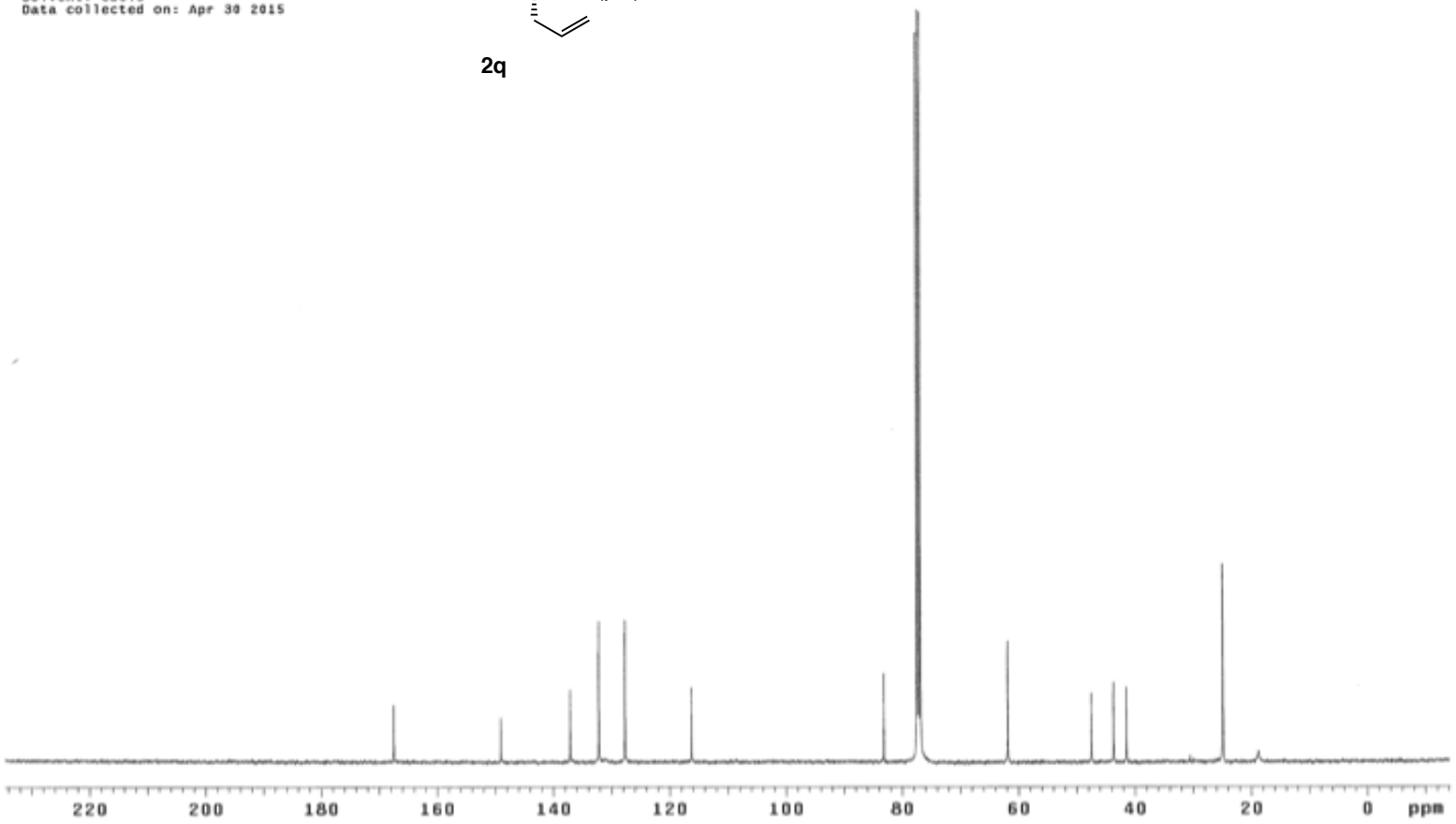
Sample directory:

FidFile: SR-V-114-carbon

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 30 2015



2q

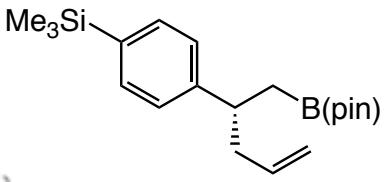


Sample Name:
SR-V-189
Data Collected on:
vnmr13-vnmrs400
Archive directory:

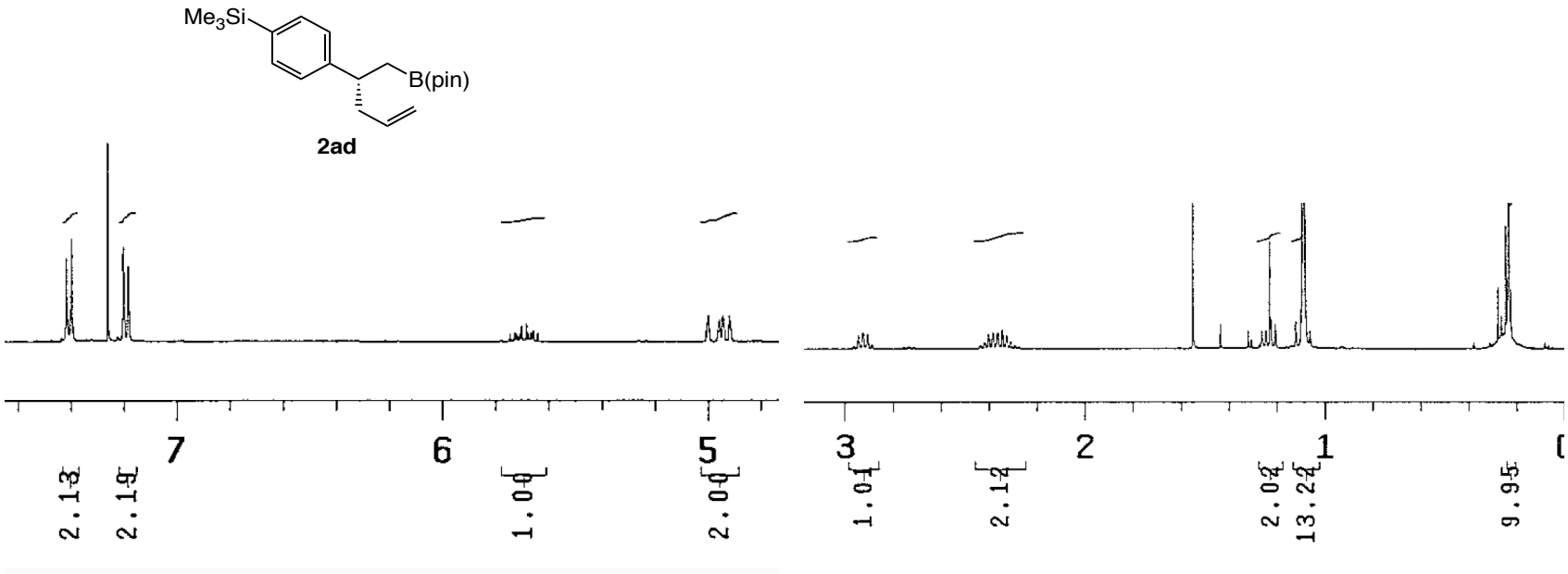
Sample directory:

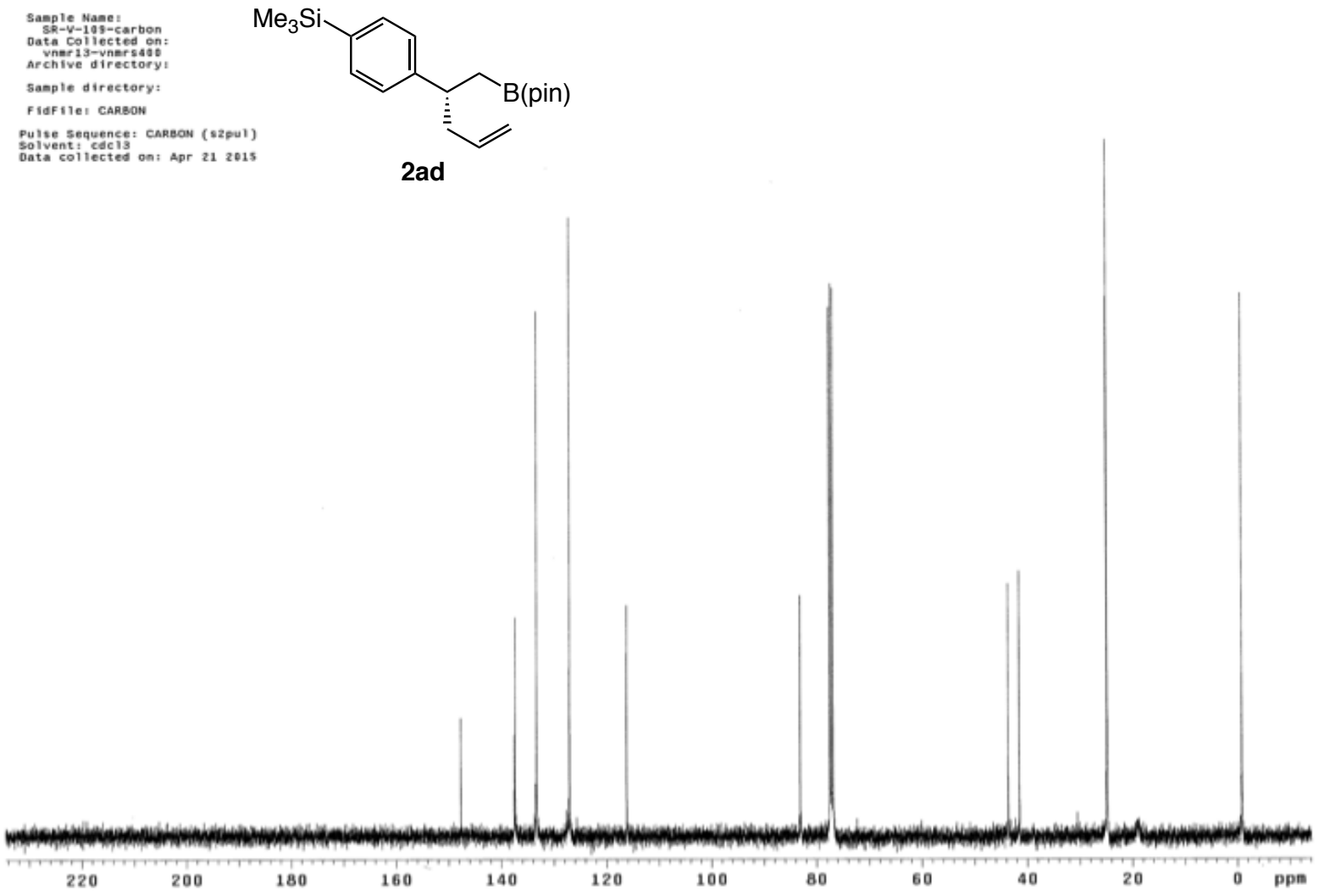
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 22 2015



2ad


Me3Si
B(pin)
2ad
7
6
5
3
2
1
2.13
2.19
1.00
2.00
1.01
2.12
2.02
13.24
9.95


Sample Name:
SR-V-109-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 21 2015
Me3Si
B(pin)
2ad
220
200
180
160
140
120
100
80
60
40
20
0
ppm

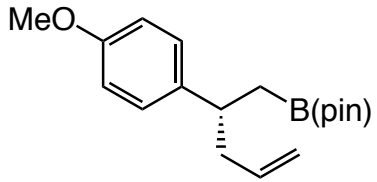
Sample Name:

Data Collected on:
vnmr13-vnmrs600
Archive directory:

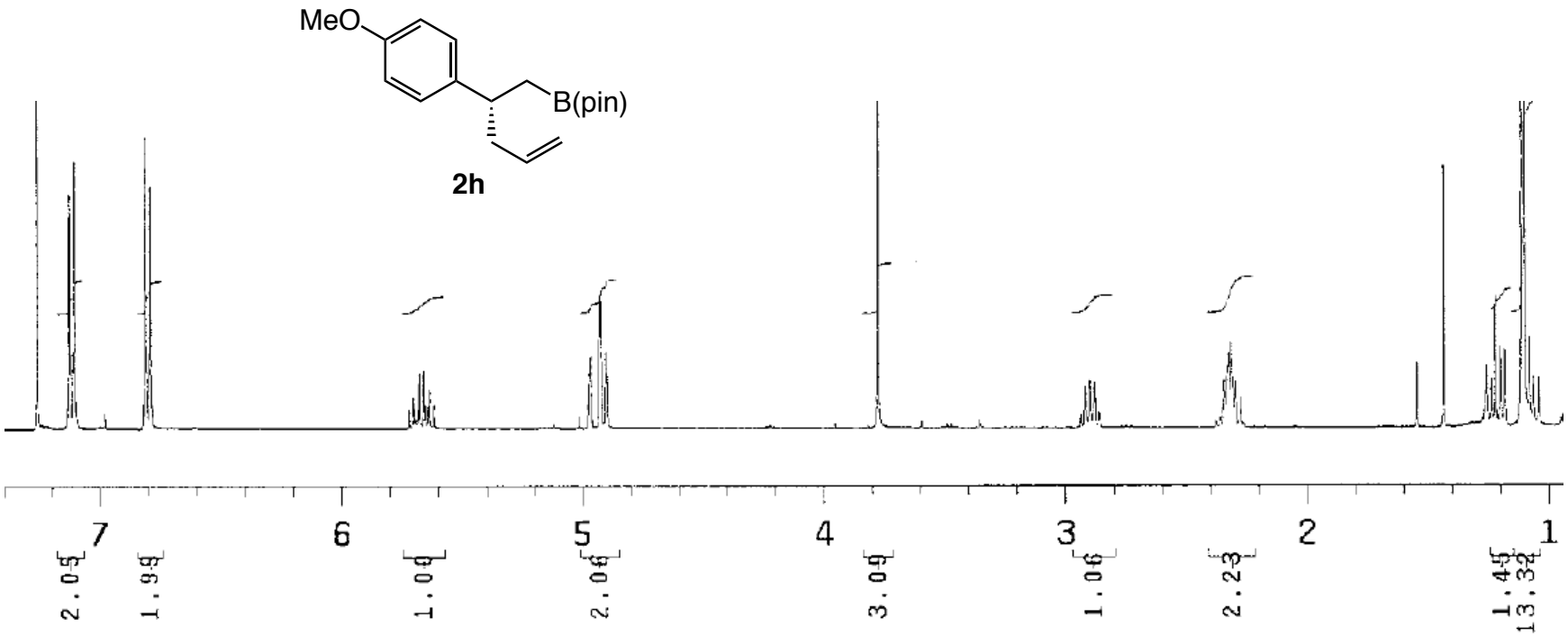
Sample directory:

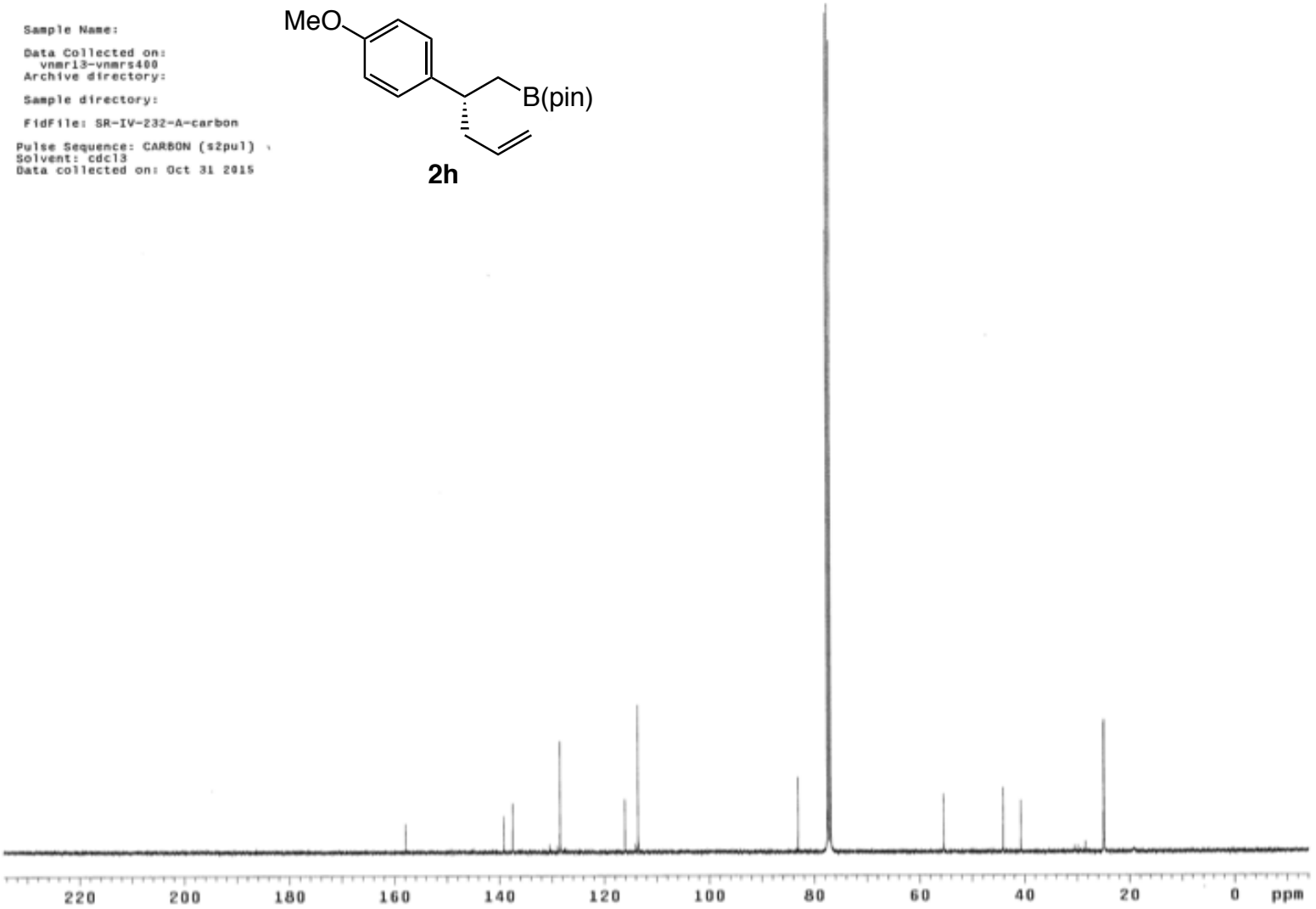
Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 14 2015



2h


MeO
B(pin)
2h
7
6
5
4
3
2
1
2.05
1.99
1.00
2.06
3.09
1.06
2.23
1.45
13.32

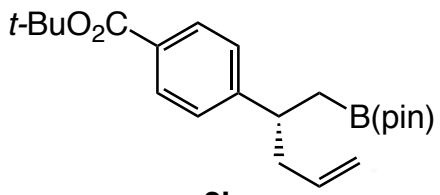

Sample Name:
Data Collected on:
vnmrl3-vnmrs400
Archive directory:
Sample directory:
FidFile: SR-IV-232-A-carbon
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 31 2015
MeO
B(pin)
2h
220
200
180
160
140
120
100
80
60
40
20
0
ppm

Sample Name:
SR-V-153-B-pTLC
Data Collected on:
vnmr13-vnmrs400
Archive directory:

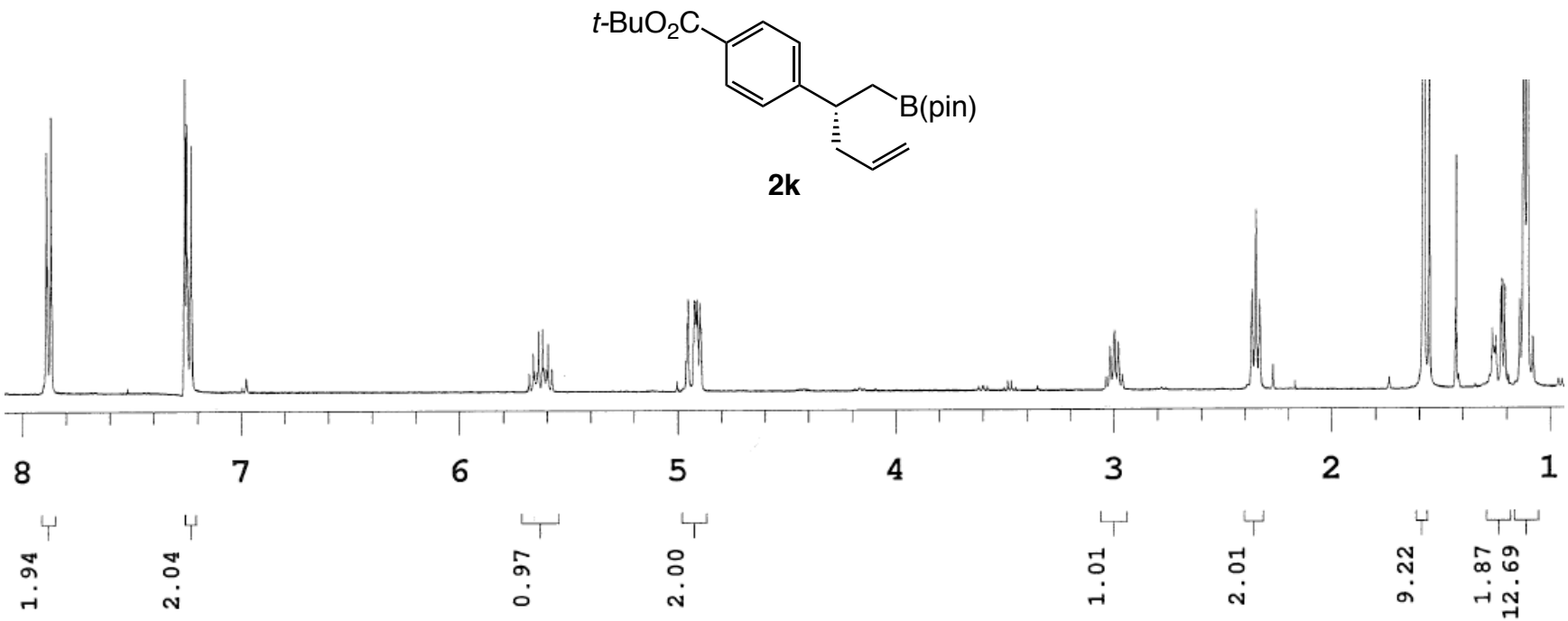
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2015



2k

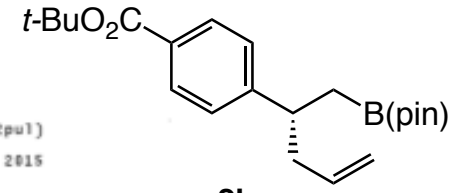

t-BuO2C
B(pin)
2k
8
7
6
5
4
3
2
1
1.94
2.04
0.97
2.00
1.01
2.01
9.22
1.87
12.69

Sample Name:
SR-V-153-B-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: SR-V-153-carbon

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2015



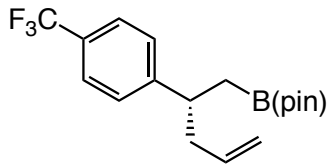
2k

Sample Name:
SR-IV-278-D-rac
Data Collected on:
vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 9 2014



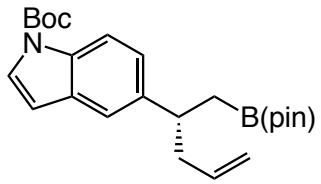
2l

Sample Name:
JL-III-237PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

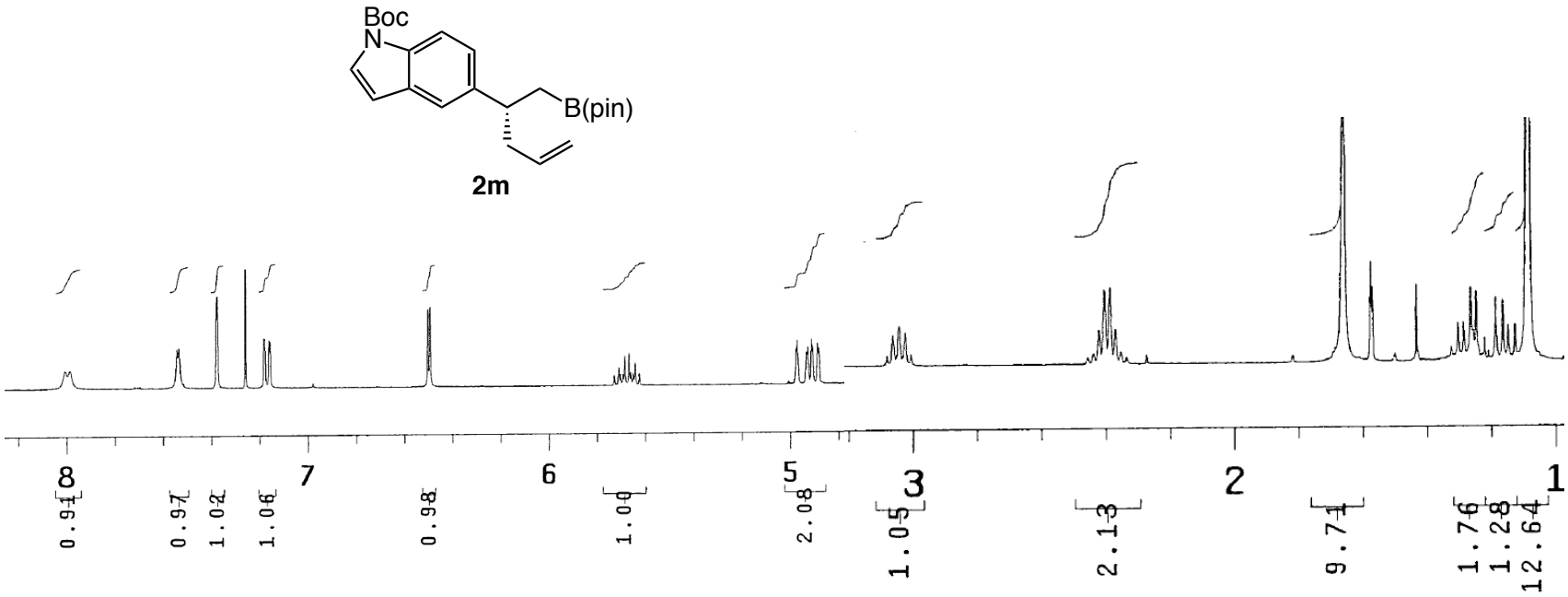
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 24 2015



2m


Boc
N
B(pin)
2m
8
7
6
5
4
3
2
1
0.94
0.97
1.02
1.06
0.98
1.00
2.08
1.05
2.13
9.71
1.76
1.28
12.64

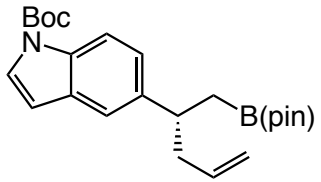
JL-III-237C-PD

Sample Name:
JL-III-237C-PD
Data Collected on:
vnmr13-vnmrs480
Archive directory:

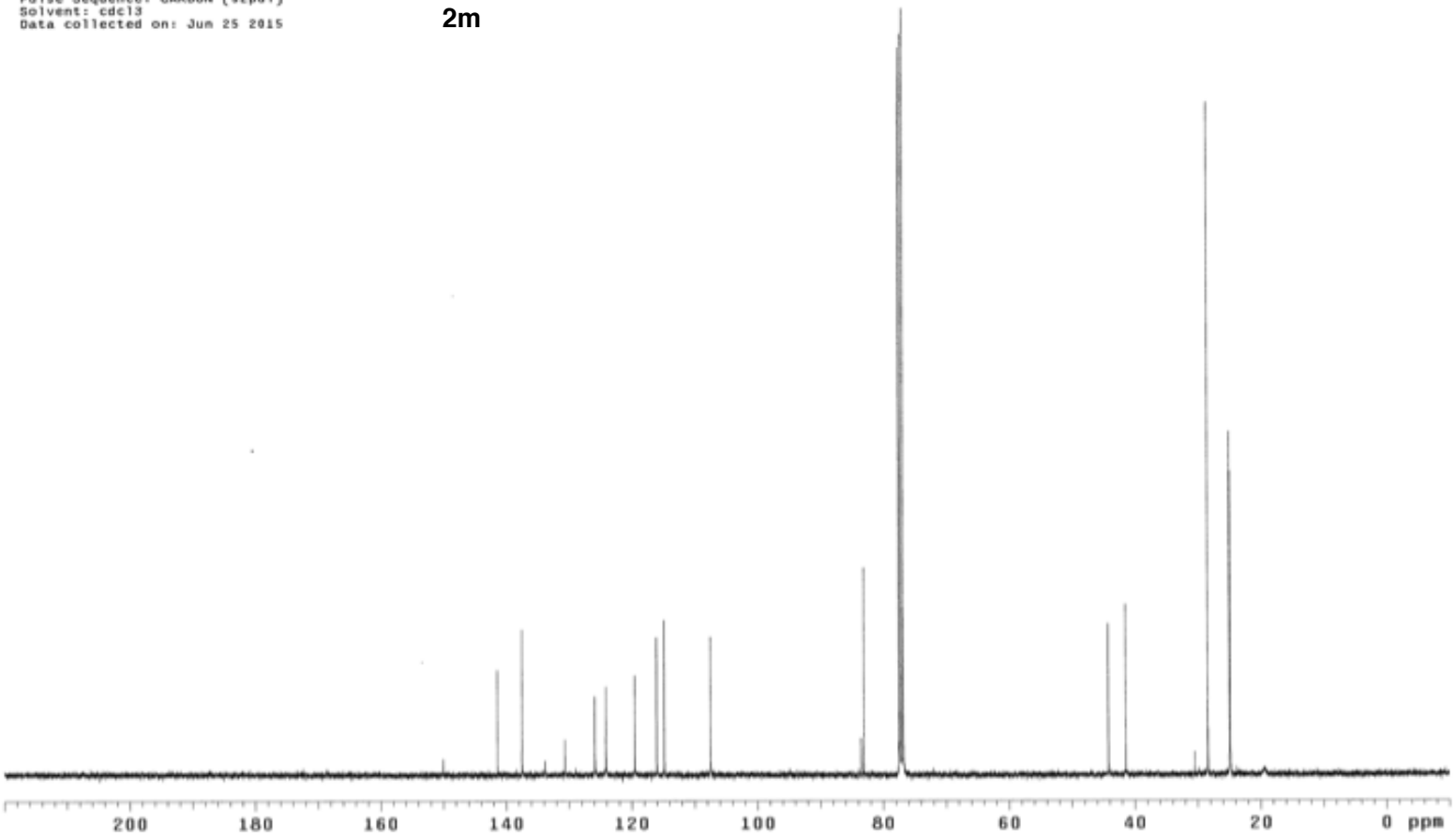
Sample directory:

FidFile: JL-III-237C-PD2

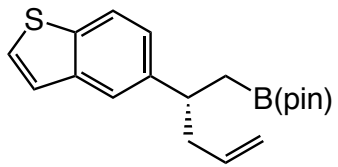
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 25 2015



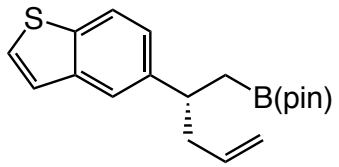
2m



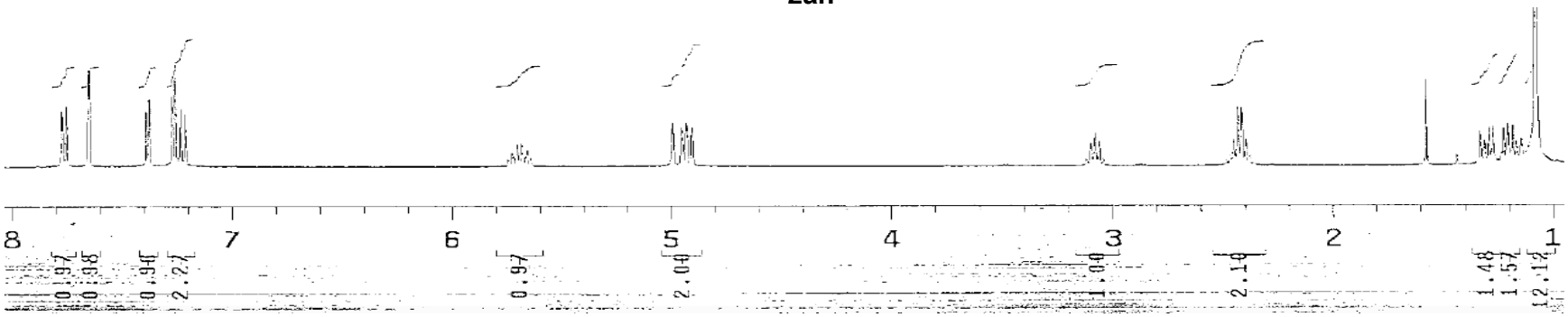
```
Sample Name:
  SR-V-139
Data Collected on:
  nmr14-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 23 2015
```



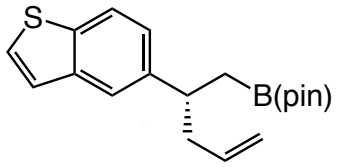
2ah



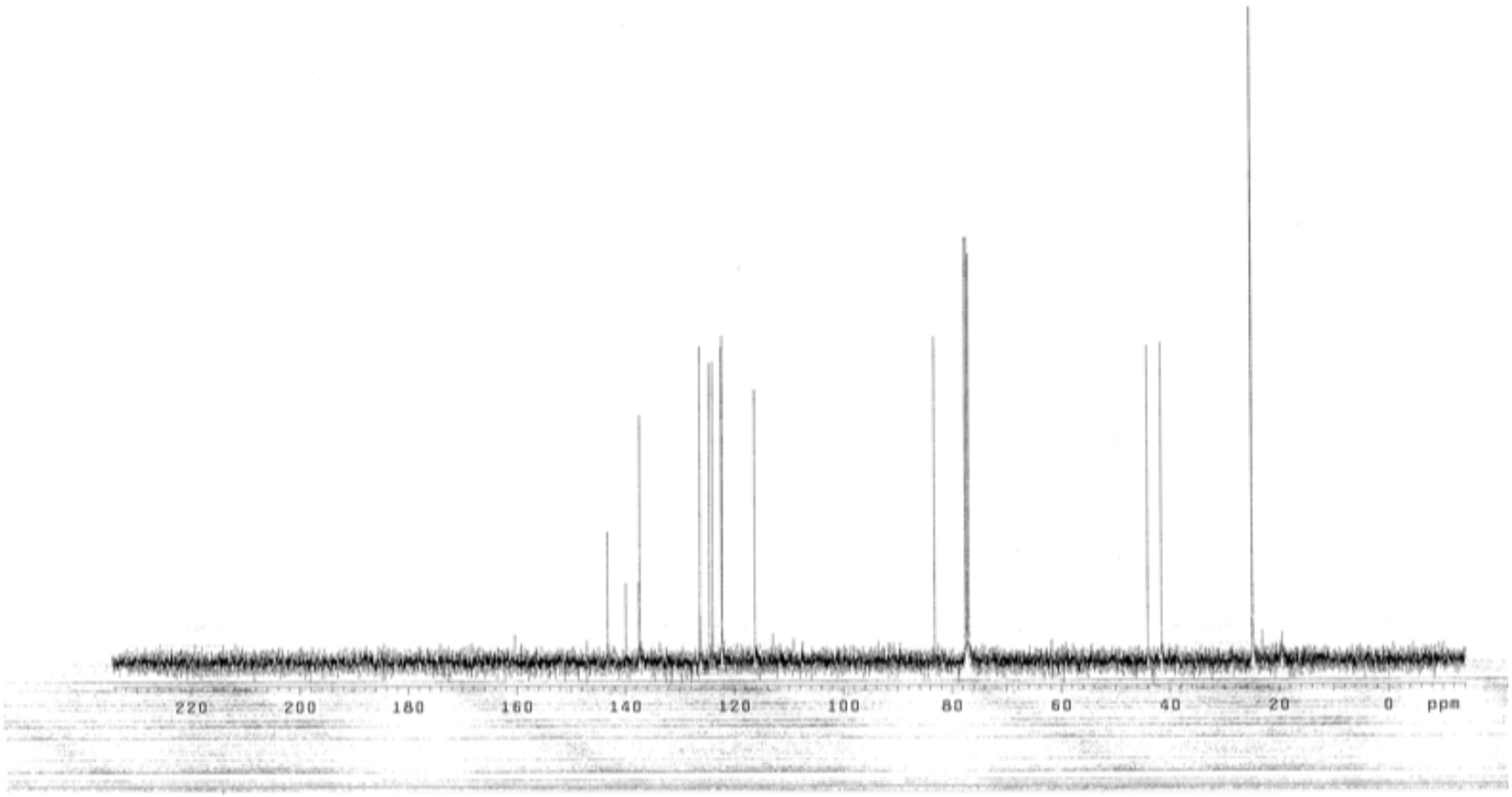
2ah



```
Sample Name:
  SR-V-133-carbon
Data Collected on:
  nmr14-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 20 2015
```



2ah

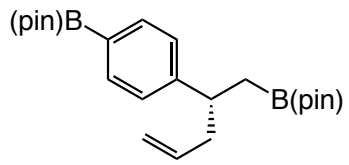


Sample Name:
SR-V-104
Data Collected on:
vnmr13-vnmrs400
Archive directory:

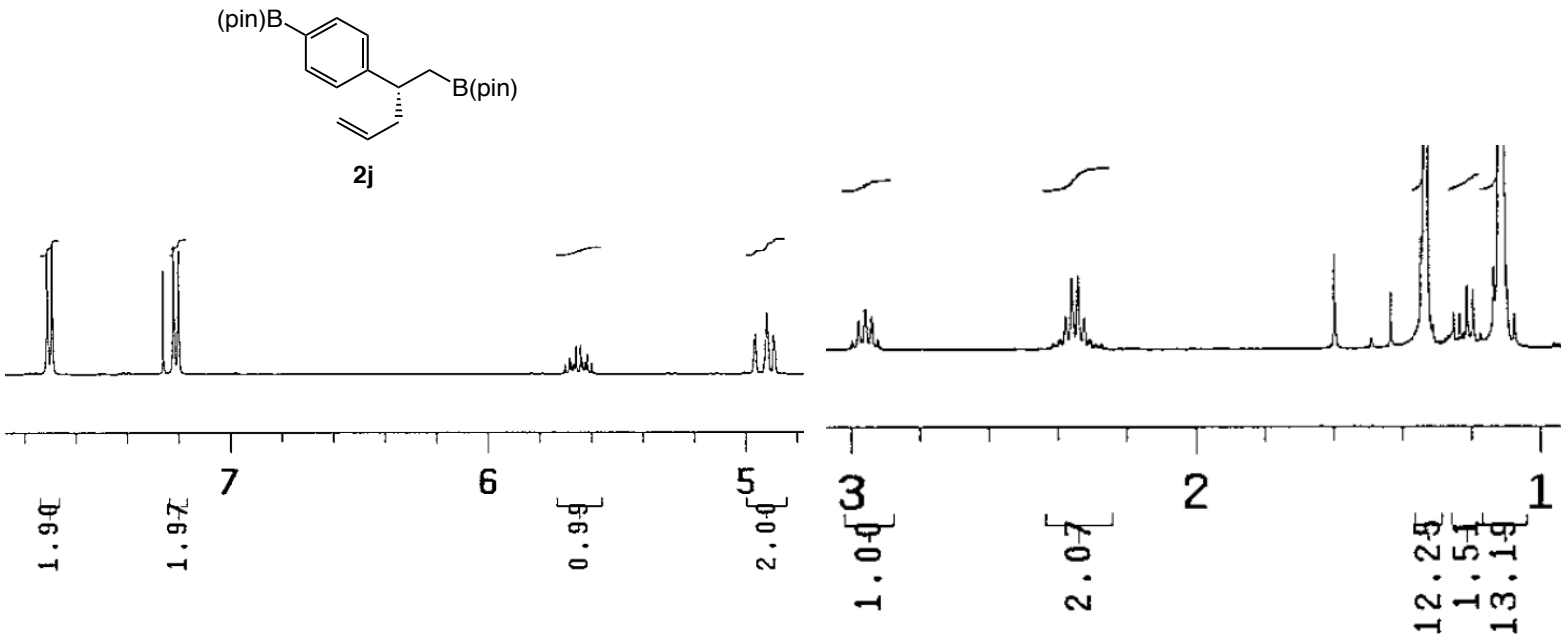
Sample directory:

Fidfile: PROTON

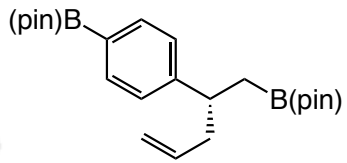
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 17 2015



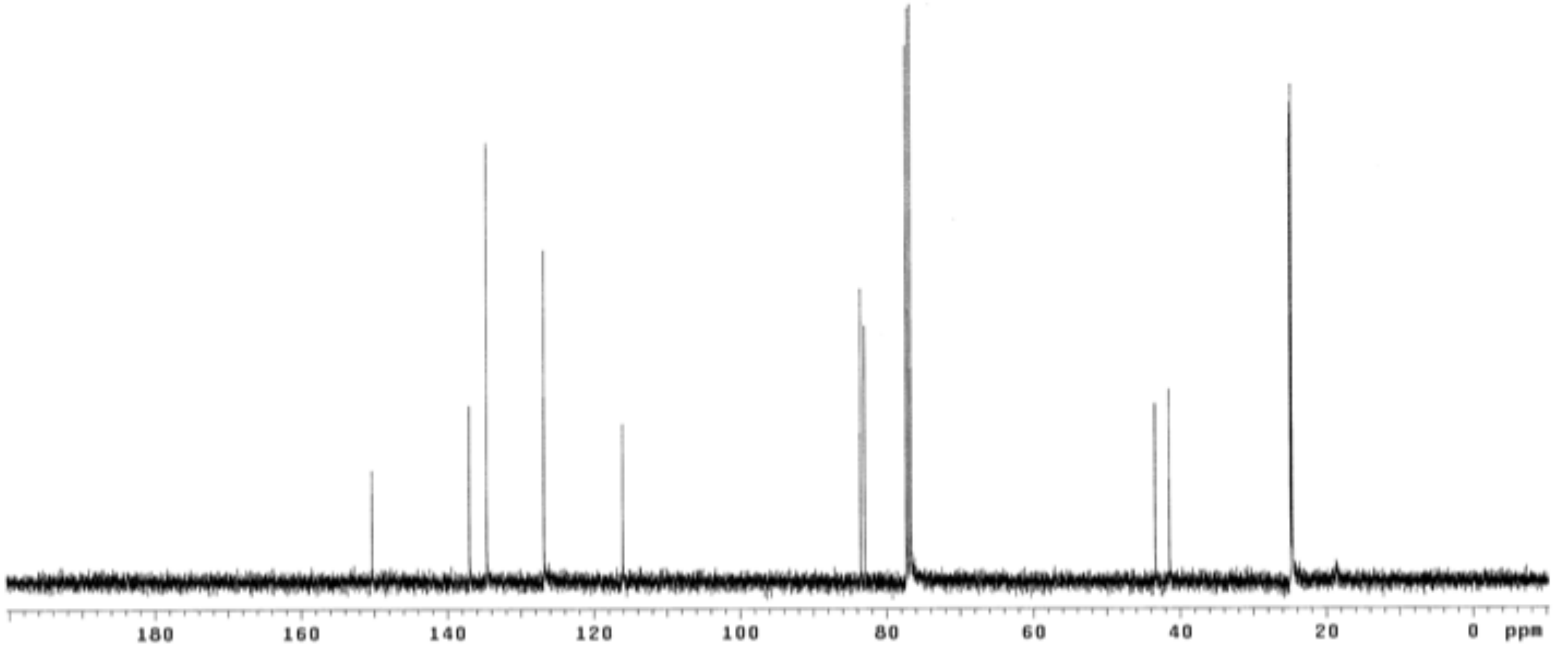
2j


(pin)B
B(pin)
2j
7
6
5
3
2
1
1.99
1.97
0.99
2.00
1.04
2.07
12.25
1.51
13.19

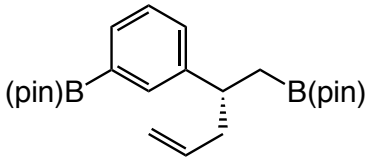
```
Sample Name:
  SR-V-104-carbon
Data Collected on:
  vnmr13-vnmrs409
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 17 2015
```



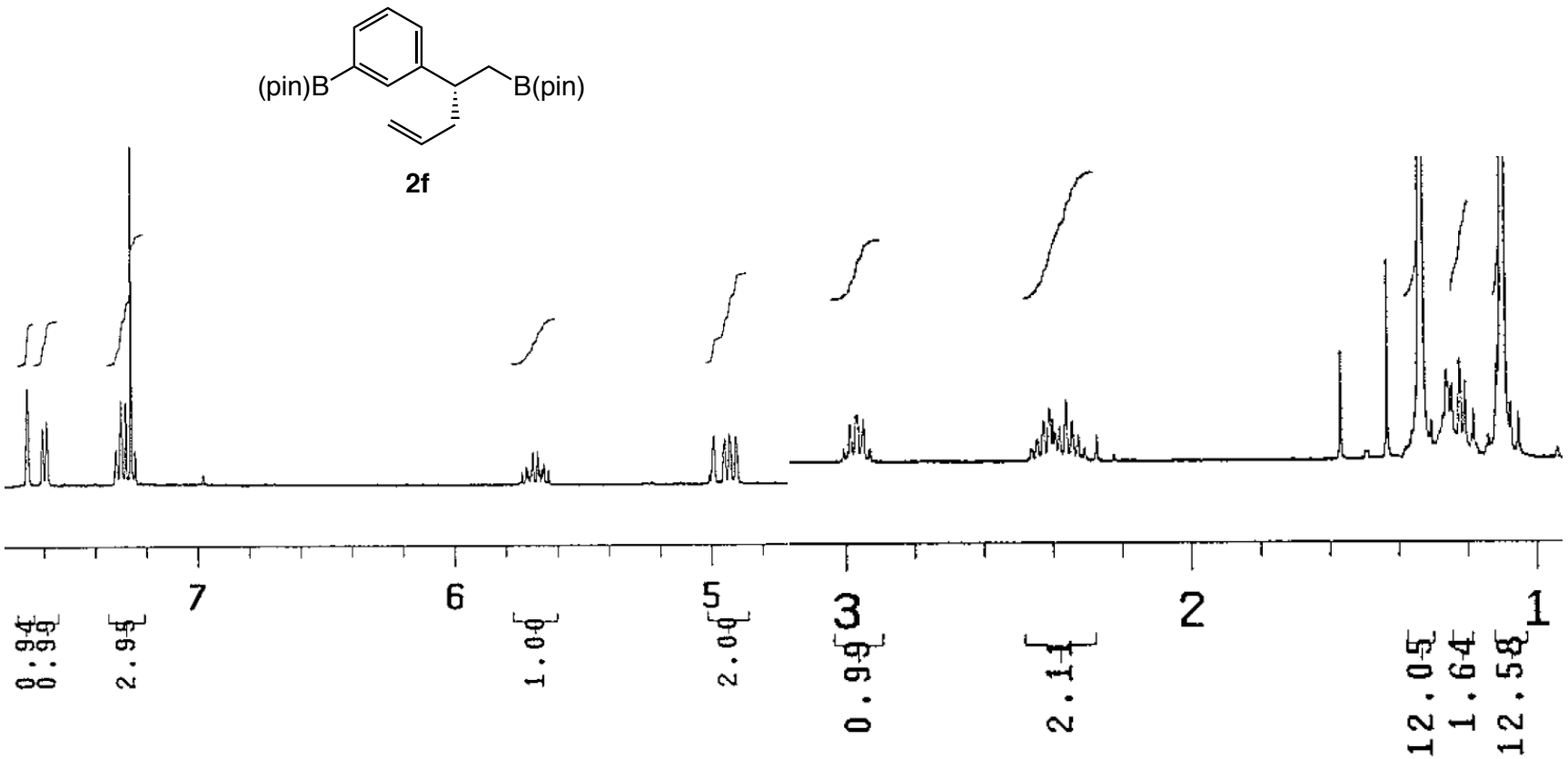
2j



```
Sample Name:
  SR-V-111-pTLC
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: SR-V-111-pTLC

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 25 2015
```



2f

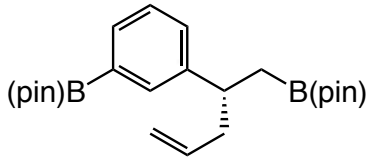

(pin)B
B(pin)
2f
7
6
5
3
2
1
0.94
0.99
2.95
1.00
2.00
0.99
2.11
12.05
1.64
12.58

Sample Name:
SR-V-111-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:

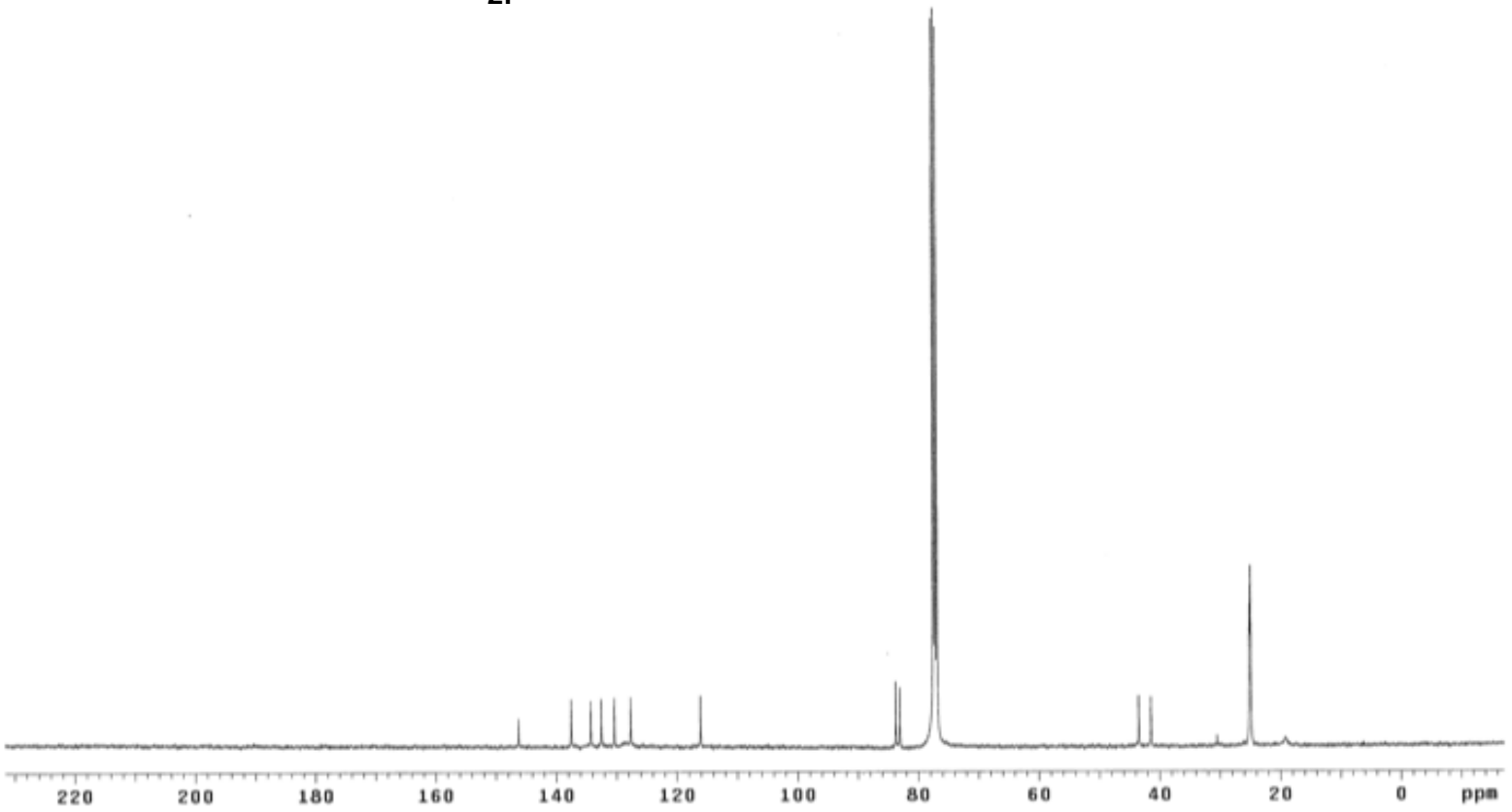
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 25 2015



2f

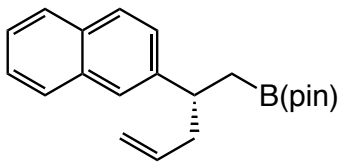


Sample Name:
JL-III-195PD-1
Data Collected on:
vnmri3-vnmrs400
Archive directory:

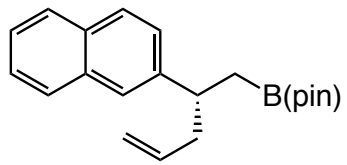
Sample directory:

FidFile: PROTON

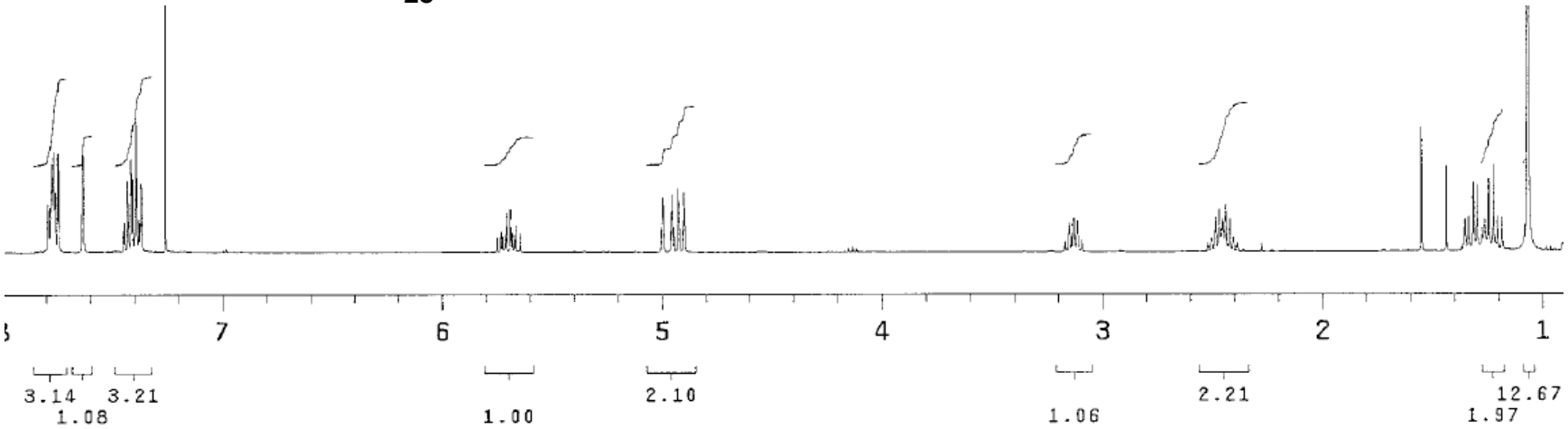
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 21 2015



2e



2e



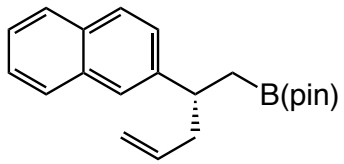
JL-III-195-C-PD

Sample Name:
JL-III-195-C-PD
Data Collected on:
vnmr13-vnmrs480
Archive directory:

Sample directory:

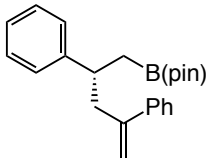
FidFile: JL-III-195PD-C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 22 2015

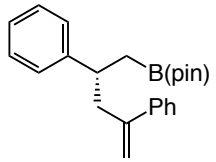


2e

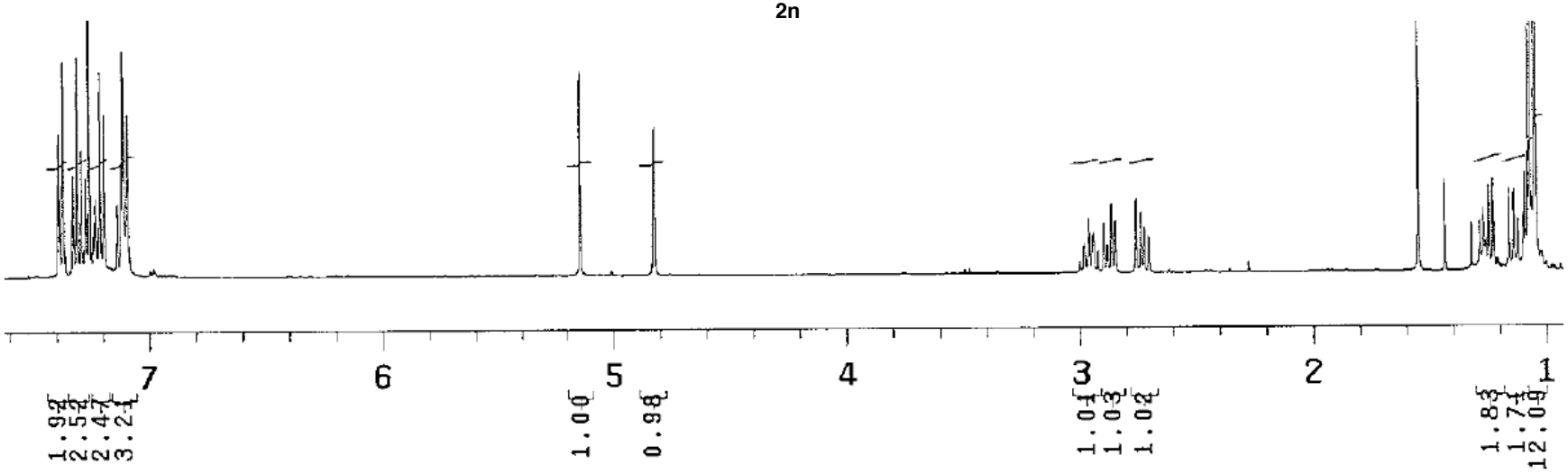
```
Sample Name:
  SR-IV-292
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 28 2014
```

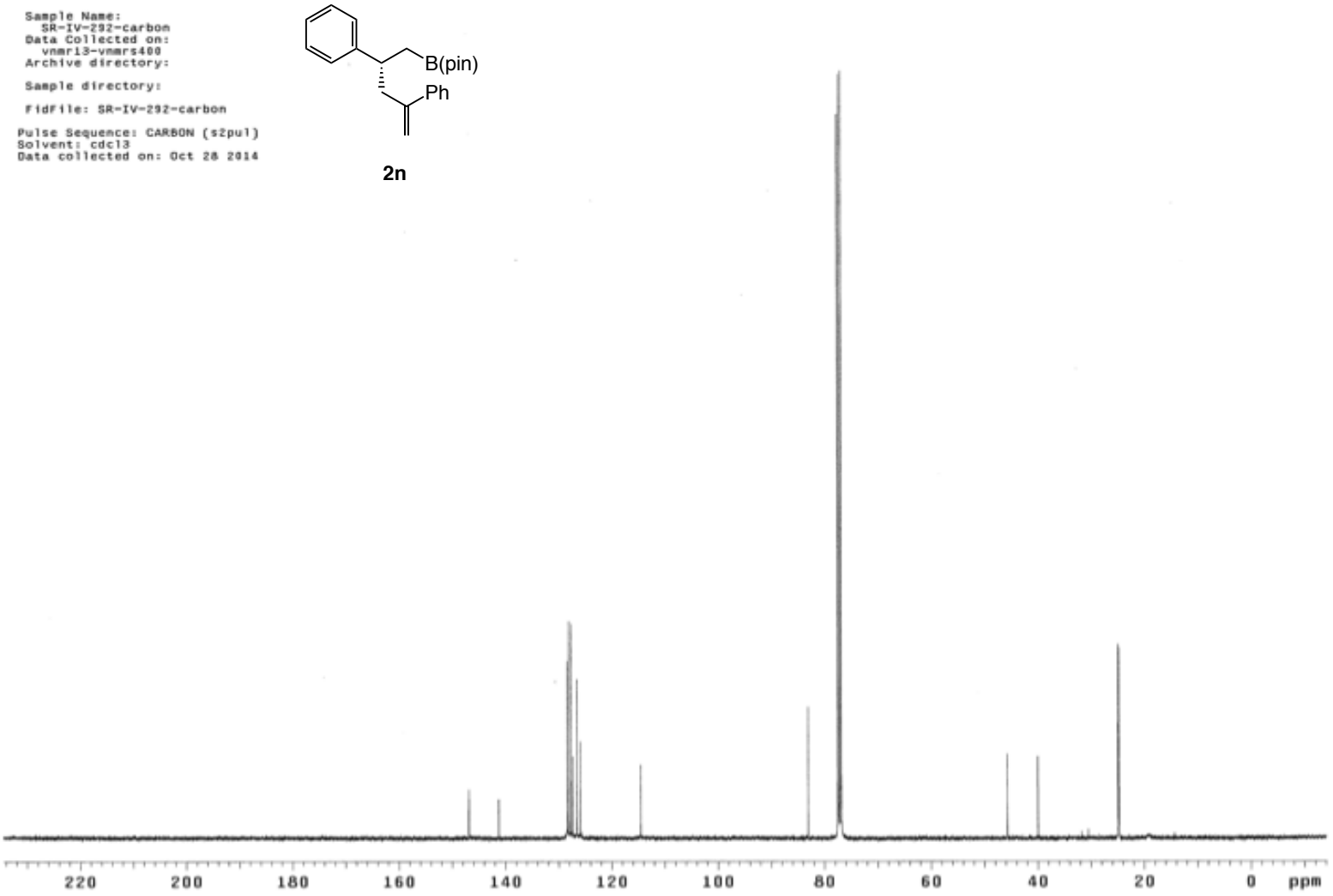


2n


B(pin)
Ph

2n


7
6
5
4
3
2
1
1.92
2.58
2.47
3.24
1.00
0.98
1.04
1.03
1.02
1.83
1.74
12.09


Sample Name:
SR-IV-292-carbon
Data Collected on:
vnmr13-vmmrs400
Archive directory:
Sample directory:
FidFile: SR-IV-292-carbon
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 28 2014
B(pin)
Ph
220
200
180
160
140
120
100
80
60
40
20
0
ppm

2n

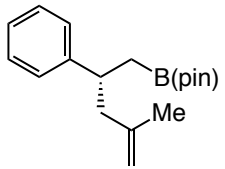
Sample Name:

Data Collected on:
vnmr13-vnmrs400
Archive directory:

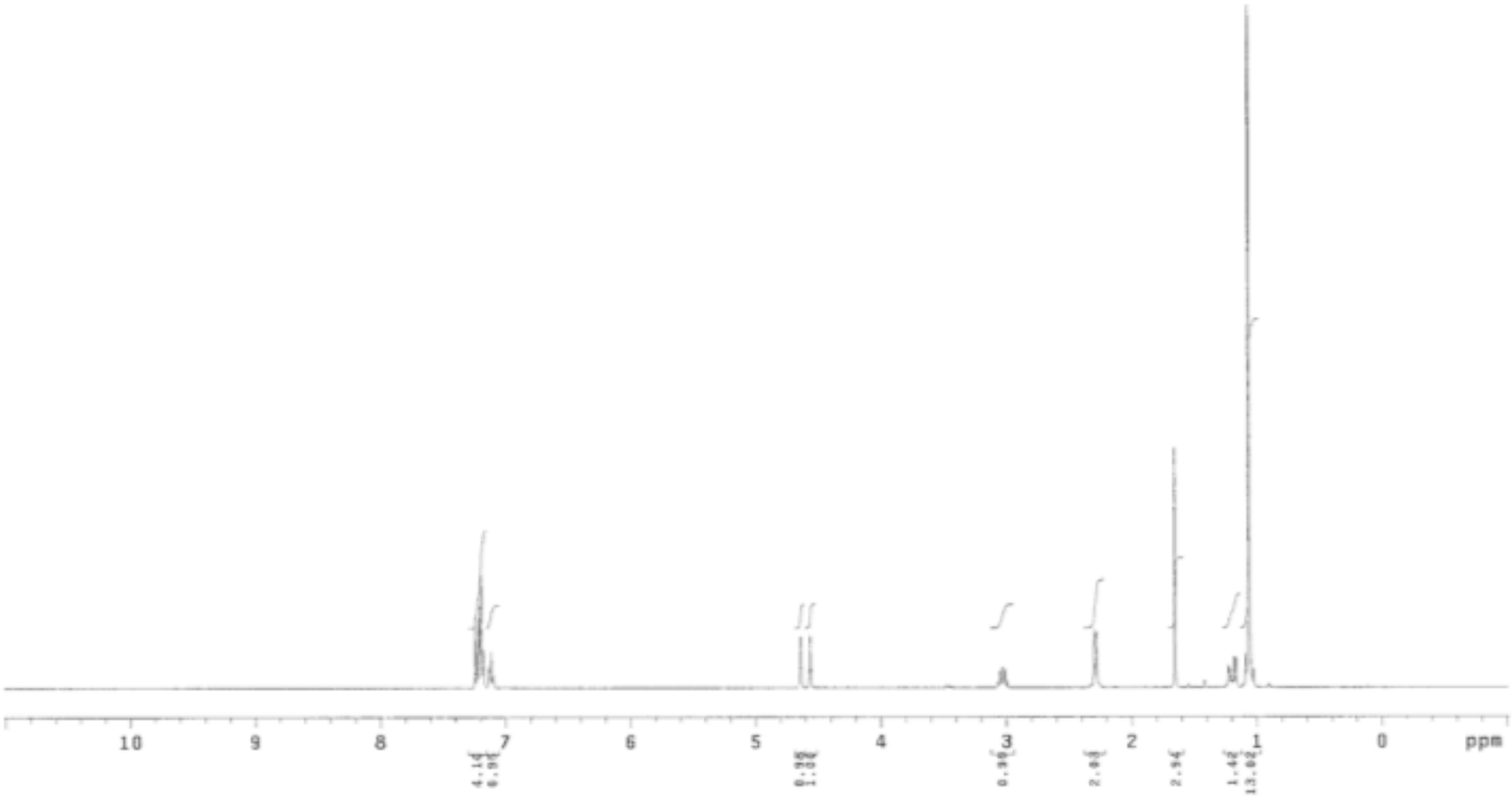
Sample directory:

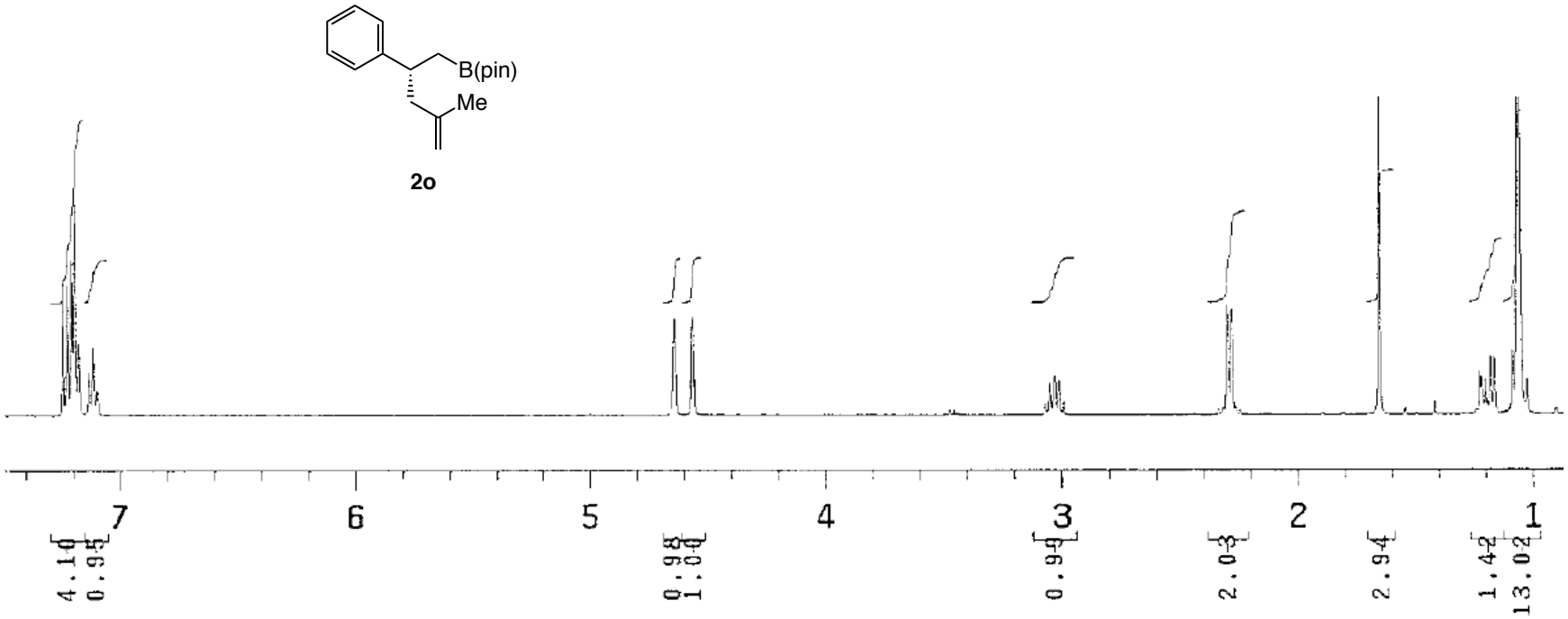
FidFile: Ph-Me-product

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 13 2015



2o





2o

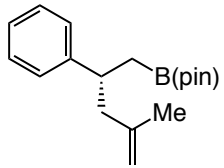
Sample Name:

Data Collected on:
vnmr13-vnmrs400
Archive directory:

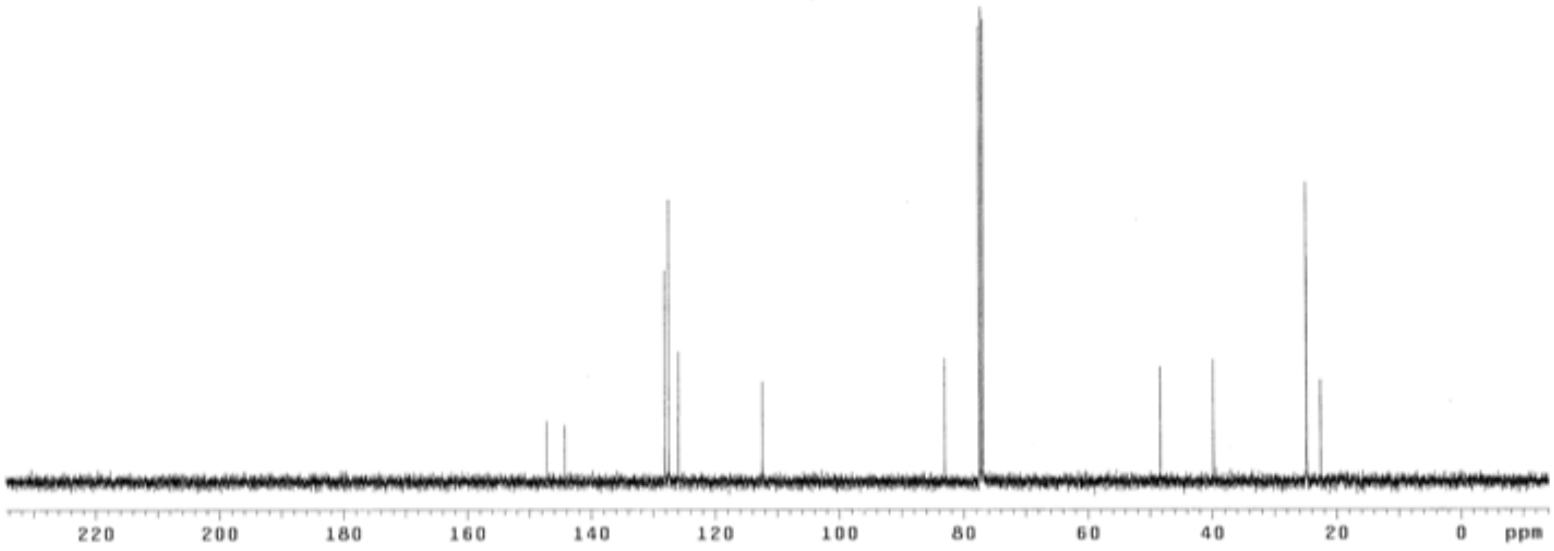
Sample directory:

FidFile: CARBON

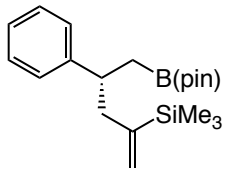
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 13 2015



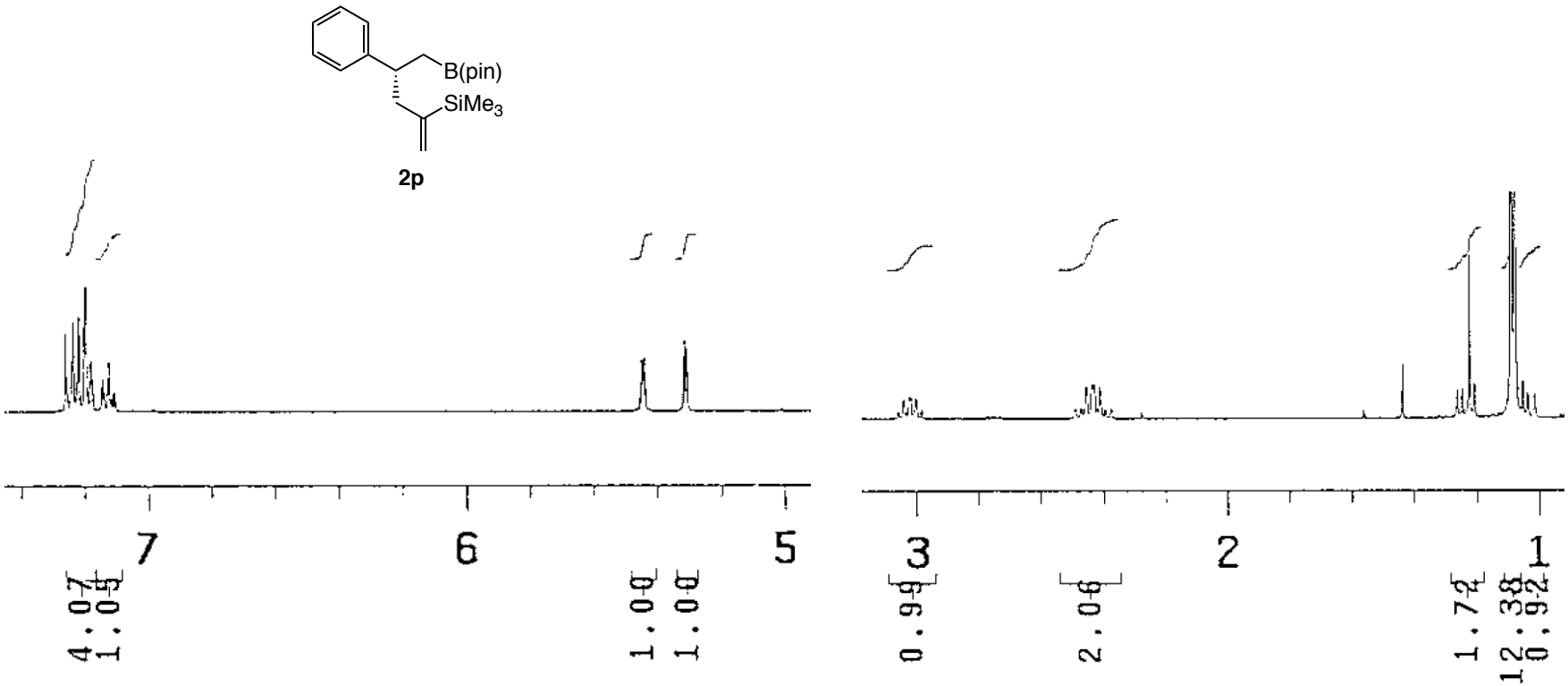
2o



```
Sample Name:
  SR-IV-302
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 14 2015
```

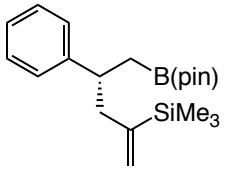


2p

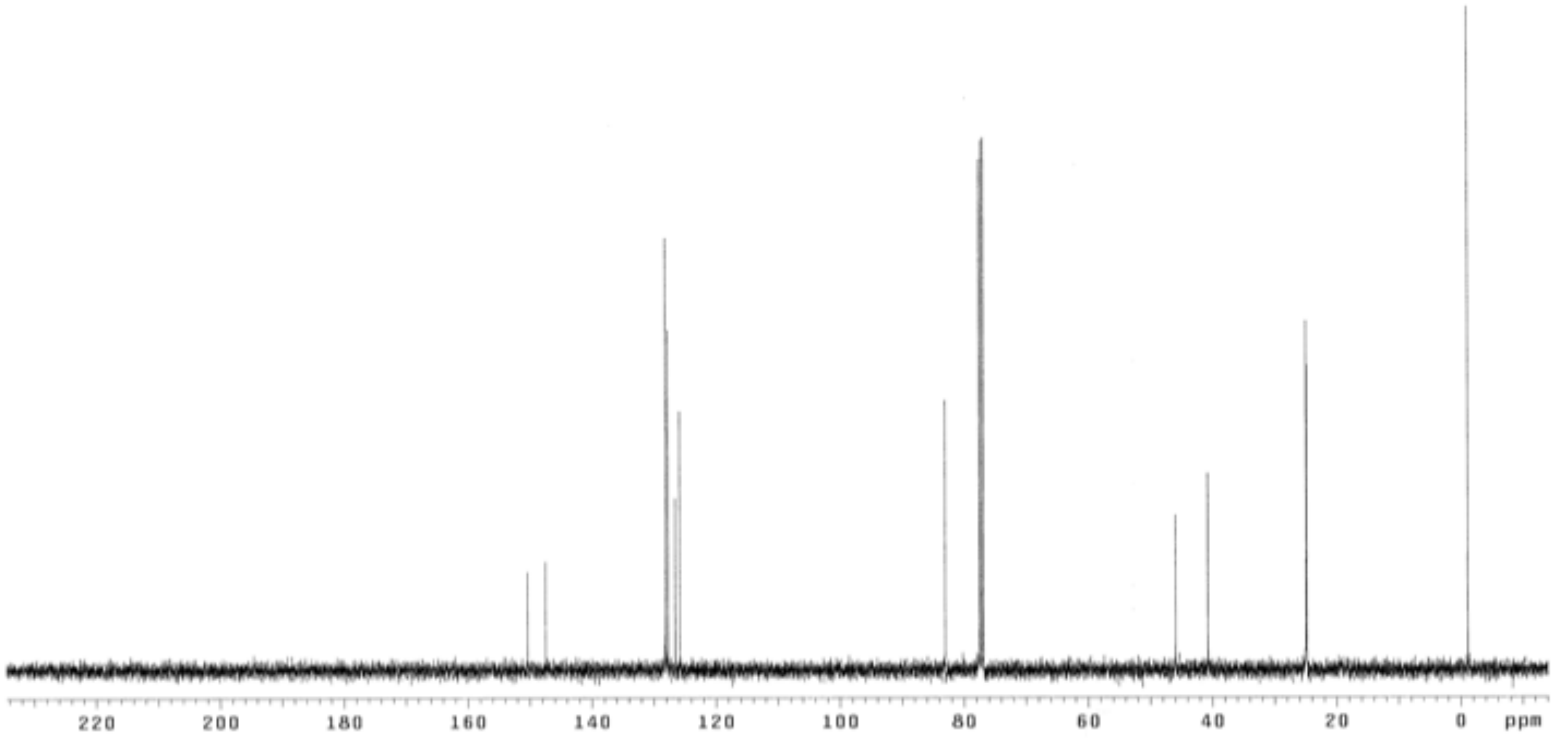


2p

```
Sample Name:
  SR-IV-302-carbon
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 14 2015
```



2p

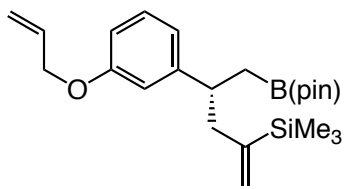


Sample Name:
SR-V-46
Data Collected on:
nmr18-vnmrs500
Archive directory:

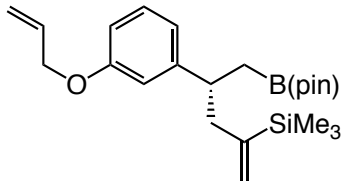
Sample directory:

FidFile: PROTON

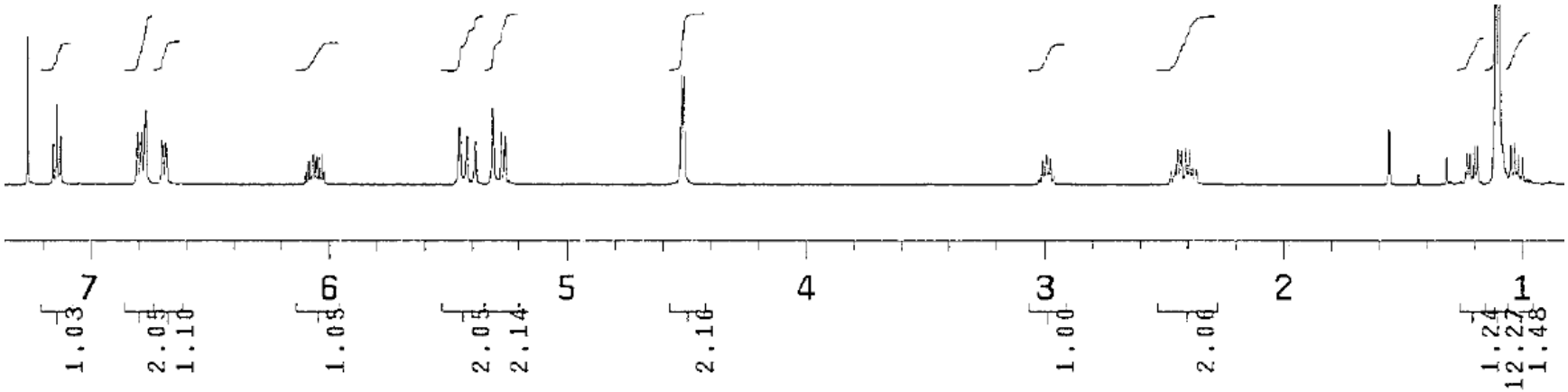
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 18 2015



2ak


O
B(pin)
SiMe3

2ak

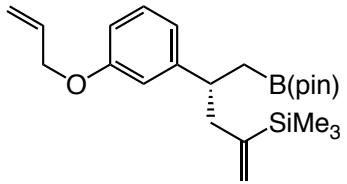

7
6
5
4
3
2
1
1.03
2.05
1.10
1.05
2.05
2.14
2.16
1.00
2.06
1.24
12.27
1.48

Sample Name:
SR-V-46-carbon
Data Collected on:
nmr18-vnmrs500
Archive directory:

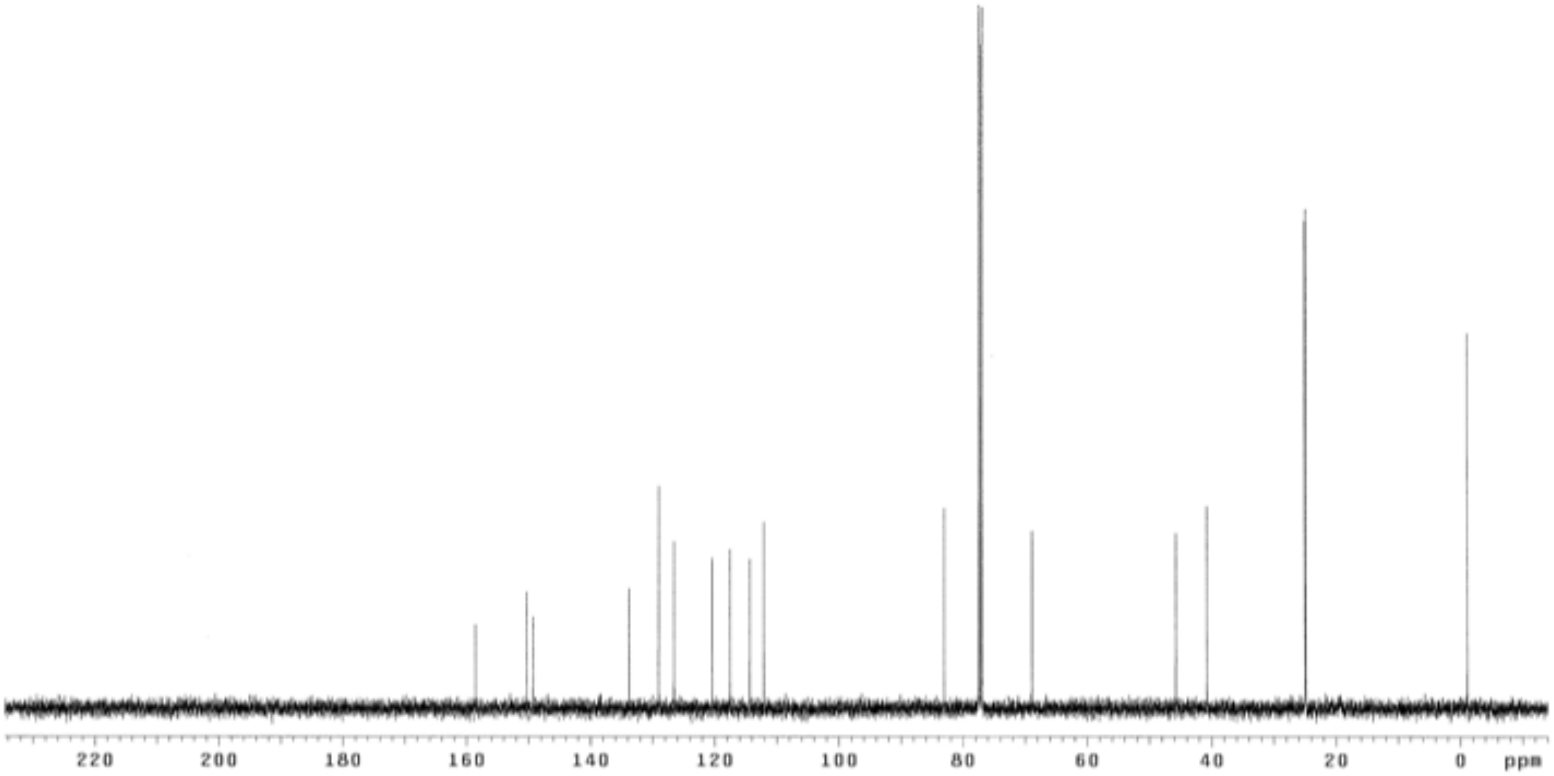
Sample directory:

FidFile: CARBON

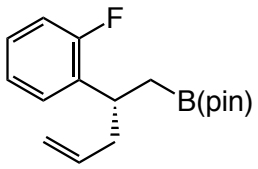
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 18 2015



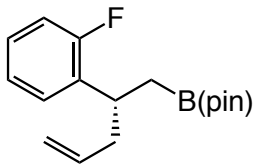
2ak



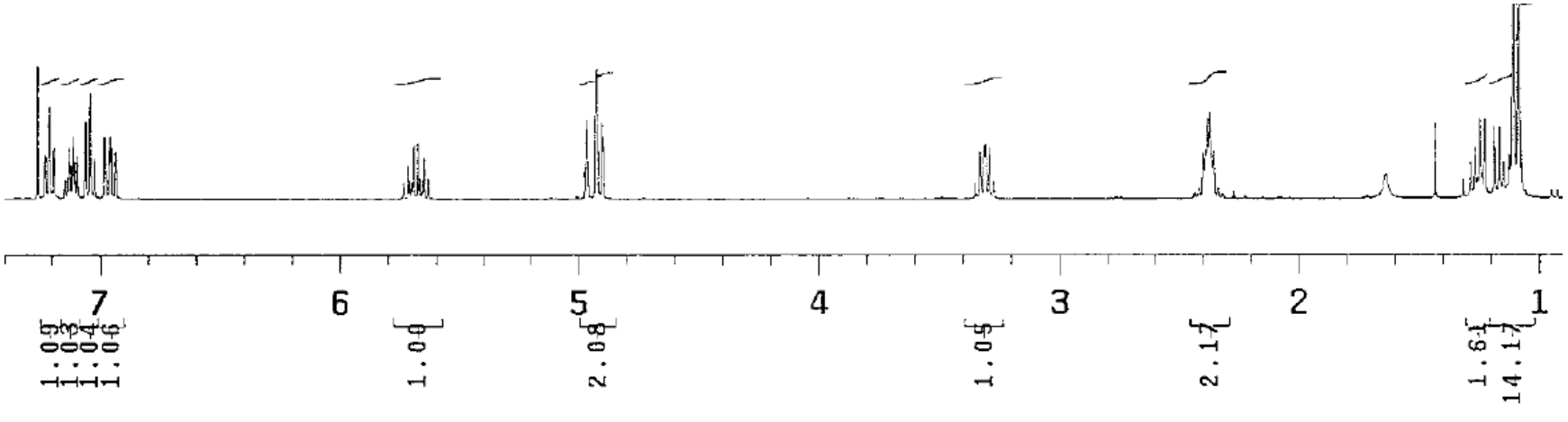
```
Sample Name:
  SR-IV-265-A
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct  1 2014
```



2c



2c

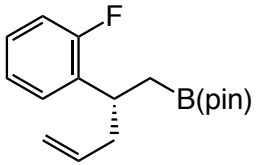


Sample Name:
SR-IV-265-A-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:

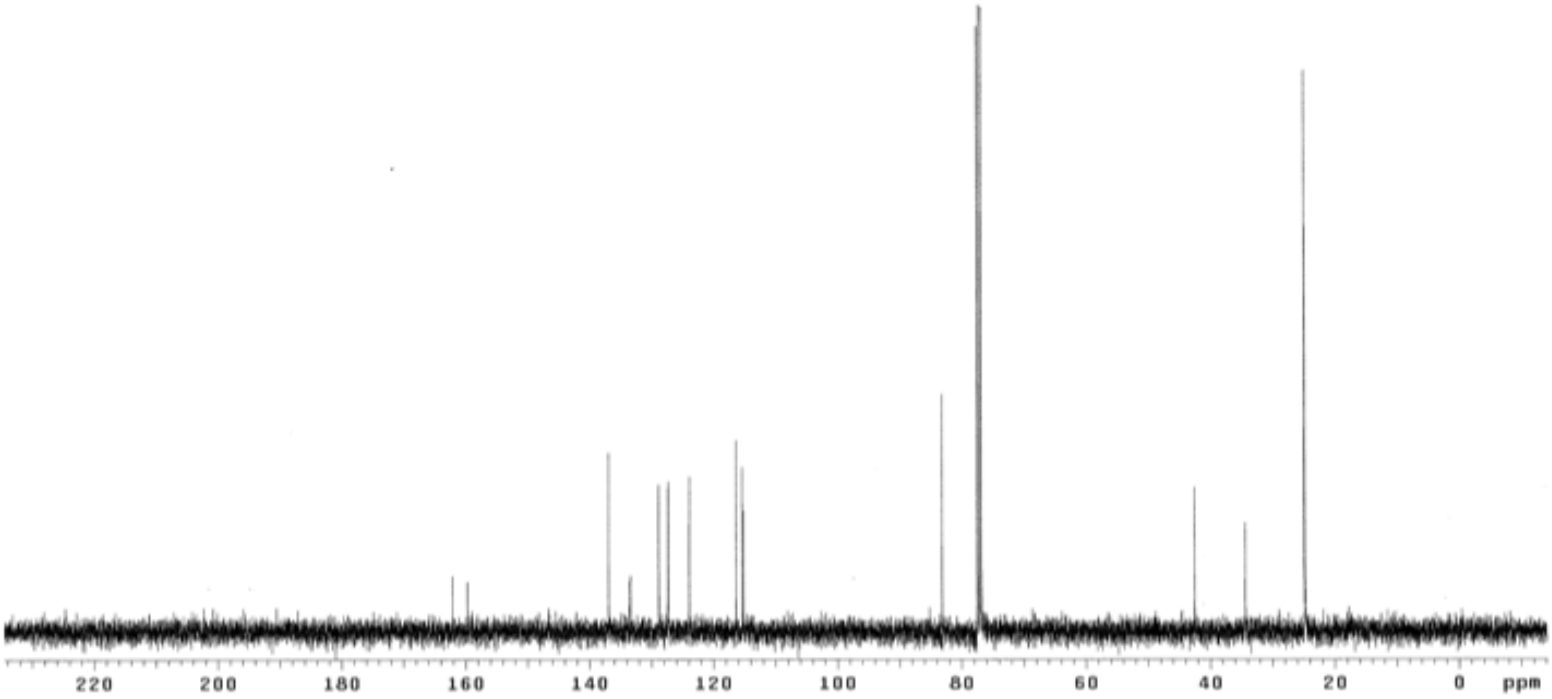
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 1 2014



2c

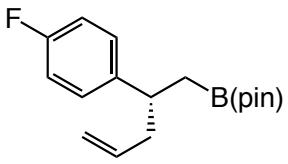


Sample Name:
SR-IV-252-A
Data Collected on:
vnmr13-vnmrs400
Archive directory:

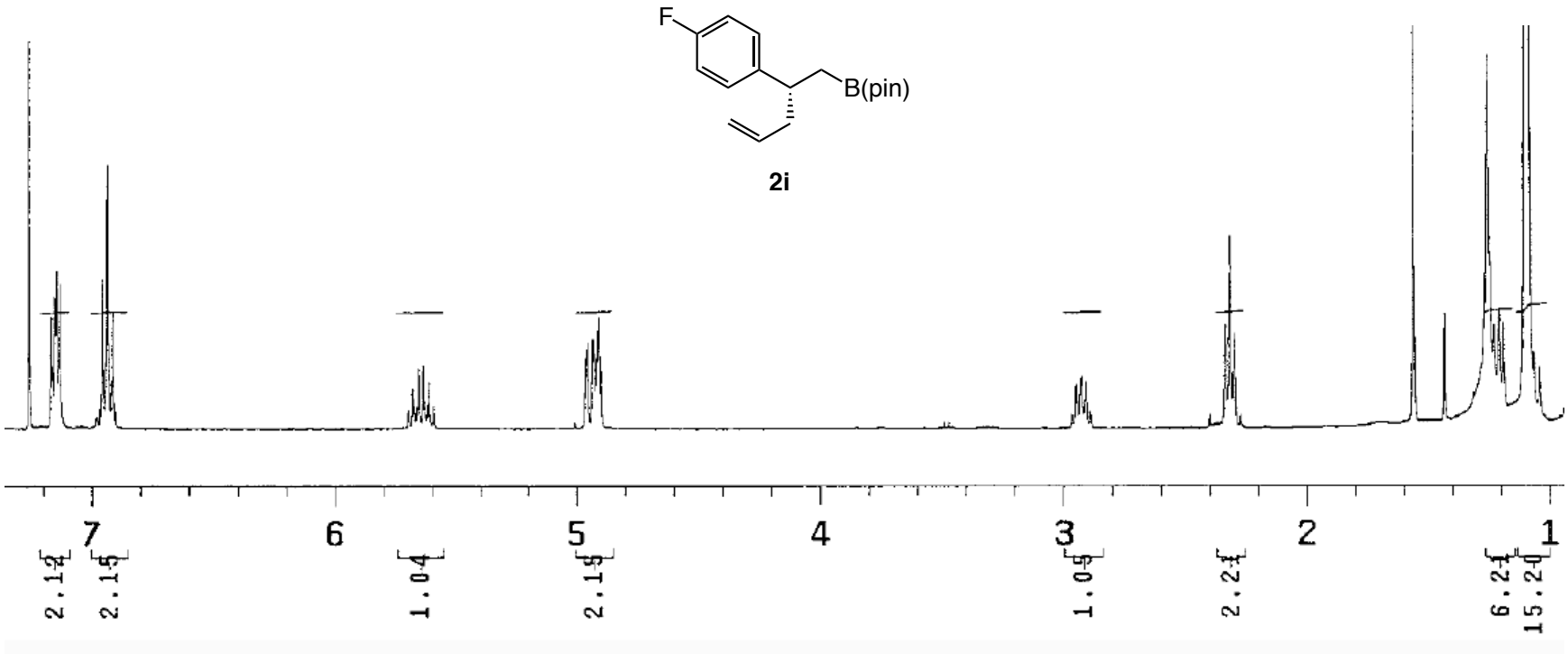
Sample directory:

FidFile: PROTON

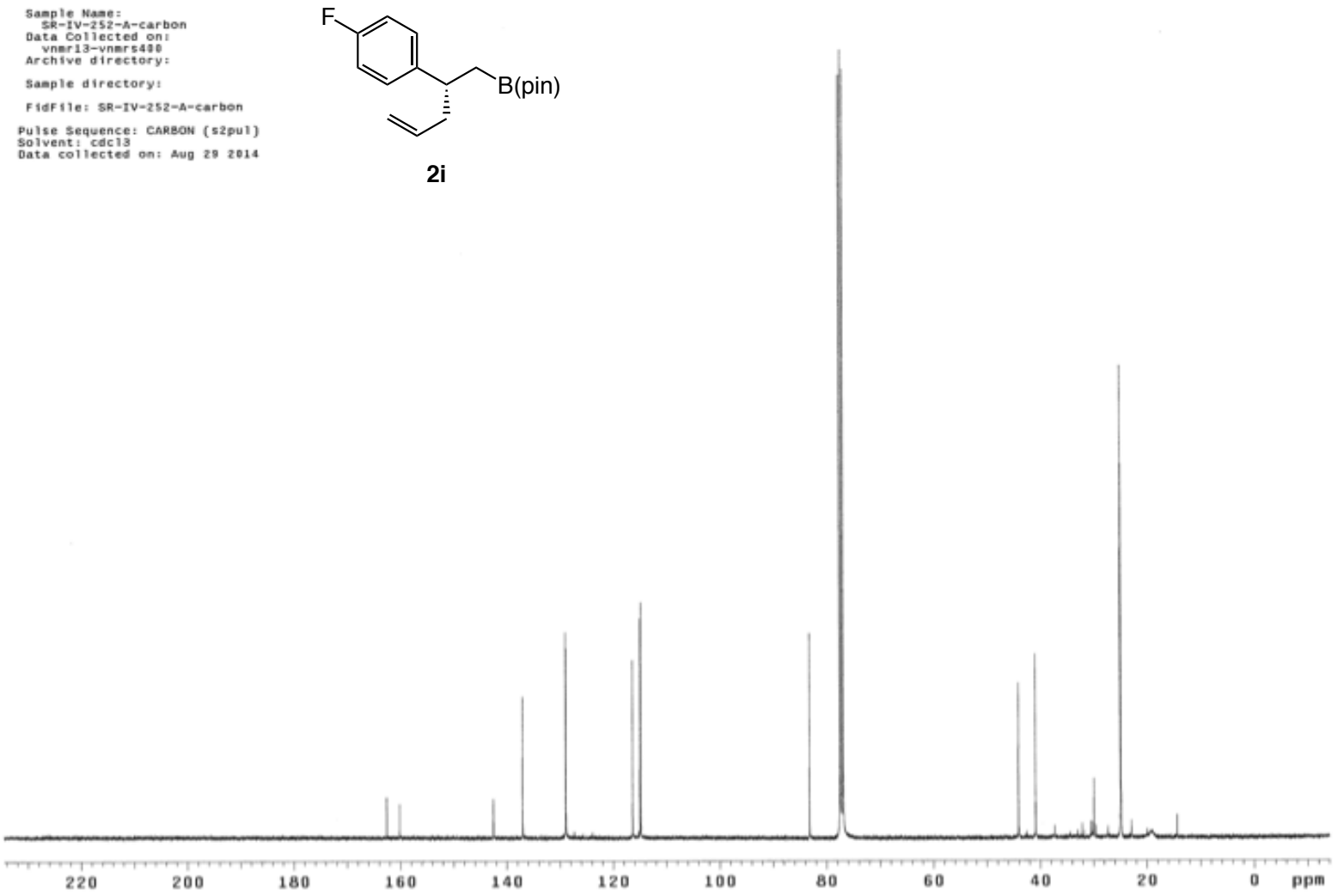
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 29 2014



2i



2i


Sample Name:
SR-IV-252-A-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: SR-IV-252-A-carbon
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 29 2014
F
B(pin)
220
200
180
160
140
120
100
80
60
40
20
0
ppm

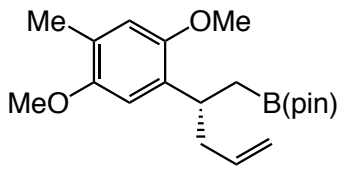
2i

Sample Name:
SR-V-34
Data Collected on:
vnmr13-vnmrs400
Archive directory:

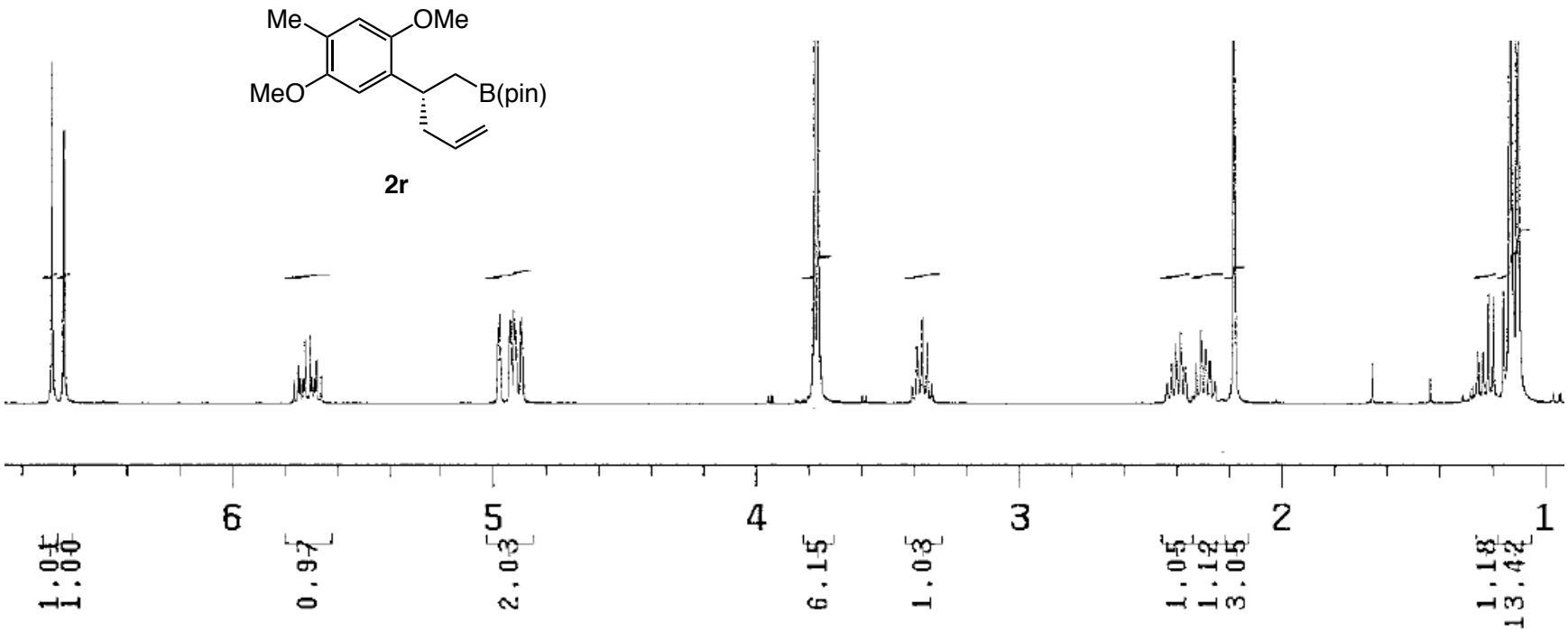
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 28 2014



2r

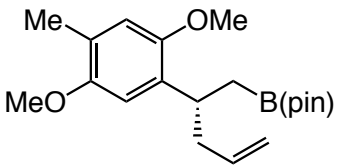

Me
OMe
MeO
B(pin)
2r
6
5
4
3
2
1
1,05
1,00
0,97
2,03
6,15
1,03
1,05
1,12
3,05
1,18
13,42

Sample Name:
SR-V-34-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:

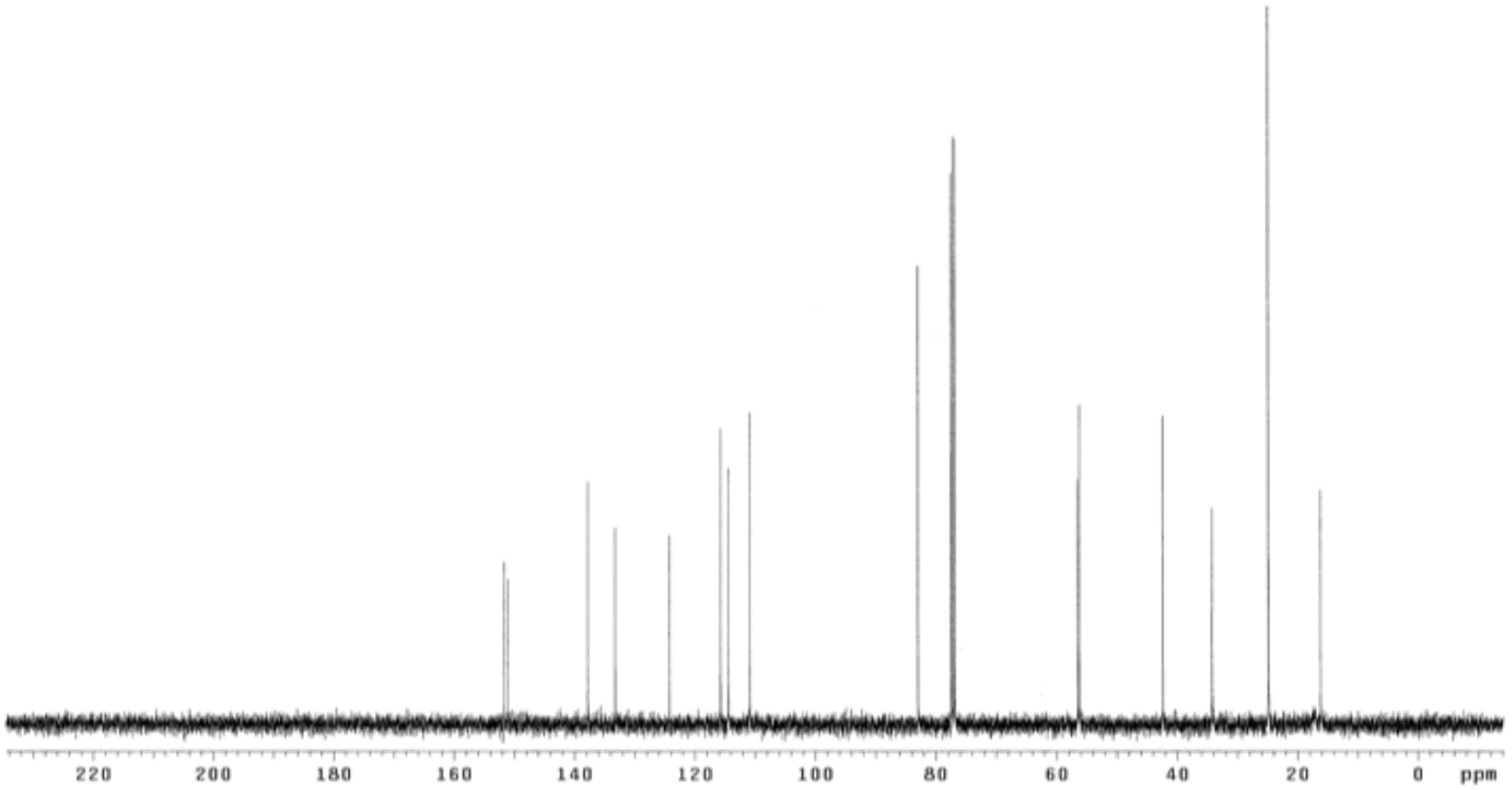
Sample directory:

FidFile: CARBON

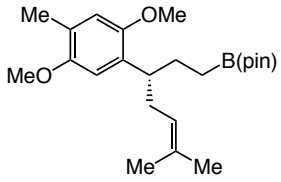
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 28 2014



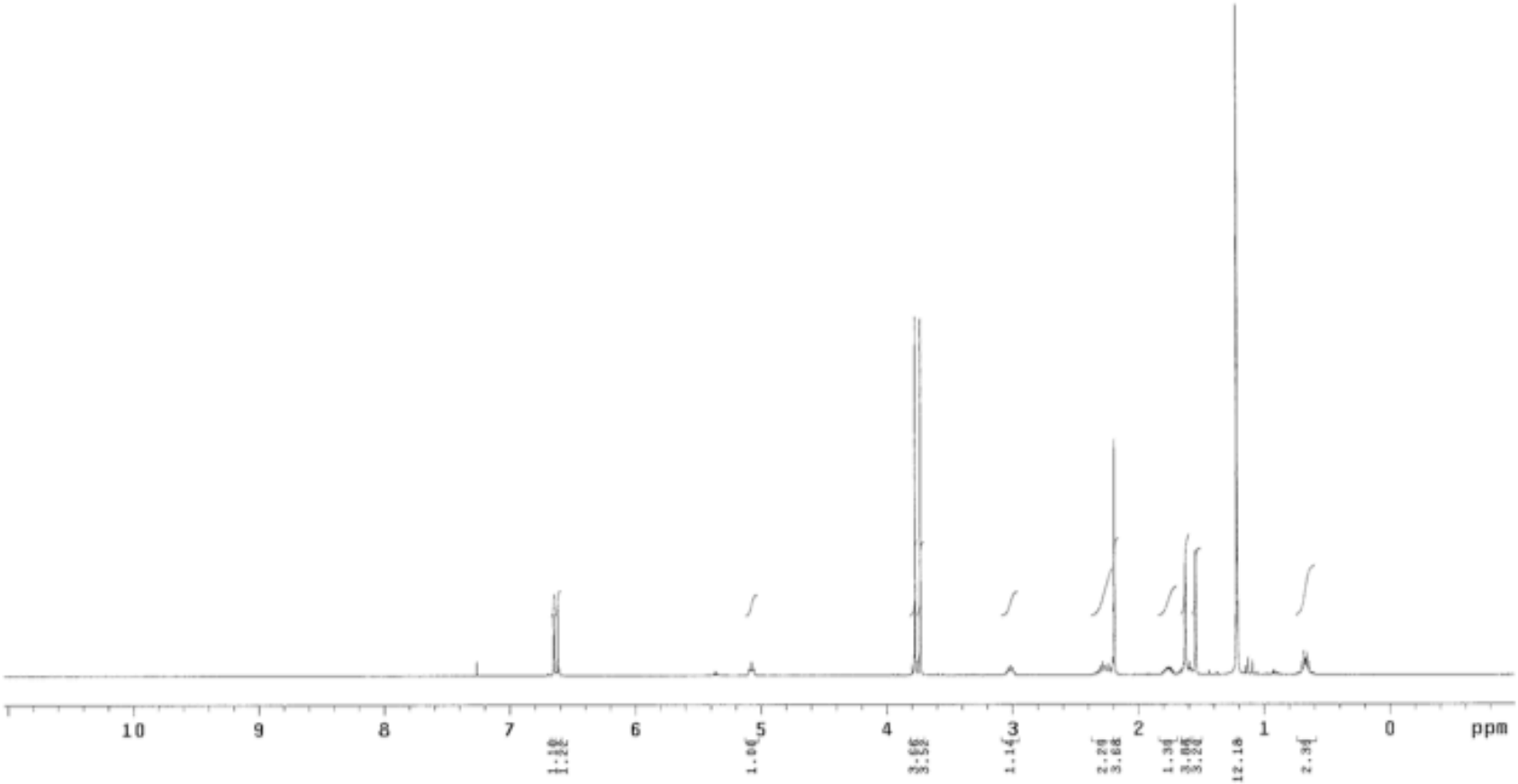
2r

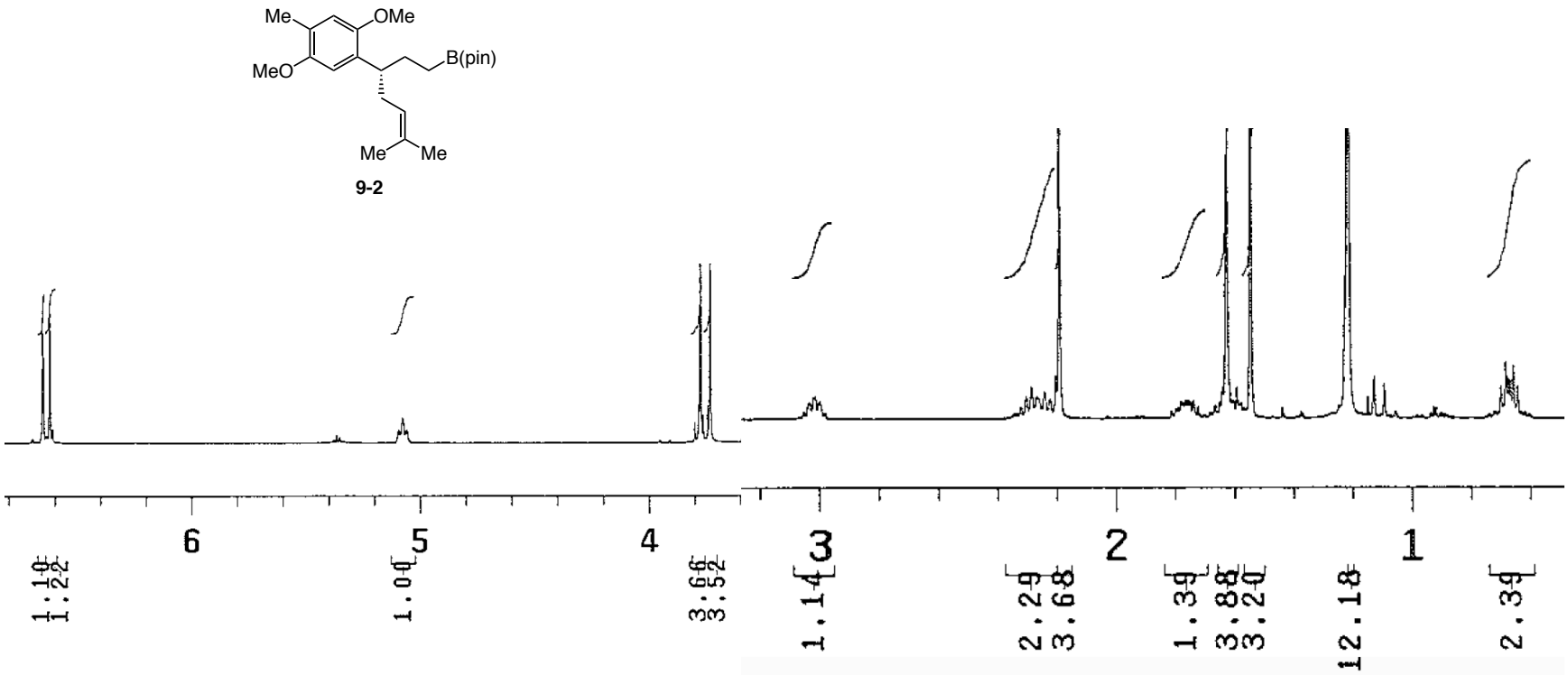


```
Sample Name:
  SR-V-36
Data Collected on:
  nmr14-vnmrs480
Archive directory:

Sample directory:

FidFile: SR-V-36

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 18 2015
```

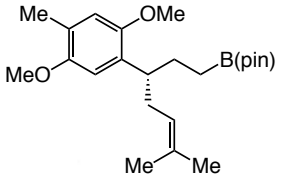


9-2

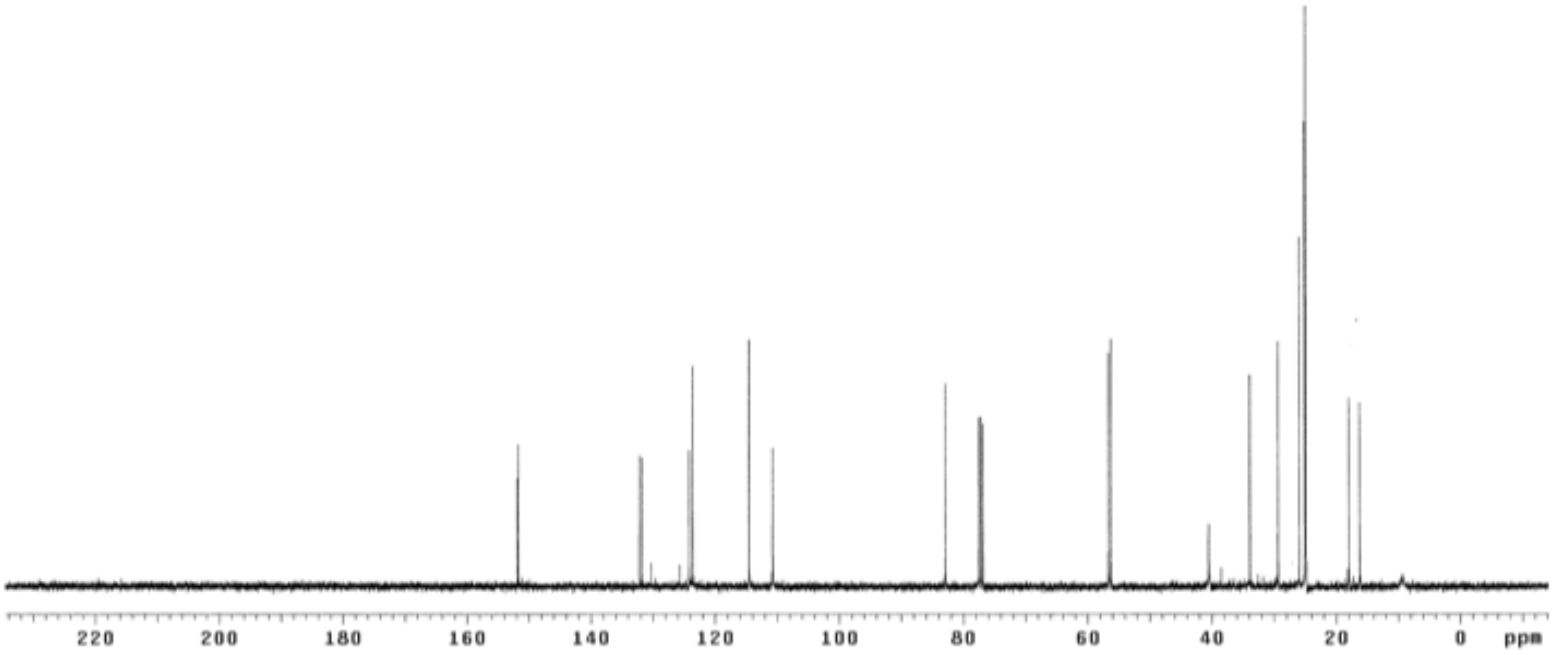



Me
OMe
MeO
B(pin)
Me
Me
9-2
6
5
4
3
2
1
1.10
1.22
1.00
3.66
3.52
1.14
2.29
3.68
1.39
3.88
3.20
12.18
2.39

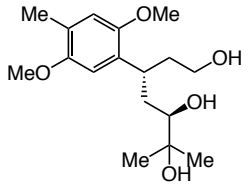
```
Sample Name:
  SR-V-36-carbon
Data Collected on:
  nmrl4-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 18 2015
```



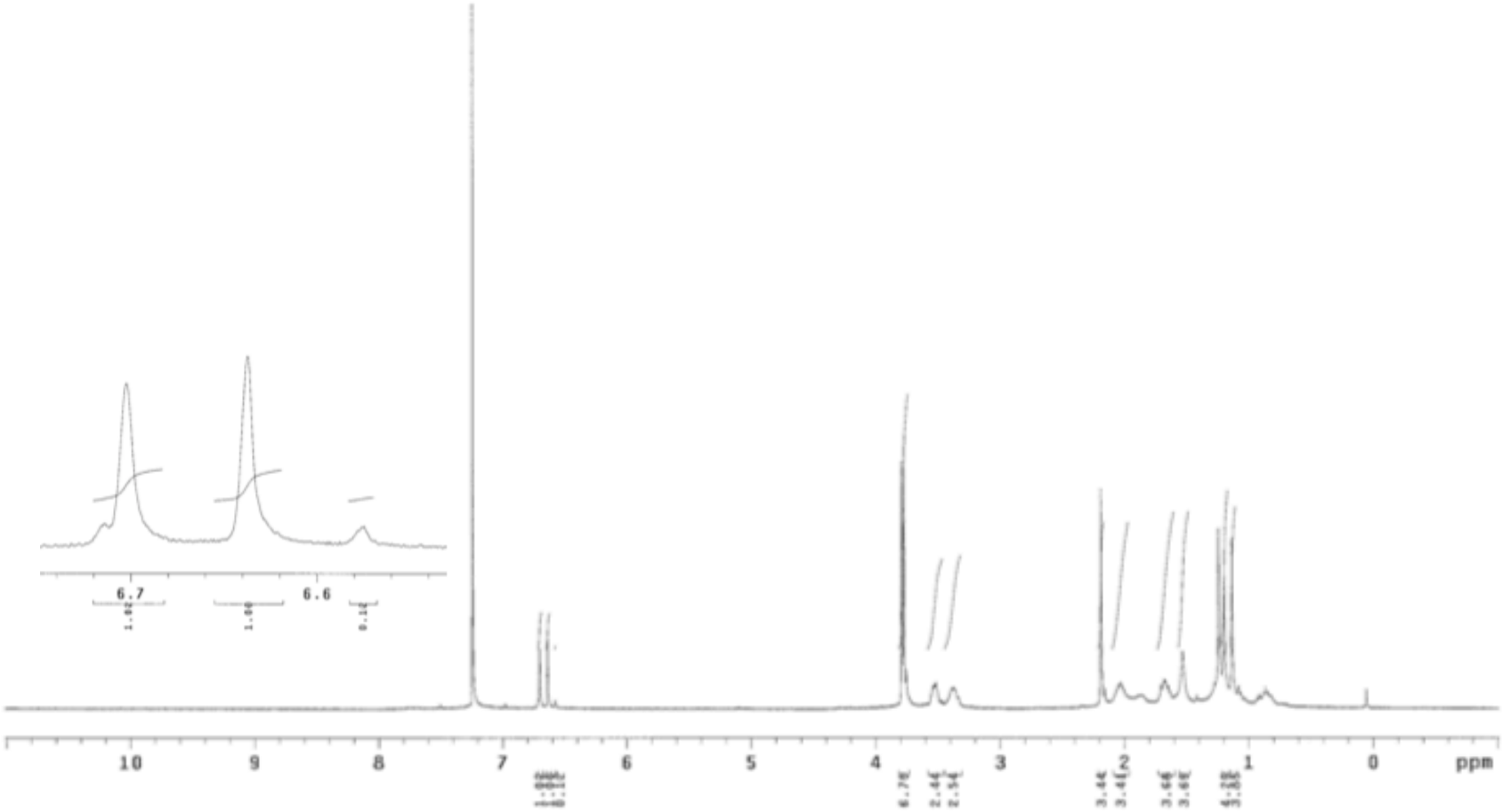
9-2



```
Sample Name:
  SR-V-69-5
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 20 2015
```



10



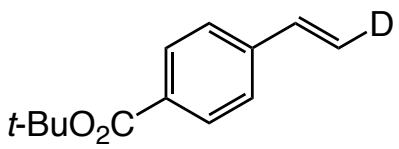
JL-IV-44PD

Sample Name:
JL-IV-44PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

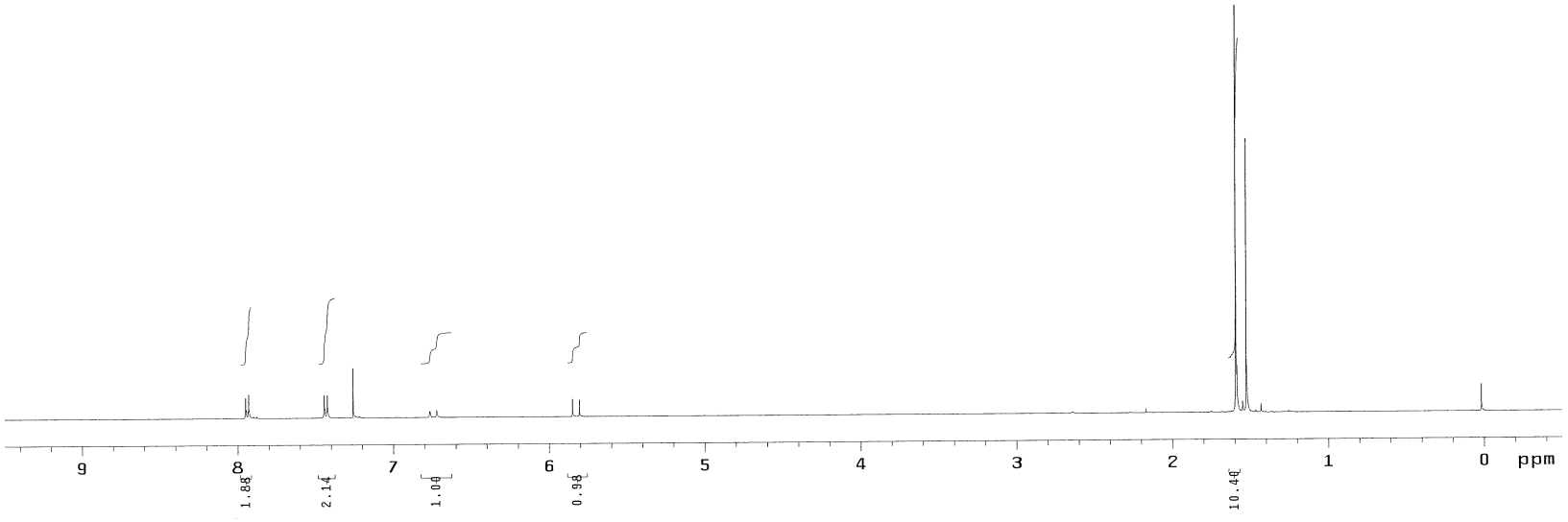
Sample directory:

FidFile: JL-IV-44PD

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 7 2015



15



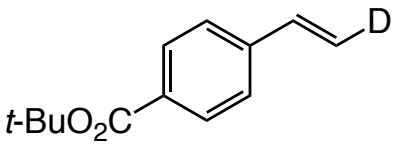
JL-IV-50PD

Sample Name:
JL-IV-50PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

Sample directory:

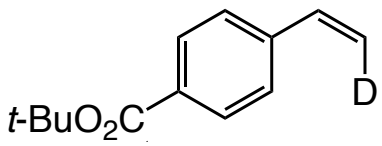
FidFile: JL-IV-50PD-1-C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 15 2015

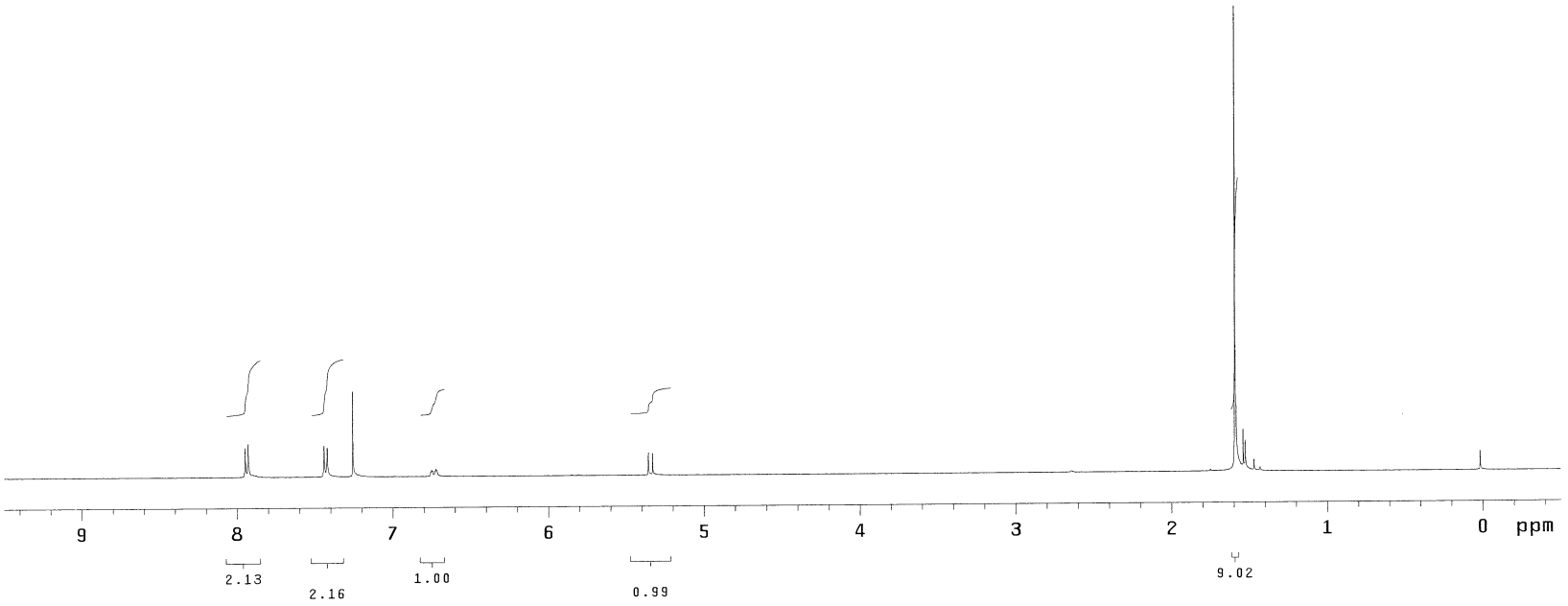


15

```
JL-IV-45PD

 Sample Name:
   JL-IV-45PD
 Data Collected on:
   vnmr13-vnmrs400
 Archive directory:

 Sample directory:

 FidFile: JL-IV-45PD

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct  7 2015
```



16



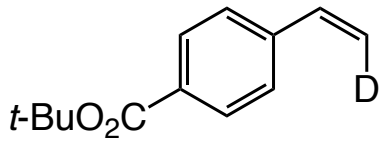
JL-IV-45PD-C

Sample Name:
JL-IV-45PD-C
Data Collected on:
vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: JL-IV-45PD-C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 13 2015



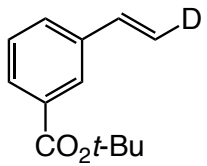
16

JL-IV-179PD

Sample Name:
JL-IV-179PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

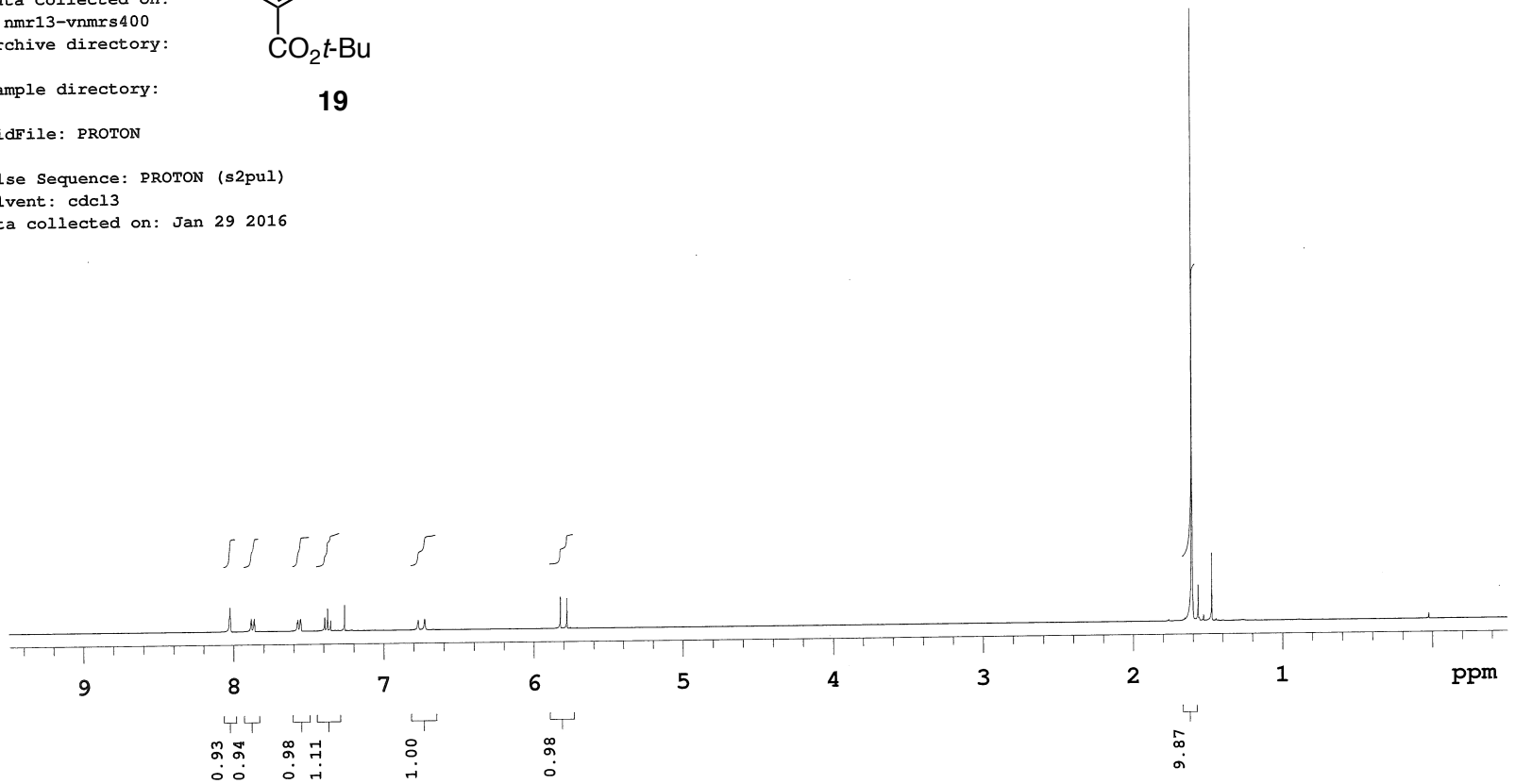
Sample directory:

FidFile: PROTON



19

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 29 2016

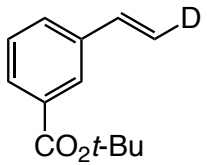


JL-IV-179PD-C

Sample Name:
JL-IV-179PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

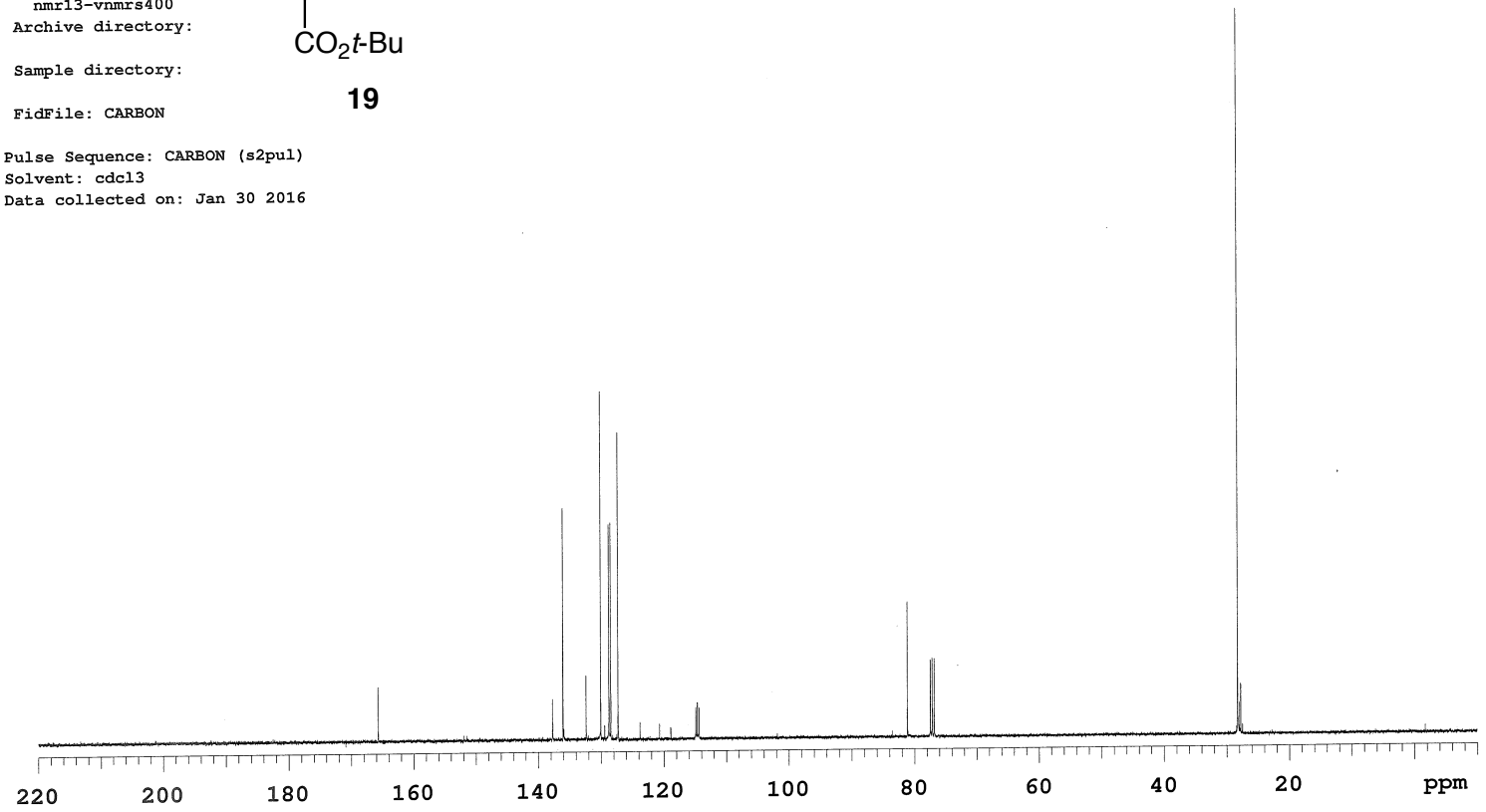
Sample directory:

FidFile: CARBON



19

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 30 2016



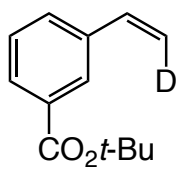
JL-IV-180PD

Sample Name:
JL-IV-180PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: JL-IV-180PD

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 29 2016



20

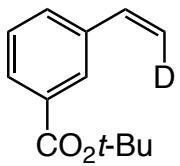
JL-IV-180PD-C

Sample Name:
JL-IV-180PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

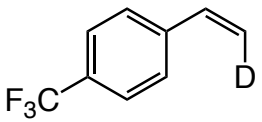
Sample directory:

FidFile: CARBON

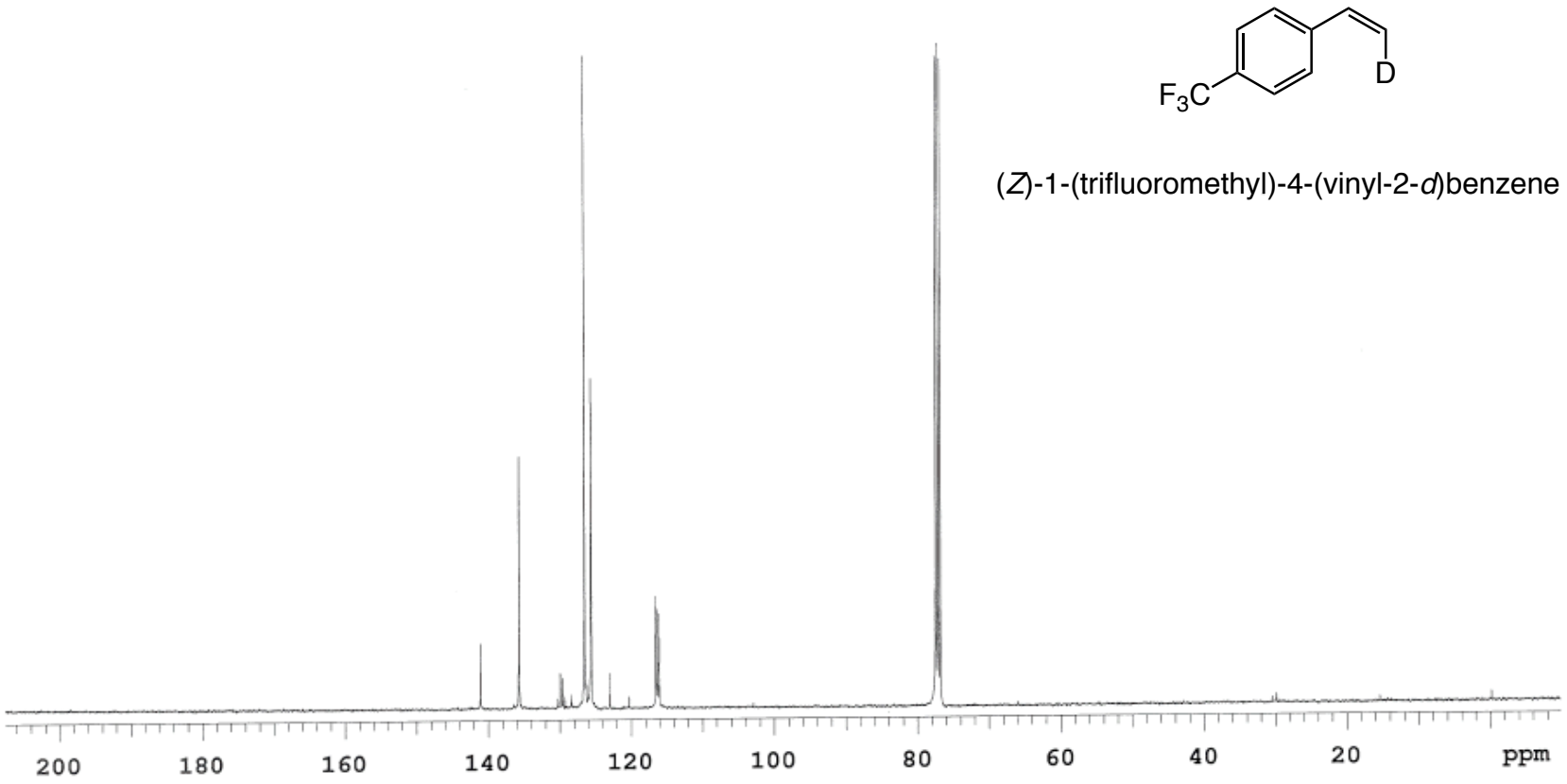
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 30 2016



20



(*Z*)-1-(trifluoromethyl)-4-(vinyl-2-*d*)benzene



(*Z*)-1-(trifluoromethyl)-4-(vinyl-2-*d*)benzene

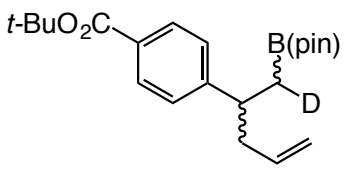
JL-IV-46PD

Sample Name:
JL-IV-46PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

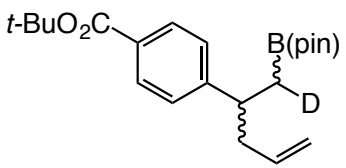
Sample directory:

FidFile: JL-IV-46-2PD

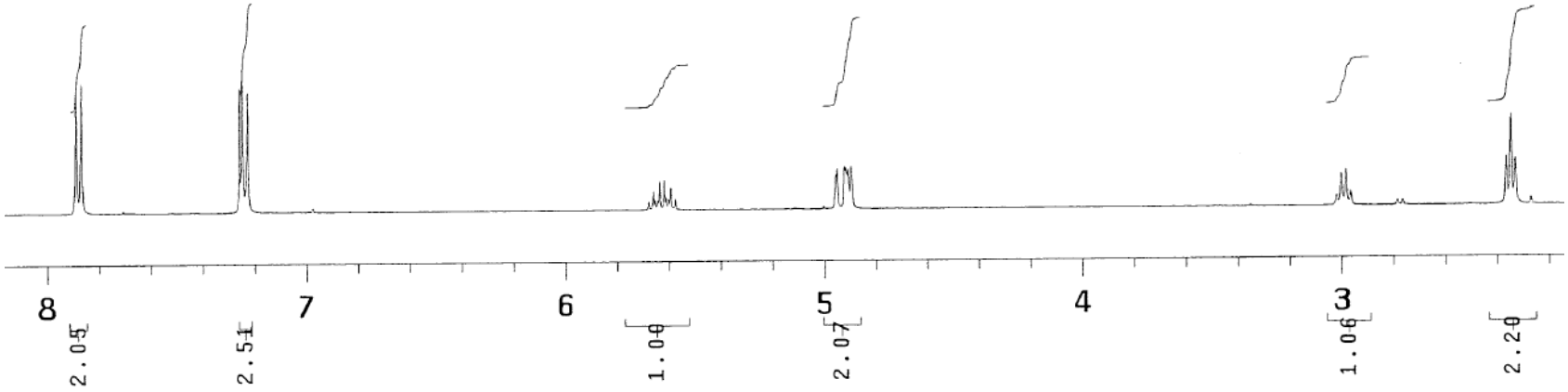
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 10 2015



2k-d
from *E* olefin



2k-d
from *E* olefin



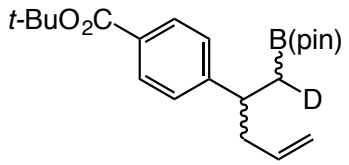
JL-IV-46PD

Sample Name:
JL-IV-46PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

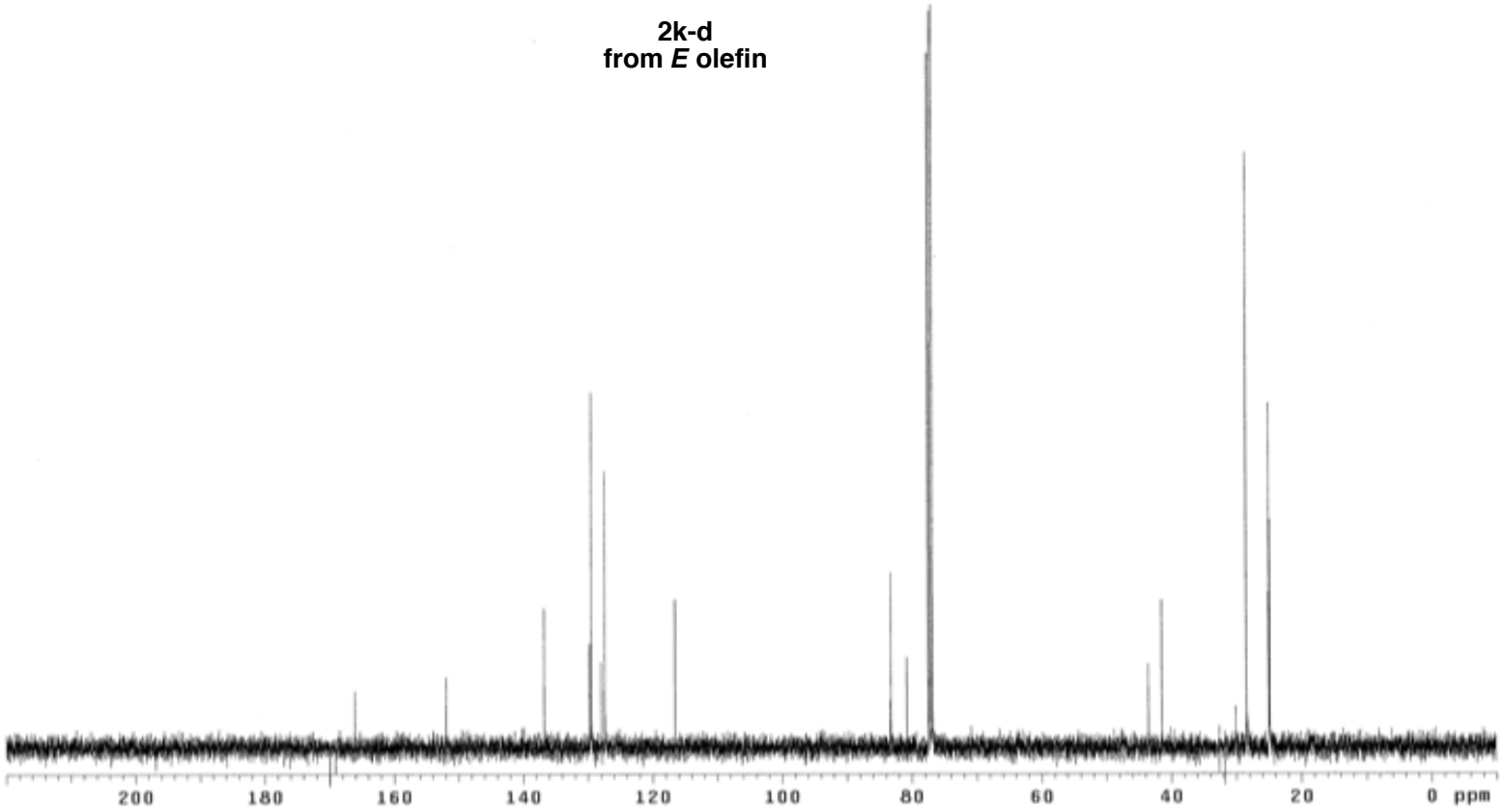
Sample directory:

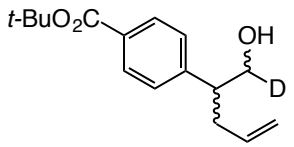
FidFile: JL-IV-46PD-C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 10 2015



2k-d
from *E* olefin





oxidation product of 2k-d from *E* olefin 60:40 d.r.

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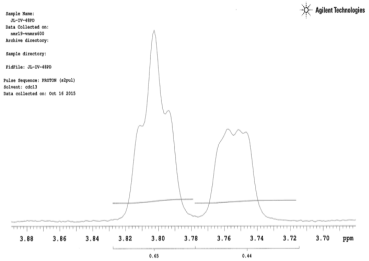
```
Sample Name:
  JL-IV-48PD
Data Collected on:
  nmr19-vnmrs600
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 16 2015
```



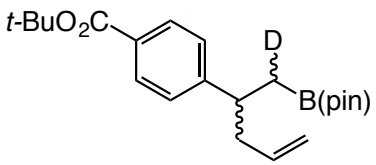
JL-IV-47PD

Sample Name:
JL-IV-47PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

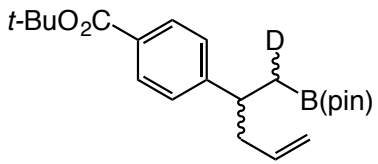
Sample directory:

FidFile: JL-IV-47PD-1

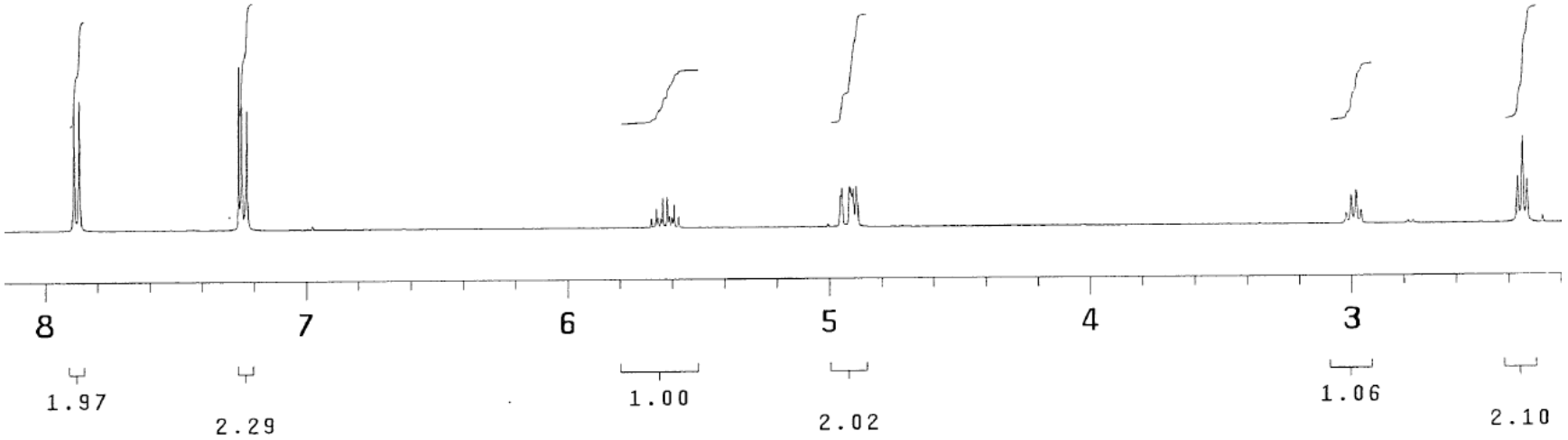
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 10 2015



2k-d
from *Z* olefin



2k-d
from *Z* olefin



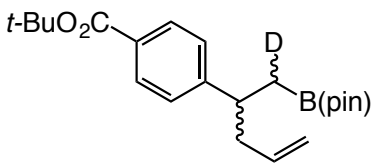
JL-IV-47PD

Sample Name:
JL-IV-47PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: JL-IV-47PD-C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 10 2015



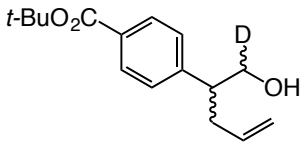
2k-d
from *Z* olefin

Sample Name:
JL-IV-49PD
Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

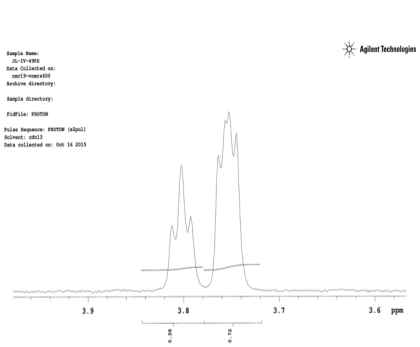
FidFile: PROTON

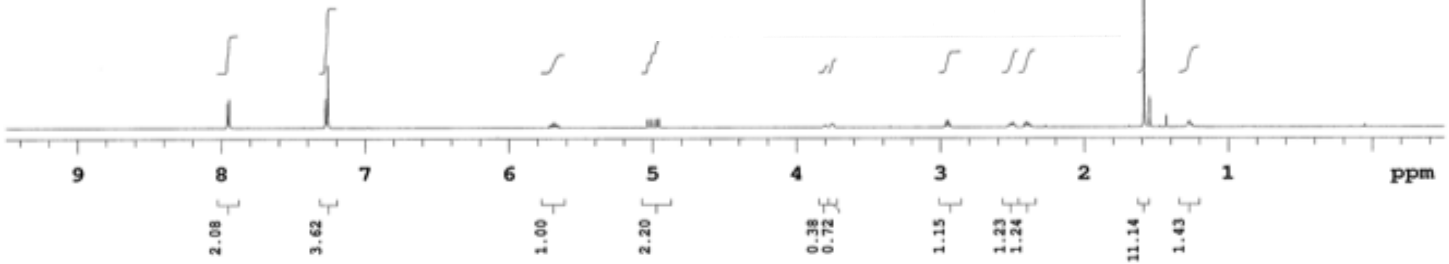
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 16 2015



oxidation product of 2k-d from *Z* olefin 35:65 d.r.

Agilent Technologies



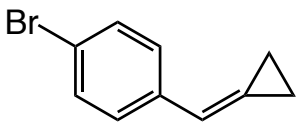


JL-IV-57PD

Sample Name:
JL-IV-57PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

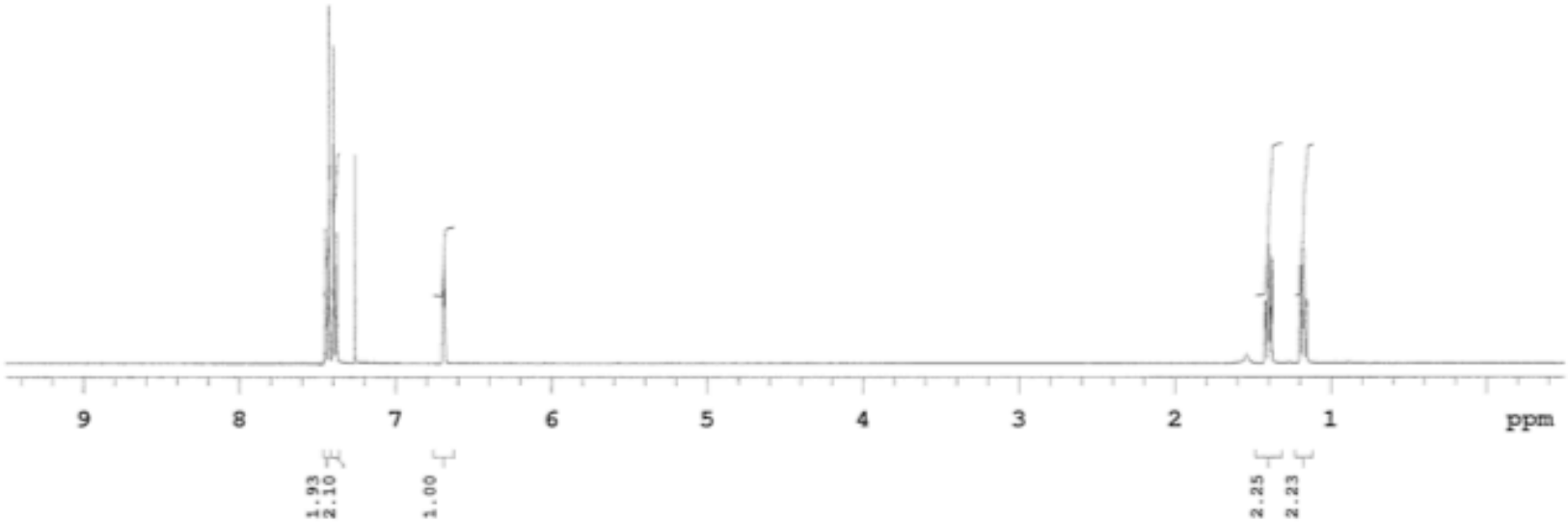
Sample directory:

FidFile: JL-IV-57PD



27

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 30 2015



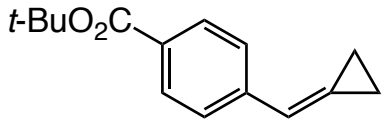
JL-IV-67CD

Sample Name:
JL-IV-67CD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

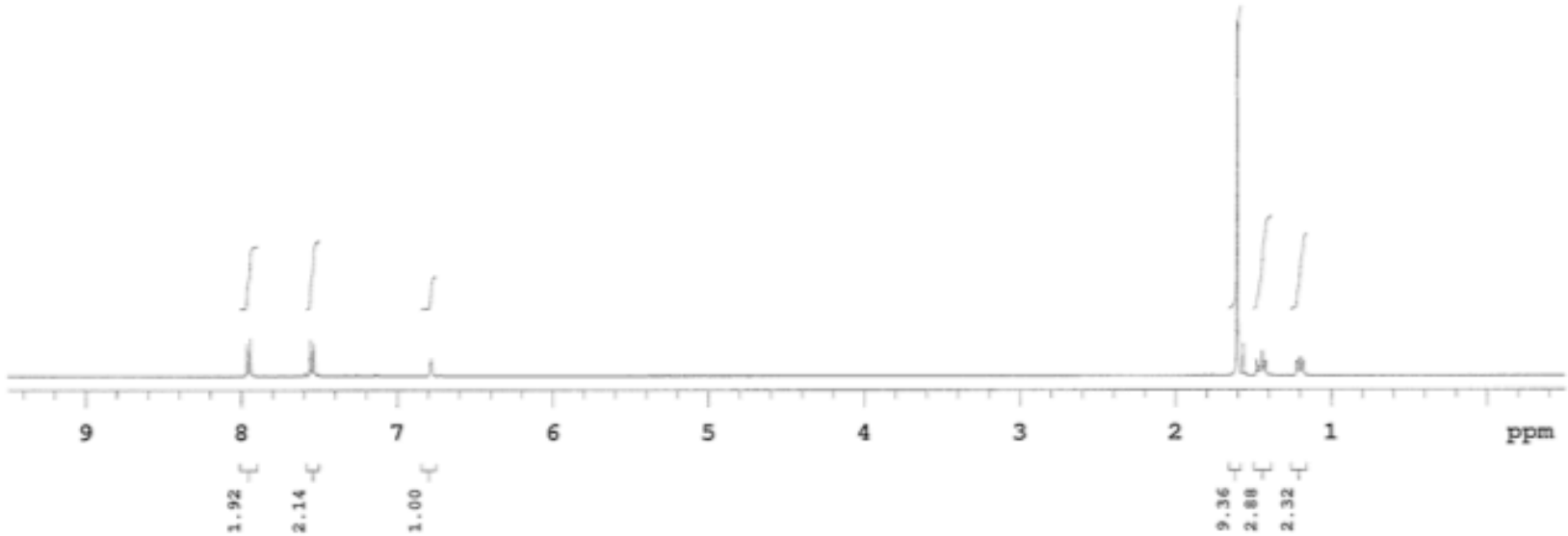
Sample directory:

FidFile: JL-IV-67PD

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 5 2015



28



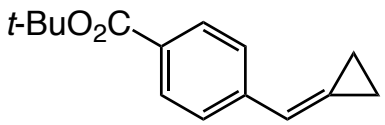
JL-IV-67CD

Sample Name:
JL-IV-67CD
Data Collected on:
vnmrl3-vnmrs400
Archive directory:

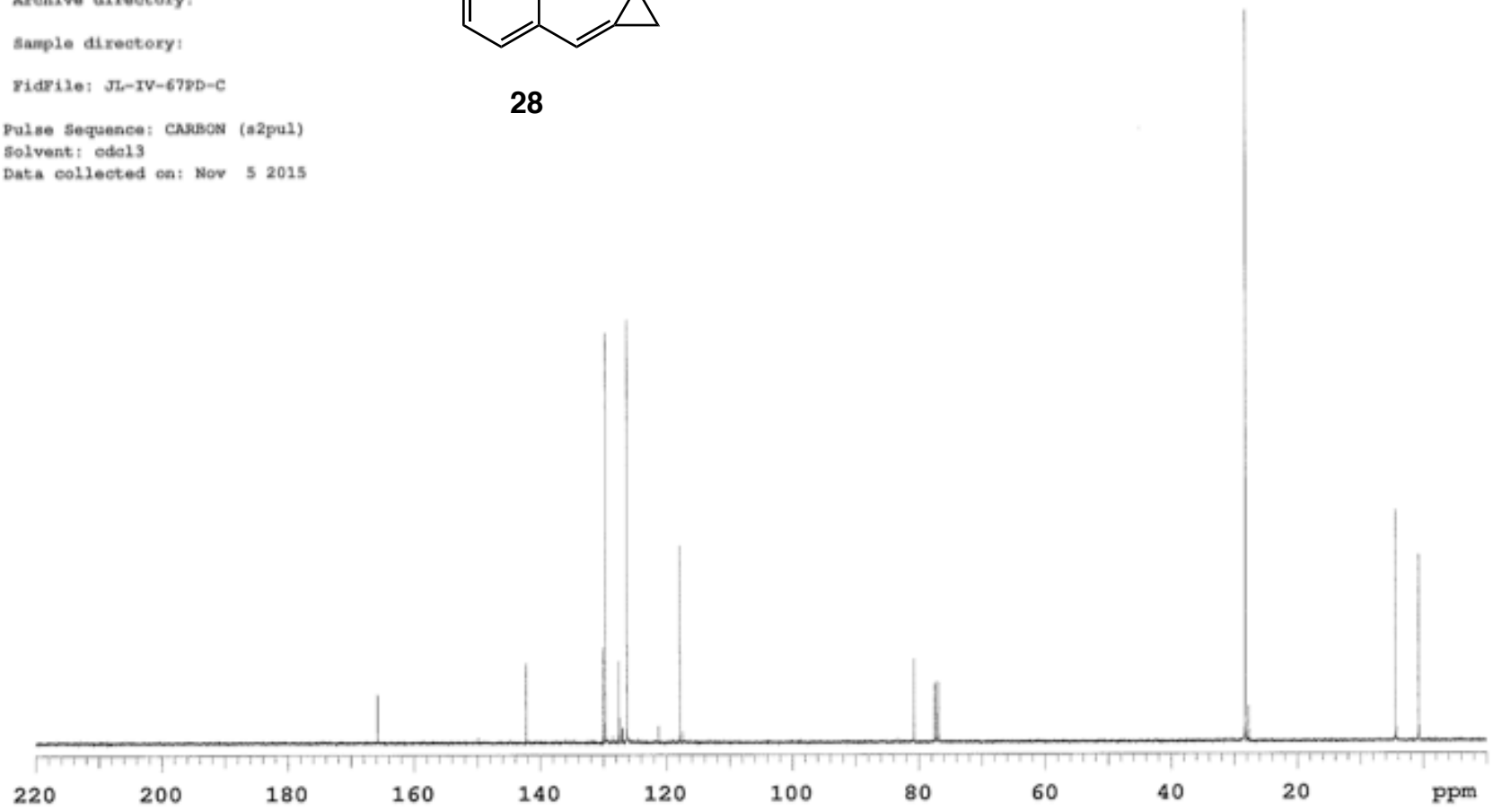
Sample directory:

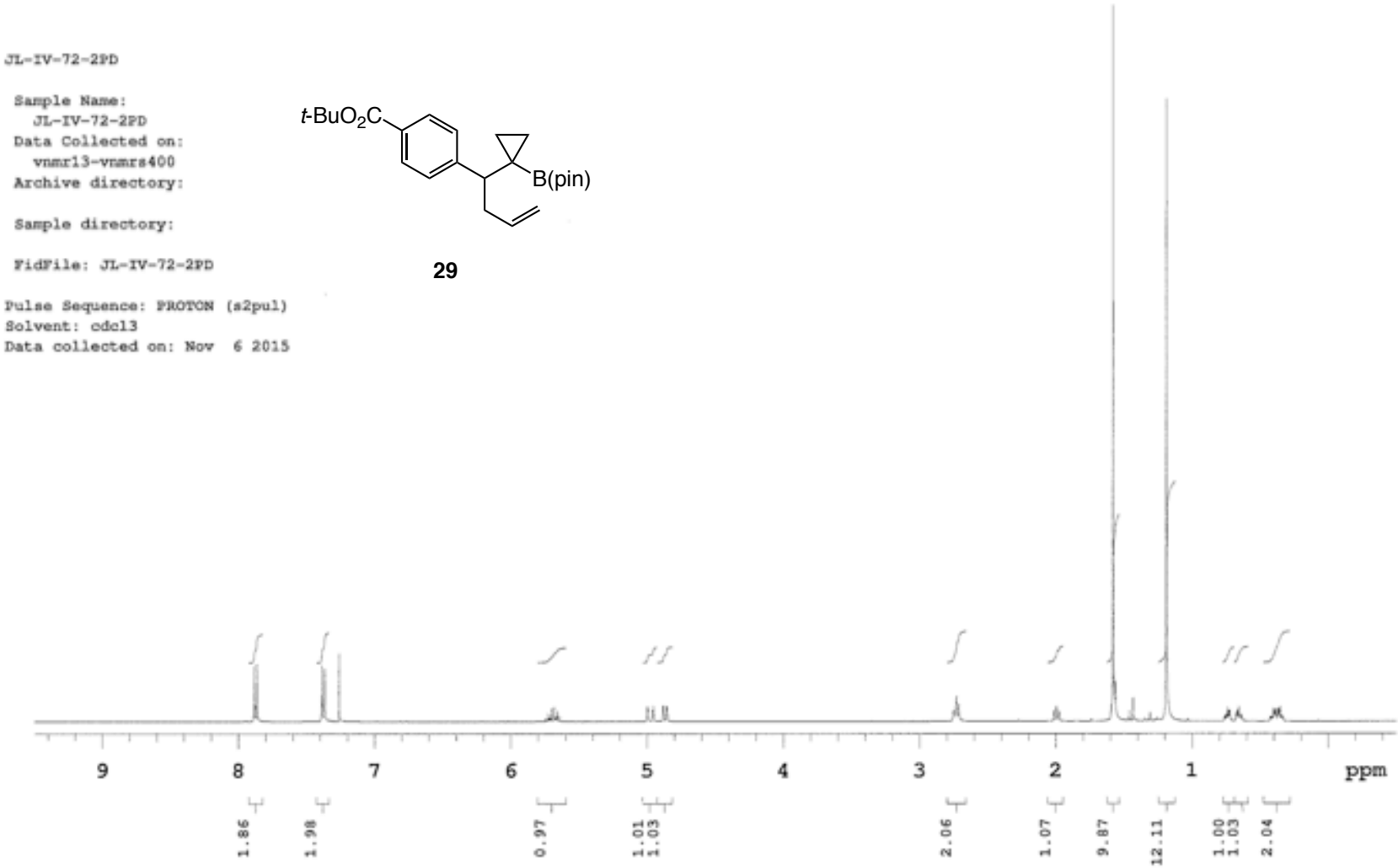
FidFile: JL-IV-67PD-C

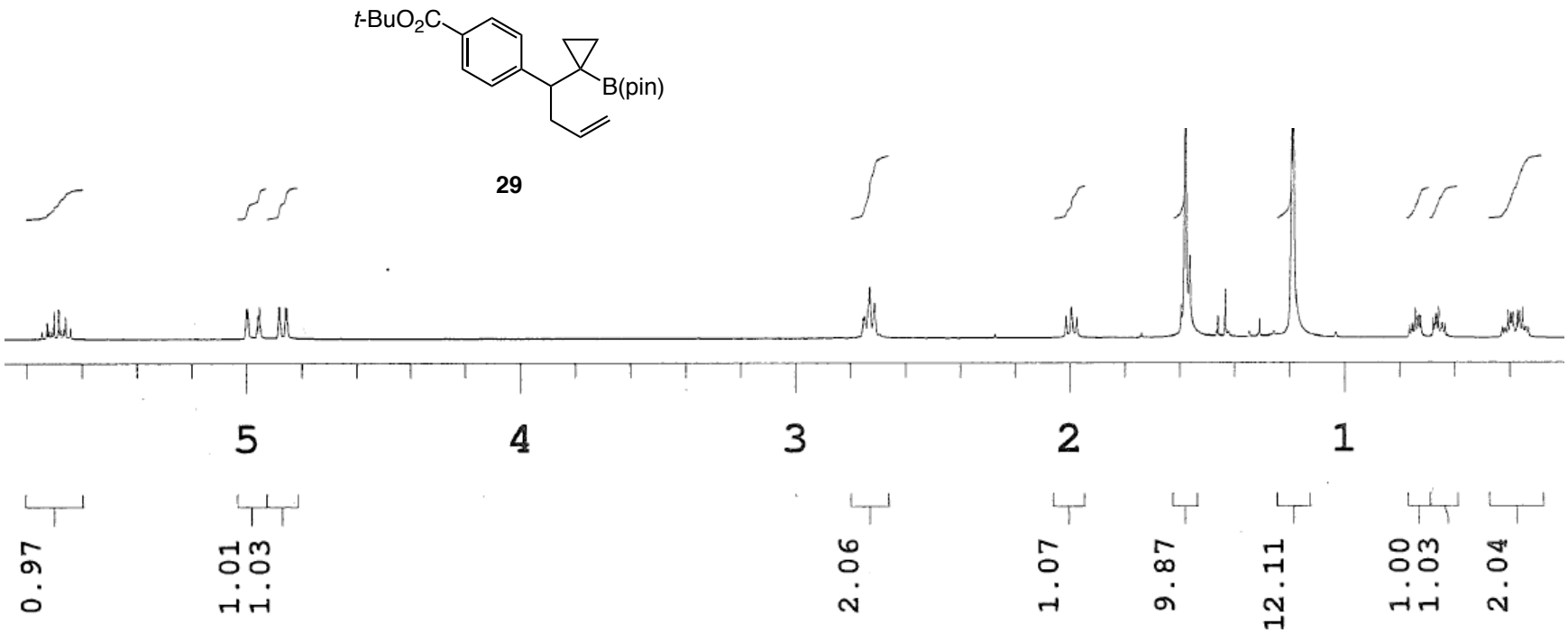
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 5 2015



28




JL-IV-72-2PD
Sample Name:
JL-IV-72-2PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: JL-IV-72-2PD
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 6 2015
t-BuO2C
B(pin)
29
9
8
7
6
5
4
3
2
1
ppm
1.86
1.98
0.97
1.01
1.03
2.06
1.07
9.87
12.11
1.00
1.03
2.04


t-BuO2C
B(pin)
29
5
4
3
2
1
0.97
1.01
1.03
2.06
1.07
9.87
12.11
1.00
1.03
2.04

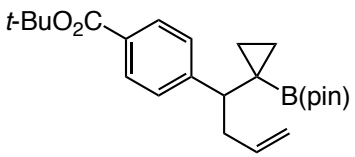
JL-IV-72PD-C

Sample Name:
JL-IV-72PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

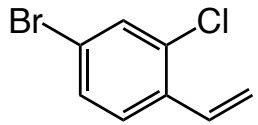
Sample directory:

FidFile: CARBON

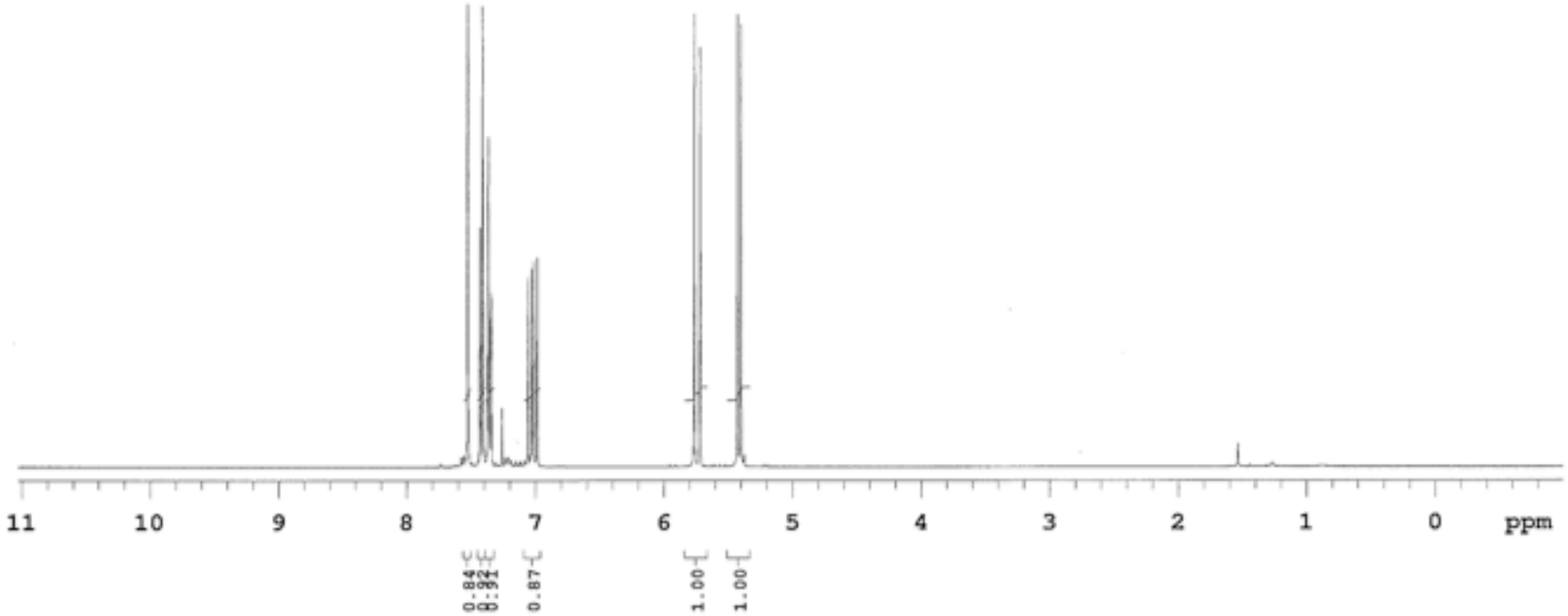
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 12 2015

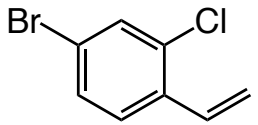


29

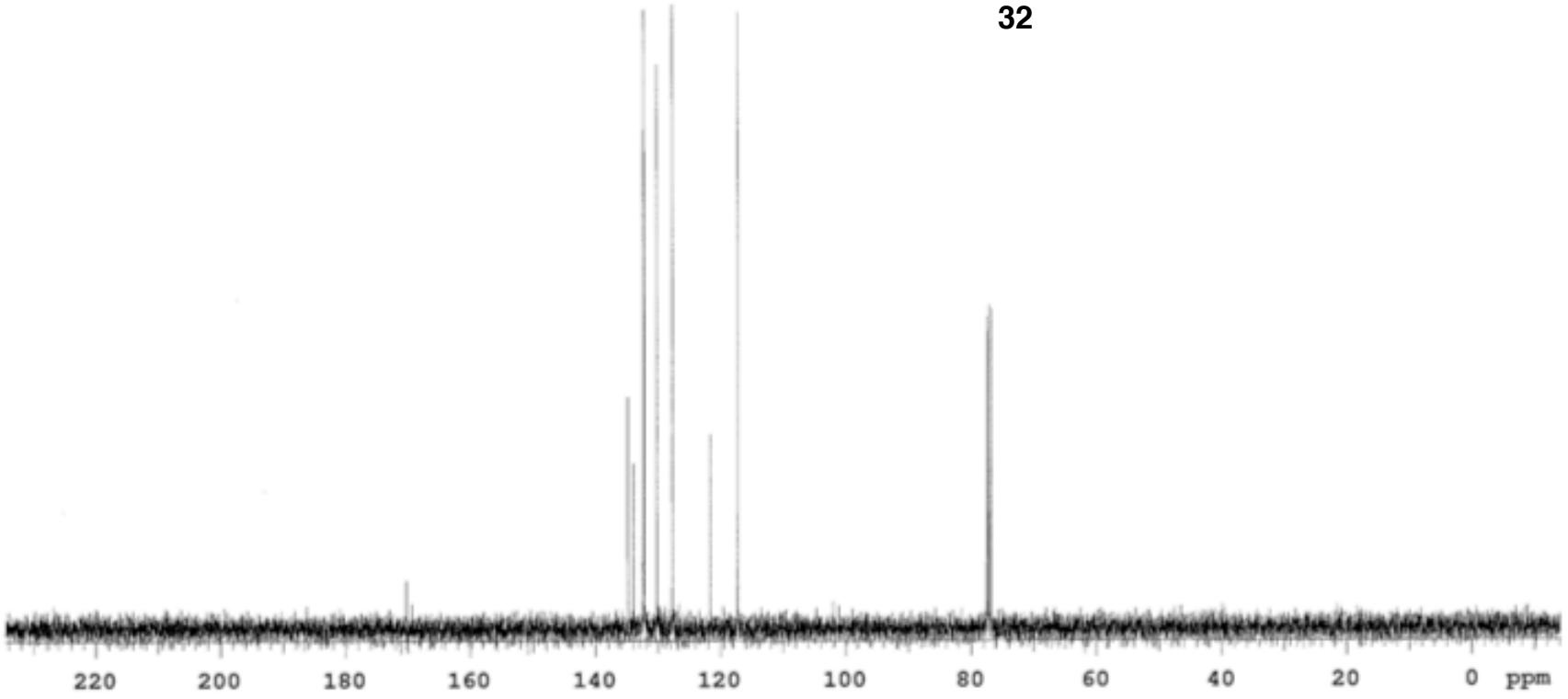


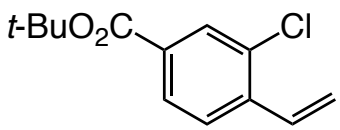
32



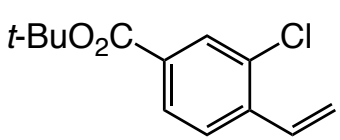


32

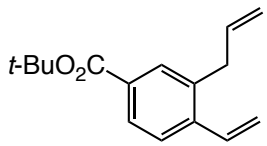




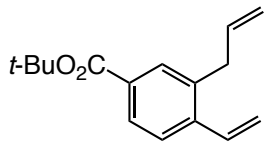
33



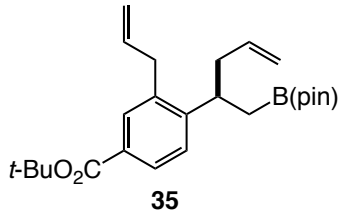
33



34

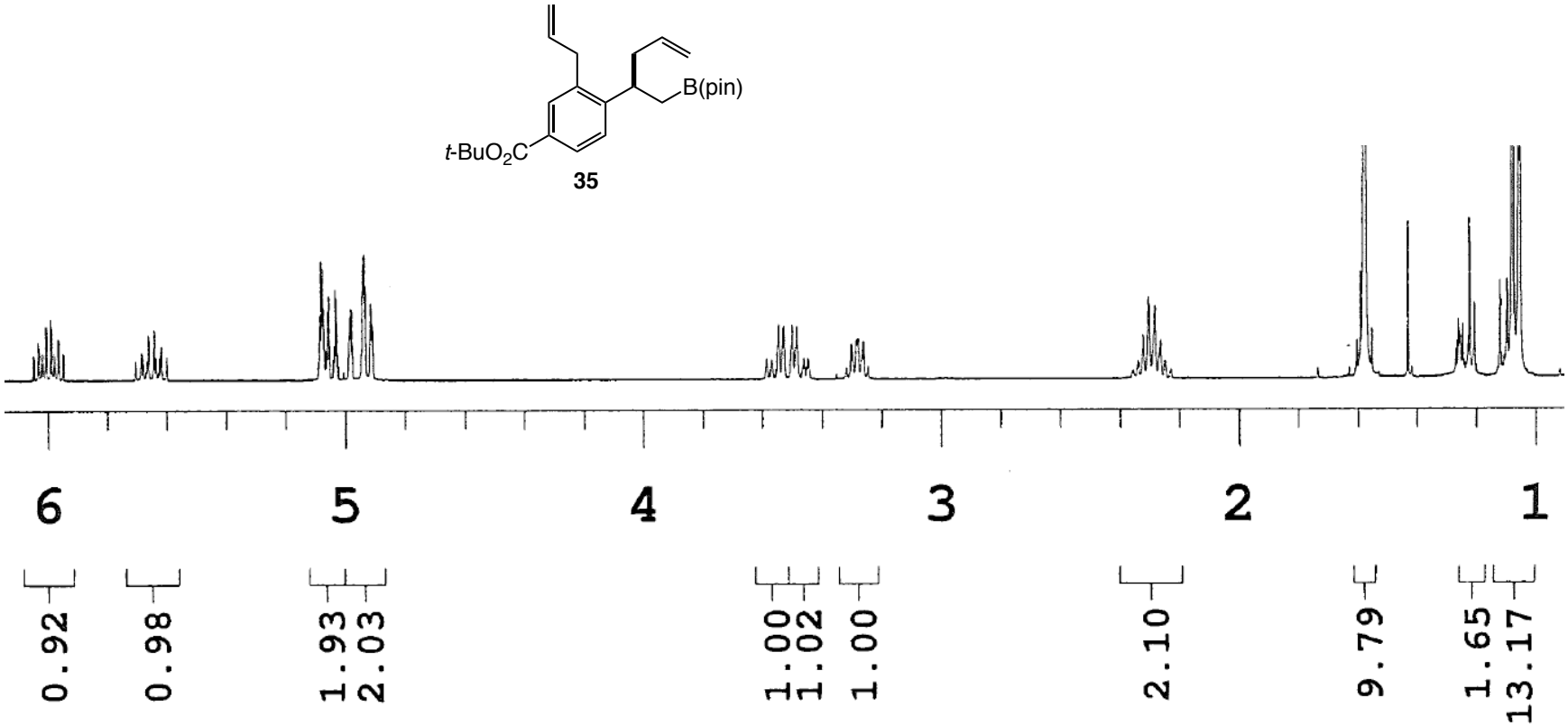


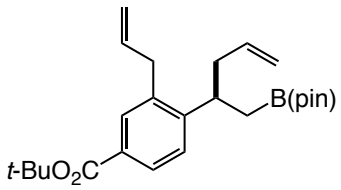
34


B(pin)
t-BuO2C

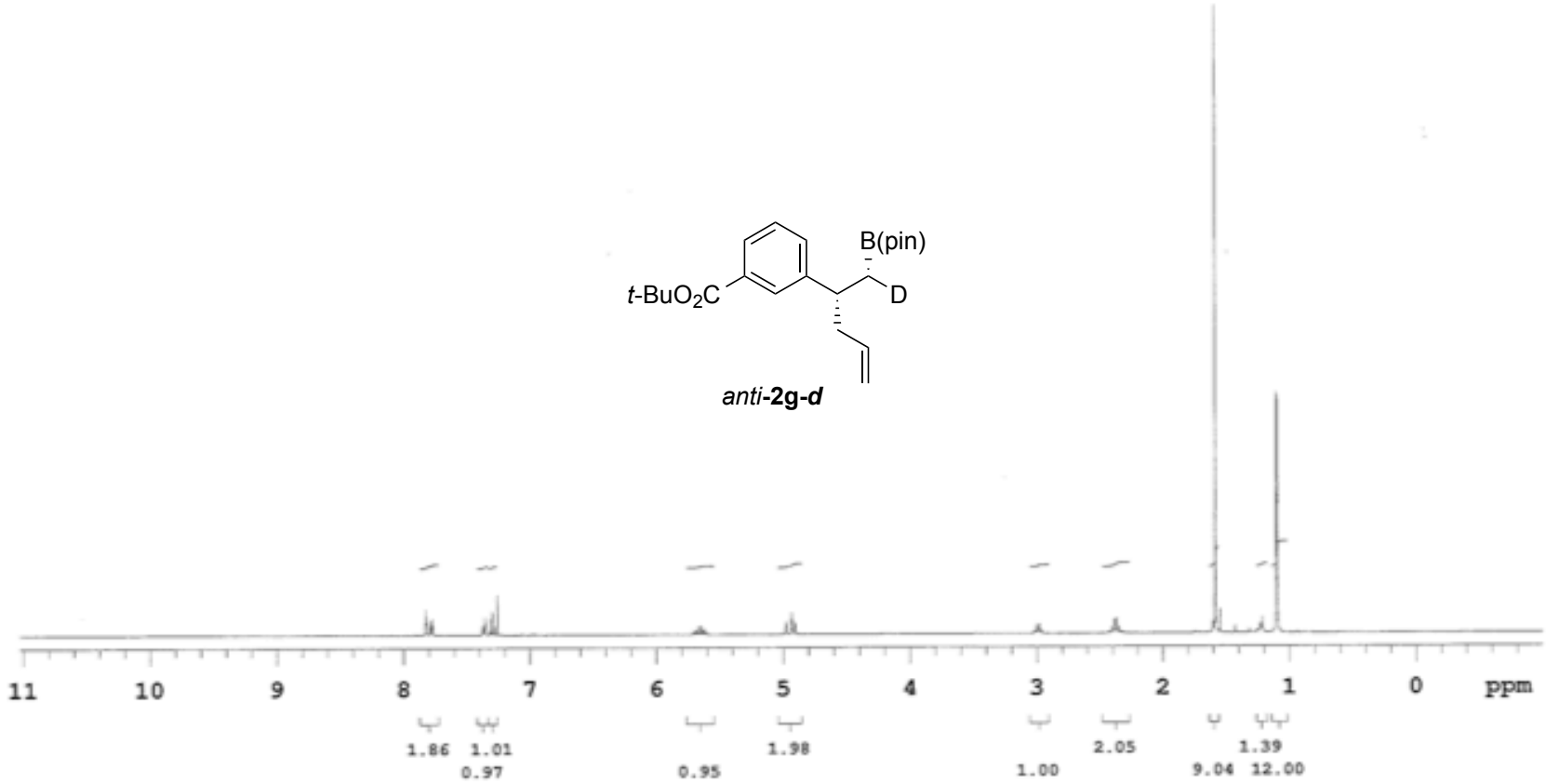
35

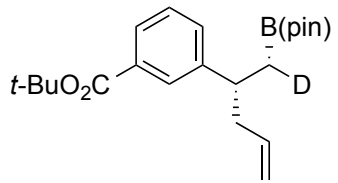
10
9
8
7
6
5
4
3
2
1
0
ppm
1.45
0.92
0.98
1.93
2.03
1.00
1.02
1.00
2.10
9.79
1.65
13.17


B(pin)
t-BuO2C
35
6
5
4
3
2
1
0.92
0.98
1.93
2.03
1.00
1.02
1.00
2.10
9.79
1.65
13.17

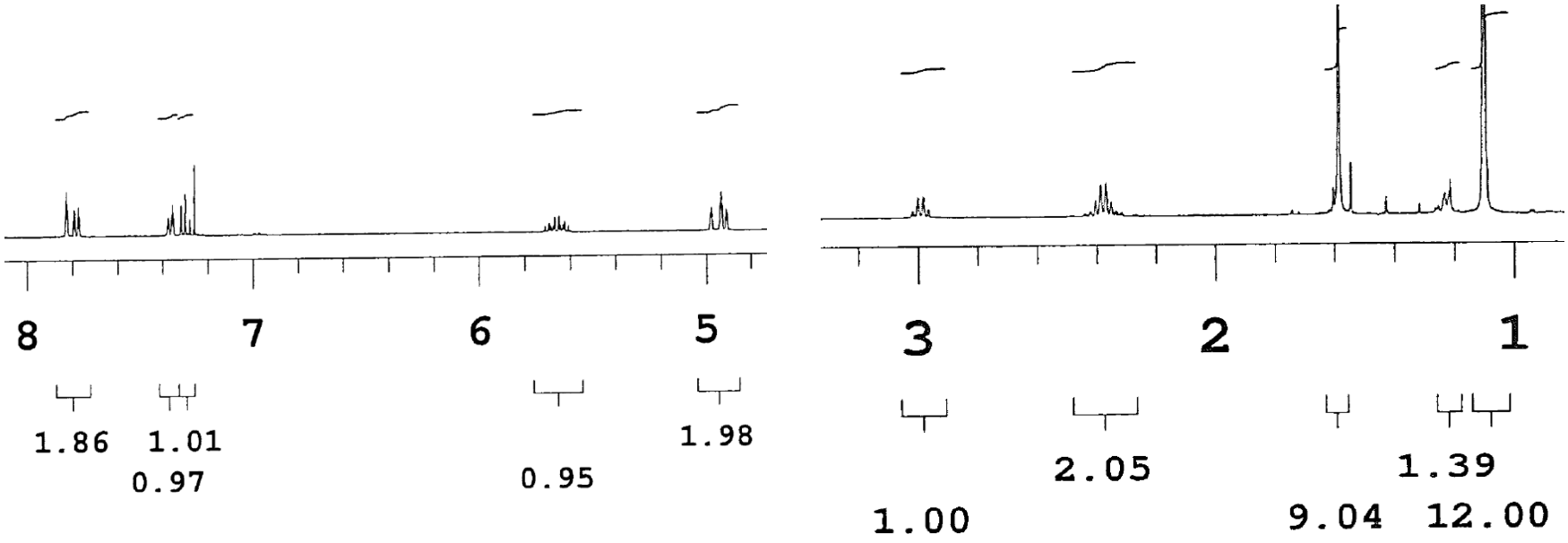


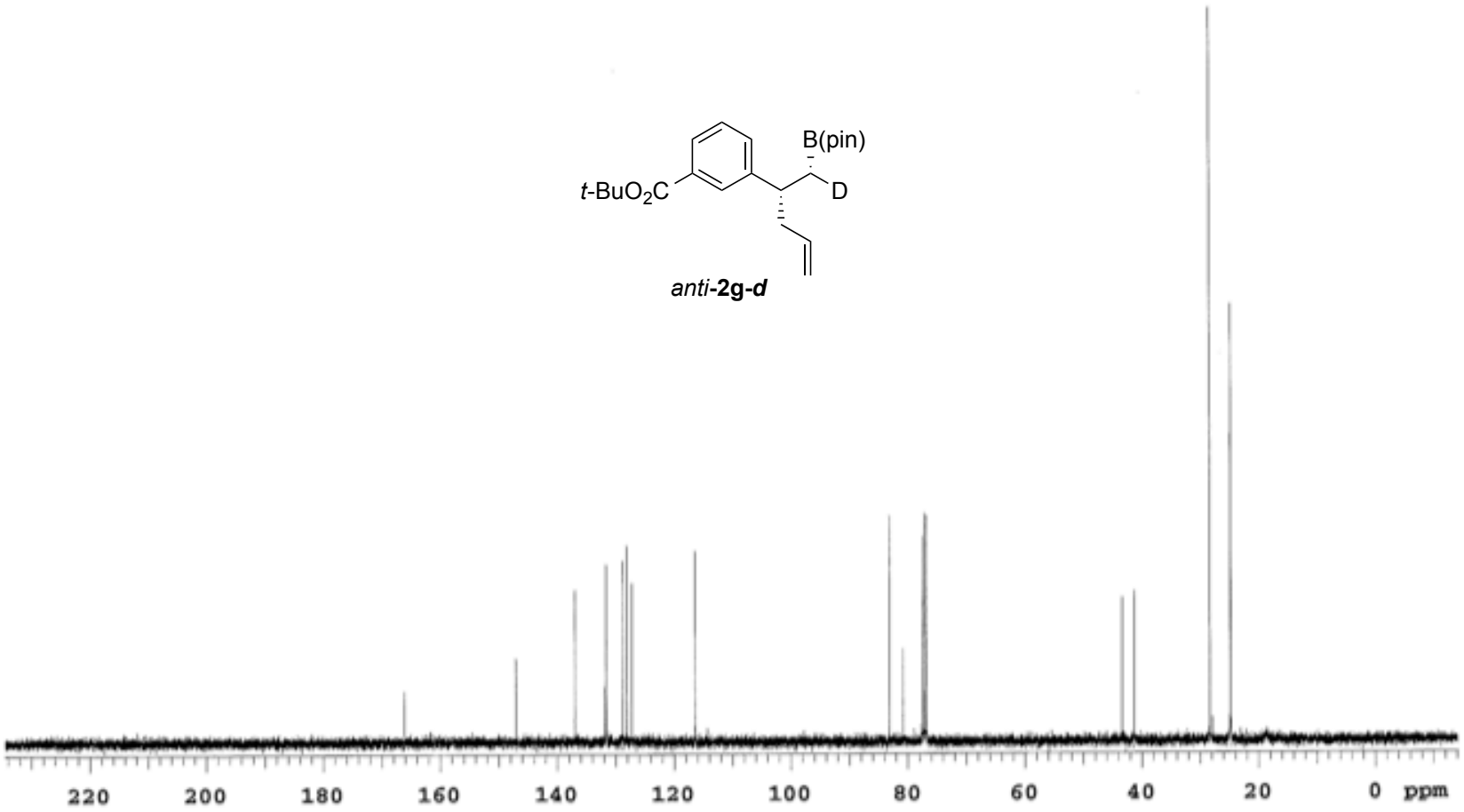
35


B(pin)
t-BuO2C
D
anti-2g-d
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.86
1.01
0.97
0.95
1.98
1.00
2.05
9.04
1.39
12.00

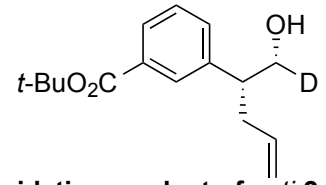


anti-**2g-*d***

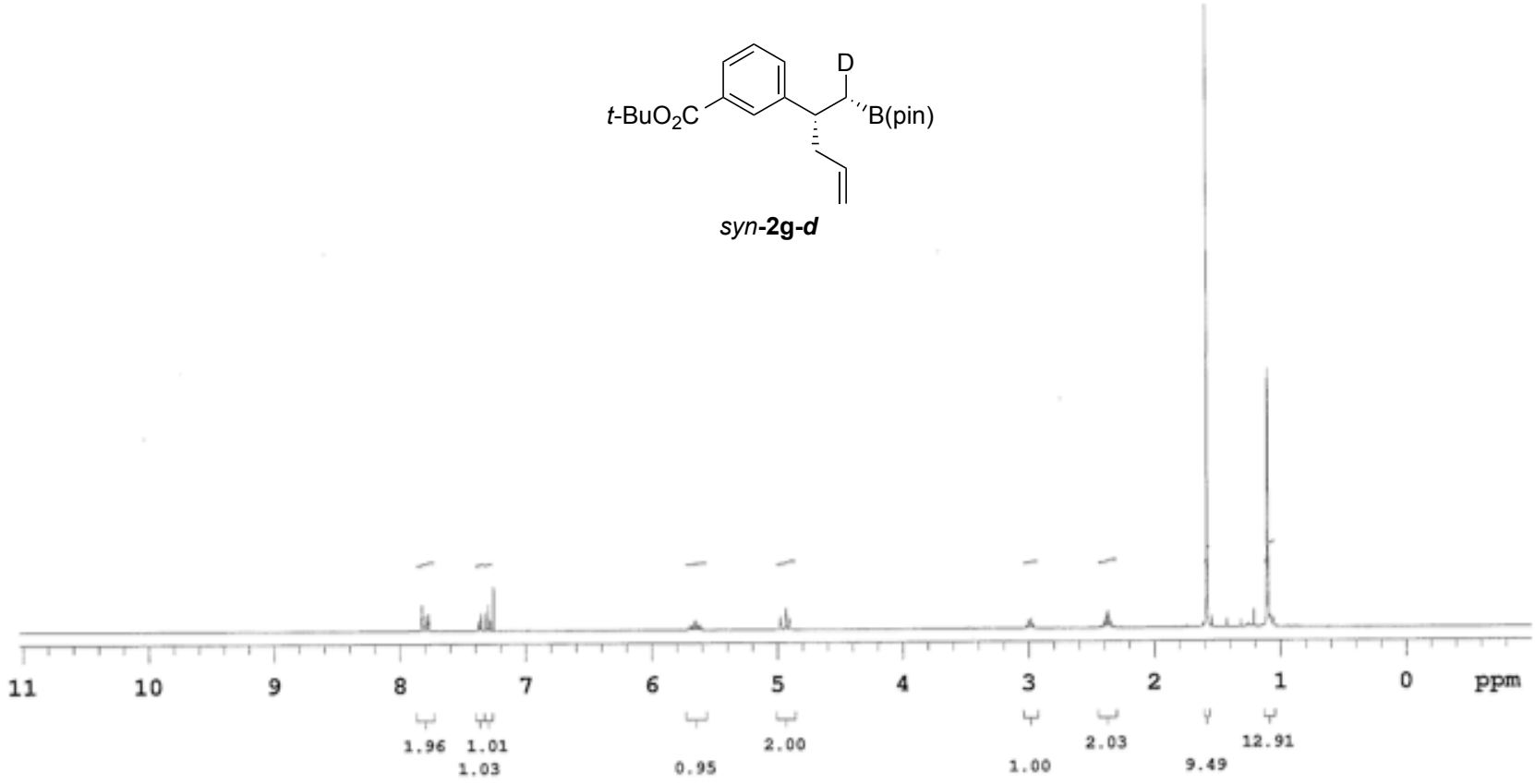


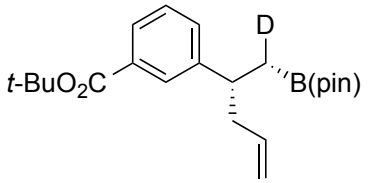


anti-**2g**-***d***

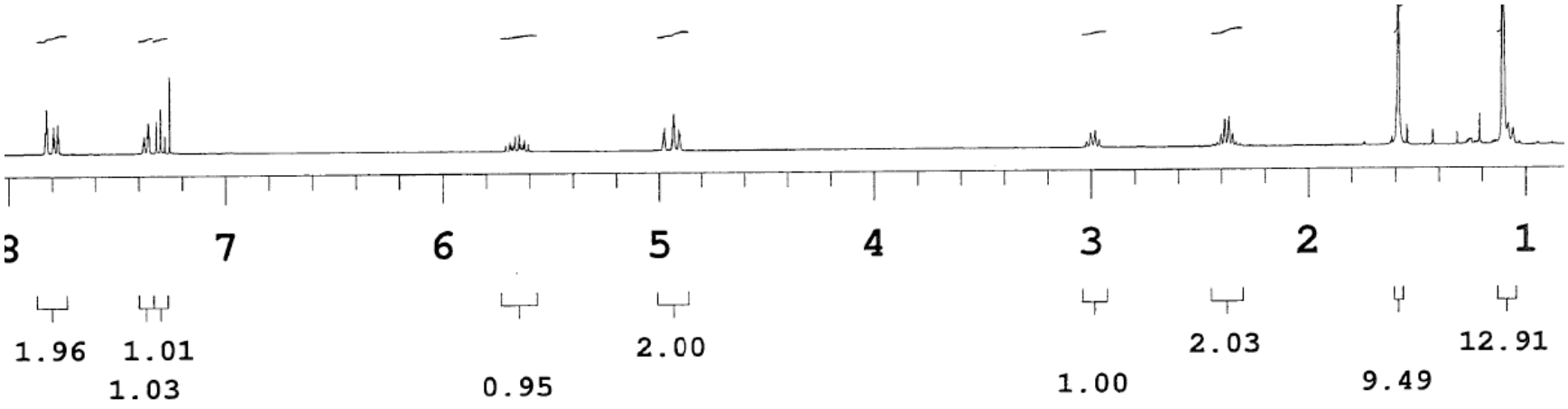


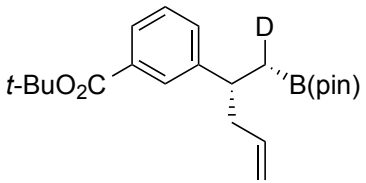
oxidation product of *anti*-2g-*d*
>98:2 d.r.


D
t-BuO2C
B(pin)
syn-2g-d
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.96
1.01
1.03
0.95
2.00
1.00
2.03
9.49
12.91

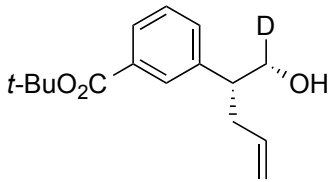


syn-**2g-*d***

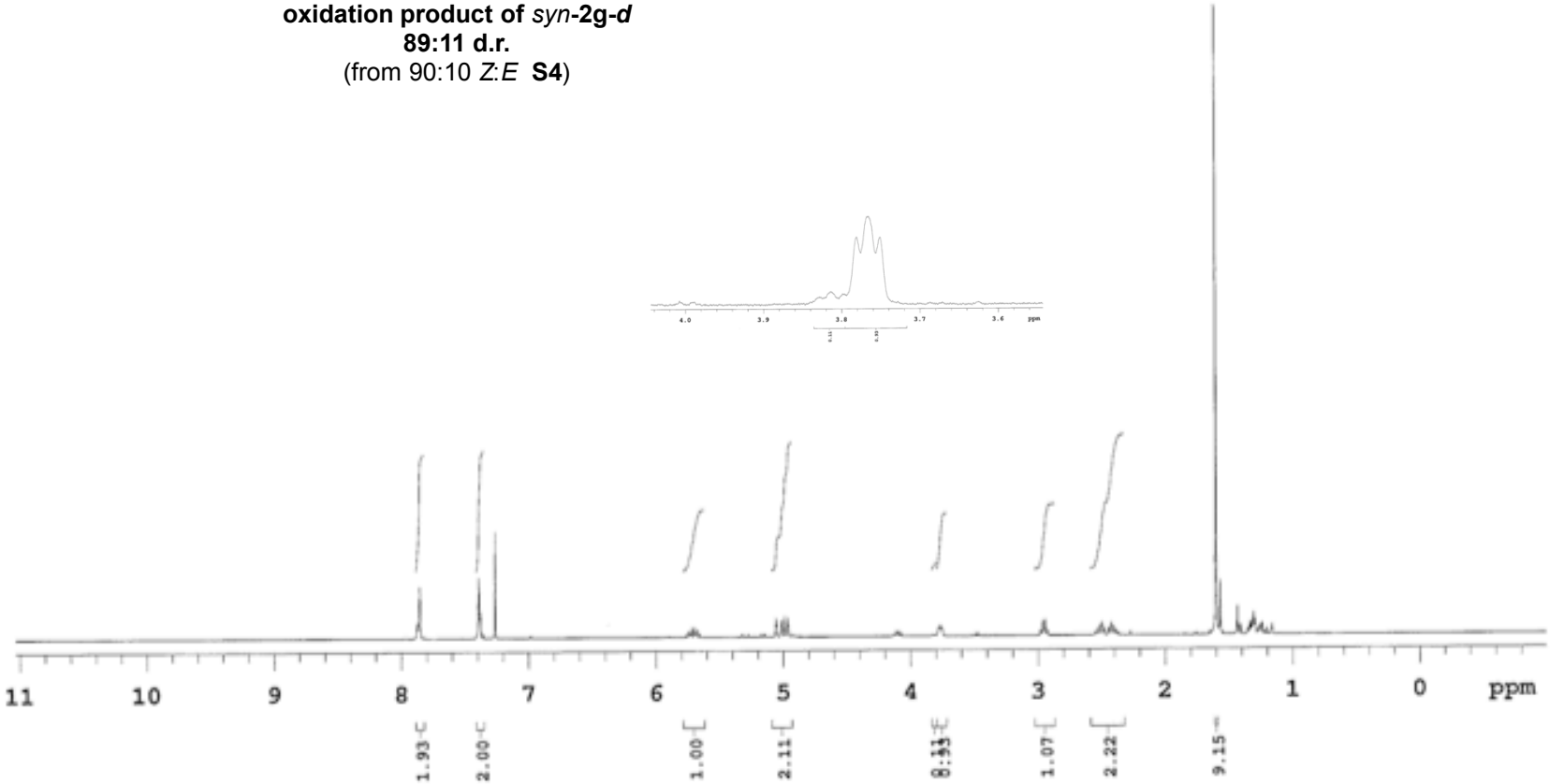


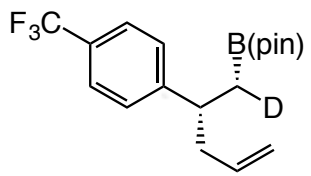


syn-**2g**-***d***



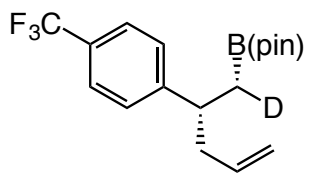
oxidation product of *syn*-2g-*d*
89:11 d.r.
(from 90:10 *Z*:*E* **S4**)



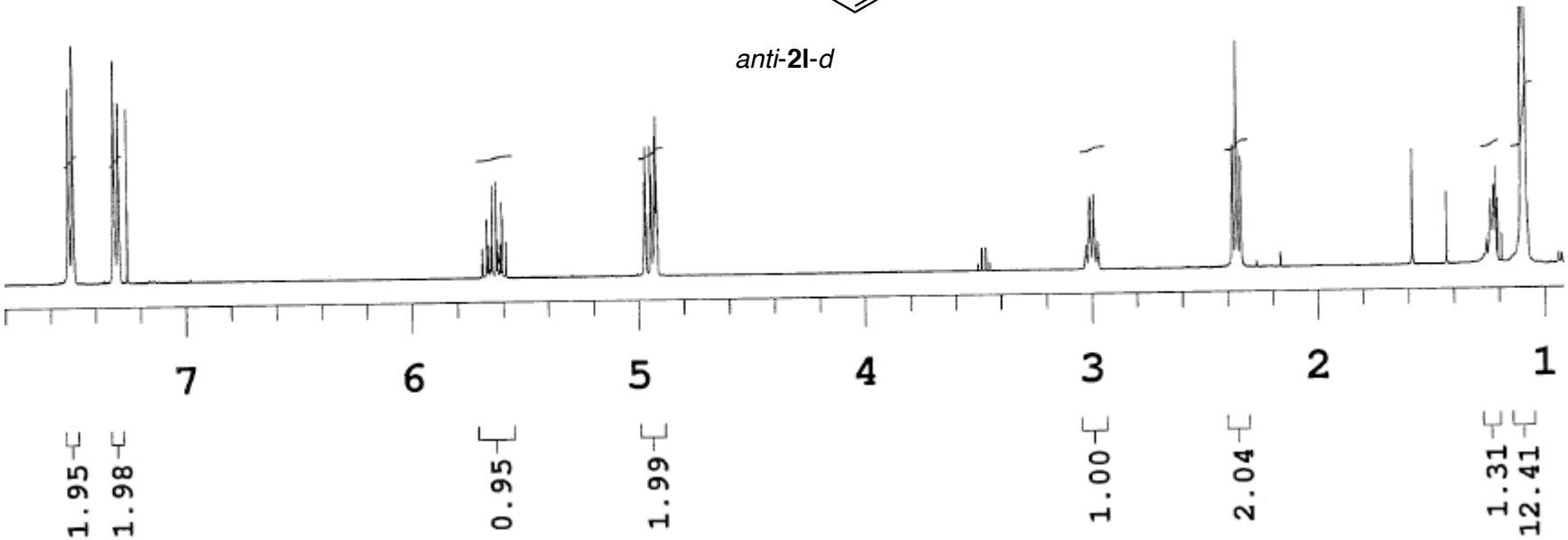

F3C
B(pin)
D

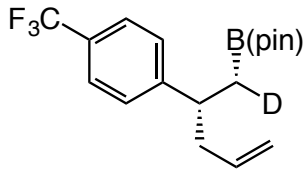
anti-**2l**-*d*

11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.95
1.98
0.95
1.99
1.00
2.04
1.31
12.41

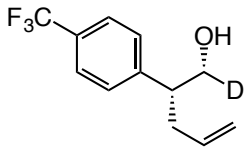


anti-**2l**-*d*

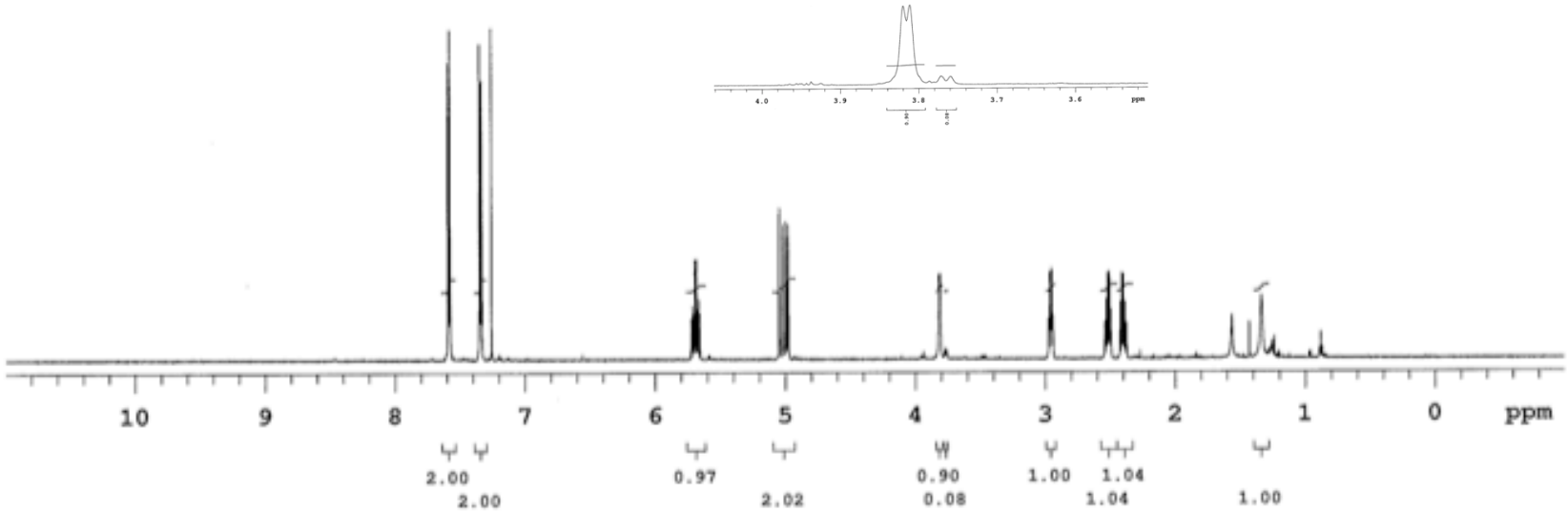


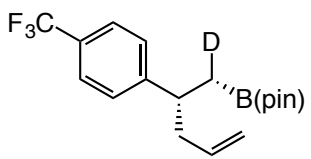


anti-**2l**-*d*



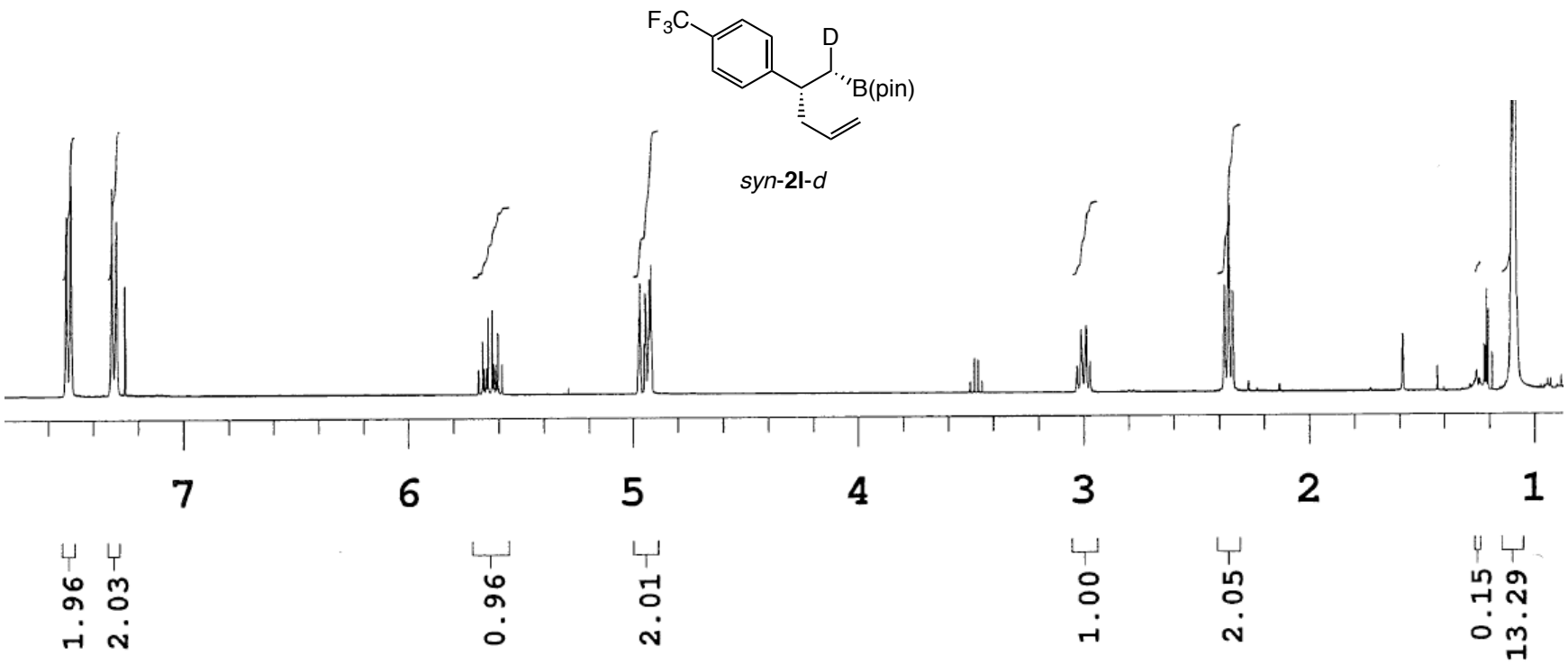
oxidation product of *anti*-**2l**-*d*
92:8 d.r.
(from 91:9 *E:Z alkene)*



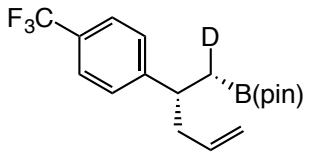

F3C
D
B(pin)

syn-**2l**-*d*

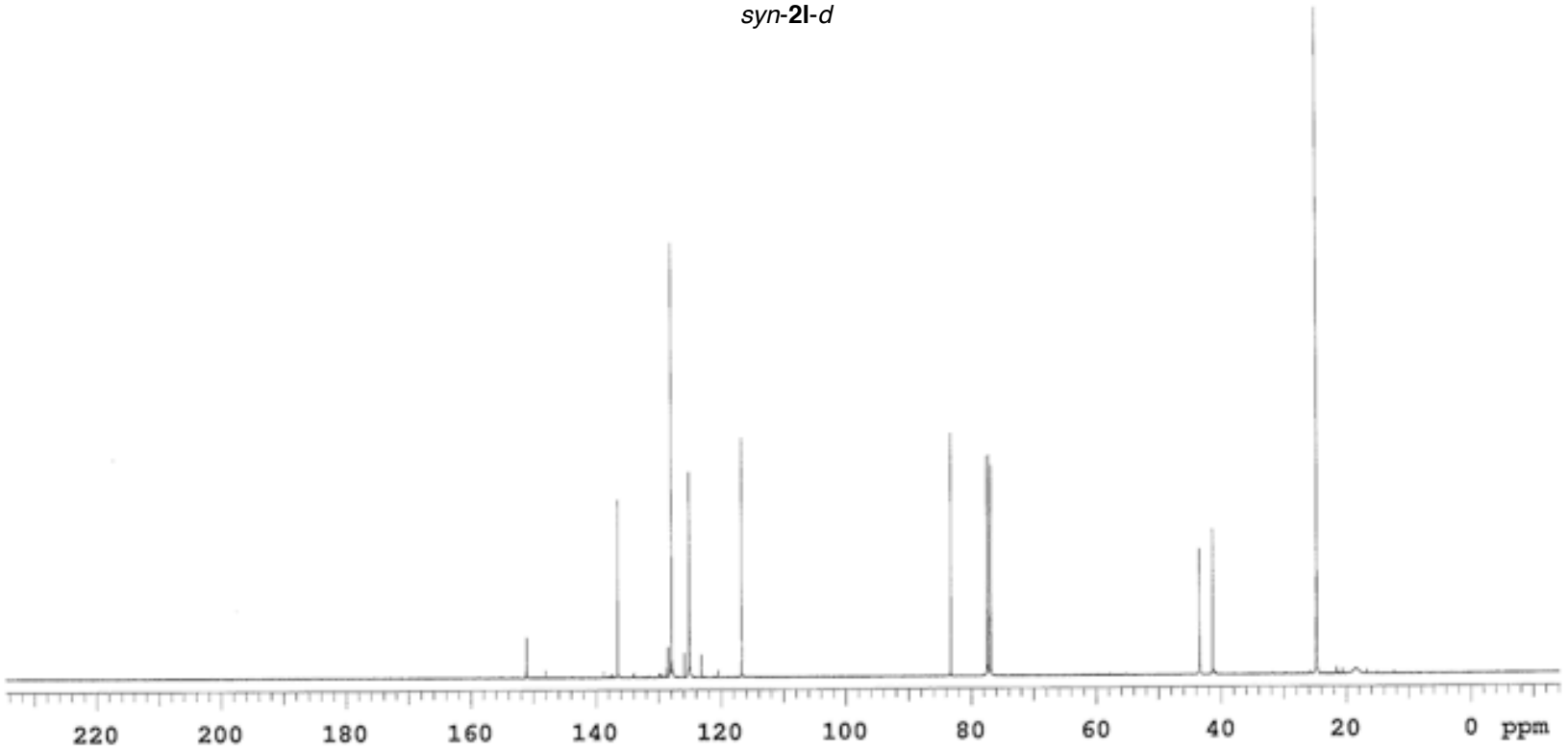
1.101
1.089
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.96
2.03
0.96
2.01
1.00
2.05
0.15
13.29

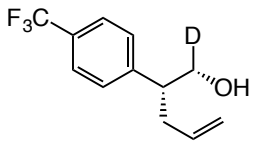


syn-**2l**-*d*

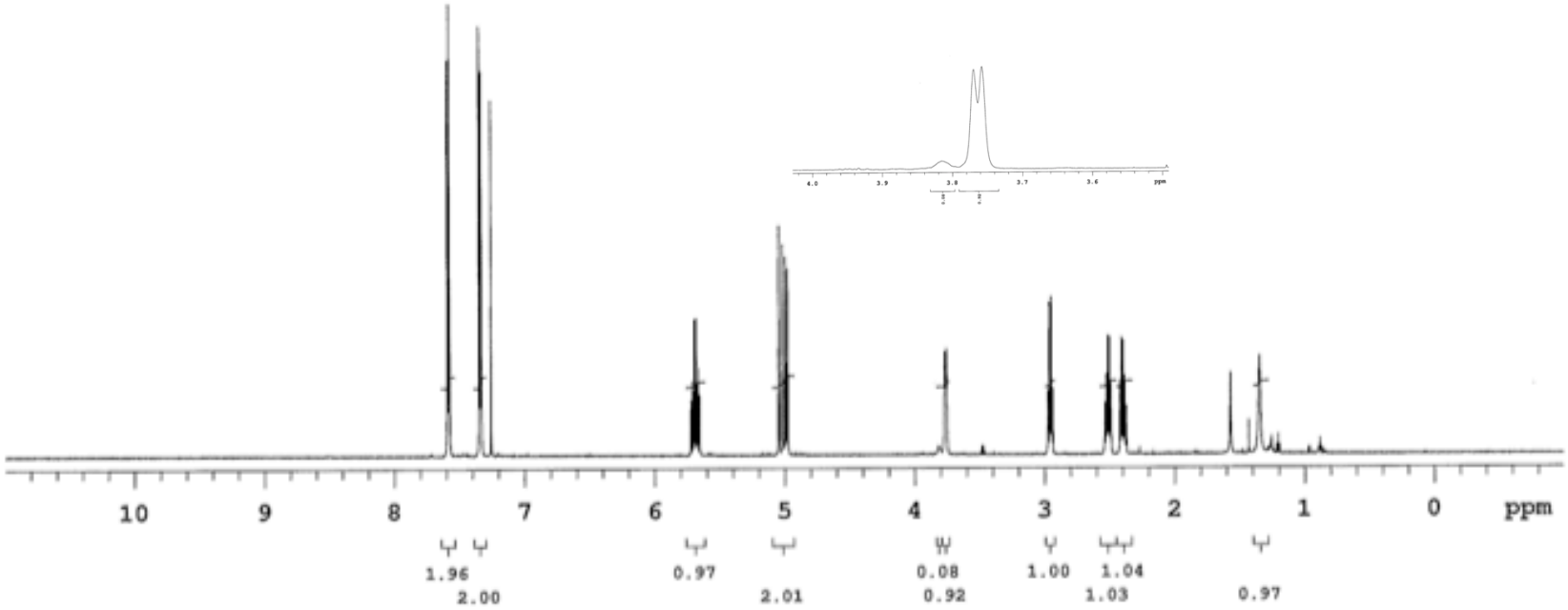


syn-**2l**-*d*





oxidation product of *syn*-**2l**-*d*
92:8 d.r.
(from 90:10 *Z:E alkene)*



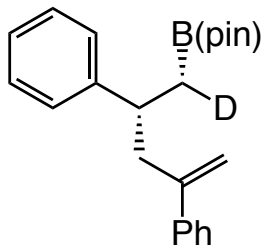
JL-III-251PD

Sample Name:
JL-III-251PD
Data Collected on:
nmr19-vnmrs60$
Archive directory:

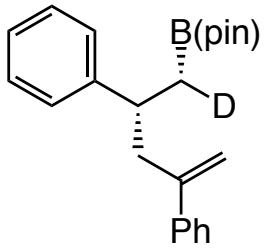
Sample directory:

FidFile: PROTON

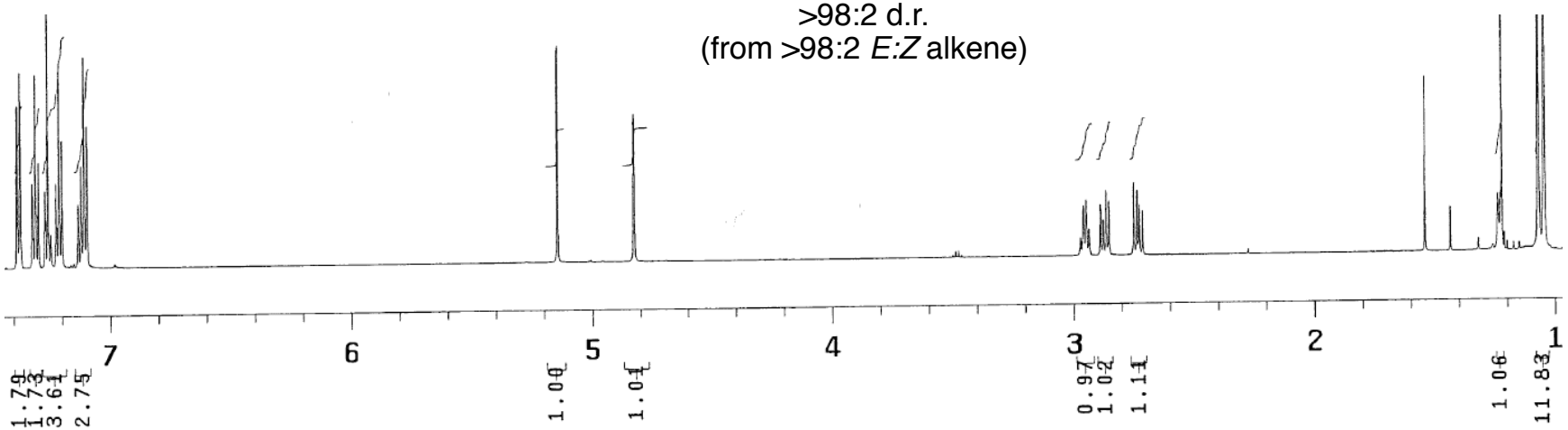
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 15 2015



anti-**2n**-*d*
>98:2 d.r.
(from >98:2 *E:Z* alkene)



anti-**2n**-*d*
>98:2 d.r.
(from >98:2 *E:Z* alkene)



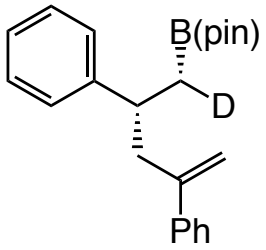
JL-III-106-C-PD

Sample Name:
JL-III-106-C-PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

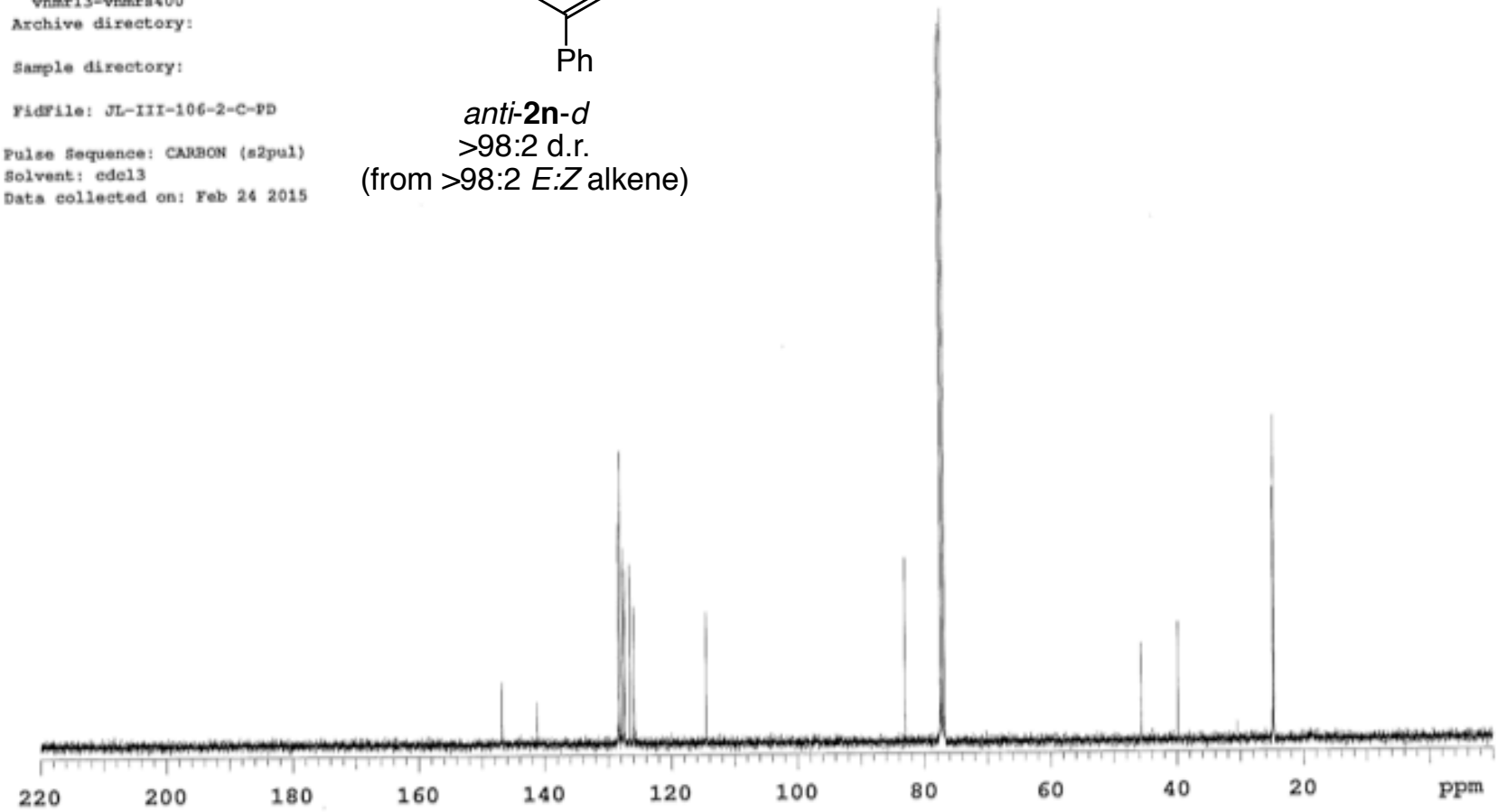
Sample directory:

FidFile: JL-III-106-2-C-PD

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 24 2015



anti-**2n**-*d*
>98:2 d.r.
(from >98:2 *E:Z* alkene)



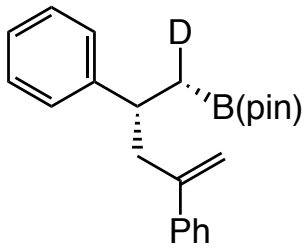
JL-III-252PD

Sample Name:
JL-III-252PD
Data Collected on:
nmr19-vnmrs600
Archive directory:

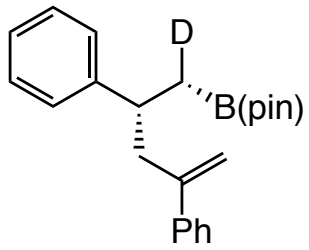
Sample directory:

FidFile: PROTON

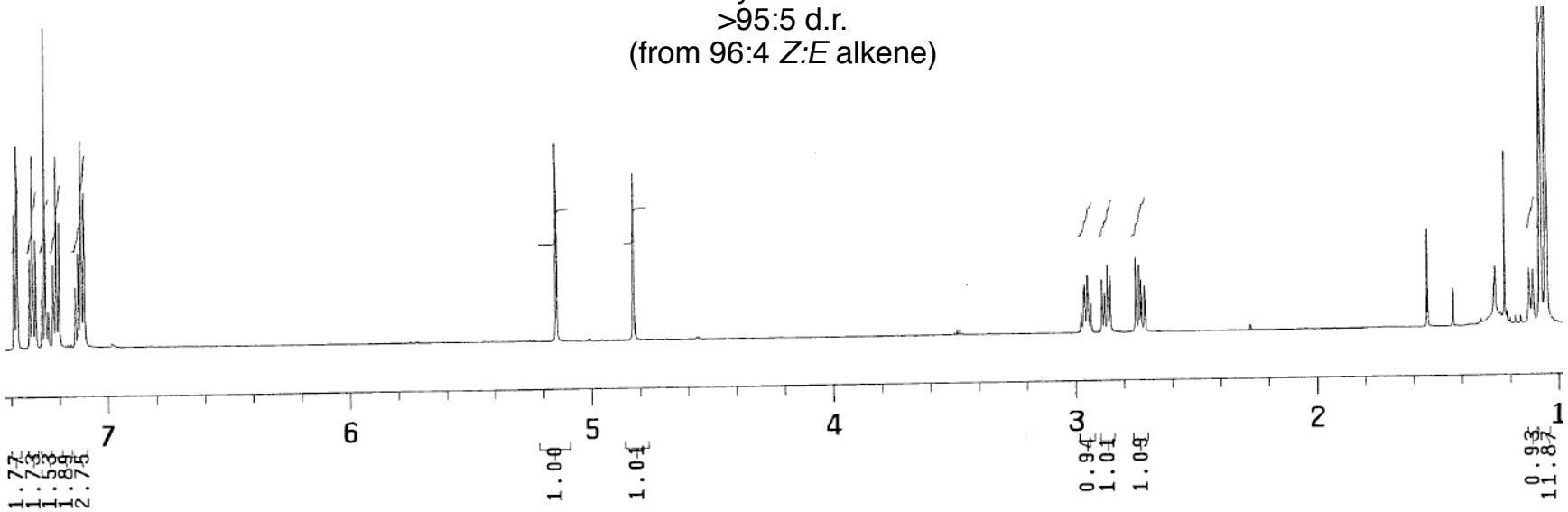
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 15 2015



syn-**2n**-*d*
>95:5 d.r.
(from 96:4 *Z:E* alkene)



syn-**2n**-*d*
>95:5 d.r.
(from 96:4 *Z:E* alkene)



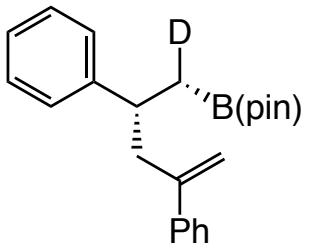
JL-III-107-PD-C

Sample Name:
JL-III-107-PD-C
Data Collected on:
vnmr13-vnmrs400
Archive directory:

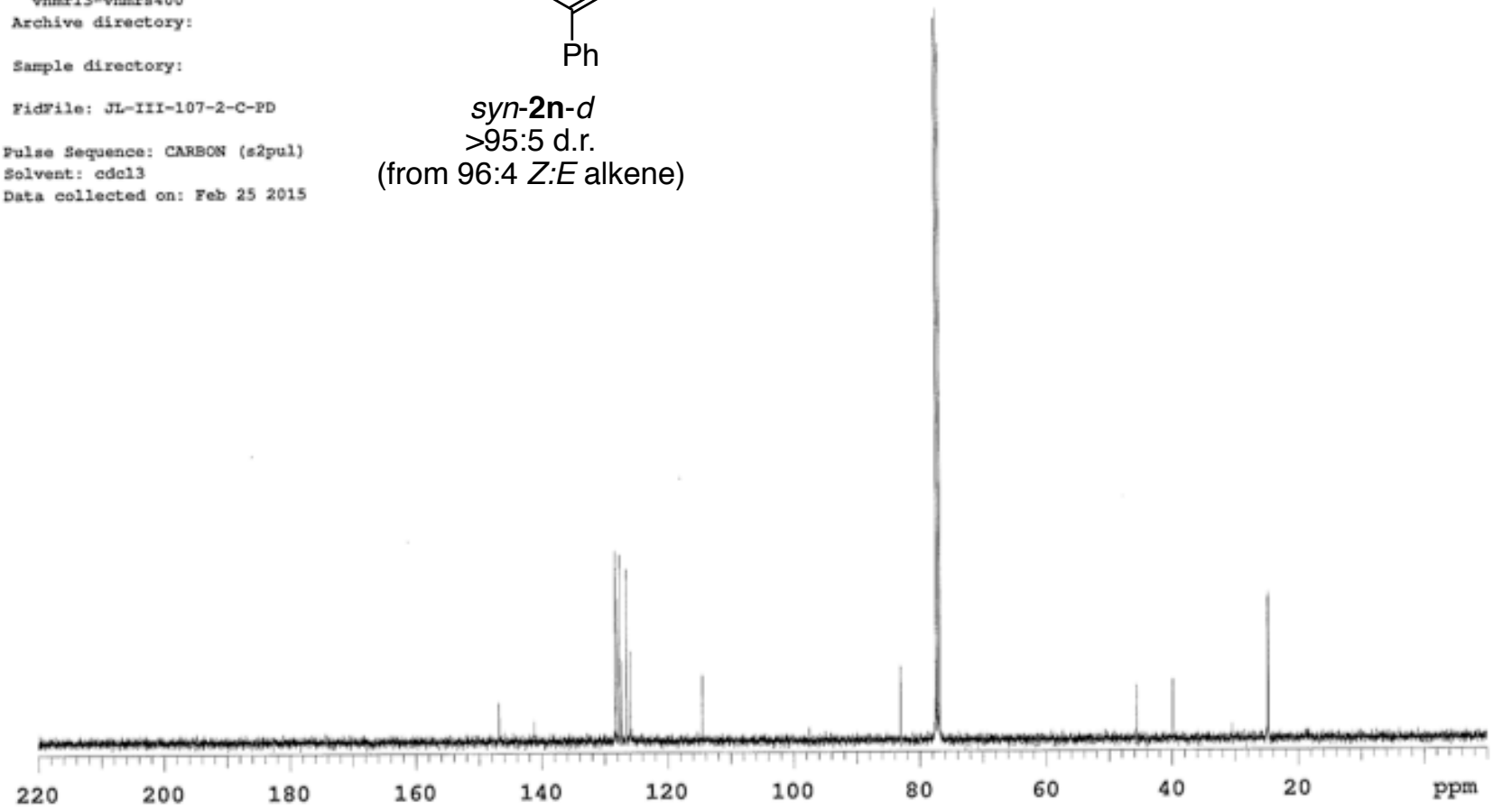
Sample directory:

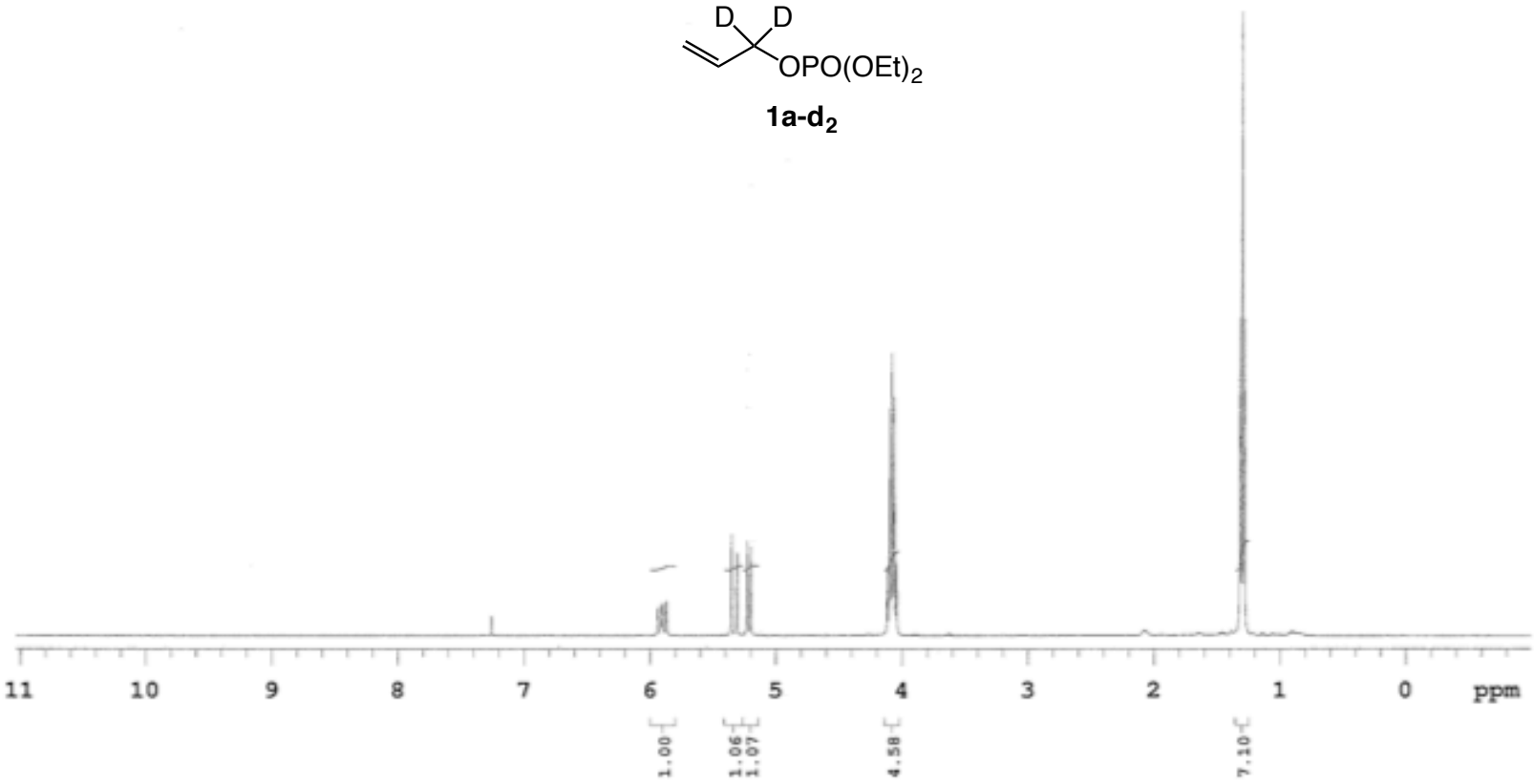
FidFile: JL-III-107-2-C-PD

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 25 2015



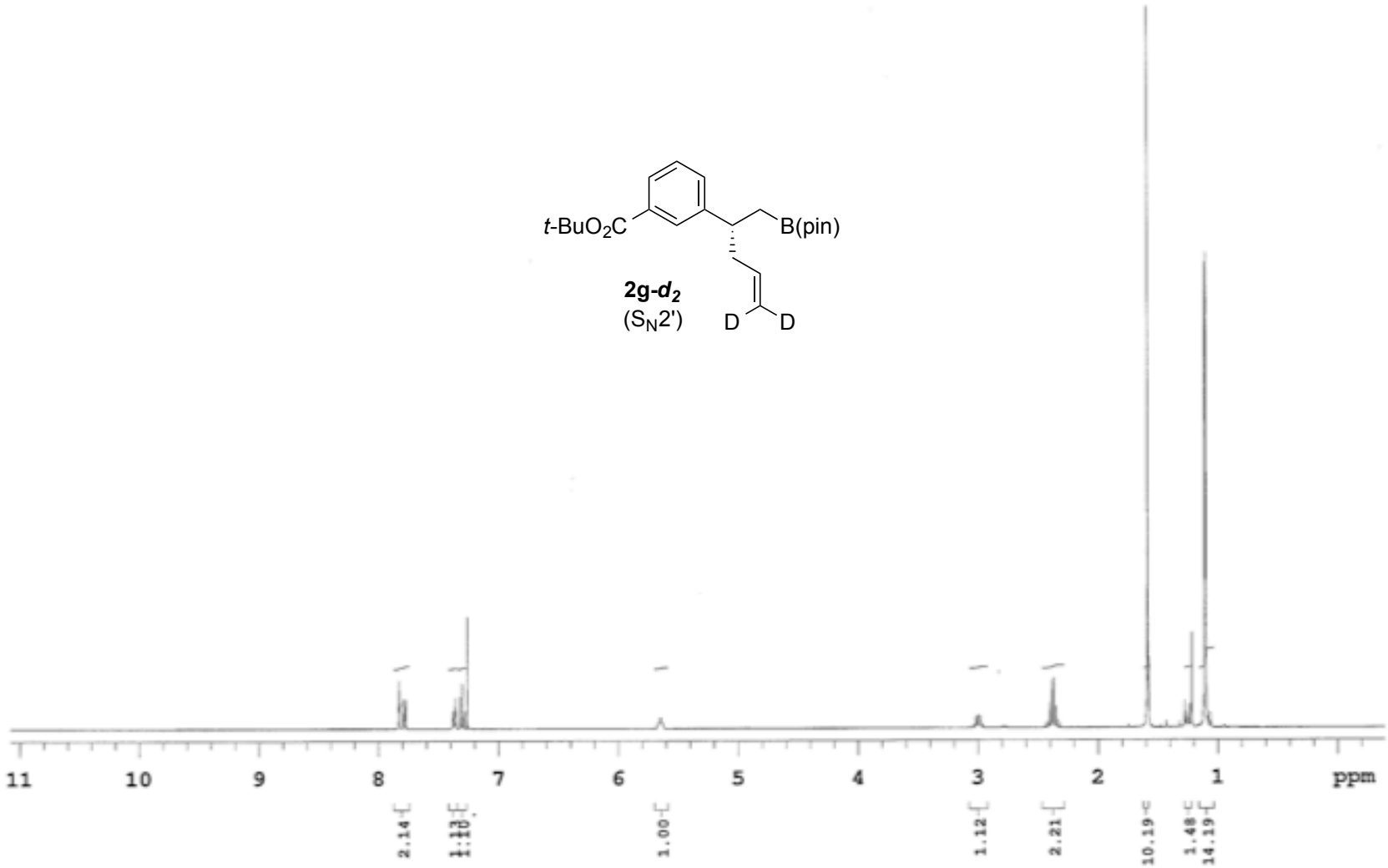
syn-**2n**-*d*
>95:5 d.r.
(from 96:4 *Z:E* alkene)

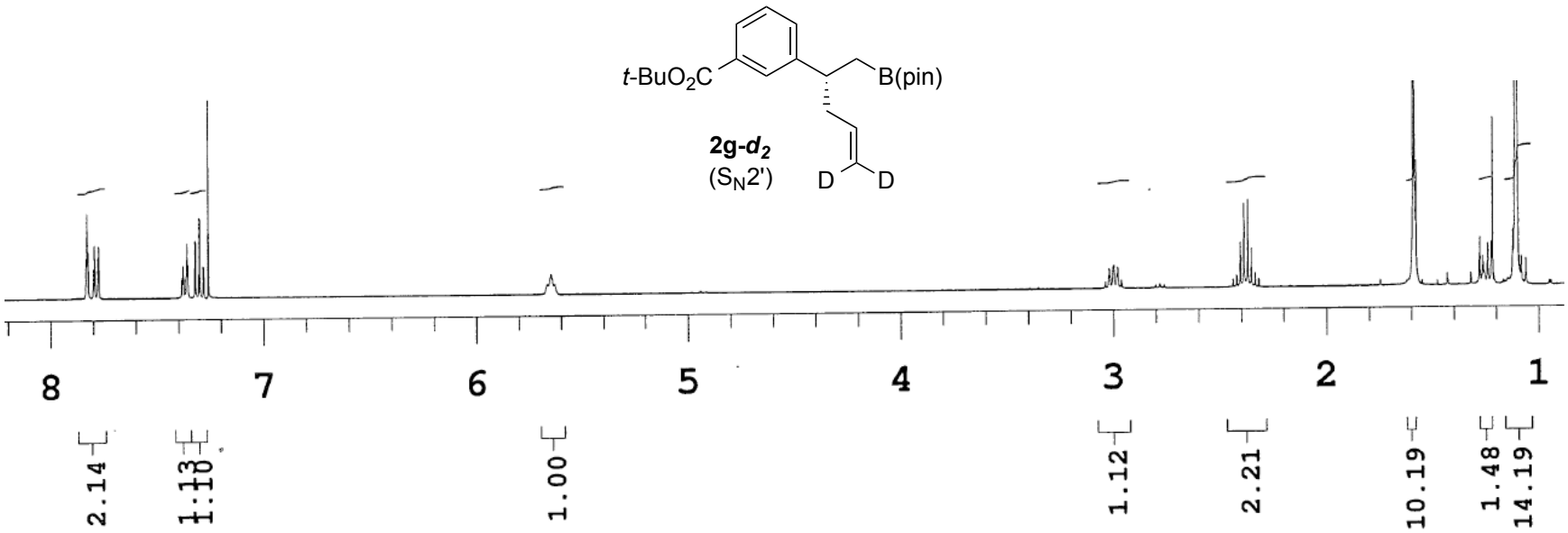


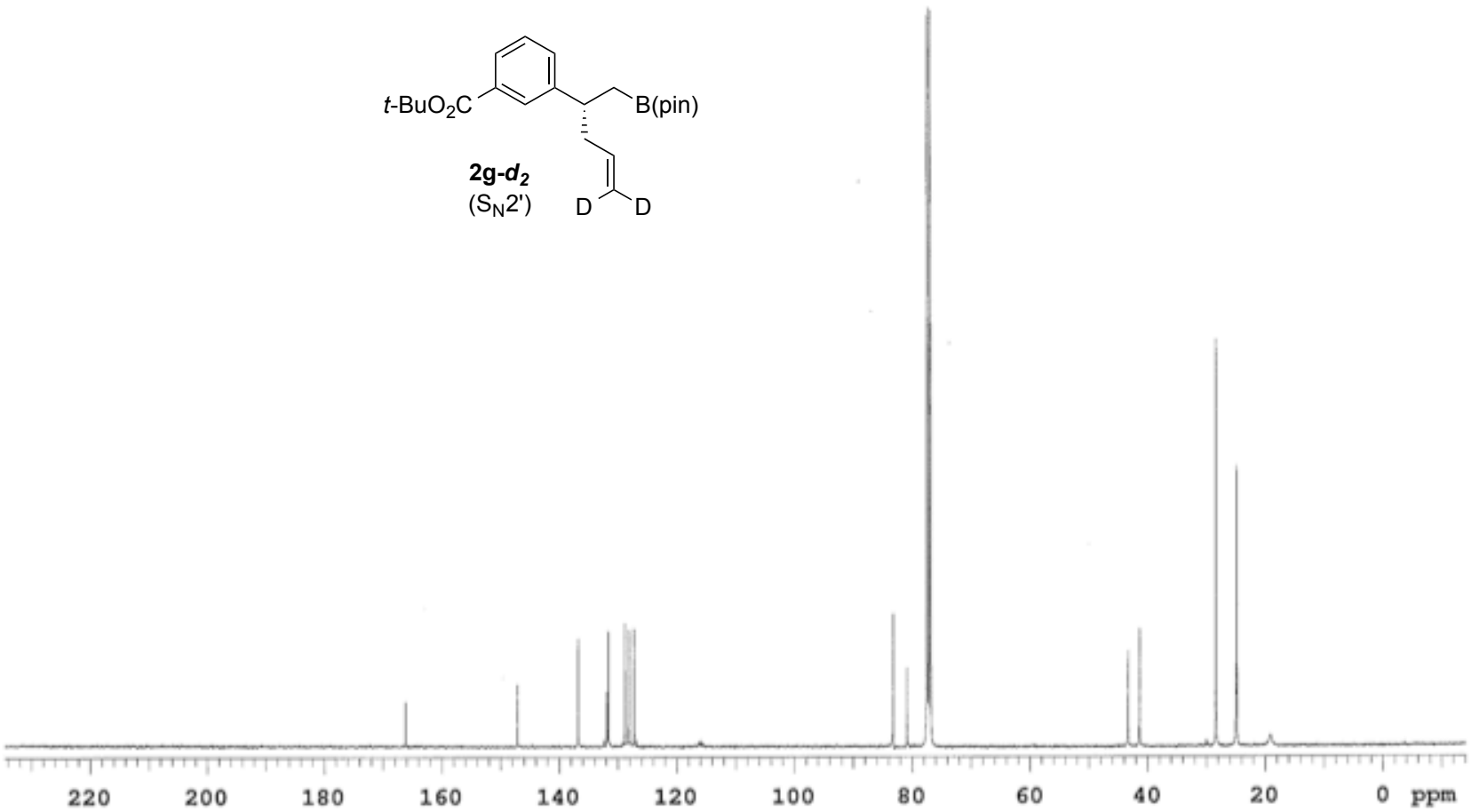


1a-d$_2$

1a-d_2


t-BuO2C
B(pin)
2g-d2
(SN2')
D
D
11
10
9
8
7
6
5
4
3
2
1
ppm
2.14
1.13
1.10
1.00
1.12
2.21
10.19
1.48
14.19


t-BuO2C
B(pin)
2g-d2
(SN2')
D
D
8
7
6
5
4
3
2
1
2.14
1.13
1.00
1.12
2.21
10.19
1.48
14.19


t-BuO2C
B(pin)
2g-d2
(SN2')
D
D
220
200
180
160
140
120
100
80
60
40
20
0
ppm

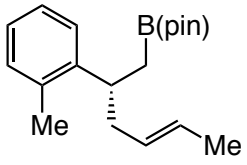
JL-IV-169-2PD

Sample Name:
JL-IV-169-2PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: JL-IV-169PD-2

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 21 2016



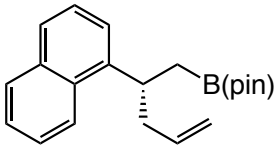
2ai

Sample Name:
JL-II-252PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

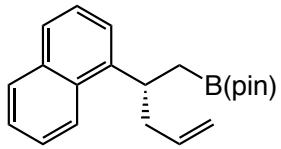
Sample directory:

FidFile: PROTON

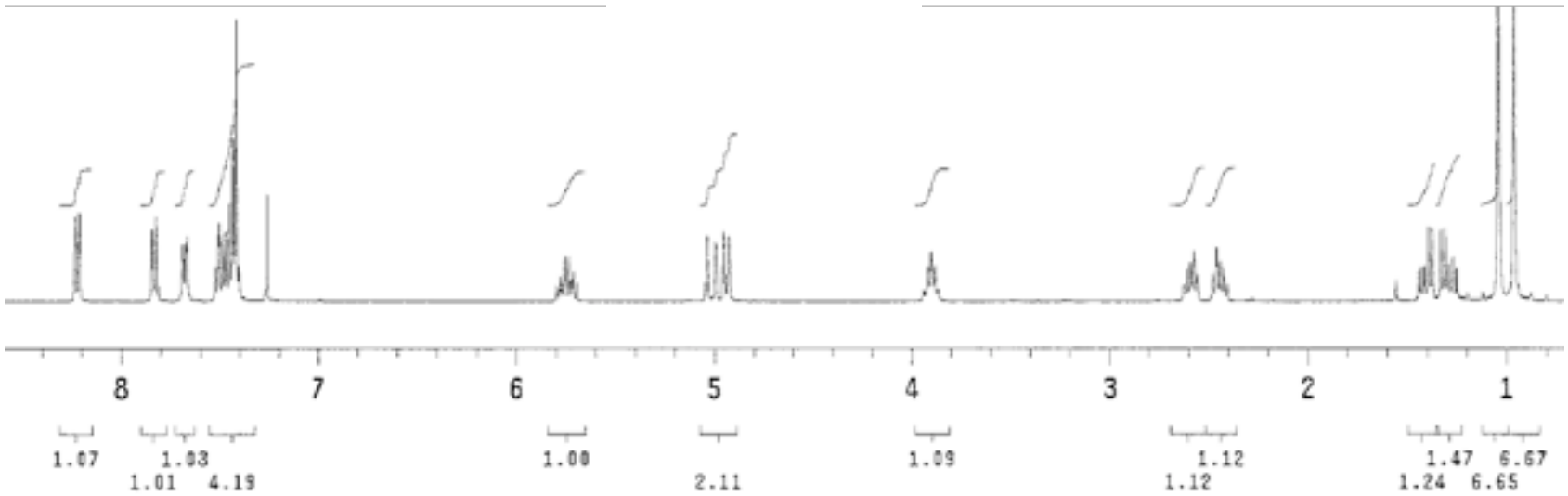
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 4 2014



2af


B(pin)

2af


8
7
6
5
4
3
2
1
1.07
1.03
1.01
4.19
1.00
2.11
1.09
1.12
1.12
1.47
6.67
1.24
6.65

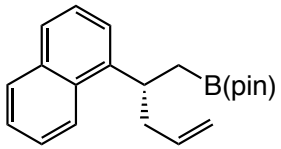
JL-II-252PD-C

Sample Name:
JL-II-252PD-C
Data Collected on:
vnmrj5-vnmrs408
Archive directory:

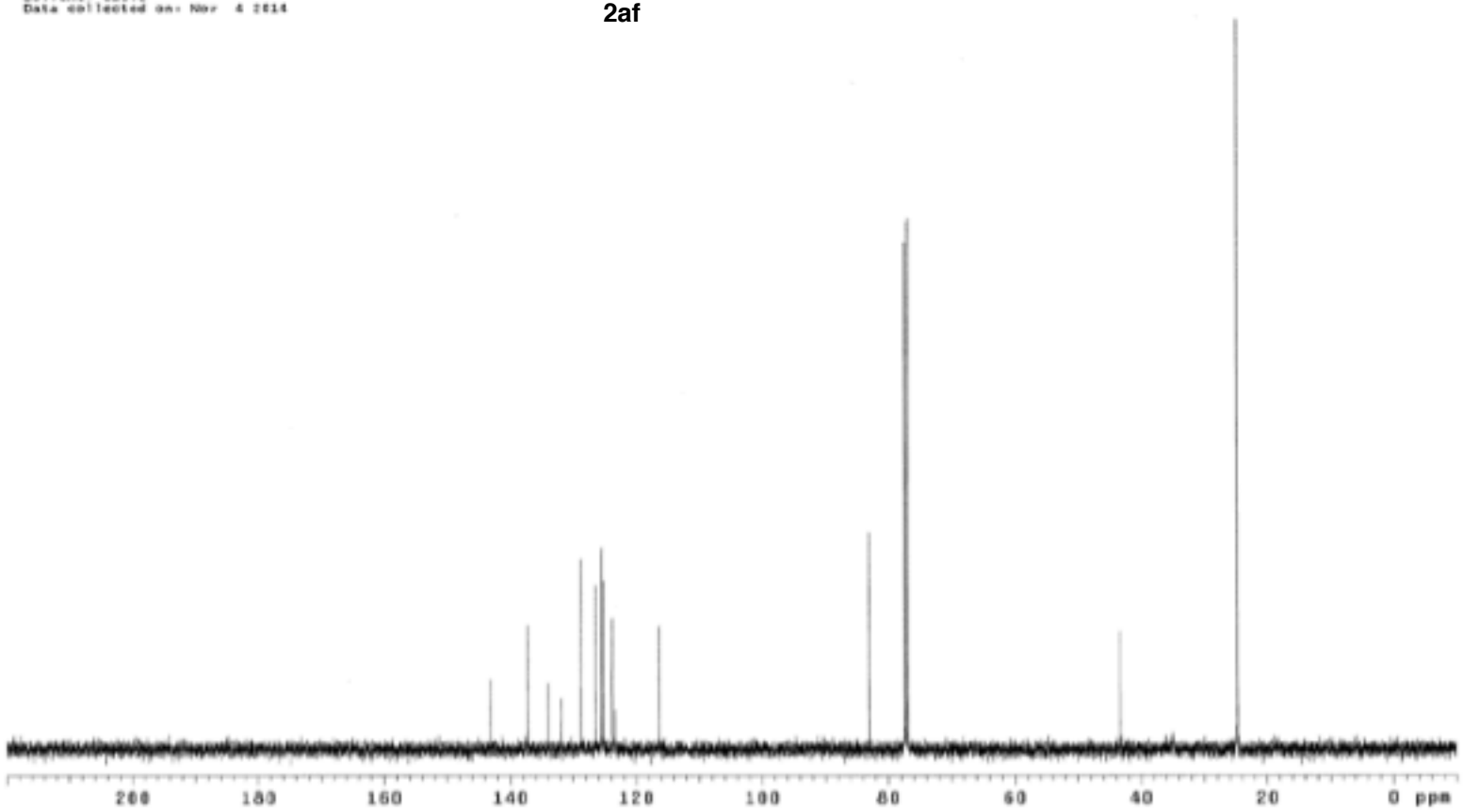
Sample directory:

FidFile: JL-II-252PD-C

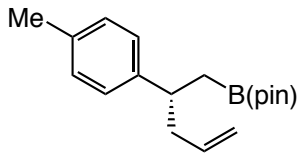
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 4 2014



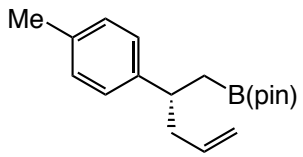
2af



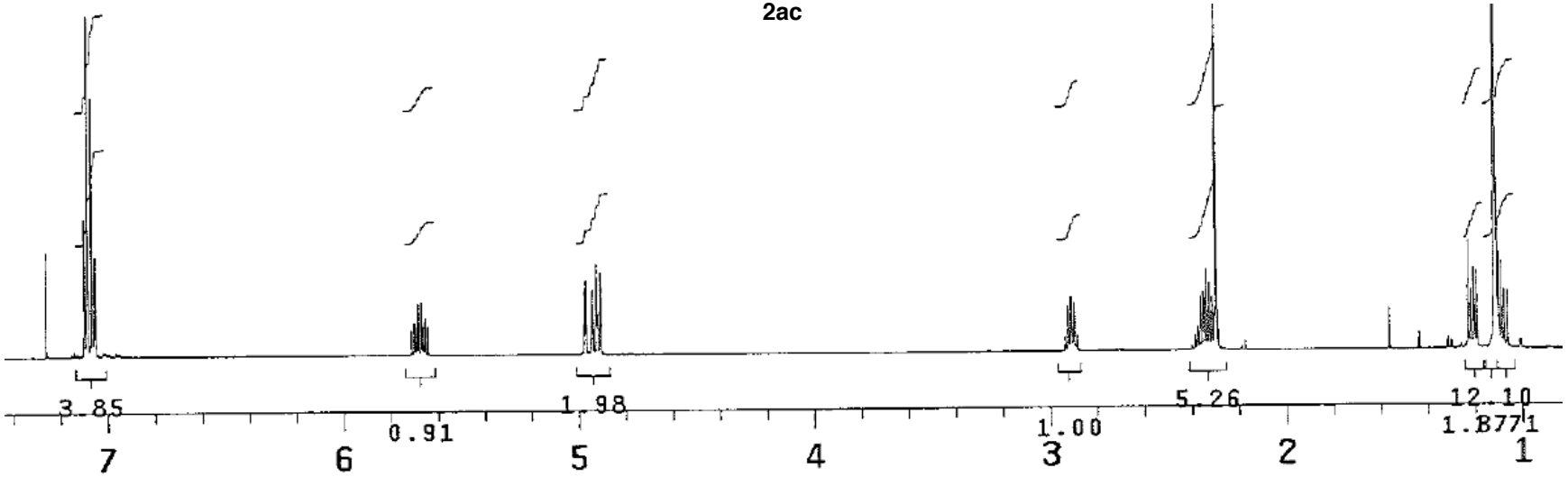
```
Sample Name:
  SR-V-48
Data Collected on:
  nmr19-vnmrs600
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 23 2015
```



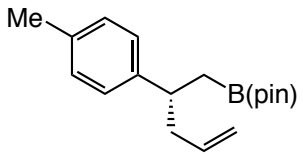
2ac



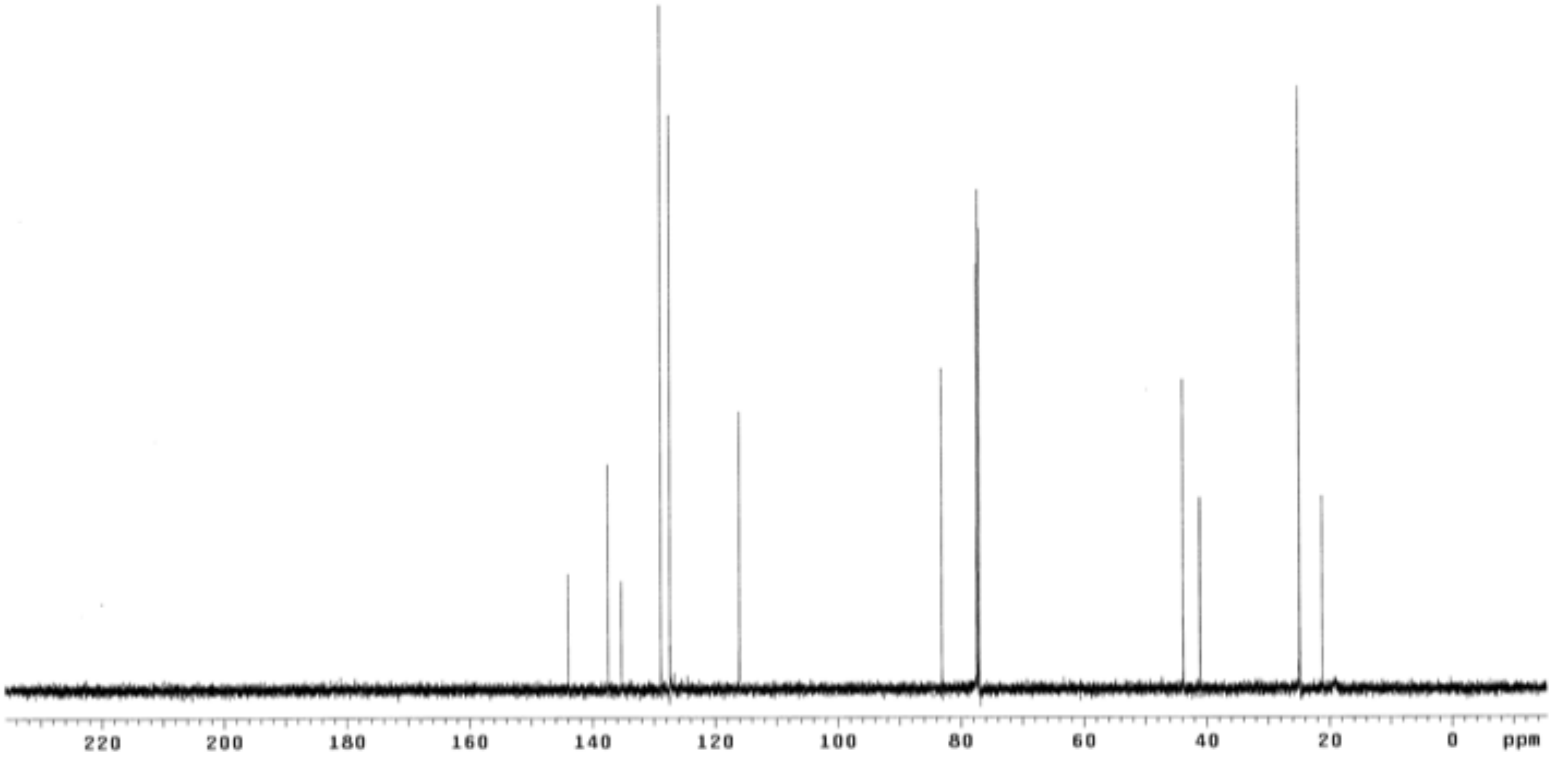
2ac



```
Sample Name:
  SR-V-48-carbon
Data Collected on:
  nmr19-vnmrs600
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 23 2015
```



2ac

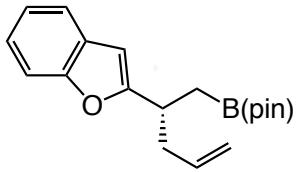


Sample Name:
JL-II-257PD
Data Collected on:
vnmr13-vnmrs400
Archive directory:

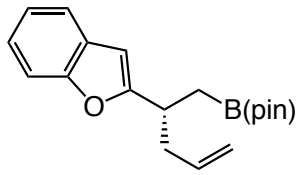
Sample directory:

FidFile: JL-III-275-5PD

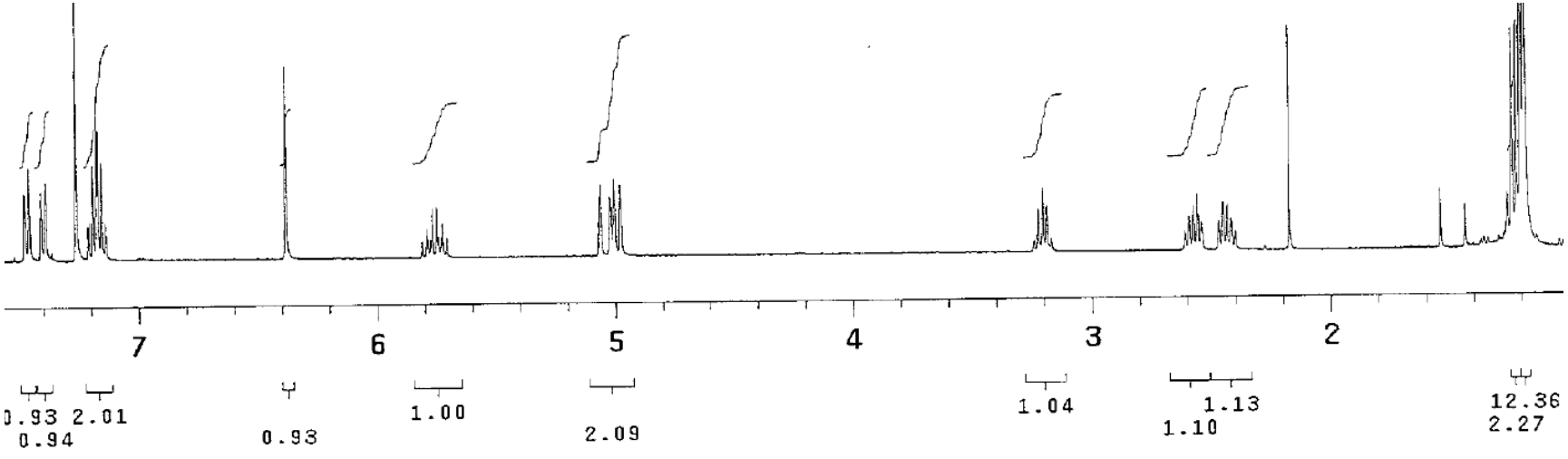
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 20 2015



2ag



2ag



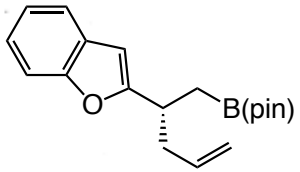
JL-III-127PD-C

Sample Name:
JL-III-127PD-C
Data Collected on:
vnmr13-vnmrs400
Archive directory:

Sample directory:

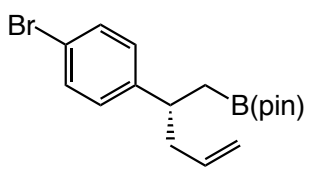
FidFile: JL-III-127PD-C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 20 2015

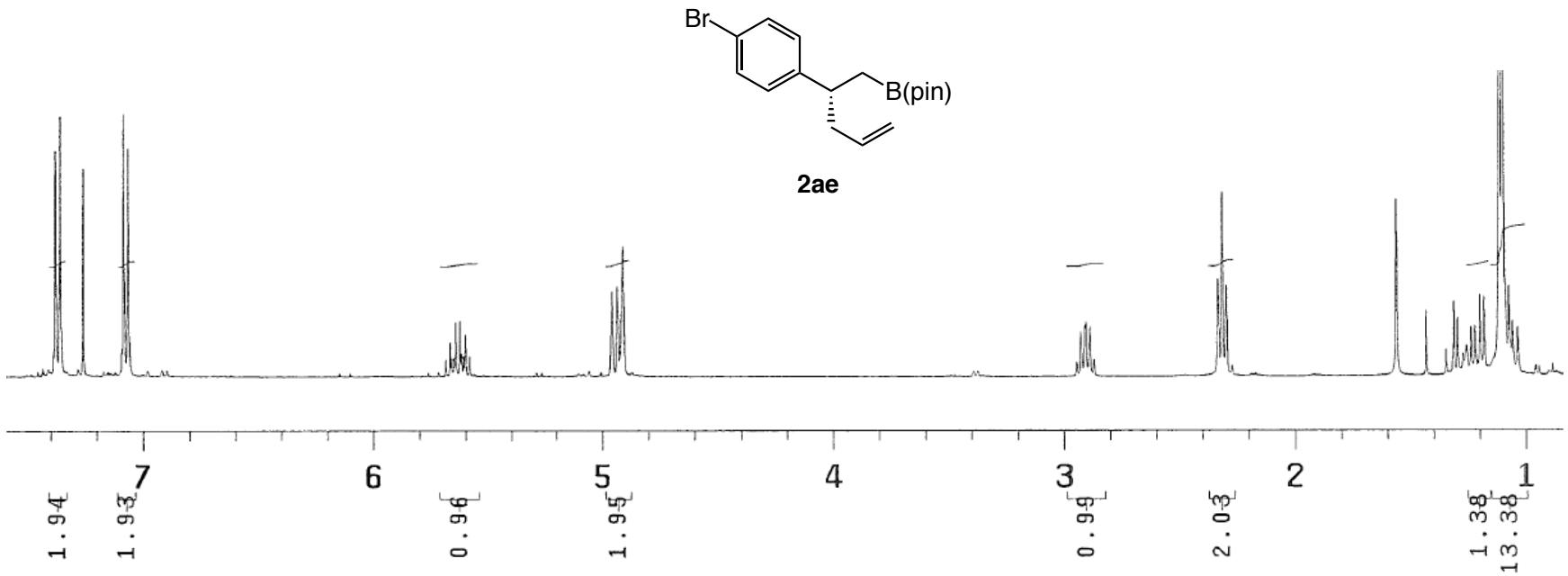


2ag

```
Sample Name:
  SR-IV-263-3
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 26 2014
```

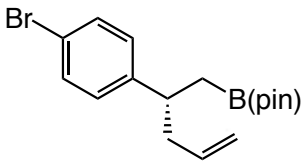


2ae

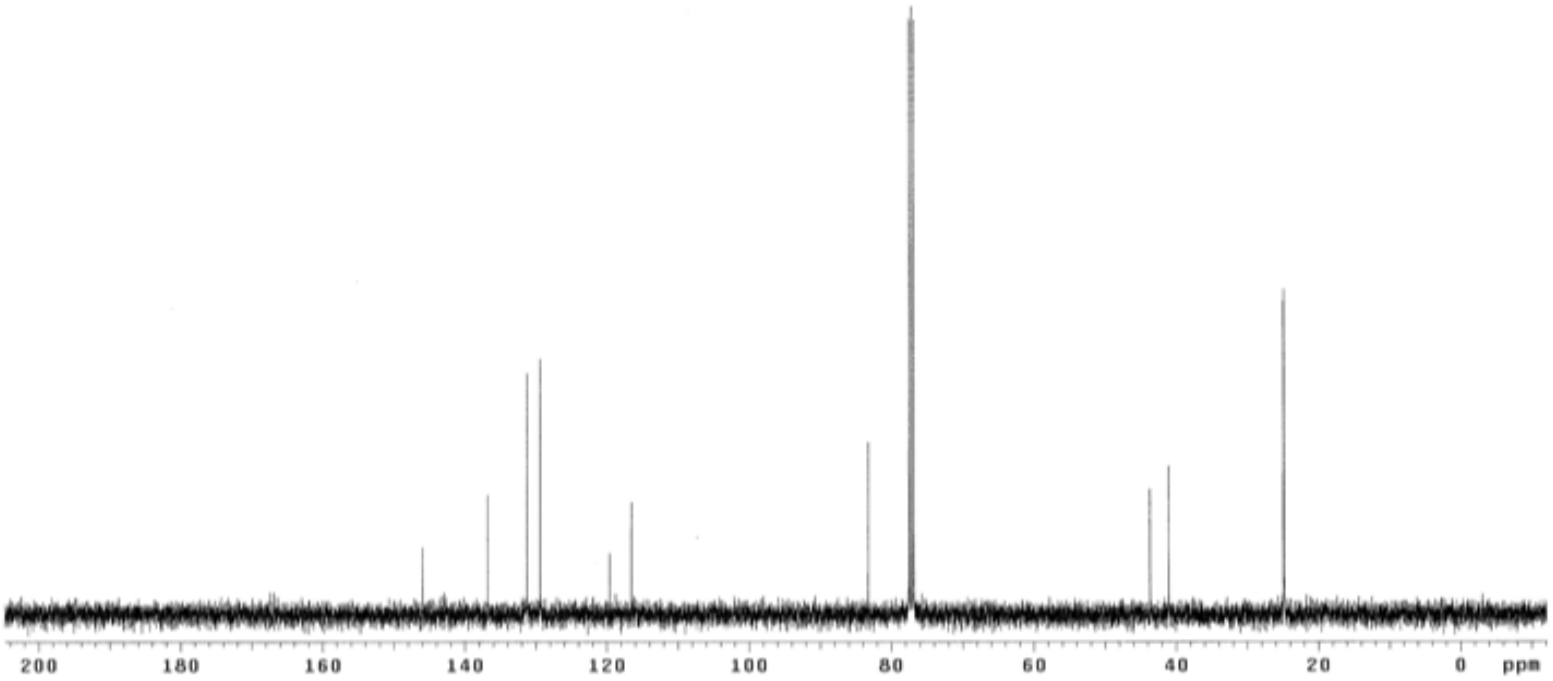


2ae

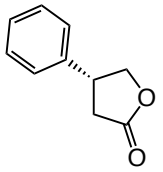
```
Sample Name:
  SR-IV-263-3-carbon
Data Collected on:
  vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: SR-IV-263-3-carbon

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 26 2014
```



2ae



```
Sample Name:
  SR-IV-266-oxid
Data Collected on:
  nmr14-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 26 2015
```



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