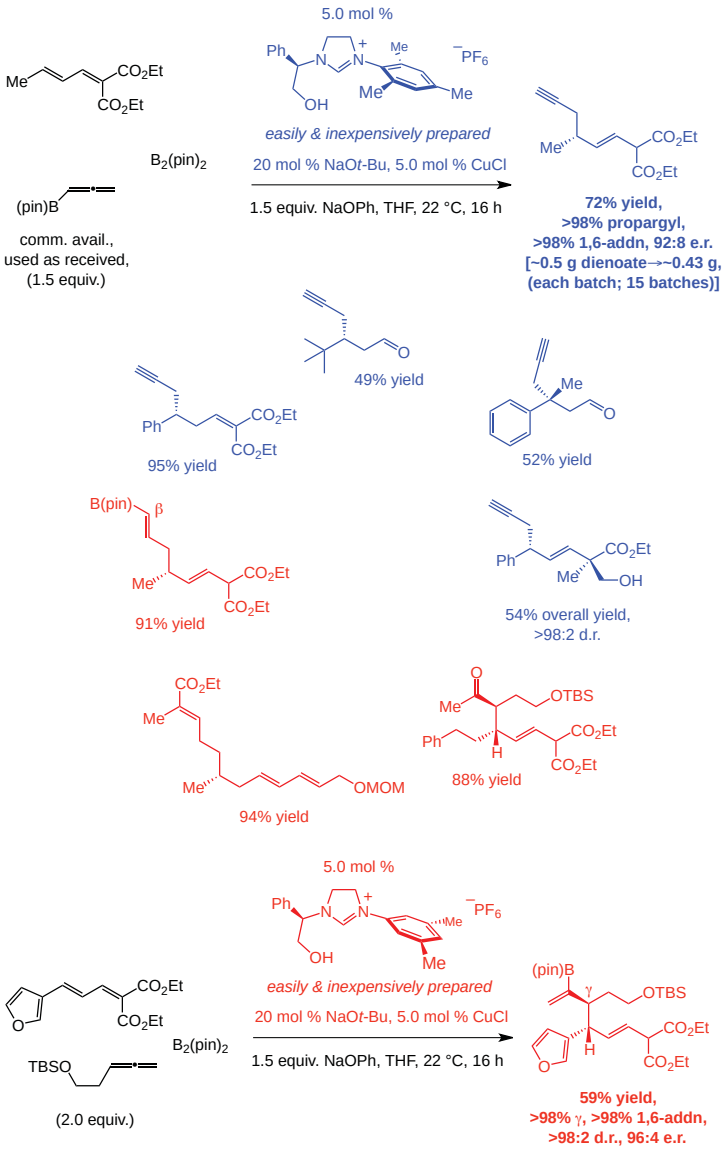
Catalytic Enantioselective 1,6-Conjugate Additions of Propargyl and Allyl Groups

Fanke Meng, Xiben Li, Sebastian Torker, Ying Shi, Xiao Shen & Amir H. Hoveyda

Department of Chemistry, Merkert Chemistry Center, Boston College, Chestnut Hill, Massachusetts 02467, USA

SUPPLEMENTARY INFORMATION



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1. Extended Bibliography

Additional citation regarding competition between 1,6- and 1,4-conjugate addition:

Hénon, H., Mauduit, M. & Alexakis, A. Regiodivergent 1,4 versus 1,6 asymmetric copper-catalyzed conjugate addition. *Angew. Chem. Int. Edn* **47**, 9122–9124 (2008).

Additional citations on auxiliary-controlled catalytic enantioselective 1,6-conjugate addition:

Okada, S., Arayama, K., Murayama, R., Ishizuka, T., Hara, K., Hirone, N., Hata, T. & Urabe, H. Iron-catalyst-switched selective conjugate addition of Grignard reagents: α,β,γ,δ-Unsaturated amides as versatile templates for asymmetric three-component coupling process. *Angew. Chem. Int. Edn.* **47**, 6860–6864 (2008).

Additional citations on catalytic enantioselective Claisen rearrangement processes:

(a) Maruoka, K., Banno, H. & Yamamoto, H. Asymmetric Claisen rearrangement catalyzed by chiral organoaluminum reagent. *J. Am. Chem. Soc.* **112**, 7791–7793 (1990).

(b) Abraham, L., Czerwonka, R. & Hiersemann, M. The catalytic enantioselective Claisen rearrangement of an allyl vinyl ether. *Angew. Chem. Int. Edn* **40**, 4700–4703 (2001).

(c) Akiyama, K. & Mikami, K. Enantioselective catalysis of Claisen rearrangement by DABNTf–Pd(II) complex. *Tetrahedron Lett.* **45**, 7217–7220 (2004).

(d) Geherty, M. E., Dura, R. D. & Nelson, S. G. Catalytic asymmetric Claisen rearrangement of unactivated allyl vinyl ethers. *J. Am. Chem. Soc.* **132**, 11875–11877 (2010).

(e) Uyeda, C. & Jacobsen, E. N. Enantioselective Claisen rearrangements with a hydrogen-bond donor catalyst. *J. Am. Chem. Soc.* **130**, 9228–9229 (2008).

(f) Uyeda, C., Rötheli, A. R. & Jacobsen, E. N. Catalytic enantioselective Claisen rearrangement of *O*-allyl β-ketoesters. *Angew. Chem. Int. Edn* **49**, 9753–9756 (2010).

(g) Uyeda, C. & Jacobsen, E. N. Transition-state charge stabilization through multiple non-covalent interactions in the guanidinium-catalyzed enantioselective Claisen rearrangement. *J. Am. Chem. Soc.* **133**, 5062–5075 (2011).

(h) Tan, J., Cheon, C.-H. & Yamamoto, H. Catalytic asymmetric Claisen rearrangement of enolphosphonates: Construction of vicinal tertiary and all-carbon quaternary centers. *Angew. Chem. Int. Edn* **51**, 8264–8267 (2012).

Additional citations on applications of catalytic enantioselective Claisen rearrangement in natural product synthesis:

(a) Pollex, A. & Hiersemann, M. Catalytic asymmetric Claisen rearrangement in natural product synthesis: Synthetic studies toward (-)-Xeniolide F. *Org. Lett.* **7**, 5705–5708 (2005).

(b) Becker, J., Butt, L., Kiedrowski, V., Mischler, E., Quentin, F. & Hiersemann, M. Catalytic asymmetric Claisen rearrangement of Gosteli-type allyl vinyl ether: Total synthesis of (-)-9,10-Dihydroecklonialactone B. *J. Org. Chem.* **79**, 3040–3051 (2014).

2. Experimental

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 a Varian Unity INOVA 400 (400 MHz) spectrometer. 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, br s = broad singlet, m = multiplet, app. = apparent), and coupling constant (Hz). ^{13}C NMR spectra were recorded on a Varian Unity INOVA 400 (100 MHz) spectrometer 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. Enantiomer ratios were determined by high-performance liquid chromatography (HPLC) with a Shimadzu chromatograph (Chiral Technologies Chiralcel OD-H (4.6 x 250 mm), Chiralcel OJ-H (4.6 x 250 mm), Chiralcel OZ-H (4.6 x 250 mm), Chiralcel OZ-3 (4.6 x 150 mm), 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.

Unless otherwise noted, all reactions were carried out with distilled and degassed solvents under an atmosphere of dry N_2 in oven- (135 °C) or flame-dried glassware with standard dry box or vacuum-line techniques. Solvents were purified under a positive pressure of dry argon by a modified Innovative Technologies purification system: toluene, benzene and hexanes were purified through a copper oxide and alumina column; CH_2Cl_2 and Et_2O were purged with Ar and purified by passage through two alumina columns. Tetrahydrofuran (THF; Aldrich Chemical Co.) was purified by distillation from sodium benzophenone ketyl immediately prior to use unless otherwise specified. Methanol (Aldrich Chemical Co.) was distilled over CaH_2. All work-up and purification procedures were carried out with reagent grade solvents (purchased from Fisher Scientific) in air.

Reagents and Ligands

Allenes (11): prepared according to previously reported procedures.[1]

Allenylboronic acid pinacol ester: purchased from Aldrich Chemical Co. and used as received.

Alkenyl-substituted dienoates: prepared according to previously reported procedures.[2]

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(1) (a) Crabbé, P., Fillion, H., André, D. & Luche, J.-L. *J. Chem. Soc., Chem. Commun.* 859–860 (1979). (b) Searles, S., Li, Y., Nassim, B., Lopes, M-T. R., Tran, P. T. & Crabbé, P. *J. Chem. Soc., Perkin Trans. 1* 747–751 (1984). (c) Inoue, A., Kondo, J., Shinokubo, H. & Oshima, K. *Chem. Eur. J.* **8**, 1730–1740 (2002). (d) Baird, M. S., Nizovtsev, A. V. & Bolesov, I. G. *Tetrahedron* **58**, 1581–1593 (2002).

Aryl-substituted dienoates: prepared according to previously reported procedures.[3]

Barium hydroxide octahydrate: purchased from Aldrich Chemical Co. and used as received.

[1,1'-Bis(diphenylphosphino)ferrocene]dichloropalladium (II), complex with dichloromethane: purchased from Strem Chemicals Inc. and used as received.

Bis(pinacolato)diboron: purchased from Frontier Scientific, Inc. and recrystallized from pentane.

(Carbethoxyethylidene)triphenylphosphorane: purchased from Aldrich Chemical Co. and used as received.

Chromium(II) chloride: purchased from Alfa Aesar Co. and used as received.

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

1,4-Diazabicyclo[2.2.2]octane (DABCO): purchased from Aldrich Chemical Co. and used as received.

1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU): purchased from Aldrich Chemical Co. and used as received.

2-Dichloromethyl-4,4,5,5-tetramethyl-[1,3,2]dioxaborolane: prepared according to previously reported procedures[4].

Diethyl bromomalonate: purchased from Alfa Aesar Co. and used as received.

Dimethyl sulfoxide: purchased from Aldrich Chemical Co. and used as received.

Iodomethane: purchased from Aldrich Chemical Co. and used as received.

Imidazolinium salt 3a and Imidazolium salt 3b: purchased from Aldrich Chemical Co. and used as received.

Imidazolinium salts 9a-g: prepared according to previously reported procedures[5].

Lithium iodide: purchased from Aldrich Chemical Co. and used as received.

Methyl chloroformate: purchased from Aldrich Chemical Co. and used as received.

***N*,*N*-Diisopropylamine:** purchased from Aldrich Chemical Co. and used as received.

***N*,*N*-Dimethylformamide:** purchased from Aldrich Chemical Co. and used as received.

Phosphines (8a-e): purchased from Strem Chemicals Inc. and used as received.

Porcine liver esterase: purchased from Aldrich Chemical Co. and used as received.

Potassium carbonate: purchased from Aldrich Chemical Co. and used as received.

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(2) Singh, R. & Ghosh, S. K. *Tetrahedron* **66**, 2284–2292 (2010).

(3) Liu, L., Sarkisian, R., Xu, Z. & Wang, H. *J. Org. Chem.* **77**, 7693–7699 (2012).

(4) Raheem, I. T., Goodman, S. N. & Jacobsen, E. N. *J. Am. Chem. Soc.* **126**, 706–707 (2004).

(5) Meng, F., McGrath, K. P. & Hoveyda, A. H. *Nature* **513**, 367–374 (2014).

Sodium borohydride: purchased from Alfa Aesar Co. and used as received.

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

Sodium hydride: purchased from Strem Chemicals Inc. and used as received.

Sodium perborate tetrahydrate: purchased from Aldrich Chemical Co. and used as received.

Sodium phenoxide: purchased from Alfa Aesar Co. and used as received.

Triethylamine: purchased from Aldrich Chemical Co. and used as received.

Imidazolinium salts 9e and 9g:

9e: IR (neat): 2954 (m), 2929 (m), 2858 (m), 1635 (s), 1471 (m), 1382 (w), 1252 (m), 1140 (m), 1032 (w), 835 (s), 782 (m), 703 (m), 558 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.01 (1H, s), 7.43–7.35 (5H, m), 6.95 (2H, s), 4.97–4.94 (1H, m), 4.27–4.07 (6H, m), 2.30 (3H, s), 2.29 (6H, s), 0.83 (9H, s), –0.02 (3H, s), –0.07 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.8, 140.7, 133.7, 130.6, 130.2, 129.7, 129.6, 127.9, 64.0, 63.3, 50.8, 48.3, 25.9, 21.2, 18.3, 17.6, –5.6, –5.7; HRMS (ESI+): Calcd for $C_{26}H_{39}N_2O_1Si_1$ $[M–PF_6]^+$: 423.28316 m/z, Found: 423.28234 m/z. Specific rotation: $[\alpha]_D^{20}$ –24.7 (*c* 1.08, acetone).

9g: IR (neat): 2953 (m), 2928 (m), 2857 (m), 1631 (s), 1598 (s), 1471 (m), 1378 (m), 1331 (m), 1289 (m), 1201 (m), 1106 (m), 1006 (w), 827 (s), 779 (s), 684 (m), 557 (s) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.66 (1H, s), 7.42–7.35 (5H, m), 6.93–6.86 (3H, m), 4.96–4.94 (1H, m), 4.37–4.32 (2H, m), 4.23–4.20 (1H, m), 4.16–4.11 (1H, m), 4.03–3.98 (2H, m), 2.31 (6H, s), 0.86 (9H, s), 0.06 (3H, s), 0.04 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 171.7, 153.6, 140.5, 135.0, 133.0, 129.6, 129.5, 128.0, 116.1, 64.5, 63.1, 48.5, 47.8, 25.8, 21.3, 18.2, –5.6, –5.7; HRMS (ESI+): Calcd for $C_{25}H_{37}N_2O_1Si_1$ $[M–PF_6]^+$: 409.26751 m/z, Found: 409.26824 m/z. Specific rotation: $[\alpha]_D^{20}$ –25.2 (*c* 1.26, acetone).

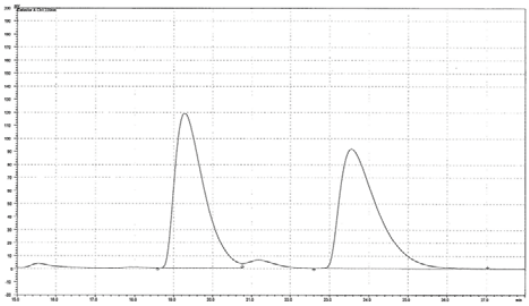
NHC–Cu-Catalyzed Enantioselective Propargyl 1,6-Conjugate; Tertiary Centers

In an N_2-filled glove box, imidazolinium salt **9b** (2.3 mg, 0.0050 mmol), CuCl (0.5 mg, 0.0050 mmol), NaO*t*-Bu (0.9 mg, 0.010 mmol) and NaOPh (17.4 mg, 0.15 mmol) and thf (0.5 mL) are added into an oven-dried vial equipped with a stirring bar. The mixture is allowed to premix for 2 h at 22 °C. The resulting mixture is then added into a separate oven-dried vial containing allenylboronic acid pinacol ester (36.0 μL, 0.20 mmol). The vial is sealed with a Teflon screw cap and removed from the glove box. The mixture is allowed to stir at 22 °C for 30 min. Dienoate **1a** (27.4 mg, 0.10 mmol) is subsequently added into the solution by a syringe, and the resulting mixture is allowed to stir at 22 °C for 16 h. The mixture is filtered through a short plug of Celite and silica gel eluting with diethyl ether. The filtrate is washed with 1M solution of aqueous NaOH, dried over $MgSO_4$ and concentrated *in vacuo*. The resulting yellow oily residue is purified by silica gel chromatography (hexanes:ethyl acetate = 20:1) to obtain **4a** (23.3 mg, 0.074 mmol, 74% yield) as colorless oil.

(*R*,*E*)-Diethyl 2-(3-phenylhex-1-en-5-yn-1-yl)malonate (4a):

IR (neat): 3288 (m), 2982 (m), 2935 (m), 1729 (s), 1601 (w), 1494 (m), 1452 (m), 1368 (m), 1266 (s), 1173 (s), 1030 (s), 970 (m), 863 (m), 700 (s), 637 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.33–7.30 (2H, m), 7.24–7.22 (3H, m), 5.94 (1H, dd, *J* = 15.0, 6.6 Hz), 5.82 (1H, dd, *J* = 15.0, 9.0 Hz), 4.23–4.18 (4H, m), 4.03 (1H, *J* = 9.0 Hz), 3.59 (1H, td, *J* = 7.2, 7.2 Hz), 2.65–2.57 (2H, m), 1.96 (1H, t, *J* = 3.0 Hz), 1.27 (3H, t, *J* = 7.2 Hz), 1.24 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.2, 168.1, 142.1, 137.6, 128.6, 127.8, 127.0, 122.9, 82.1, 70.3, 61.8, 61.7, 55.7, 47.1, 25.4, 14.2, 14.1; HRMS (ESI+): Calcd for $C_{19}H_{23}O_4$ $[M+H]^+$: 315.15963 m/z, Found: 315.16119 m/z. Specific rotation: $[\alpha]_D^{20}$ –4.7 (*c* 0.69, $CHCl_3$).

Enantiomeric purity of **4a** was determined by HPLC analysis in comparison with authentic racemic material (97.5:2.5 e.r. shown; Chiralcel OD–H column, 99.5:0.5 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm).



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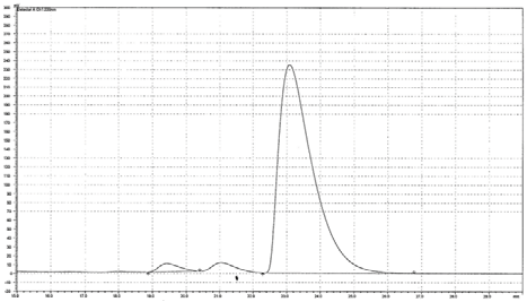

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1	19.430	410774	9605	2.437	3.928
2	23.078	16447193	234907	97.563	96.072

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	19.272	50.259	1	19.430	2.437
2	23.551	49.741	2	23.078	97.563

Determination of Stereochemical Identity:

The corresponding (*R*)-3-phenylhexan-1-ol was obtained after one-pot isomerization and retro-aldol and hydrogenation of the corresponding aldehyde **16a**. Specific rotation for (*R*)-3-phenylhexan-1-ol: $[\alpha]_D^{20}$ –6.0 (*c* 1.69, $CHCl_3$). Literature value: $[\alpha]_D^{20}$ –6.7 (*c* 2.00, $CHCl_3$)[6].

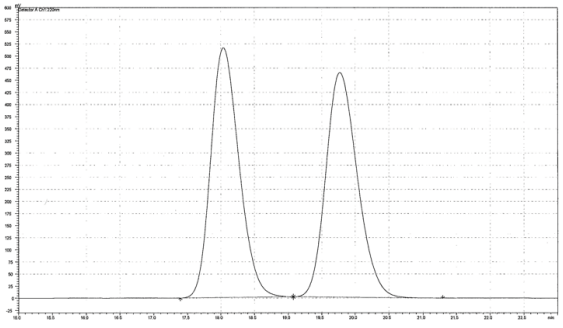
(*R*,*E*)-Diethyl 2-(3-(2-methoxyphenyl)hex-1-en-5-yn-1-yl)malonate (4b):

IR (neat): 3292 (w), 2982 (w), 2938 (w), 1729 (s), 1599 (w), 1492 (m), 1439 (m), 1240 (s), 1148 (s), 1027 (s), 970 (m), 861 (w), 754 (s), 637 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.21 (1H, td, *J* = 7.8, 1.8 Hz), 7.16 (1H, dd, *J* = 7.8, 1.8 Hz), 6.91 (1H, td, *J* = 7.8, 1.2 Hz), 6.86 (1H, dd, *J* = 7.8, 1.2 Hz), 5.99 (1H, dd, *J* = 15.6, 6.8 Hz), 5.83 (1H, dd, *J* = 15.6, 9.0 Hz), 4.20 (2H, q, *J* = 7.2 Hz), 4.17 (2H, q, *J* = 7.2 Hz), 4.03 (1H, d, *J* = 9.0 Hz), 4.00 (1H, td, *J* = 6.6, 6.6 Hz), 3.82 (3H, s), 2.62–2.60 (2H, m), 1.92 (1H, t, *J* = 3.0 Hz), 1.27 (3H, t, *J* = 7.2 Hz), 1.24 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.3, 168.2, 157.0, 137.0, 130.5, 128.4, 128.0, 122.7, 120.6, 110.8, 82.7, 69.8, 61.7, 61.6, 55.8, 55.5,

(6) Reyes, E., Vicario, J. L., Carrillo, L., Badía, D., Uria, U. & Iza, A. *J. Org. Chem.* **71**, 7763–7772 (2006).

40.9, 23.9, 14.2, 14.1; HRMS (ESI+): Calcd for $C_{20}H_{25}O_5$ $[M+H]^+$: 345.17020 m/z, Found: 345.17007 m/z. Specific rotation: $[\alpha]_D^{20}$ –3.9 (*c* 1.69, $CHCl_3$).

Enantiomeric purity of **4b** was determined by HPLC analysis in comparison with authentic racemic material (97:3 e.r. shown; Chiralcel OZ–H column, 99:1 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm).



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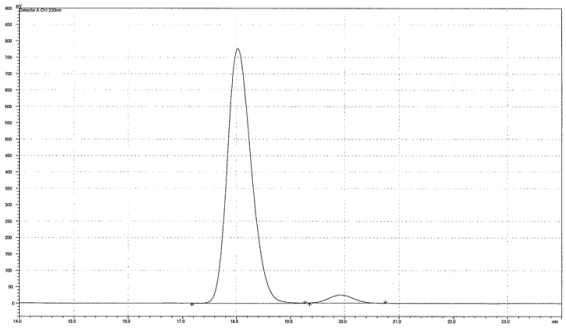
2	19.769	15166318	464026	49.989	47.372



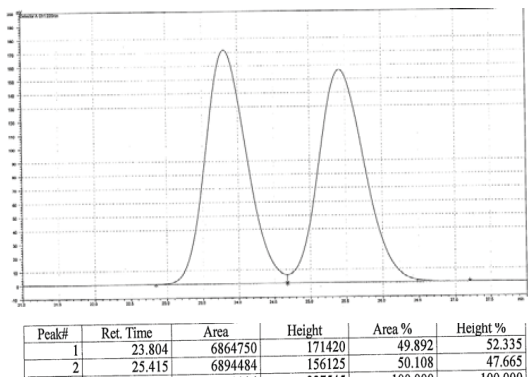
Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.023	23841299	777595	96.791	96.936
2	19.925	790436	24583	3.209	3.064

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	18.035	50.011	1	18.023	96.791
2	19.769	49.989	2	19.925	3.209

(*R*,*E*)-Diethyl 2-(3-(*o*-tolyl)hex-1-en-5-yn-1-yl)malonate (4c):

IR (neat): 3288 (m), 2982 (m), 2937 (m), 1729 (s), 1463 (m), 1368 (m), 1265 (s), 1148 (s), 1096 (m), 1029 (s), 970 (m), 863 (m), 757 (m), 638 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.19–7.11 (4H, m), 5.86 (1H, dd, *J* = 15.6, 6.8 Hz), 5.75 (1H, dd, *J* = 15.6, 8.8 Hz), 4.20 (2H, q, *J* = 6.8 Hz), 4.17 (2H, q, *J* = 6.8 Hz), 4.01 (1H, d, *J* = 8.8 Hz), 3.85 (1H, td, *J* = 6.8, 7.2 Hz), 2.63–2.59 (2H, m), 2.35 (3H, s), 1.95 (1H, t, *J* = 2.8 Hz), 1.27 (3H, t, *J* = 6.8 Hz), 1.23 (3H, t, *J* = 6.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.2, 168.1, 140.1, 137.4, 136.2, 130.7, 126.8, 126.5, 126.4, 122.8, 82.3, 70.0, 61.8, 61.7, 55.7, 42.8, 24.5, 19.7, 14.2, 14.1; HRMS (ESI+): Calcd for $C_{20}H_{25}O_4$ $[M+H]^+$: 329.17528 m/z, Found: 329.17450 m/z. Specific rotation: $[\alpha]_D^{20}$ –11.0 (*c* 1.36, $CHCl_3$).

Enantiomeric purity of **4c** was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OZ–H column, 99.5:0.5 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm).



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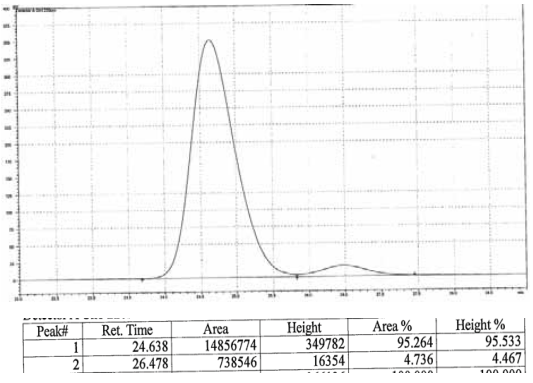


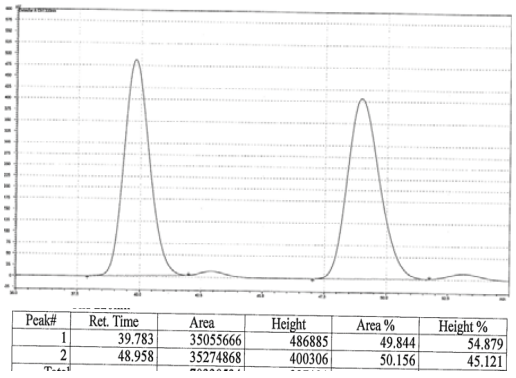
Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.638	14856774	349782	95.264	95.533
2	26.478	738546	16354	4.736	4.467

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	23.804	49.892	1	24.638	95.264
2	25.415	50.108	2	26.478	4.736

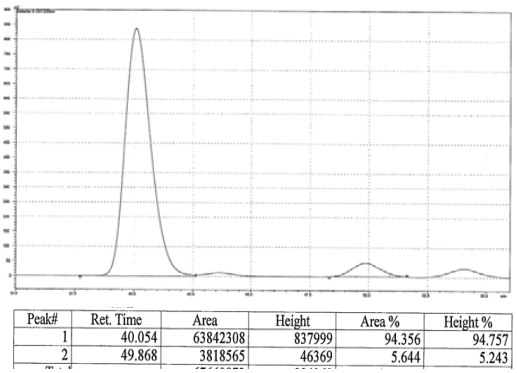
(*R*,*E*)-Diethyl 2-(3-(naphthalen-1-yl)hex-1-en-5-yn-1-yl)malonate (4d):

IR (neat): 3293 (w), 2982 (w), 2935 (w), 1728 (s), 1368 (m), 1258 (m), 1173 (m), 1095 (m), 1030 (m), 971 (m), 861 (w), 779 (s), 639 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.08 (1H, d, *J* = 8.4 Hz), 7.87 (1H, d, *J* = 8.8 Hz), 7.76 (1H, d, *J* = 8.0 Hz), 7.54–7.39 (4H, m), 6.07 (1H, dd, *J* = 15.6, 6.8 Hz), 5.90 (1H, dd, *J* = 15.6, 8.8 Hz), 4.46 (1H, td, *J* = 6.8, 6.4 Hz), 4.20 (2H, q, *J* = 7.2 Hz), 4.16 (2H, q, *J* = 7.2 Hz), 4.06 (1H, d, *J* = 8.8 Hz), 2.80–2.77 (2H, m), 1.98 (1H, t, *J* = 2.8 Hz), 1.26 (3H, t, *J* = 7.2 Hz), 1.21 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.2, 168.1, 138.0, 137.4, 134.1, 131.4, 129.1, 127.7, 126.2, 125.7, 125.5, 124.5, 123.4, 123.3, 82.3, 70.5, 61.8, 61.7, 55.8, 42.2, 24.8, 14.2, 14.1; HRMS (ESI+): Calcd for $C_{23}H_{25}O_4$ $[M+H]^+$: 365.17528 m/z, Found: 365.17471 m/z. Specific rotation: $[\alpha]_D^{20}$ +23.8 (*c* 1.81, $CHCl_3$).

Enantiomeric purity of **4d** was determined by HPLC analysis in comparison with authentic racemic material (94:6 e.r. shown; Chiralcel OZ–H column, 99.5:0.5 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	39.783	35055666	486885	49.844	54.879
2	48.958	35274868	400306	50.156	45.121



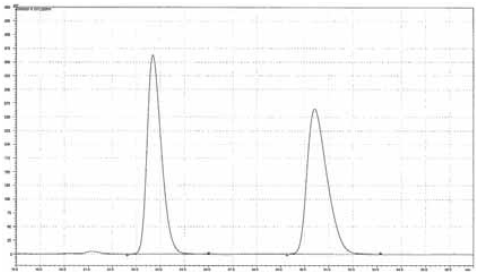
Peak#	Ret. Time	Area	Height	Area %	Height %
1	40.054	63842308	837999	94.356	94.757
2	49.868	3818565	46369	5.644	5.243

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	39.783	49.844	1	40.054	94.356
2	48.958	50.156	2	49.868	5.644

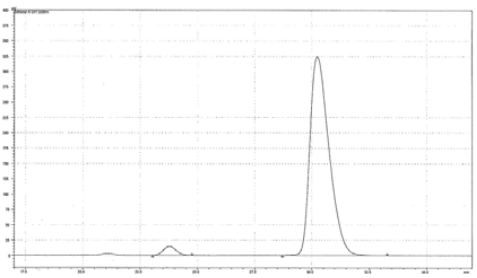
(*R*,*E*)-Diethyl 2-(3-(4-methoxyphenyl)hex-1-en-5-yn-1-yl)malonate (4e):

IR (neat): 3286 (m), 2982 (m), 2935 (m), 1728 (s), 1610 (m), 1512 (s), 1464 (m), 1246 (s), 1176 (s), 1096 (m), 1030 (s), 971 (m), 830 (m), 640 (m), 545 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.14 (2H, d, *J* = 8.4 Hz), 6.85 (2H, d, *J* = 8.4 Hz), 5.91 (1H, dd, *J* = 15.6, 7.2 Hz), 5.78 (1H, dd, *J* = 15.6, 8.4 Hz), 4.20 (2H, q, *J* = 7.2 Hz), 4.18 (2H, q, *J* = 7.2 Hz), 4.02 (1H, d, *J* = 8.4 Hz), 3.79 (3H, s), 3.55 (1H, td, *J* = 7.2, 6.8 Hz), 2.60–2.56 (2H, m), 1.95 (1H, t, *J* = 2.8 Hz), 1.27 (3H, t, *J* = 7.2 Hz), 1.25 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.3, 168.2, 158.6, 138.0, 134.1, 128.7, 122.6, 114.0, 82.3, 70.3, 61.8, 61.7, 55.7, 55.4, 46.2, 25.5, 14.2, 14.1; HRMS (ESI+): Calcd for $C_{20}H_{25}O_5$ $[M+H]^+$: 345.17020 m/z, Found: 345.17107 m/z. Specific rotation: $[\alpha]_D^{20}$ –10.0 (*c* 1.24, $CHCl_3$).

Enantiomeric purity of **4e** was determined by HPLC analysis in comparison with authentic racemic material (97:3 e.r. shown; Chiralcel OZ–H column, 98.5:1.5 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.684	15096524	362409	49.975	57.796
2	30.414	15111662	264640	50.025	42.204



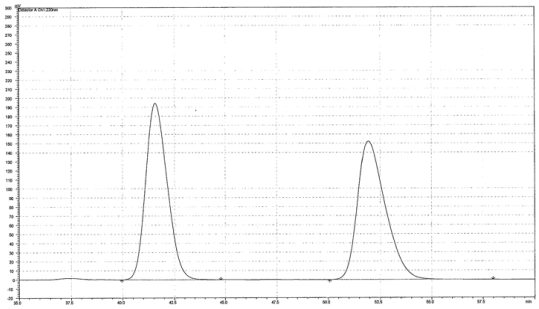
Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.772	574518	14902	2.990	4.399
2	30.233	18642376	323885	97.010	95.601

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	23.684	49.975	1	23.772	2.990
2	30.414	50.025	2	30.233	97.010

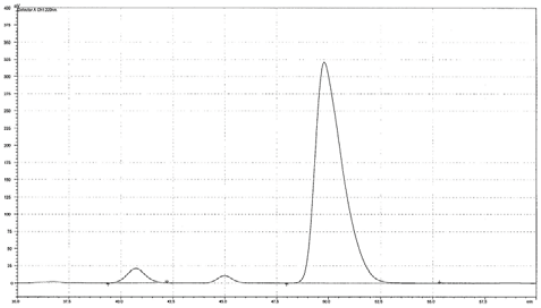
(*R*,*E*)-Diethyl 2-(3-(4-bromophenyl)hex-1-en-5-yn-1-yl)malonate (4f):

IR (neat): 3297 (w), 2982 (w), 2935 (w), 1728 (s), 1488 (m), 1368 (m), 1264 (m), 1150 (m), 1030 (m), 971 (m), 822 (m), 642 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.43 (2H, d, *J* = 8.4 Hz), 7.11 (2H, d, *J* = 8.4 Hz), 5.89 (1H, dd, *J* = 15.0, 7.2 Hz), 5.79 (1H, dd, *J* = 15.0, 9.0 Hz), 4.21 (2H, q, *J* = 7.2 Hz), 4.18 (2H, q, *J* = 7.2 Hz), 4.02 (1H, d, *J* = 9.0 Hz), 3.55 (1H, td, *J* = 6.6, 7.2 Hz), 2.61 (1H, ddd, *J* = 16.8, 7.2, 2.4 Hz), 1.95 (1H, t, *J* = 2.4 Hz), 1.27 (3H, t, *J* = 7.2 Hz), 1.24 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.1, 168.0, 141.0, 137.1, 131.7, 129.6, 123.4, 120.9, 81.6, 70.7, 61.9, 61.8, 55.6, 46.5, 25.2, 14.2, 14.1; HRMS (ESI+): Calcd for $C_{19}H_{22}Br_1O_4$ $[M+H]^+$: 393.07015 m/z, Found: 393.06864 m/z. Specific rotation: $[\alpha]_D^{20}$ –11.9 (*c* 1.80, $CHCl_3$).

Enantiomeric purity of **4f** was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OZ–H column, 99.5:0.5 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	41.563	14035442	194262	49.971	56.045
2	51.939	14051794	152358	50.029	43.955



Peak#	Ret. Time	Area	Height	Area %	Height %
1	40.713	1273265	20462	4.156	5.996
2	49.791	29364916	320785	95.844	94.004

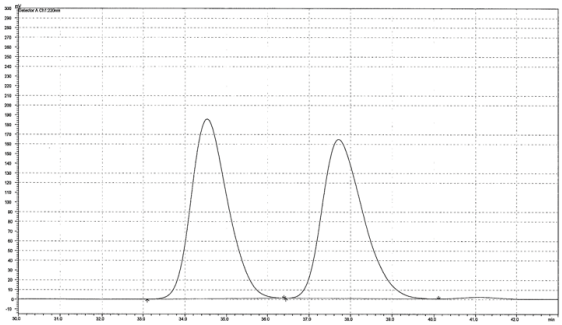
Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	41.563	49.971	1	40.713	4.156
2	51.939	50.029	2	49.791	95.844

(*R*,*E*)-Diethyl 2-(3-(4-(trifluoromethyl)phenyl)hex-1-en-5-yn-1-yl)malonate (4g):

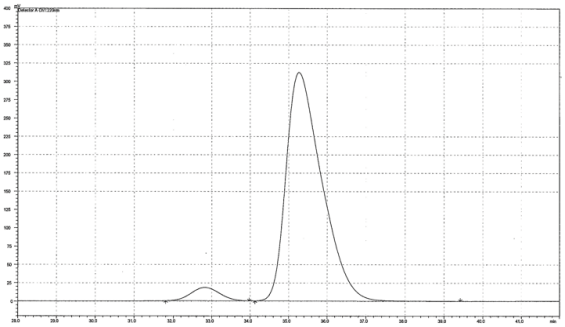
IR (neat): 3299 (w), 2984 (w), 2940 (w), 1730 (s), 1619 (w), 1447 (w), 1324 (s), 1269 (m), 1161 (s), 1113 (s), 1067 (s), 1018 (s), 971 (m), 837 (m), 638 (m), 606 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.57 (2H, d, *J* = 8.0 Hz), 7.35 (2H, d, *J* = 8.0 Hz), 5.92 (1H, dd, *J* = 15.6, 6.8 Hz), 5.82 (1H, dd, *J* = 15.6, 8.4 Hz), 4.24–4.16 (4H, m), 4.03 (1H, d, *J* = 8.4 Hz), 2.66 (1H, ddd, *J* = 16.8, 7.2, 2.8 Hz), 1.96

(1H, t, *J* = 2.8 Hz), 1.27 (3H, t, *J* = 6.8 Hz), 1.24 (3H, t, *J* = 6.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.1, 168.0, 146.0, 136.7, 129.3 (q, *J* = 32.6 Hz), 127.9, 125.6 (q, *J* = 3.8 Hz), 124.3 (q, *J* = 270.2 Hz), 123.8, 81.4, 70.9, 61.9, 61.8, 55.6, 46.8, 25.2, 14.2, 14.1; HRMS (ESI+): Calcd for $C_{20}H_{22}F_3O_4$ $[M+H]^+$: 383.14702 m/z, Found: 383.14610 m/z. Specific rotation: $[\alpha]_D^{20}$ –9.5 (*c* 2.16, $CHCl_3$).

Enantiomeric purity of **4g** was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OZ–H column, 99.5:0.5 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	34.527	11307932	185229	50.175	53.039
2	37.702	11228926	164005	49.825	46.961



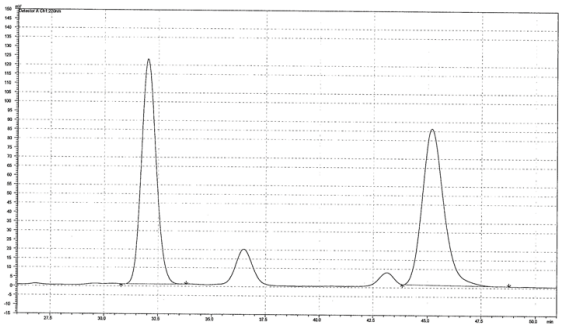
Peak#	Ret. Time	Area	Height	Area %	Height %
1	32.815	874585	17574	4.170	5.334
2	35.266	20098864	311865	95.830	94.666

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	34.527	50.175	1	32.815	4.170
2	37.702	49.825	2	35.266	95.830

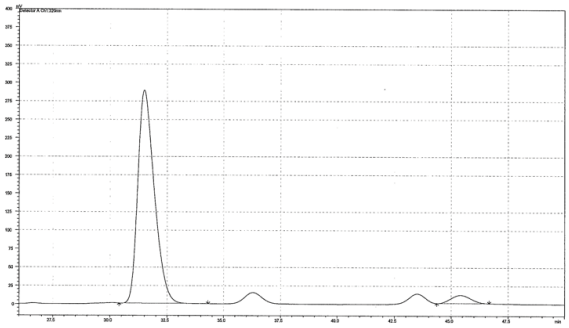
(*R*,*E*)-Diethyl 2-(3-(furan-3-yl)hex-1-en-5-yn-1-yl)malonate (4h):

IR (neat): 3291 (w), 2982 (w), 2936 (w), 1729 (s), 1465 (w), 1368 (m), 1252 (m), 1174 (m), 1113 (m), 1030 (m), 970 (m), 862 (w), 784 (m), 648 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.28–7.26 (1H, m), 7.08–7.07 (1H, m), 7.00–6.98 (1H, m), 5.90 (1H, dd, *J* = 15.6, 7.2 Hz), 5.82 (1H, dd, *J* = 15.6, 8.4 Hz), 4.21 (2H, q, *J* = 7.2 Hz), 4.20 (2H, q, *J* = 7.2 Hz), 4.03 (1H, d, *J* = 8.4 Hz), 3.69 (1H, td, *J* = 7.2, 6.8 Hz), 2.62–2.59 (2H, m), 1.98 (1H, t, *J* = 2.8 Hz), 1.27 (3H, t, *J* = 7.2 Hz), 1.26 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.21, 168.19, 142.7, 137.3, 127.2, 125.8, 123.1, 121.0, 82.0, 70.5, 61.8, 55.6, 42.7, 25.2, 14.18, 14.16; HRMS (ESI+): Calcd for $C_{17}H_{21}O_5$ $[M+H]^+$: 305.13890 m/z, Found: 305.13793 m/z. Specific rotation: $[\alpha]_D^{20}$ –30.6 (*c* 1.01, $CHCl_3$).

Enantiomeric purity of **4h** was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OJ–H column, 98.5:1.5 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	32.014	5777857	122124	49.710	58.999
2	45.177	5845352	84869	50.290	41.001



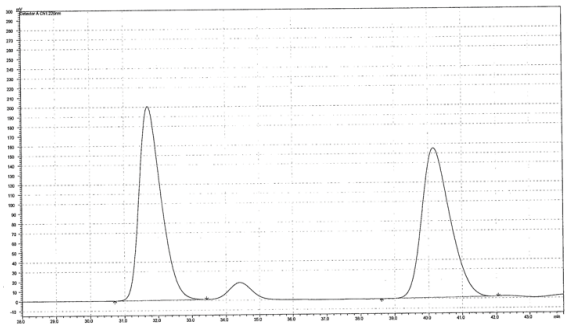
Peak#	Ret. Time	Area	Height	Area %	Height %
1	31.489	14372396	288383	95.638	96.339
2	45.411	655568	10958	4.362	3.661

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	32.014	49.710	1	31.489	95.638
2	45.177	50.290	2	45.411	4.362

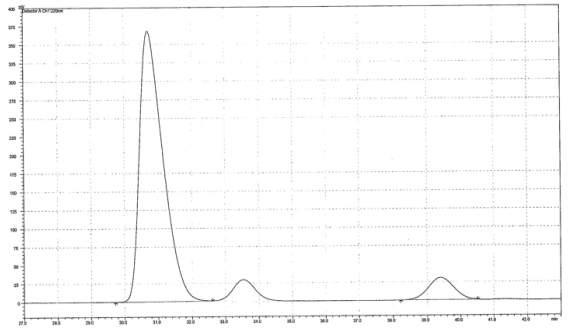
(*R*,*E*)-Diethyl 2-(3-(thiophen-3-yl)hex-1-en-5-yn-1-yl)malonate (4i):

IR (neat): 3293 (w), 2983 (w), 2937 (w), 1728 (s), 1505 (w), 1369 (m), 1259 (m), 1152 (s), 1113 (m), 1069 (m), 1026 (s), 969 (m), 876 (m), 790 (m), 731 (m), 639 (m), 600 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.36–7.35 (1H, m), 7.30–7.29 (1H, m), 6.32–6.31 (1H, m), 5.88–5.78 (2H, m), 4.20 (2H, q, *J* = 7.2 Hz), 4.19 (2H, q, *J* = 7.2 Hz), 4.03 (1H, d, *J* = 7.6 Hz), 3.50 (1H, td, *J* = 6.4, 6.4 Hz), 2.54–2.51 (2H, m), 1.98 (1H, t, *J* = 2.8 Hz), 1.27 (3H, t, *J* = 7.2 Hz), 1.26 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.2, 143.1, 139.3, 137.0, 126.1, 123.2, 110.0, 81.9, 70.4, 61.8, 55.5, 38.2, 24.9, 14.2; HRMS (ESI+): Calcd for $C_{17}H_{21}O_4S_1$ $[M+H]^+$: 321.11605 m/z, Found: 321.11658 m/z. Specific rotation: $[\alpha]_D^{20}$ –21.2 (*c* 1.97, $CHCl_3$).

Enantiomeric purity of **4i** was determined by HPLC analysis in comparison with authentic racemic material (92:8 e.r. shown; Chiralcel OJ–H column, 99:1 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	31.705	9047214	200145	50.286	56.440
2	40.151	8944392	154471	49.714	43.560



Peak#	Ret. Time	Area	Height	Area %	Height %
1	30.710	17708934	367655	91.707	92.439
2	39.398	1601337	30071	8.293	7.561

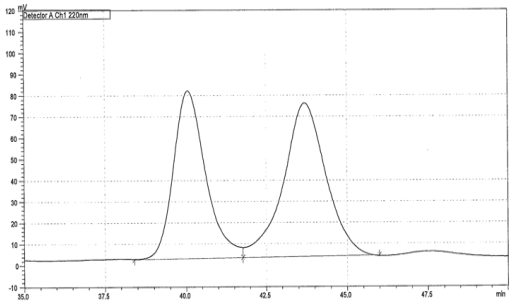
Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	31.705	50.286	1	30.710	91.707
2	40.151	49.714	2	39.398	8.293

(*R*,*E*)-Diethyl 2-((*R*,*E*)-3-((*E*)-styryl)hex-1-en-5-yn-1-yl)malonate (4j):

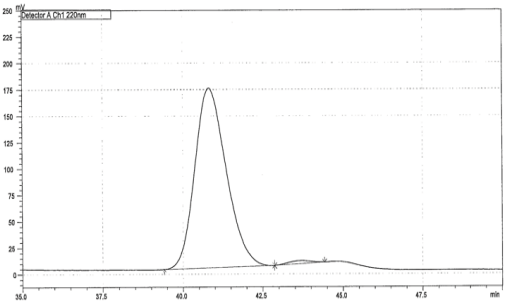
IR (neat): 3292 (m), 2982 (m), 2935 (w), 1732 (s), 1598 (w), 1391 (m), 1248 (m), 1174 (m), 1020 (m), 969 (m), 863 (w), 750 (m), 694 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.38–7.35 (2H, m), 7.32–7.28

(2H, m), 7.24–7.20 (1H, m), 6.45 (1H, d, *J* = 16.0 Hz), 6.20 (1H, dd, *J* = 16.0, 7.2 Hz), 5.88–5.77 (2H, m), 4.21 (4H, q, *J* = 7.2 Hz), 4.05 (1H, d, *J* = 8.0 Hz), 3.22–3.15 (1H, m), 2.45–2.42 (2H, m), 2.01 (1H, t, *J* = 2.4 Hz), 1.28 (3H, t, *J* = 7.2 Hz), 1.27 (3H, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.2, 137.2, 137.0, 131.3, 130.3, 128.7, 127.5, 126.4, 123.1, 81.8, 70.4, 61.8, 55.7, 44.4, 24.7, 14.2; HRMS (ESI+): Calcd for $C_{21}H_{25}O_4$ $[M+H]^+$: 341.17528 m/z, Found: 341.17565 m/z. Specific rotation: $[\alpha]_D^{20}$ –31.7 (*c* 0.65, $CHCl_3$).

Enantiomeric purity of **4j** was determined by HPLC analysis in comparison with authentic racemic material (99:1 e.r. shown; Chiralcel OJ–H column, 94:6 hexanes/*i*-PrOH, 0.6 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Conc.
1	40.058	6072150	79286	49.239
2	43.698	6259807	72845	50.761



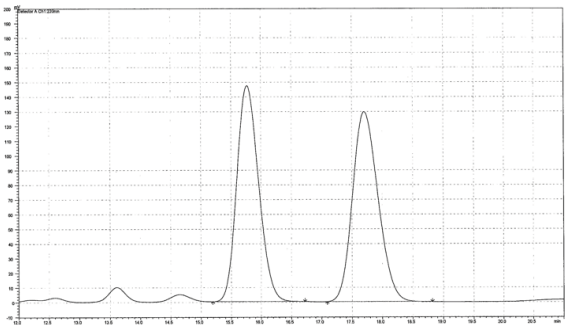
Peak#	Ret. Time	Area	Height	Conc.
1	40.828	11703471	170373	98.834
2	43.694	138083	2862	1.166

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	40.058	49.239	1	40.828	98.834
2	43.698	50.761	2	43.694	1.166

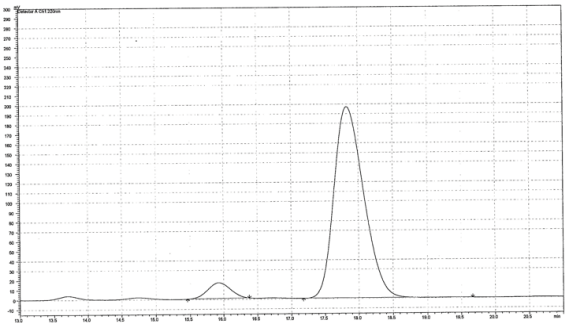
(*R*,*E*)-Diethyl 2-(3-phenethylhex-1-en-5-yn-1-yl)malonate (4k):

IR (neat): 3286 (w), 2982 (w), 2934 (w), 1730 (s), 1454 (w), 1368 (m), 1262 (m), 1147 (s), 1113 (m), 1030 (s), 971 (m), 862 (w), 748 (m), 700 (m), 639 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.30–7.26 (2H, m), 7.20–7.17 (3H, m), 5.79 (1H, dd, *J* = 15.6, 8.4 Hz), 5.63 (1H, dd, *J* = 15.6, 8.4 Hz), 4.23 (2H, q, *J* = 7.2 Hz), 4.22 (2H, q, *J* = 7.2 Hz), 4.04 (1H, d, *J* = 8.8 Hz), 2.70–2.62 (1H, m), 2.60–2.51 (1H, m), 2.35–2.27 (3H, m), 1.97 (1H, t, *J* = 2.4 Hz), 1.94–1.85 (1H, m), 1.76–1.67 (1H, m), 1.28 (6H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.4, 168.3, 142.1, 138.5, 128.6, 128.5, 125.9, 123.2, 82.0, 70.0, 61.8, 61.7, 55.8, 40.8, 35.3, 33.3, 24.5, 14.21, 14.19; HRMS (ESI+): Calcd for $C_{21}H_{27}O_4$ $[M+H]^+$: 343.19093 m/z, Found: 343.19021 m/z. Specific rotation: $[\alpha]_D^{20}$ +7.8 (*c* 1.26, $CHCl_3$).

Enantiomeric purity of **4k** was determined by HPLC analysis in comparison with authentic racemic material (94:6 e.r. shown; Chiralcel OZ–H column, 99.5:0.5 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.762	3725084	146976	49.610	53.241
2	17.699	3783631	129081	50.390	46.759



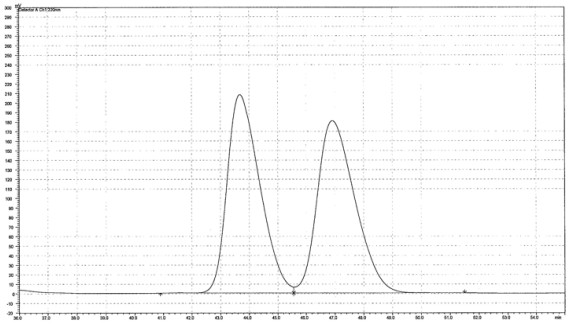
Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.923	369836	15984	5.831	7.517
2	17.826	5972981	196652	94.169	92.483

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	15.762	49.610	1	15.923	5.831
2	17.699	50.390	2	17.826	94.169

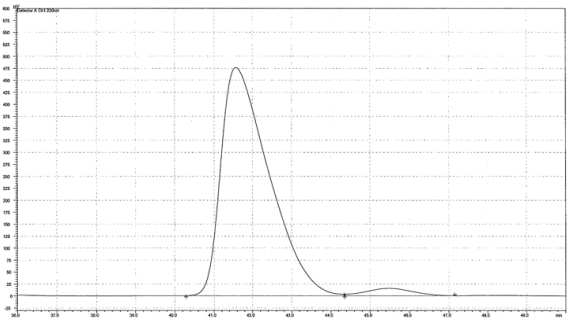
(*S*,*E*)-Diethyl 2-(3-cyclohexylhex-1-en-5-yn-1-yl)malonate (4l):

IR (neat): 3288 (w), 2982 (w), 2924 (m), 2852 (m), 1732 (s), 1448 (m), 1368 (m), 1265 (m), 1148 (m), 1032 (m), 972 (m), 862 (w), 630 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 5.70 (1H, dd, *J* = 15.2, 8.4 Hz), 5.59 (1H, dd, *J* = 15.2, 8.8 Hz), 4.19 (4H, q, *J* = 7.6 Hz), 4.00 (1H, d, *J* = 8.8 Hz), 2.30–2.26 (2H, m), 2.09–2.02 (1H, m), 1.93 (1H, t, *J* = 2.8 Hz), 1.76–1.62 (5H, m), 1.49–1.40 (1H, m), 1.26 (3H, t, *J* = 7.2 Hz), 1.25 (3H, t, *J* = 7.2 Hz), 1.22–1.06 (3H, m), 1.00–0.80 (2H, m); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.5, 168.4, 137.7, 123.0, 82.7, 69.7, 61.7, 61.6, 55.8, 47.2, 40.0, 31.0, 29.8, 26.6, 26.53, 26.46, 21.7, 14.2; HRMS (ESI+): Calcd for $C_{19}H_{29}O_4$ $[M+H]^+$: 321.20658 m/z, Found: 321.20727 m/z. Specific rotation: $[\alpha]_D^{20}$ +4.7 (*c* 1.53, $CHCl_3$).

Enantiomeric purity of **4l** was determined by HPLC analysis in comparison with authentic racemic material (97:3 e.r. shown; Chiralcel OZ–H column, 99.6:0.4 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	43.676	16409594	207685	50.166	53.523
2	46.912	16301064	180344	49.834	46.477



Peak#	Ret. Time	Area	Height	Area %	Height %
1	41.569	41059492	476161	96.996	96.849
2	45.483	1271710	15491	3.004	3.151

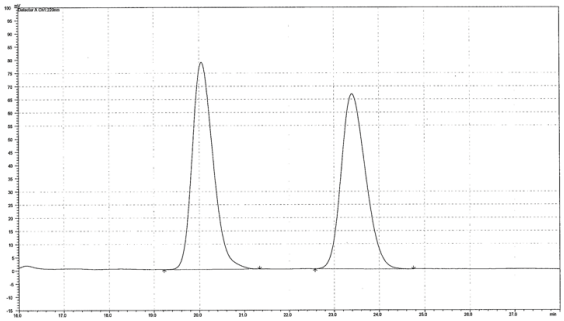
Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	43.676	50.166	1	41.569	96.996
2	46.912	49.834	2	45.483	3.004

(*R*,*E*)-Diethyl 2-(3-(*tert*-butyl)hex-1-en-5-yn-1-yl)malonate (4m):

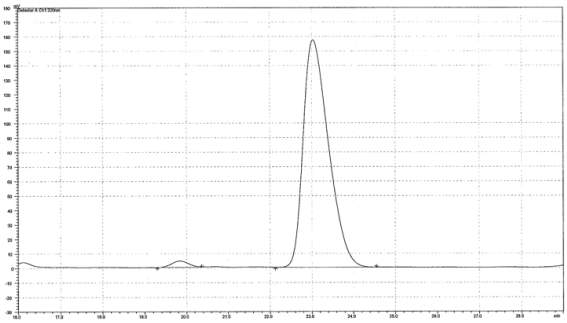
IR (neat): 3289 (w), 2962 (m), 2872 (w), 1733 (s), 1468 (w), 1368 (m), 1260 (m), 1148 (m), 1033 (m), 971 (m), 862 (w), 628 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 5.75 (1H, dd, *J* = 15.6, 8.8 Hz), 5.57 (1H, dd, *J* = 15.6, 8.8 Hz), 4.19 (4H, q, *J* =7.2 Hz), 4.03 (1H, d, *J* = 8.8 Hz), 2.41 (1H, dt, *J* = 15.6, 2.8

Hz), 2.13–2.00 (2H, m), 1.89 (1H, t, J = 2.8 Hz), 1.26 (3H, t, J = 7.2 Hz), 1.25 (3H, t, J = 7.2 Hz), 0.88 (9H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.5, 168.4, 136.2, 124.2, 83.7, 69.5, 61.7, 61.6, 55.8, 52.6, 33.3, 27.7, 19.6, 14.2; HRMS (ESI+): Calcd for $C_{17}H_{27}O_4$ $[M+H]^+$: 295.19093 m/z, Found: 295.19175 m/z. Specific rotation: $[\alpha]_D^{20}$ –2.3 (*c* 1.49, $CHCl_3$).

Enantiomeric purity of **4m** was determined by HPLC analysis in comparison with authentic racemic material (98:2 e.r. shown; Chiralcel OZ–H column, 99.6:0.4 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.048	2524539	78646	50.148	54.186
2	23.399	2509688	66496	49.852	45.814

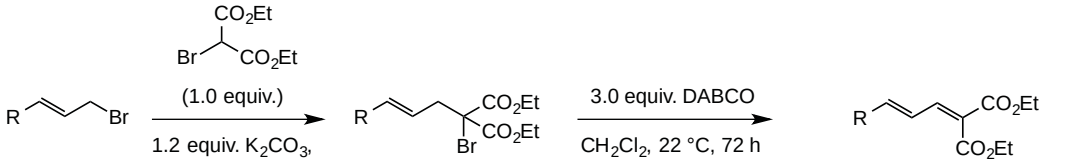


Peak#	Ret. Time	Area	Height	Area %	Height %
1	19.832	125019	4329	1.840	2.682
2	23.031	6668277	157079	98.160	97.318

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	20.048	50.148	1	19.832	1.840
2	23.399	49.852	2	23.031	98.160

Synthesis of Alkyl-Substituted Dienoates

Scheme S1: Preparation of Alkyl-Substituted Dienoates



S1, R = $PhCH_2CH_2$, 95% yield;
S2, R = Cy, >98% yield;
S3, R = *t*-Bu, 93% yield

S4, R = $PhCH_2CH_2$, 82% yield based on rec. s. m.;
S5, R = Cy, 66% yield based on rec. s. m.;
S6, R = *t*-Bu, 80% yield based on rec. s. m.

Representative Procedure for Alkylation of Diethyl Bromomalonate

To a solution of allyl bromide[7] (4.00 g, 17.8 mmol) and diethyl bromomalonate (2.10 mL, 14.8 mmol) in *N*,*N*'-dimethylformamide (DMF, 30 mL) was added K_2CO_3 (2.25 g, 16.3 mmol) at 22 °C. The mixture was allowed to stir at 22 °C for 16 h, after which water (20 mL) and diethyl ether (30 mL) was added to quench the reaction. The aqueous layer was washed with diethyl ether (2 × 30 mL), and the combined organic layers were washed with a solution of brine (2 × 30 mL), dried over $MgSO_4$ and concentrated under vacuum. The resulting colorless oil was purified by silica gel column

(7) Fañanás-Mastral, M., Pérez, M., Bos, P. H., Rudolph, A., Harutyunyan, S. R. & Feringa, B. L. *Angew. Chem. Int. Edn* **51**, 1922–1925 (2012).

chromatography (hexanes:ethyl acetate = 50:1) to afford 5.44 g **S1** (14.2 mmol, 95% yield) as colorless oil.

(*E*)-Diethyl 2-bromo-2-(5-phenylpent-2-en-1-yl)malonate (S1):

IR (neat): 2983 (w), 2936 (w), 1739 (s), 1454 (m), 1367 (m), 1233 (s), 1191 (m), 1096 (m), 1030 (m), 969 (m), 857 (m), 746 (m), 698 (m), 650 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.30–7.26 (2H, m), 7.20–7.16 (3H, m), 5.65 (1H, dt, *J* = 15.6, 6.4 Hz), 5.48 (1H, dt, *J* = 15.6, 6.8 Hz), 4.26 (4H, q, *J* = 7.2 Hz), 2.99 (2H, d, *J* = 6.8 Hz), 2.69–2.65 (2H, m), 2.34 (2H, dt, *J* = 7.6, 7.2 Hz), 1.28 (6H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ166.7, 141.7, 135.9, 128.5, 128.4, 125.9, 123.4, 63.0, 62.7, 41.7, 35.8, 34.4, 14.0; HRMS (ESI+): Calcd for $C_{18}H_{24}Br_1O_4$ $[M+H]^+$: 383.08580 m/z, Found: 383.08507 m/z.

(*E*)-Diethyl 2-bromo-2-(3-cyclohexylallyl)malonate (S2):

IR (neat): 2981 (w), 2923 (m), 2851 (m), 1741 (s), 1447 (m), 1367 (w), 1232 (s), 1187 (m), 1095 (m), 1022 (m), 971 (m), 858 (m), 649 (w) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 5.52 (1H, dd, *J* = 15.2, 6.4 Hz), 5.37 (1H, dt, *J* = 15.2, 7.2 Hz), 4.24 (4H, q, *J* = 7.2 Hz), 2.94 (2H, d, *J* = 7.2 Hz), 1.97–1.88 (1H, m), 1.72–1.60 (6H, m), 1.27 (6H, t, *J* = 7.2 Hz), 1.25–0.97 (5H, m); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.7, 142.8, 120.2, 63.0, 41.8, 40.9, 32.9, 26.2, 26.0, 14.0; HRMS (ESI+): Calcd for $C_{16}H_{26}Br_1O_4$ $[M+H]^+$: 361.10145 m/z, Found: 361.10139 m/z.

(*E*)-Diethyl 2-bromo-2-(4,4-dimethylpent-2-en-1-yl)malonate (S3):

IR (neat): 2959 (m), 2867 (w), 1741 (s), 1446 (w), 1365 (m), 1256 (s), 1175 (s), 1095 (m), 1022 (m), 974 (m), 858 (m), 650 (w) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 5.60 (1H, d, *J* = 15.6 Hz), 5.32 (1H, dt, *J* = 15.6, 7.2 Hz), 4.24 (4H, q, *J* = 7.2 Hz), 2.95 (2H, d, *J* = 7.2 Hz), 1.28 (3H, t, *J* = 7.2 Hz), 0.98 (9H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.7, 147.8, 117.5, 63.00, 62.96, 41.8, 33.3, 29.5, 14.1; HRMS (ESI+): Calcd for $C_{14}H_{24}Br_1O_4$ $[M+H]^+$: 335.08580 m/z, Found: 335.08415 m/z.

Representative Procedure for Elimination of Bromo-malonates

To a solution of bromo-malonate **S1** (5.44 g, 14.2 mmol) in CH_2Cl_2 (50 mL) was added 1,4-diazabicyclo[2.2.2]octane (DABCO) (2.39 g, 21.3 mmol) at 22 °C. The solution was allowed to stir at 22 °C for 72 h. Water (30 mL) was then added to quench the reaction, and the aqueous layer was washed with CH_2Cl_2 (2 × 30 mL). The combined organic layers were dried over $MgSO_4$ and concentrated under vacuum. The resulting yellow oil was purified by silica gel column chromatography (hexanes:ethyl acetate = 30:1 to 10:1) to afford 885 mg **S4** (2.9 mmol, 21% yield) and 4.07g of recovered **S1** (10.6 mmol, 75% yield) as yellow oil.

(*E*)-Diethyl 2-(5-phenylpent-2-en-1-ylidene)malonate (S4):

IR (neat): 2983 (w), 2937 (w), 1715 (s), 1636 (m), 1454 (m), 1241 (s), 1211 (s), 1094 (m), 1025 (m), 982 (w), 748 (m), 700 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.32–7.27 (3H, m), 7.22–7.16 (3H, m), 6.54 (1H, dd, *J* = 15.2, 11.6 Hz), 6.32 (1H, dt, *J* = 15.2, 7.2 Hz), 4.31 (2H, q, *J* = 7.2 Hz), 4.25 (2H, q, *J* = 7.2 Hz), 2.78–2.75 (2H, m), 2.57–2.52 (2H, m), 1.33 (3H, t, *J* = 7.2 Hz), 1.30 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.5, 164.9, 148.2, 145.2, 141.0, 128.6, 128.5, 126.4, 126.3, 124.3, 61.39,

61.36, 35.1, 35.0, 14.31, 14.29; HRMS (ESI+): Calcd for $C_{18}H_{23}O_4$ $[M+H]^+$: 303.15963 m/z, Found: 303.16021 m/z.

(*E*)-Diethyl 2-(3-cyclohexylallylidene)malonate (S5):

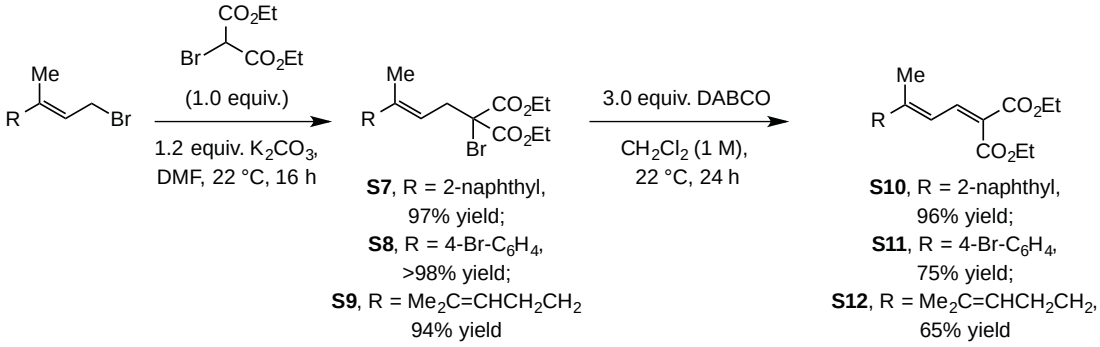
IR (neat): 2982 (m), 2925 (m), 2852 (m), 1712 (s), 1632 (m), 1448 (m), 1377 (m), 1239 (s), 1122 (m), 1025 (s), 982 (m), 862 (m), 734 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.32 (1H, d, *J* = 11.2 Hz), 6.48 (1H, ddd, *J* = 15.2, 11.2, 1.2 Hz), 6.25 (1H, dd, *J* = 15.2, 6.8 Hz), 4.32 (2H, q, *J* = 7.2 Hz), 4.24 (2H, q, *J* = 7.2 Hz), 2.18–2.11 (1H, m), 1.79–1.62 (5H, m), 1.34 (3H, t, *J* = 7.2 Hz), 1.29 (3H, t, *J* = 7.2 Hz), 1.25–1.08 (6H, m); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.6, 165.0, 155.1, 146.1, 123.8, 123.4, 61.31, 61.28, 41.6, 32.2, 26.1, 25.8, 14.35, 14.31; HRMS (ESI+): Calcd for $C_{16}H_{25}O_4$ $[M+H]^+$: 281.17528 m/z, Found: 281.17653 m/z.

(*E*)-Diethyl 2-(4,4-dimethylpent-2-en-1-ylidene)malonate (S6):

IR (neat): 2962 (m), 2904 (w), 2870 (w), 1715 (s), 1632 (m), 1463 (m), 1366 (m), 1235 (s), 1195 (s), 1144 (m), 1060 (s), 1030 (m), 985 (m), 865 (w), 799 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.34 (1H, d, *J* = 11.2 Hz), 6.46 (1H, dd, *J* = 15.6, 11.6 Hz), 6.31 (1H, d, *J* = 15.2 Hz), 4,33 (2H, q, *J* = 7.2 Hz), 4.24 (2H, q, *J* = 7.2 Hz), 1.34 (3H, t, *J* = 7.2 Hz), 1.30 (3H, t, *J* = 7.2 Hz), 1.07 (9H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.6, 165.0, 160.0, 146.3, 124.0, 120.9, 61.3, 34.5, 29.0, 14.35, 14.31; HRMS (ESI+): Calcd for $C_{14}H_{23}O_4$ $[M+H]^+$: 255.15963 m/z, Found: 255.16064 m/z.

Synthesis of Dienoates with a Trisubstituted Alkene

Scheme S2: Synthesis of Dienoates for Formation of All-Carbon Quaternary Stereogenic Centers



S7, R = 2-naphthyl, 97% yield;
S8, R = 4-Br-C_6H_4, >98% yield;
S9, R = $Me_2C{=}CHCH_2CH_2$ 94% yield

S10, R = 2-naphthyl, 96% yield;
S11, R = 4-Br-C_6H_4, 75% yield;
S12, R = $Me_2C{=}CHCH_2CH_2$, 65% yield

Representative Procedure for Alkylation of Diethyl Bromomalonate with Allyl Bromide

Bromo-malonates **S7-9** were prepared following a procedure described above (*Page S16*).

(*E*)-Diethyl 2-bromo-2-(3-(naphthalen-2-yl)but-2-en-1-yl)malonate (S7):

IR (neat): 3055 (w), 2982 (m), 2938 (w), 1740 (s), 1445 (m), 1367 (m), 1260 (s), 1183 (m), 1095 (m), 1036 (m), 892 (w), 858 (m), 748 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.84–7.77 (4H, m), 7.55 (1H, dd, *J* = 8.4, 2.0 Hz), 7.49–7.42 (2H, m), 5.91 (1H, t, *J* = 7.2 Hz), 4.31 (4H, q, *J* = 7.2 Hz), 2.19 (3H, s), 1.31 (6H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.9, 140.6, 139.5, 133.5, 132.8, 128.2, 127.9, 127.6, 126.2, 125.8, 124.6, 124.5, 121.3, 63.2, 62.6, 37.9, 16.7, 14.0; HRMS (ESI+): Calcd for $C_{21}H_{24}Br_1O_4$ $[M+H]^+$: 419.08580 m/z, Found: 419.08399 m/z.

(*E*)-Diethyl 2-bromo-2-(3-(4-bromophenyl)but-2-en-1-yl)malonate (S8):

IR (neat): 2982 (w), 2937 (w), 1738 (s), 1587 (w) 1465 (m), 1400 (m), 1367 (m), 1256 (s), 1182 (s), 1076 (m), 1007 (s), 895 (m), 813 (m), 743 (w), 651 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.57 (2H, d, *J* = 8.4 Hz), 6.37 (2H, d, *J* = 8.4 Hz), 4.88 (1H, t, *J* = 6.8 Hz), 3.44 (4H, q, *J* = 7.2 Hz), 2.38 (1H, d, *J* = 6.8 Hz), 1.19 (3H, s), 0.44 (6H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.8, 142.3, 138.7, 131.4, 127.7, 127.6, 121.4, 63.2, 62.4, 37.7, 16.5, 14.0; HRMS (ESI+): Calcd for $C_{17}H_{21}Br_2O_4$ $[M+H]^+$: 448.97861 m/z, Found: 448.97983 m/z.

(*E*)-Diethyl 2-bromo-2-(3,7-dimethylocta-2,6-dien-1-yl)malonate (S9):

IR (neat): 2981 (m), 2926 (m), 1741 (s), 1445 (m), 1367 (m), 1235 (s), 1175 (m), 1096 (m), 1023 (m), 892 (m), 650 (w) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 5.14 (1H, t, *J* = 7.2 Hz), 5.06 (1H, t, *J* = 6.8 Hz), 4.25 (2H, q, *J* = 7.2 Hz), 4.24 (2H, q, *J* = 7.2 Hz), 3.01 (1H, d, *J* = 6.8 Hz), 2.09–1.93 (4H, m), 1.66 (3H, s), 1.63 (3H, s), 1.58 (3H, s), 1.27 (6H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.9, 140.6, 131.7, 124.0, 117.1, 63.1, 63.0, 39.9, 37.1, 26.6, 25.8, 17.8, 16.7, 14.0; HRMS (ESI+): Calcd for $C_{17}H_{28}Br_1O_4$ $[M+H]^+$: 375.11710 m/z, Found: 375.11615 m/z.

Representative Procedure for Elimination of Bromomalonate

To a solution of bromo-malonate **S9** (3.54 g, 9.4 mmol) in CH_2Cl_2 (10 mL) was added DABCO (3.18 g, 28.3 mmol) at 22 °C. The solution was allowed to stir at 22 °C for 24 h, after which water (30 mL) was added to quench the reaction. The aqueous layer was then washed with CH_2Cl_2 (2 × 30 mL). The combined organic layers were dried over $MgSO_4$ and concentrated under vacuum. The resulting yellow oil was purified by silica gel chromatography (hexanes:ethyl acetate = 12:1) to afford 1.81 g **S12** (6.1 mmol, 65% yield) as yellow oil.

(*E*)-Diethyl 2-(3-(naphthalen-2-yl)but-2-en-1-ylidene)malonate (S10):

IR (neat): 3058 (w), 2981 (m), 2937 (w), 1710 (s), 1604 (s), 1466 (m), 1366 (m), 1244 (s), 1164 (s), 1062 (s), 1023 (m), 857 (m), 749 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.95–7.81 (5H, m), 7.64 (1H, dd, *J* = 8.4, 1.6 Hz), 7.52–7.47 (2H, m), 7.06 (1H, d, *J* = 12.0 Hz), 4.38 (2H, q, *J* = 7.2 Hz), 4.31 (2H, q, *J* = 7.2 Hz), 2.46 (3H, d, *J* = 1.6 Hz), 1.39 (3H, t, *J* = 7.2 Hz), 1.35 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.9, 165.1, 149.6, 140.1, 139.0, 133.6, 133.3, 128.6, 128.3, 127.7, 126.8, 126.6, 126.0, 125.3, 123.9, 122.2, 61.44, 61.41, 16.8, 14.4, 14.3; HRMS (ESI+): Calcd for $C_{21}H_{23}O_4$ $[M+H]^+$: 339.15963 m/z, Found: 339.15929 m/z.

(*E*)-Diethyl 2-(3-(4-bromophenyl)but-2-en-1-ylidene)malonate (S11):

IR (neat): 2981 (w), 2937 (w), 2906 (w), 1707 (s), 1610 (m), 1581 (m), 1445 (m), 1367 (m), 1275 (m), 1234 (s), 1211 (s), 1165 (s), 1062 (s), 1006 (m), 948 (w), 863 (w), 821 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.79 (1H, d, *J* = 12.4 Hz), 7.49 (2H, d, *J* = 8.4 Hz), 7.35 (2H, d, *J* = 8.4 Hz), 6.86 (1H, d, *J* = 12.4 Hz), 4.34 (2H, q, *J* = 7.2 Hz), 4.28 (2H, q, *J* = 7.2 Hz), 2.31 (3H, s), 1.35 (3H, t, *J* = 7.2 Hz), 1.32 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.8, 165.0, 148.4, 140.8, 139.8, 131.8, 127.9, 125.9, 123.2, 122.1, 61.5, 16.7, 14.4, 14.3; HRMS (ESI+): Calcd for $C_{17}H_{20}Br_1O_4$ $[M+H]^+$: 367.05450 m/z, Found: 367.05310 m/z.

(*E*)-Diethyl 2-(3,7-dimethylocta-2,6-dien-1-ylidene)malonate (S12):

IR (neat): 2980 (m), 2932 (m), 1715 (s), 1627 (m), 1446 (m), 1380 (m), 1246 (s), 1204 (s), 1143 (m), 1026 (s), 864 (w), 797 (w) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.65 (1H, d, *J* = 12.0 Hz), 6.26 (1H, d, *J* = 12.0 Hz), 5.05 (1H, t, *J* = 6.8 Hz), 4.31 (2H, q, *J* = 7.2 Hz), 4.24 (2H, q, *J* = 7.2 Hz), 2.21–2.10 (4H, m), 1.93 (3H, s), 1.67 (3H, s), 1.58 (3H, s), 1.33 (3H, t, *J* = 7.2 Hz), 1.29 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.0, 165.2, 155.2, 140.4, 132.6, 123.4, 123.2, 120.5, 61.24, 61.21, 40.9, 26.3, 25.8, 17.8, 17.7, 14.31, 14.30; HRMS (ESI+): Calcd for $C_{17}H_{27}O_4$ $[M+H]^+$: 295.19093 m/z, Found: 295.19105 m/z.

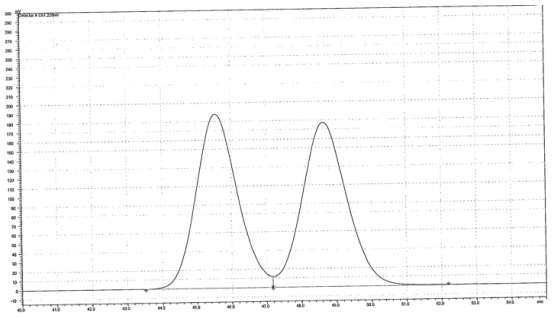
Representative Procedure for Catalytic Enantioselective 1,6-Conjugate Propargyl Additions; Quaternary Carbon Centers

In an N_2-filled glove box, imidazolinium salt **9b** (4.6 mg, 0.010 mmol), CuCl (1.0 mg, 0.010 mmol), NaO*t*-Bu (1.9 mg, 0.020 mmol) and NaOPh (17.4 mg, 0.15 mmol) and THF (0.5 mL) are added into an oven-dried vial equipped with a stirring bar. The mixture is allowed to premix for 2 h at 22 °C. The resulting mixture is then added into a separate oven-dried vial containing allenylboronic acid pinacol ester (36.0 μL, 0.20 mmol). The vial is sealed with a Teflon screw cap and removed from the glove box. The mixture is then allowed to stir at 22 °C for 30 min. Then dienoate **S10** (33.8 mg, 0.10 mmol) is added into the solution by a syringe, and the solution is allowed to stir at 22 °C for 24 h. The mixture is filtered through a short plug of Celite and silica gel eluting with diethyl ether. The filtrate is washed with a 1M aqueous solution of NaOH, dried over $MgSO_4$ and concentrated *in vacuo*. The resulting yellow oil is purified by silica gel chromatography (hexanes:ethyl acetate = 20:1) to give 30.2 mg **10a** (0.080 mmol, 80% yield) as colorless oil.

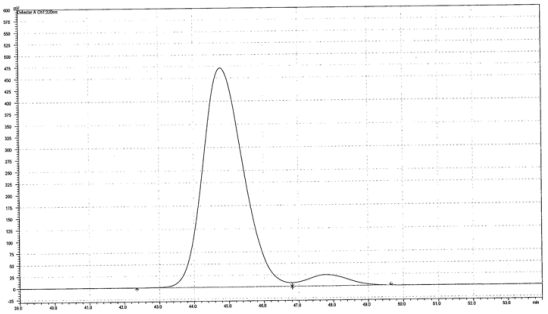
(*R*,*E*)-Diethyl 2-(3-methyl-3-(naphthalen-2-yl)hex-1-en-5-yn-1-yl)malonate (10a):

IR (neat): 3293 (w), 2980 (m), 2937 (w), 1731 (s), 1600 (w), 1463 (w), 1368 (m), 1249 (m), 1175 (m), 1096 (m), 975 (w), 858 (m), 819 (m), 750 (m), 645 (w) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.83–7.78 (4H, m), 7.49–7.43 (3H, m), 6.05 (1H, d, *J* = 16.0 Hz), 5.85 (1H, dd, *J* = 16.0, 8.8 Hz), 4.24 (4H, q, *J* = 7.2 Hz), 4.10 (1H, d, *J* = 8.8 Hz), 2.80 (1H, dd, *J* = 16.4, 2.8 Hz), 2.73 (1H, dd, *J* = 16.4, 2.8 Hz), 1.95 (1H, t, *J* = 2.8 Hz), 1.64 (3H, s), 1.292 (3H, t, *J* = 7.2 Hz), 1.289 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.3, 142.9, 142.8, 133.3, 132.2, 128.2, 127.9, 127.5, 126.1, 125.9, 125.4, 125.0, 120.9, 81.4, 71.2, 61.8, 55.8, 44.1, 31.3, 25.8, 14.2; HRMS (ESI+): Calcd for $C_{24}H_{27}O_4$ $[M+H]^+$: 379.19093 m/z, Found: 379.19093 m/z. Specific rotation: $[\alpha]_D^{20}$ –9.1 (*c* 2.03, $CHCl_3$).

Enantiomeric purity of **10a** was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OZ–H column, 99.5:0.5 hexanes/*i*-PrOH, 0.6 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	45.548	15591793	187885	49.869	51.455
2	48.646	15673561	177262	50.131	48.545



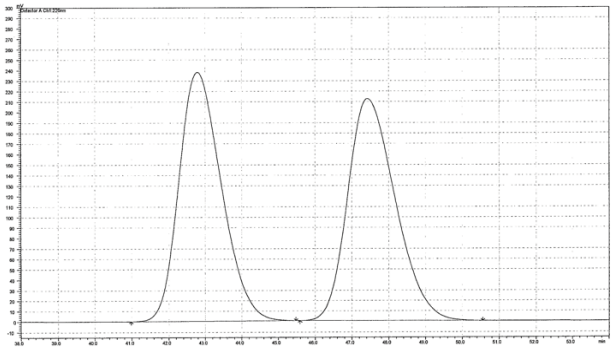
Peak#	Ret. Time	Area	Height	Area %	Height %
1	44.781	37739365	470979	94.989	95.149
2	47.791	1991026	24011	5.011	4.851

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	45.548	49.869	1	44.781	94.989
2	48.646	50.131	2	47.791	5.011

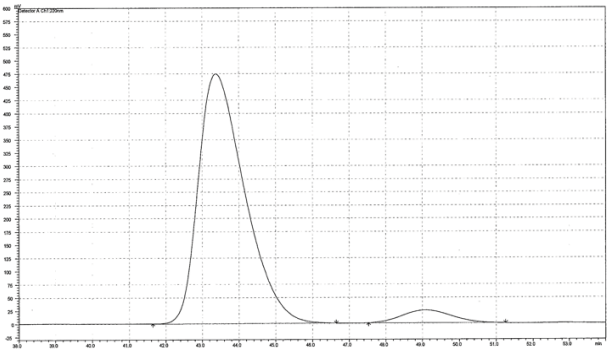
(*R*,*E*)-Diethyl 2-(3-(4-bromophenyl)-3-methylhex-1-en-5-yn-1-yl)malonate (10b):

IR (neat): 3294 (m), 2980 (m), 2936 (w), 1732 (s), 1490 (m), 1369 (m), 1262 (m), 1177 (m), 1009 (m), 861 (w), 824 (w), 647 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.42 (2H, d, *J* = 8.0 Hz), 7.21 (2H, d, *J* = 8.0 Hz), 5.93 (1H, d, *J* = 16.4 Hz), 5.78 (1H, dd, *J* = 16.4, 8.4 Hz), 4.22 (4H, q, *J* = 7.2 Hz), 4.05 (1H, d, *J* = 8.8 Hz), 2.65 (1H, dd, *J* = 16.4, 2.8 Hz), 2.58 (1H, dd, *J* = 16.8, 2.4 Hz), 1.94 (1H, t, *J* = 2.8 Hz), 1.49 (3H, s), 1.28 (6H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.3, 144.5, 142.4, 131.4, 128.6, 121.0, 120.6, 81.0, 71.3, 61.8, 55.7, 43.7, 31.3, 25.9, 14.2; HRMS (ESI+): Calcd for $C_{20}H_{24}Br_1O_4$ $[M+H]^+$: 407.08580 m/z, Found: 407.08427 m/z. Specific rotation: $[\alpha]_D^{20}$ –6.9 (*c* 1.67, $CHCl_3$).

Enantiomeric purity of **10b** was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OZ–H column, 99.5:0.5 hexanes/*i*-PrOH, 0.6 mL/min, 220 nm).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	42.784	19252139	237716	50.242	52.853
2	47.421	19066824	212053	49.758	47.147



Peak#	Ret. Time	Area	Height	Area %	Height %
1	43.371	41482003	473954	94.848	95.134
2	49.083	2253434	24243	5.152	4.866

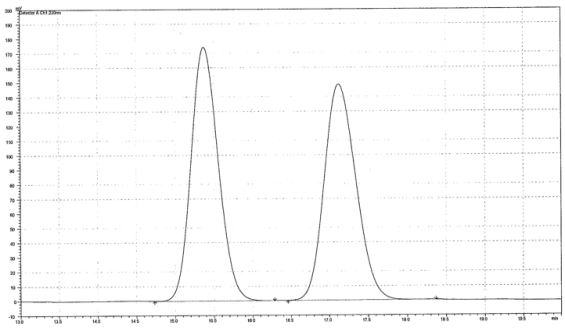
Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	42.784	50.242	1	43.371	94.848
2	47.421	49.758	2	49.083	5.152

(*R*,*E*)-Diethyl 2-(3,7-dimethyl-3-(prop-2-yn-1-yl)octa-1,6-dien-1-yl)malonate (10c):

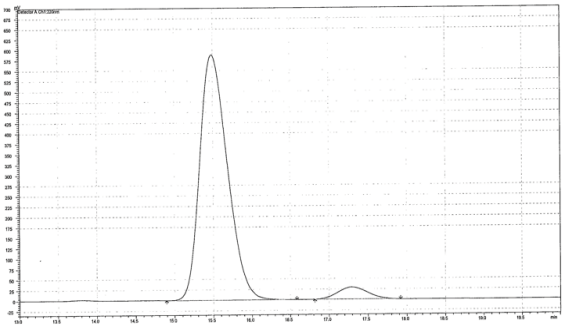
IR (neat): 3291 (m), 2968 (m), 2918 (m), 1734 (s), 1447 (m), 1369 (m), 1255 (m), 1176 (m), 1149 (m), 1033 (m), 974 (m), 863 (w), 636 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 5.70–5.61 (2H, m), 5.07 (1H, t, *J* = 7.2 Hz), 4.19 (4H, q, *J* = 7.2 Hz), 3.99 (1H, dd, *J* = 5.6, 2.4 Hz), 2.21–2.20 (2H, m), 1.96

(1H, t, *J* = 2.8 Hz), 1.90–1.82 (2H, m), 1.66 (3H, s), 1.57 (3H, s), 1.51–1.38 (2H, m), 1.26 (3H, t, *J* = 7.2 Hz), 1.25 (3H, t, *J* = 7.2 Hz), 1.11 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.5, 143.2, 131.6, 124.5, 120.1, 81.6, 70.5, 61.7, 55.9, 39.9, 39.2, 30.5, 25.8, 23.6, 23.0, 17.7, 14.2; HRMS (ESI+): Calcd for $C_{20}H_{31}O_4$ $[M+H]^+$: 335.22223 m/z, Found: 335.22233 m/z.

Enantiomeric purity of **10c** was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralpak AD–H column, 99.9:0.1 hexanes/*i*-PrOH, 0.6 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ –3.1 (*c* 1.28, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.371	4238862	174308	50.108	54.023
2	17.122	4220548	148345	49.892	45.977



Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.481	14698508	587349	95.067	95.354
2	17.289	762765	28620	4.933	4.646

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	15.371	50.108	1	15.481	95.067
2	17.122	49.892	2	17.289	4.933

Catalytic Multicomponent Cu–B Additions to Allenes/1,6-Conjugate Additions

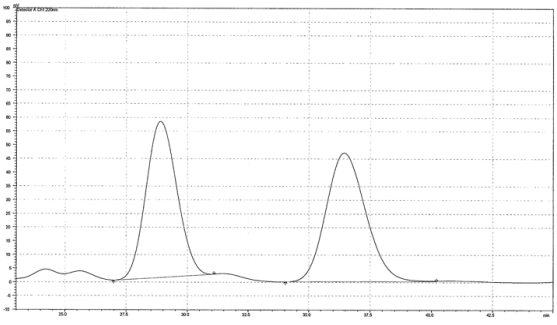
In an N_2-filled glove box, imidazolinium salt **9d** (2.2 mg, 0.0050 mmol), CuCl (0.5 mg, 0.0050 mmol), NaO*t*-Bu (0.9 mg, 0.010 mmol) and NaOPh (17.4 mg, 0.15 mmol) and THF (0.5 mL) are added into an oven-dried vial equipped with a stirring bar. The mixture is allowed to premix for 2 h at 22 °C. The resulting mixture is then added into a separate oven-dried vial containing bis(pinacolato)diboron (38.1 mg, 0.15 mmol). The vial is sealed with a Teflon screw cap and removed from the glove box. The mixture is allowed to stir at 22 °C for 30 min, after which allene **11** (29.8 mg, 0.15 mmol) and dienoate **1a** (27.4 mg, 0.10 mmol) are added into the solution by syringe. The solution is allowed to stir at 22 °C for 16 h. The mixture is then filtered through a short plug of Celite and silica gel eluting with diethyl ether. The filtrate is washed with a 1M aqueous solution of NaOH, dried over $MgSO_4$ and concentrated *in vacuo*. The resulting yellow oil is purified by silica gel chromatography (hexanes:ethyl acetate = 25:1) to furnish 37.4 mg **12a** (0.062 mmol, 62% yield) as colorless oil.

(*E*)-Diethyl 2-(4-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-3-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexa-1,5-dien-1-yl)malonate (12a):

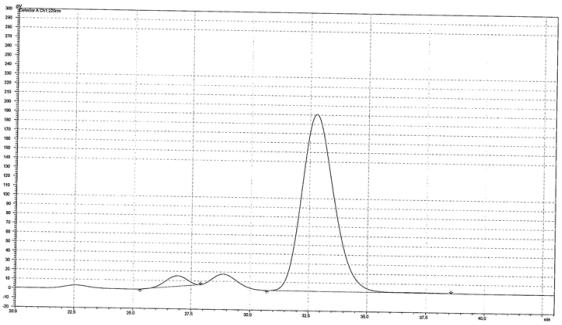
IR (neat): 3028 (m), 2978 (m), 2955 (m), 2857 (m), 1734 (s), 1417 (m), 1305 (m), 1252 (m), 1141 (s), 1094 (s), 1032 (m), 968 (m), 834 (s), 775 (s), 699 (s), 619 (w) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.21–7.17 (2H, m), 7.10–7.06 (3H, m), 5.80–5.78 (2H, m), 5.63 (1H, d, *J* = 3.2 Hz), 5.32 (1H, d, *J* = 3.6 Hz), 4.21 (2H, q, *J* = 7.2 Hz), 4.13 (2H, q, *J* = 7.2 Hz), 3.99–3.97 (1H, m), 3.63–3.58 (1H, m),

3.55–3.50 (1H, m), 3.44–3.38 (1H, m), 2.60 (1H, td, *J* = 11.2, 2.8 Hz), 1.97–1.88 (1H, m), 1.70–1.61 (1H, m), 1.28 (3H, t, *J* = 7.2 Hz), 1.23 (6H, s), 1.18 (3H, t, *J* = 7.2 Hz), 1.18 (6H, s), 0.88 (9H, s), 0.002 (3H, s), –0.003 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.5, 168.3, 143.7, 139.6, 132.2, 128.5, 128.3, 126.0, 122.4, 83.2, 61.8, 61.7, 61.6, 55.8, 53.5, 48.2, 35.0, 26.1, 25.0, 24.8, 18.4, 14.2, 14.1, –5.12, –5.11; HRMS (ESI+): Calcd for $C_{33}H_{54}B_1O_7Si_1$ $[M+H]^+$: 601.37318 m/z, Found: 601.37467 m/z.

Enantiomeric purity of **12a** was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OZ–H column, 99.9:0.1 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ –10.6 (*c* 1.56, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	28.882	5273415	57996	50.058	55.288
2	36.440	5261123	46901	49.942	44.712



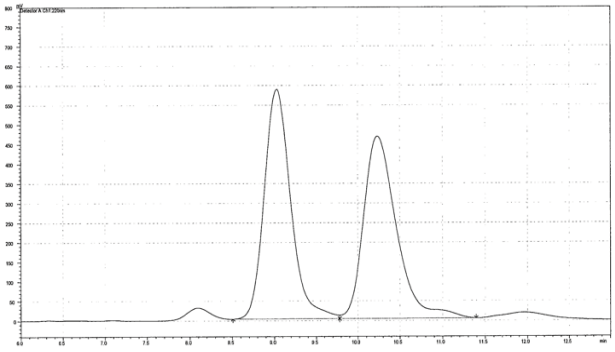
Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.905	693529	11232	3.668	5.584
2	32.781	18213360	189912	96.332	94.416

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	28.882	50.058	1	26.905	3.668
2	36.440	49.942	2	32.781	96.332

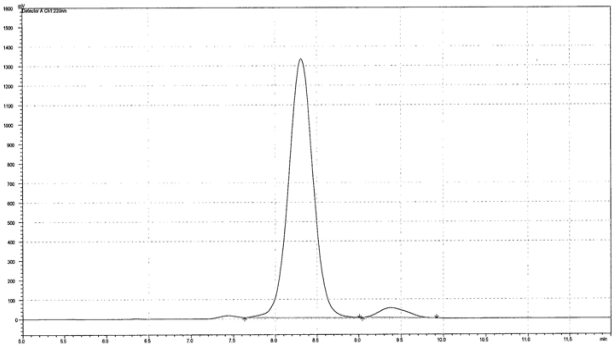
Diethyl 2-((3*S*,4*S*,*E*)-4-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-3-(2-methoxyphenyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexa-1,5-dien-1-yl)malonate (12b):

IR (neat): 2978 (m), 2955 (m), 2931 (m), 2857 (m), 1734 (s), 1598 (w), 1464 (m) 1367 (m), 1305 (m), 1243 (s), 1142 (s), 1095 (s), 1031 (s), 970 (m), 835 (s), 775 (m), 751 (m), 701 (w) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.09–7.03 (2H, m), 6.79–6.71 (2H, m), 5.94 (1H, dd, *J* = 15.2, 9.2 Hz), 5.79 (1H, dd, *J* = 15.2, 9.2 Hz), 5.58 (1H, d, *J* = 4.0 Hz), 5.38 (1H, d, *J* = 3.6 Hz), 4.20 (2H, q, *J* = 7.2 Hz), 4.10 (2H, q, *J* = 7.2 Hz), 3.97 (1H, d, *J* = 9.2 Hz), 3.83–3.76 (1H, m), 3.75 (3H, s), 3.56–3.49 (1H, m), 3.45–3.36 (1H, m), 2.87 (1H, td, *J* = 6.8, 2.8 Hz), 1.94–1.85 (1H, m), 1.72–1.63 (1H, m), 1.27 (3H, t, *J* = 7.2 Hz), 1.21 (6H, s), 1.18 (3H, t, *J* = 7.2 Hz), 1.16 (6H, s), 0.88 (9H, s), 0.01 (3H, s), 0.00 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.6, 168.4, 157.3, 138.8, 131.6, 131.3, 130.1, 127.1, 122.2, 120.2, 110.6, 83.0, 62.0, 61.6, 61.4, 55.9, 55.0, 45.6, 35.4, 26.1, 24.9, 24.7, 18.4, 14.2, 14.1, –5.10, –5.15; HRMS (ESI+): Calcd for $C_{34}H_{56}B_1O_8Si_1$ $[M+H]^+$: 631.38375 m/z, Found: 631.38424 m/z.

Enantiomeric purity of **12b** was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OZ–3 column, 99.6:0.4 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ –6.1 (*c* 1.88, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.028	12872367	585119	50.464	55.730
2	10.229	12635656	464801	49.536	44.270



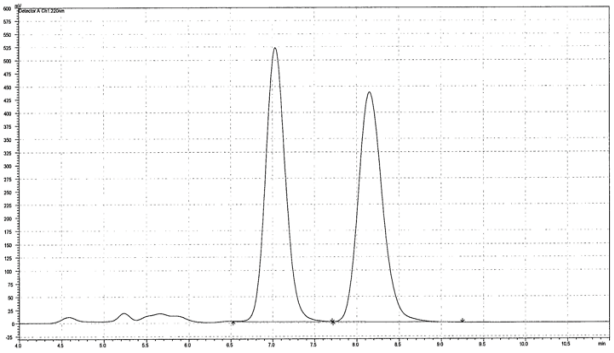
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.311	27043857	1329289	95.993	96.382
2	9.375	1128780	49898	4.007	3.618

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	9.028	50.464	1	8.311	95.993
2	10.229	49.536	2	9.375	4.007

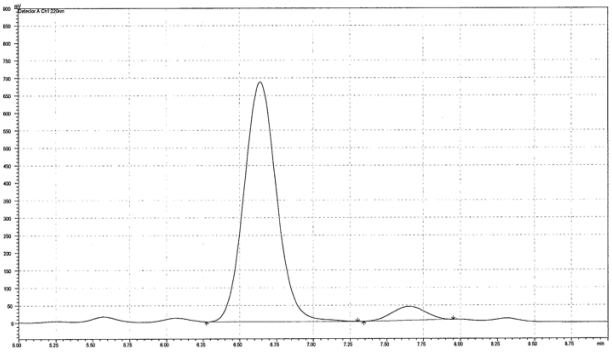
Diethyl 2-((3*S*,4*S*,*E*)-4-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-(*o*-tolyl)hexa-1,5-dien-1-yl)malonate (12c):

IR (neat): 2978 (m), 2956 (m), 2931 (m), 2857 (m), 1734 (s), 1612 (w), 1463 (m), 1368 (m), 1306 (m), 1216 (m), 1143 (s), 1097 (m), 1033 (m), 969 (m), 836 (m), 776 (m), 728 (m), 702 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.13–6.97 (4H, m), 5.78 (1H, dd, *J* = 15.2, 9.2 Hz), 5.72 (1H, d, *J* = 3.2 Hz), 5.59 (1H, dd, *J* = 15.2, 9.6 Hz), 5.48 (1H, d, *J* = 3.2 Hz), 4.20 (2H, q, *J* = 7.2 Hz), 4.12 (2H, q, *J* = 7.2 Hz), 3.94 (1H, d, *J* = 8.8 Hz), 3.83 (1H, app. t, *J* = 10.0 Hz), 3.59–3.53 (1H, m), 3.49–3.42 (1H, m), 2.77 (1H, td, *J* = 10.4, 2.8 Hz), 2.30 (3H, s), 2.01–1.93 (1H, m), 1.70–1.61 (1H, m), 1.27 (3H, 7.2 Hz), 1.18 (3H, t, *J* = 7.2 Hz), 1.18 (6H, s), 1.13 (6H, s), 0.88 (9H, s), 0.01 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.4, 168.3, 140.9, 139.1, 136.5, 132.2, 130.3, 128.0, 125.8, 125.7, 122.2, 83.2, 61.72, 61.70, 61.5, 55.8, 48.8, 45.8, 35.6, 26.1, 25.1, 24.4, 19.8, 18.4, 14.2, 14.0, –5.12, –5.14; HRMS (ESI+): Calcd for $C_{34}H_{56}B_1O_7Si_1$ $[M+H]^+$: 615.38883 m/z, Found: 615.38940 m/z.

Enantiomeric purity of **12c** was determined by HPLC analysis in comparison with authentic racemic material (94:6 e.r. shown; Chiralcel OZ–3 column, 99.6:0.4 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ –8.1 (*c* 1.26, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.030	8585573	521342	49.813	54.400
2	8.149	8649996	437011	50.187	45.600



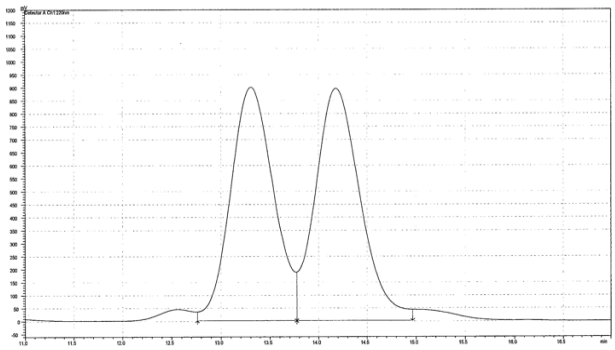
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.636	10470940	685591	94.358	94.525
2	7.648	626092	39711	5.642	5.475

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	7.030	49.813	1	6.636	94.358
2	8.149	50.187	2	7.648	5.642

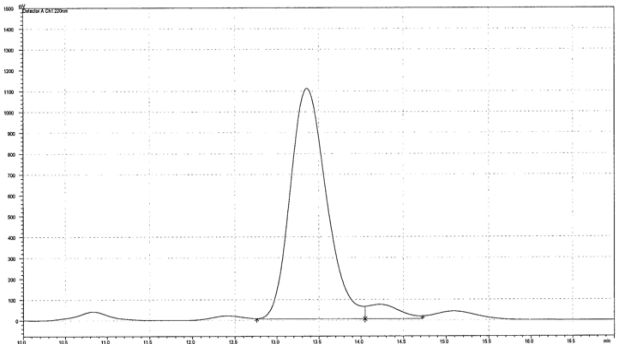
Diethyl 2-((3*S*,4*S*,*E*)-4-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-3-(naphthalen-1-yl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexa-1,5-dien-1-yl)malonate (12d):

IR (neat): 2979 (m), 2956 (m), 2857 (m), 1734 (s), 1597 (w), 1471 (m), 1390 (m), 1306 (m), 1255 (m), 1142 (s), 1096 (m), 1033 (m), 968 (m), 836 (m), 778 (s), 703 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.27 (1H, d, *J* = 8.4 Hz), 7.77 (1H, d, *J* = 8.0 Hz), 7.63 (1H, d, *J* = 8.0 Hz), 7.46–7.32 (4H, m), 5.89–5.87 (2H, m), 5.61 (1H, d, *J* = 3.2 Hz), 5.42 (1H, d, *J* = 3.2 Hz), 4.56–4.49 (1H, m), 4.20 (2H, q, *J* = 7.2 Hz), 4.04 (2H, q, *J* = 7.2 Hz), 3.97–3.94 (1H, m), 3.61–3.56 (1H, m), 3.49–3.43 (1H, m), 2.98–2.93 (1H, m), 2.08–2.02 (1H, m), 1.84–1.75 (1H, m), 1.27 (3H, t, *J* = 7.2 Hz), 1.13 (6H, s), 1.06 (3H, t, *J* = 7.2 Hz), 1.03 (6H, s), 0.88 (9H, s), 0.01 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.4, 168.2, 139.4, 139.0, 134.1, 132.1, 131.9, 128.8, 126.5, 125.9, 125.42, 125.38, 125.1, 124.3, 122.7, 83.2, 61.7, 61.5, 55.7, 46.9, 34.9, 26.1, 25.0, 24.4, 18.4, 14.2, 13.9, –5.12, –5.15; HRMS (ESI+): Calcd for $C_{37}H_{56}B_1O_7Si_1$ $[M+H]^+$: 651.38883 m/z, Found: 651.38849 m/z.

Enantiomeric purity of **12d** was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OZ–3 column, 99.6:0.4 hexanes/*i*-PrOH, 0.5 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ +9.6 (*c* 1.81, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.301	27823421	898956	49.664	50.128
2	14.176	28199904	894359	50.336	49.872



Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.355	33193505	1106366	94.852	94.133
2	14.219	1801445	68958	5.148	5.867

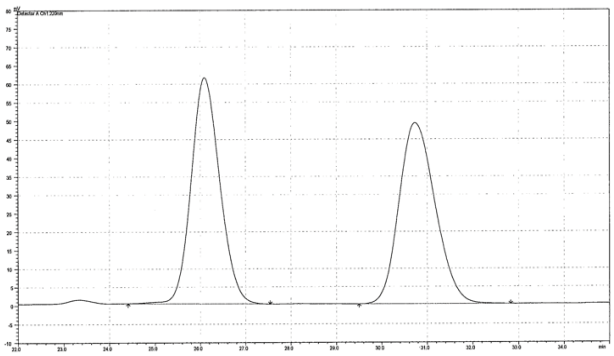
Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	13.301	49.664	1	13.355	94.852
2	14.176	50.336	2	14.219	5.148

Diethyl 2-((3*S*,4*S*,*E*)-3-(4-bromophenyl)-4-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexa-1,5-dien-1-yl)malonate (12e):

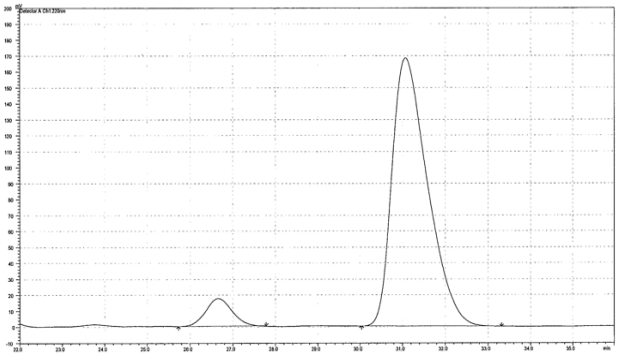
IR (neat): 2979 (m), 2956 (m), 2931 (m), 2857 (m), 1733 (s), 1610 (w), 1471 (m), 1368 (m), 1306 (m), 1252 (m), 1142 (s), 1096 (s), 1033 (m), 968 (m), 835 (s), 776 (m), 700 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.31 (2H, d, *J* = 8.4 Hz), 6.95 (2H, d, *J* = 8.4 Hz), 5.82–5.70 (2H, m), 5.65 (1H, d, *J* = 3.6 Hz), 5.33 (1H, d, *J* = 3.6 Hz), 4.20 (2H, q, *J* = 7.2 Hz), 4.13 (2H, q, *J* = 7.2 Hz), 3.97 (1H, d, *J* = 8.0 Hz), 3.60–3.49 (2H, m), 3.43–3.37 (1H, m), 2.56 (1H, td, *J* = 11.2, 3.2 Hz), 1.94–1.86 (1H, m), 1.67–1.58 (1H, m), 1.27 (3H, t, *J* = 7.2 Hz), 1.22 (6H, s), 1.19 (3H, t, *J* = 7.2 Hz), 1.18 (6H, s), 0.87 (9H, s),

0.00 (3H, s), –0.01 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.3, 168.2, 142.8, 139.0, 132.6, 131.3, 130.2, 122.8, 119.7, 83.3, 61.8, 61.7, 61.6, 55.7, 52.9, 48.0, 34.9, 26.1, 24.9, 24.8, 18.4, 14.2, 14.1, –5.1, –5.2; HRMS (ESI+): Calcd for $C_{33}H_{53}B_1Br_1O_7Si_1$ $[M+H]^+$: 679.28370 m/z, Found: 679.28266 m/z.

Enantiomeric purity of **12e** was determined by HPLC analysis in comparison with authentic racemic material (93:7 e.r. shown; Chiralcel OZ–H column, 99.5:0.5 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ –5.6 (*c* 1.98, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.094	2691709	61244	49.673	55.526
2	30.730	2727182	49053	50.327	44.474



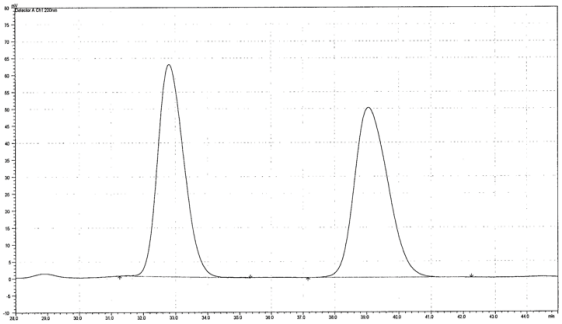
Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.654	737669	17243	7.058	9.304
2	31.070	9713709	168075	92.942	90.696

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	26.094	49.673	1	26.654	7.058
2	30.730	50.327	2	31.070	92.942

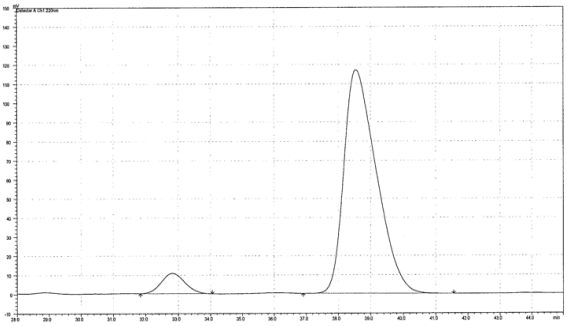
Diethyl 2-((3*S*,4*S*,*E*)-4-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-3-(4-methoxyphenyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexa-1,5-dien-1-yl)malonate (12f):

IR (neat): 2978 (m), 2955 (m), 2931 (m), 2857 (m), 1734 (s), 1610 (w), 1511 (m), 1417 (m), 1367 (m), 1303 (m), 1247 (s), 1141 (s), 1094 (s), 1034 (s), 968 (m), 833 (s), 775 (s), 700 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.99 (2H, d, *J* = 8.4 Hz), 6.74 (2H, d, *J* = 8.4 Hz), 5.77–5.75 (2H, m), 5.64 (1H, d, *J* = 3.6 Hz), 5.33 (1H, d, *J* = 3.6 Hz), 4.20 (2H, q, *J* = 7.6 Hz), 4.13 (2H, q, *J* = 7.6 Hz), 3.98–3.96 (1H, m), 3.74 (3H, s), 3.58–3.49 (2H, m), 3.41 (1H, dt, *J* = 10.0, 7.6 Hz), 2.56 (1H, td, *J* = 11.2, 2.8 Hz), 1.96–1.87 (1H, m), 1.69–1.62 (1H, m), 1.27 (3H, t, *J* = 7.2 Hz), 1.23 (6H, s), 1.19 (3H, t, *J* = 7.2 Hz), 1.19 (6H, s), 0.88 (9H, s), 0.00 (3H, s), –0.01 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.5, 168.4, 157.7, 139.9, 135.8, 132.1, 129.3, 122.0, 113.7, 83.2, 61.8, 61.7, 61.6, 55.8, 55.2, 52.6, 48.2, 35.0, 26.1, 25.0, 24.8, 18.4, 14.2, 14.1, –5.12, –5.15; HRMS (ESI+): Calcd for $C_{34}H_{56}B_1O_8Si_1$ $[M+H]^+$: 631.38375 m/z, Found: 631.38476 m/z.

Enantiomeric purity of **12f** was determined by HPLC analysis in comparison with authentic racemic material (94:6 e.r. shown; Chiralcel OZ–H column, 99.6:0.4 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ –11.0 (*c* 1.91, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	32.798	3561219	62636	49.638	55.566
2	39.059	3613144	50088	50.362	44.434



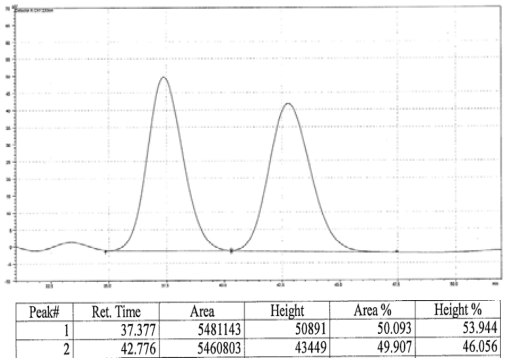
Peak#	Ret. Time	Area	Height	Area %	Height %
1	32.823	532921	10585	6.149	8.303
2	38.538	8133549	116901	93.851	91.697

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	26.094	49.673	1	26.654	7.058
2	30.730	50.327	2	31.070	92.942

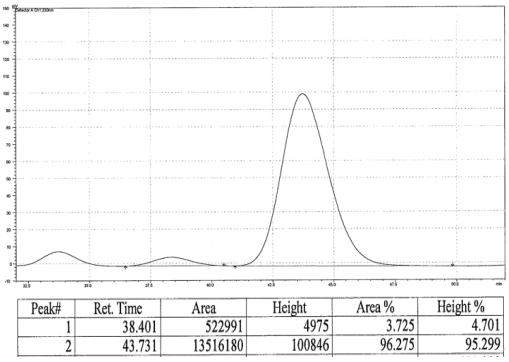
Diethyl 2-((3*S*,4*S*,*E*)-4-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-3-(furan-3-yl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexa-1,5-dien-1-yl)malonate (12g):

IR (neat): 2978 (m), 2955 (m), 2930 (m), 2857 (m), 1734 (s), 1610 (w), 1471 (m), 1368 (m), 1305 (m), 1253 (m), 1216 (m), 1141 (s), 1095 (s), 1034 (m), 968 (m), 834 (s), 775 (s), 701 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.16–7.14 (1H, m), 6.87–6.85 (2H, m), 5.77–5.74 (2H, m), 5.69 (1H, d, *J* = 3.6 Hz), 5.37 (1H, d, *J* = 3.6 Hz), 4.20 (2H, q, *J* = 7.2 Hz), 4.15 (2H, q, *J* = 7.2 Hz), 4.00–3.98 (1H, m), 3.76–3.72 (1H, m), 3.55–3.49 (1H, m), 3.43–3.38 (1H, m), 2.57 (1H, td, *J* = 11.2, 3.2 Hz), 1.91–1.83 (1H, m), 1.65–1.57 (1H, m), 1.27 (3H, t, *J* = 7.2 Hz), 1.23 (6H, s), 1.21 (3H, t, *J* = 7.2 Hz), 1.20 (6H, s), 0.87 (9H, s), –0.007 (3H, s), –0.009 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.4, 168.3, 144.1, 138.6, 131.6, 127.5, 125.0, 122.5, 120.7, 83.2, 61.72, 61.67, 61.63, 55.7, 48.7, 47.8, 34.6, 26.1, 25.0, 24.8, 18.4, 14.2, 14.1, –5.1, –5.2; HRMS (ESI+): Calcd for $C_{31}H_{52}B_1O_8Si_1$ $[M+H]^+$: 591.35245 m/z, Found: 591.35110 m/z.

Enantiomeric purity of **12g** was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; Chiralcel OZ–H column, 99.5:0.5 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ –15.3 (*c* 2.65, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	37.377	5481143	50891	50.093	53.944
2	42.776	5460803	43449	49.907	46.056



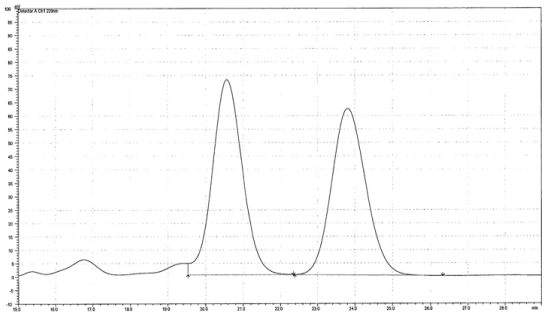
Peak#	Ret. Time	Area	Height	Area %	Height %
1	38.401	522991	4975	3.725	4.701
2	43.731	13516180	100846	96.275	95.299

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	37.377	50.093	1	38.401	3.725
2	42.776	49.907	2	43.731	96.275

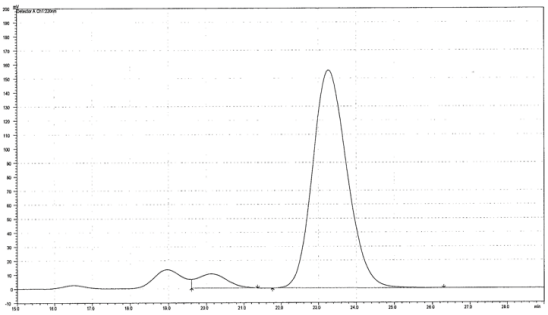
Diethyl 2-((3*S*,4*S*,*E*)-4-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-(thiophen-3-yl)hexa-1,5-dien-1-yl)malonate (12h):

IR (neat): 2979 (m), 2955 (m), 2931 (m), 2857 (m), 1735 (s), 1610 (w), 1471 (m), 1369 (m), 1307 (m), 1254 (m), 1215 (m), 1143 (s), 1096 (m), 1028 (m), 969 (m), 836 (m), 777 (m), 701 (w) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.26 (1H, s), 7.11 (1H, s), 6.20 (1H, s), 5.79–5.66 (3H, m), 5.42 (1H, d, *J* = 3.2 Hz), 4.21 (2H, q, *J* = 7.2 Hz), 4.17 (2H, q, *J* = 7.2 Hz), 3.99 (1H, d, *J* = 8.0 Hz), 3.55 (2H, m), 3.43–3.35 (1H, m), 2.47 (1H, td, *J* = 11.2, 2.8 Hz), 1.89–1.81 (1H, m), 1.66–1.57 (1H, m), 1.27 (3H, t, *J* = 7.2 Hz), 1.23 (3H, t, *J* = 7.2 Hz), 1.22 (6H, s), 1.21 (6H, s), 0.87 (9H, s), –0.01 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.41, 168.36, 142.5, 139.2, 138.4, 131.6, 127.0, 110.3, 83.3, 61.73, 61.68, 55.7, 47.2, 43.6, 34.4, 26.1, 24.9, 24.8, 18.4, 14.2, 14.1, –5.1, –5.2; HRMS (ESI+): Calcd for $C_{31}H_{52}B_1O_7S_1Si_1$ $[M+H]^+$: 607.32960 m/z, Found: 607.33019 m/z.

Enantiomeric purity of **12h** was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OZ–H column, 99.7:0.3 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ –6.2 (*c* 2.01, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.564	3991746	72543	50.295	53.921
2	23.807	3944913	61993	49.705	46.079



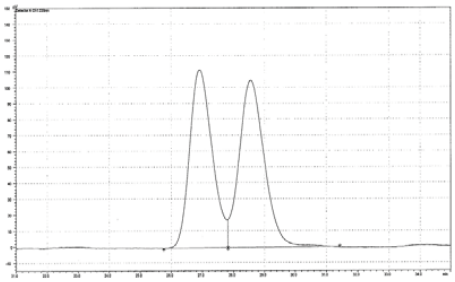
Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.131	558394	10222	5.358	6.168
2	23.264	9862334	155494	94.642	93.832

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	20.564	50.295	1	20.131	5.358
2	23.807	49.705	2	23.264	94.642

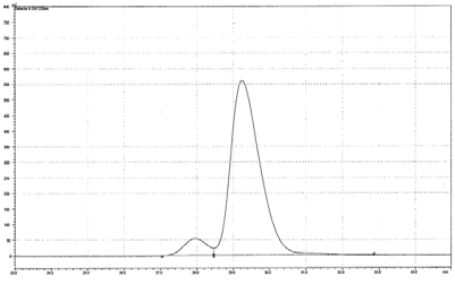
Diethyl 2-((3*S*,4*S*,*E*)-4-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-3-phenethyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexa-1,5-dien-1-yl)malonate (12i):

IR (neat): 2978 (m), 2955 (m), 2930 (m), 2857 (m), 1735 (s), 1606 (w), 1496 (m), 1369 (m), 1306 (m), 1253 (m), 1142 (s), 1195 (s), 1033 (m), 970 (m), 835 (s), 775 (m), 700 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.24–7.22 (2H, m), 7.15–7.09 (3H, m), 5.84 (1H, d, *J* = 3.6 Hz), 5.73 (1H, dd, *J* = 15.6, 9.2 Hz), 5.51 (1H, d, *J* = 3.6 Hz), 5.41 (1H, dd, *J* = 15.6, 9.6 Hz), 4.22 (4H, q, *J* = 7.2 Hz), 4.06 (1H, d, *J* = 9.2 Hz), 3.51–3.44 (1H, m), 3.40–3.33 (1H, m), 2.66–2.56 (1H, m), 2.43–2.33 (1H, m), 2.32–2.25 (1H, m), 2.10 (1H, td, *J* = 11.2, 3.2 Hz), 1.76–1.67 (2H, m), 1.61–1.52 (1H, m), 1.36–1.30 (1H, m), 1.29 (3H, t, *J* = 7.2 Hz), 1.28 (3H, t, *J* = 7.2 Hz), 1.20 (6H, s), 1.18 (6H, s), 0.86 (9H, s), –0.01 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.64, 168.55, 143.0, 140.2, 131.4, 128.6, 128.3, 125.6, 123.4, 83.2, 61.9, 61.71, 61.68, 56.0, 47.8, 46.1, 35.2, 34.8, 33.6, 26.1, 24.83, 24.76, 18.4, 14.2, –5.10, –5.14; HRMS (ESI+): Calcd for $C_{35}H_{58}B_1O_7Si_1$ $[M+H]^+$: 629.40448 m/z, Found: 629.40555 m/z.

Enantiomeric purity of **12i** was determined by HPLC analysis in comparison with authentic racemic material (93:7 e.r. shown; Chiralcel OZ–3 column, 99.6:0.4 hexanes/*i*-PrOH, 0.5 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ +1.2 (*c* 2.14, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.904	5622610	111450	49.519	51.688
2	28.551	5731937	104170	50.481	48.312



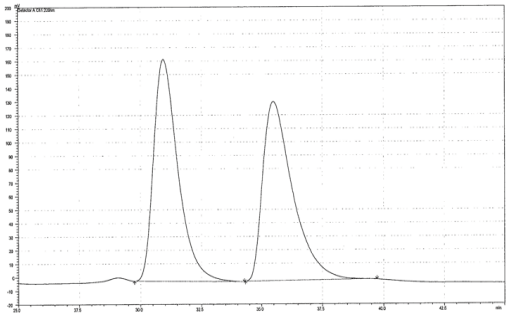
Peak#	Ret. Time	Area	Height	Area %	Height %
1	27.944	2330925	53714	6.945	8.744
2	29.238	31231665	560562	93.055	91.256

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	26.904	49.519	1	27.944	6.945
2	28.551	50.481	2	29.238	93.055

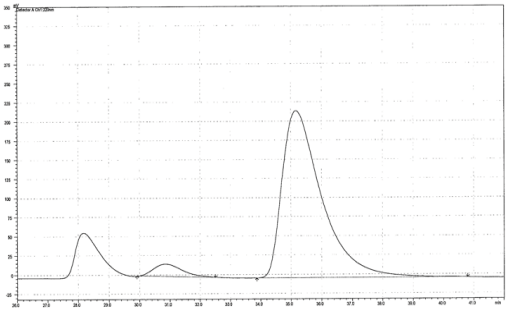
Diethyl 2-((1*E*,3*S*,4*S*,6*E*)-3,7-diphenyl-4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)hepta-1,6-dien-1-yl)malonate (12j):

IR (neat): 3026 (m), 2978 (m), 2934 (m), 1733 (s), 1600 (w), 1447 (m), 1369 (m), 1305 (m), 1141 (s), 1031 (m), 966 (m), 858 (m), 743 (m), 699 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.32–7.27 (3H, m), 7.24–7.14 (4H, m), 7.13–7.09 (3H, m), 6.31 (1H, d, *J* = 16.0 Hz), 6.10 (1H, dt, *J* = 16.0, 7.6 Hz), 5.88–5.86 (2H, m), 5.69 (1H, d, *J* = 3.6 Hz), 5.36 (1H, d, *J* = 3.6 Hz), 4.23 (2H, q, *J* = 7.2 Hz), 4.16 (2H, q, *J* = 7.2 Hz), 4.04–4.02 (1H, m), 3.71–3.66 (1H, m), 2.74–2.60 (2H, m), 2.48–2.40 (1H, m), 1.29 (3H, t, *J* = 7.2 Hz), 1.22 (6H, s), 1.21 (3H, t, *J* = 7.2 Hz), 1.20 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.5, 168.3, 143.3, 139.6, 138.1, 132.4, 130.7, 130.0, 128.5, 128.4, 128.3, 126.8, 126.1, 122.4, 83.2, 61.8, 61.6, 55.7, 53.4, 51.3, 36.3, 25.0, 24.7, 14.2, 14.1; HRMS (ESI+): Calcd for $C_{34}H_{44}B_1O_6$ $[M+H]^+$: 559.32309 m/z, Found: 559.32510 m/z.

Enantiomeric purity of **12j** was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; Chiralcel OD–H column, 99:1 hexanes/*i*-PrOH, 0.5 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ –18.0 (*c* 3.34, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	30.936	11401869	164195	50.078	55.344
2	35.492	11366271	132484	49.922	44.656



Peak#	Ret. Time	Area	Height	Area %	Height %
1	30.845	1058992	16095	5.146	6.875
2	35.160	19521928	217999	94.854	93.125

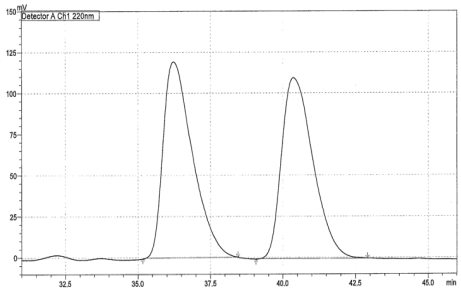
Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	30.936	50.078	1	30.845	5.146

2	35.492	49.922	2	35.160	94.854

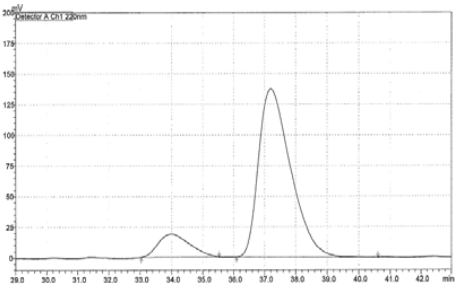
Diethyl 2-((3*S*,4*S*,*E*)-4-acetyl-8-(*tert*-butyldimethylsilyl)-3-phenyloct-1-en-7-yn-1-yl)malonate (12k):

IR (neat): 2954 (m), 2930 (m), 2856 (m), 2173 (m), 1733 (s), 1713 (s), 1463 (m), 1363 (m), 1250 (s), 1152 (s), 1032 (s), 970 (m), 837 (s), 775 (s), 701 (s), 680 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.30–7.26 (2H, m), 7.21–7.14 (3H, s), 5.86–5.76 (2H, m), 4.21 (2H, q, *J* = 7.2 Hz), 4.15 (2H, q, *J* = 7.2 Hz), 4.00–3.98 (1H, m), 3.50–3.45 (1H, m), 3.26–3.20 (1H, m), 2.30–2.23 (1H, m), 2.15–2.06 (1H, m), 1.83–1.79 (1H, m), 1.78 (3H, s), 1.27 (3H, t, *J* = 7.2 Hz), 1.21 (3H, t, *J* = 7.2 Hz), 0.95 (9H, s), 0.095 (3H, s), 0.091 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 211.9, 168.1, 167.9, 141.5, 136.4, 128.9, 127.9, 127.1, 124.0, 106.6, 84.1, 61.9, 61.8, 56.0, 55.6, 51.9, 32.4, 29.2, 26.2, 18.1, 16.7, 14.2, 14.1, –4.3; HRMS (ESI+): Calcd for $C_{29}H_{43}O_5Si_1$ $[M+H]^+$: 499.28797 m/z, Found: 499.28813 m/z.

Enantiomeric purity of **12k** was determined by HPLC analysis in comparison with authentic racemic material (88:12 e.r. shown; Chiralcel OZ–3 column, 99:1 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ –19.8 (*c* 0.50, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Conc.
1	36.225	8379336	119339	50.247
2	40.365	8296947	110102	49.753



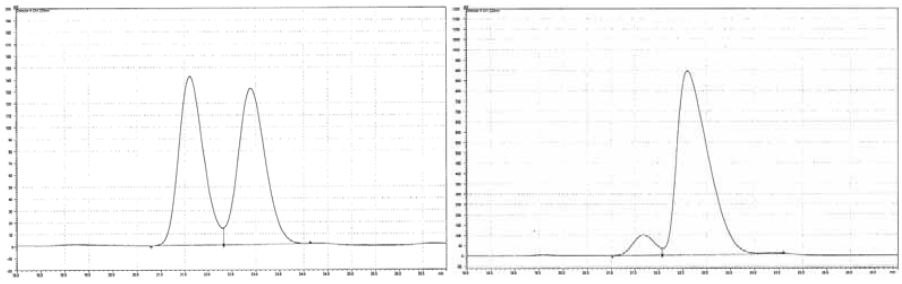
Peak#	Ret. Time	Area	Height	Conc.
1	33.987	1319370	18836	11.873
2	37.199	9792585	137375	88.127

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	36.225	50.247	1	33.987	11.873
2	40.365	49.753	2	37.199	88.127

Diethyl 2-((3*S*,4*S*,*E*)-7-(methoxy(methyl)amino)-7-oxo-3-phenyl-4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)hept-1-en-1-yl)malonate (12l):

IR (neat): 2978 (m), 2937 (m), 1732 (s), 1664 (s), 1445 (m), 1368 (s), 1305 (s), 1273 (m), 1140 (s), 1030 (s), 967 (s), 861 (m), 765 (m), 700 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.19–7.15 (2H, m), 7.09–7.05 (3H, m), 5.85 (1H, dd, *J* = 15.6, 8.4 Hz), 5.78 (1H, dd, *J* = 15.6, 8.4 Hz), 5.66 (1H, d, *J* = 3.6 Hz), 5.34 (1H, d, *J* = 3.6 Hz), 4.19 (2H, q, *J* = 7.2 Hz), 4.11 (2H, q, *J* = 7.2 Hz), 3.98 (1H, d, *J* = 7.6 Hz), 3.65–3.60 (1H, m), 3.61 (3H, s), 3.12 (3H, s), 2.54 (1H, dt, *J* = 10.8, 2.8 Hz), 2.37–2.29 (1H, m), 2.27–2.19 (1H, m), 2.09–2.01 (1H, m), 1.78–1.69 (1H, m), 1.25 (3H, t, *J* = 7.2 Hz), 1.22 (6H, s), 1.18 (6H, s), 1.16 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.4, 168.3, 143.7, 139.4, 132.4, 128.5, 128.2, 125.9, 122.4, 83.2, 61.7, 61.5, 61.2, 55.6, 53.5, 51.1, 26.9, 25.0, 24.7, 14.1, 14.0; HRMS (ESI+): Calcd for $C_{30}H_{45}B_1N_1O_8$ $[M+H]^+$: 558.32382 m/z, Found: 558.32521 m/z.

Enantiomeric purity of **12l** was determined by HPLC analysis in comparison with authentic racemic material (93:7 e.r. shown; Chiralcel OZ–3 column, 95:5 hexanes/*i*-PrOH, 0.5 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ –14.8 (*c* 2.14, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.605	5183810	141743	49.945	51.936
2	22.889	5195310	131174	50.055	48.064

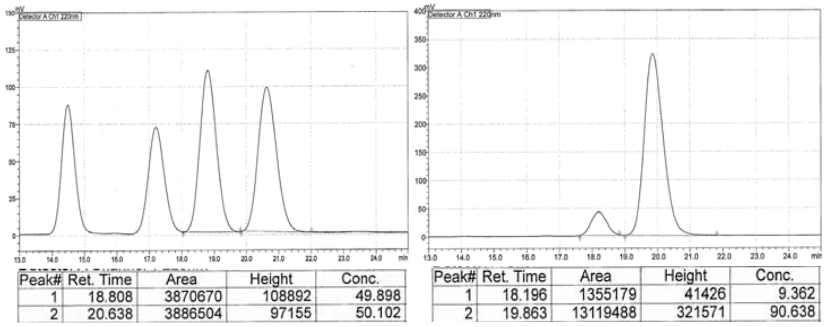
Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.676	3231853	100979	7.296	10.145
2	22.602	41067312	894396	92.704	89.855

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	21.605	49.945	1	21.676	7.296
2	22.889	50.055	2	22.602	92.704

(*R*,*E*)-Diethyl 2-(3-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexa-1,5-dien-1-yl)malonate (12m):

IR (neat): 2979 (m), 2934 (w), 1732 (s), 1616 (w), 1446 (m), 1367 (m), 1307 (m), 1211 (m), 1138 (s), 1030 (m), 969 (m), 862 (m), 758 (m), 699 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 600 MHz): δ 7.27–7.25 (2H, m), 7.18–7.15 (3H, m), 5.84 (1H, dd, *J* = 15.6, 7.2 Hz), 5.76 (1H, d, *J* = 3.6 Hz), 5.69 (1H, dd, *J* = 15.6, 7.2 Hz), 5.49 (1H, d, *J* = 3.6 Hz), 4.19 (2H, q, *J* = 7.2 Hz), 4.16 (2H, q, *J* = 7.2 Hz), 3.97 (1H, d, *J* = 9.0 Hz), 3.65 (1H, dt, *J* = 7.2, 7.2 Hz), 2.62–2.56 (2H, m), 1.27 (3H, t, *J* = 7.2 Hz), 1.24 (12H, s), 1.23 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 168.37, 168.36, 143.7, 139.9, 131.7, 128.4, 128.1, 126.2, 121.5, 83.4, 61.62, 61.57, 55.8, 47.9, 41.5, 24.9, 14.13, 14.08; HRMS (ESI+): Calcd for $C_{25}H_{36}B_1O_6$ $[M+H]^+$: 443.26049 m/z, Found: 443.26111 m/z.

Enantiomeric purity of **12m** was determined by HPLC analysis in comparison with authentic racemic material (91:9 e.r. shown; Chiralcel OZ–H column, 99.5:0.5 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ +5.9 (*c* 1.29, $CHCl_3$).



Peak#	Ret. Time	Area	Height	Conc.
1	18.808	3870670	108892	49.898
2	20.638	3886504	97155	50.102

Peak#	Ret. Time	Area	Height	Conc.
1	18.196	1355179	41426	9.362
2	19.863	13119488	321571	90.638

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	18.808	49.898	1	18.196	9.362
2	20.638	50.102	2	19.863	90.638

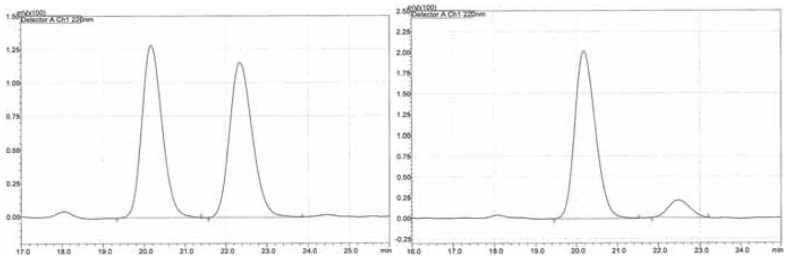
Determination of Stereochemical Identity

The absolute stereochemistry was determined by comparison of the ketone **S13** formed from oxidation of alkenylboron **12m** with $NaBO_3$•$4H_2O$ and hydration of alkyne **7a** in the presence of $Hg(OAc)_2$ and PPTS[8] and assigned as *R* enantiomer.

(*R*,*E*)-Diethyl 2-(5-oxo-3-phenylhex-1-en-1-yl)malonate (S13):

IR (neat): 2982 (m), 2936 (m), 1730 (s), 1602 (w), 1419 (m), 1367 (m), 1154 (s), 1030 (s), 971 (m), 861 (m), 756 (m), 701 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.31–7.26 (2H, m), 7.22–7.17 (3H, m), 5.84 (1H, dd, *J* = 15.6, 6.8 Hz), 5.71 (1H, dd, *J* = 15.6, 8.8 Hz), 4.19 (2H, q, *J* = 6.8 Hz), 4.17 (2H, q, *J* = 6.8 Hz), 3.97 (1H, d, *J* = 8.8 Hz), 3.96 (1H, td, *J* = 7.2, 6.8 Hz), 2.89 (1H, dd, *J* = 16.0, 7.2 Hz), 2.83 (1H, dd, *J* = 16.0, 7.2 Hz), 2.07 (3H, s), 1.26 (3H, t, *J* = 7.2 Hz), 1.23 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 206.7, 168.2, 168.1, 142.4, 138.3, 128.8, 127.8, 126.9, 122.0, 61.80, 61.75, 55.6, 49.1, 43.4, 30.8, 14.14, 14.11; HRMS (ESI+): Calcd for $C_{19}H_{25}O_5$ $[M+H]^+$: 333.17020 m/z, Found: 333.17047 m/z.

Enantiomeric purity of **S13** generated from oxidation of **12m** was determined by HPLC analysis in comparison with authentic racemic material (90:10 e.r. shown; Chiralcel OZ–H column, 95:5 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ +14.9 (*c* 1.28, $CHCl_3$).



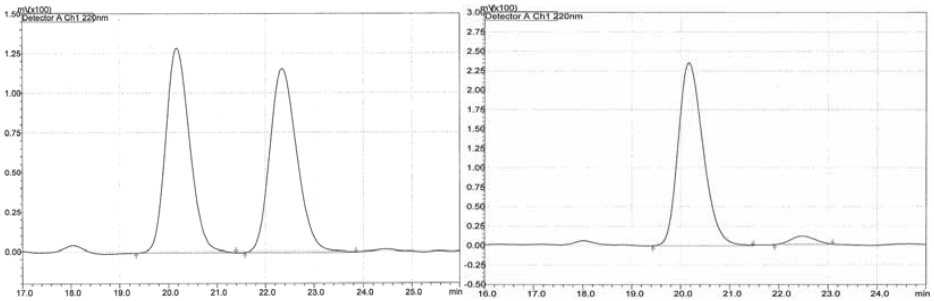
Peak#	Ret. Time	Area	Height	Conc.
1	20.170	4434161	129067	50.145
2	22.346	4408604	115382	49.855

Peak#	Ret. Time	Area	Height	Conc.
1	20.184	7113957	202532	90.279
2	22.486	765976	21024	9.721

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	20.170	50.145	1	20.184	90.279
2	22.346	49.855	2	22.486	9.279

Enantiomeric purity of **S13** generated from hydration of **7m** with $Hg(OAc)_2$ and PPTS was determined by HPLC analysis in comparison with authentic racemic material (97:3 e.r. shown; Chiralcel OZ–H column, 95:5 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm).

(8) Guérinot, A., Lepesqueux, G., Sablé, S., Reymond, S. & Cossy, J. *J. Org. Chem.* **75**, 5151–5163 (2010).



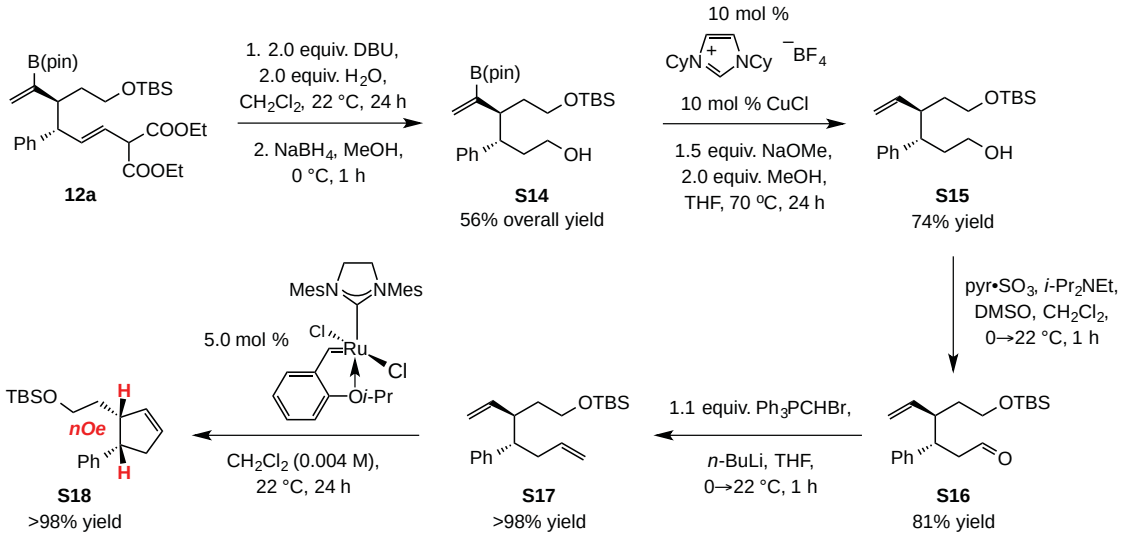
Peak#	Ret. Time	Area	Height	Conc.
1	20.170	4434161	129067	50.145
2	22.346	4408604	115382	49.855

Peak#	Ret. Time	Area	Height	Conc.
1	20.166	8379164	235854	97.061
2	22.475	253760	8791	2.939

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	20.170	50.145	1	20.166	97.061
2	22.346	49.855	2	22.475	2.939

The relative stereochemistry as illustrated below.

Scheme S3: Determination of Relative Stereochemistry of Products of Catalytic Multicomponent Reactions



(3*S*,4*S*)-4-(2-((*tert*-Butyldimethylsilyl)oxy)ethyl)-3-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-5-en-1-ol (S14):

To a solution of **12a** (1.41 g, 2.35 mmol) in CH_2Cl_2 (10 mL) is added DBU (703 µL, 4.70 mmol) and water (85 µL, 4.70 mmol) at 22 °C. The resulting solution is allowed to stir at 22 °C for 24 h. After this time, the solvent is evaporated under vacuum. The resulting yellow oil is purified by silica gel column chromatography (hexanes:ethyl acetate = 25:1) to afford 1.322 g aldehyde mixed with diethyl malonate as yellow oil. The yellow oil was dissolved in methanol (20 mL) followed by addition of $NaBH_4$ (202 mg, 5.33 mmol) at 0 °C. The resulting solution was allowd to stir at 22 °C for 2 h. The solvent was evaporated under vacuum and the resulting yellow oil was purified by silica gel column chromatography (hexanes:ethyl acetate = 8:1) to afford 612 mg alcohol **S14** (1.33 mmol, 56% yield) as yellow oil. IR (neat): 3464 (br), 2953 (m), 2929 (m), 2857 (m), 1608 (w), 1388 (m), 1306 (m), 1142 (s), 1093 (s), 969 (m), 835 (s), 775 (m), 701 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.22–7.16 (2H, m), 7.12–7.06 (3H, m), 5.66 (1H, d, *J* = 3.6 Hz), 5.29 (1H, d, *J* = 3.6 Hz), 3.59–3.53 (1H, m), 3.51–

3.39 (3H, m), 2.97–2.91 (1H, m), 2.56–2.50 (1H, m), 2.21–2.13 (1H, m), 1.97–1.89 (1H, m), 1.78–1.69 (2H, m), 1.57 (1H, br s), 1.22 (6H, s), 1.19 (6H, s), 0.88 (9H, s), 0.02 (3H, s), 0.01 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.0, 131.6, 128.9, 128.1, 126.0, 83.2, 62.0, 61.8, 48.6, 46.3, 36.4, 34.5, 26.1, 25.0, 24.7, 18.4, –5.1; HRMS (ESI+): Calcd for $C_{26}H_{46}B_1O_4Si_1$ $[M+H]^+$: 461.32584 m/z, Found: 461.32602 m/z.

(3*S*,4*R*)-4-(2-((*tert*-Butyldimethylsilyl)oxy)ethyl)-3-phenylhex-5-en-1-ol (S15):

S15 was prepared according to a previously reported procedure.[9] IR (neat): 3346 (br), 2952 (m), 2929 (m), 2857 (m), 1602 (w), 1420 (w), 1254 (m), 1094 (s), 937 (m), 834 (s), 774 (s), 701 (s), 663 (s) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.28–7.25 (2H, m), 7.21–7.17 (1H, m), 7.13–7.11 (2H, m), 5.41 (1H, dt, *J* = 16.8, 10.0 Hz), 5.01 (1H, dd, *J* = 10.0, 2.0 Hz), 4.94 (1H, dd, *J* = 17.2, 2.0 Hz), 3.62–3.44 (4H, m), 2.81–2.76 (1H, m), 2.45–2.38 (1H, m), 2.04–1.91 (2H, m), 1.76–1.68 (1H, m), 1.30 (1H, br s), 1.31–1.23 (1H, m), 0.88 (9H, s), 0.02 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.9, 139.5, 129.1, 128.1, 126.4, 116.6, 61.30, 61.26, 46.3, 45.7, 36.4, 35.8, 26.1, 18.4, –5.1, –5.2; HRMS (ESI+): Calcd for $C_{20}H_{35}O_2Si_1$ $[M+H]^+$: 335.24063 m/z, Found: 335.24137 m/z.

(3*S*,4*R*)-4-(2-((*tert*-Butyldimethylsilyl)oxy)ethyl)-3-phenylhex-5-enal (S16):

S16 was prepared according to a previously reported procedure.[8] IR (neat): 2953 (m), 2929 (m), 2856 (m), 1725 (s), 1603 (w), 1454 (m), 1253 (m), 1093 (s), 1031 (m), 918 (m), 833 (s), 774 (s), 701 (s), 662 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.65 (1H, t, *J* = 2.0 Hz), 7.30–7.26 (2H, m), 7.24–7.18 (1H, m), 7.15–7.12 (2H, m), 5.39 (1H, dt, *J* = 17.2, 10.0 Hz), 5.08 (1H, dd, *J* = 10.0, 2.0 Hz), 4.98 (1H, dd, *J* = 17.2, 2.0 Hz), 2.83–2.81 (2H, m), 2.48–2.41 (1H, m), 1.74–1.66 (1H, m), 1.32–1.23 (1H, m), 0.88 (9H, s), 0.01 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 202.1, 140.7, 138.5, 129.0, 128.3, 126.8, 117.6, 61.0, 47.5, 45.3, 43.8, 35.7, 26.1, 18.4, –5.18, –5.21; HRMS (ESI+): Calcd for $C_{20}H_{33}O_2Si_1$ $[M+H]^+$: 333.22498 m/z, Found: 333.22592 m/z.

***tert*-Butyldimethyl(((3*R*,4*S*)-4-phenyl-3-vinylhept-6-en-1-yl)oxy)silane (S17):**

S17 was prepared according to a previously reported procedure.[8] IR (neat): 2953 (m), 2928 (m), 2857 (m), 1603 (w), 1453 (m), 1388 (m), 1253 (m), 1097 (s), 1004 (m), 912 (s), 833 (s), 773 (s), 701 (s), 662 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.30–7.26 (2H, m), 7.22–7.17 (1H, m), 7.14–7.12 (2H, m), 5.73–5.63 (1H, m), 5.40 (1H, dt, *J* = 16.8, 10.0 Hz), 5.07–4.92 (4H, m), 3.64–3.58 (1H, m), 3.54–3.48 (1H, m), 2.75–2.70 (1H, m), 2.56–2.44 (3H, m), 1.76–1.68 (1H, m), 1.34–1.25 (1H, m), 0.91 (9H, s), 0.04 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 142.1, 139.3, 137.4, 129.3, 127.9, 126.2, 116.7, 116.1, 61.3, 49.7, 44.6, 37.8, 36.1, 26.1, 18.4, –5.12, –5.14; HRMS (ESI+): Calcd for $C_{21}H_{35}O_1Si_1$ $[M+H]^+$: 331.24572 m/z, Found: 331.24422 m/z.

***tert*-Butyldimethyl(2-((1*R*,5*S*)-5-phenylcyclopent-2-en-1-yl)ethoxy)silane (S18):**

To a solution of **S17** (74 mg, 0.245 mmol) in CH_2Cl_2 (50 mL) is added Ru complex (7.7 mg, 0.0122 mmol) at 22 °C and the mixture was allowed to stir at 22 °C for 24 h. After this time, the solution is concentrated under vacuum and the resulting dark green oil is purified by silica gel chromatography

(9) Meng, F., McGrath, K. P. & Hoveyda, A. H. *Nature* **513**, 367–374 (2014).

(hexanes:diethyl ether = 100:1) to afford 67.4 mg **S18** (0.222 mmol, 99% yield) as colorless oil. IR (neat): 2953 (m), 2928 (m), 2956 (m), 1493 (m), 1360 (w), 1254 (m), 1096 (s), 1006 (w), 982 (w), 834 (s), 774 (s), 699 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.31–7.18 (5H, m), 5.92–5.87 (2H, m), 3.61–3.55 (1H, m), 3.51–3.42 (2H, m), 3.05–2.99 (1H, m), 2.74–2.64 (2H, m), 1.30–1.24 (1H, m), 1.20–1.11 (1H, m), 0.87 (9H, s), –0.02 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 143.1, 135.1, 130.1, 128.5, 128.2, 126.1, 62.2, 47.5, 45.9, 37.7, 34.2, 26.1, 18.4, –5.2; HRMS (ESI+): Calcd for $C_{19}H_{31}O_1Si_1$ $[M+H]^+$: 303.21442 m/z, Found: 303.21426 m/z.

Procedure for Isomerization of 1,6-Conjugate Addition Products

To a solution of substrate **4a** (15.0 mg, 0.049 mmol) in CH_2Cl_2 (1 mL) is added DABCO (11.0 mg, 0.098 mmol) at 22 °C. The resulting solution is allowed to stir at 22 °C for 16 h. After this time, the solvent is evaporated. The resulting yellow oil is purified by silica gel chromatography (hexanes:ethyl acetate = 15:1) to afford 14.2 mg **14** (0.045 mmol, 95% yield) as colorless oil.

(*S*)-Diethyl 2-(3-phenylhex-5-yn-1-ylidene)malonate (14):

IR (neat): 3290 (m), 2982 (m), 2936 (w), 1722 (s), 1453 (m), 1376 (m), 1254 (s), 1224 (s), 1096 (m), 1024 (m), 863 (w), 760 (m), 701 (m), 642 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.34–7.30 (2H, m), 7.26–7.20 (3H, m), 6.87 (1H, t, *J* = 7.6 Hz), 4.29 (2H, q, *J* = 7.2 Hz), 4.19 (2H, q, *J* = 7.2 Hz), 3.03–2.98 (1H, m), 2.92–2.85 (1H, m), 2.74–2.62 (1H, m), 2.53–2.50 (2H, m), 1.98 (1H, t, *J* = 2.8 Hz), 1.32 (3H, t, *J* = 7.2 Hz), 1.25 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.4, 163.9, 146.8, 142.3, 130.0, 128.8, 127.5, 127.2, 82.0, 70.6, 61.4, 44.0, 34.9, 26.0, 14.3, 14.2; HRMS (ESI+): Calcd for $C_{19}H_{23}O_4$ $[M+H]^+$: 315.15963 m/z, Found: 315.16105 m/z. Specific rotation: $[\alpha]_D^{20}$ –4.2 (*c* 1.13, $CHCl_3$).

Procedure for Conversion to Aldehydes

To a solution of **4a** (400 mg, 1.27 mmol) in CH_2Cl_2 (5 mL) is added DBU (380 μL, 2.54 mmol) and water (46 μL, 2.54 mmol) at 22 °C. The resulting solution is allowed to stir at 22 °C for 24 h. After this time, the solvent is evaporated under vacuum. The resulting yellow oil is purified by silica gel column chromatography (hexanes:ethyl acetate = 25:1) to afford 128 mg aldehyde **15a** (0.74 mmol, 58% overall yield) as yellow oil.

(*R*)-3-Phenylhex-5-ynal (15a):

IR (neat): 3288 (m), 2920 (m), 2832 (m), 2728 (m), 1721 (s), 1495 (m), 1390 (w), 1283 (m), 1181 (m), 1068 (m), 1029 (m), 762 (m), 701 (s), 642 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 9.73 (1H, t, *J* = 1.6 Hz), 7.34–7.30 (2H, m), 7.26–7.22 (3H, m), 3.50–3.43 (1H, m), 3.04 (1H, ddd, *J* = 17.2, 6.0, 1.6 Hz), 2.84 (1H, ddd, *J* = 17.2, 8.0, 1.6 Hz), 2.59 (1H, ddd, *J* = 16.8, 6.4, 2.4 Hz), 2.51 (1H, ddd, *J* = 16.8, 7.6, 2.8 Hz), 2.02 (1H, t, *J* = 2.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 201.1, 142.5, 128.8, 127.4, 127.3, 81.8, 71.0, 48.5, 38.6, 26.1; HRMS (ESI+): Calcd for $C_{12}H_{13}O_1$ $[M+H]^+$: 173.09664 m/z, Found: 173.09651 m/z. Specific rotation: $[\alpha]_D^{20}$ –8.3 (*c* 0.60, $CHCl_3$).

(*R*)-3-(2-Methoxyphenyl)hex-5-ynal (15b):

IR (neat): 3288 (m), 2919 (m), 2838 (m), 2726 (m), 1721 (s), 1600 (m), 1493 (s), 1463 (m), 1292 (m), 1242 (s), 1120 (m), 1028 (m), 935 (w), 755 (s), 644 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 9.72 (1H,

t, *J* = 2.0 Hz), 7.25–7.19 (2H, m), 6.92 (1H, td, *J* = 7.6, 1.2 Hz), 6.87 (1H, d, *J* = 8.0 Hz), 3.88–3.81 (1H, m), 3.84 (3H, s), 3.00 (1H, ddd, *J* = 16.8, 6.4, 2.0 Hz), 2.84 (1H, ddd, *J* = 16.8, 8.0, 2.0 Hz), 2.63 (1H, ddd, *J* = 16.8, 6.4, 2.0 Hz), 2.56 (1H, ddd, *J* = 16.8, 8.0, 2.0 Hz), 1.99 (1H, t, *J* = 2.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 202.0, 157.0, 130.2, 128.2, 128.0, 120.8, 110.8, 82.4, 70.6, 55.4, 47.3, 32.9, 24.0; HRMS (ESI+): Calcd for $C_{13}H_{15}O_2$ $[M+H]^+$: 203.10720 m/z, Found: 203.10803 m/z. Specific rotation: $[\alpha]_D^{20}$ –9.1 (*c* 0.56, $CHCl_3$).

(*R*)-3-(*tert*-Butyl)hex-5-ynal (15c):

IR (neat): 3289 (m), 2962 (m), 2872 (m), 2719 (m), 1724 (s), 1471 (m), 1397 (m), 1290 (m), 1227 (m), 1074 (w), 1018 (w), 639 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.86 (1H, t, *J* = 2.0 Hz), 2.61–2.49 (2H, m), 2.47–2.41 (1H, m), 2.15–2.07 (2H, m), 1.98 (1H, t, *J* = 2.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 202.7, 83.6, 70.8, 44.9, 42.2, 33.4, 27.7, 20.0; HRMS (ESI+): Calcd for $C_{13}H_{15}O_2$ $[M+H]^+$: 153.12794 m/z, Found: 153.12811 m/z. Specific rotation: $[\alpha]_D^{20}$ –5.7 (*c* 0.37, $CHCl_3$).

(*R*)-3-methyl-3-phenylhex-5-ynal (16):

IR (neat): 3289 (m), 2970 (m), 2927 (m), 2848 (m), 2740 (m), 1719 (s), 1601 (w), 1498 (m), 1382 (m), 1248 (m), 1157 (m), 1032 (m), 912 (w), 763 (m), 700 (s), 643 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.54 (1H, t, *J* = 2.8 Hz), 7.40–7.34 (4H, m), 7.27–7.23 (1H, m), 2.95 (1H, dd, *J* = 16.0, 2.4 Hz), 2.80 (1H, dd, *J* = 16.0, 2.8 Hz), 2.67 (1H, dd, *J* = 16.8, 2.8 Hz), 2.60 (1H, dd, *J* = 16.8, 2.8 Hz), 2.03 (1H, t, *J* = 2.8 Hz), 1.59 (3H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 202.2, 144.9, 128.8, 127.0, 126.0, 81.0, 71.7, 53.6, 39.6, 32.9, 25.9; HRMS (ESI+): Calcd for $C_{13}H_{15}O_1$ $[M+H]^+$: 187.11229 m/z, Found: 187.11313 m/z. Specific rotation: $[\alpha]_D^{20}$ –4.3 (*c* 0.48, $CHCl_3$).

Procedure for Methylation of 1,6-Conjugate Addition Product

To a solution of diester **4a** (200 mg, 0.64 mmol) in thf (3 mL) is added NaH (31 mg, 0.76 mmol) at 0 °C. The mixture is allowed to stir at 0 °C for 1 h, after which MeI (119 μL, 1.91 mmol) is added through a syringe at 0 °C. After the solution is allowed to stir at 22 °C for 18 h, the reaction is then quenched by addition of a saturated solution of aqueous NH_4Cl (3 mL). The water layer is washed with Et_2O (2 × 3 mL), and the combined organic layers are dried over $MgSO_4$ and concentrated under vacuum. The resulting yellow oil is purified by silica gel chromatography (hexanes:ethyl acetate = 15:1) to afford 150 mg **17** (0.48 mmol, 75% yield) as yellow oil.

(*R*,*E*)-Diethyl 2-methyl-2-(3-phenylhex-1-en-5-yn-1-yl)malonate (17):

IR (neat): 3294 (m), 2983 (m), 2938 (m), 2911 (w), 1730 (s), 1601 (w), 1453 (m), 1377 (m), 1256 (s), 1108 (s), 1021 (m), 972 (m), 862 (m), 759 (m), 700 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.33–7.29 (2H, m), 7.24–7.21 (3H, m), 6.07 (1H, dd, *J* = 16.4, 1.2 Hz), 5.82 (1H, dd, *J* = 16.0, 7.2 Hz), 4.19 (2H, q, *J* = 7.2 Hz), 4.17 (2H, q, *J* = 7.2 Hz), 3.59 (1H, td, *J* = 7.2, 6.8 Hz), 2.66–2.54 (2H, m), 1.94 (1H, t, *J* = 2.8 Hz), 1.56 (3H, s), 1.25 (3H, t, *J* = 7.2 Hz), 1.22 (3H, t, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 171.3, 171.2, 142.4, 133.2, 129.4, 128.6, 127.7, 126.9, 82.2, 70.2, 61.6, 55.6, 47.0, 25.5, 20.5, 14.15, 14.11; HRMS (ESI+): Calcd for $C_{20}H_{25}O_4$ $[M+H]^+$: 329.17528 m/z, Found: 329.17576 m/z. Specific rotation: $[\alpha]_D^{20}$ –5.2 (*c* 1.68, $CHCl_3$).

Procedure for Enantioselective Desymmetrization of Diesters

(*R*,*E*)-Diethyl 2-methyl-2-(3-phenylhex-1-en-5-yn-1-yl)malonate (**17**) (35 mg, 0.11 mmol) is first dissolved in DMSO (0.5 mL) and phosphate buffer (pH = 8, 1.5 mL) and then pig liver esterase (PLE) is introduced (11 mg). The solution is allowed to stir at 22 °C for 0.5 h after which the reaction is quenched by addition of diethyl ether (10 mL). The organic layer is washed with brine three times (3 × 5 mL), dried over $MgSO_4$ and concentrated *in vacuo*. The residue was dissolved in dry THF (1.0 mL). At 0 °C, $ClCO_2Me$ (13 μL, 0.165 mmol) and Et_3N (22 μL, 0.165 mmol) are added. The mixture is allowed to stir at 22 °C for 1 h. After filtration and removal of volatiles *in vacuo*, the residue is dissolved in MeOH (1.0 mL) and $NaBH_4$ (15 mg, 0.33 mmol) is added at 0 °C. The solution is then allowed to stir at 0 °C for 1 h. At this time, the reaction is quenched by addition of a saturated solution of NH_4Cl. The aqueous layer is washed with ethyl acetate (3 × 5 mL) and the combined organic layers are dried over $MgSO_4$, concentrated and purified by silica gel chromatography (hexanes/ethyl acetate = 8:1) to afford **18** (25 mg, 72% overall yield) as colorless oil.

(2*R*,5*R*,*E*)-Dthyl 2-(hydroxymethyl)-2-methyl-5-phenyloct-3-en-7-ynoate (18):

IR (neat): 3486 (br), 3294 (m), 2978 (m), 2925 (m), 2854 (m), 1722 (s), 1494 (m), 1453 (m), 1375 (m), 1233 (m), 1123 (m), 1041 (s), 974 (m), 864 (m), 759 (m), 699 (s), 635 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.19–7.32 (m, 5H), 5.82 (dd, 1H, *J* = 16.0, 7.2 Hz), 5.67 (dd, 1H, *J* = 16.0, 1.2 Hz), 4.16 (qd, 2H, *J* = 7.2, 3.2 Hz), 3.72 (dd, 1H, *J* = 11.2, 6.4 Hz), 3.57 (dd, 1H, *J* = 11.2, 6.4 Hz), 3.53 (td, 1H, *J* = 7.6, 7.2 Hz), 2.57 (dd, 2H, *J* = 6.8, 2.0 Hz), 2.32 (t, 1H, *J* = 6.4 Hz), 1.94 (t, 1H, *J* = 2.4 Hz); 1.31 (s, 3H), 1.24 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 175.4, 142.5, 132.9, 128.5, 127.5, 126.8, 82.2, 70.0, 68.4, 61.0, 50.0, 47.2, 25.6, 19.6, 14.1; HRMS (ESI+): Calcd for $C_{18}H_{23}O_3$ $[M+H]^+$: 287.16472 m/z, Found: 287.16536 m/z. Specific rotation: $[\alpha]_D^{20}$ –3.4 (*c* 0.41, $CHCl_3$).

Conversion to a γ,δ-unsaturated carbonyl compounds:

Diethyl 2-((3*S*,4*S*,*E*)-4-acetyl-6-((*tert*-butyldimethylsilyl)oxy)-3-phenethylhex-1-en-1-yl)malonate (19):

IR (neat): 2953 (m), 2930 (m), 2857 (m), 1733 (s), 1710 (m), 1603 (w), 1471 (m), 1366 (m), 1253 (m), 1149 (m), 1095 (m), 1032 (m), 974 (m), 834 (s), 776 (m), 700 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.28–7.24 (2H, m), 7.19–7.11 (3H, m), 5.73 (1H, dd, *J* = 15.6, 8.4 Hz), 5.39 (1H, dd, *J* = 15.6, 9.6 Hz), 4.25–4.18 (4H, m), 4.03 (1H, d, *J* = 8.4 Hz), 3.53–3.46 (2H, m), 2.70–2.61 (1H, m), 2.60–2.56 (1H, m), 2.50–2.43 (1H, m), 2.37–2.29 (1H, m), 2.06 (3H, s), 1.77–1.52 (4H, m), 1.28 (3H, t, *J* = 7.2 Hz), 1.27 (3H, t, *J* = 7.2 Hz), 0.86 (9H, s), –0.003 (6H, s); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 211.7, 168.23, 168.16, 141.8, 137.2, 128.6, 128.5, 126.0, 124.7, 61.83, 61.81, 61.4, 55.7, 54.1, 44.4, 34.3, 33.4, 32.6, 30.3, 26.0, 18.4, 14.21, 14.18, –5.36, –5.40; HRMS (ESI+): Calcd for $C_{29}H_{50}N_1O_6Si_1$ $[M+H]^+$: 536.34074 m/z, Found: 536.33899 m/z. Specific rotation: $[\alpha]_D^{20}$ +8.4 (*c* 1.25, $CHCl_3$).

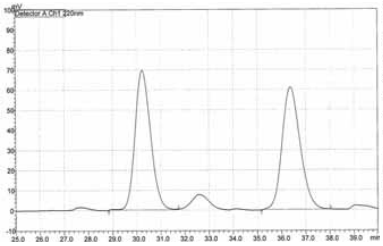
Formal Synthesis of (–)-Equisetin

(*R*,*E*)-Diethyl 2-(3-methylhex-1-en-5-yn-1-yl)malonate (4n):

IR (neat): 3290 (m), 2980 (m), 2931 (m), 1731 (s), 1459 (m), 1369 (m), 1259 (m), 1217 (m), 1150 (m), 1032 (m), 972 (m), 863 (w), 635 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 5.77–5.66 (2H, m), 4.20

(4H, q, *J* = 7.2 Hz), 3.97 (1H, d, *J* = 7.6 Hz), 2.48–2.41 (1H, m), 2.28–2.14 (2H, m), 1.97 (1H, t, *J* = 2.4 Hz), 1.26 (6H, t, *J* = 7.2 Hz), 1.12 (3H, d, *J* = 7.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 168.4, 140.2, 121.1, 82.5, 69.8, 61.7, 55.7, 35.7, 25.9, 19.2, 14.2; HRMS (ESI+): Calcd for $C_{14}H_{21}O_4$ $[M+H]^+$: 253.14398 m/z, Found: 253.14394 m/z.

Enantiomeric purity of **4n** was determined by HPLC analysis in comparison with authentic racemic material (92:8 e.r. shown; Chiralcel OZ–H column, 99:1 hexanes/*i*-PrOH, 0.8 mL/min, 220 nm). Specific rotation: $[\alpha]_D^{20}$ –3.6 (*c* 0.89, $CHCl_3$).



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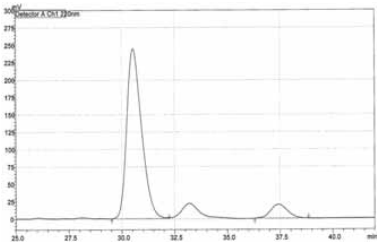

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1	30.537	11976188	244310	91.512
2	37.426	1110816	19974	8.488

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	30.235	49.909	1	30.537	91.512
2	36.374	50.091	2	37.426	8.488

Diethyl 2-((*R*,1*E*,5*E*)-3-methyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexa-1,5-dien-1-yl)malonate (20):

Alkenylboronotae **20** was prepared according to a previously reported procedure.[10] IR (neat): 2978 (m), 2932 (m), 1733 (s), 1637 (m), 1361 (s), 1318 (s), 1215 (m), 1143 (s), 1032 (m), 969 (m), 849 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.53 (1H, dt, *J* = 18.0, 6.8 Hz), 5.69–5.59 (2H, m), 5.42 (1H, dd, *J* = 18.0, 1.6 Hz), 4.19 (2H, q, *J* = 7.2 Hz), 4.18 (2H, q, *J* = 7.2 Hz), 2.36–2.30 (1H, m), 2.26–2.19 (1H, m), 2.14–2.07 (1H, m), 1.25 (12H, s), 1.00 (3H, d, *J* = 6.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 168.55, 168.53, 152.1, 141.8, 120.2, 83.1, 61.6, 55.8, 43.2, 35.8, 24.9, 19.6, 14.19, 14.17; HRMS (ESI+): Calcd for $C_{20}H_{34}B_1O_6$ $[M+H]^+$: 381.24484 m/z, Found: 381.24567 m/z. Specific rotation: $[\alpha]_D^{20}$ –5.4 (*c* 1.52, $CHCl_3$).

(*R*,*E*)-Ethyl 2,6-dimethyl-8-oxooct-2-enoate (21):

To a solution of alkyne **20** (4.61 g, 12.1 mmol) in THF (50 mL) and H_2O (50 mL) is added $NaBO_3$•$4H_2O$ (11.2 g, 36.4 mmol) at 22 °C. The resulting mixture is allowed to stir at 22 °C for 1 h after which Et_2O (30 mL) is added and the aqueous layer is washed with Et_2O (2 × 30 mL). The combined organic layers are concentrated under vacuum, affording yellow oil that is then dissolved in CH_2Cl_2 (100 mL) and treated with the Wittig reagent (4.83 g, 13.3 mmol). The resulting mixutre is allowed to stir at 22°C for 12 h. At this time, DBU (3.7 mL, 24.2 mmol) and H_2O (0.9 mL, 24.2 mmol) are added, and the mixture is allowed to stir at 22 °C for another 24 h. The solution is then concentrated under vacuum and the resulting yellow solid purified by silica gel chromatography (hexanes/ethyl acetate = 10:1) to give **21** (1.72 g, 67% overall yield) as colorless oil. The physical and spectral data

(10) Jang, H., Zhugralin, A. R., Lee, Y. & Hoveyda, A. H. *J. Am. Chem. Soc.* **133**, 7859–7871 (2011).

were identical to those previous reported.[11] ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.75 (1H, t, *J* = 2.0 Hz), 6.73–6.69 (1H, m), 4.18 (4H, q, *J* = 7.2 Hz), 2.44–2.38 (1H, m), 2.30–2.22 (1H, m), 2.18–2.06 (3H, m), 1.82 (3H, s), 1.51–1.44 (1H, m), 1.41–1.34 (1H, m), 1.28 (3H, t, *J* = 7.2 Hz), 0.98 (3H, d, *J* = 6.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 202.5, 168.2, 141.4, 128.3, 60.6, 51.0, 35.6, 27.9, 26.2, 19.8, 14.4, 12.5. Specific rotation: $[\alpha]_D^{20}$ +13.7 (*c* 2.69, $CHCl_3$).

(*R*,2*E*,8*E*)-Ethyl 2,6-dimethyl-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nona-2,8-dienoate (22):

To a suspension of $CrCl_2$ (15.9 g, 130 mmol) in THF (100 mL) is added $Cl_2CHB(pin)$ (6.83 g, 32.4 mmol) and aldehyde **21** (3.44 g, 16.2 mmol) at 22 °C; this is followed by the addition of a solution of LiI (8.67 g, 64.8 mmol) in THF (50 mL). The mixture is allowed to stir at 22 °C for 16 h, after which the reaction is quenched by addition of a saturated solution of aqueous NH_4Cl. The aqueous layer is then washed with Et_2O (2 × 80 mL) and the combined organic layers are concentrated under vacuum. The resulting green oil is purified by silica gel chromatography (hexanes/ethyl acetate = 20:1) to give the **22** (5.11 g, 94% yield) as colorless oil. IR (neat): 2977 (m), 2928 (m), 1708 (s), 1638 (m), 1459 (m), 1362 (s), 1319 (s), 1267 (s), 1143 (s), 1095 (m), 1032 (m), 970 (m), 849 (m), 744 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.72 (1H, td, *J* = 7.2, 2.0 Hz), 6.57 (1H, dt, *J* = 18.0, 7.2 Hz), 5.42 (1H, d, *J* = 18.0 Hz), 4.17 (2H, q, *J* = 7.2 Hz), 2.22–2.09 (3H, m), 2.05–1.98 (1H, m), 1.81 (3H, s), 1.64–1.55 (1H, m), 1.51–1.41 (1H, m), 1.28 (3H, t, *J* = 7.2 Hz), 1.25 (12H, s), 0.90 (3H, d, *J* = 6.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 168.4, 152.9, 142.4, 127.8, 83.1, 60.5, 43.5, 35.4, 32.3, 26.4, 24.9, 19.6, 14.4, 12.4; HRMS (ESI+): Calcd for $C_{19}H_{34}B_1O_4$ $[M+H]^+$: 337.25501 m/z, Found: 337.25570 m/z. Specific rotation: $[\alpha]_D^{20}$ +4.1 (*c* 4.46, $CHCl_3$).

(*R*,2*E*,8*E*,10*E*)-Ethyl 12-(methoxymethoxy)-2,6-dimethyldodeca-2,8,10-trienoate (24):

To a solution of alkenylboronate **22** at 22 °C (100 mg, 0.297 mmol) and iodide **23** (102 mg, 0.446 mmol) in DMF (3 mL) is added $Ba(OH)_2•8H_2O$ (141 mg, 0.446 mmol) and $Pd(dppf)Cl_2$ (12.1 mg, 0.0149 mmol). The mixture is allowed to stir at 22 °C for 16 h and then the reaction is quenched by addition of water (5 mL) and Et_2O (5 mL). The aqueous layer is washed with Et_2O (2 × 5 mL) and the combined organic layer are concentrated under vacuum and the resulting yellow oil is purified by silica gel chromatography (hexanes/ethyl acetate = 10:1) to afford **24** (90.6 g, 94% yield) as colorless oil. IR (neat): 2952 (m), 2927 (m), 1707 (s), 1650 (m), 1459 (m), 1379 (m), 1263 (m), 1147 (s), 1099 (s), 1038 (s), 990 (s), 922 (m), 745 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.72 (1H, td, *J* = 7.2, 1.2 Hz), 6.23 (1H, dd, *J* = 15.2, 10.4 Hz), 6.03 (1H, dd, *J* = 15.2, 10.4 Hz), 5.69–5.60 (2H, m), 4.63 (2H, s), 4.17 (2H, q, *J* = 7.2 Hz), 4.07–4.05 (2H, m), 3.36 (3H, s), 2.20–2.05 (3H, m), 1.98–1.91 (1H, m), 1.81 (3H, s), 1.56–1.40 (2H, m), 1.28 (3H, t, *J* = 7.2 Hz), 0.88 (2H, d, *J* = 6.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 168.4, 142.3, 133.8, 133.4, 131.0, 127.8, 126.7, 95.6, 67.7, 60.5, 55.3, 40.1, 35.3, 33.0, 26.4, 19.4, 14.4, 12.4; HRMS (ESI+): Calcd for $C_{18}H_{34}N_1O_4$ $[M+NH_4]^+$: 328.24878 m/z, Found: 328.24770 m/z. Specific rotation: $[\alpha]_D^{20}$ –0.9 (*c* 2.53, $CHCl_3$).

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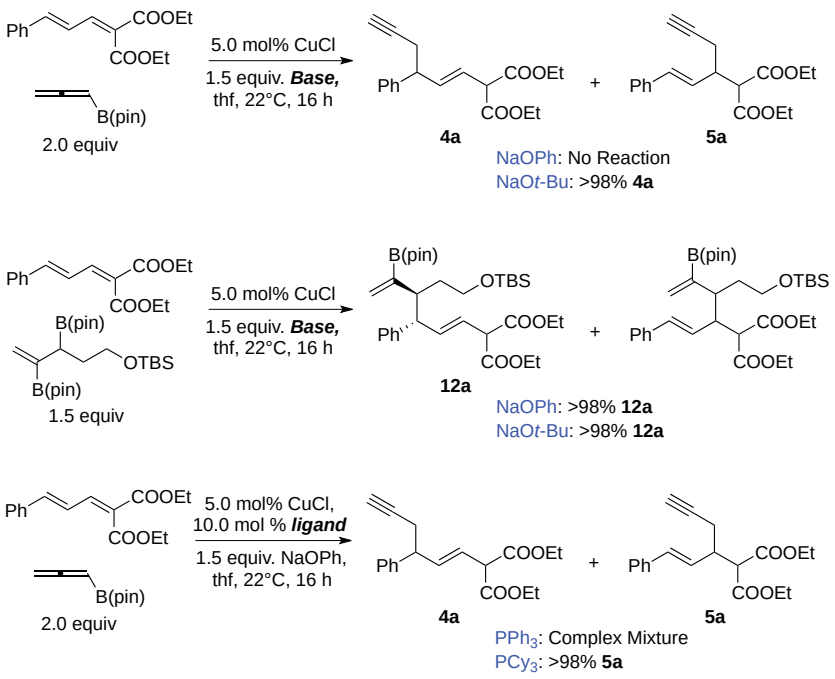
(11) Yin, J., Wang, C., Kong, L., Cai, S. & Gao, S. *Angew. Chem. Int. Edn* **51**, 7786–7789 (2012).

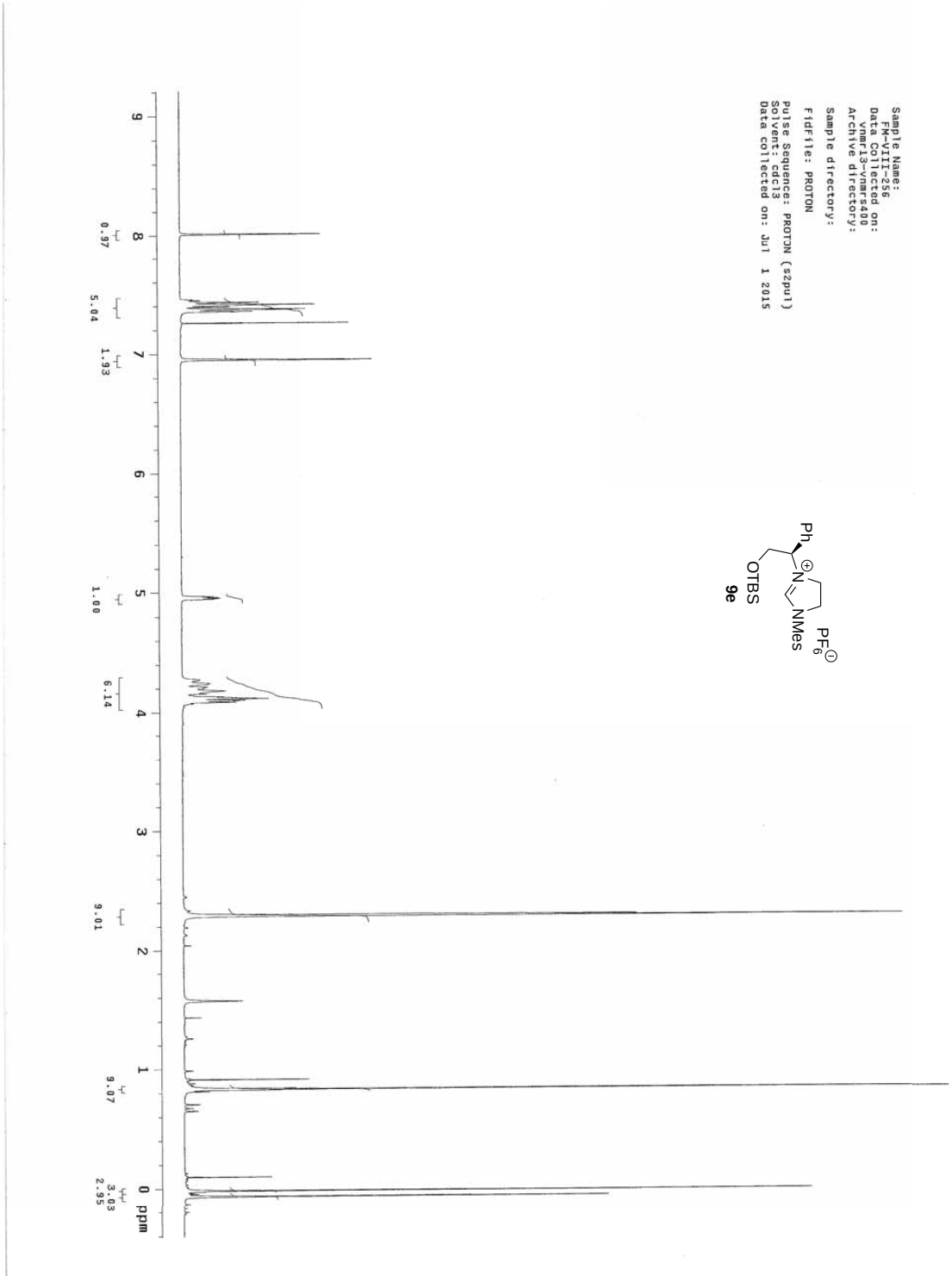
Data for Background and Control Experiments

Scheme S4: Background and Control Experiments



3. NMR Spectra

The ^{1}H and ^{13}C NMR spectra of the compounds mentioned above are shown in the following pages: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Archive directory:
Sample directory:
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Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 1 2015
Ph
N
NMes
OTBS
9e
$PF_6^{\ominus}$
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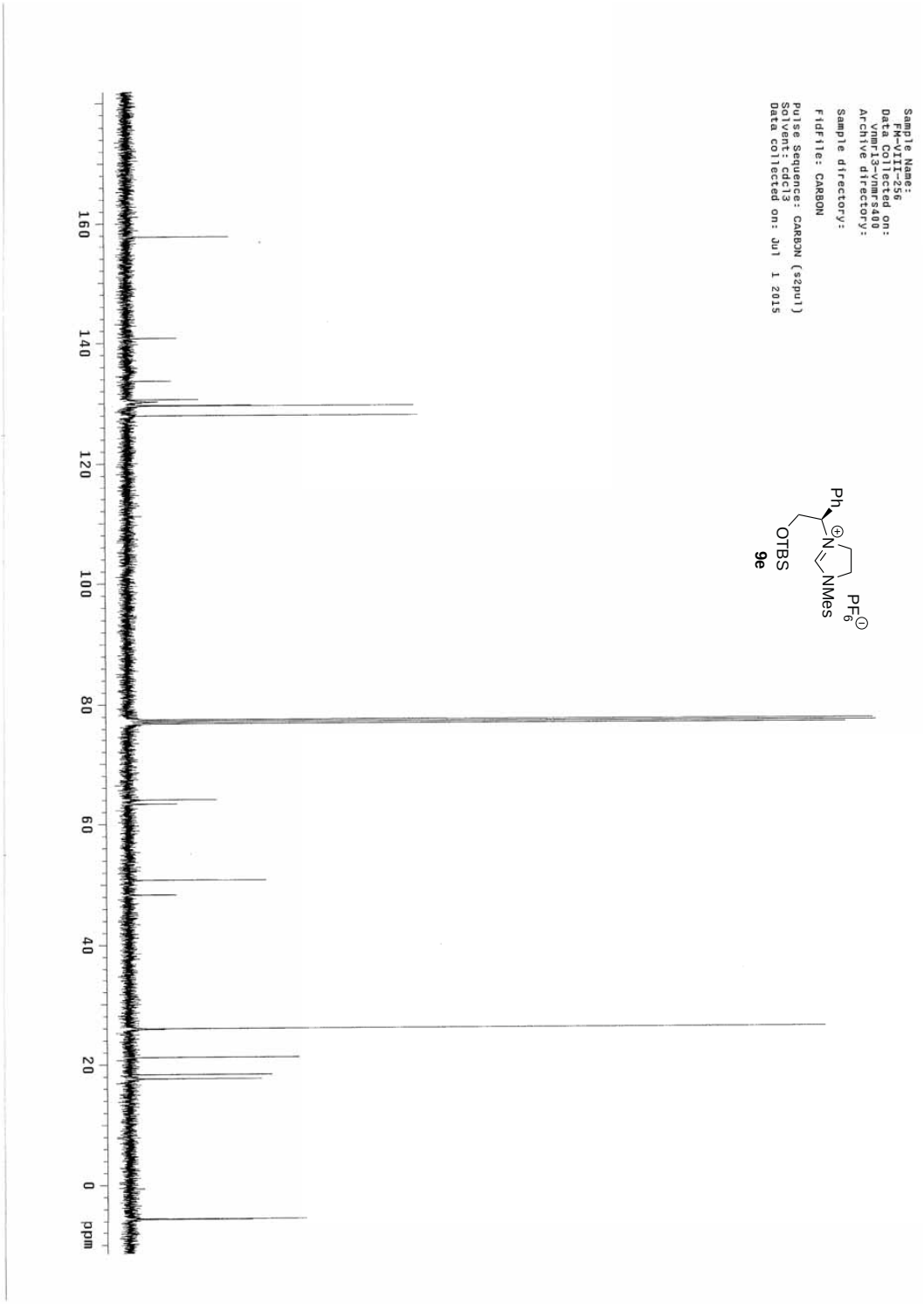
0.97
5.04
1.93
1.00
6.14
9.01
9.07
3.03
2.95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Archive directory:
Sample directory:
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Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 1 2015
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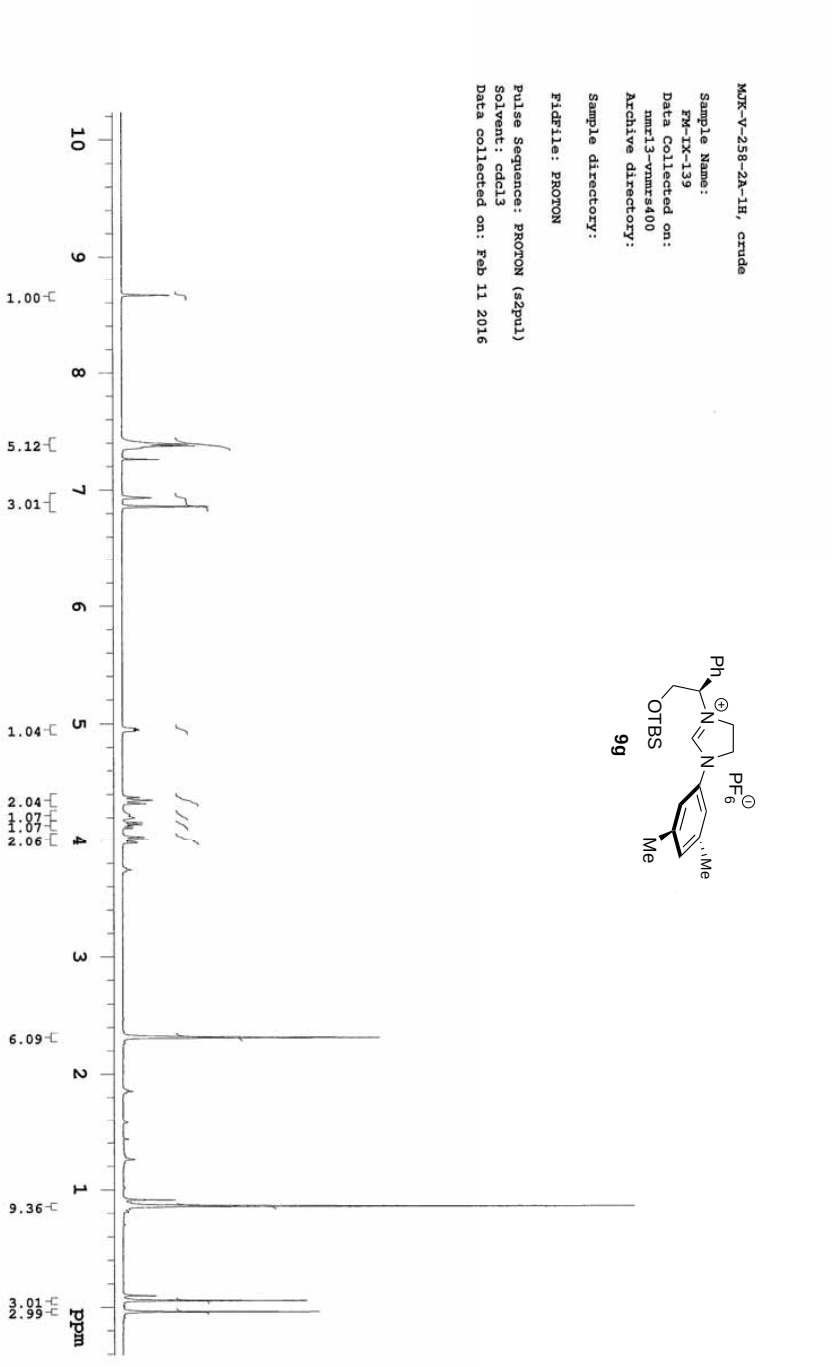
OTBS
NMes
PF6
9e
160
140
120
100
80
60
40
20
0
ppm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Archive directory:
Sample directory:
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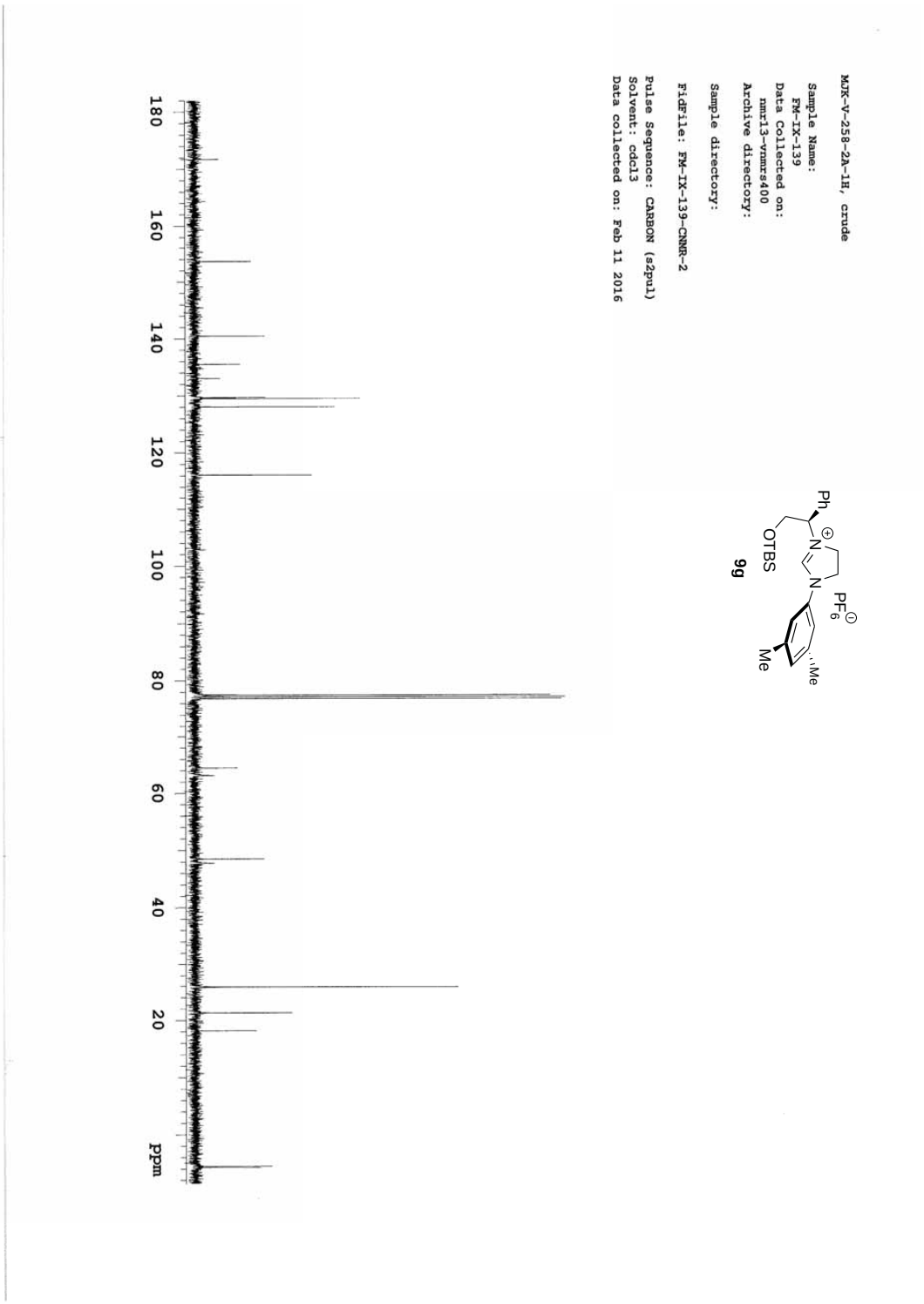
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 11 2016
Ph
OTBS
Me
Me
PF6
9g
1.00
5.12
3.01
1.04
2.04
1.07
1.07
2.06
6.09
9.36
3.01
2.99
ppm


MJK-V-258-2A-1H, crude
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Sample directory:
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Solvent: cdcl3
Data collected on: Feb 11 2016
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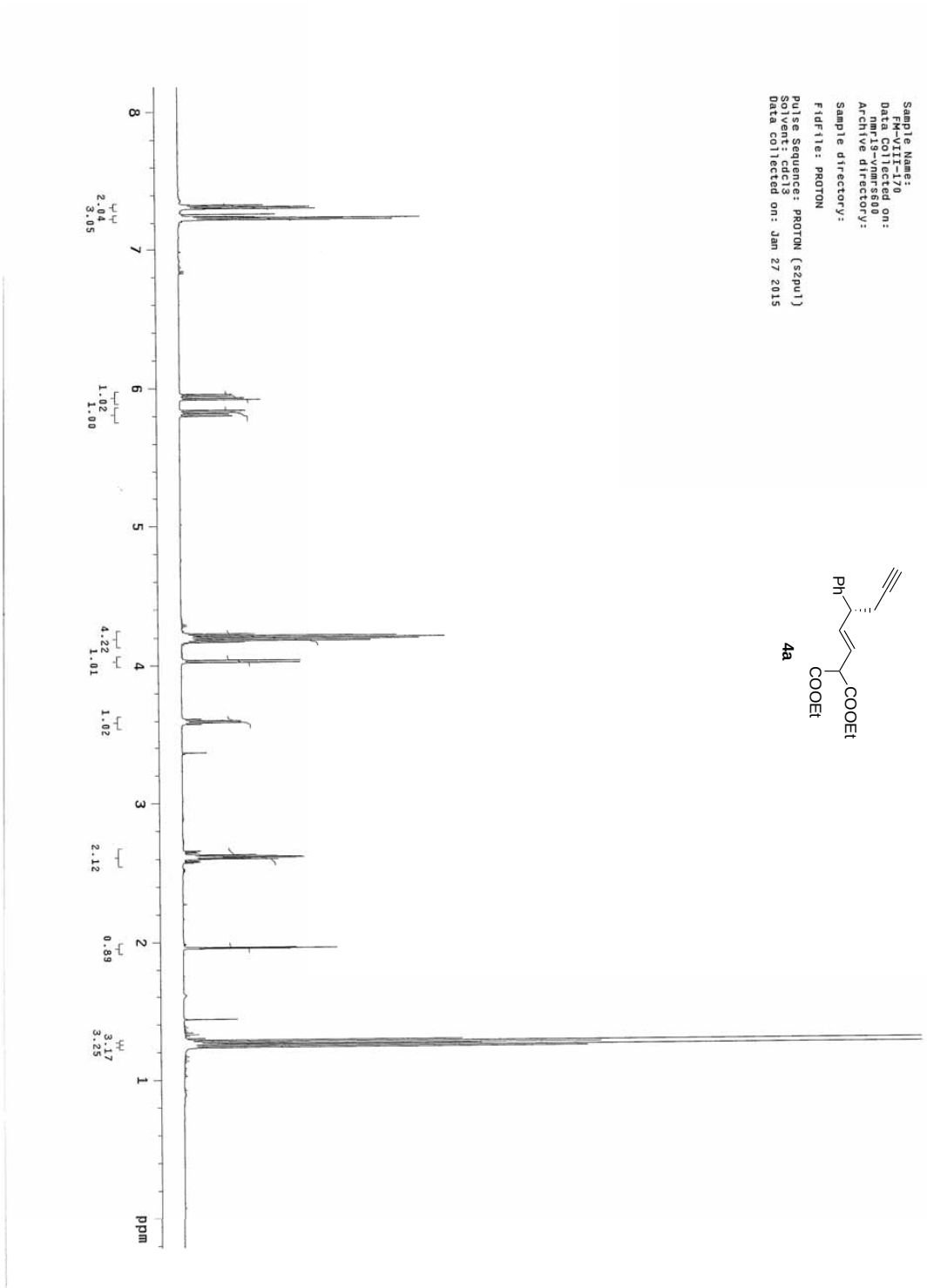
OTBS
Me
Me
PF6
9g
180
160
140
120
100
80
60
40
20
ppm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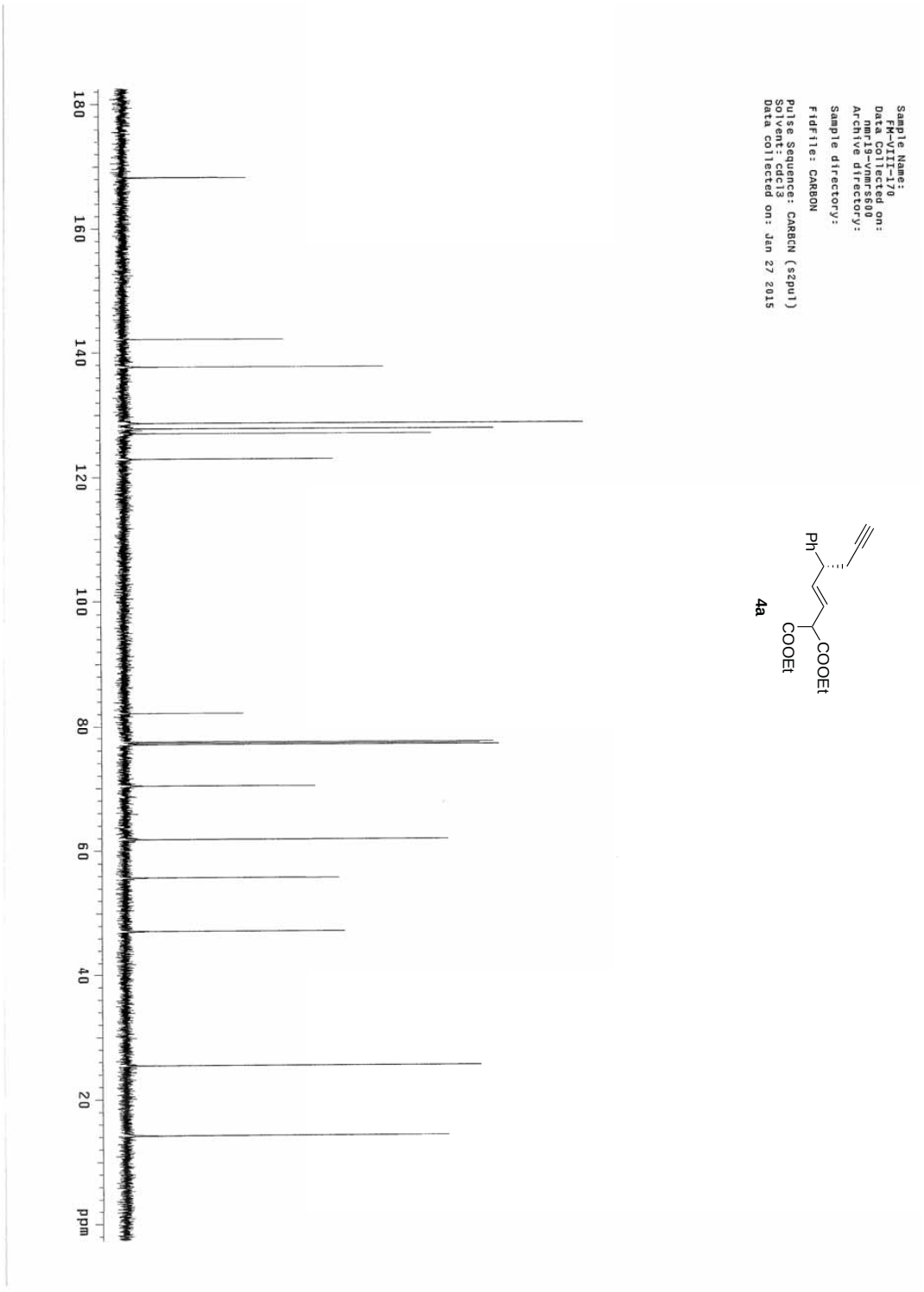
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 27 2015
Ph
COOEt
COOEt
4a
8
7
6
5
4
3
2
1
ppm
2.04
3.05
1.02
1.00
4.22
1.01
1.02
2.12
0.89
3.17
3.25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nmrig-vnmrs600
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBCN (s2pul)
Solvent: cdcl3
Data collected on: Jan 27 2015
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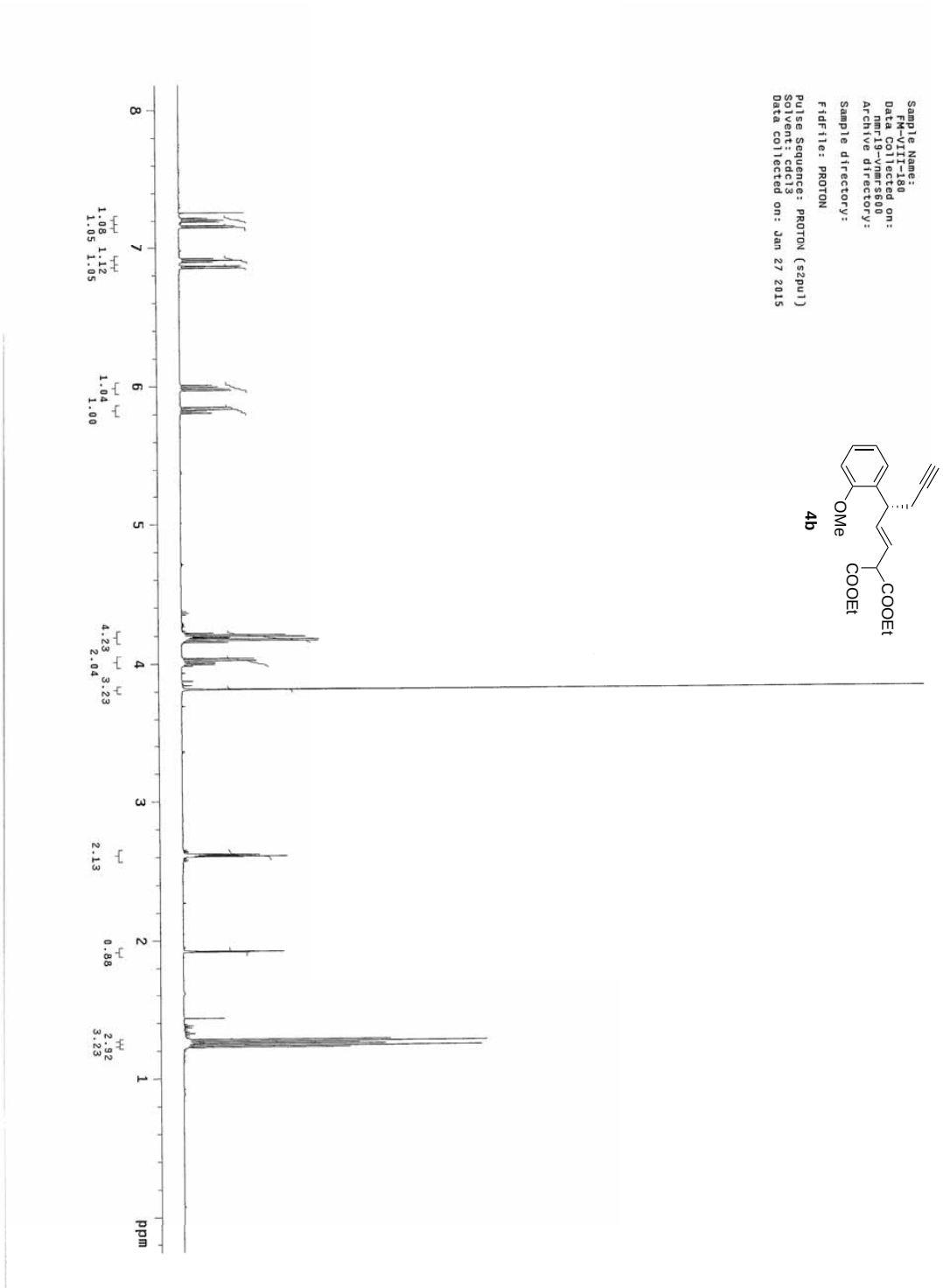
COOEt
COOEt
4a
180
160
140
120
100
80
60
40
20
ppm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Archive directory:
Sample directory:
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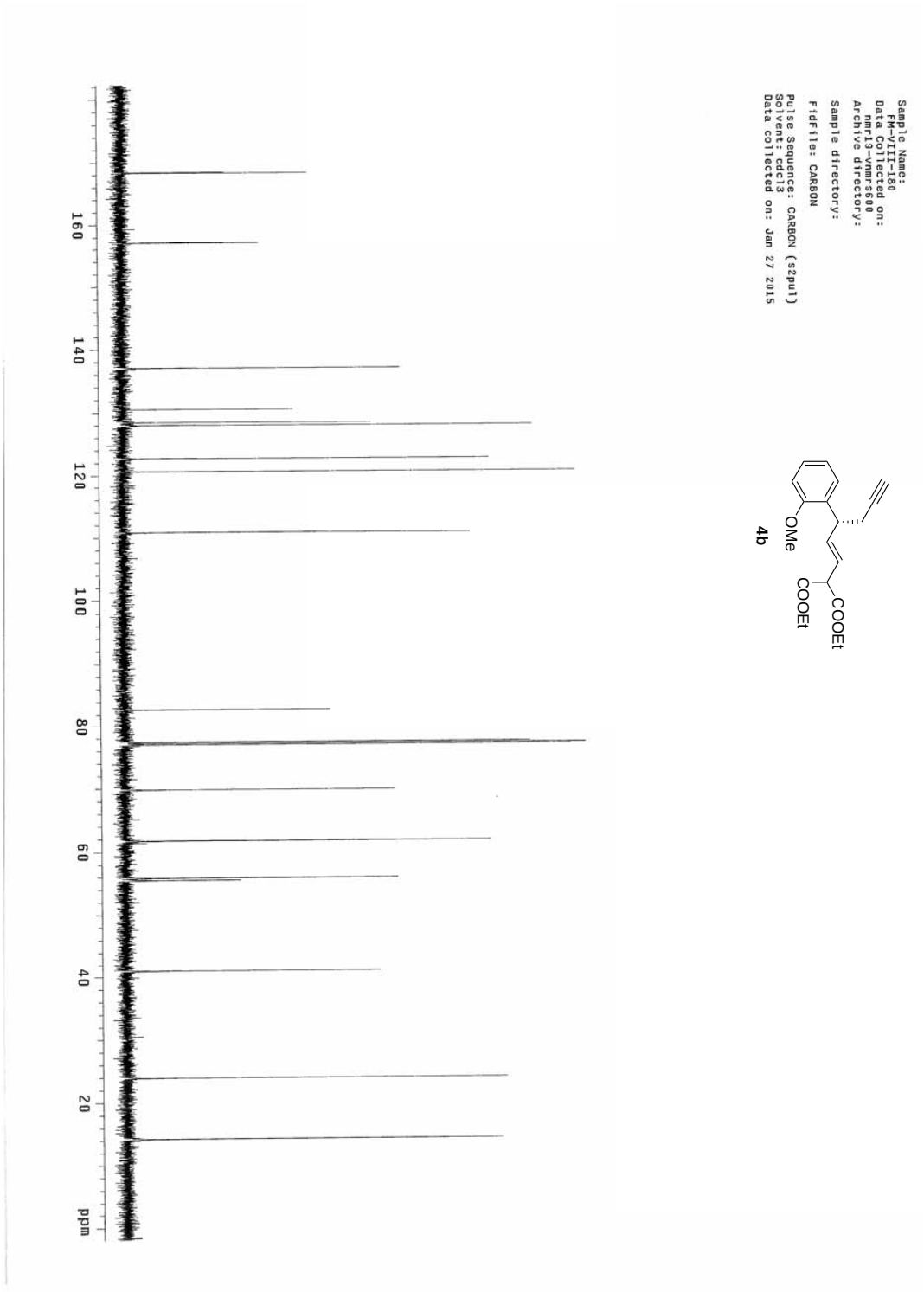
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 27 2015
OMe
COOEt
COOEt
4b
8
7
6
5
4
3
2
1
ppm
1.08
1.12
1.05
1.05
1.04
1.00
4.23
3.23
2.04
2.13
0.88
2.92
3.23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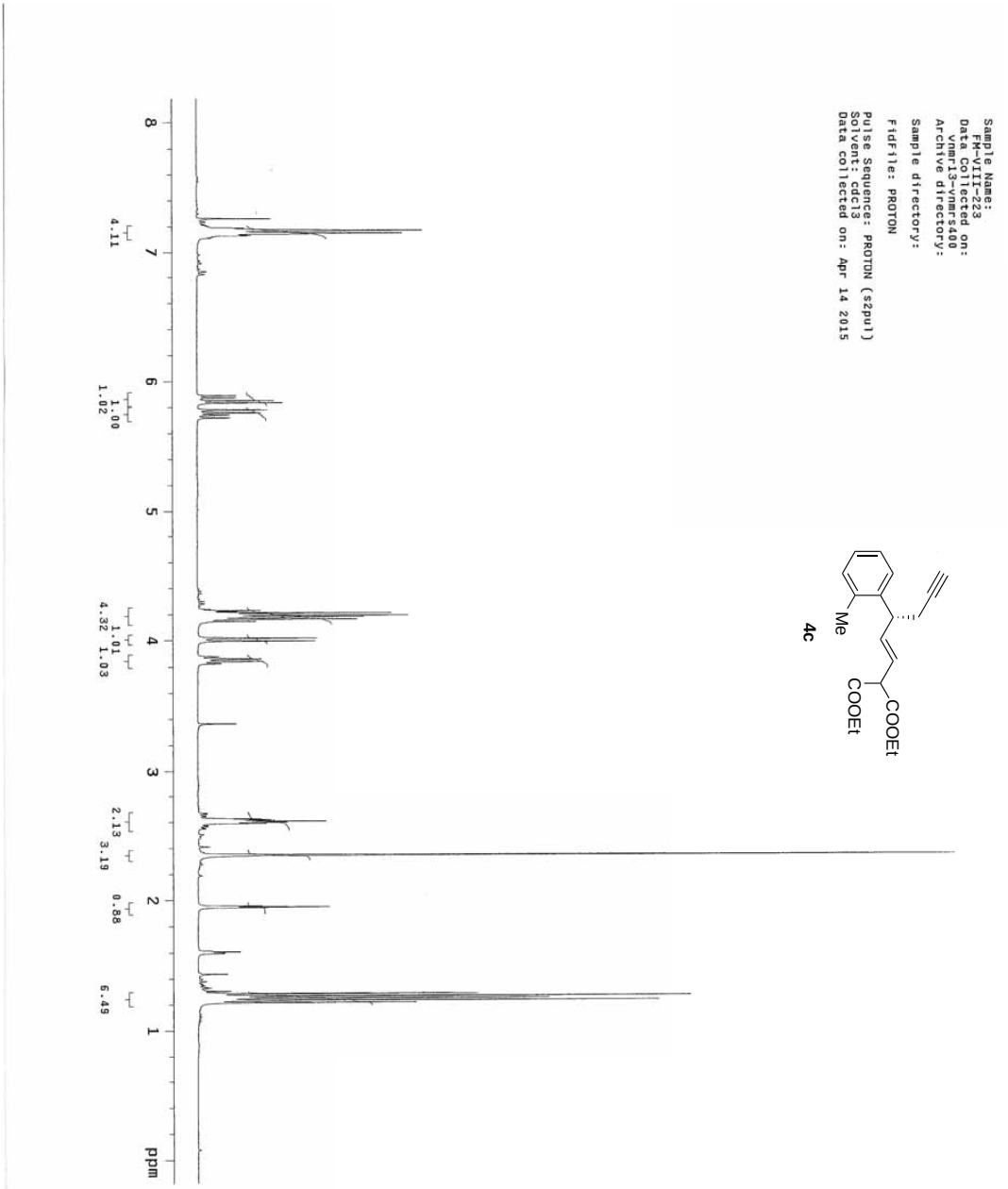
Pulse Sequence: CARBON (s2pul)
Solvent: CDCl3
Data collected on: Jan 27 2015
OMe
COOEt
COOEt
4b
160
140
120
100
80
60
40
20
ppm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Archive directory:
Sample directory:
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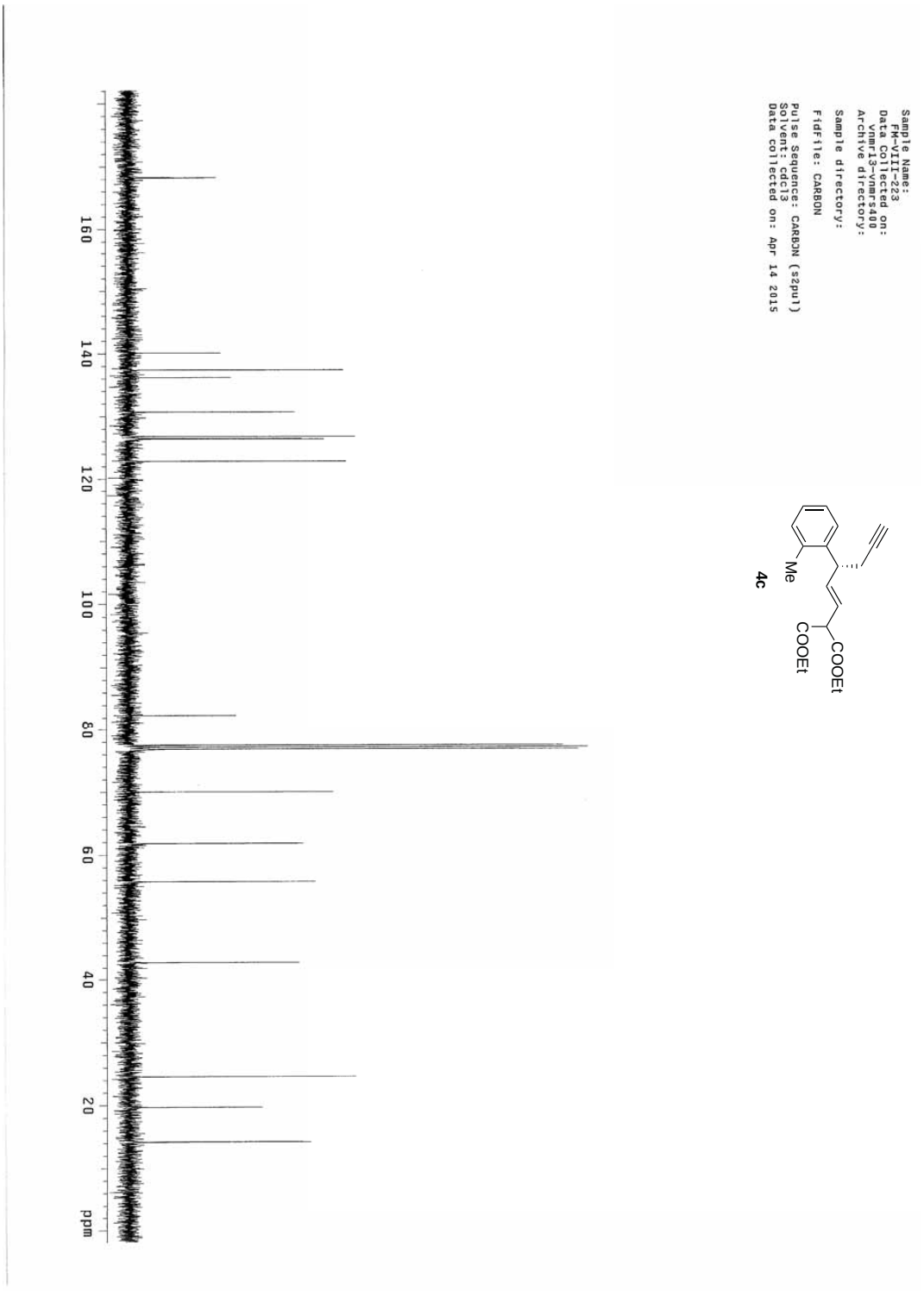
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 14 2015
Me
COOEt
COOEt
4c
8
7
6
5
4
3
2
1
ppm
4.11
1.00
1.02
1.01
4.32
1.03
2.13
3.19
0.88
6.49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Archive directory:
Sample directory:
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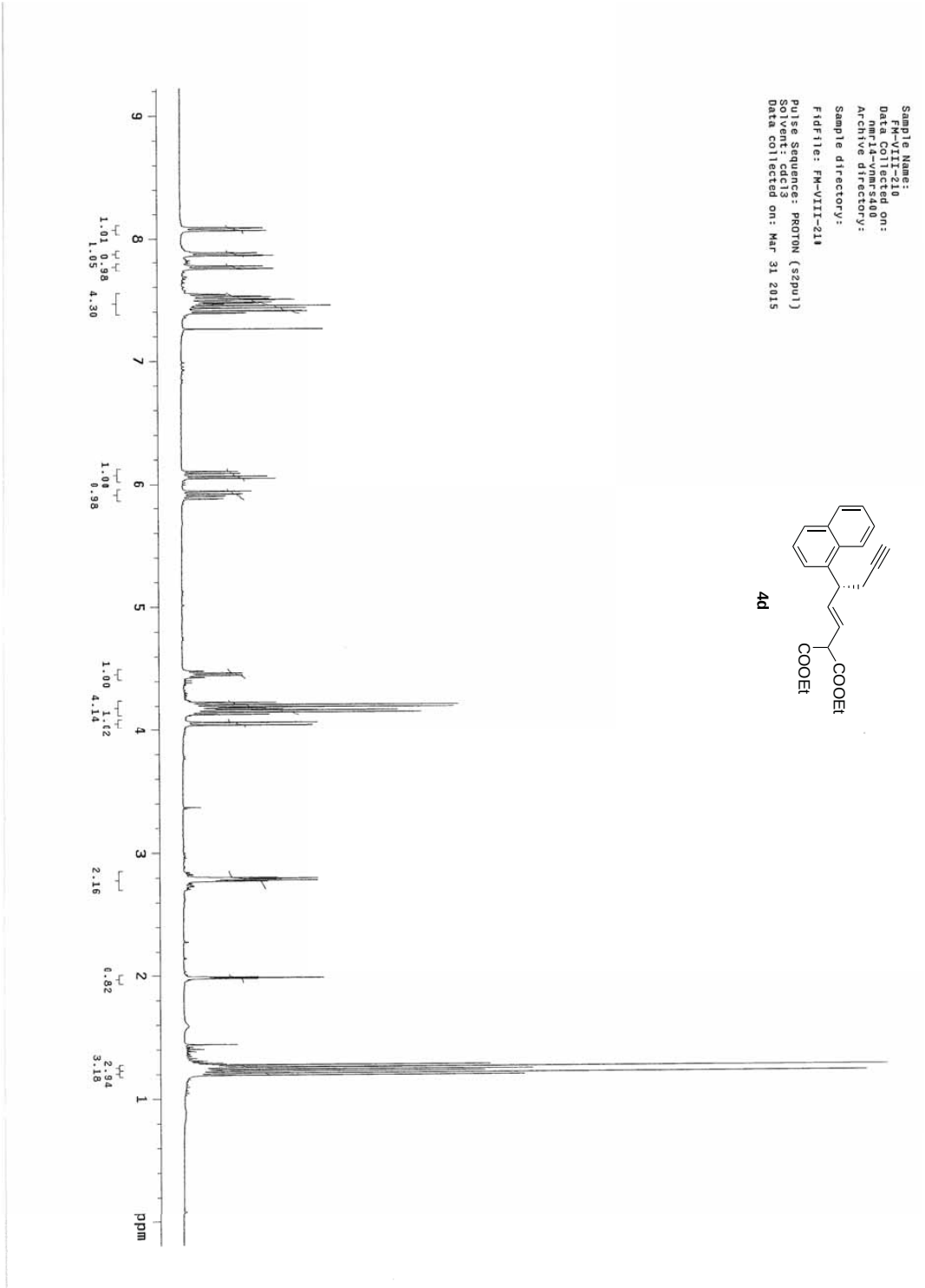
Pulse Sequence: CARBJN (s2pul)
Solvent: cdcl3
Data collected on: Apr 14 2015
Me
COOEt
COOEt
4c
160
140
120
100
80
60
40
20
ppm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Archive directory:
Sample directory:
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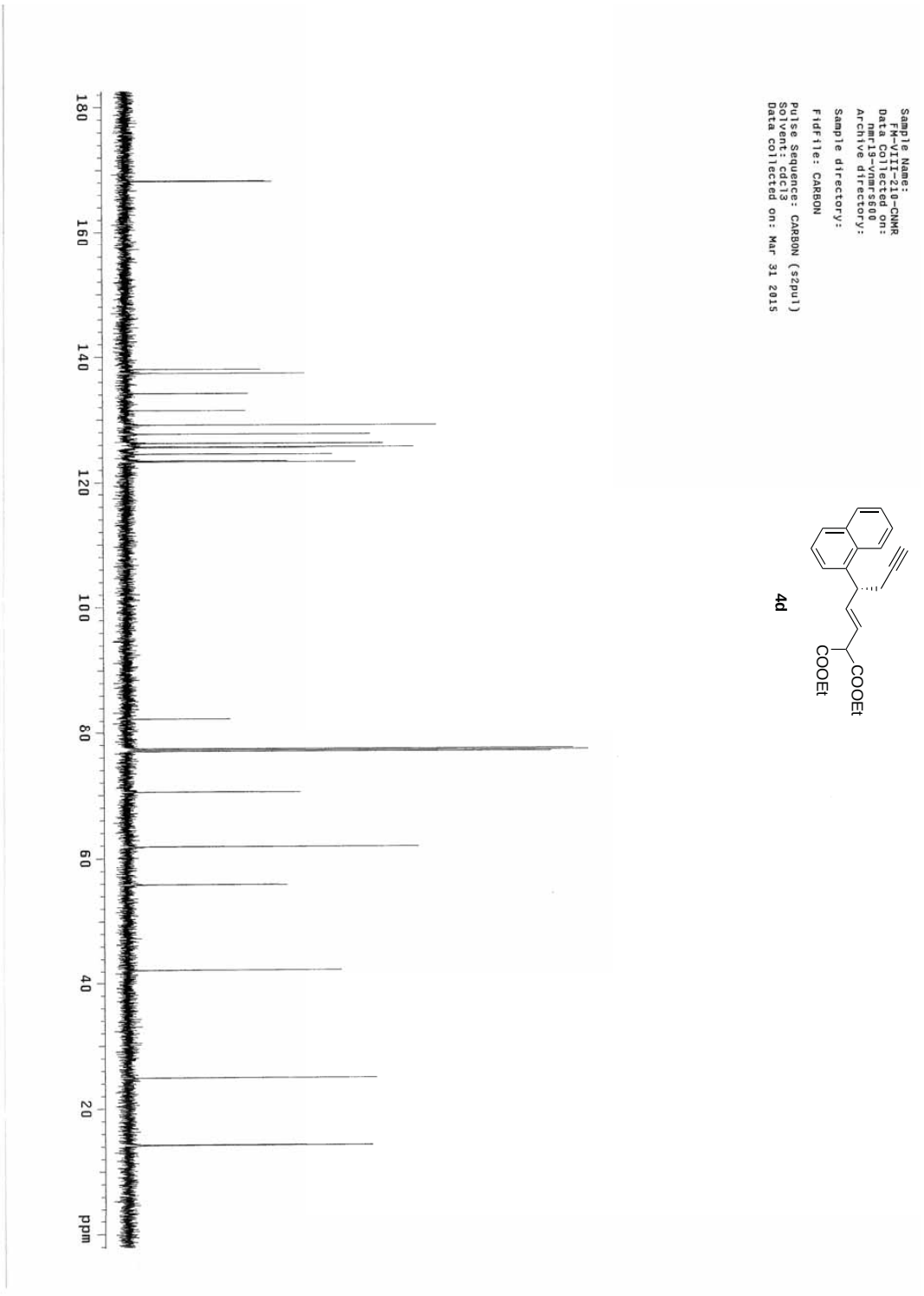
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 31 2015
COOEt
COOEt
4d
ppm
1.01
0.98
1.05
4.30
1.08
0.98
1.00
1.62
4.14
2.16
0.82
2.94
3.18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nmr19-vnmrs600
Archive directory:
Sample directory:
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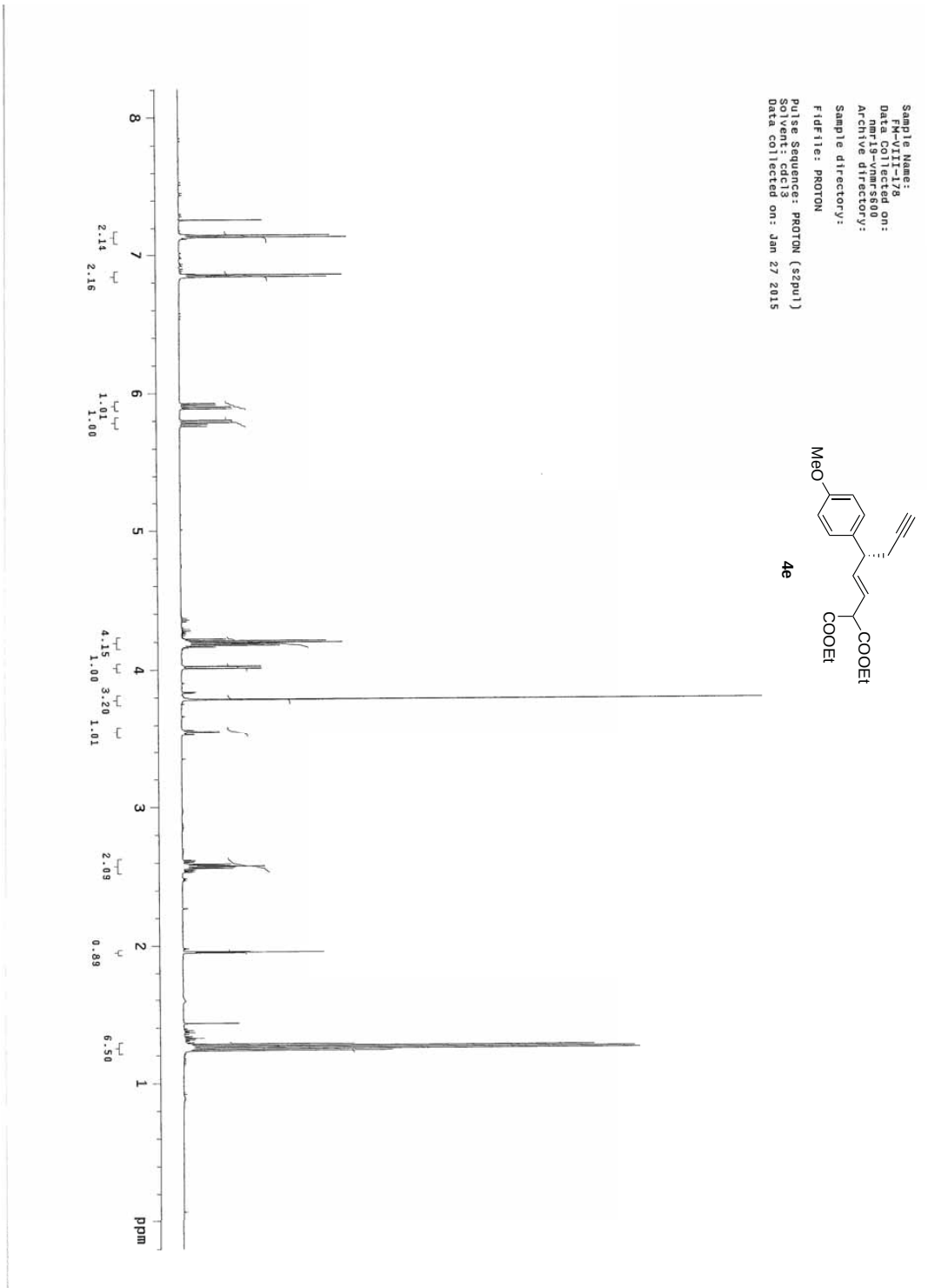
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 31 2015
COOEt
COOEt
4d
180
160
140
120
100
80
60
40
20
ppm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Sample directory:
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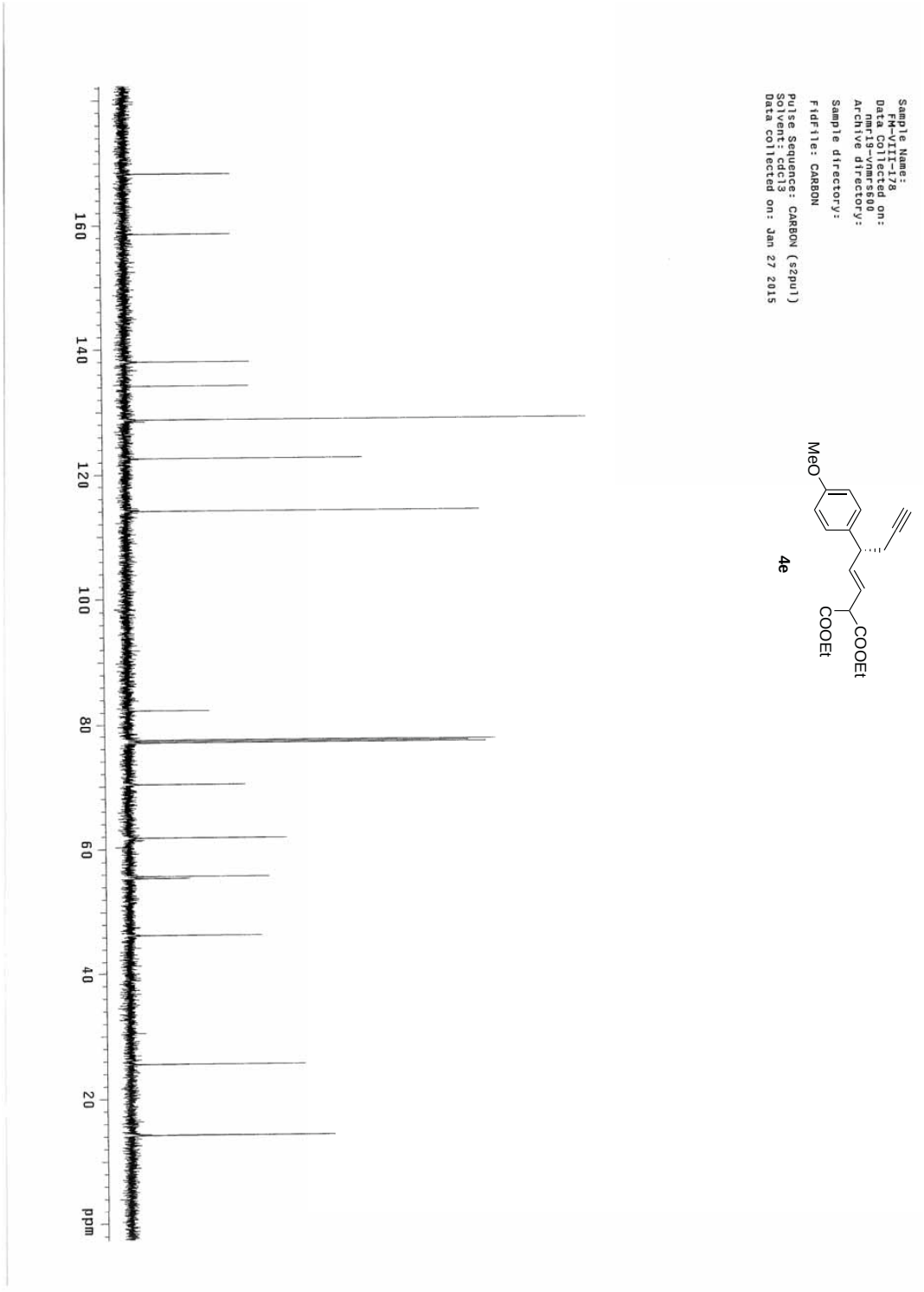
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 27 2015
MeO
COOEt
COOEt
4e
8
7
6
5
4
3
2
1
ppm
2.14
2.16
1.01
1.00
4.15
1.00
3.20
1.01
2.09
0.89
6.50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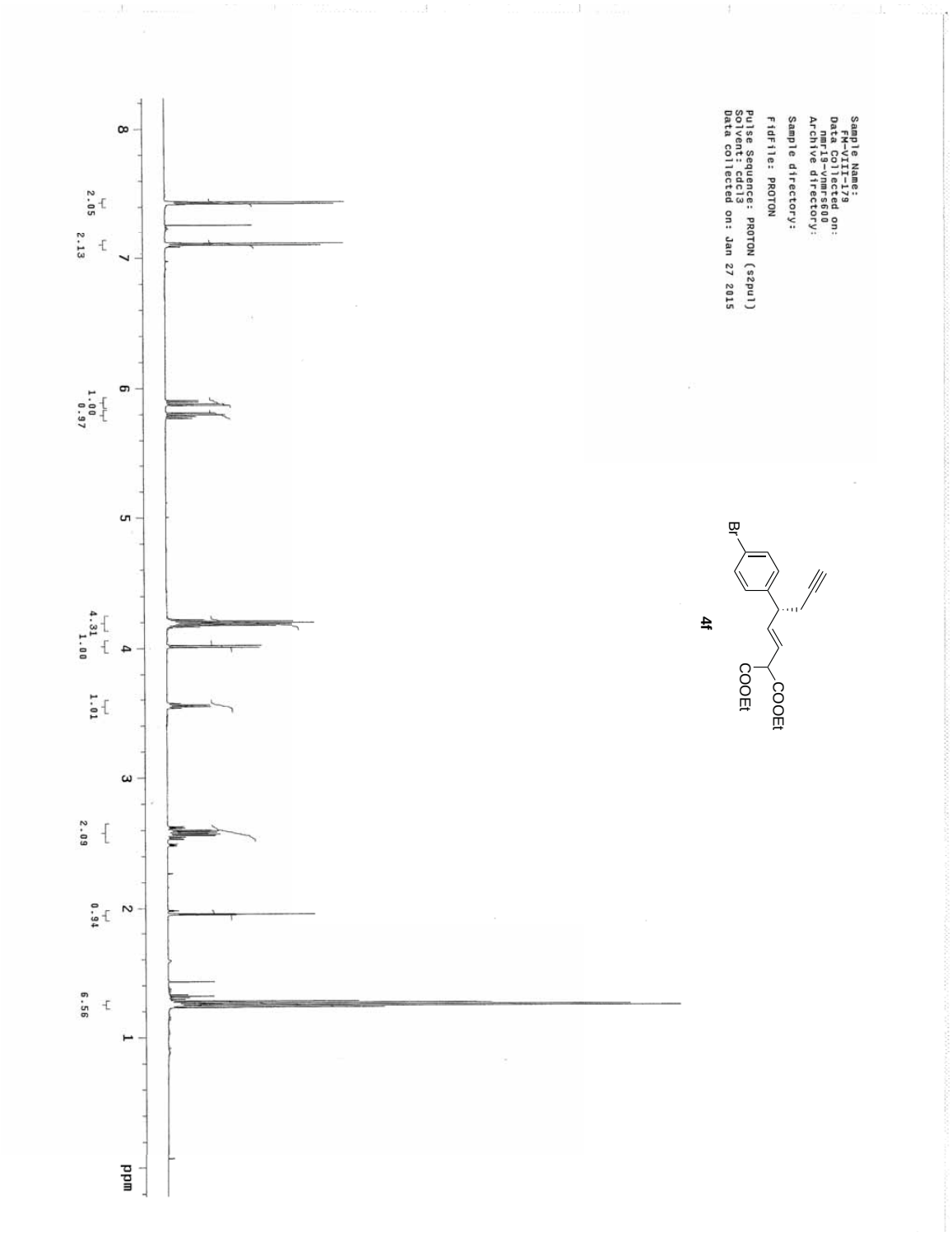
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 27 2015
MeO
COOEt
COOEt
4e
160
140
120
100
80
60
40
20
ppm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Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 27 2015
Br
COOEt
COOEt
4f
ppm
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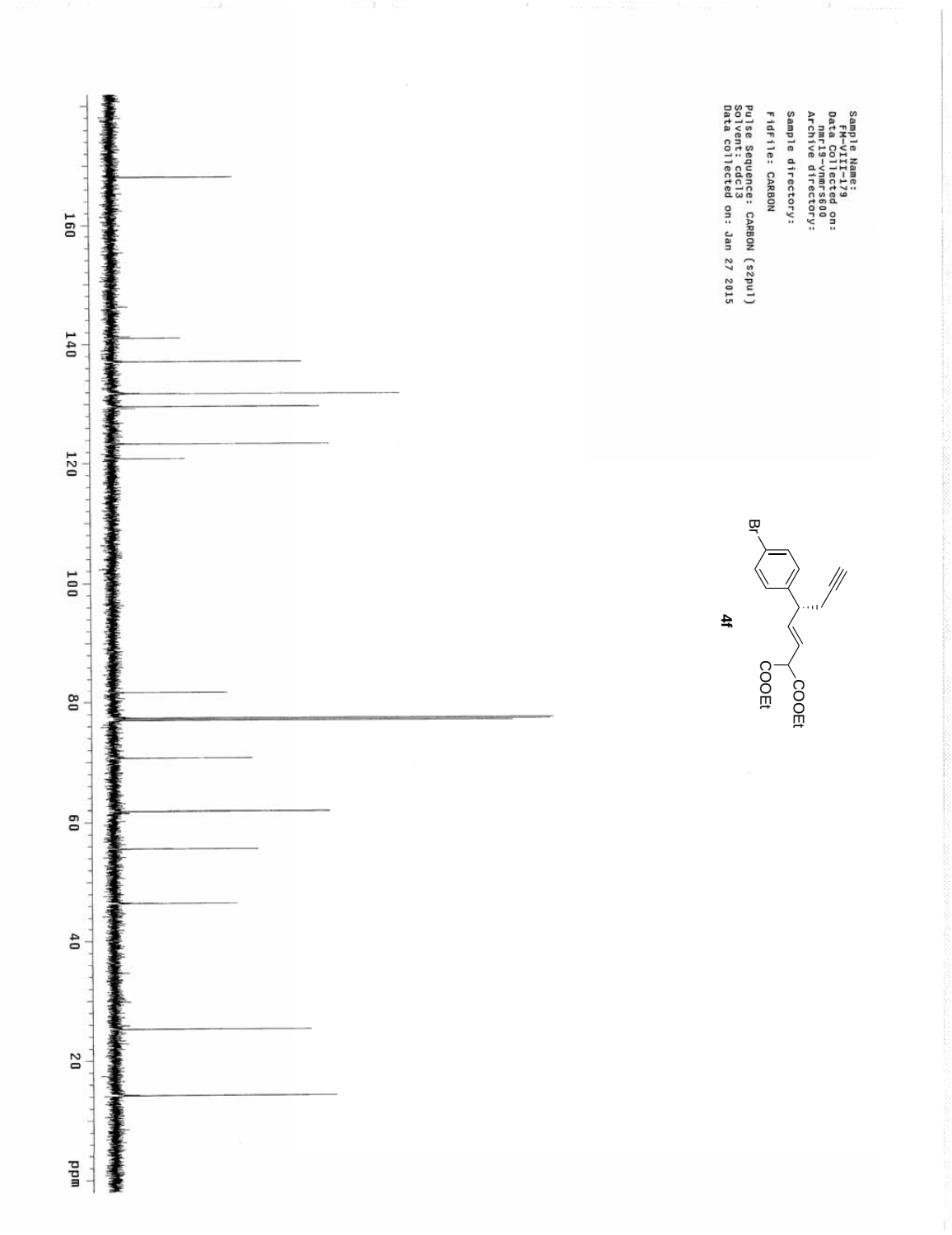
2.13
1.00
0.97
4.31
1.00
1.01
2.09
0.94
6.56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Archive directory:
Sample directory:
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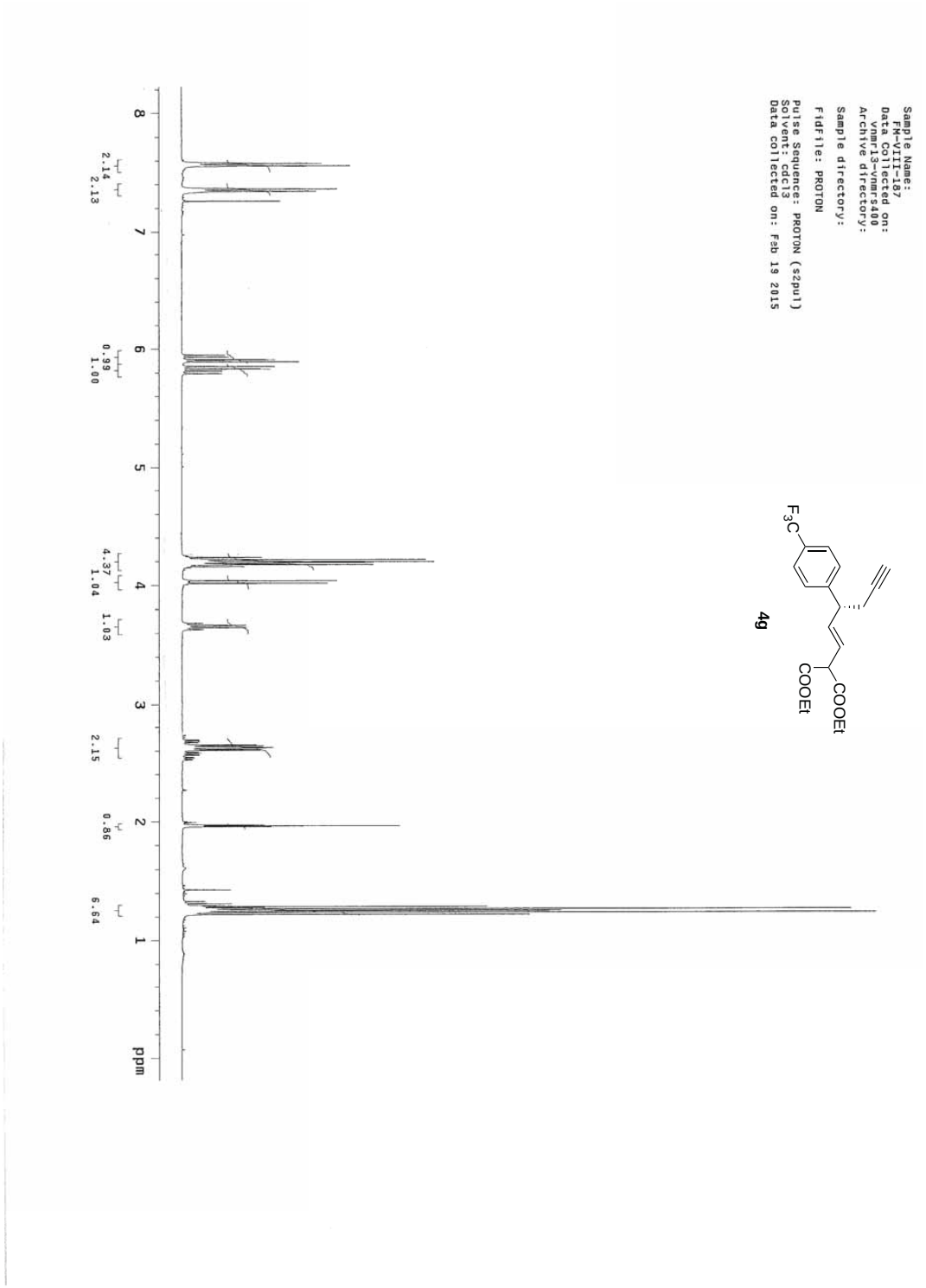
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 27 2015
Br
COOEt
COOEt
4f
160
140
120
100
80
60
40
20
ppm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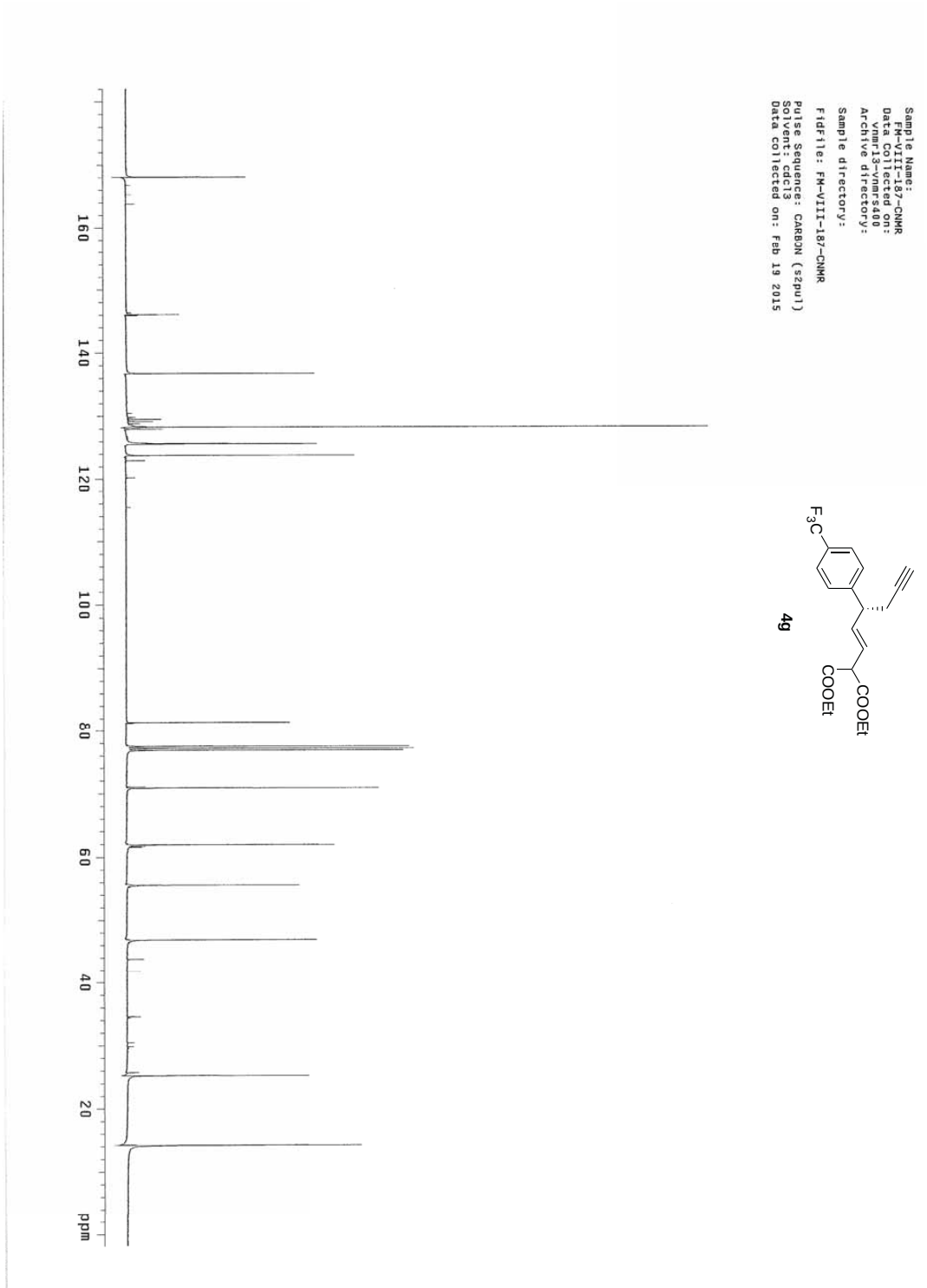
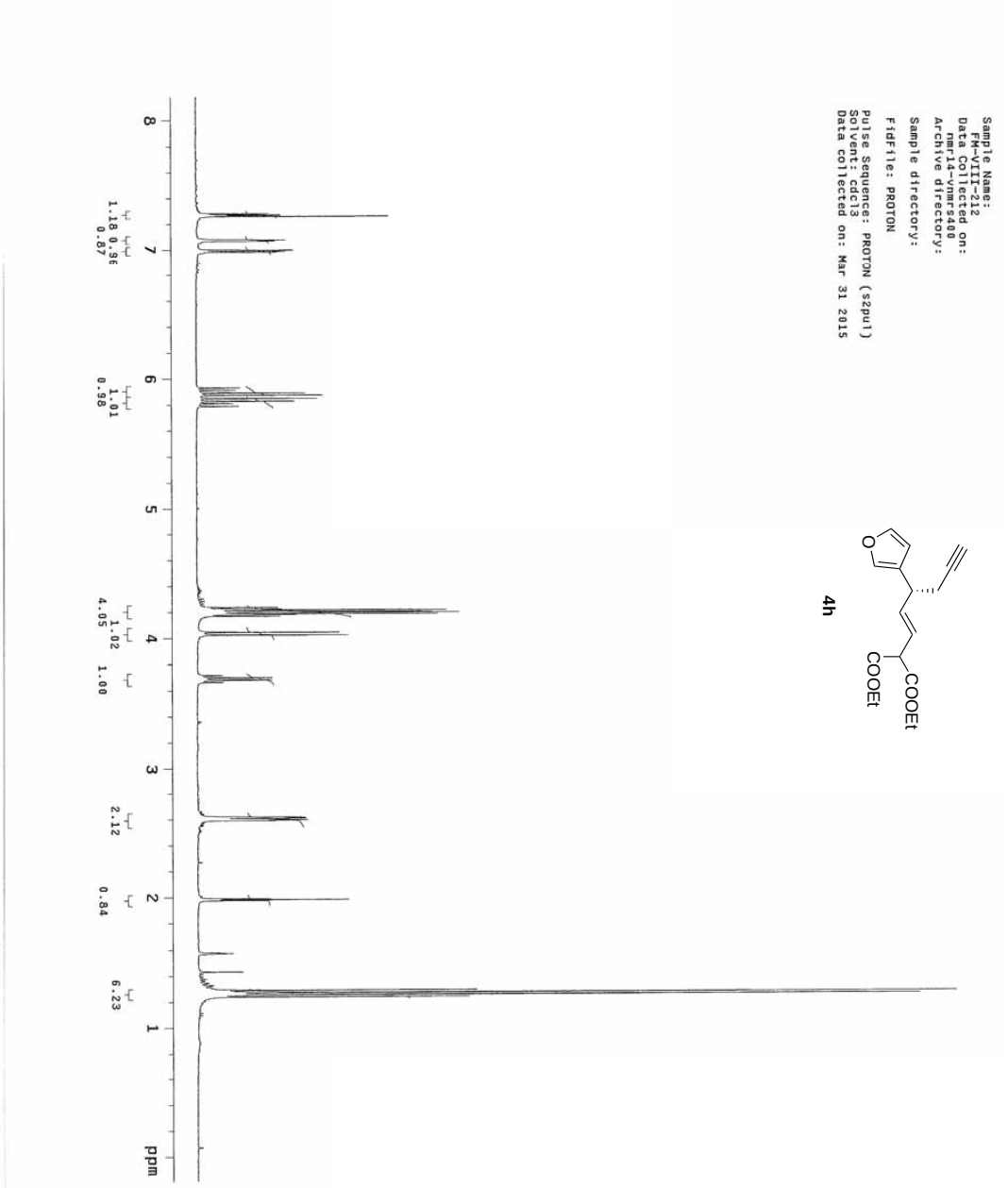
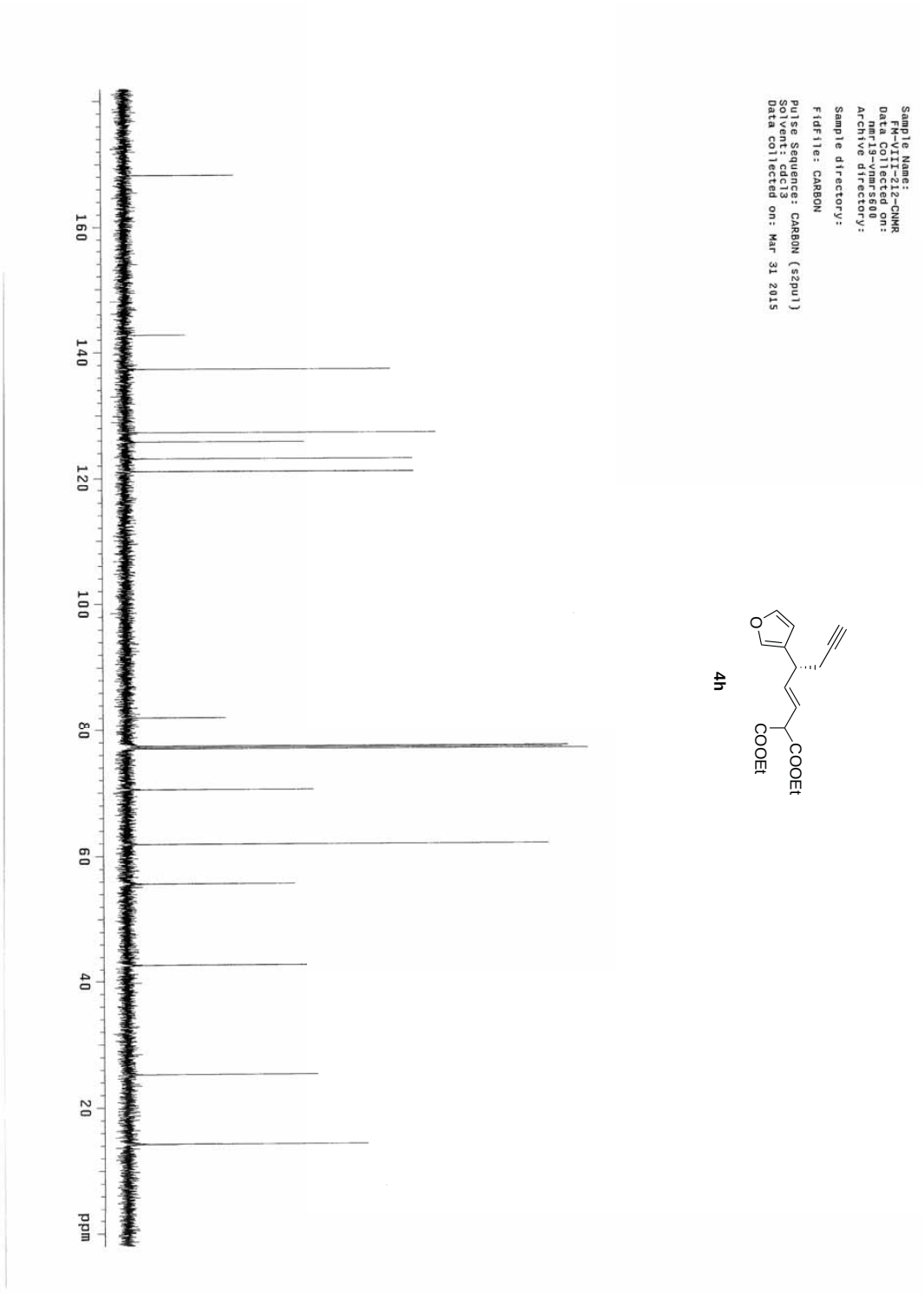
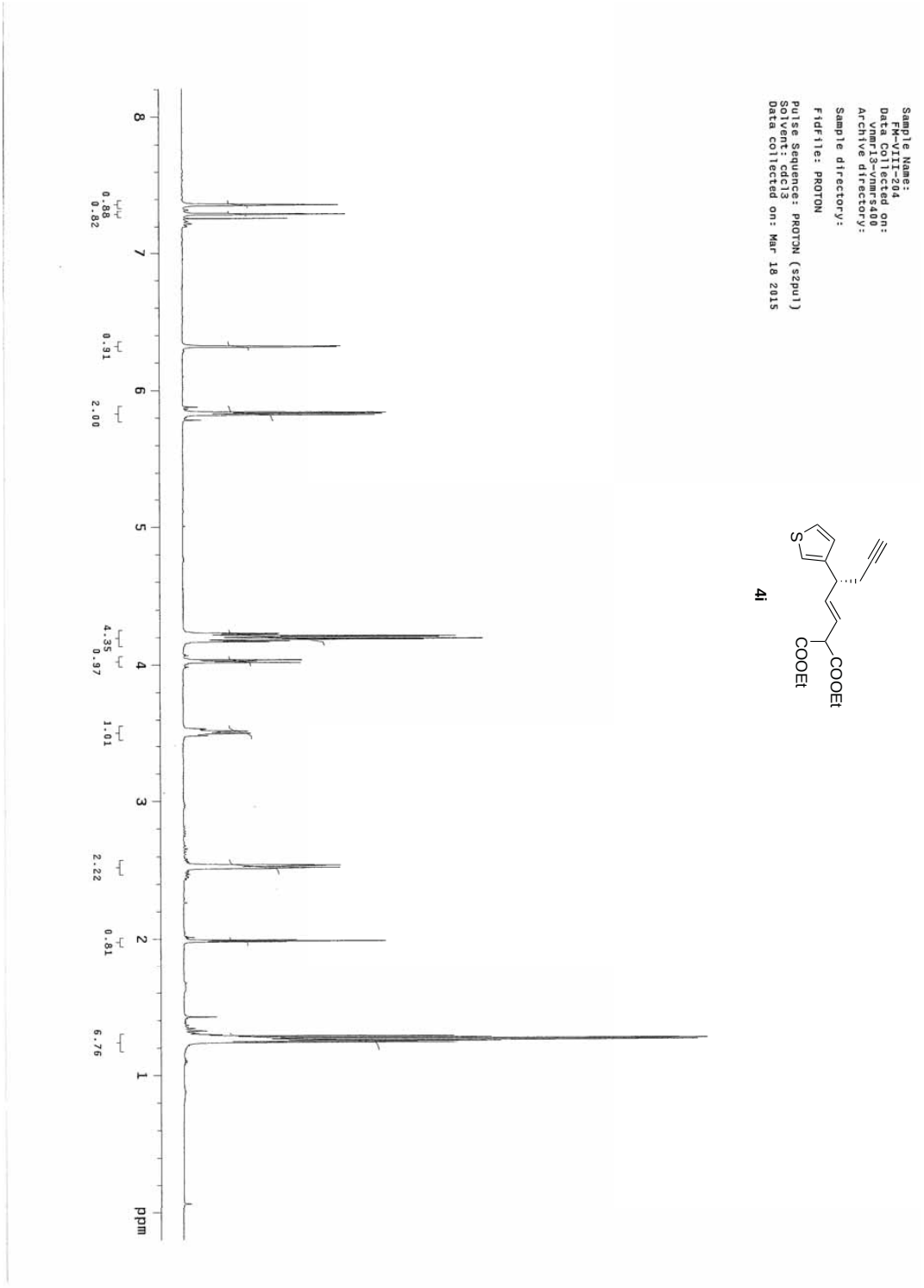
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 19 2015
F3C
COOEt
COOEt
4g
8
7
6
5
4
3
2
1
ppm
2.14
2.13
0.99
1.00
4.37
1.04
1.03
2.15
0.86
6.64

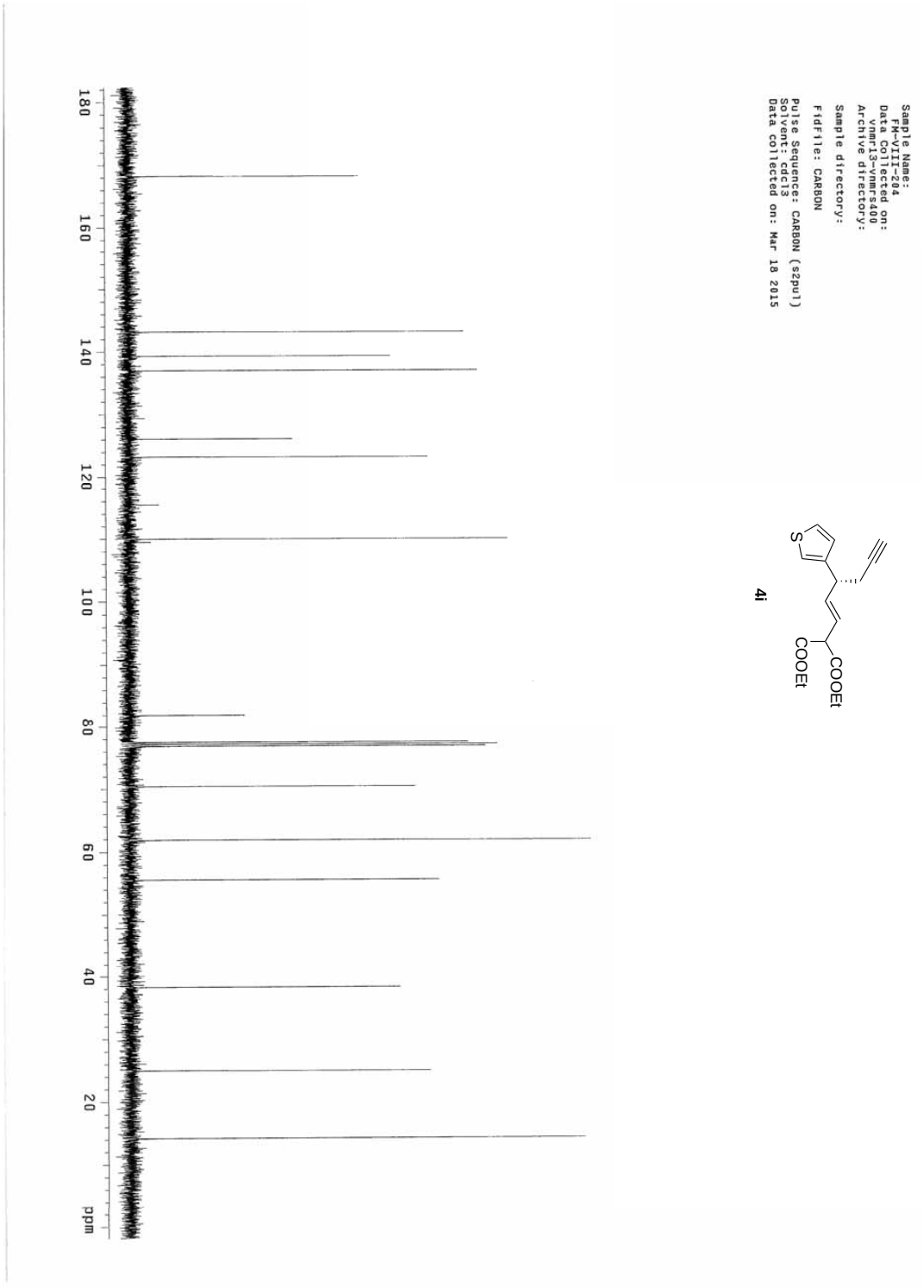

Sample Name:
FM-VIII-187-CNMR
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: FM-VIII-187-CNMR
Pulse Sequence: CARBJN (s2pul)
Solvent: cdcl3
Data collected on: Feb 19 2015
F3C
COOEt
COOEt
4g
160
140
120
100
80
60
40
20
ppm

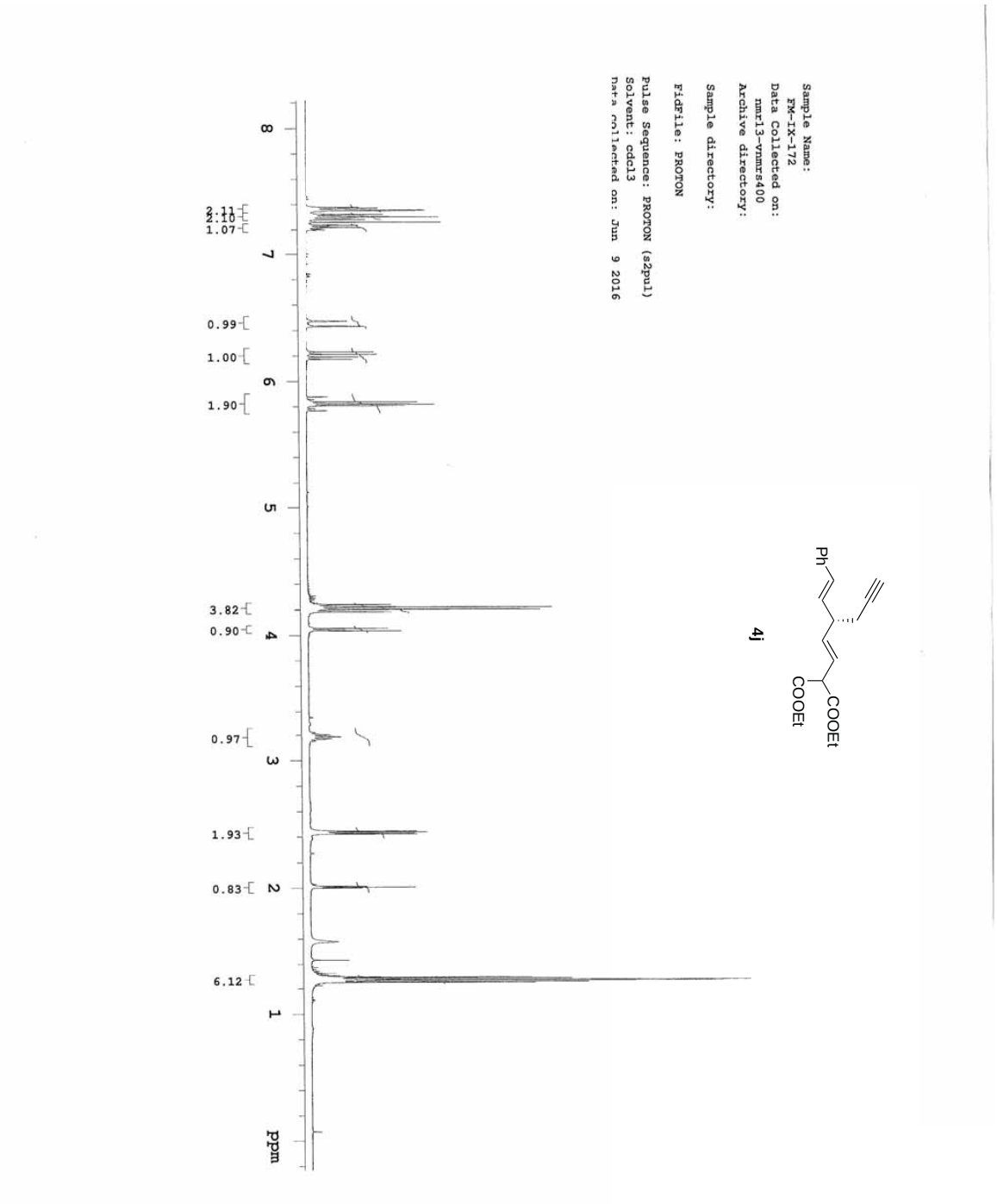

Sample Name:
FM-VIII-212
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 31 2015
4h
COOEt
COOEt
O
8
7
6
5
4
3
2
1
ppm
1.18
0.96
0.87
1.01
0.98
1.02
4.05
1.00
2.12
0.84
6.23

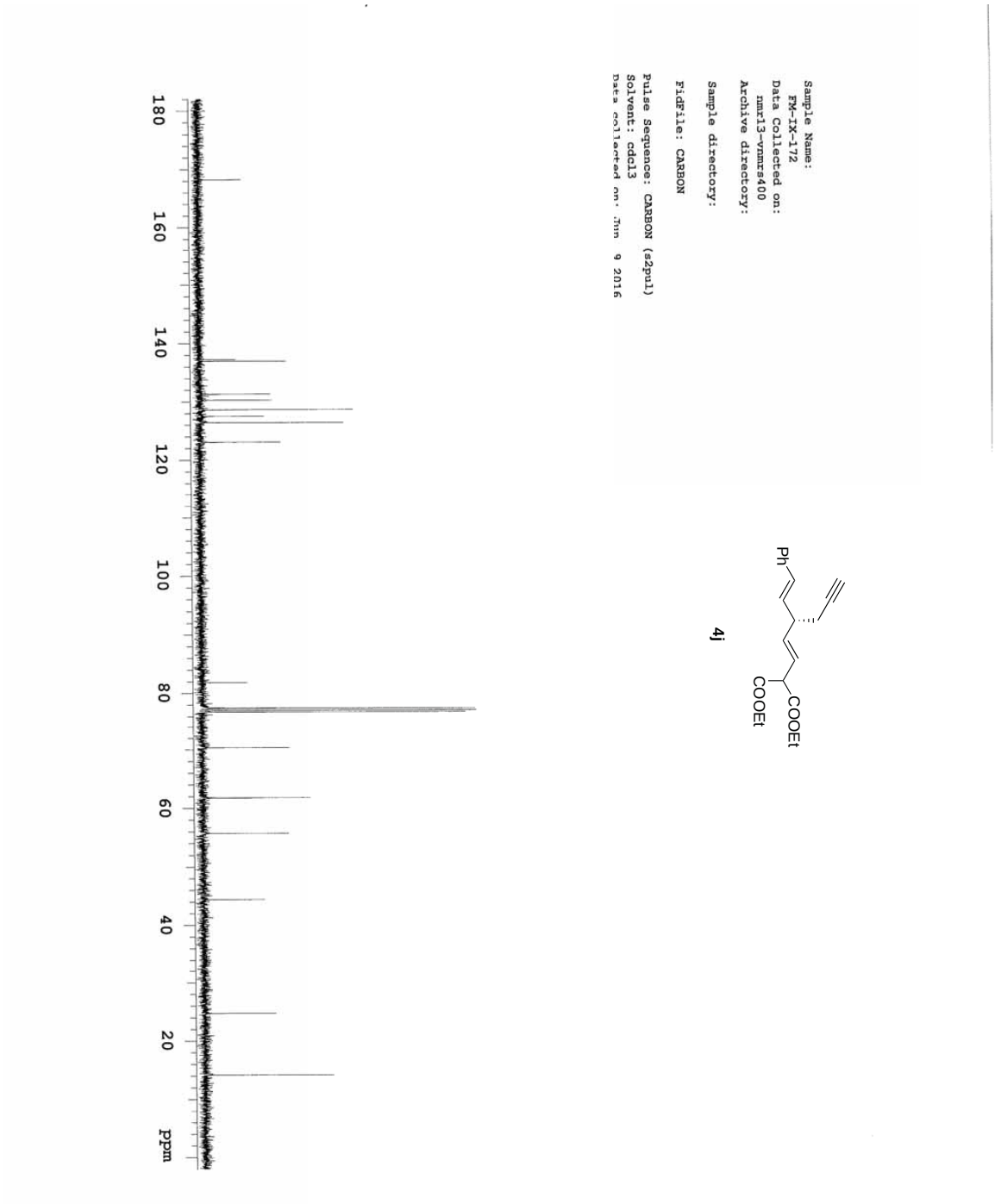

Sample Name:
FM-VIII-212-CNMR
Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 31 2015
O
COOEt
COOEt
160
140
120
100
80
60
40
20
ppm

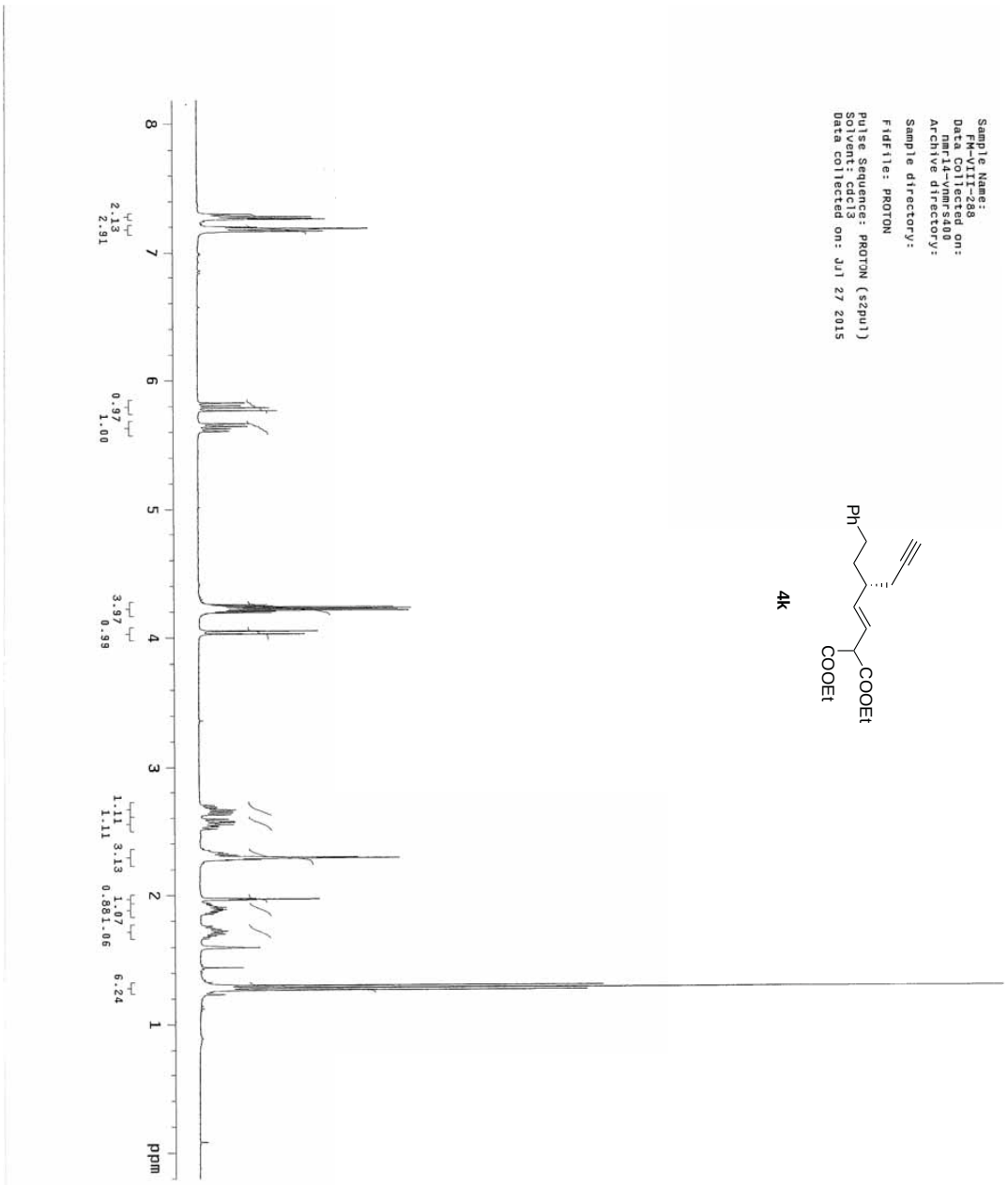
4h

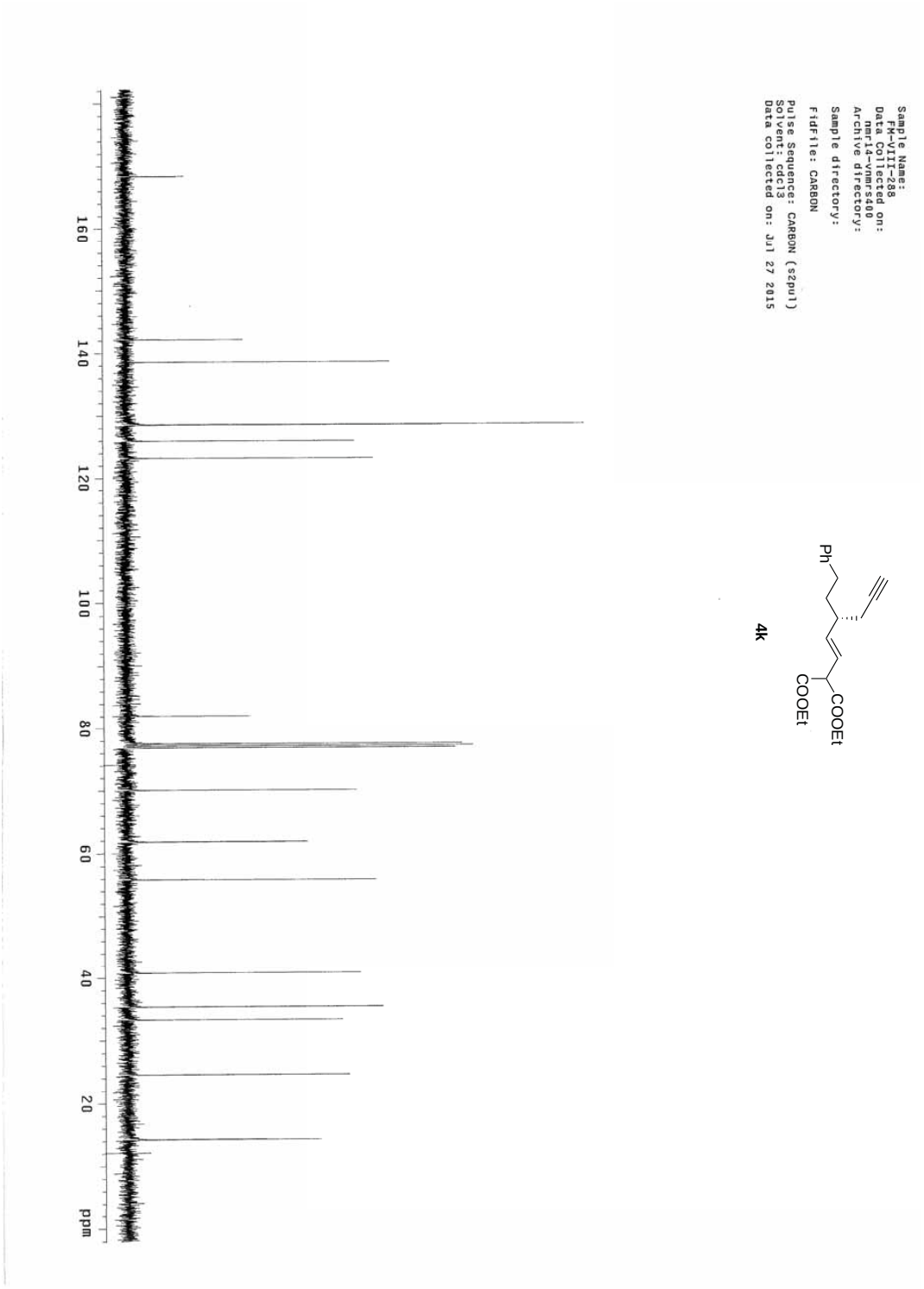

Sample Name:
FM-VIII-204
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 18 2015
S
COOEt
COOEt
4i
8
7
6
5
4
3
2
1
ppm
0.88
0.82
0.91
2.00
4.35
0.97
1.01
2.22
0.81
6.76

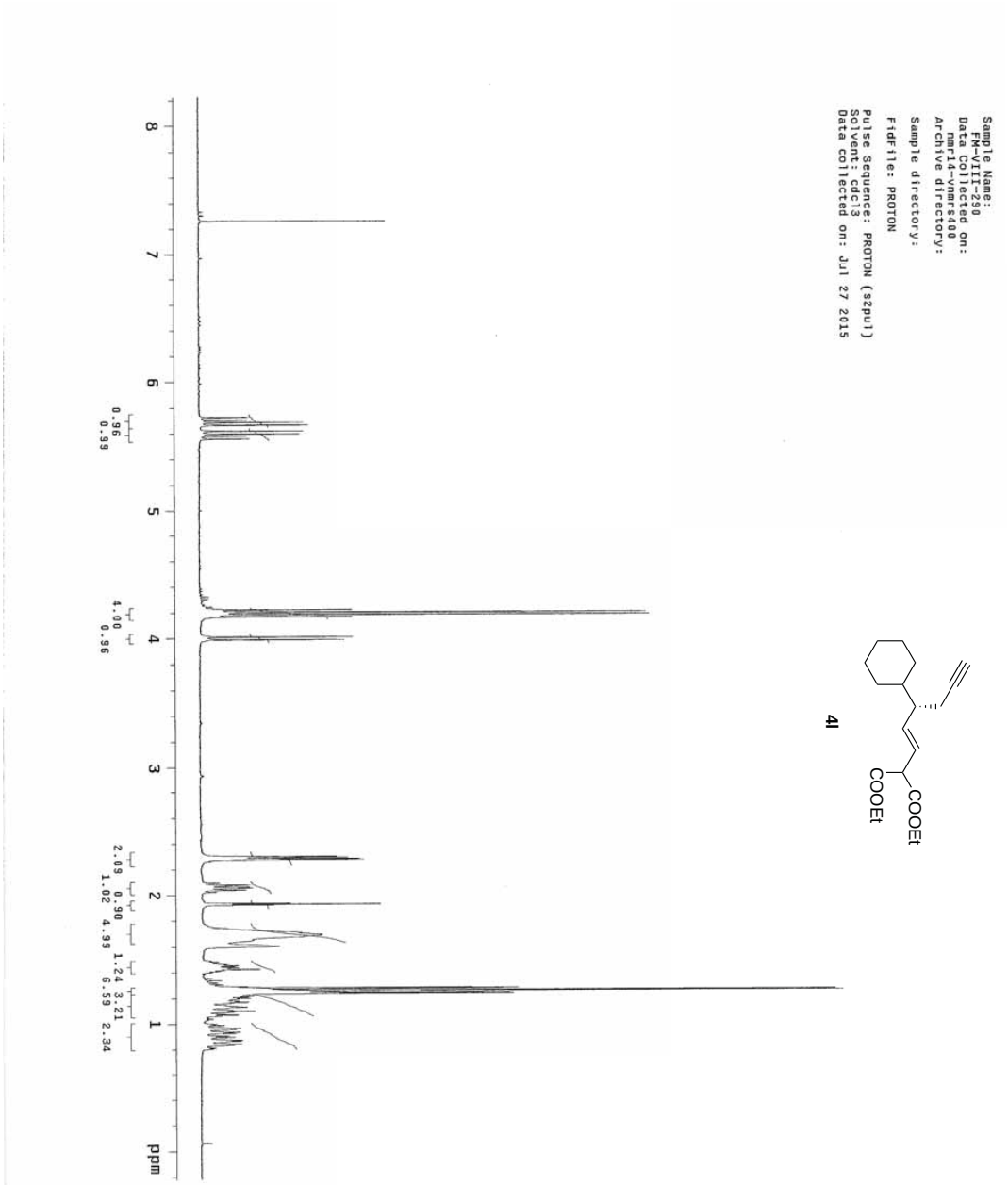

Sample Name:
FM-VIII-204
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 18 2015
S
COOEt
COOEt
4i
180
160
140
120
100
80
60
40
20
ppm

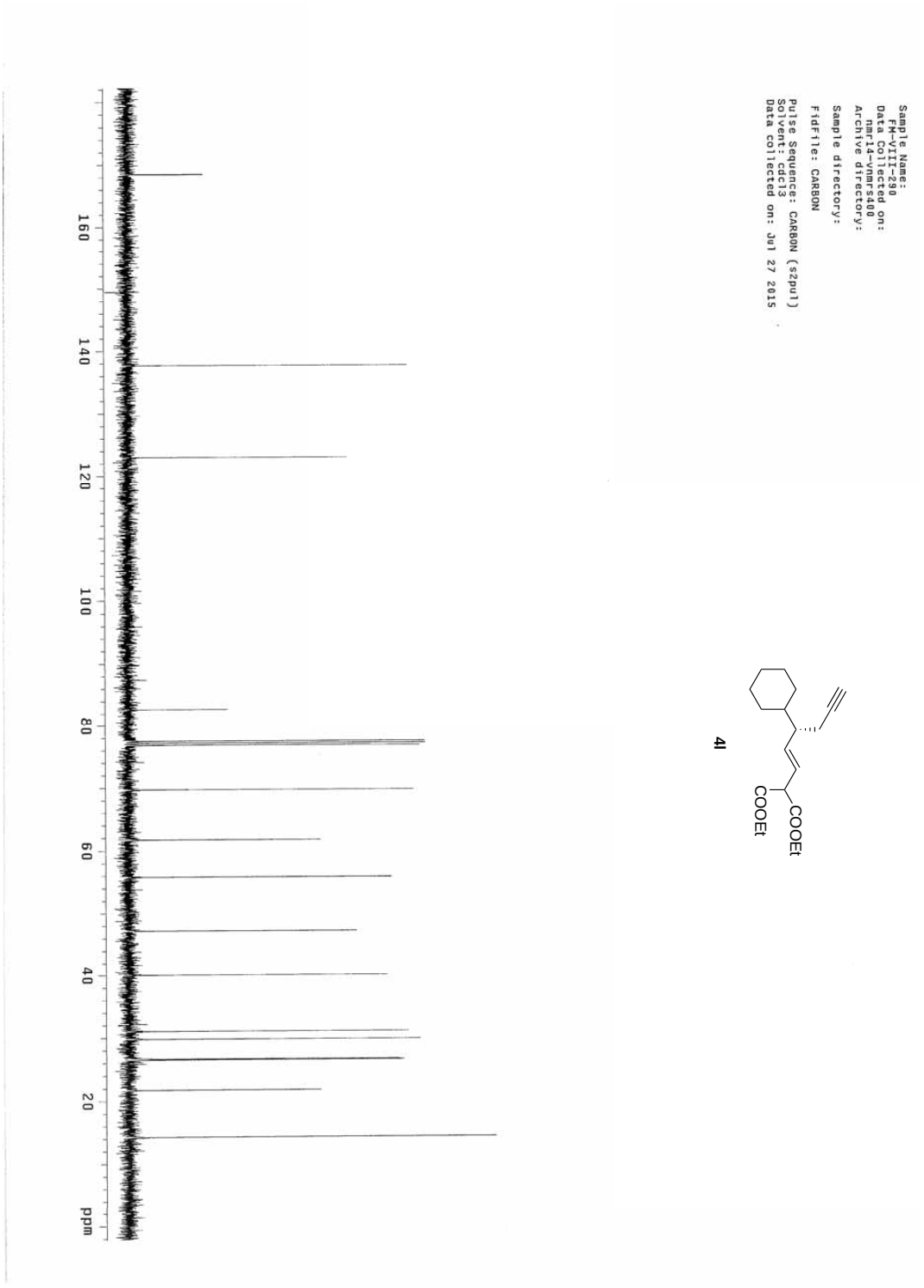

Sample Name:
FM-IX-172
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 9 2016
Ph
COOEt
COOEt
4j
2.11
2.10
1.07
0.99
1.00
1.90
3.82
0.90
0.97
1.93
0.83
6.12
8
7
6
5
4
3
2
1
ppm

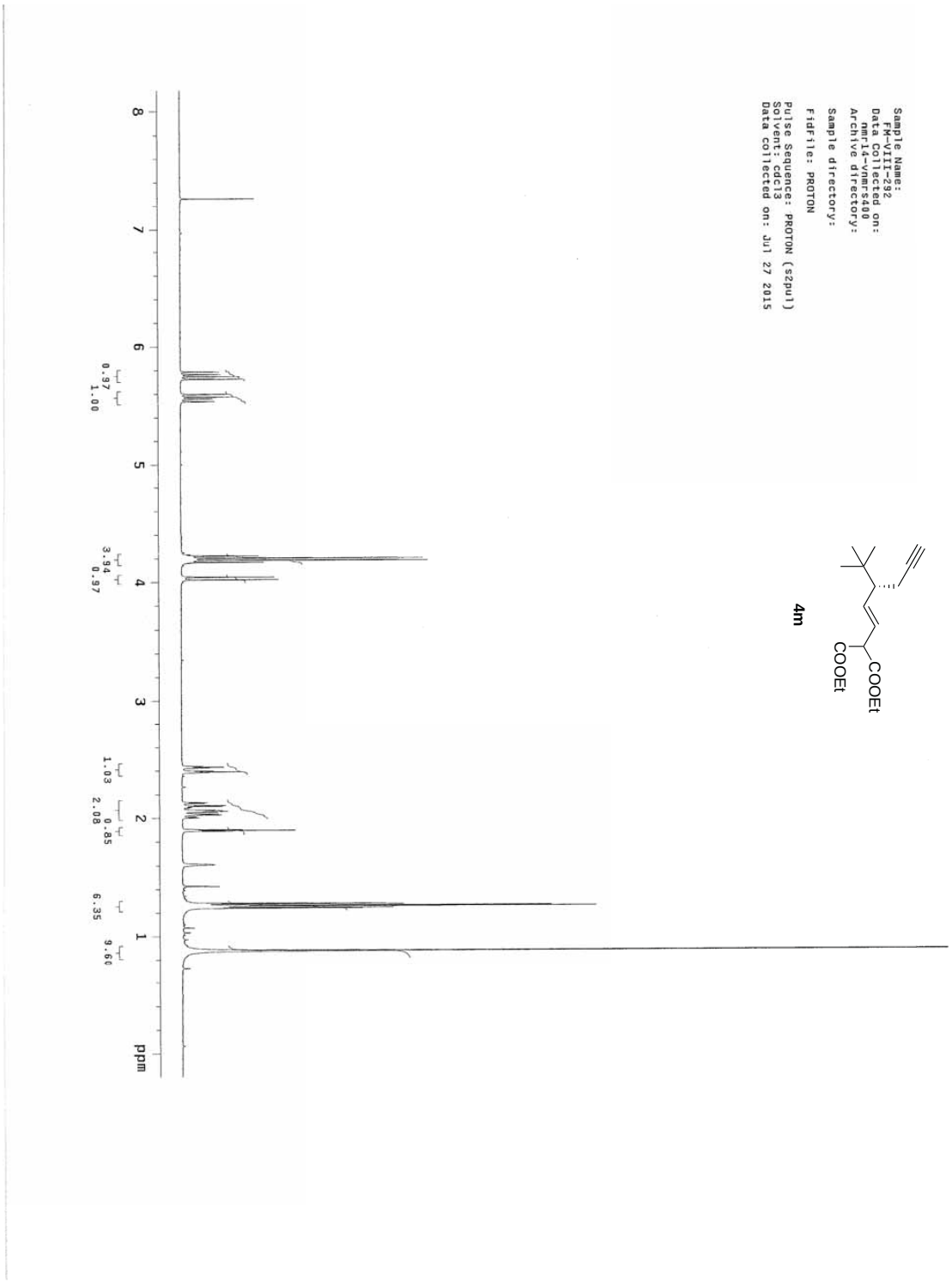

Sample Name:
FM-IX-172
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Ph
COOEt
COOEt
4j
180
160
140
120
100
80
60
40
20
ppm

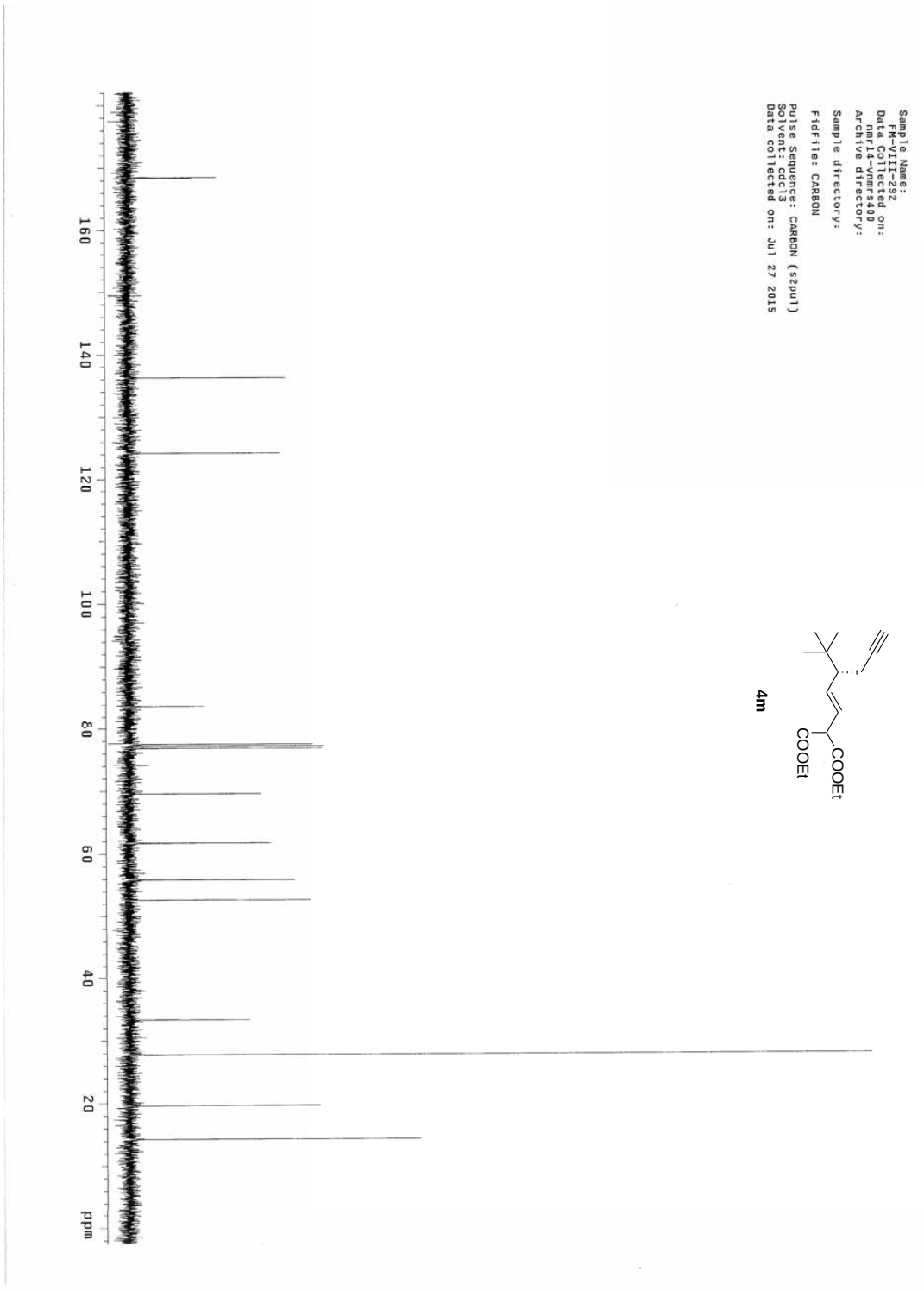

Sample Name:
FM-VIII-288
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2015
Ph
COOEt
COOEt
4k
8
7
6
5
4
3
2
1
ppm
2.13
2.91
0.97
1.00
3.97
0.99
1.11
1.11
3.13
1.07
0.88
1.06
6.24

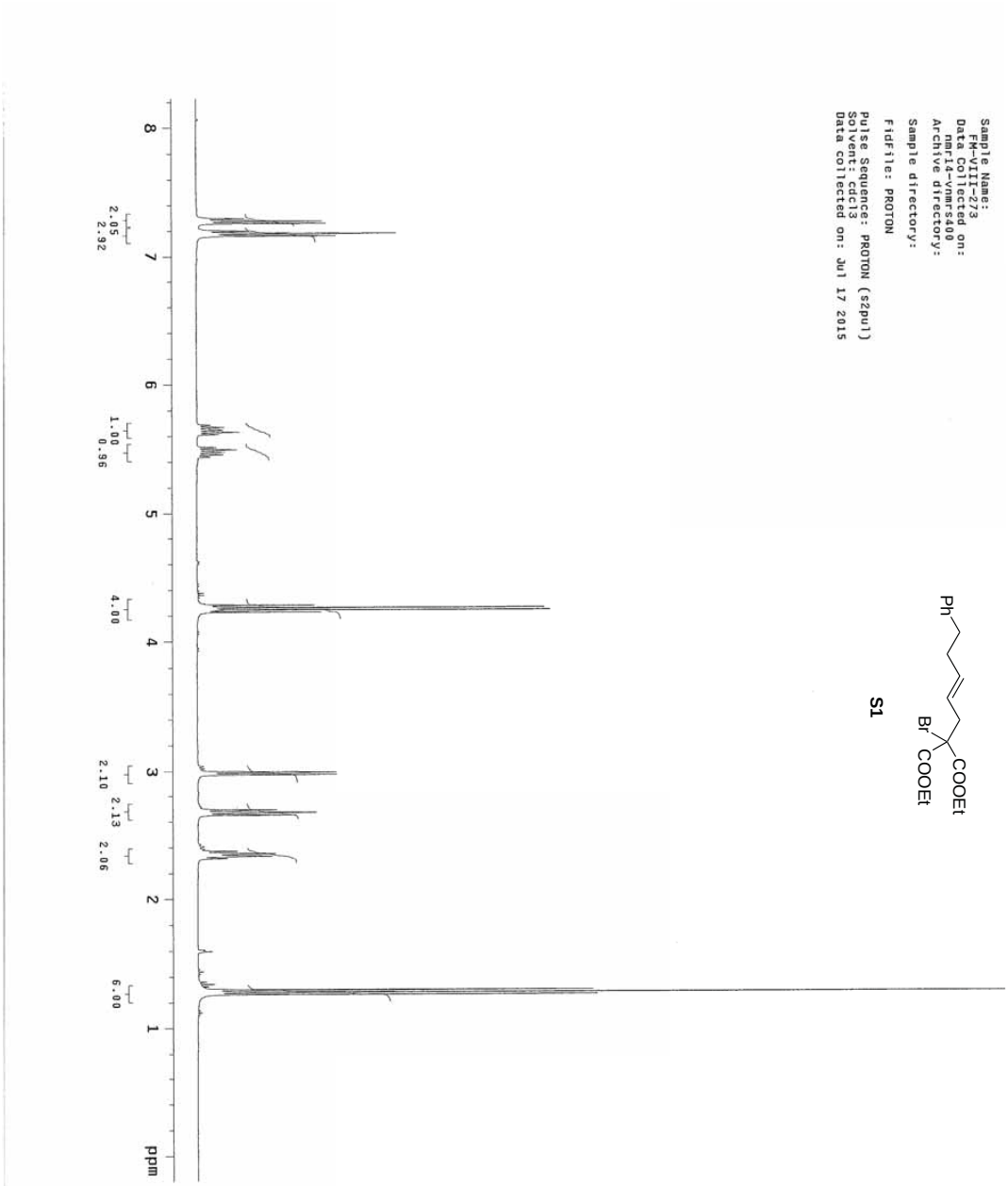

Sample Name:
FM-VIII-288
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2015
Ph
COOEt
COOEt
4k
160
140
120
100
80
60
40
20
ppm

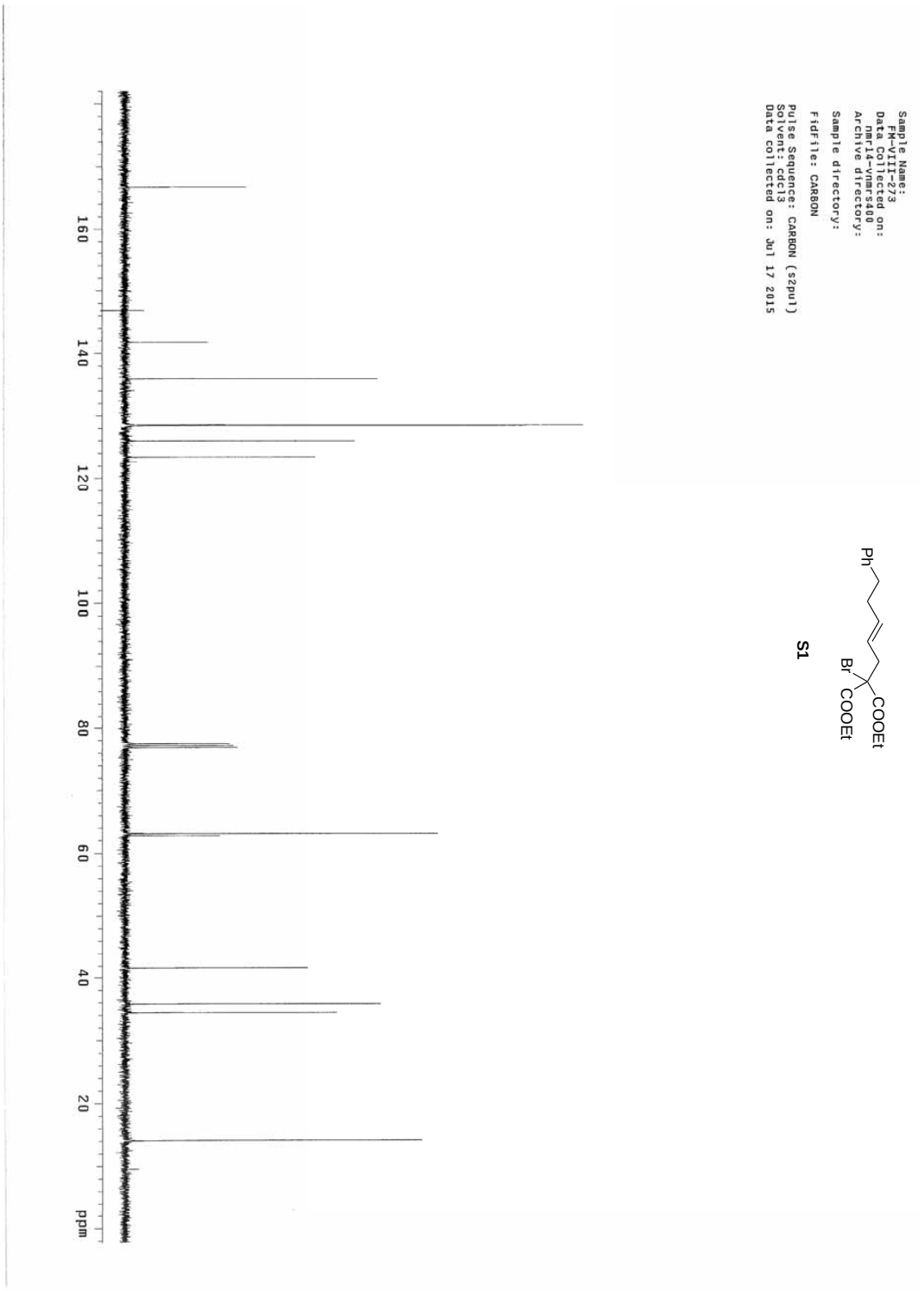

Sample Name:
FM-VIII-290
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2015
COOEt
COOEt
4l
8
7
6
5
4
3
2
1
ppm
0.96
0.99
4.00
0.96
2.09
0.90
1.02
4.99
1.24
3.21
6.59
2.34

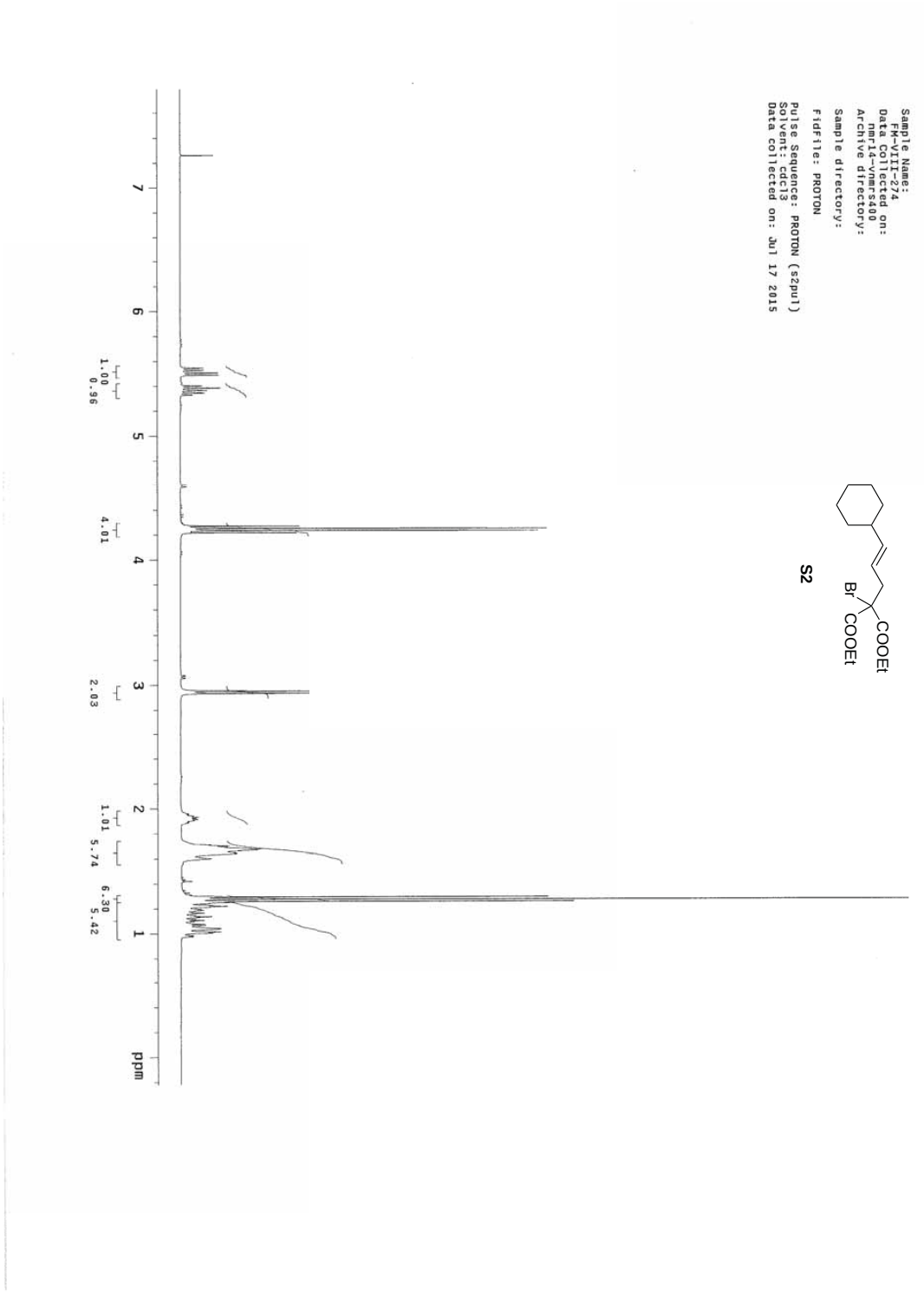

Sample Name:
FM-VIII-290
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2015
COOEt
COOEt
4l
160
140
120
100
80
60
40
20
ppm

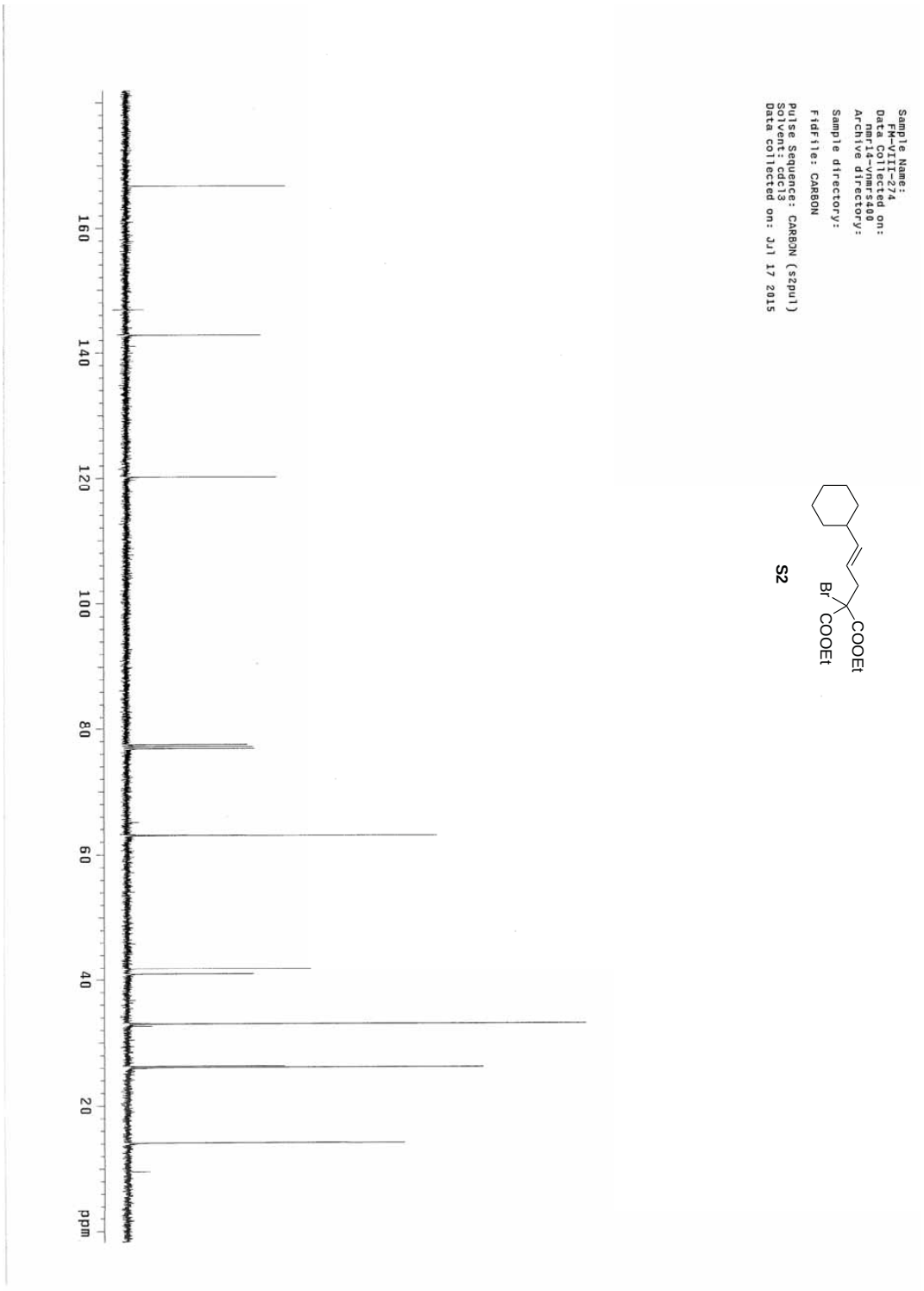

Sample Name:
FM-VIII-292
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2015
4m
COOEt
COOEt
8
7
6
5
4
3
2
1
ppm
0.97
1.00
3.94
0.97
1.03
0.85
2.08
6.35
9.66

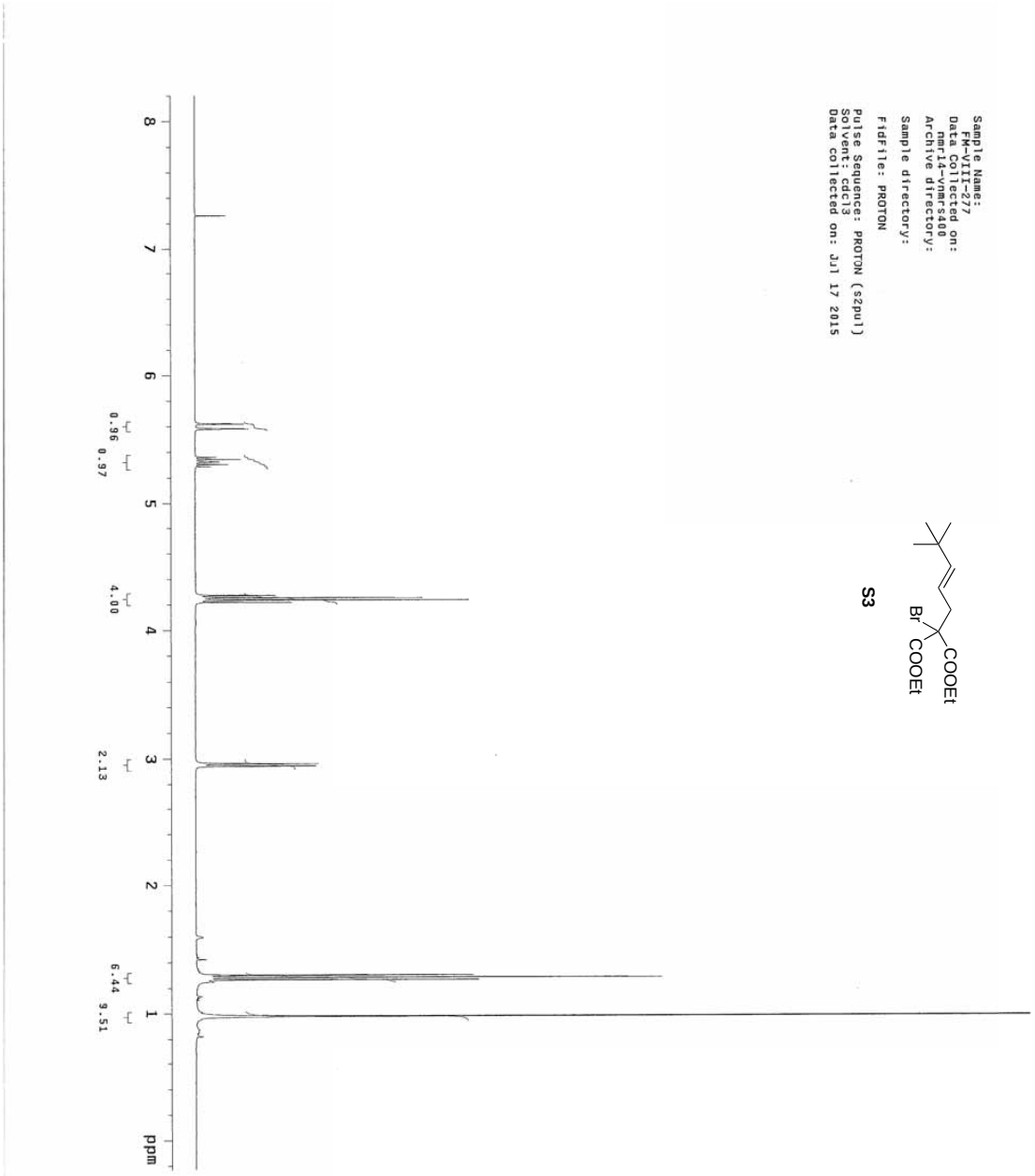

Sample Name:
FM-VIII-292
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2015
COOEt
COOEt
4m
160
140
120
100
80
60
40
20
ppm

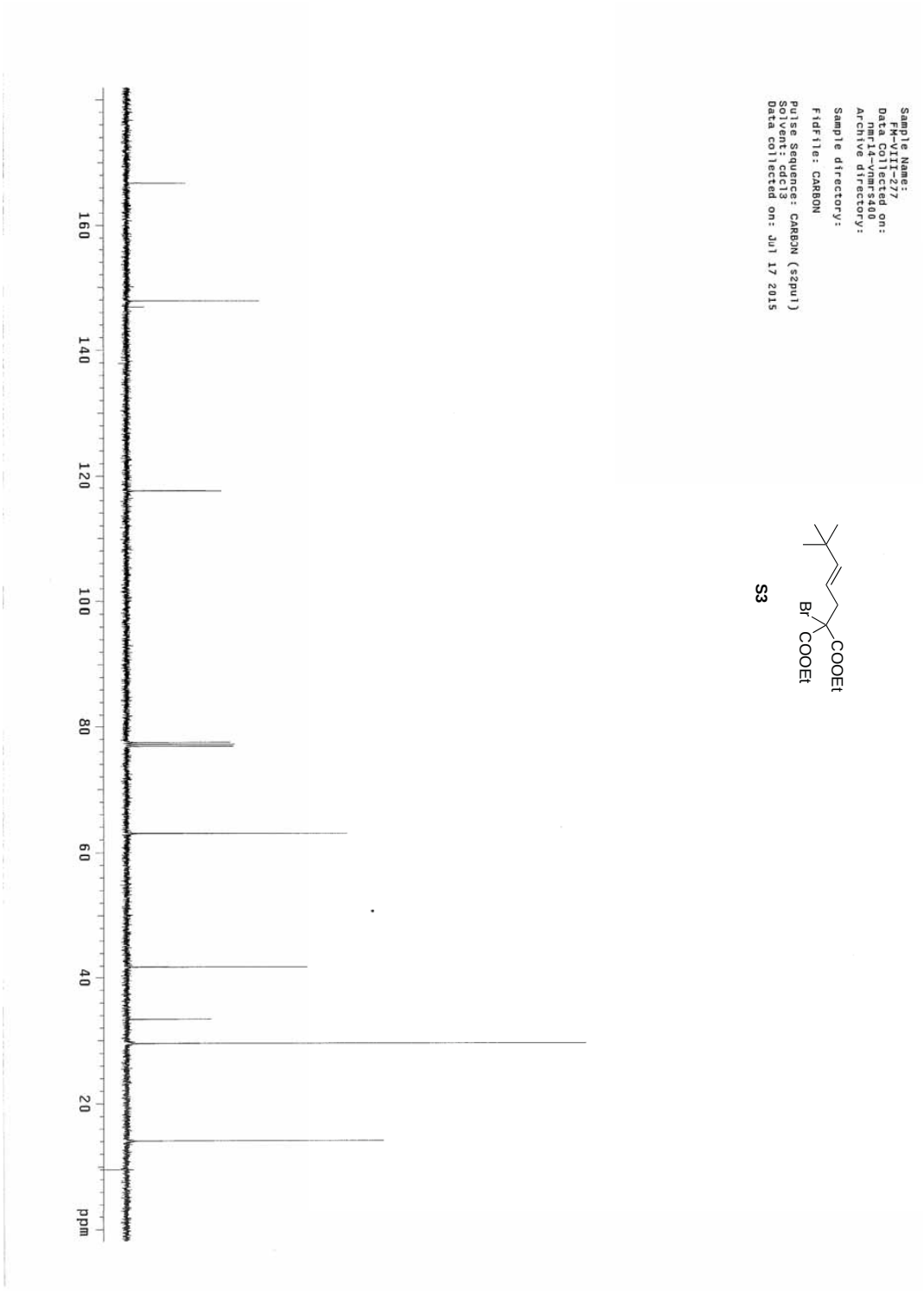

Sample Name:
FM-VIII-273
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 17 2015
Ph
Br
COOEt
COOEt
S1
8
7
6
5
4
3
2
1
ppm
2.05
2.92
1.00
0.96
4.00
2.10
2.13
2.06
6.00

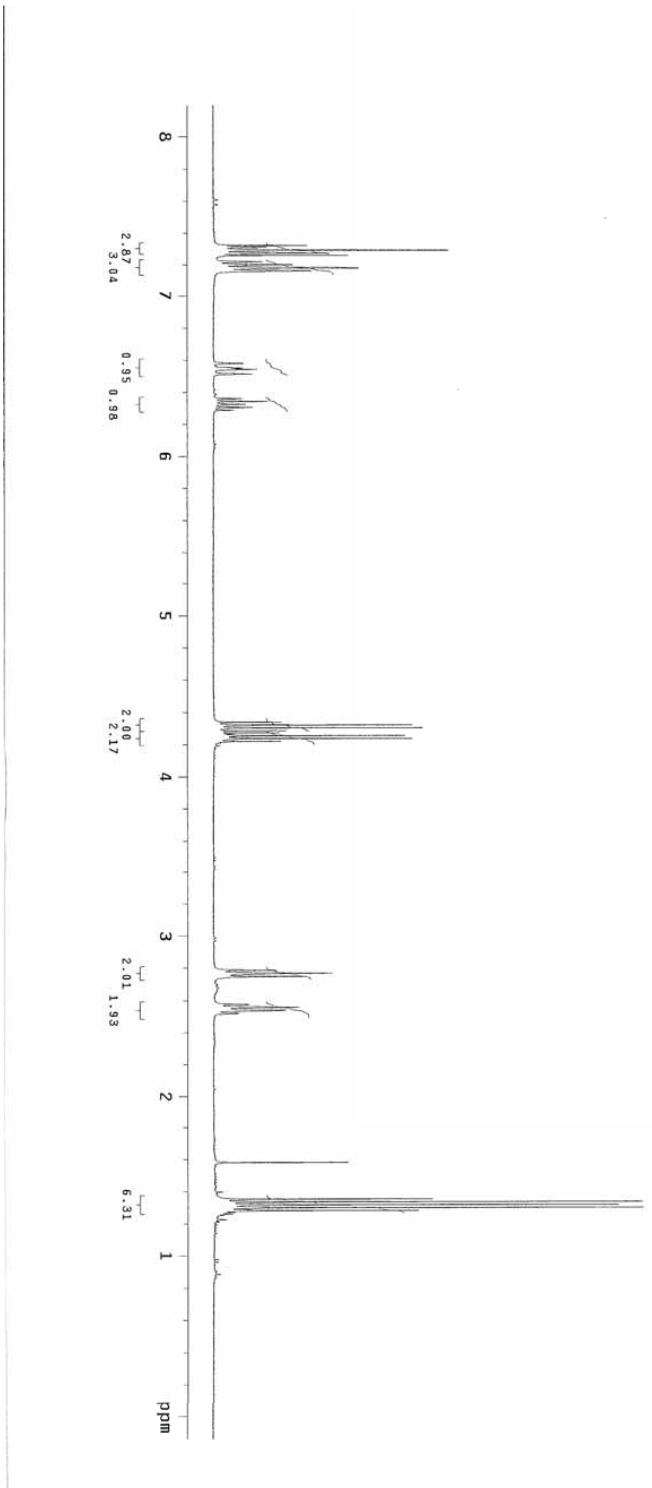

Sample Name:
FM-VIII-273
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 17 2015
Ph
Br
COOEt
COOEt
S1
160
140
120
100
80
60
40
20
ppm

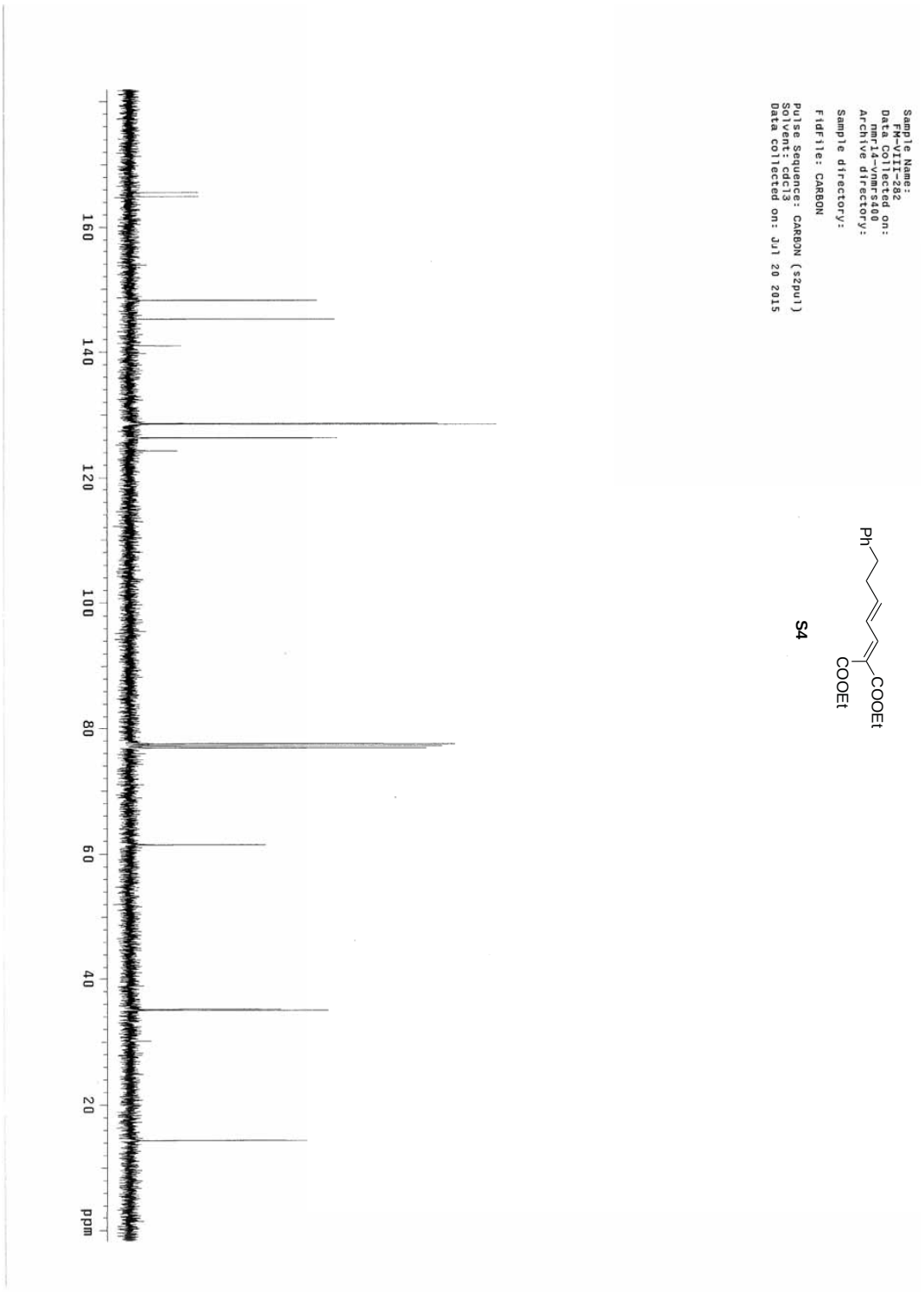

Sample Name:
FM-VIII-274
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 17 2015
Br
COOEt
COOEt
S2
7
6
5
4
3
2
1
ppm
1.00
0.96
4.01
2.03
1.01
5.74
6.30
5.42

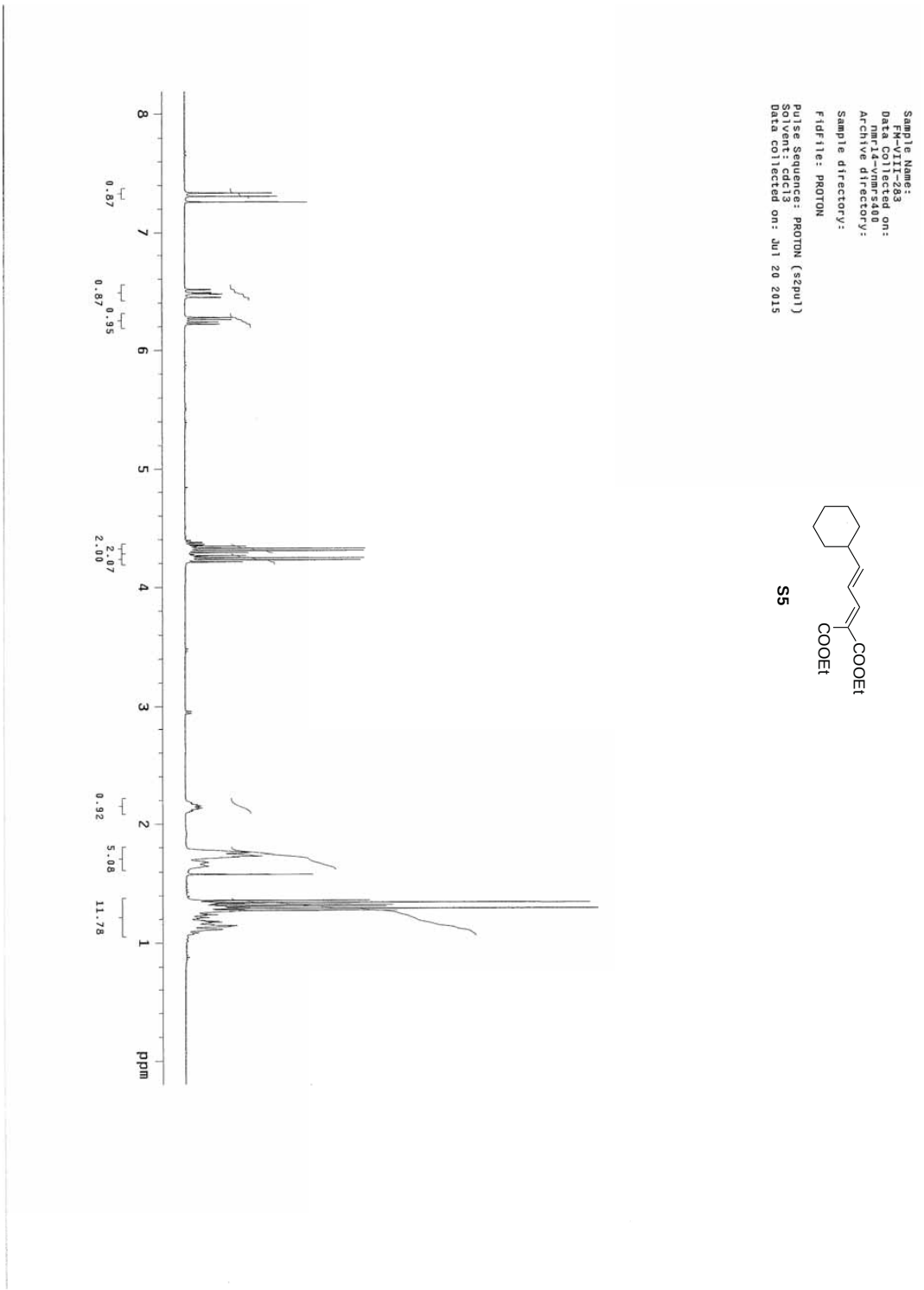

Sample Name:
FM-VIII-274
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 17 2015
Br
COOEt
COOEt
S2
160
140
120
100
80
60
40
20
ppm

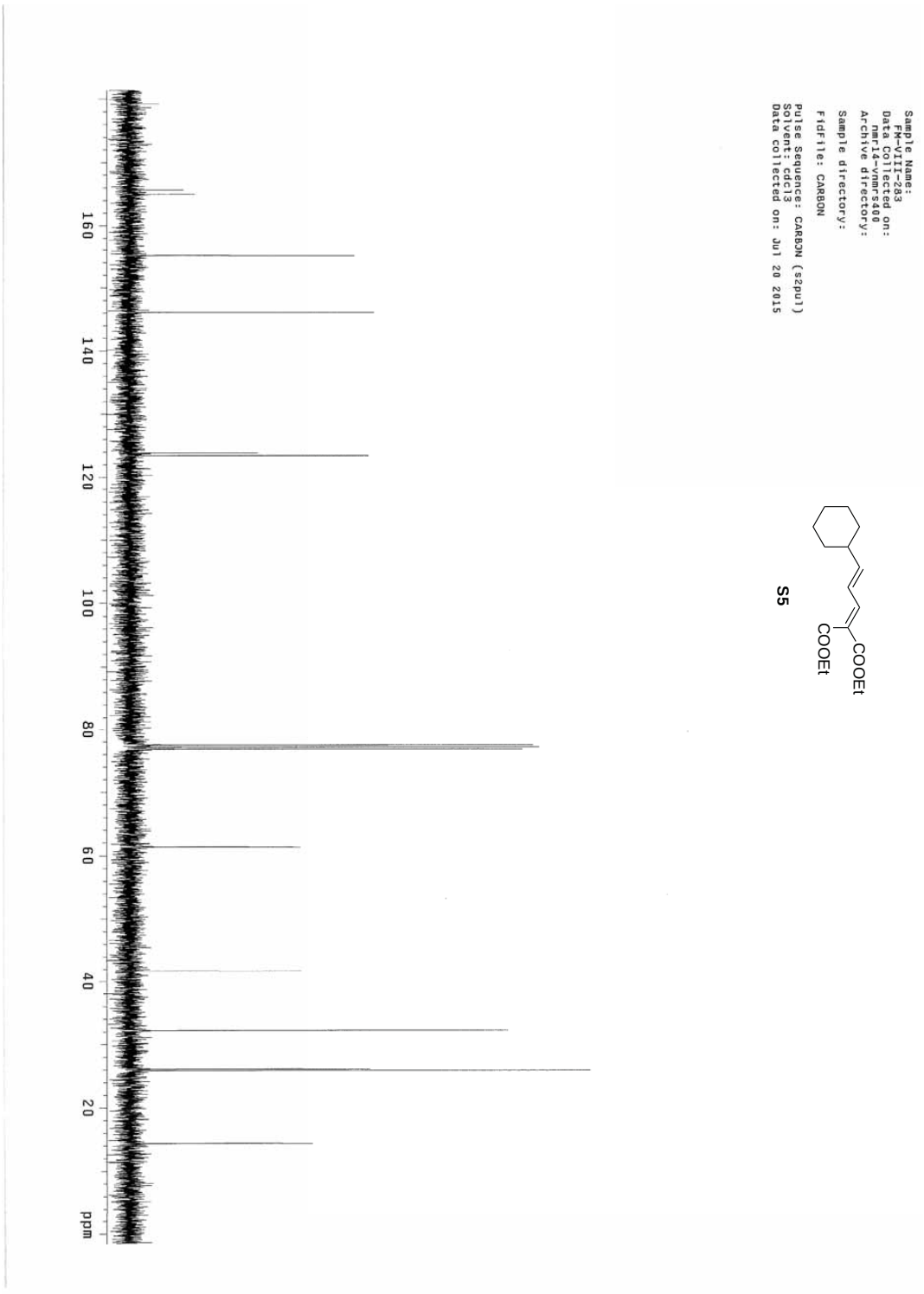

Sample Name:
FM-VIII-277
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 17 2015
Br
COOEt
COOEt
S3
8
7
6
5
4
3
2
1
ppm
0.96
0.97
4.00
2.13
6.44
9.51

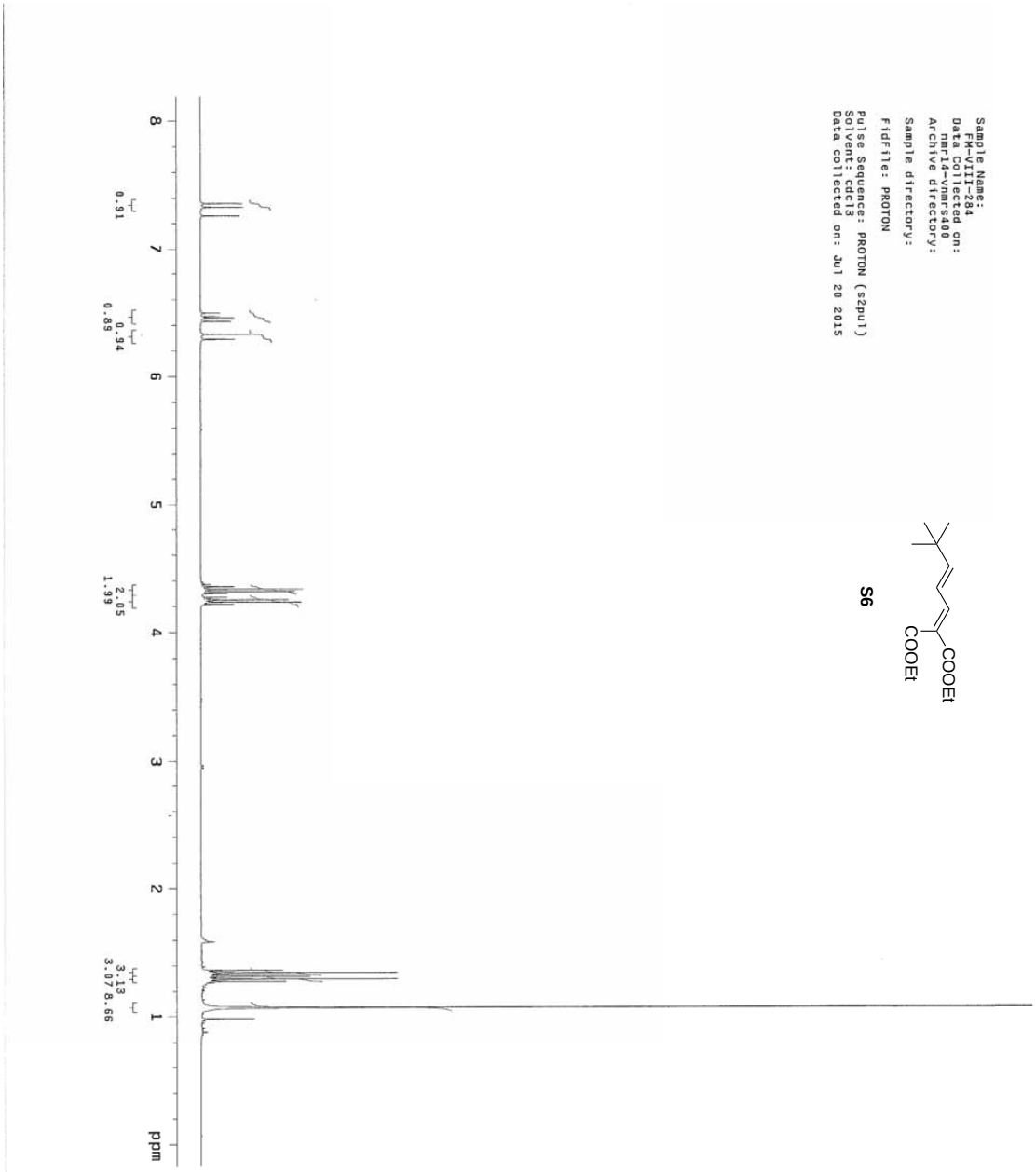

Sample Name:
FM-VIII-277
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBJN (s2pul)
Solvent: cdcl3
Data collected on: Jul 17 2015
Br
COOEt
COOEt
S3
160
140
120
100
80
60
40
20
ppm

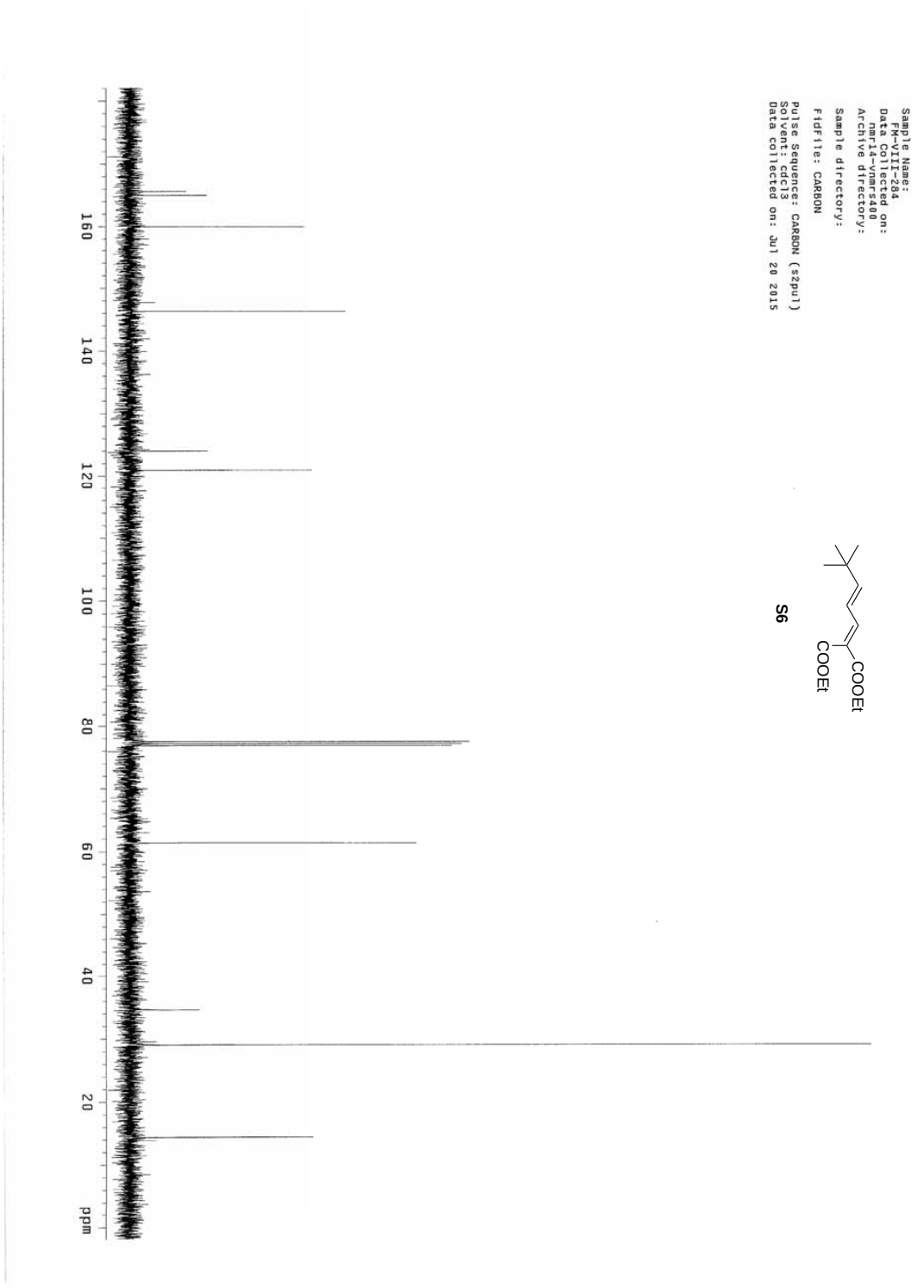

Sample Name:
FM-VIII-282
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: FM-VIII-282
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2015
Ph
COOEt
COOEt
S4
8
7
6
5
4
3
2
1
ppm
2.87
3.04
0.95
0.98
2.00
2.17
2.01
1.93
6.31

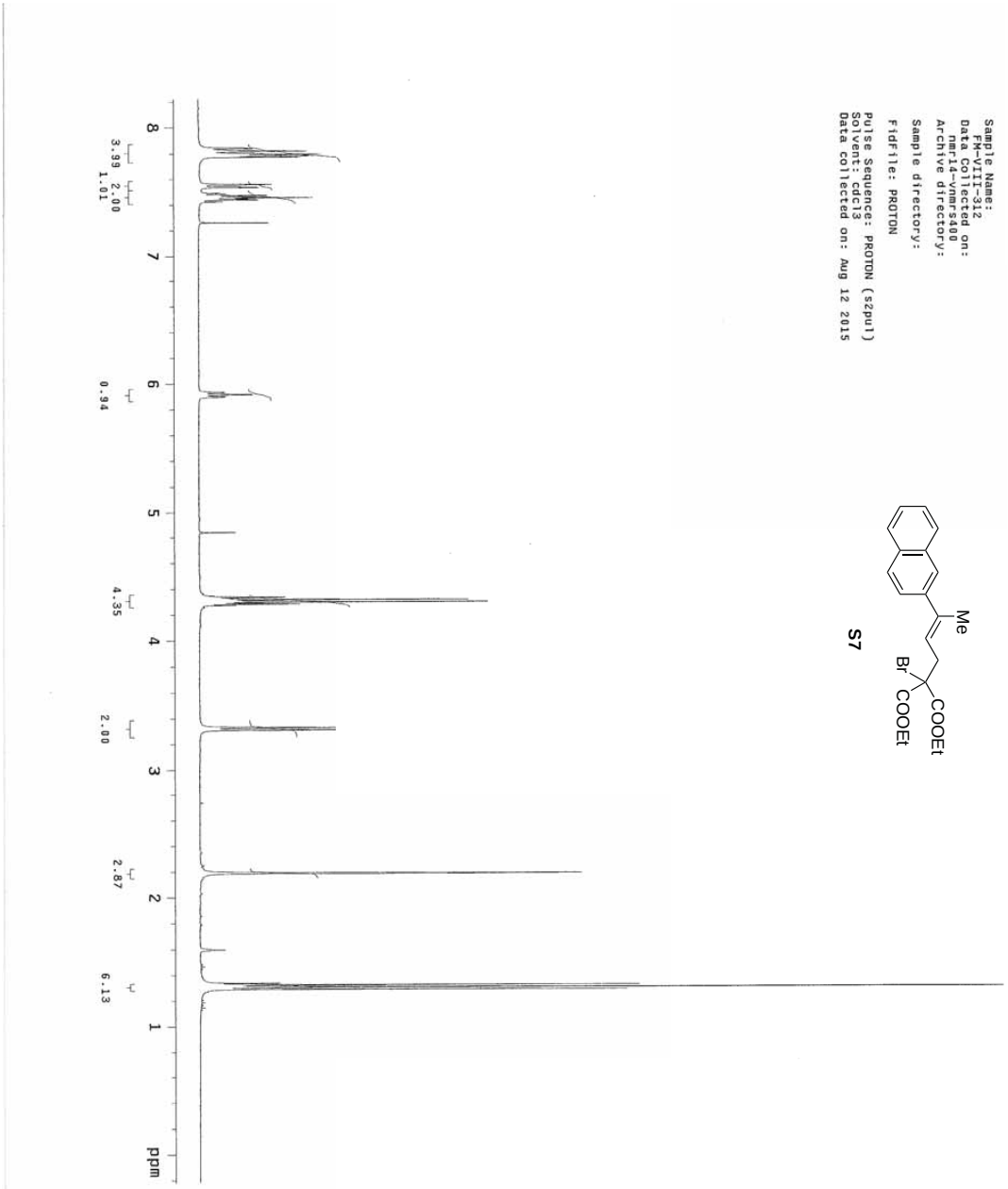

Sample Name:
FM-VIII-282
Data Collected on:
nmr14-vmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2015
Ph
COOEt
COOEt
S4
160
140
120
100
80
60
40
20
ppm

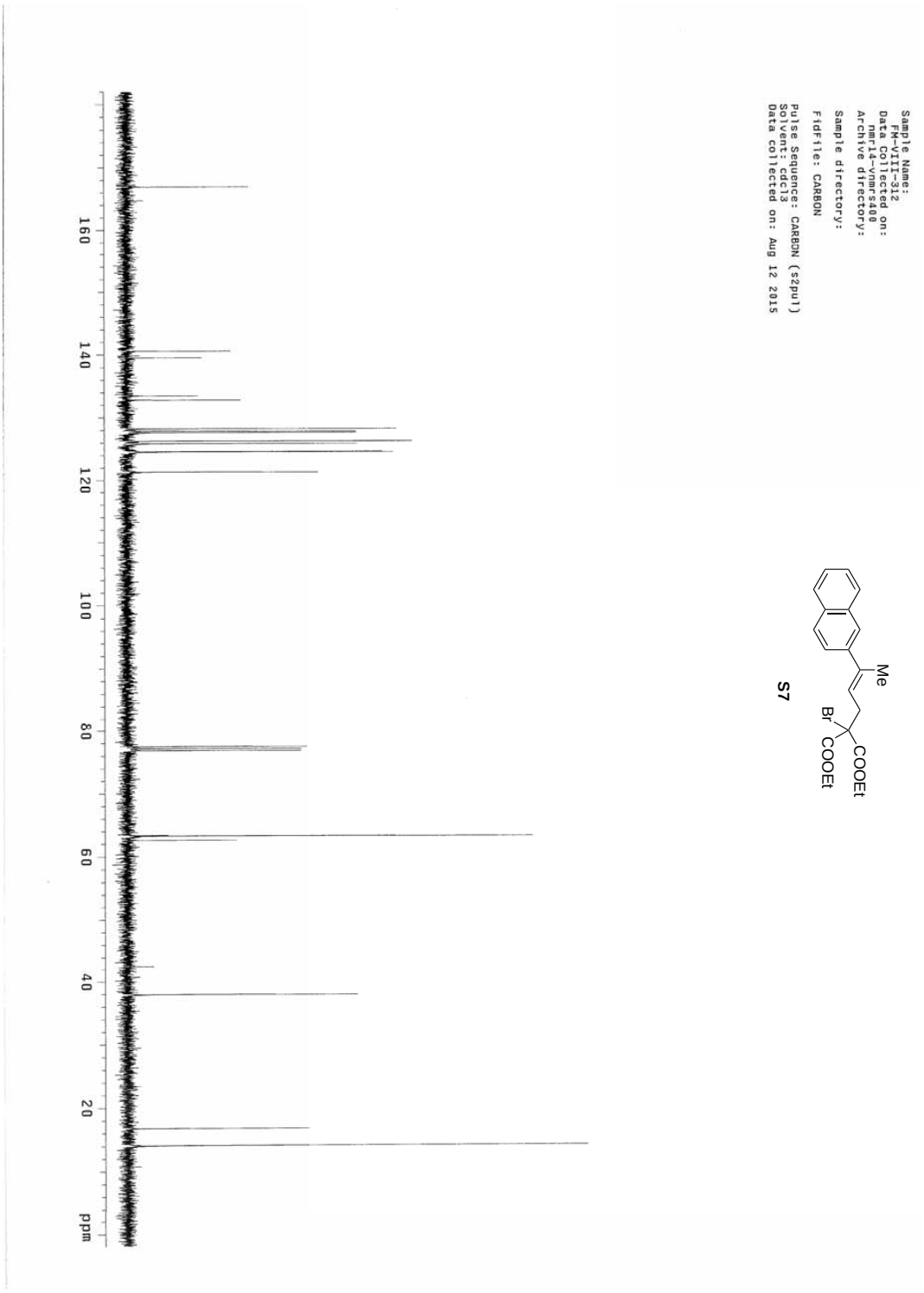

Sample Name:
FM-VIII-283
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2015
S5
COOEt
COOEt
0.87
0.87
0.95
2.07
2.00
0.92
5.08
11.78
ppm

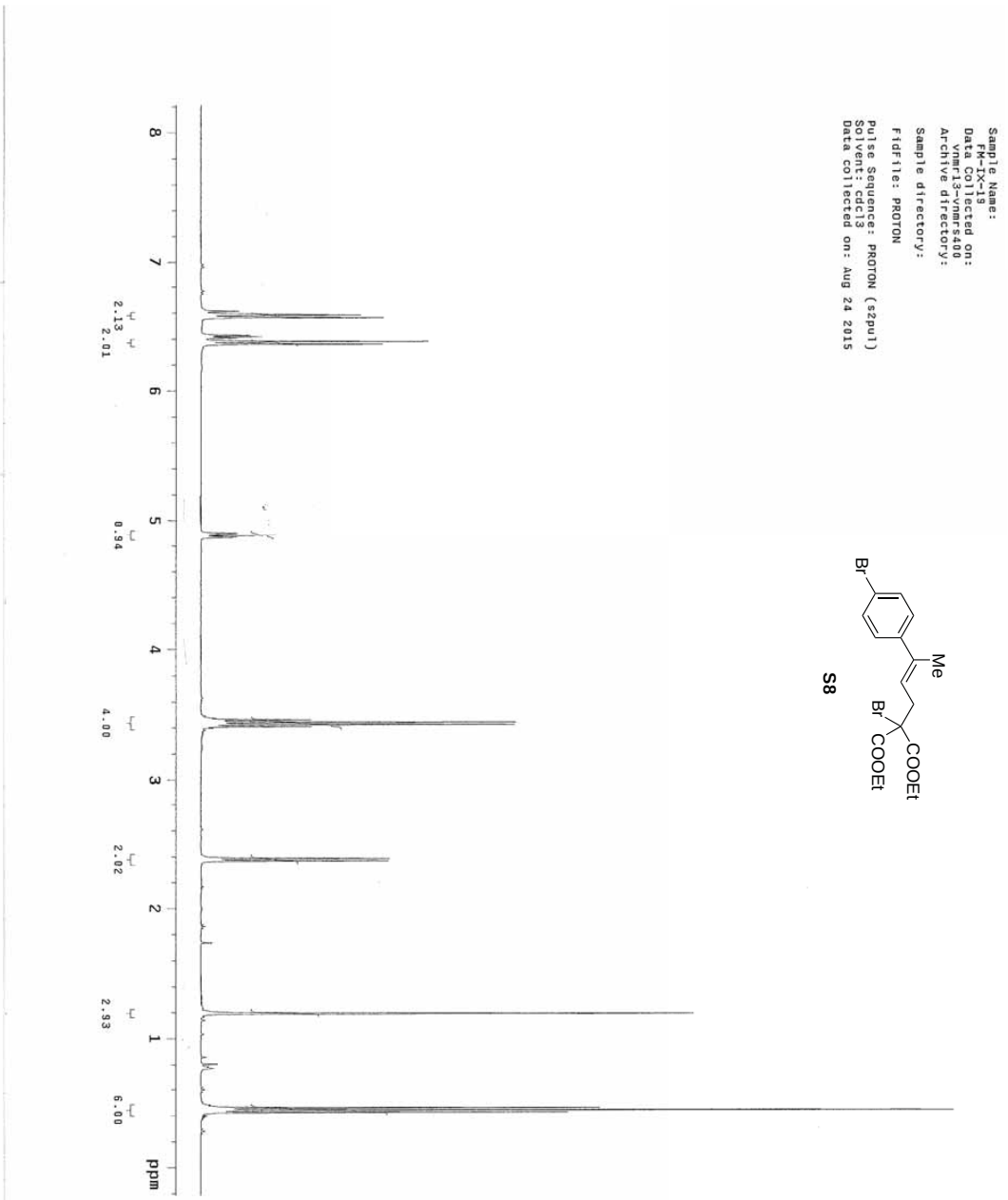

Sample Name:
FM-VIII-283
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2015
COOEt
COOEt
S5
160
140
120
100
80
60
40
20
ppm

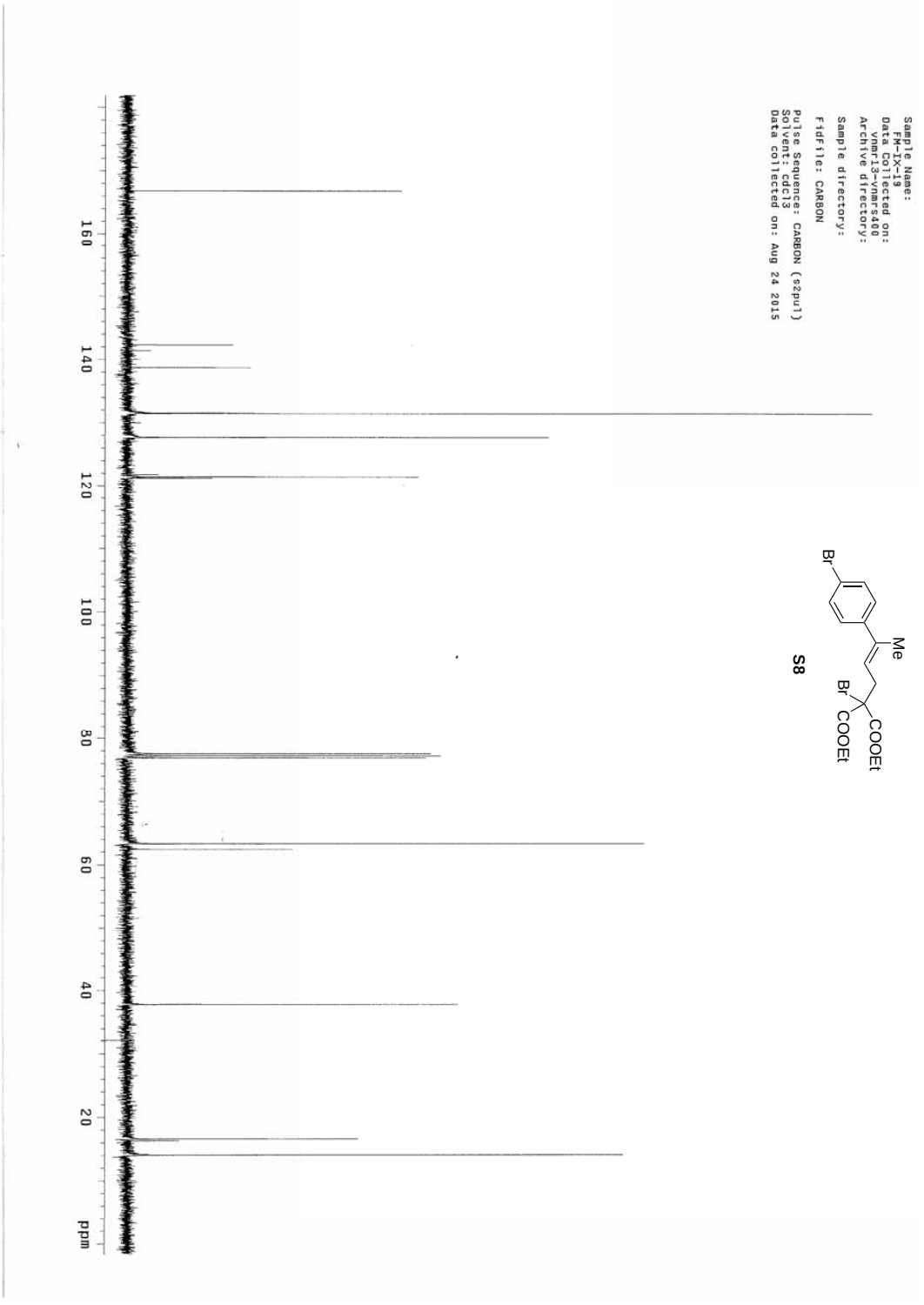

Sample Name:
FK-VIII-284
Data collected on:
nmr-pc400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2015
COOEt
COOEt
S6
0.91
0.94
0.89
2.05
1.99
3.13
3.07
8.66
8
7
6
5
4
3
2
1
ppm


Sample Name:
FM-VIII-284
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2015
COOEt
COOEt
S6
160
140
120
100
80
60
40
20
ppm

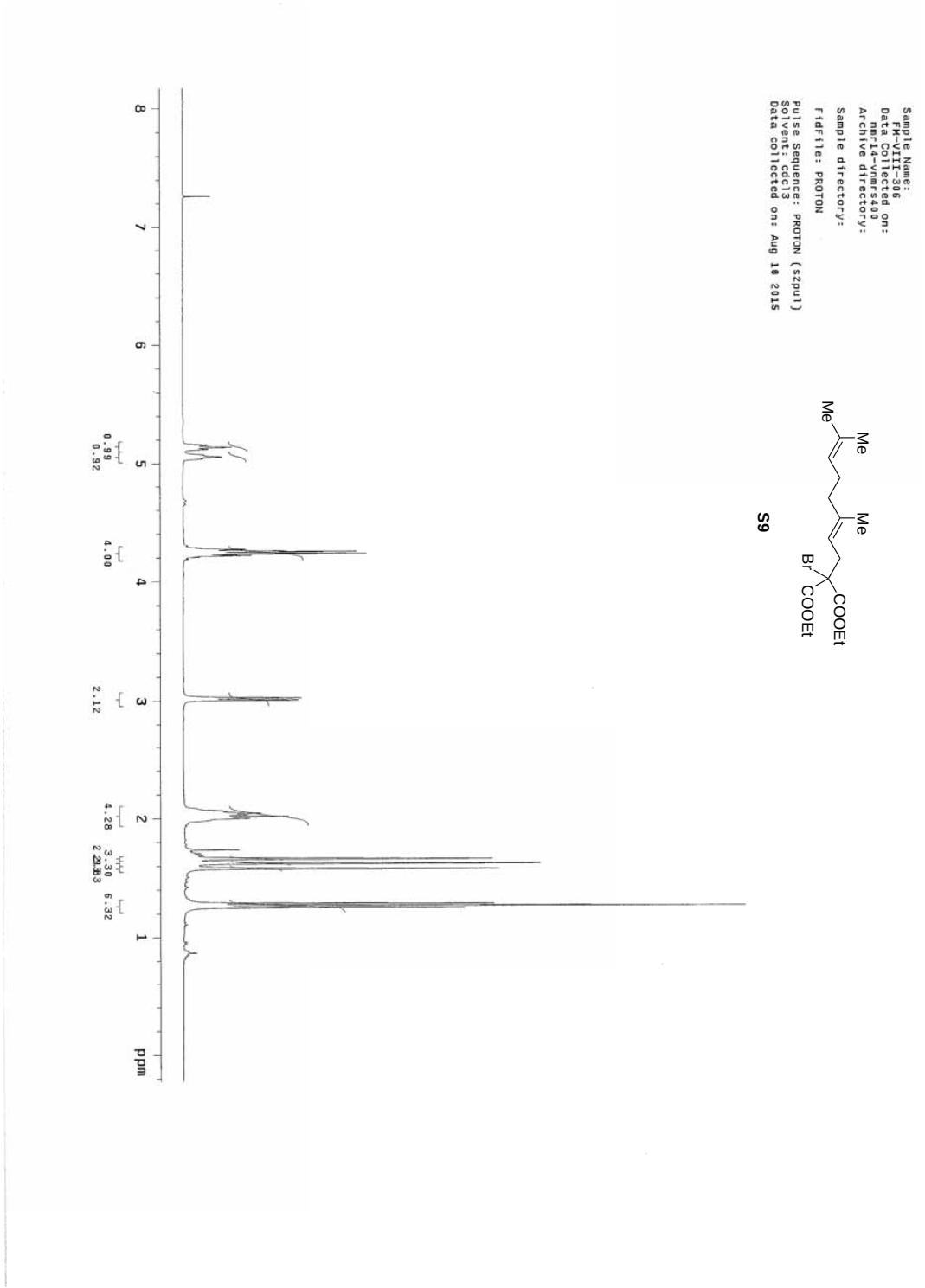

Sample Name:
FM-VIII-312
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 12 2015
Me
Br
COOEt
COOEt
S7
8
7
6
5
4
3
2
1
ppm
3.99
2.00
1.01
0.94
4.35
2.00
2.87
6.13

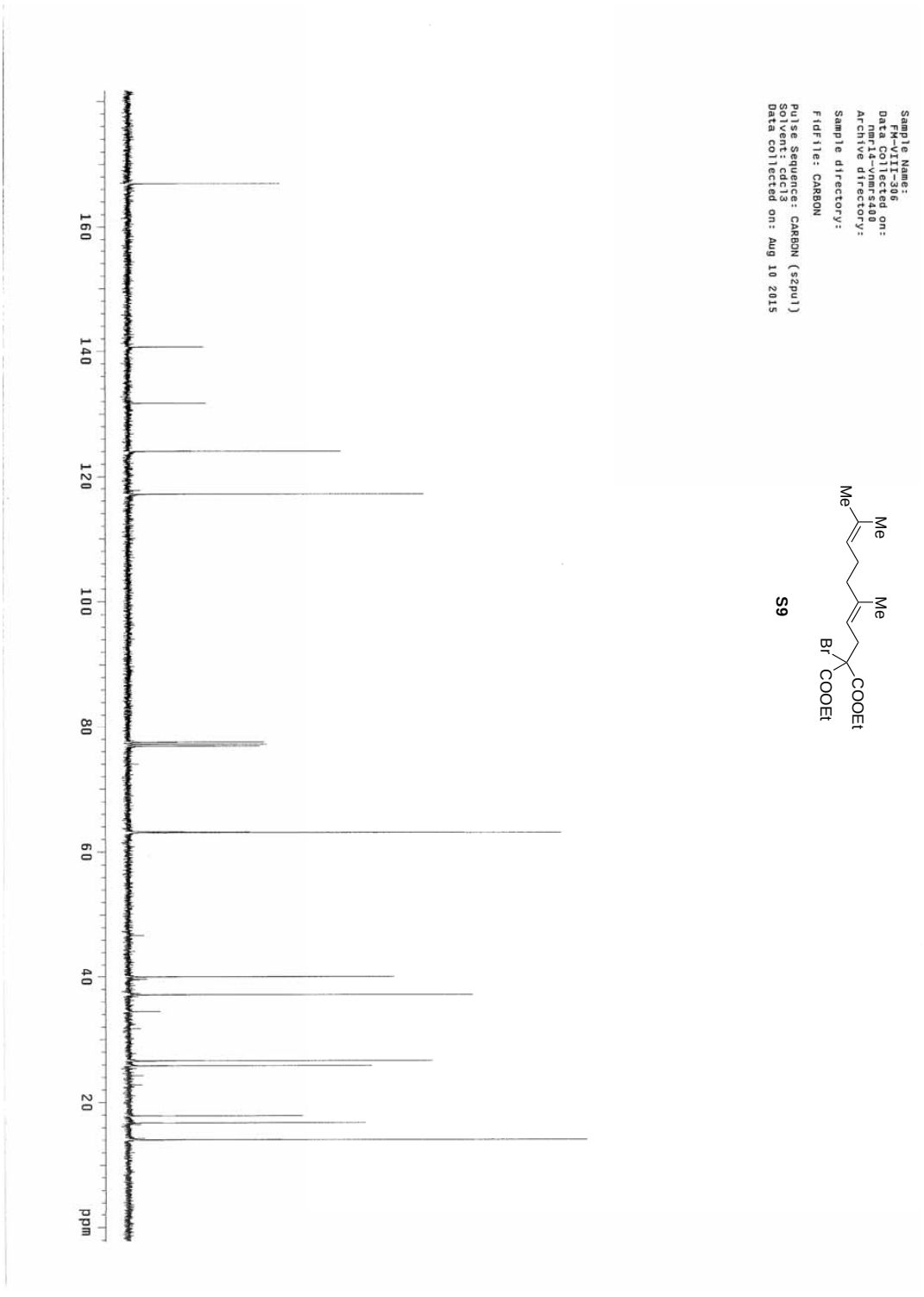

Sample Name:
FM-VIII-312
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 12 2015
Me
Br
COOEt
COOEt
S7
160
140
120
100
80
60
40
20
ppm

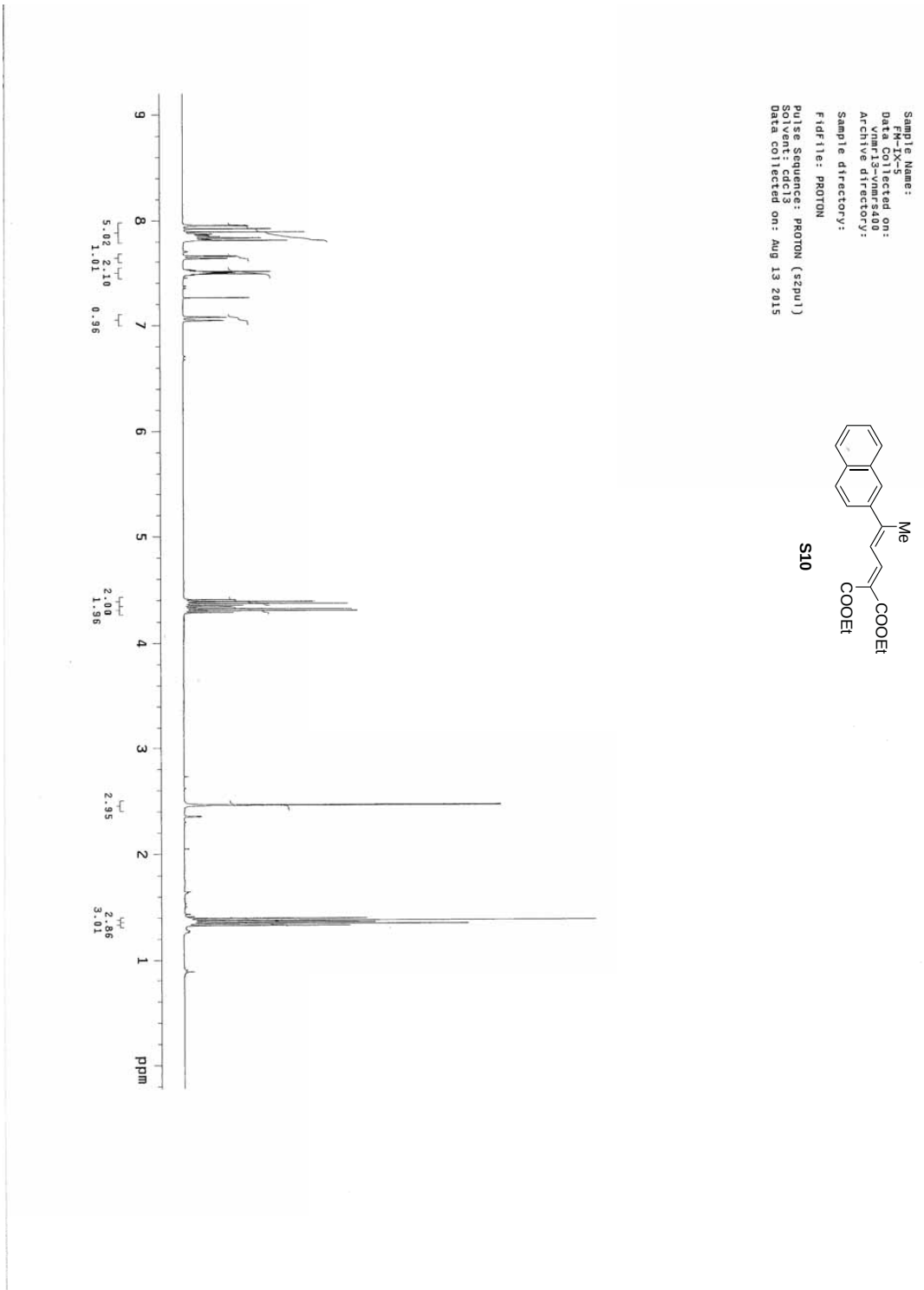

Sample Name:
FM-IX-19
Data Collected on:
Vnmrs400
Vnmrs3-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (szpul)
Solvent: cdcl3
Data collected on: Aug 24 2015
Br
Me
Br
COOEt
COOEt
S8
8
7
6
5
4
3
2
1
ppm
2.13
2.01
0.94
4.00
2.02
2.93
6.00

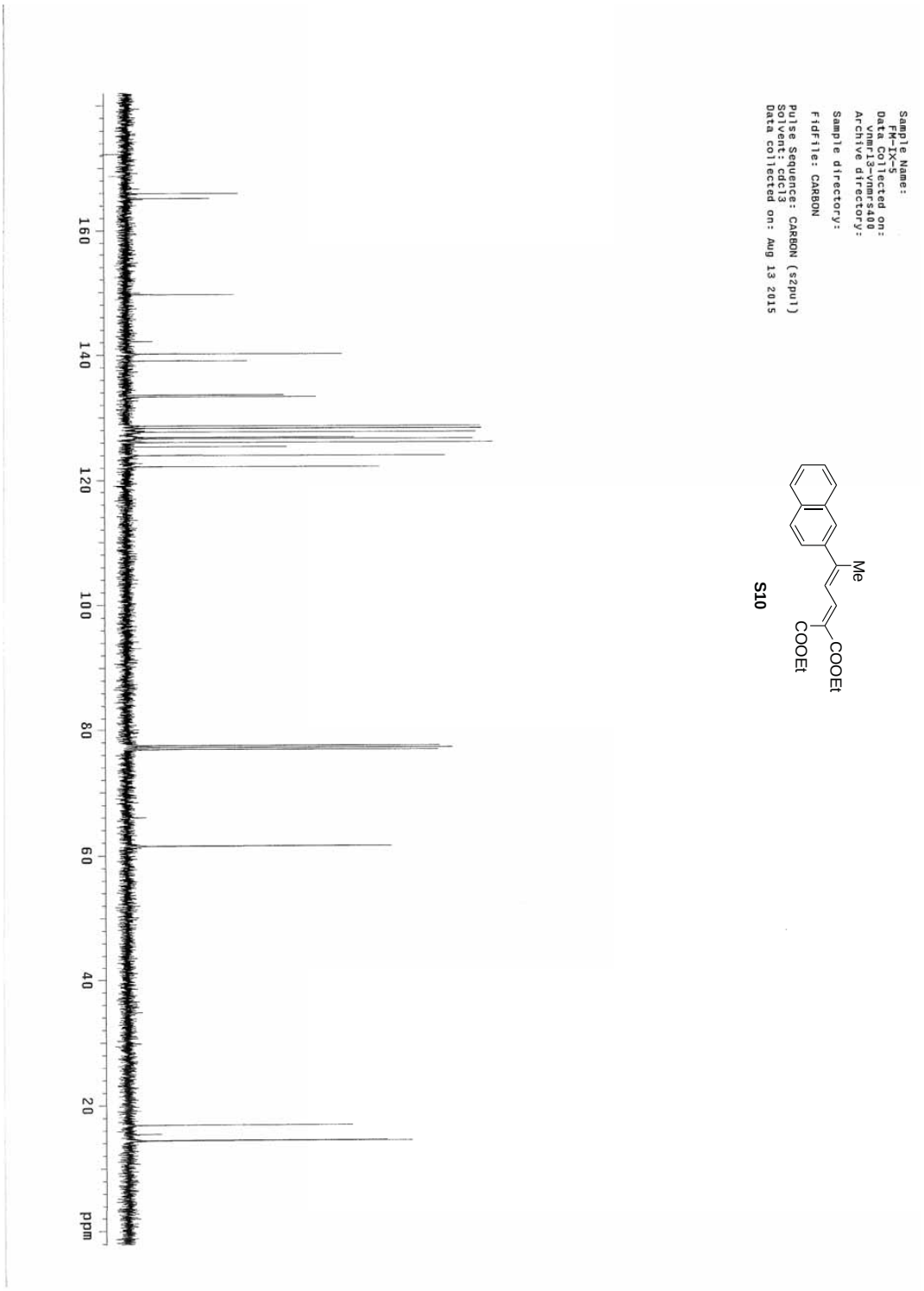

Sample Name:
Experiment:
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 24 2015
160
140
120
100
80
60
40
20
ppm
Br
Me
Br
COOEt
COOEt

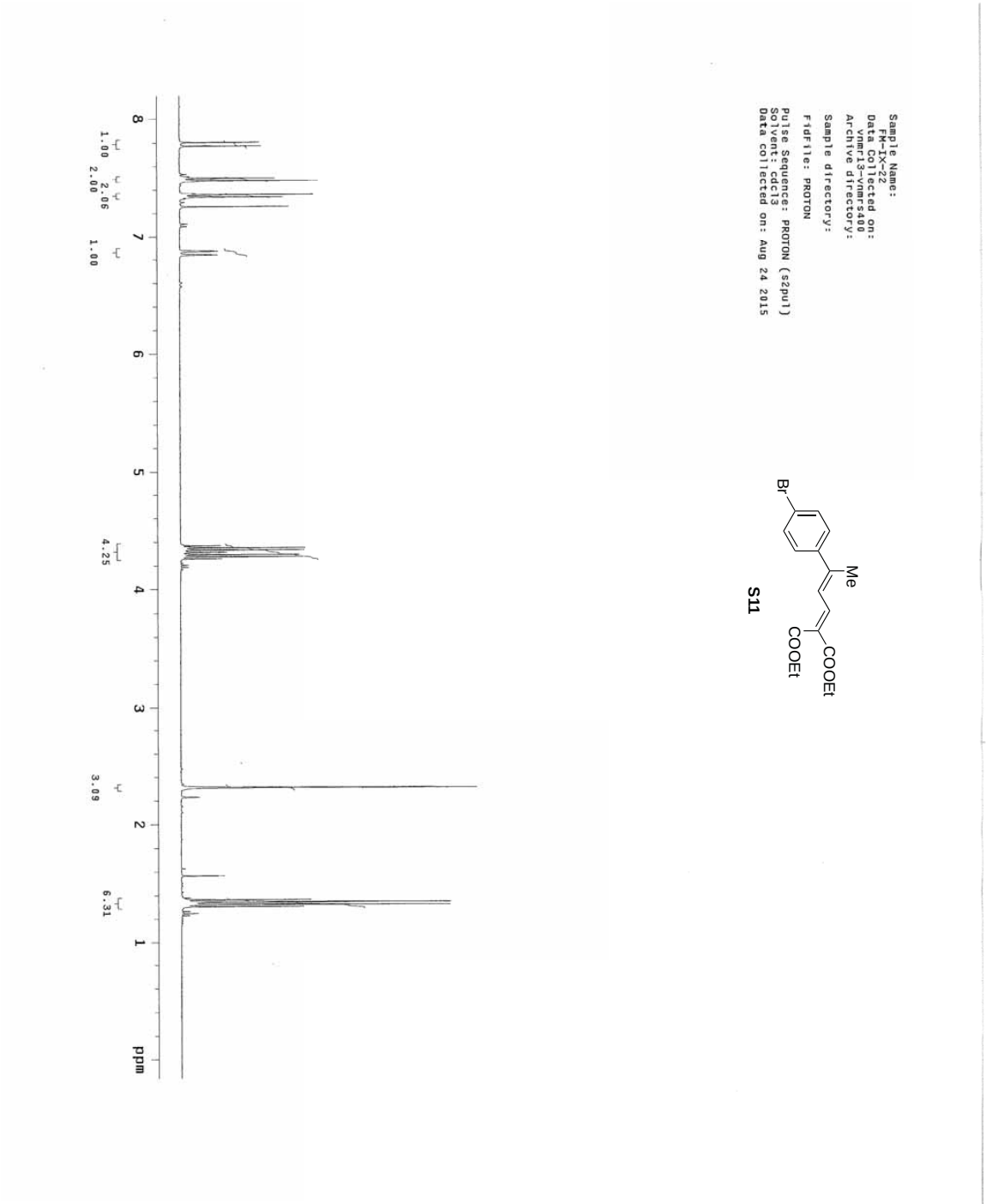
S8

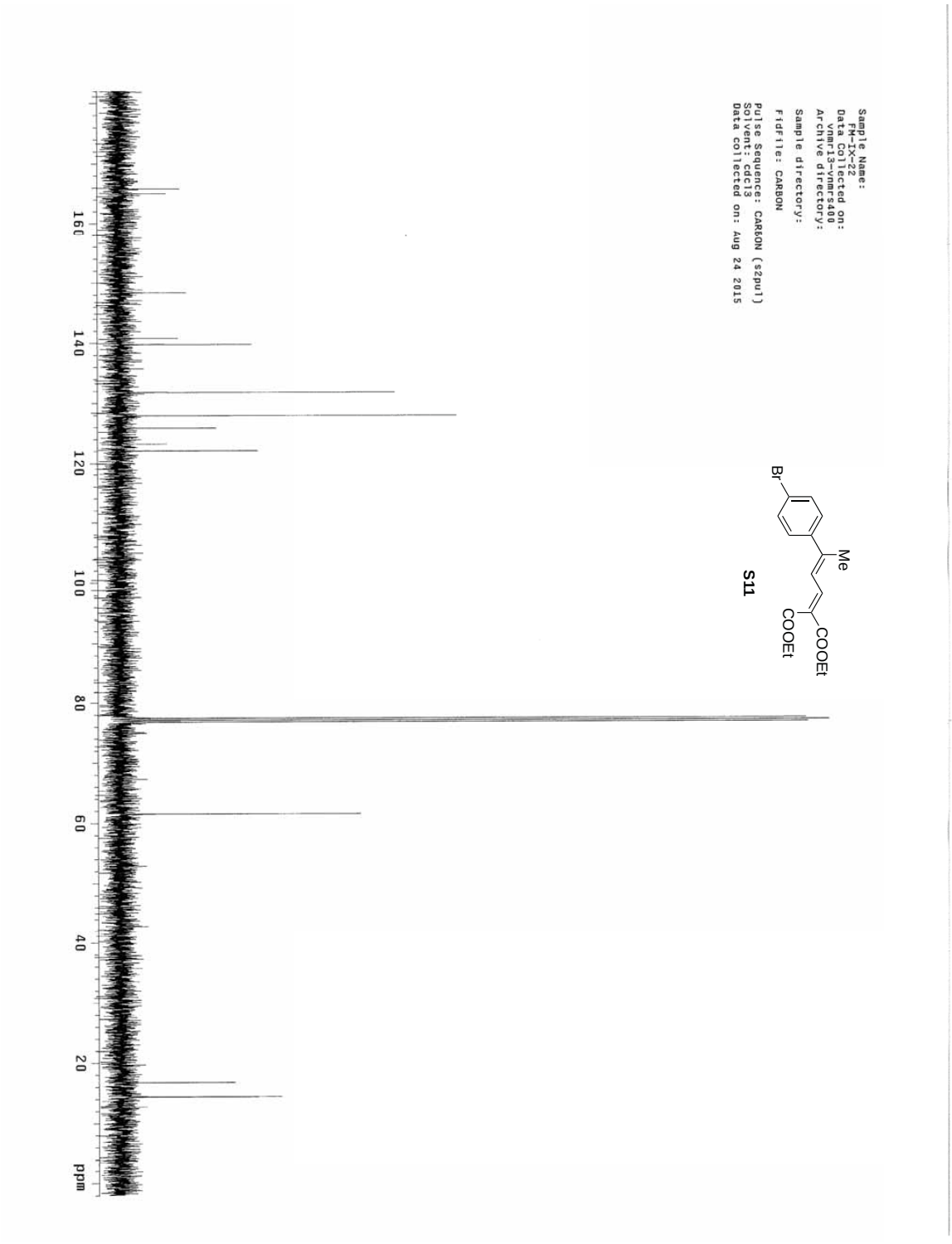

Sample Name:
FM-VIII-306
Data Collected on:
nmrl4-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 10 2015
Me
Me
Me
Br
COOEt
COOEt
S9
8
7
6
5
4
3
2
1
ppm
0.99
0.92
4.00
2.12
4.28
3.30
6.32

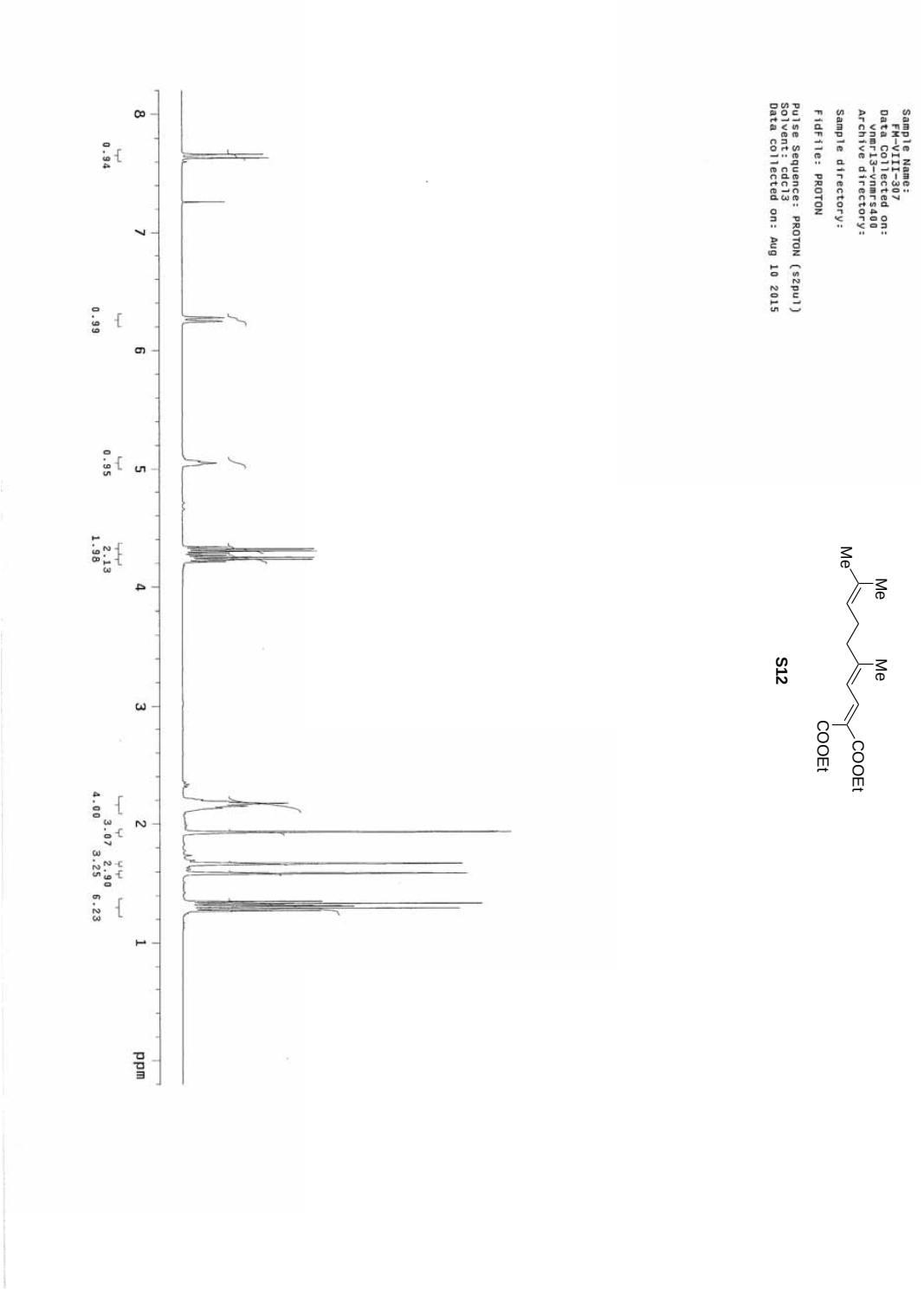

Sample Name:
FM-VIII-306
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 10 2015
Me
Me
Me
Br
COOEt
COOEt
S9
160
140
120
100
80
60
40
20
ppm

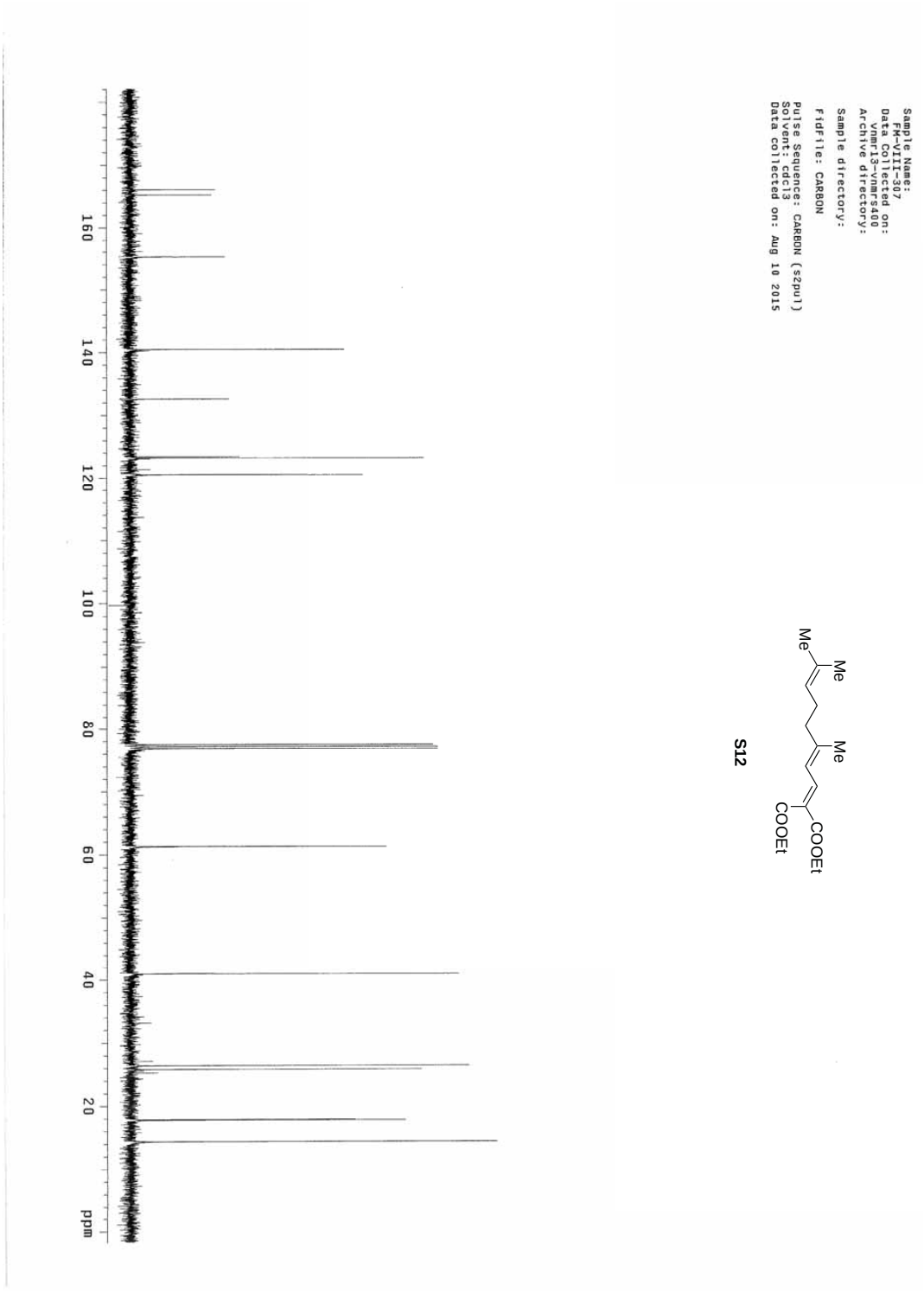

Sample Name:
FM-IX-5
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 13 2015
Me
COOEt
COOEt
S10
5.02
2.10
1.01
0.96
2.00
1.96
2.95
2.86
3.01
9
8
7
6
5
4
3
2
1
ppm


Sample Name:
FM-IX-5
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 13 2015
Me
COOEt
COOEt
S10
160
140
120
100
80
60
40
20
ppm

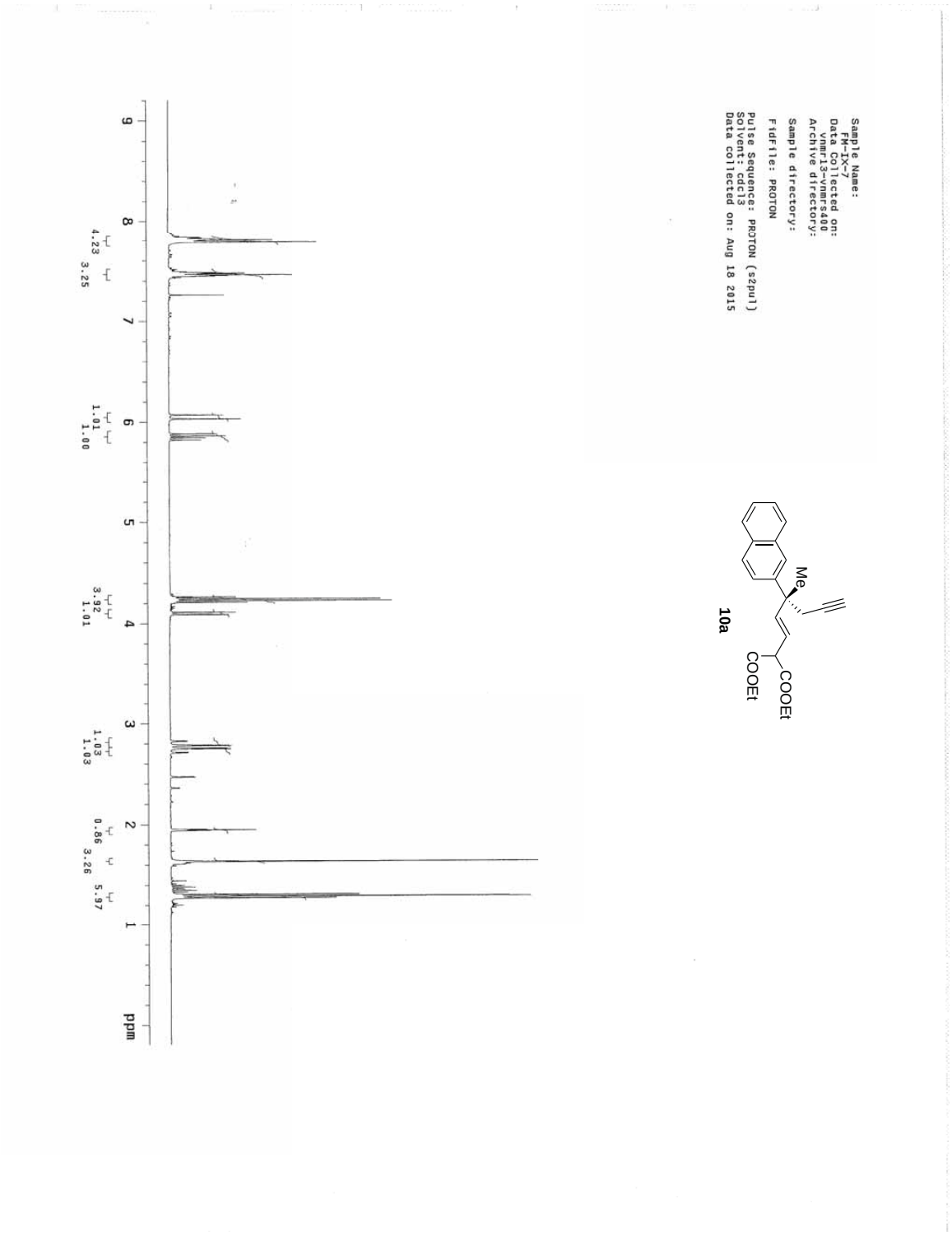

Sample Name:
FM-IX-22
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 24 2015
Br
Me
COOEt
COOEt
S11
8
7
6
5
4
3
2
1
ppm
1.00
2.06
2.00
1.00
4.25
3.09
6.31

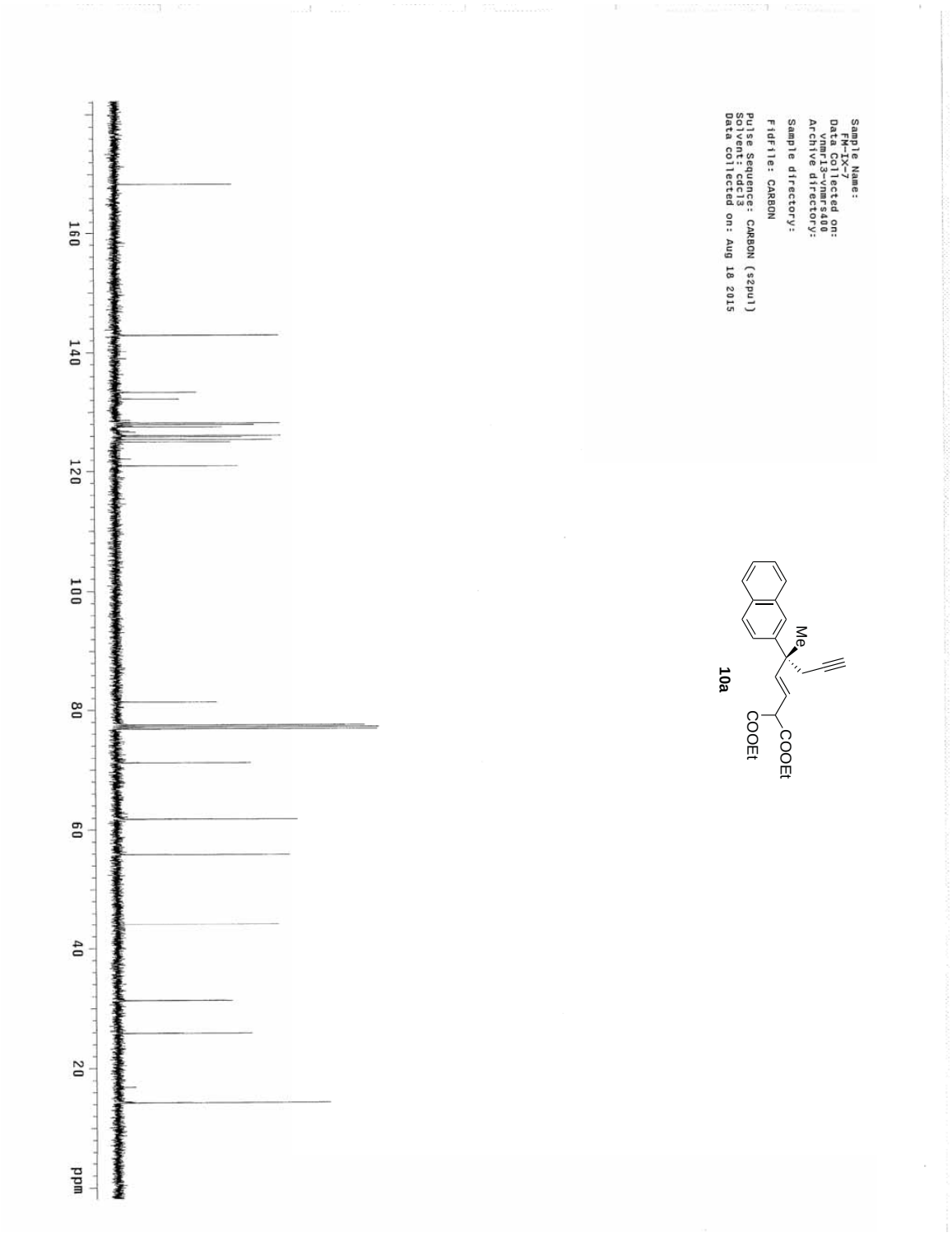

Sample Name:
FM-IX-22
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 24 2015
Br
Me
COOEt
COOEt
S11
160
140
120
100
80
60
40
20
ppm

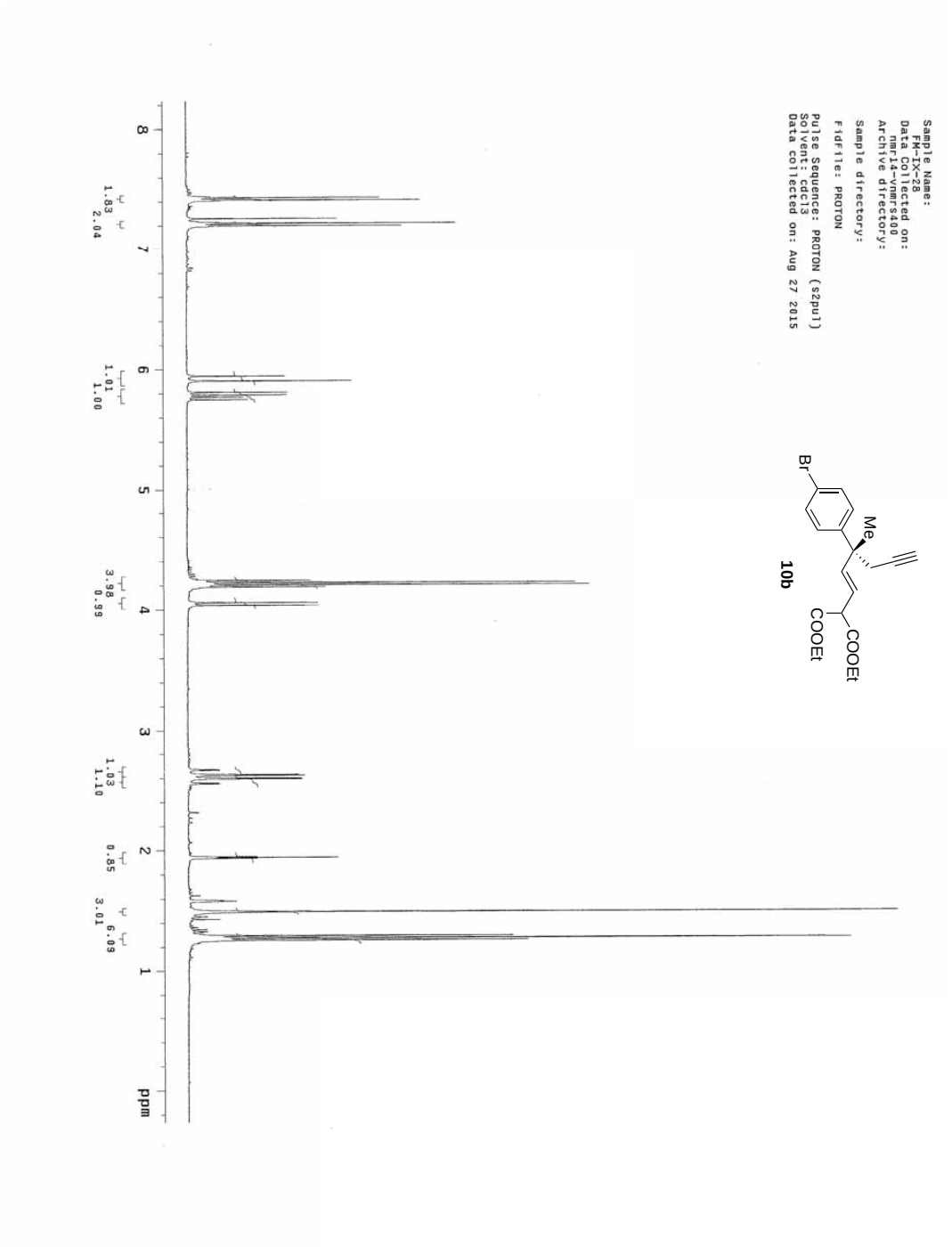

Sample Name:
FM-VIII-307
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 10 2015
Me
Me
Me
COOEt
COOEt
S12
0.94
0.99
0.85
2.13
1.98
3.07
4.00
2.90
3.25
6.23
8
7
6
5
4
3
2
1
ppm

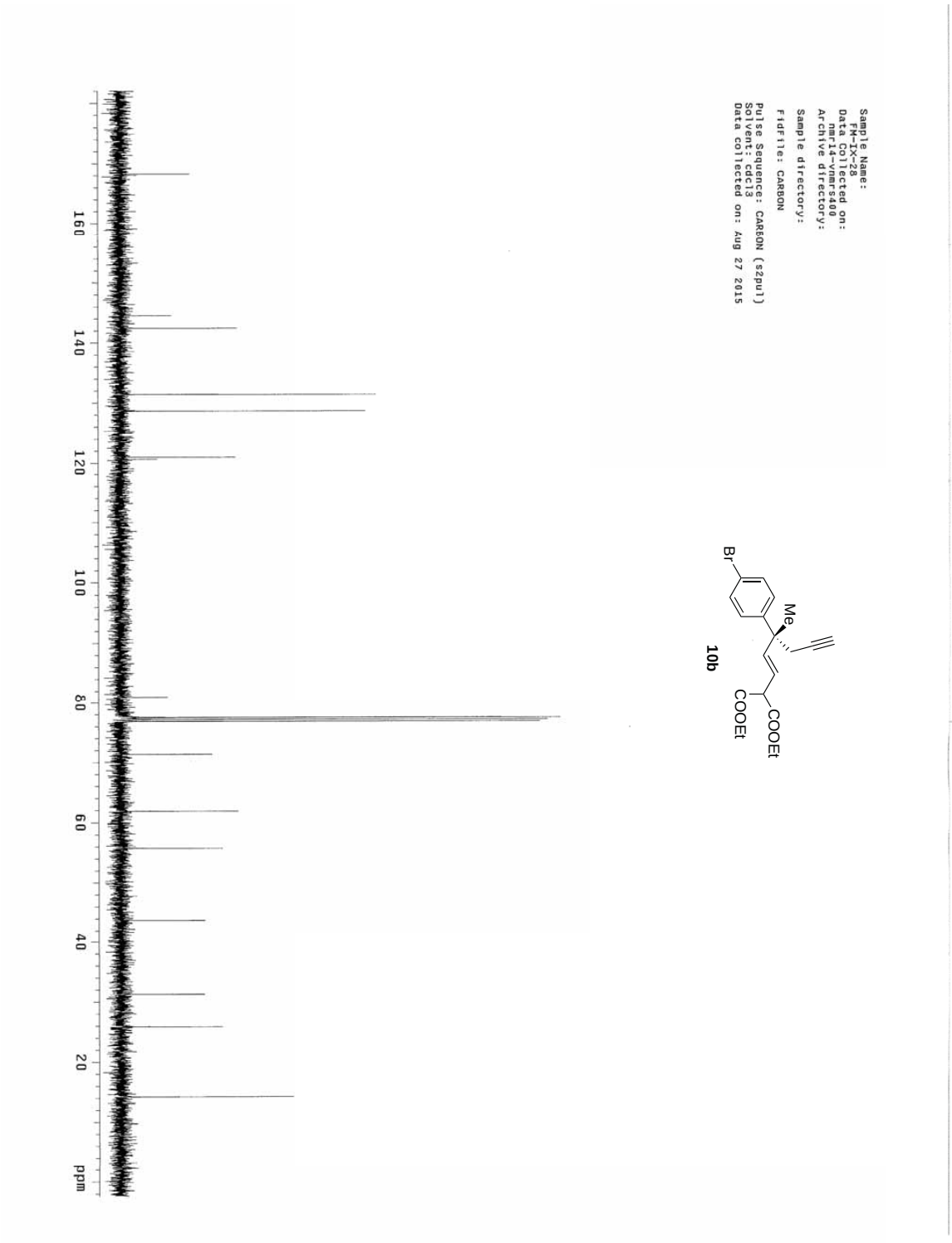

Sample Name:
FM-VIII-307
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 10 2015
Me
Me
Me
COOEt
COOEt
160
140
120
100
80
60
40
20
ppm

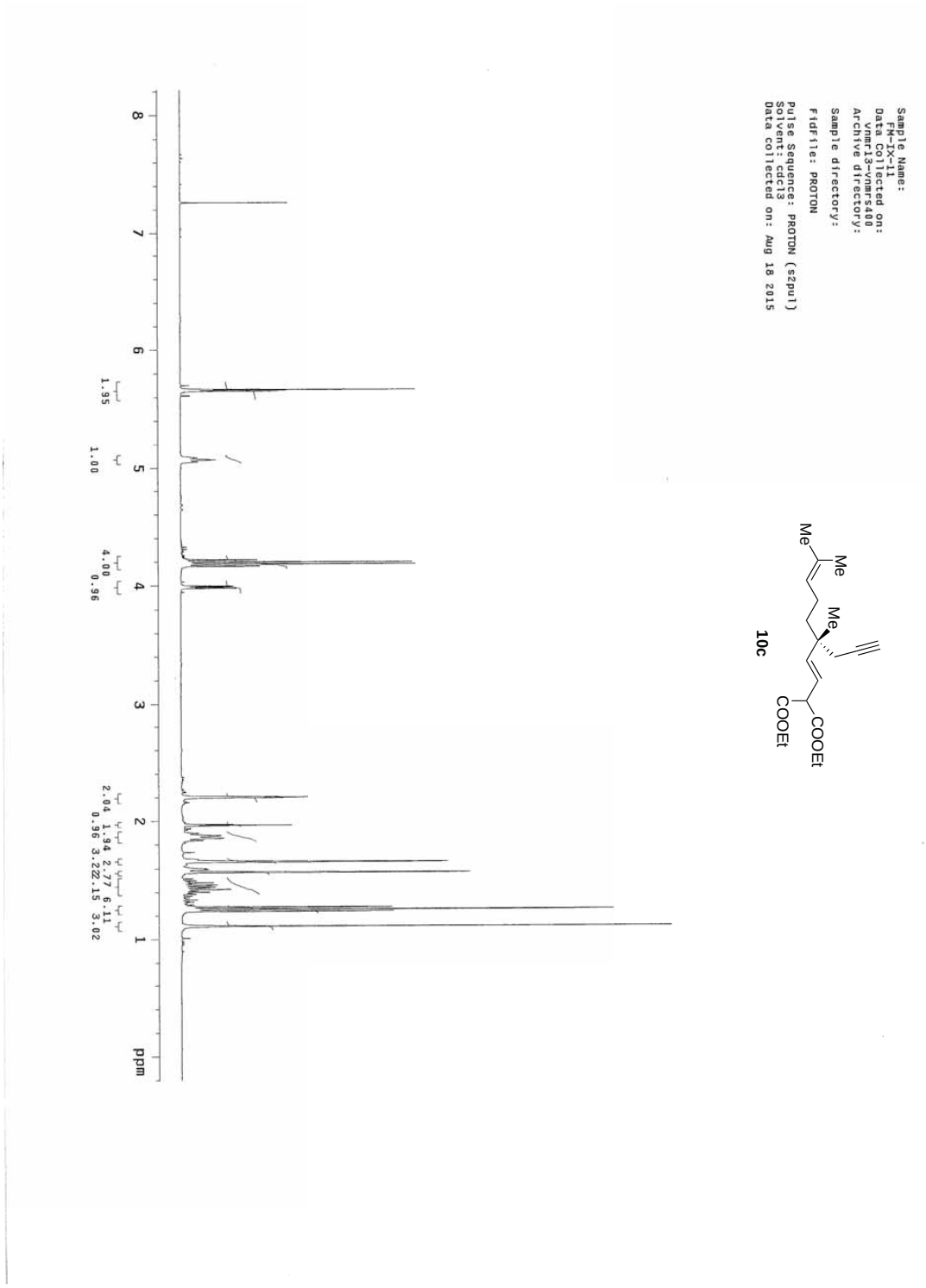
S12

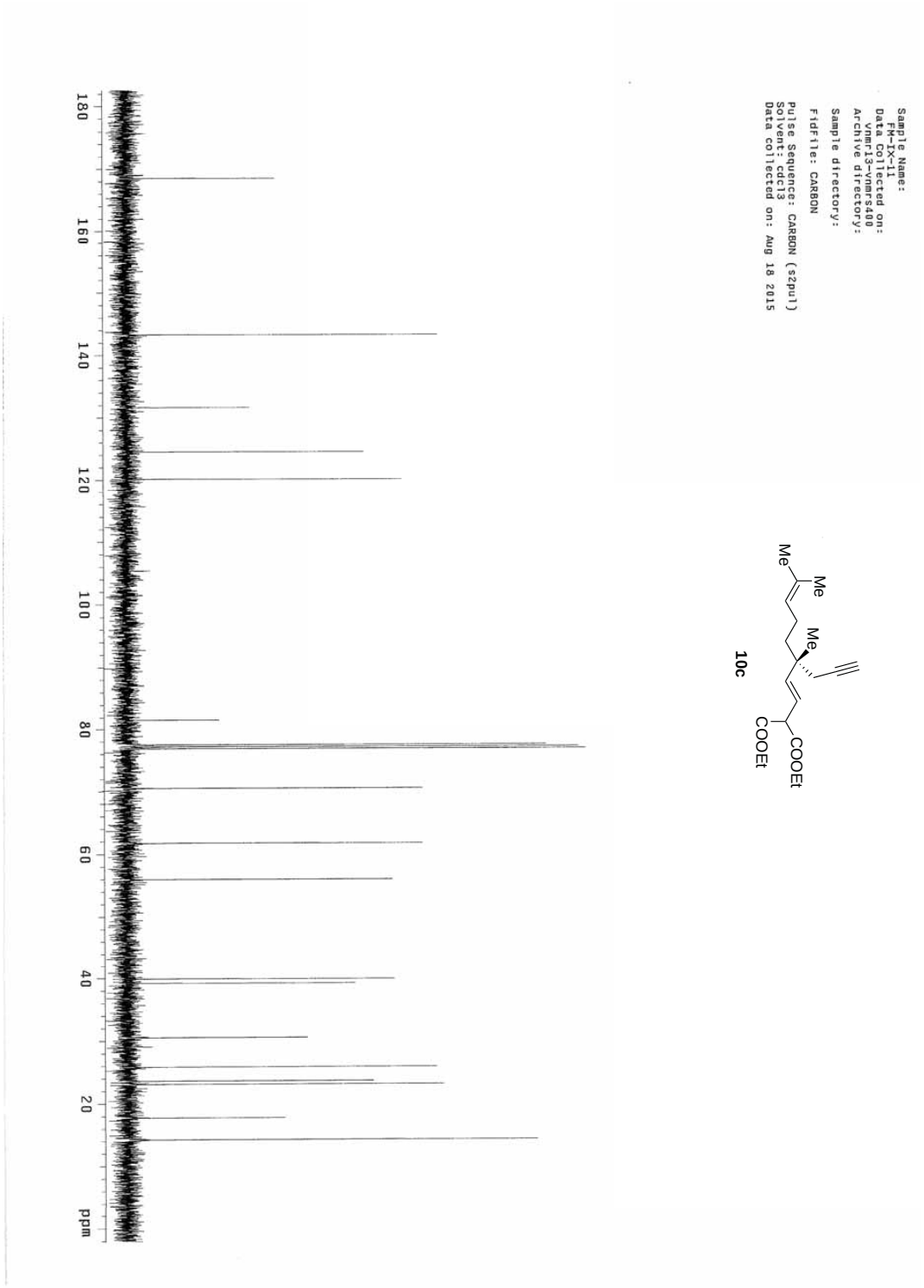

Sample Name:
PM-EX-7
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 18 2015
Me
COOEt
COOEt
10a
9
8
7
6
5
4
3
2
1
ppm
4.23
3.25
1.01
1.00
3.92
1.01
1.03
1.03
0.86
3.26
5.97

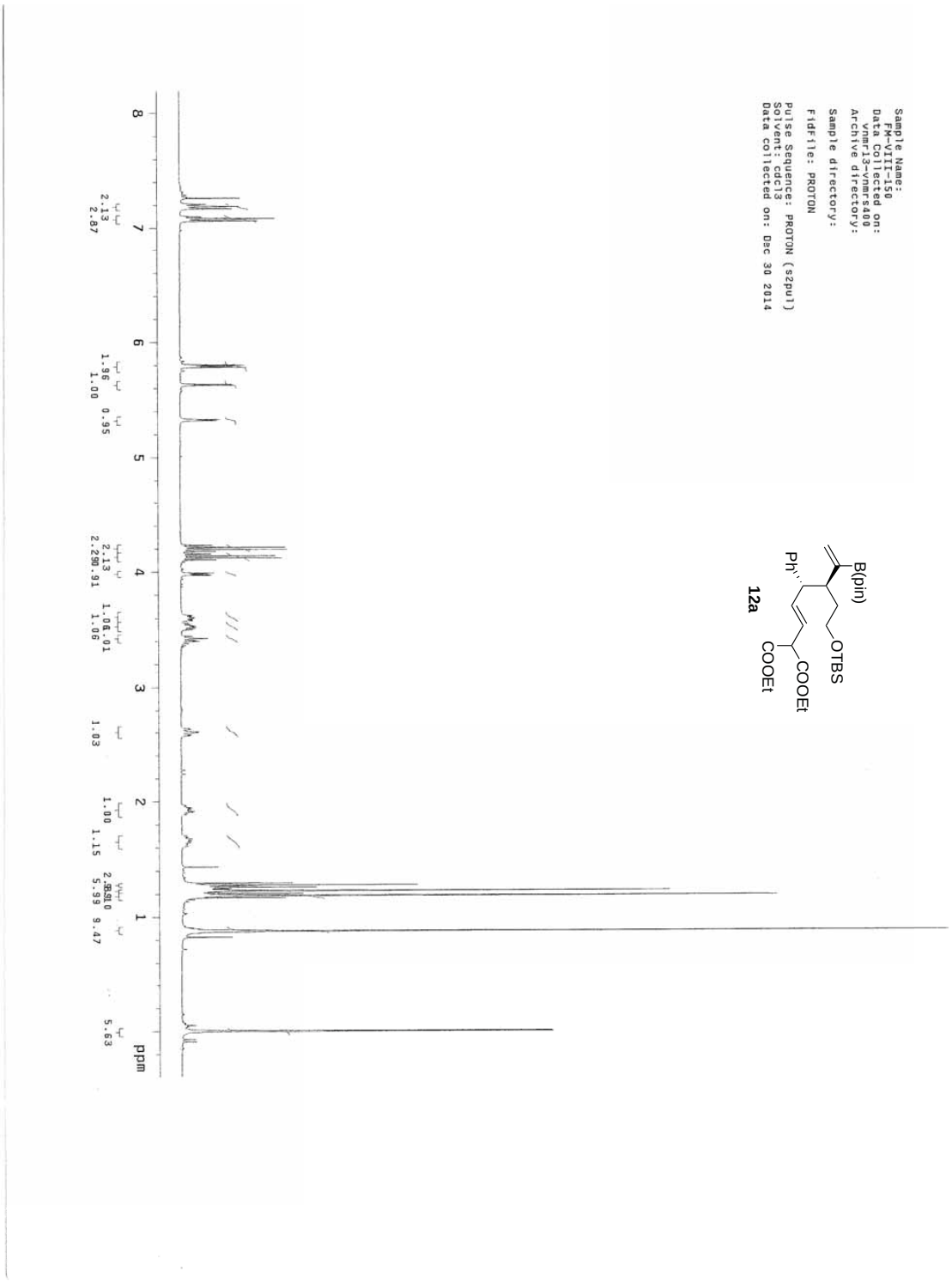

Sample Name:
FM-IX-7
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 18 2015
Me
COOEt
COOEt
10a
160
140
120
100
80
60
40
20
ppm

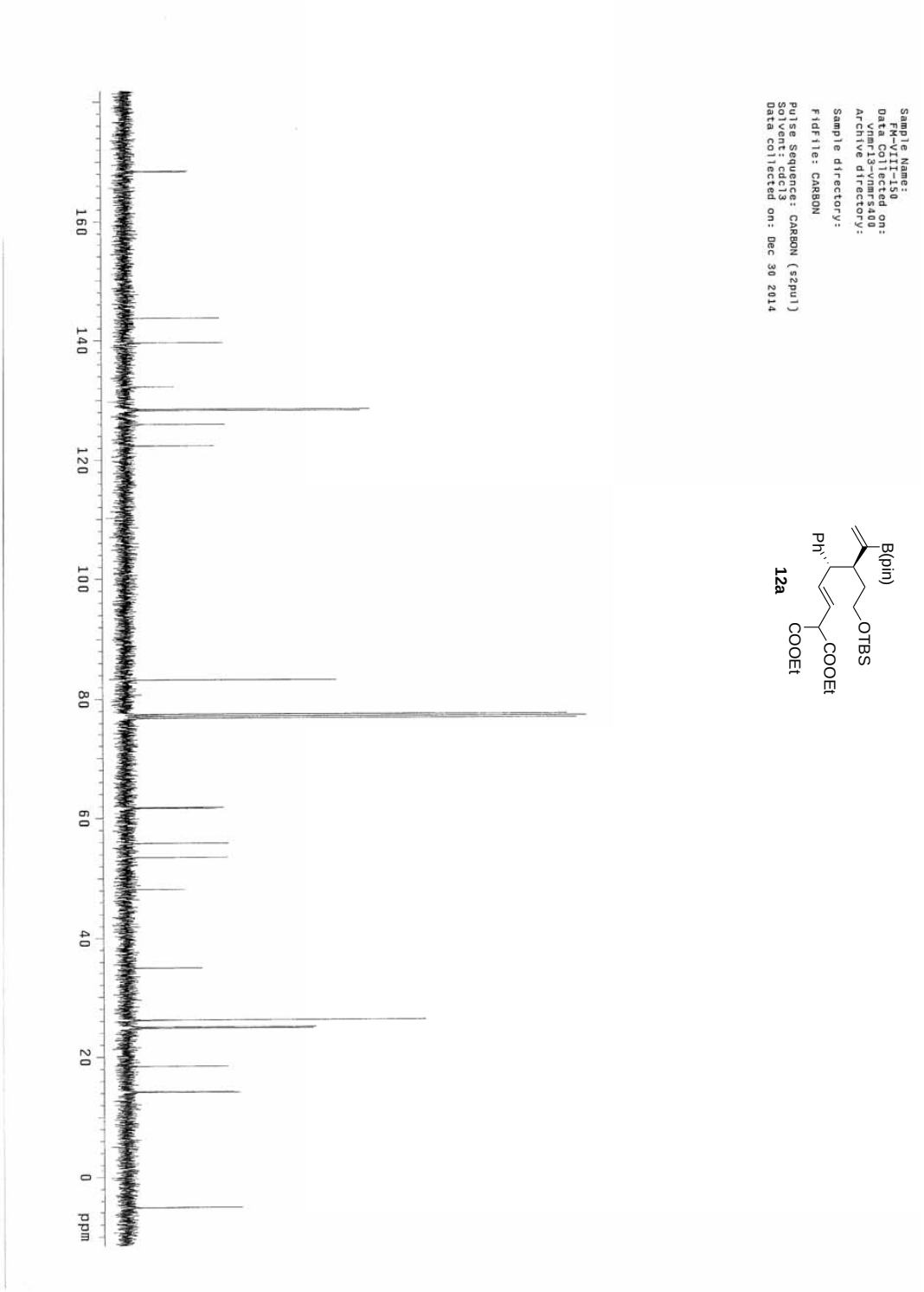

Sample Name:
PM-IX-28
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 27 2015
Br
Me
COOEt
COOEt
10b
8
7
6
5
4
3
2
1
ppm
1.83
2.04
1.01
1.00
3.98
0.99
1.03
1.10
0.85
3.01
6.09

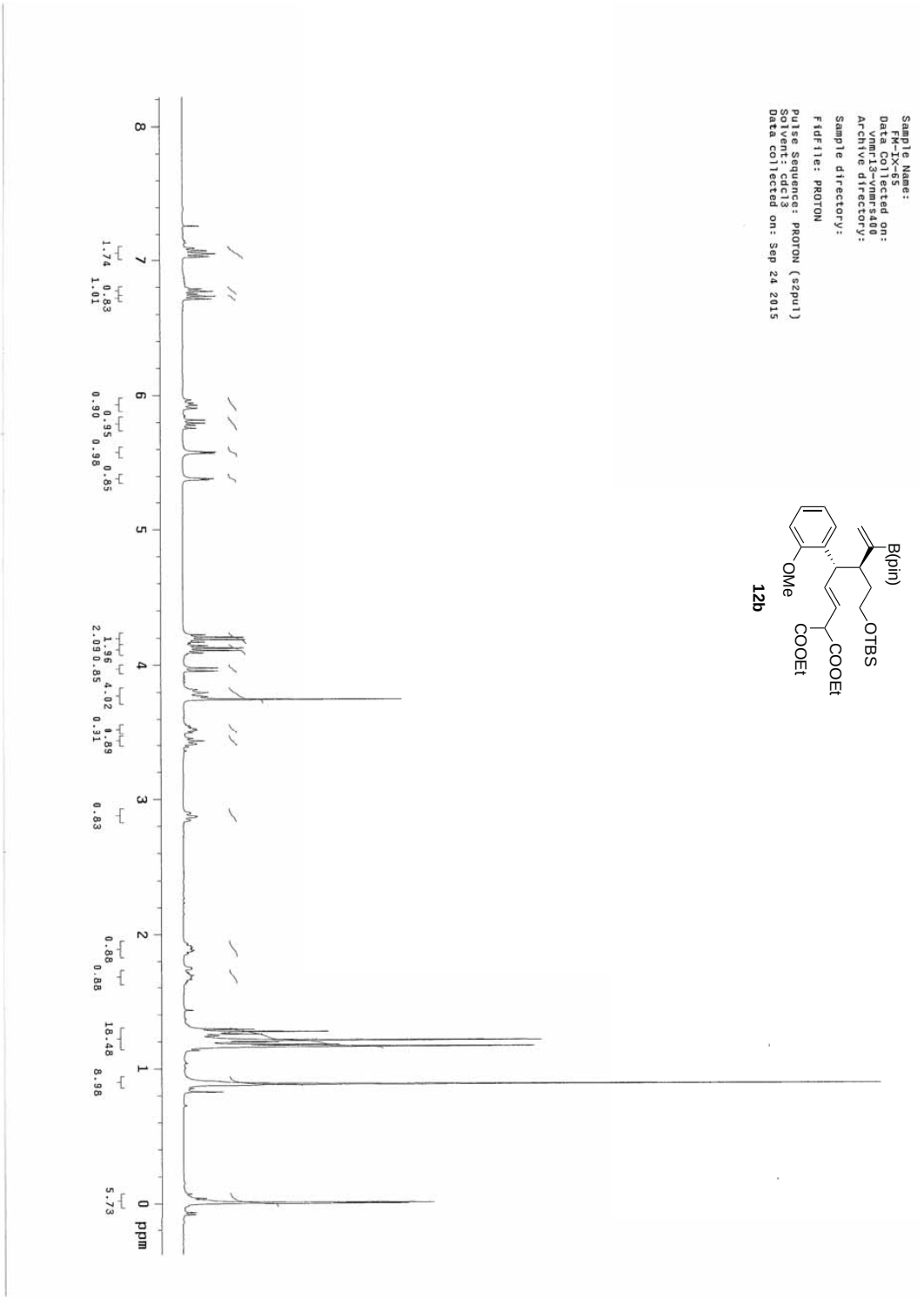

Sample Name:
FM-IX-28
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 27 2015
Br
Me
COOEt
COOEt
10b
160
140
120
100
80
60
40
20
ppm

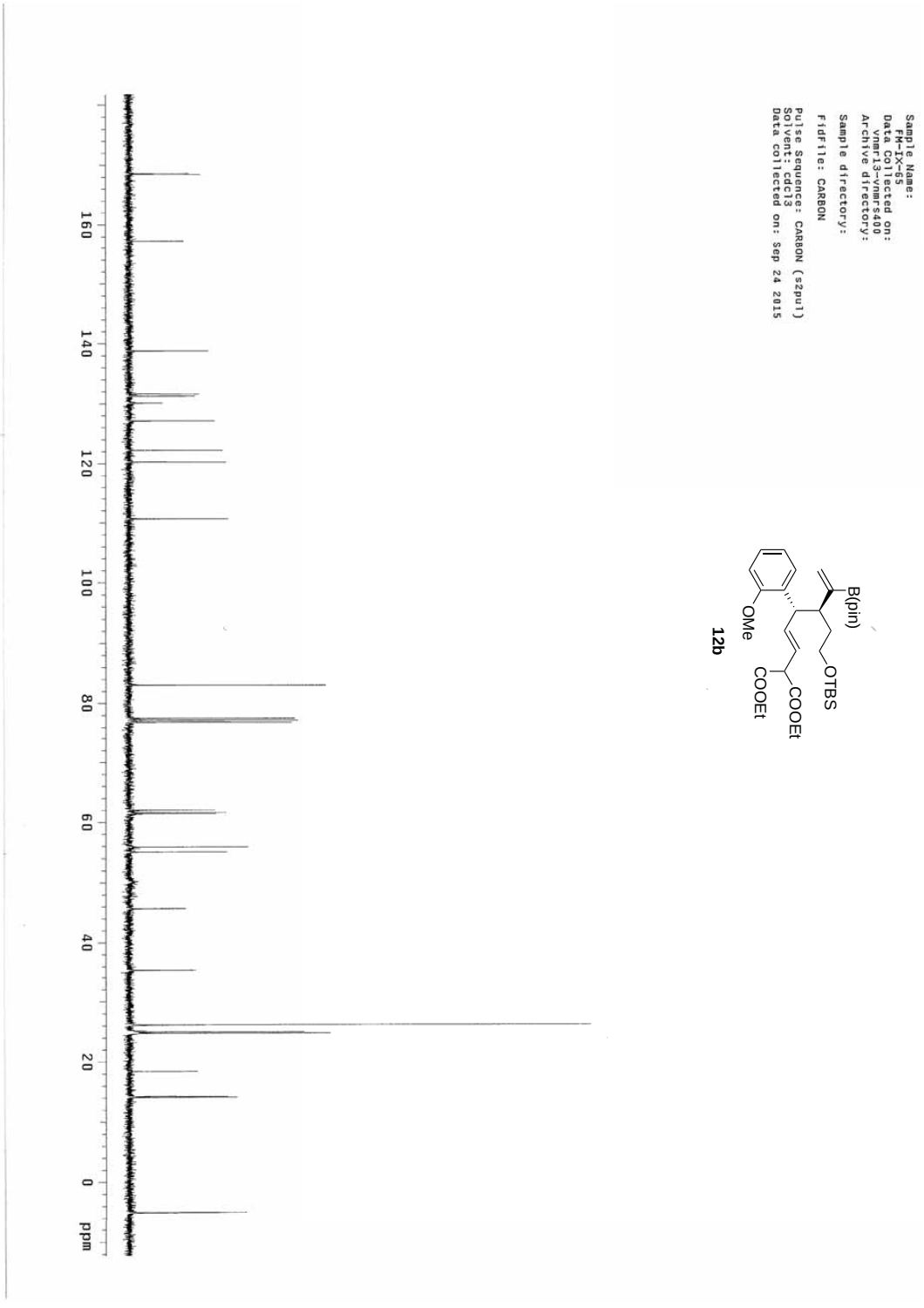

Sample Name:
FM-IX-11
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 18 2015
Me
Me
Me
COOEt
COOEt
10c
8
7
6
5
4
3
2
1
ppm
1.95
1.00
4.00
0.96
2.04 1.94 2.77 6.11
0.96 3.22 2.15 3.02

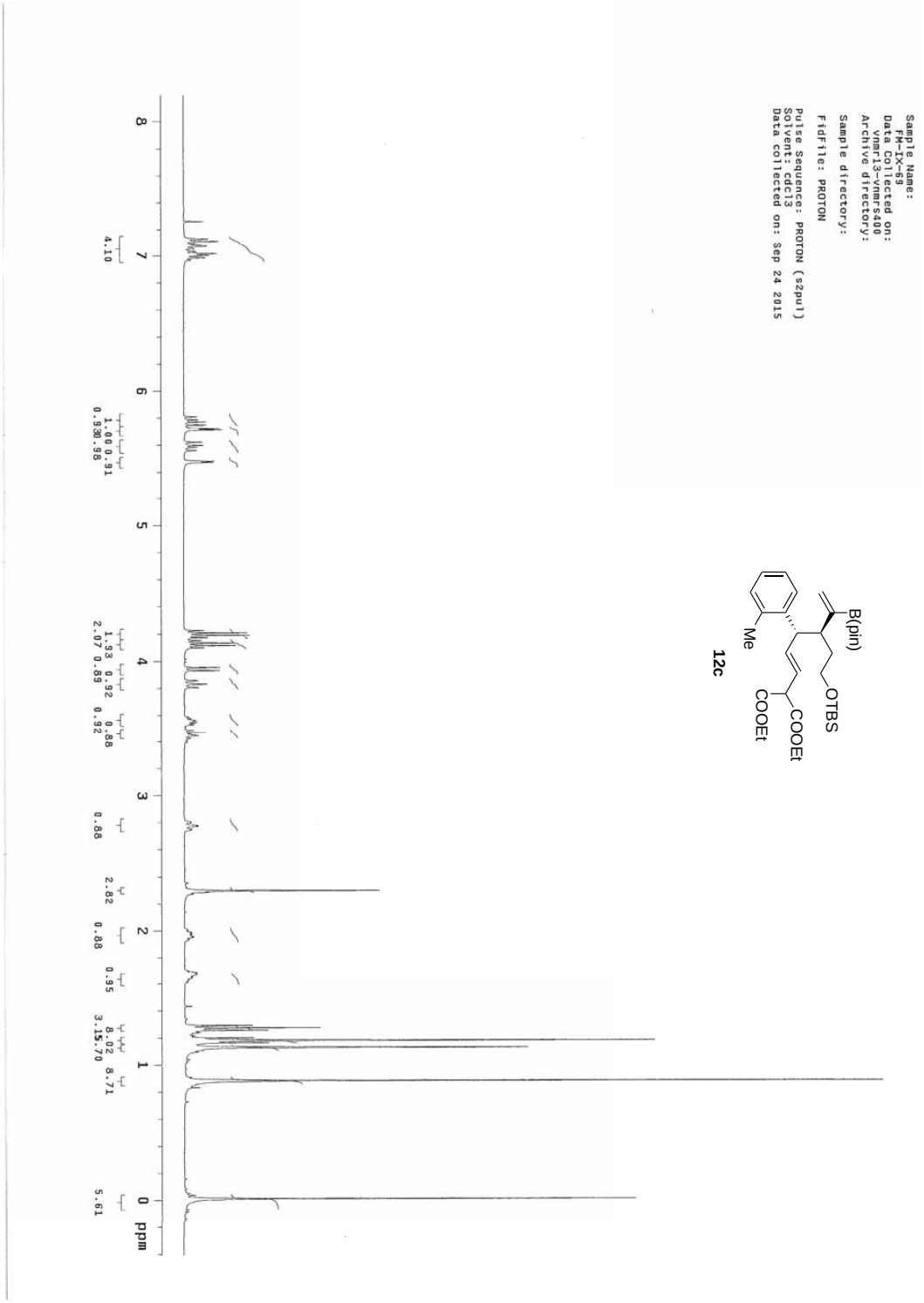

Sample Name:
FM-IX-11
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 18 2015
Me
Me
Me
COOEt
COOEt
10c
180
160
140
120
100
80
60
40
20
ppm

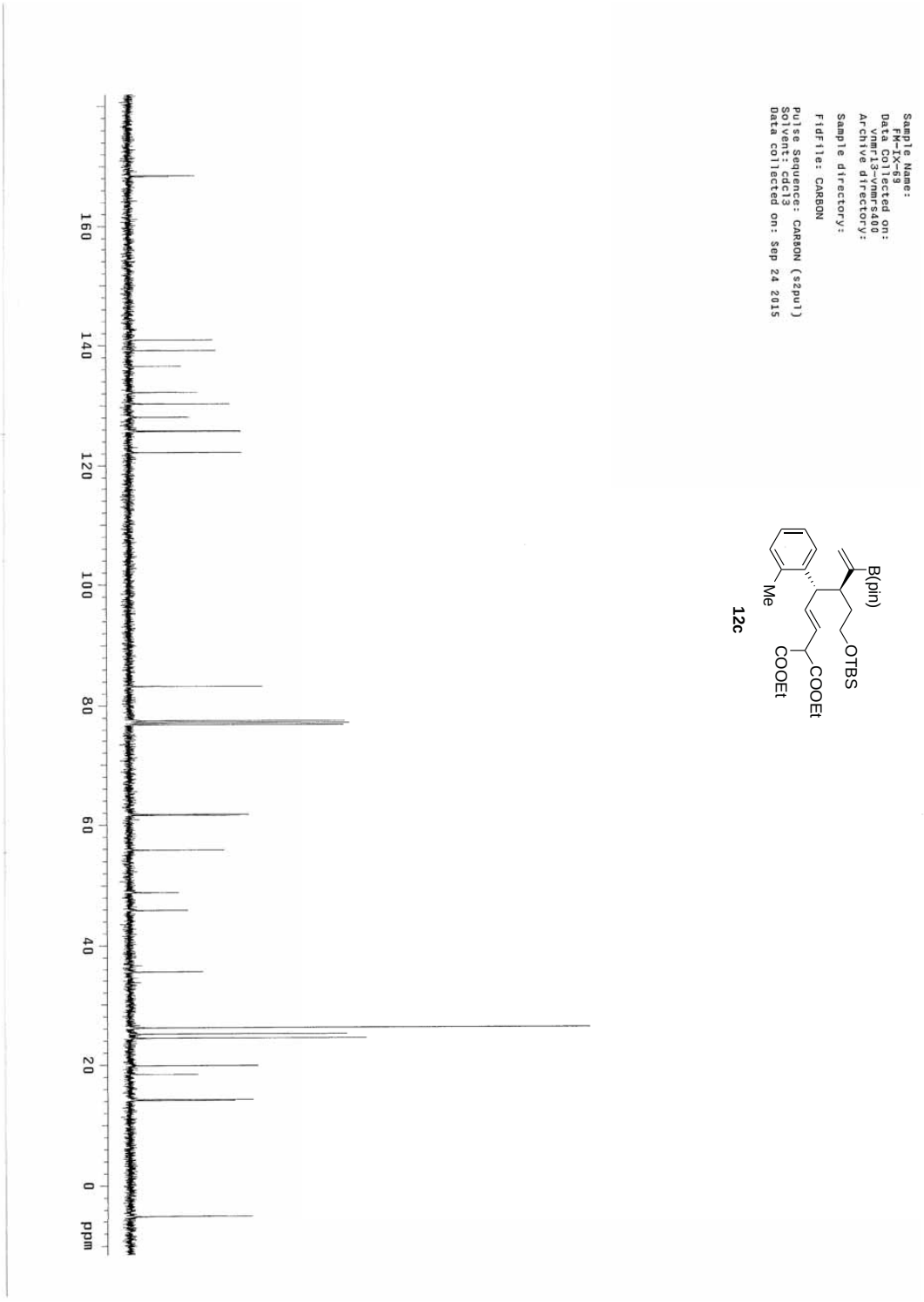

Sample Name:
FM-VIII-150
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 30 2014
B(pin)
Ph
OTBS
COOEt
COOEt
12a
ppm

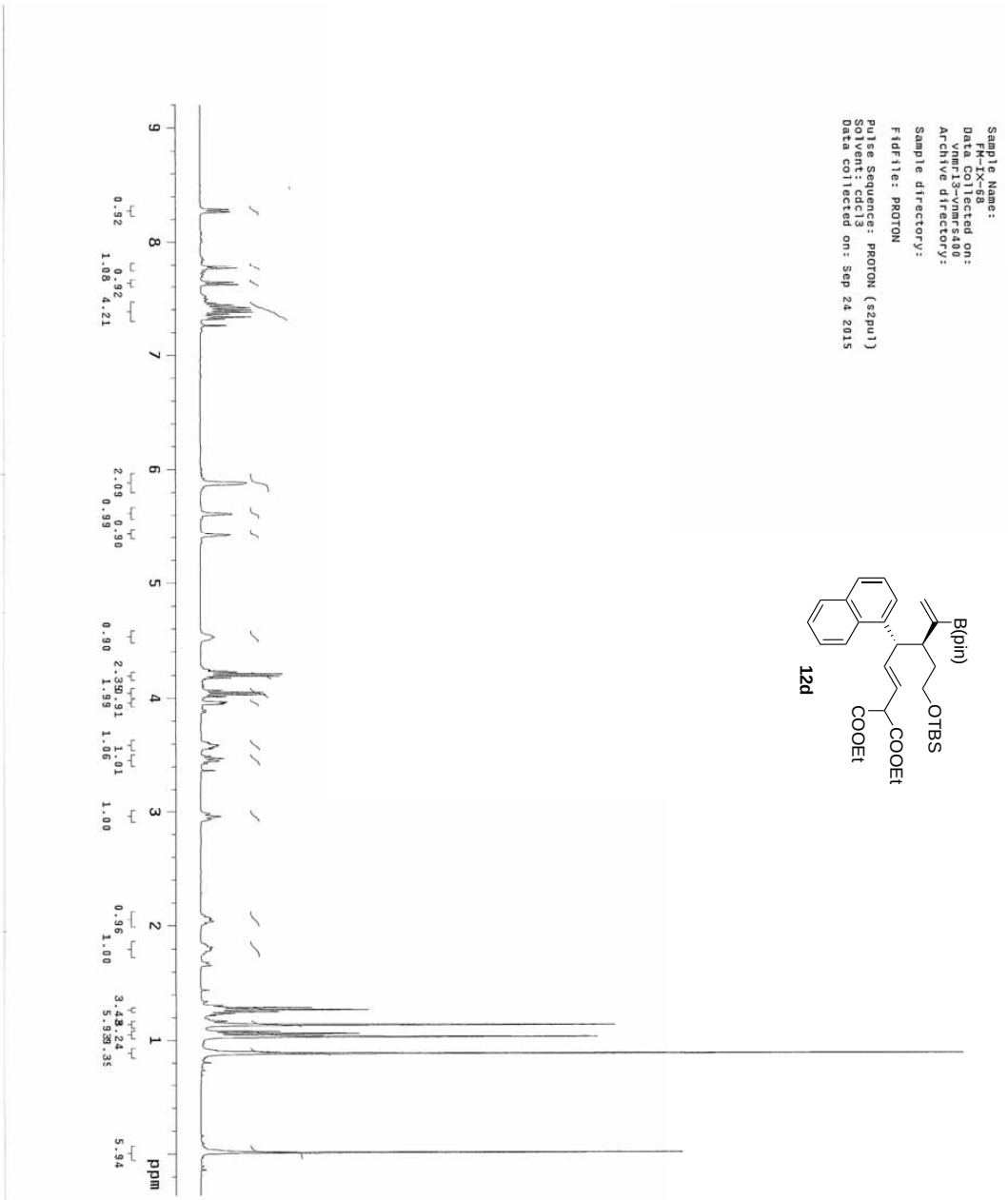

Sample Name:
FM-VIII-150
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 30 2014
B(pin)
OTBS
Ph
COOEt
COOEt
12a
160
140
120
100
80
60
40
20
0
ppm

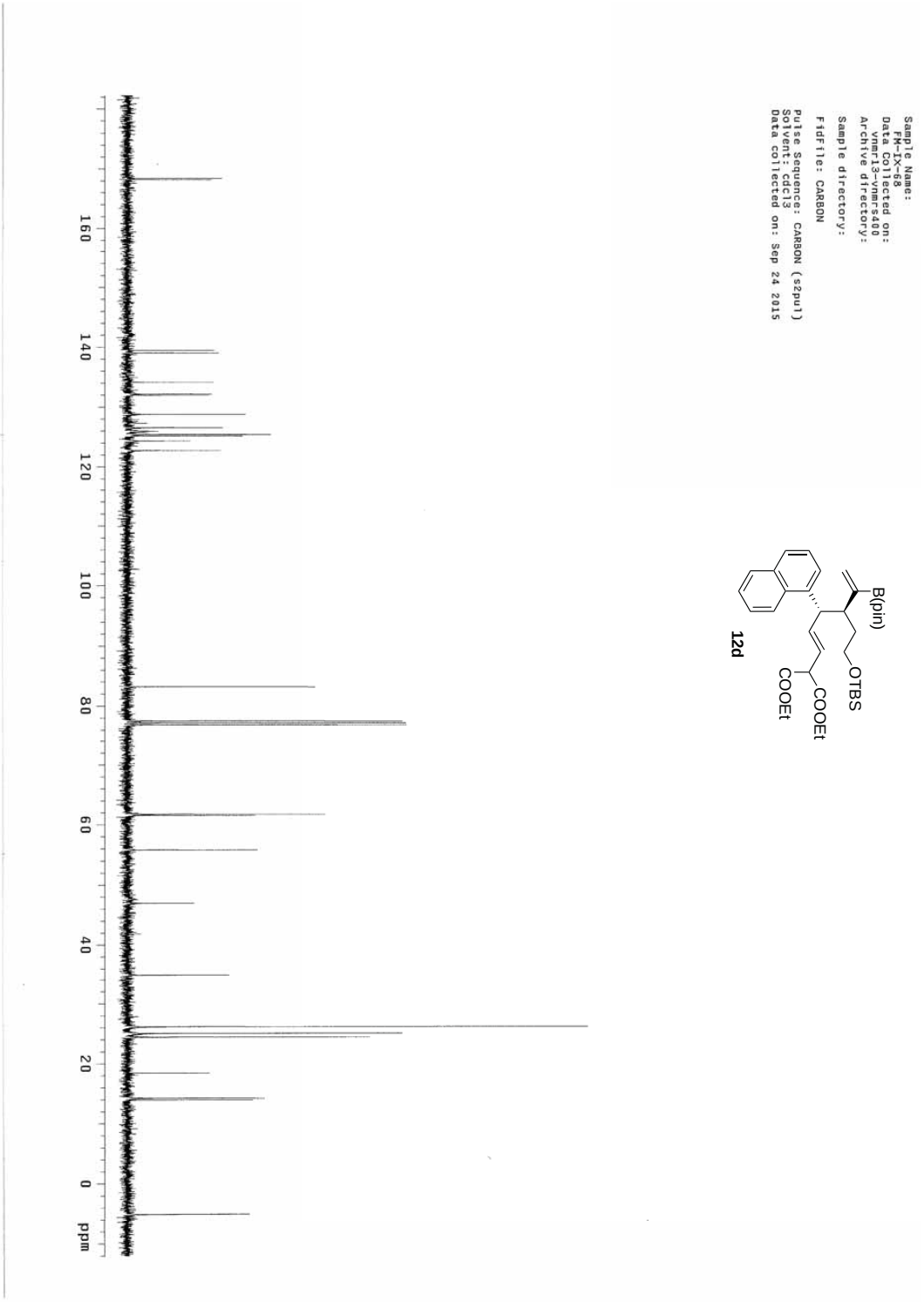

Sample Name:
FM-IX-65
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 24 2015
B(pin)
OTBS
COOEt
COOEt
OMe
12b
8
7
6
5
4
3
2
1
0 ppm
1.74 0.83 1.01
0.90 0.95 0.98 0.65
2.03 0.85 1.96 4.02 0.31 0.89
0.83
0.88 0.88
18.48 8.98
5.73

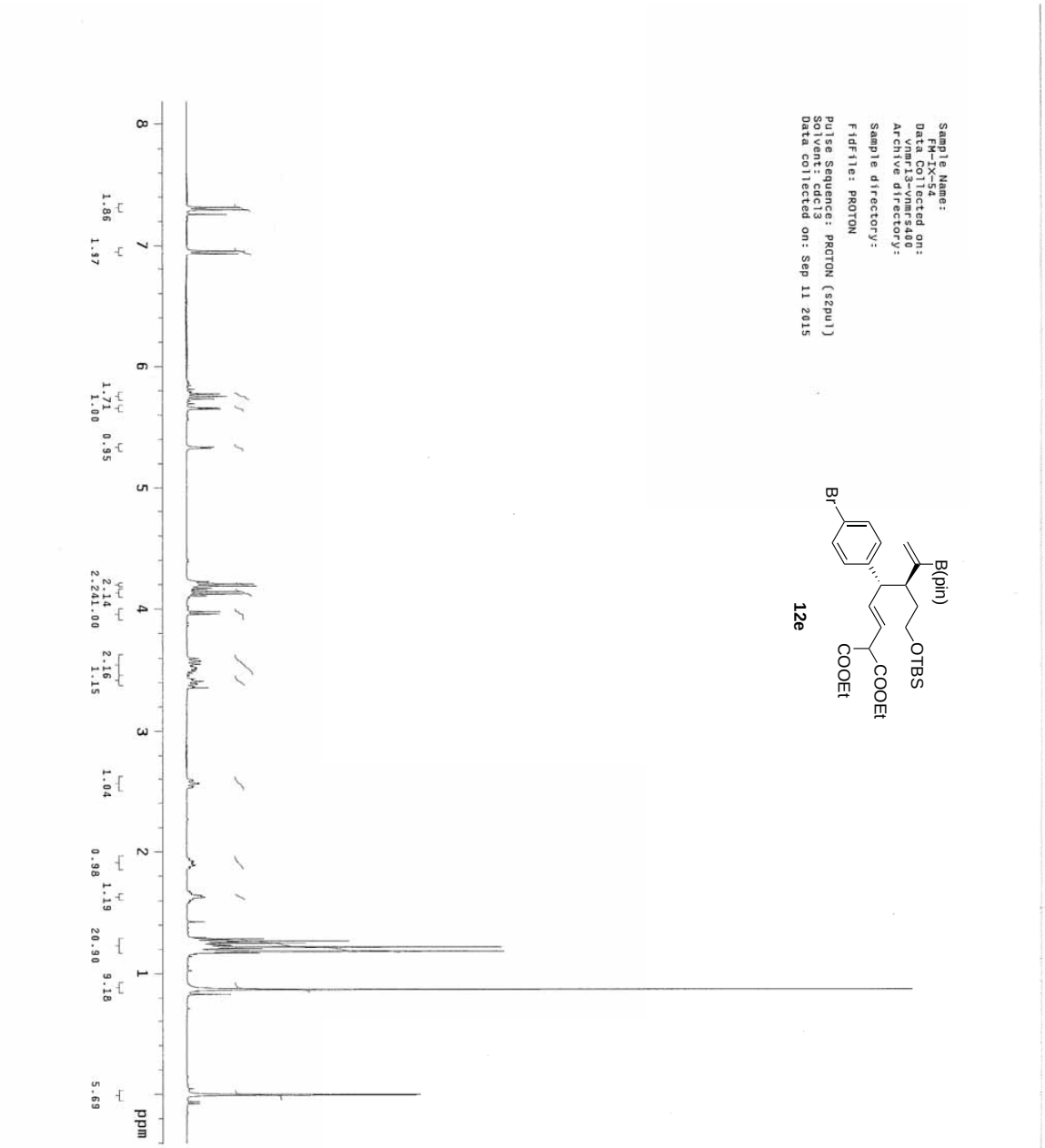

Sample Name:
FM-IX-95
Data Collected on:
Varian 3-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (szpul)
Solvent: cdcl3
Data collected on: Sep 24 2015
B(pin)
OTBS
COOEt
COOEt
OMe
12b
160
140
120
100
80
60
40
20
0
ppm

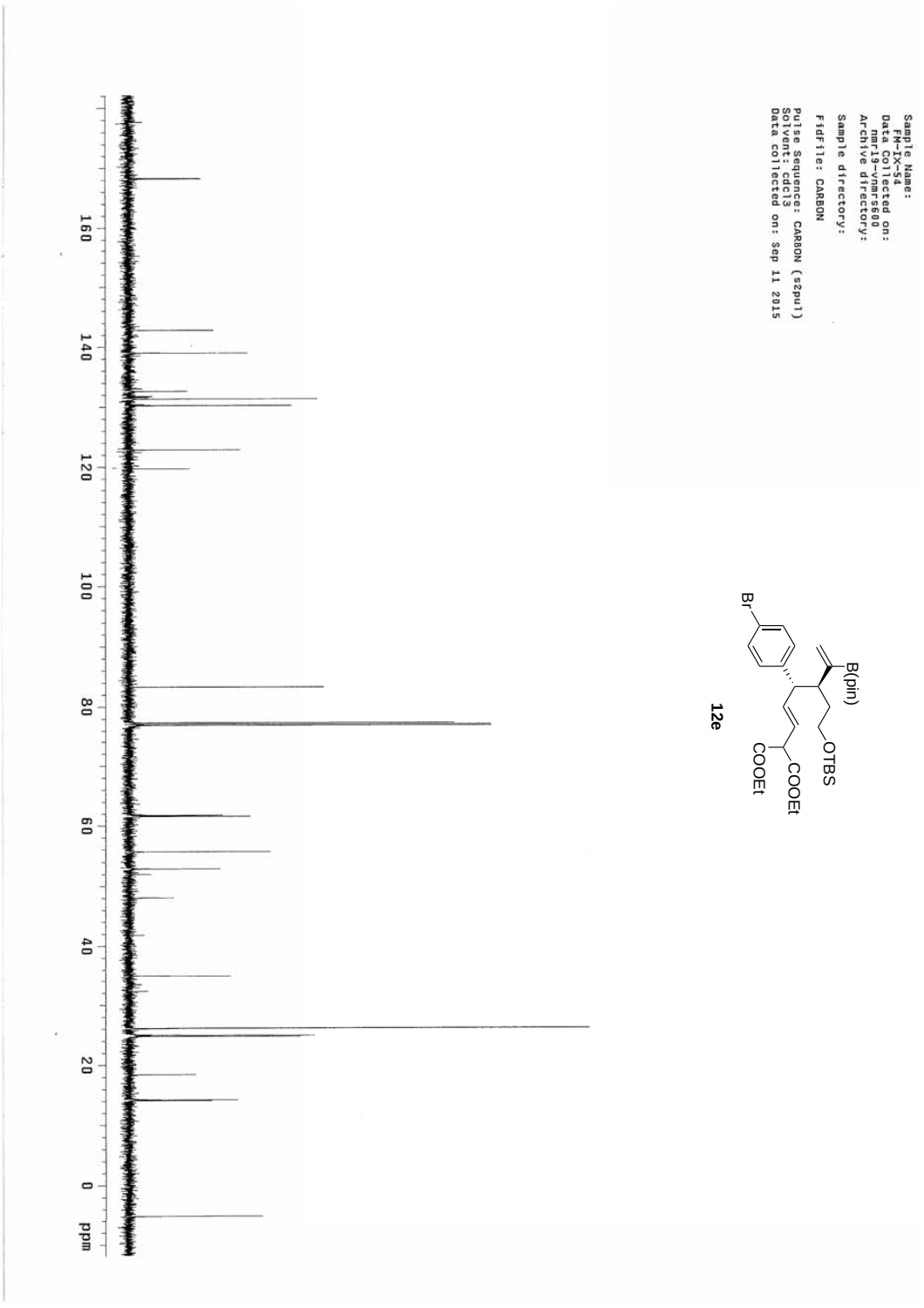

Sample Name:
FM-IX-93
Data collected on:
vnmrs13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (szpul)
Solvent: cdcl3
Data collected on: Sep 24 2015
B(pin)
OTBS
COOEt
COOEt
Me
12c
ppm

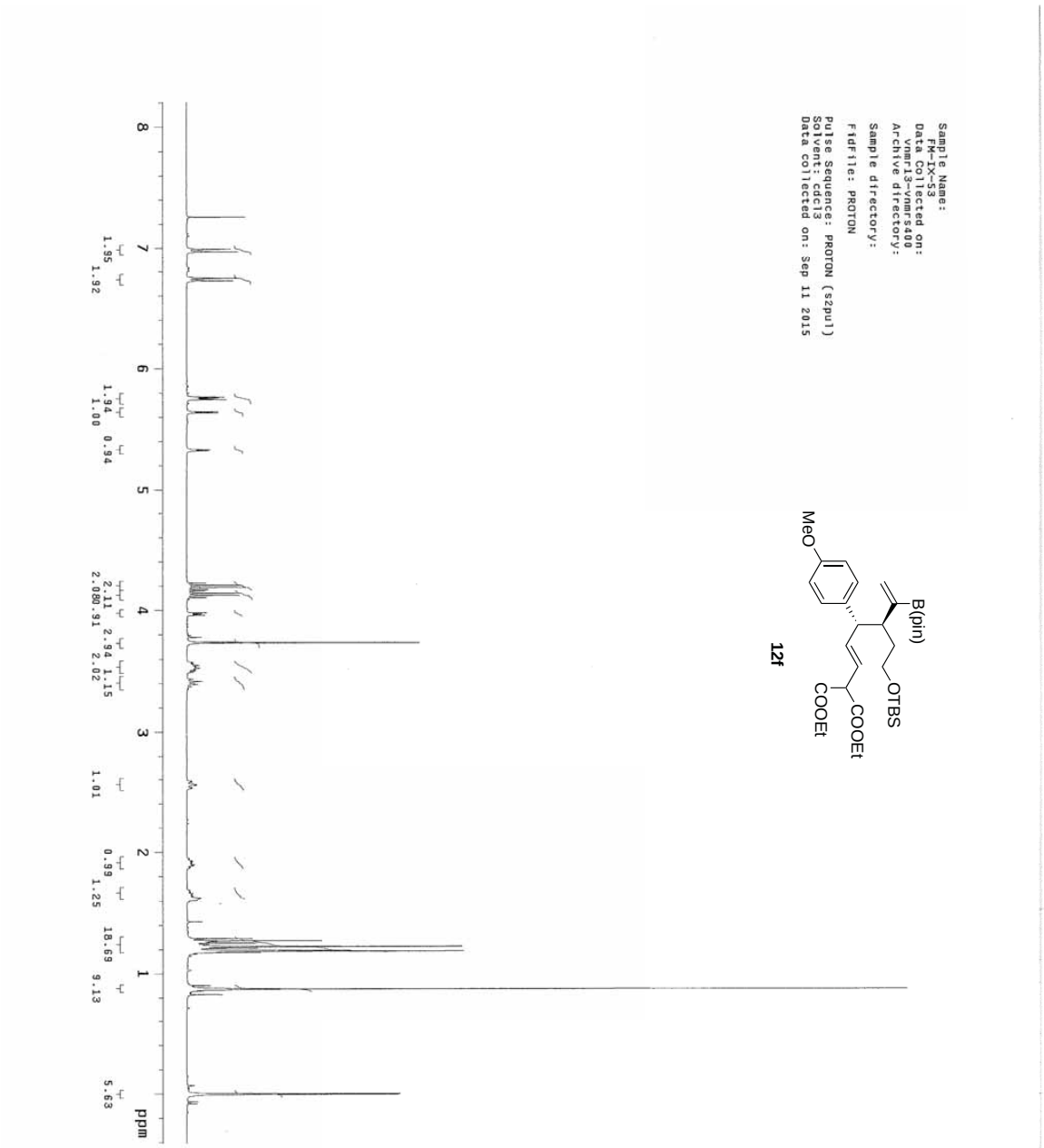

Sample Name:
FM-IX-69
Data Collected on:
Inova3-vnmrs400
Archive directory:
Sample directory:
Fidfile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 24 2015
B(pin)
OTBS
COOEt
COOEt
Me
12c
160
140
120
100
80
60
40
20
0
ppm

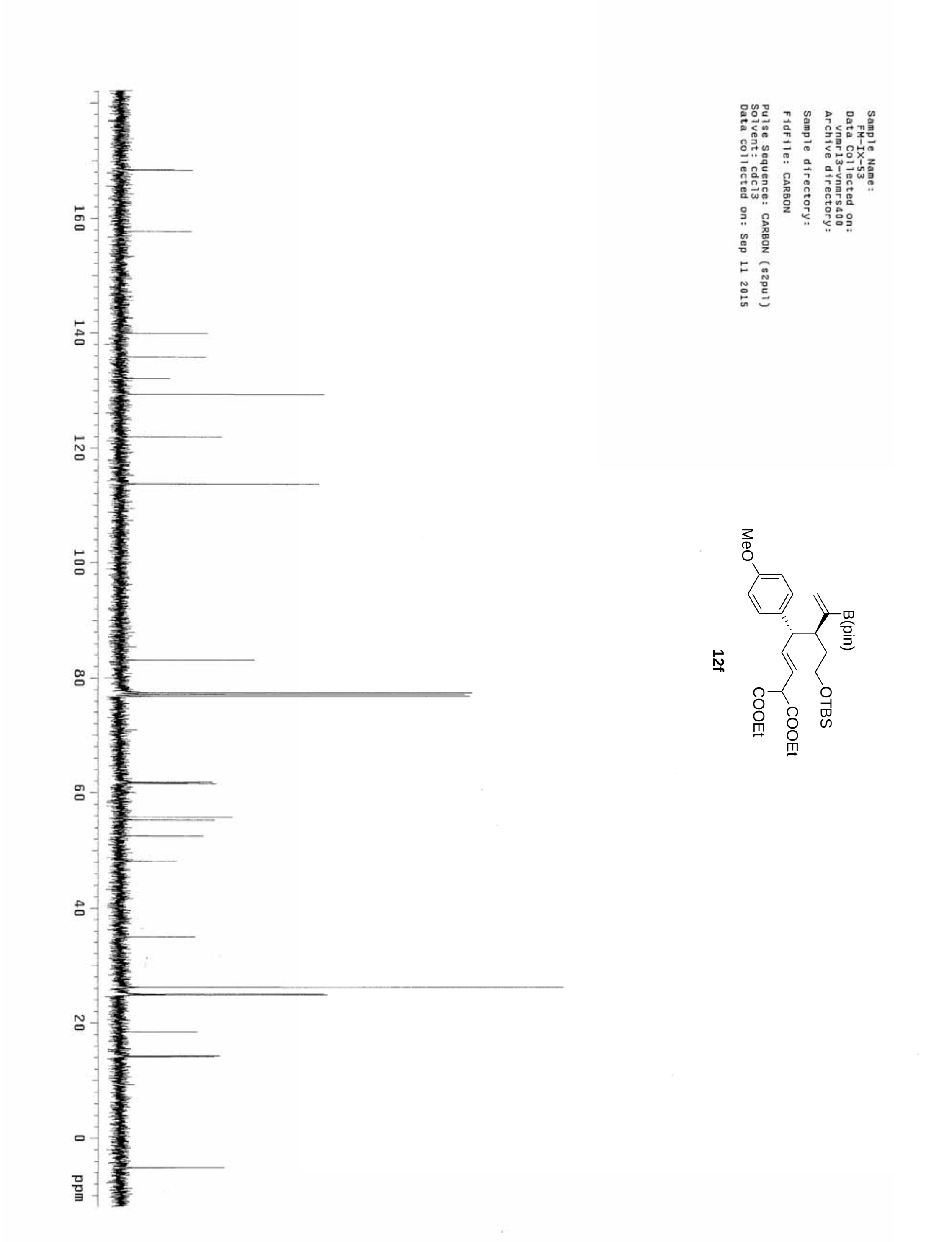

Sample Name:
FM-IX-58
Data Collected on:
vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 24 2015
B(pin)
OTBS
COOEt
COOEt
12d
ppm

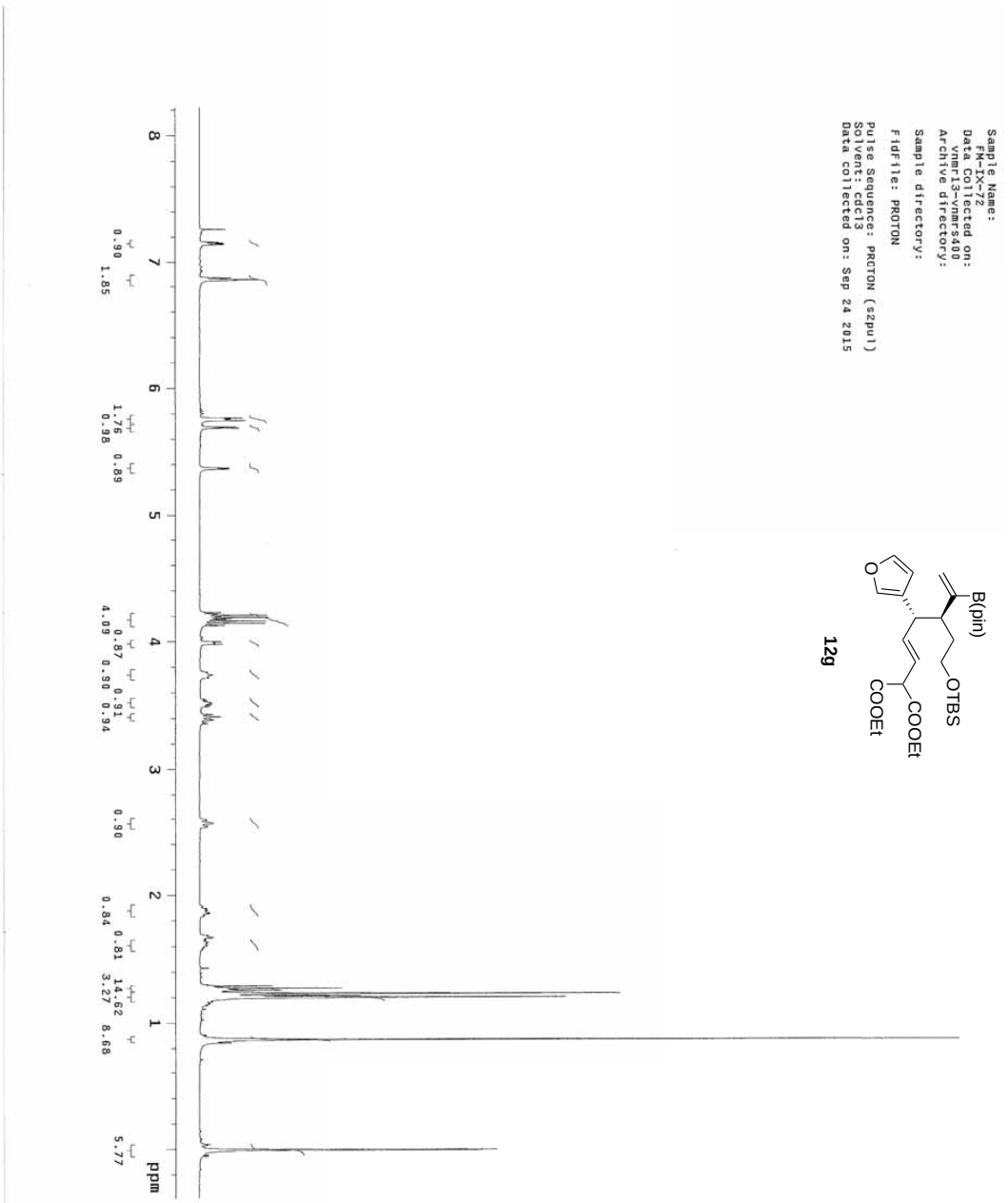

Sample Name:
FM-IX-158
Data collected on:
vnmrs13-inmr400
Archive directory:
Sample directory:
F4dFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 24 2015
B(pin)
OTBS
COOEt
COOEt
12d
160
140
120
100
80
60
40
20
0
ppm

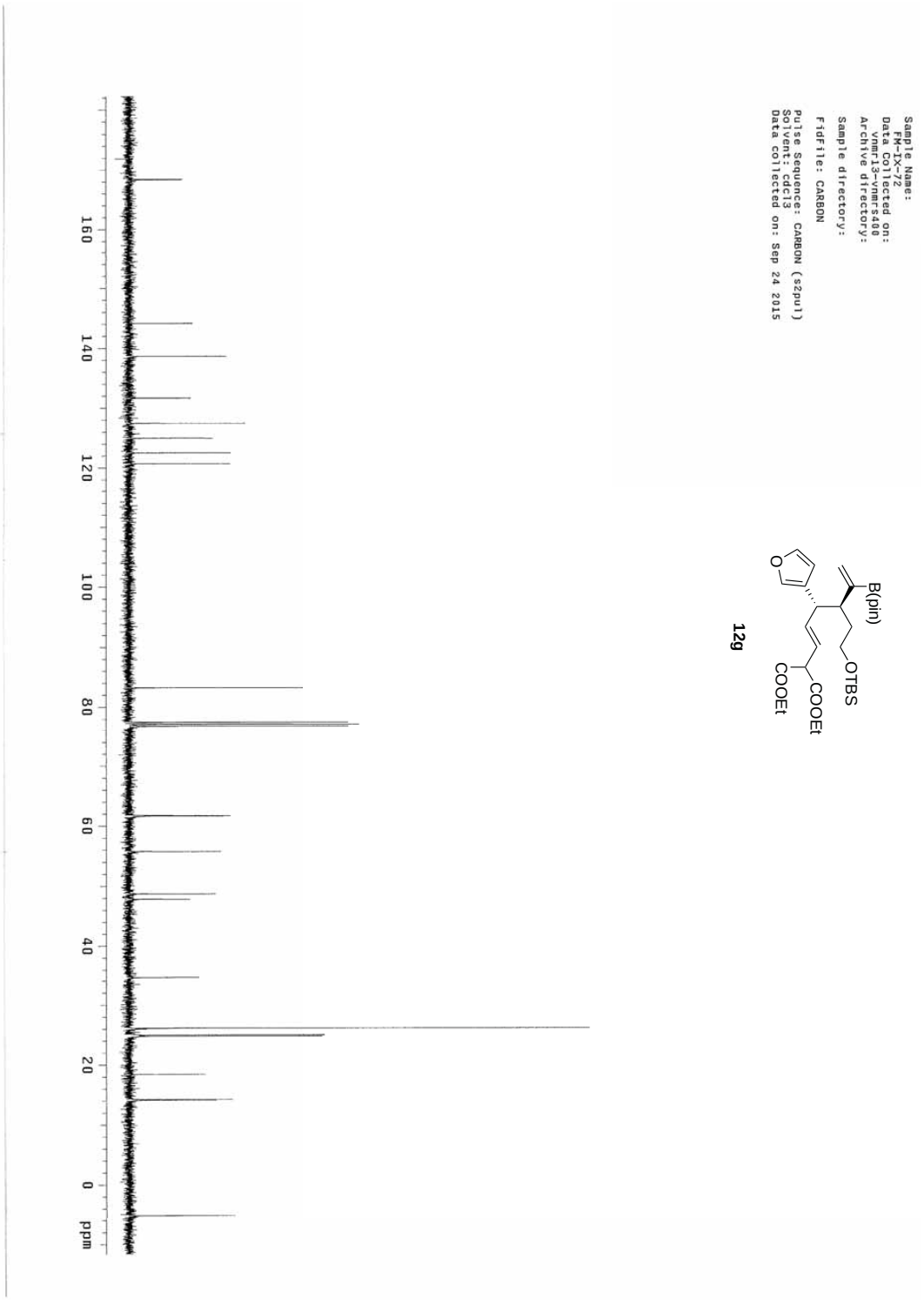

Sample Name:
FM-IX-54
Data(0) collected on:
vnmrj3-inmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 11 2015
B(pin)
OTBS
COOEt
COOEt
Br
12e
1.86
1.97
1.71
1.00
0.95
2.14
2.241.00
2.16
1.15
1.04
0.98
1.19
20.90
9.18
5.69
ppm


Sample Name:
FM-IX-34
Data Collected on:
Unity-inova500
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 11 2015
Br
B(pin)
OTBS
COOEt
COOEt
12e
160
140
120
100
80
60
40
20
0
ppm

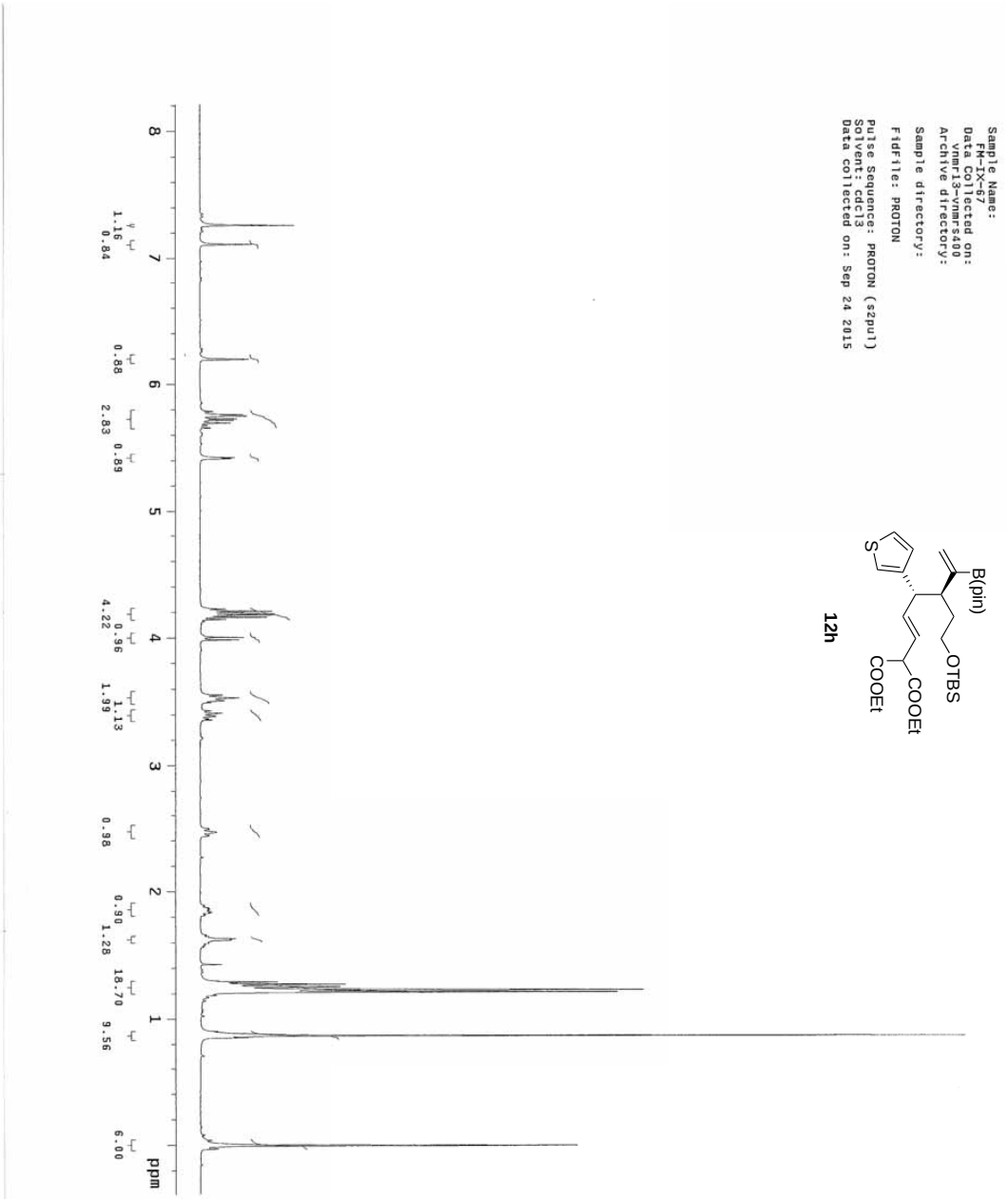

Sample Name:
Exp: proton
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: CDCl3
Data collected on: Sep 11 2015
MeO
B(pin)
OTBS
COOEt
COOEt
12f
8
7
6
5
4
3
2
1
ppm
1.95
1.92
1.94
1.00
0.94
2.11
2.00
2.94
0.91
1.15
2.02
1.01
0.99
1.25
18.69
9.13
5.63

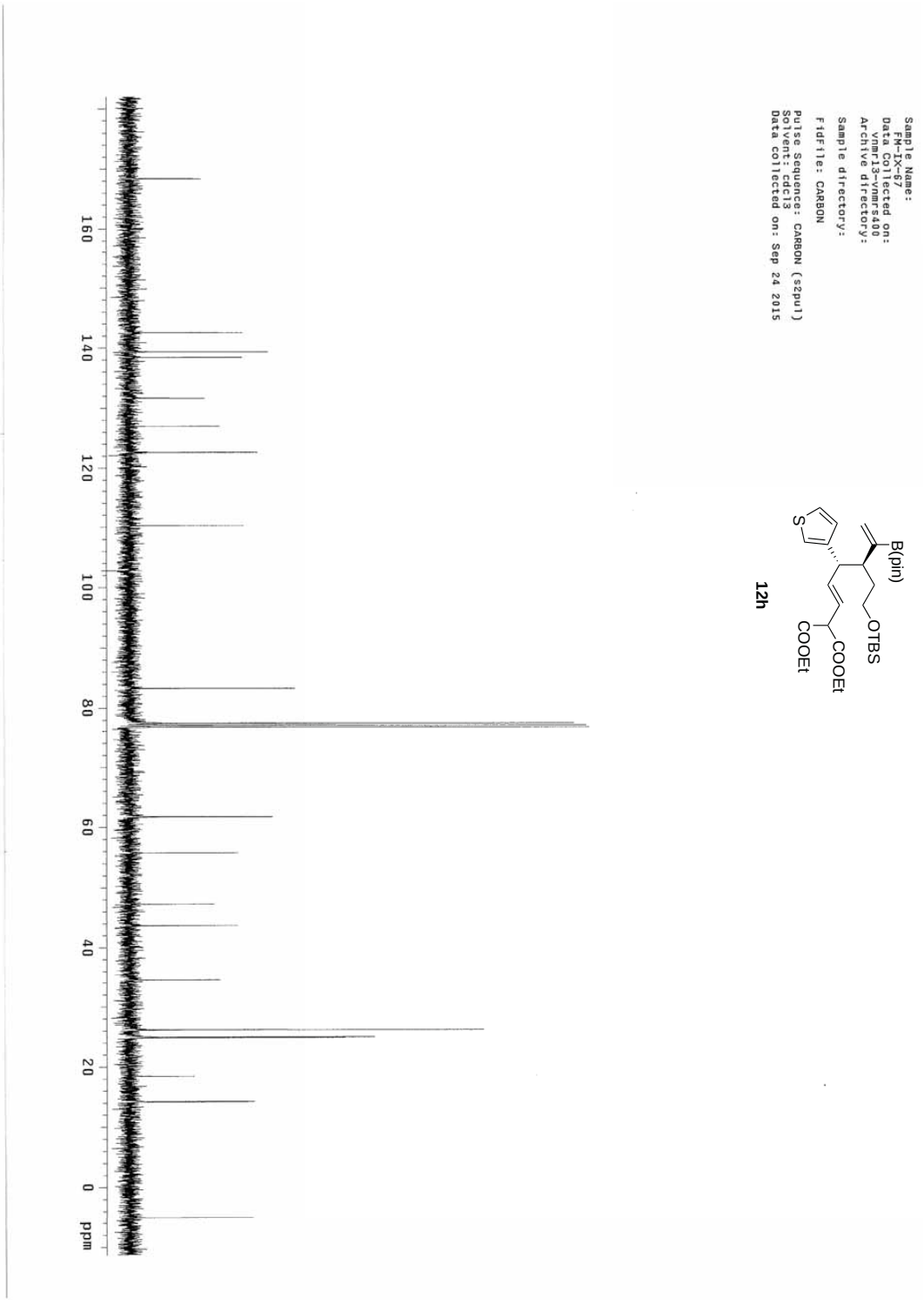

Sample Name:
FM-IX-53
Data Collected on:
vnmrl3-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 11 2015
B(pin)
OTBS
COOEt
COOEt
MeO
12f
160
140
120
100
80
60
40
20
0
ppm

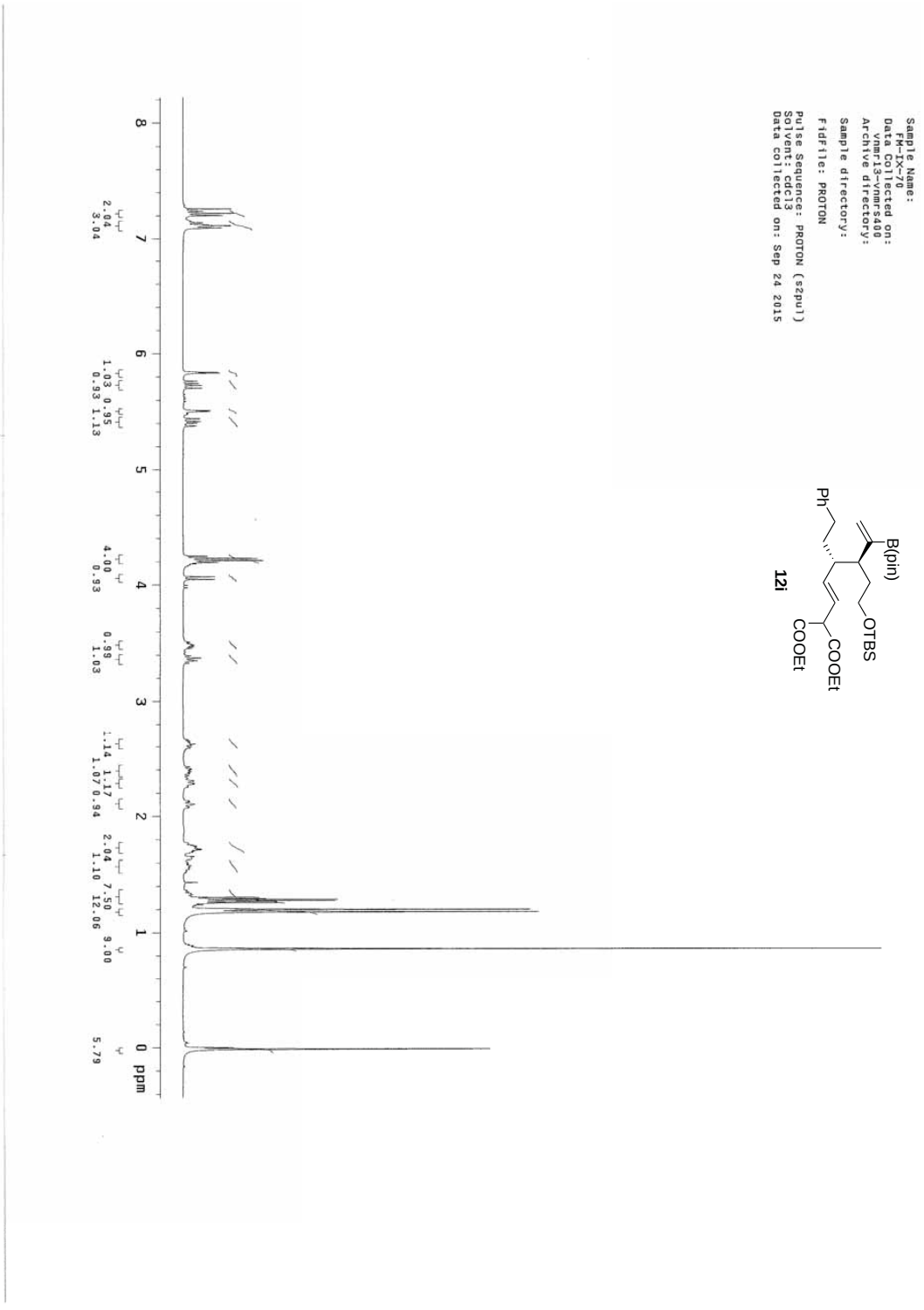

Sample Name:
FM-IX-72
Data Collected on:
vnmrs1.mercury
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 24 2015
B(pin)
OTBS
COOEt
COOEt
O
12g
ppm

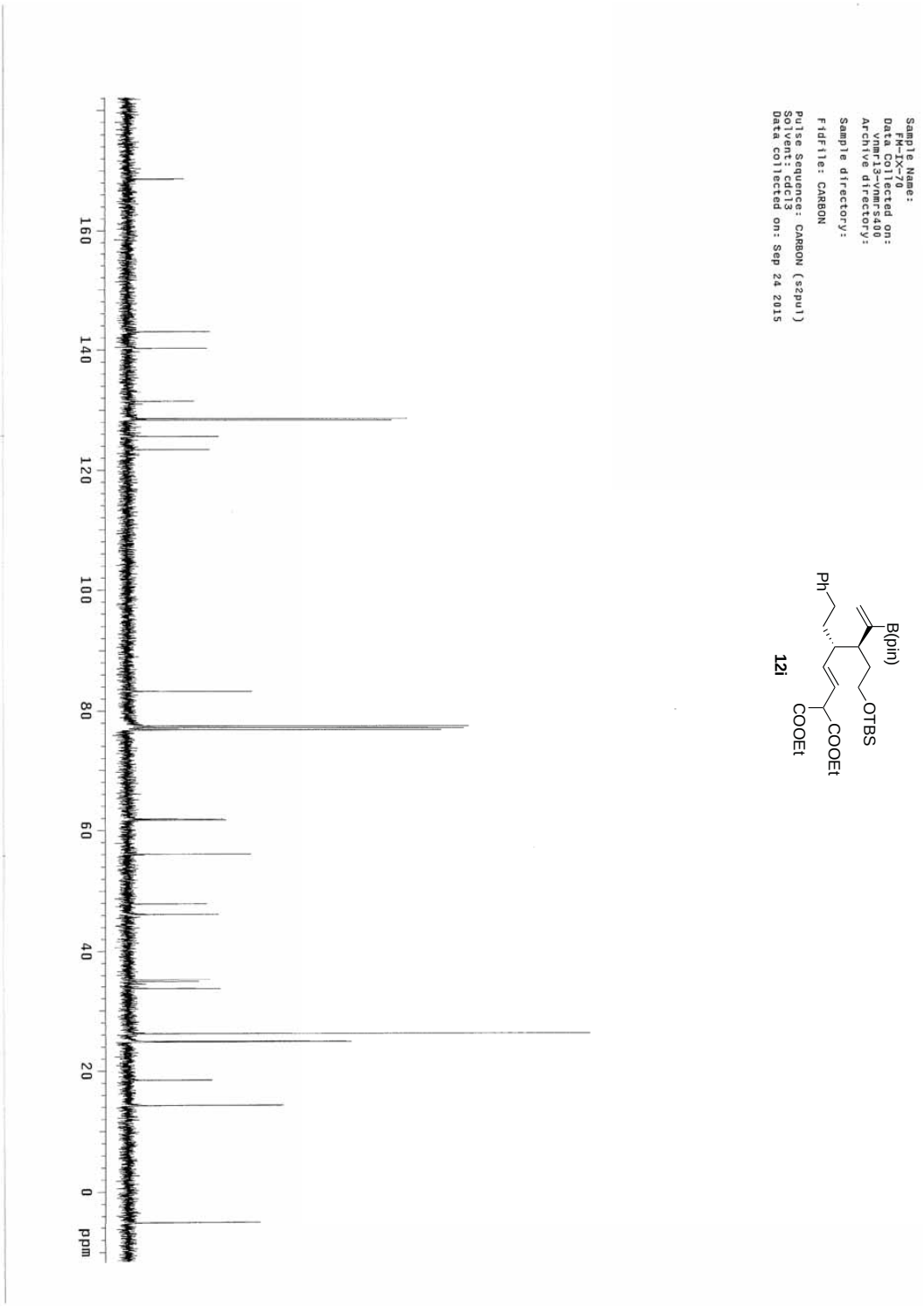

Sample Name:
FM-IX-72
Data Collected on:
vnmrs-pul3-1mmr400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 24 2015
O
B(pin)
OTBS
COOEt
COOEt
160
140
120
100
80
60
40
20
0
ppm

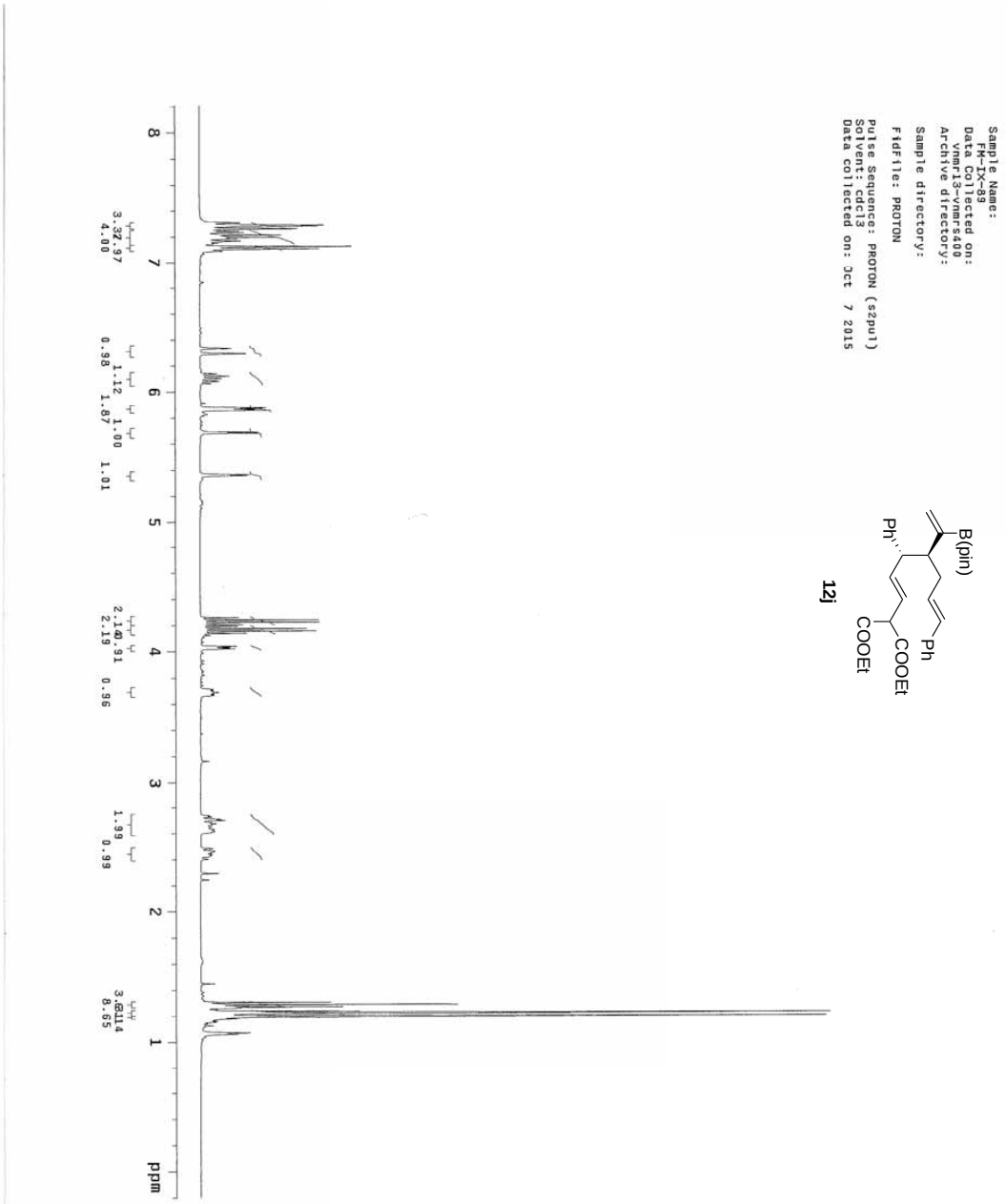
12g

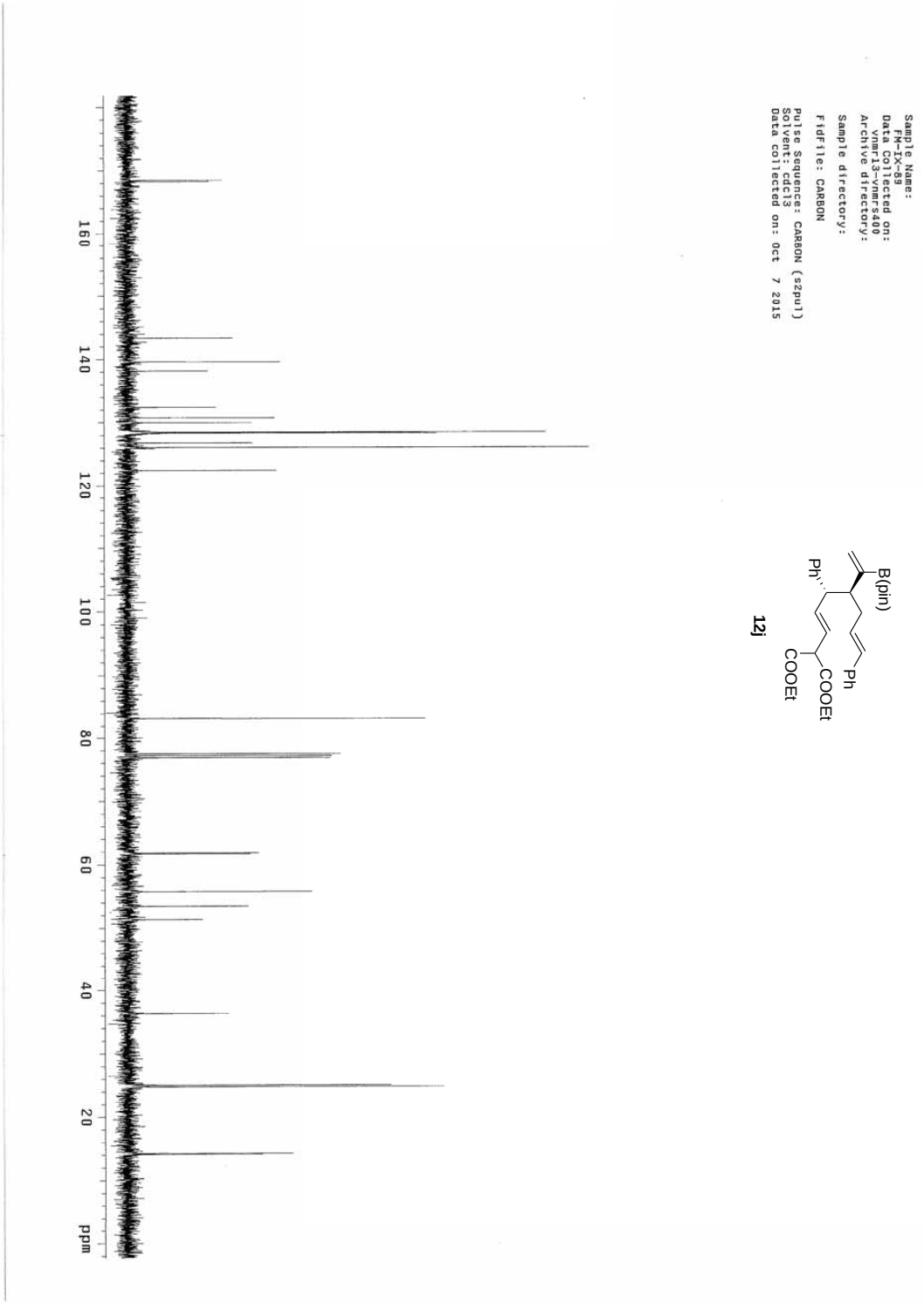

Sample Name:
FM-IX-67
Data Collected on:
vnmrs3-smp400
Archive directory:
Sample directory:
F1dF1le: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 24 2015
B(pin)
OTBS
COOEt
COOEt
S
12h
ppm

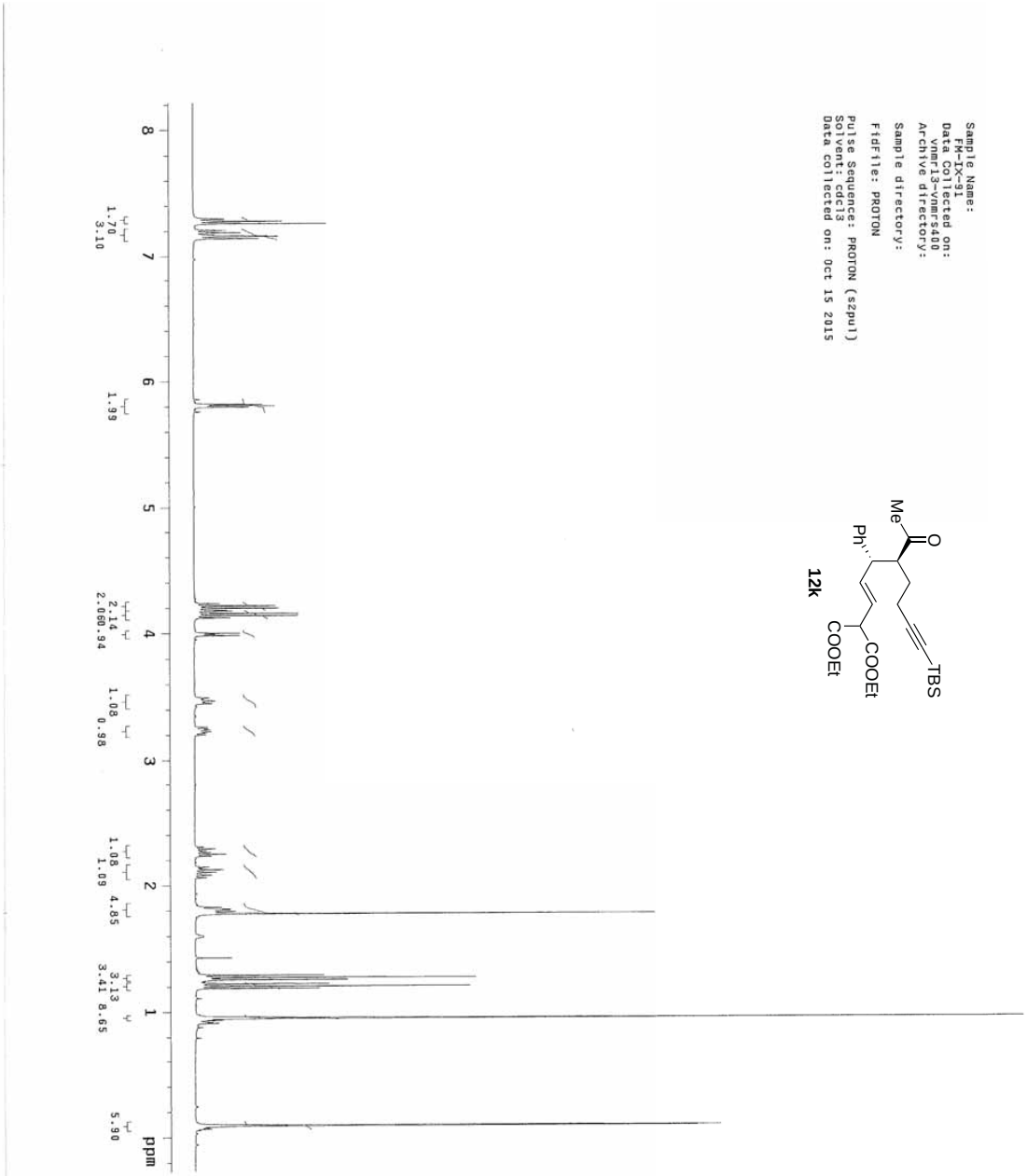

Sample Name:
FM-IX-67
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 24 2015
S
B(pin)
OTBS
COOEt
COOEt
12h
160
140
120
100
80
60
40
20
0
ppm

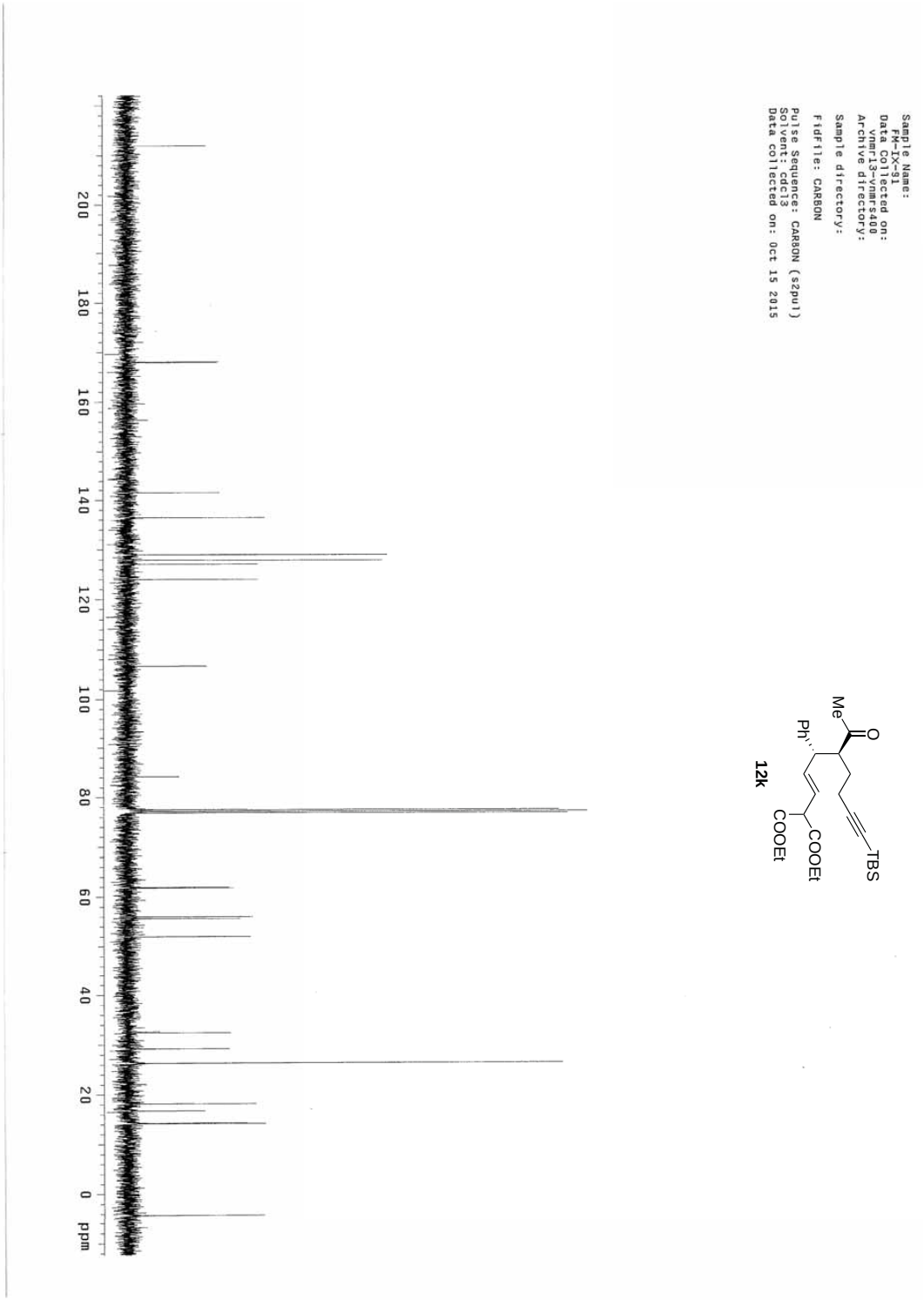

Sample Name:
TM-1-77e
Data Collected on:
vnmrj13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 24 2015
B(pin)
OTBS
COOEt
COOEt
Ph
12i
8
7
6
5
4
3
2
1
0 ppm
2.04
3.04
1.03 0.95
0.93 1.13
4.00
0.93
0.99
1.03
1.14 1.17
1.07 0.94
2.04 7.50 9.00
1.10 12.06
5.79

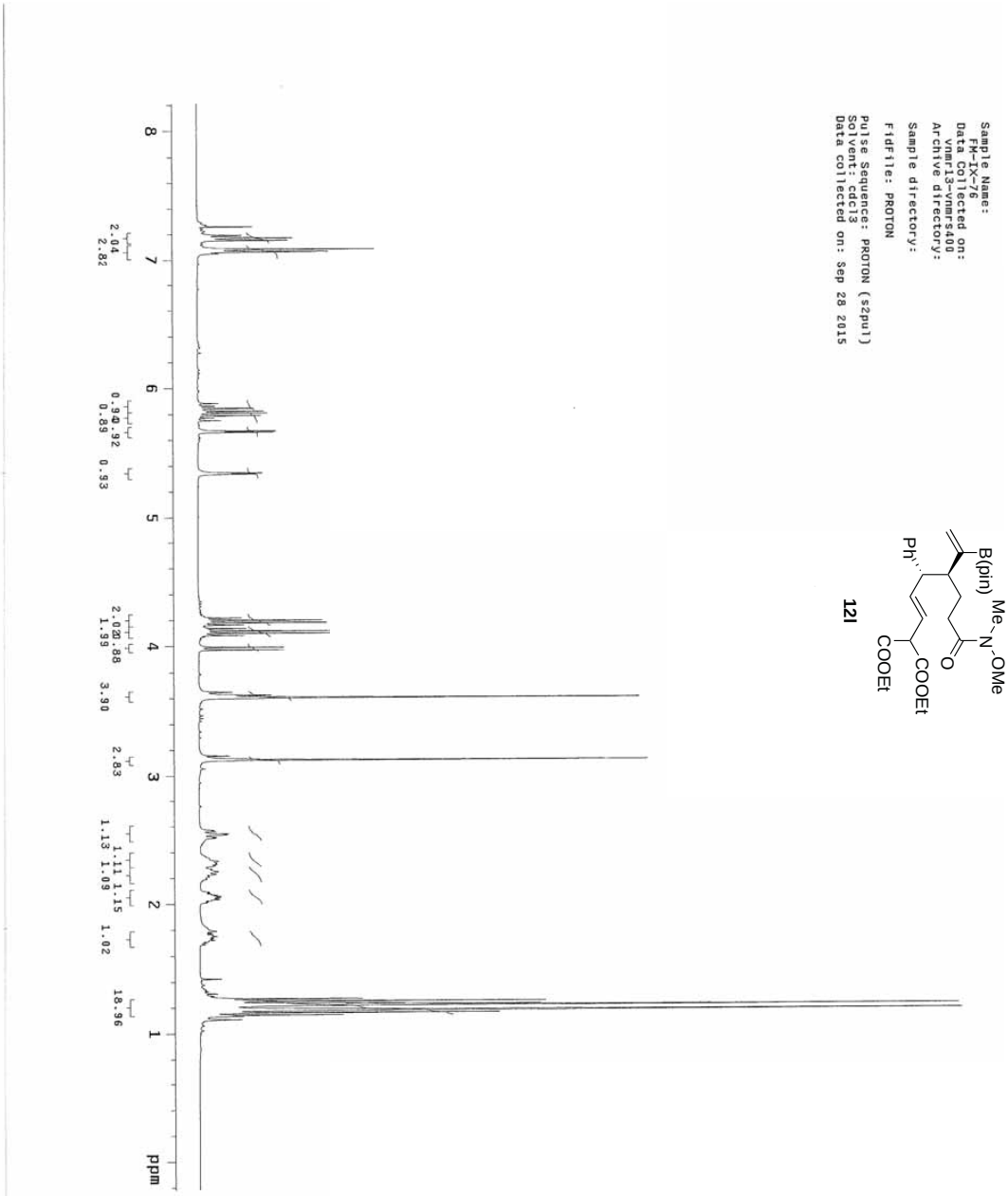

Sample Name:
FM-IX-70
Data Collected on:
Varian-13-omrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 24 2015
Ph
B(pin)
OTBS
COOEt
COOEt
12i
160
140
120
100
80
60
40
20
0
ppm

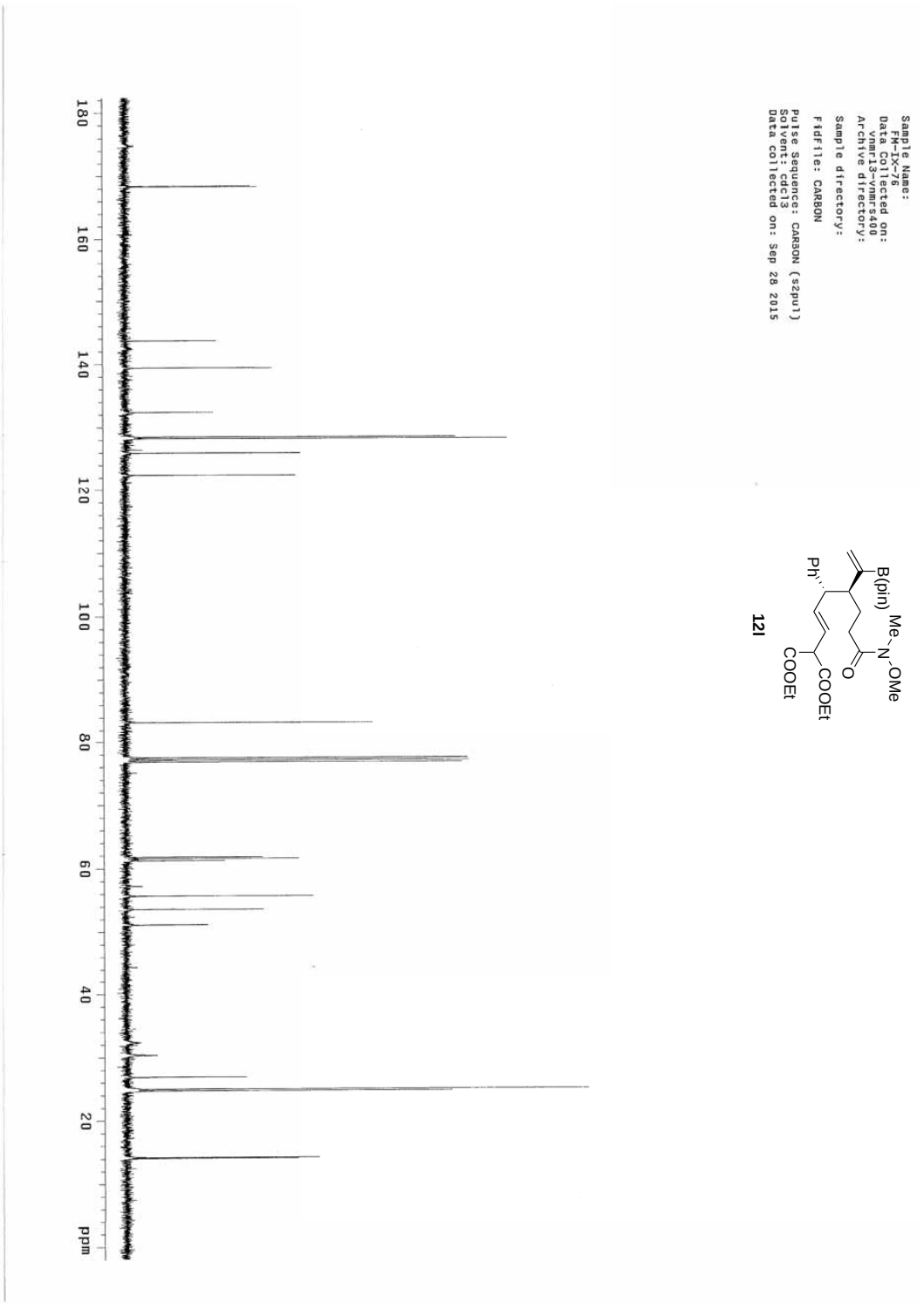

Sample Name:
FM-IX-93
Data Collected on:
vnmrs3-vnmr400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 7 2015
B(pin)
Ph
COOEt
COOEt
12j
ppm

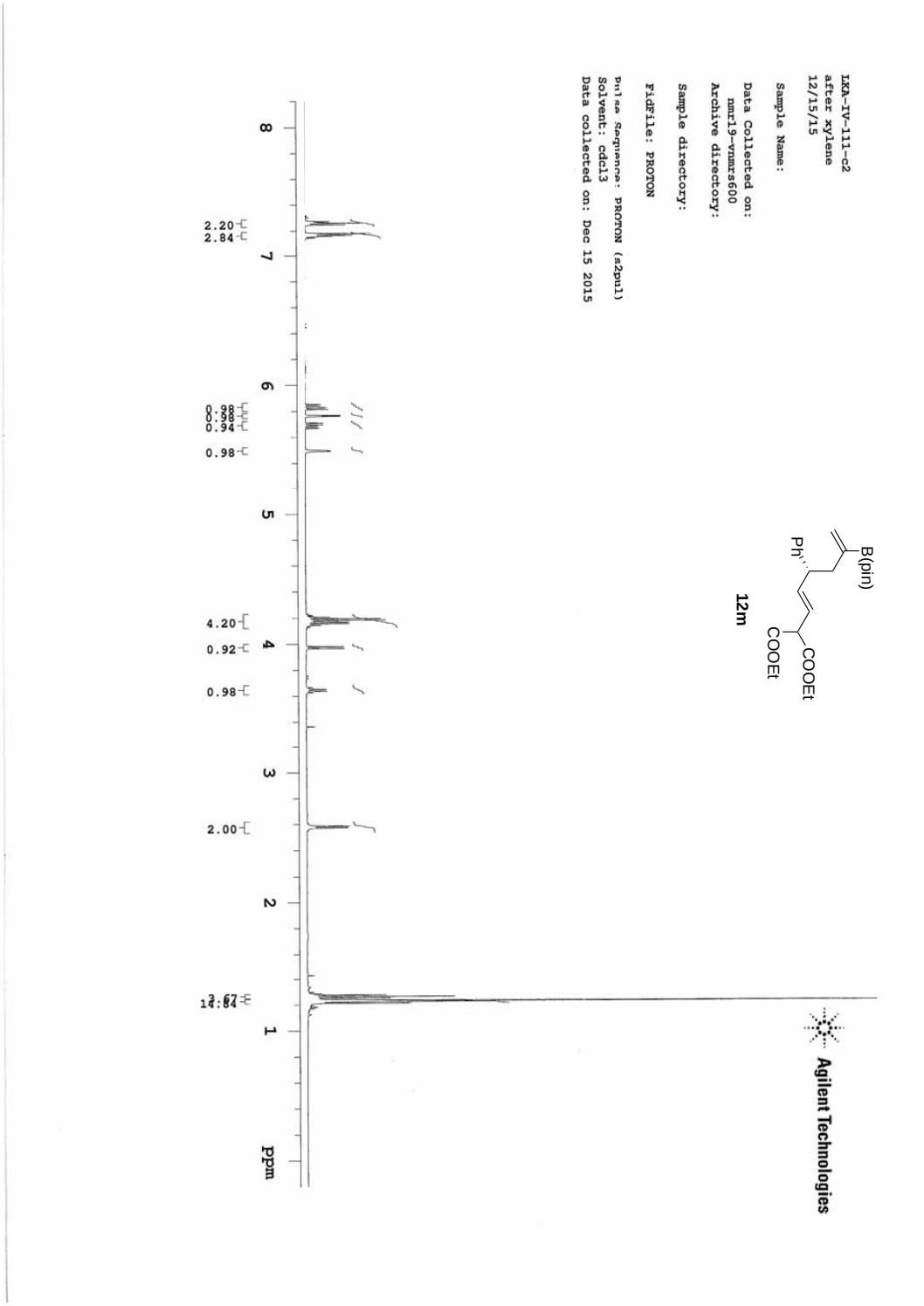

Sample Name:
FM-IX-99
Data Collected on:
vnmrs3-vnmr400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (szpul)
Solvent: cdcl3
Data collected on: Oct 7 2015
B(pin)
Ph
COOEt
COOEt
Ph
12j
160
140
120
100
80
60
40
20
ppm

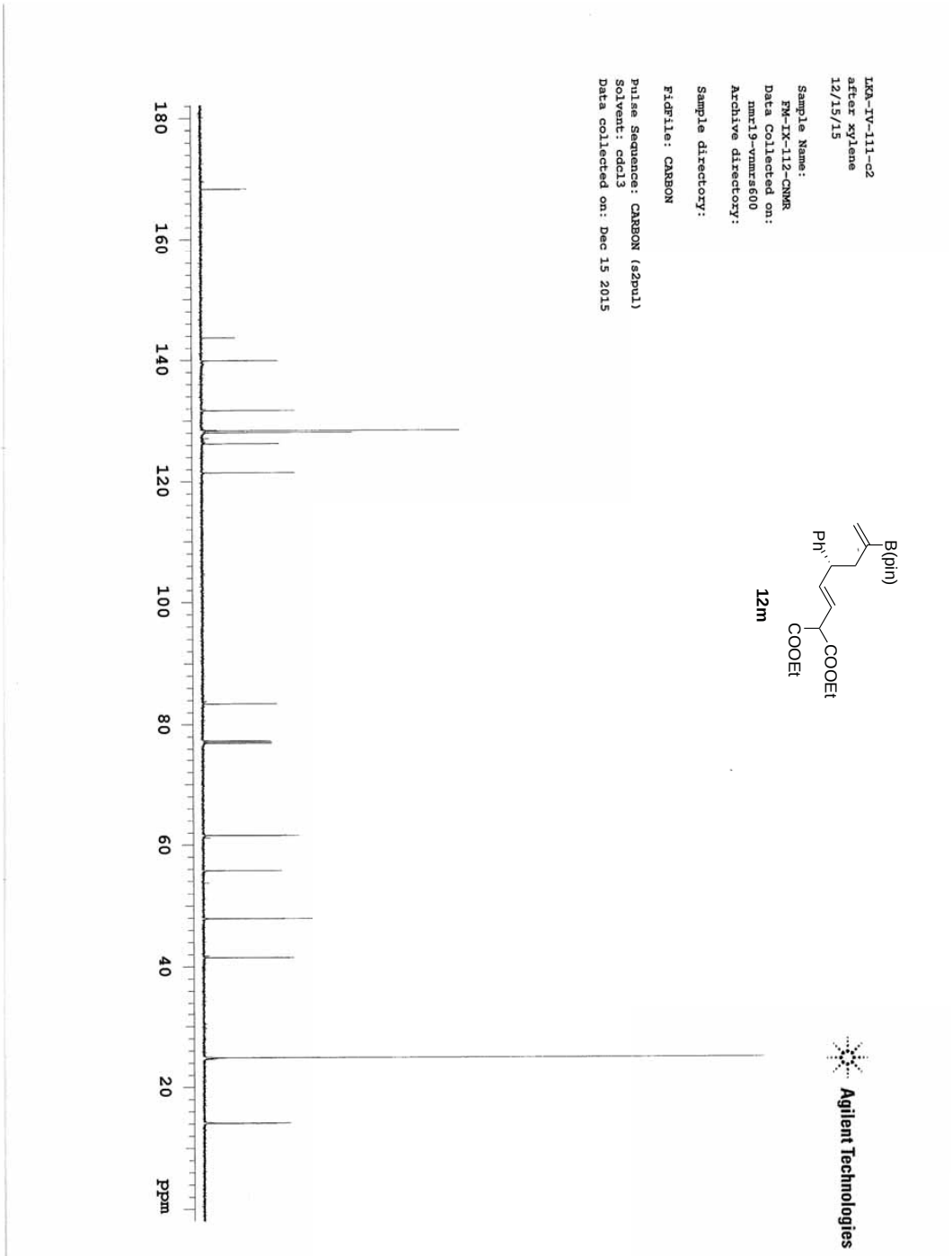

Sample Name:
FM-IX-91
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (szpul)
Solvent: cdcl3
Data collected on: Oct 15 2015
Me
O
Ph
TBS
COOEt
COOEt
12k
ppm

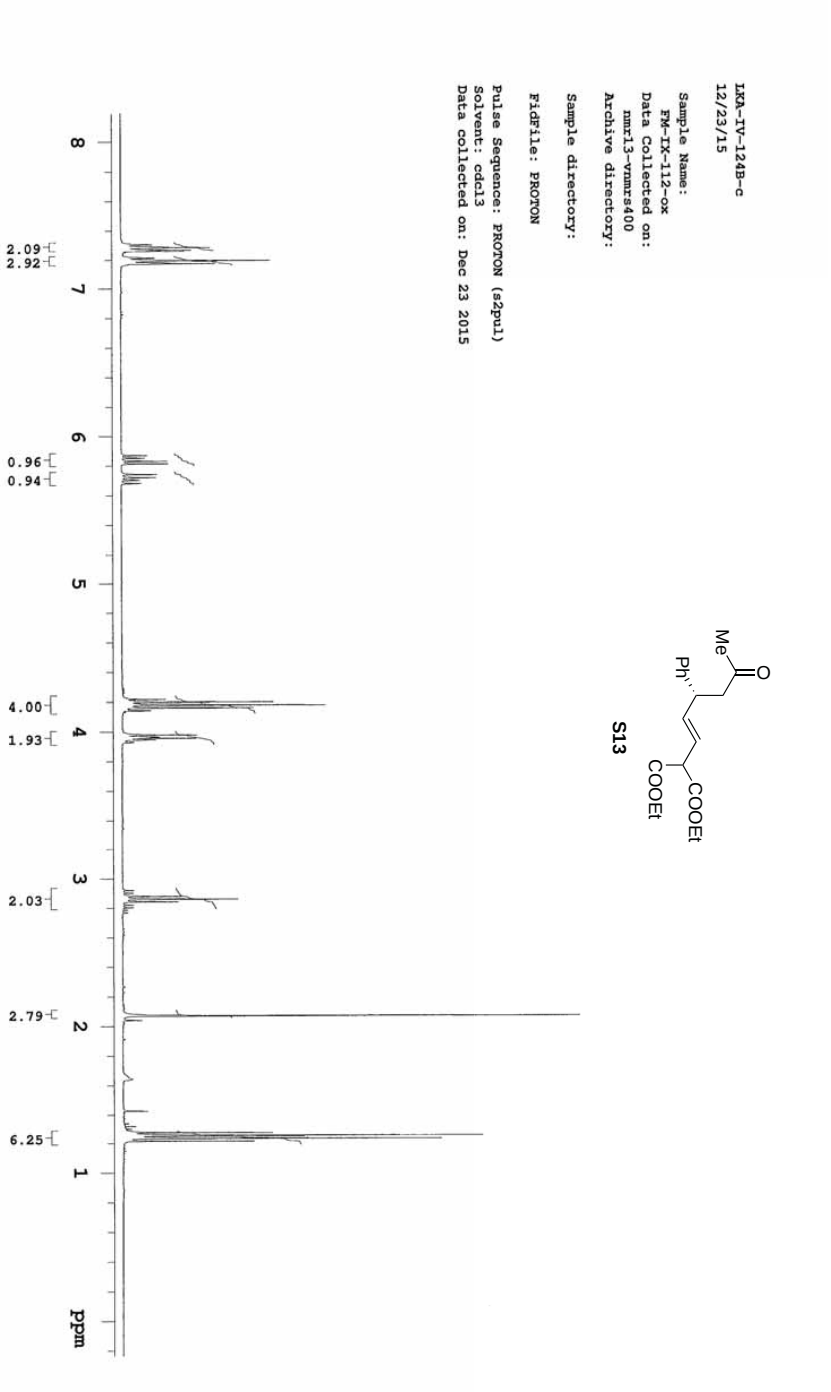

Sample Name:
FM-IX-91
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 15 2015
200
180
160
140
120
100
80
60
40
20
0
ppm
Me
O
Ph
COOEt
COOEt
TBS
12k


Sample Name:
FM-IX-76
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 28 2015
B(pin)
Me
N
OMe
Ph
COOEt
COOEt
O
12l
8
7
6
5
4
3
2
1
ppm
2.04
2.82
0.90
0.92
0.89
0.93
2.00
0.98
1.99
3.90
2.83
1.13
1.11
1.09
1.15
1.02
18.96

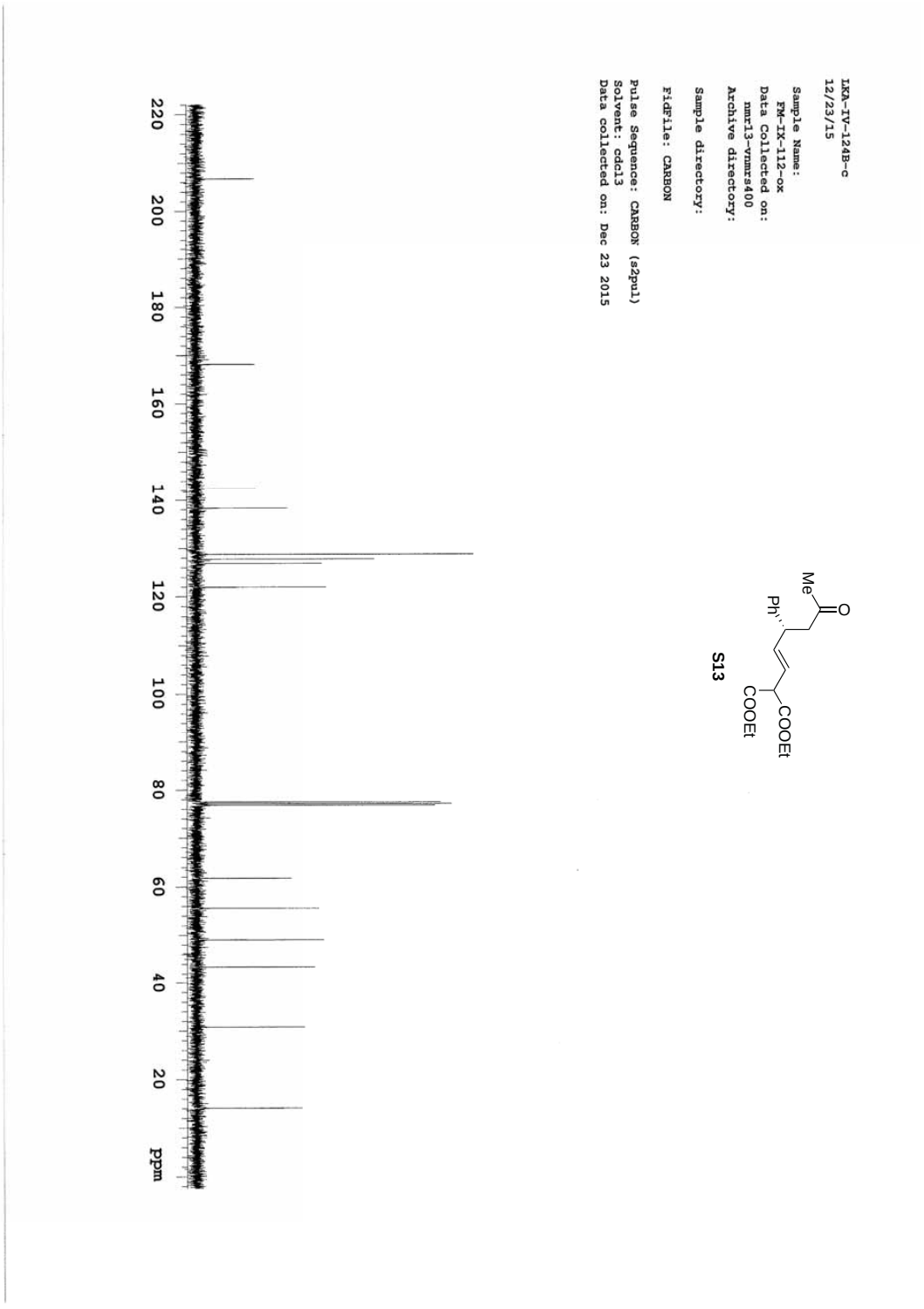

Sample Name:
FM-IX-76
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 28 2015
B(pin)
Me
N
OMe
O
Ph
COOEt
COOEt
12l
180
160
140
120
100
80
60
40
20
ppm


LKA-IV-111-c2
after xylene
12/15/15
Sample Name:
Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 15 2015
B(pin)
Ph
COOEt
COOEt
12m
Agilent Technologies
2.20
2.84
0.98
0.98
0.94
0.98
4.20
0.92
0.98
2.00
3.67
14.84
8
7
6
5
4
3
2
1
PPm

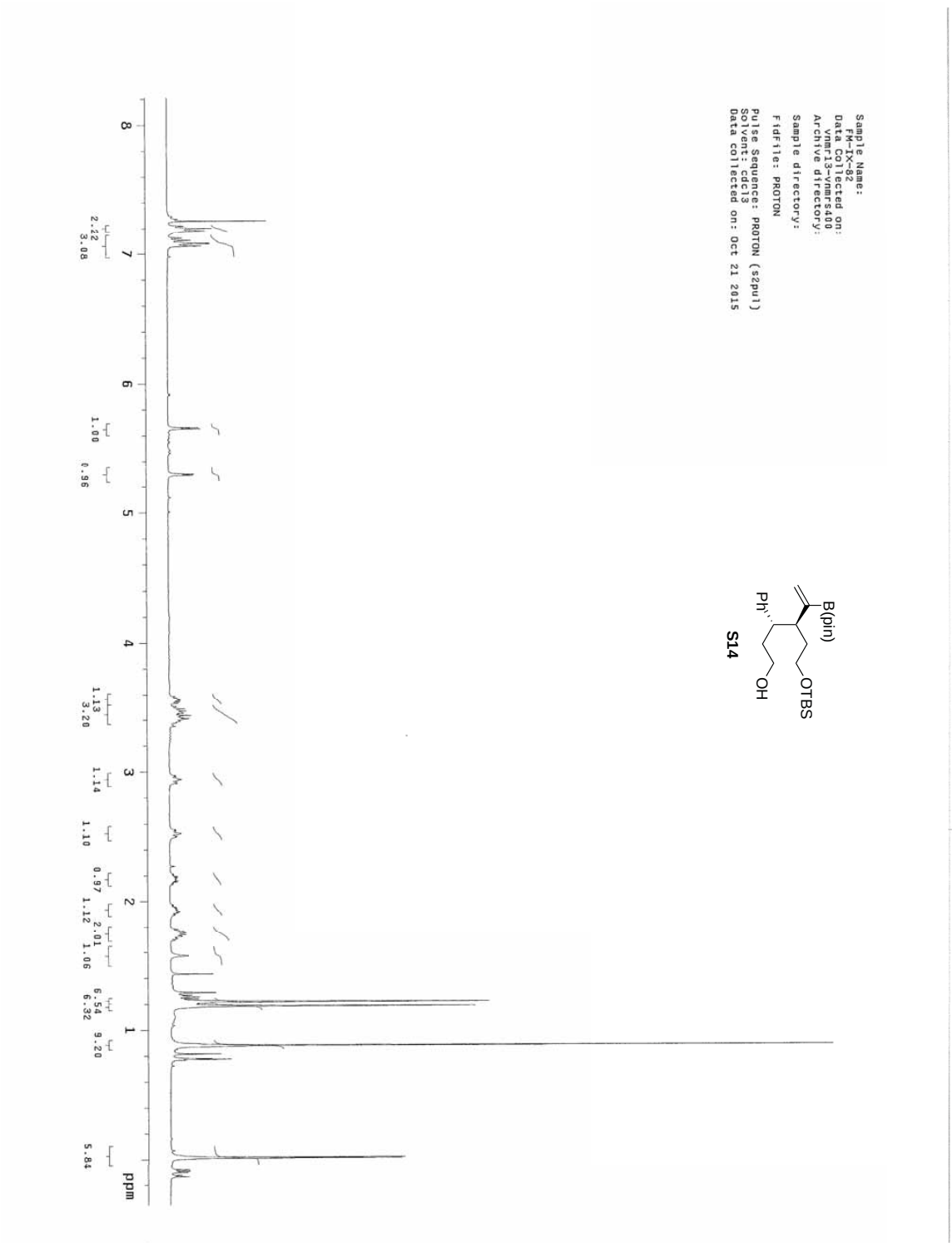

LKA-IV-111-c2
after xylene
12/15/15
Sample Name:
FM-IX-112-CNMR
Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 15 2015
B(pin)
Ph
COOEt
COOEt
12m
Agilent Technologies
180
160
140
120
100
80
60
40
20
ppm

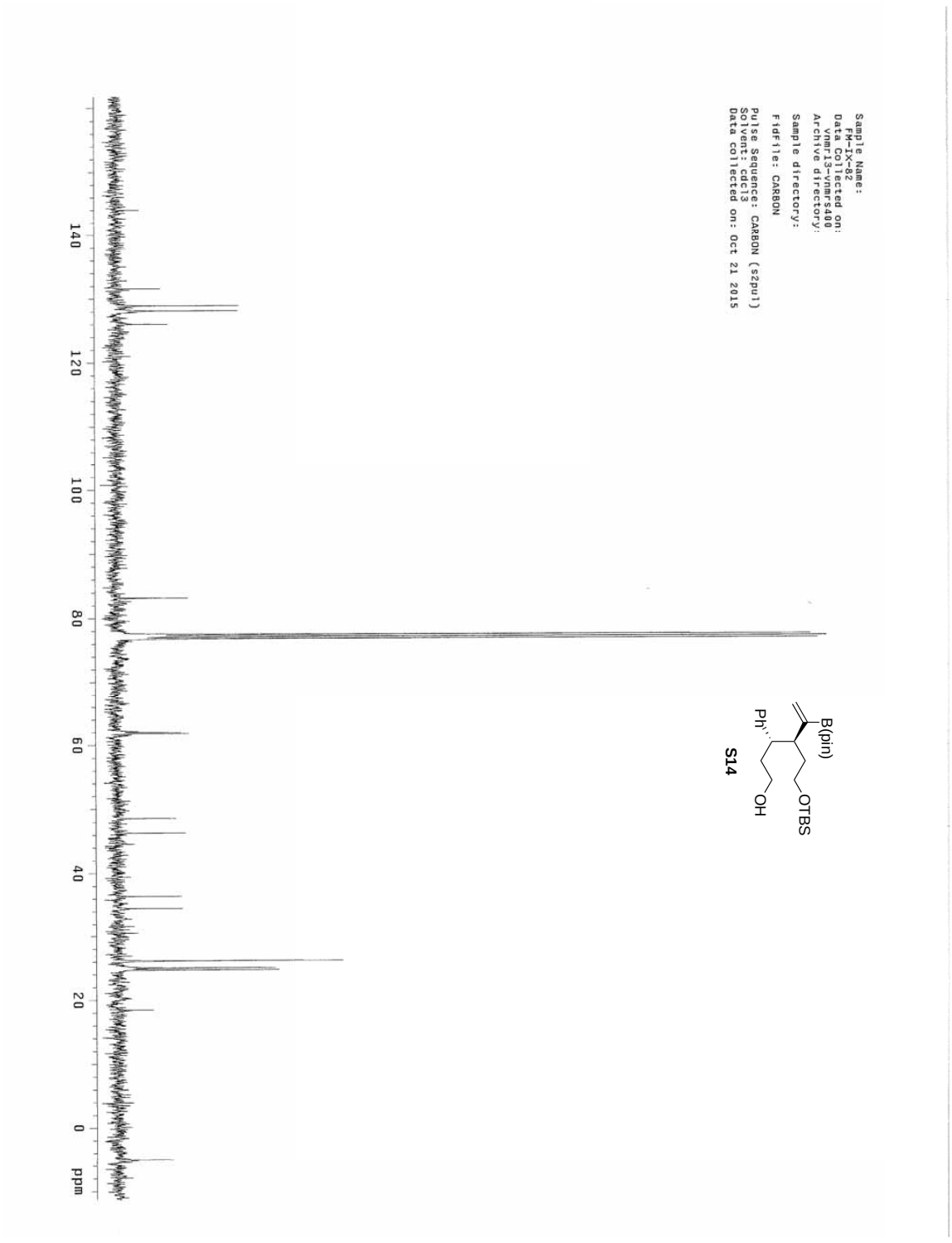

LKA-IV-124B-c
12/23/15
Sample Name:
FM-IX-112-ox
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 23 2015
2.09
2.92
0.96
0.94
4.00
1.93
2.03
2.79
6.25
8
7
6
5
4
3
2
1
ppm
Me
O
Ph
COOEt
COOEt

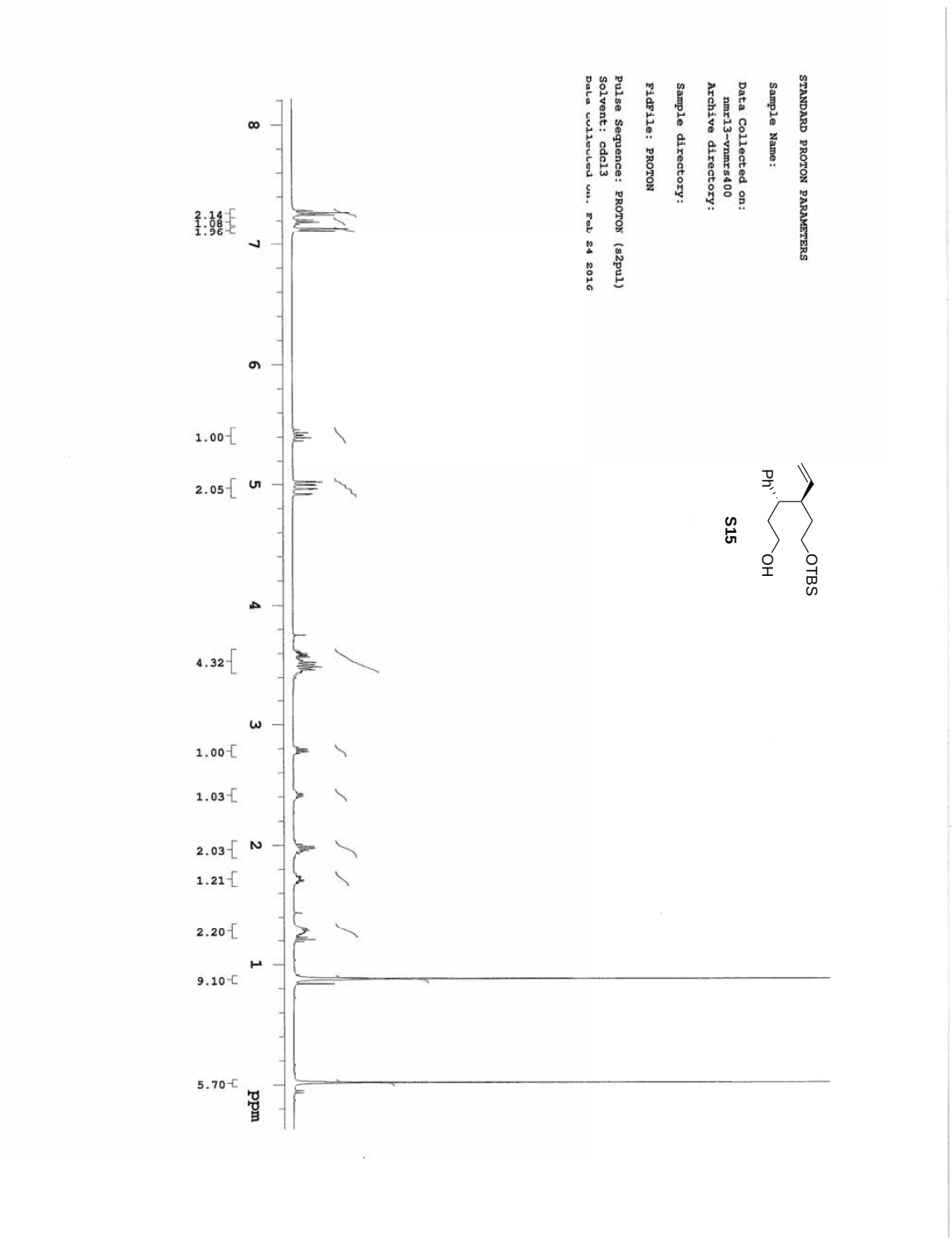
S13

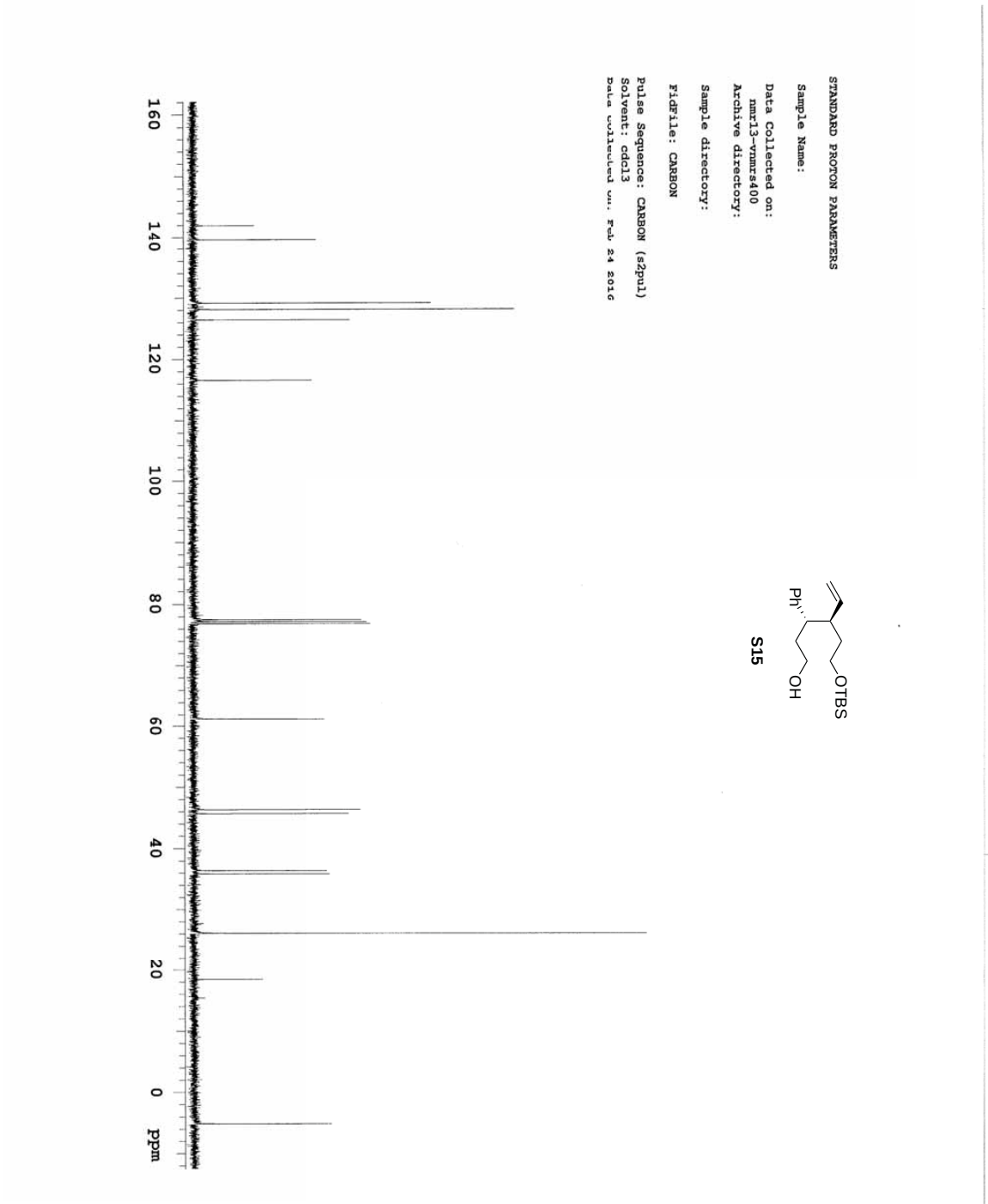

LKA-IV-124B-c
12/23/15
Sample Name:
FM-IX-112-ox
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 23 2015
Me
O
Ph
COOEt
COOEt
220
200
180
160
140
120
100
80
60
40
20
ppm

S13

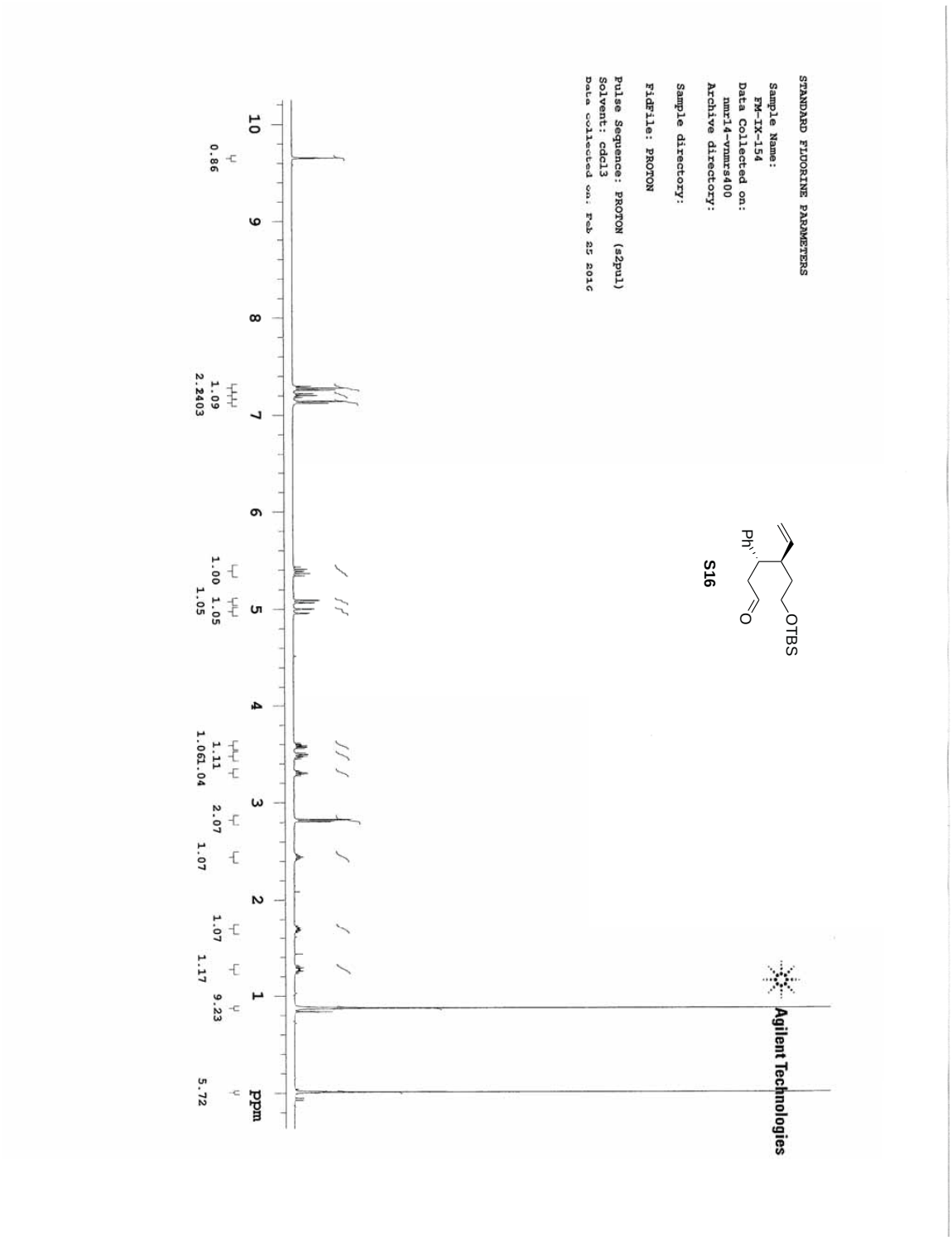

Sample Name:
FM-IX-82
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 21 2015
B(pin)
OTBS
Ph
OH
S14
ppm


Sample Name:
FM-IX-82
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 21 2015
B(pin)
Ph
OTBS
OH
S14
140
120
100
80
60
40
20
0
ppm


STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 24 2016
Ph
OH
OTBS
S15
2.14
2.08
1.96
1.00
2.05
4.32
1.00
1.03
2.03
1.21
2.20
9.10
5.70
8
7
6
5
4
3
2
1
ppm


STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
OTBS
Ph
OH
160
140
120
100
80
60
40
20
0
ppm

S15


STANDARD FLUORINE PARAMETERS
Sample Name:
FM-IX-154
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 25 2016
Ph
OTBS
O
S16
Agilent Technologies
10
9
8
7
6
5
4
3
2
1
ppm
0.86
1.09
2.2403
1.00
1.05
1.05
1.11
1.06
1.04
2.07
1.07
1.07
1.17
9.23
5.72

STANDARD FLUORINE PARAMETERS

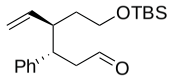
Sample Name:

Data Collected on:
nmr14-vnmrs400
Archive directory:

Sample directory:

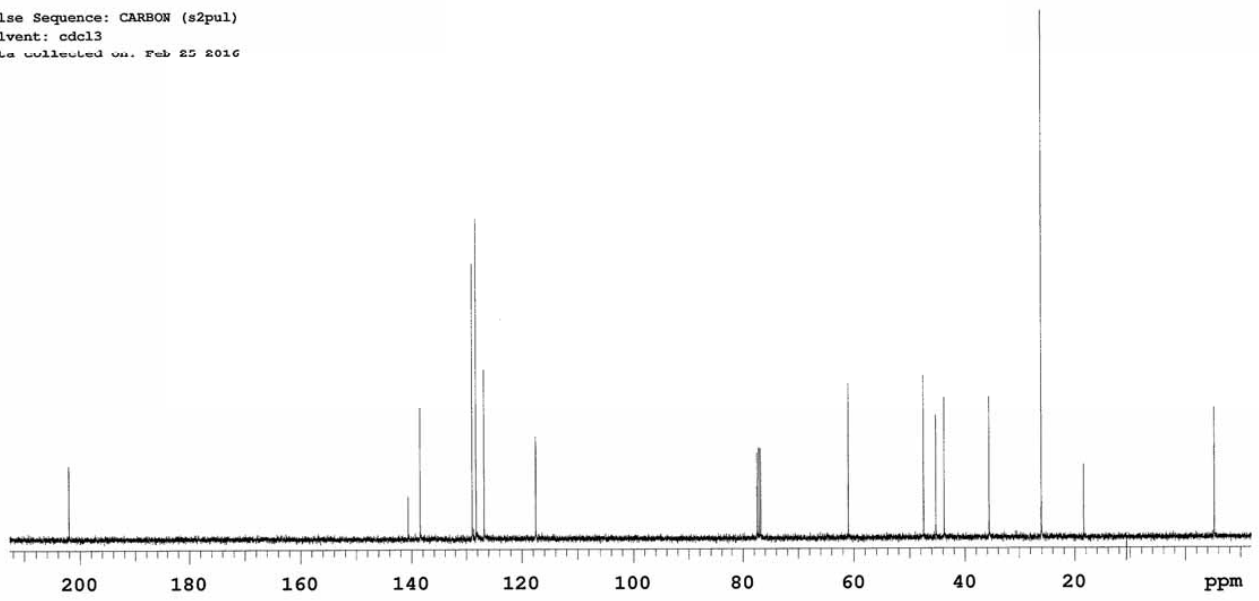
FidFile: CARBON

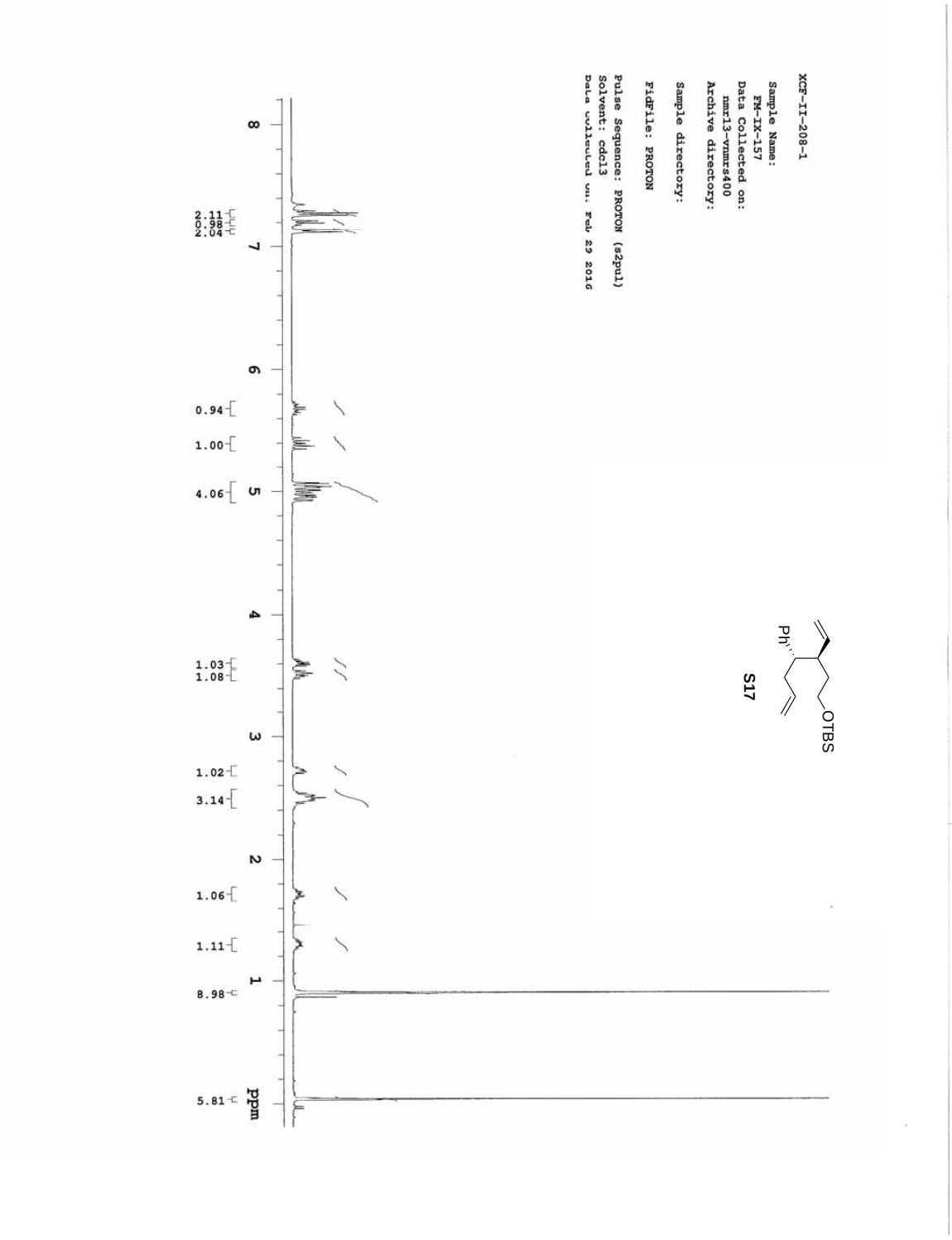
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 25 2016

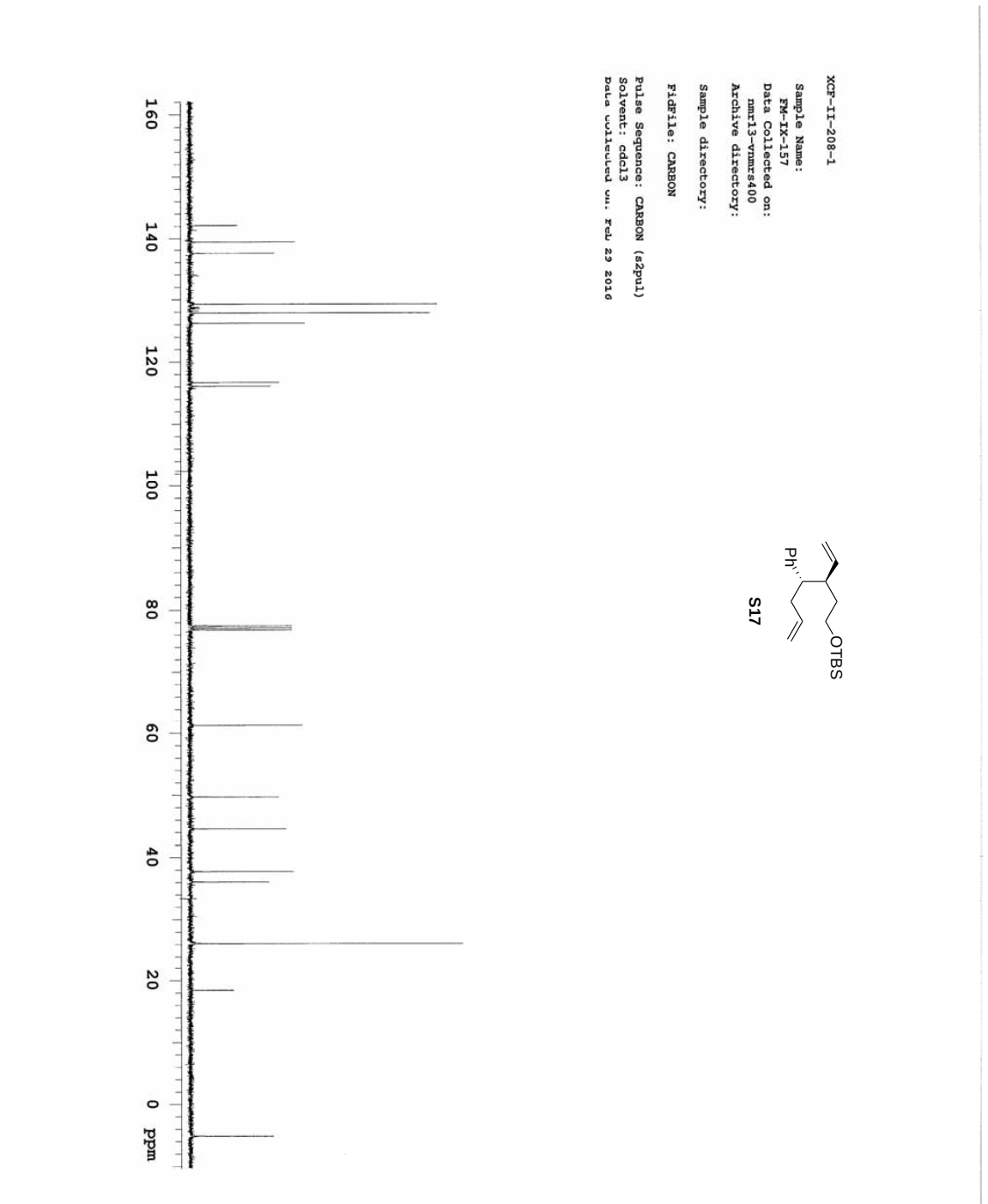


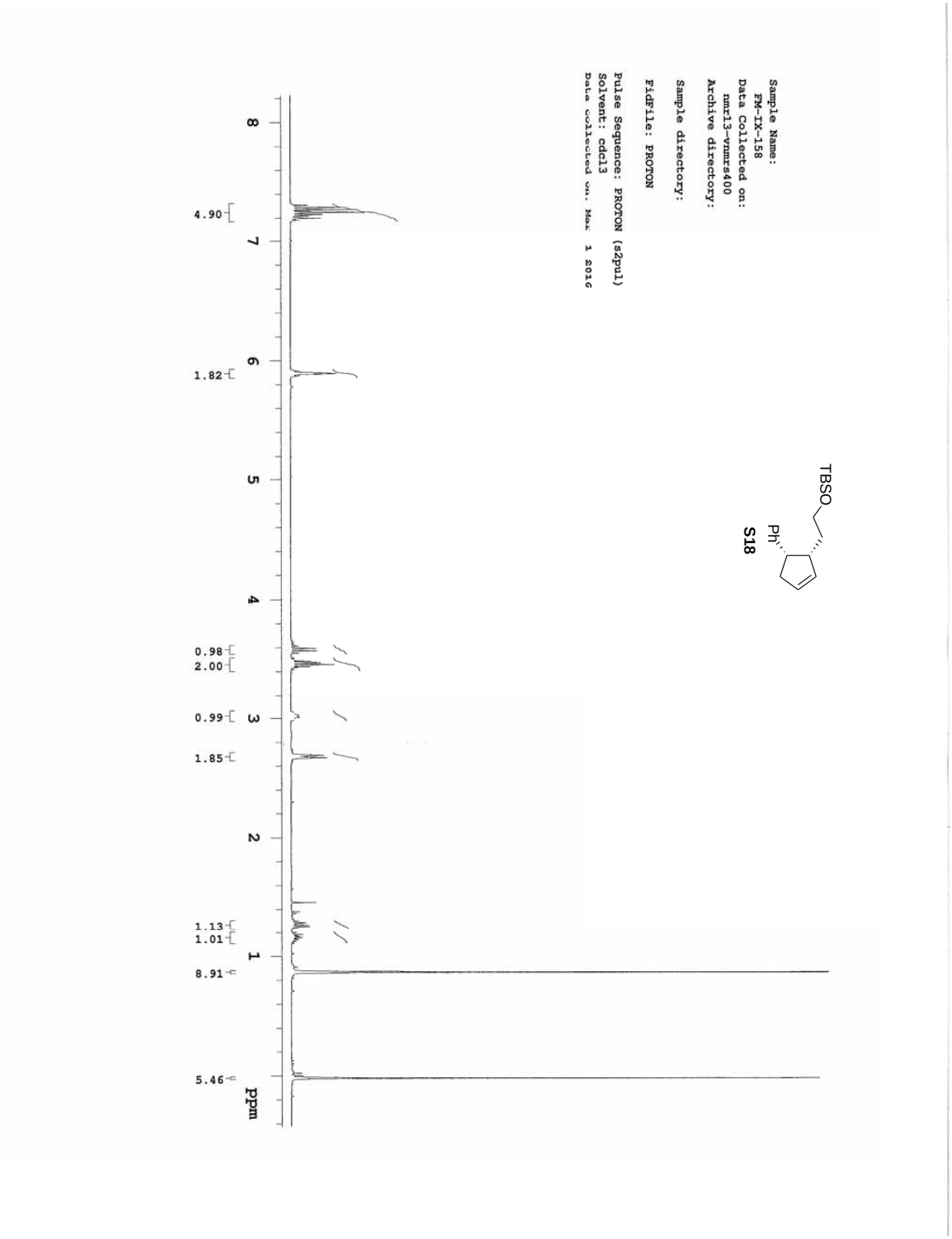
S16

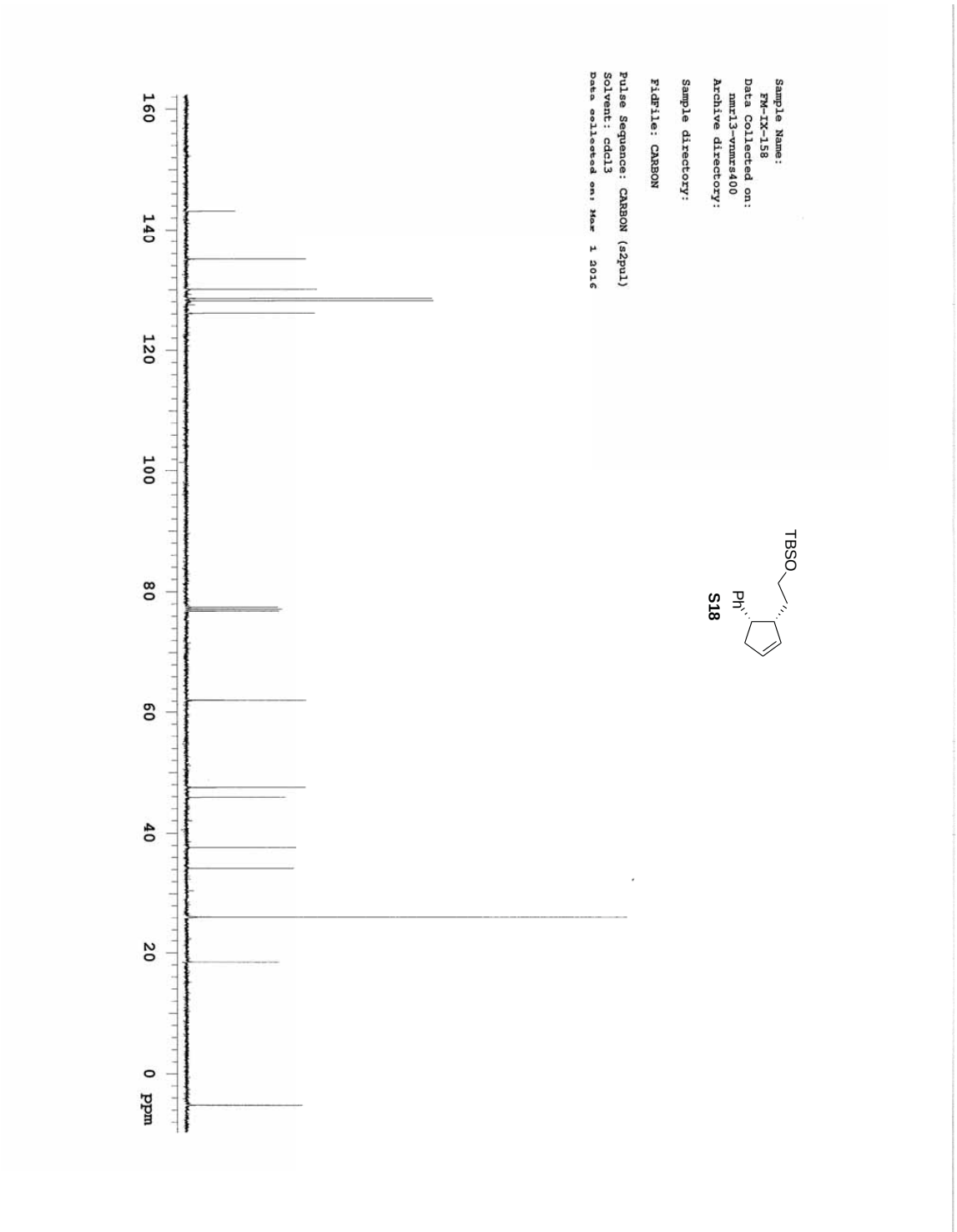
Agilent Technologies

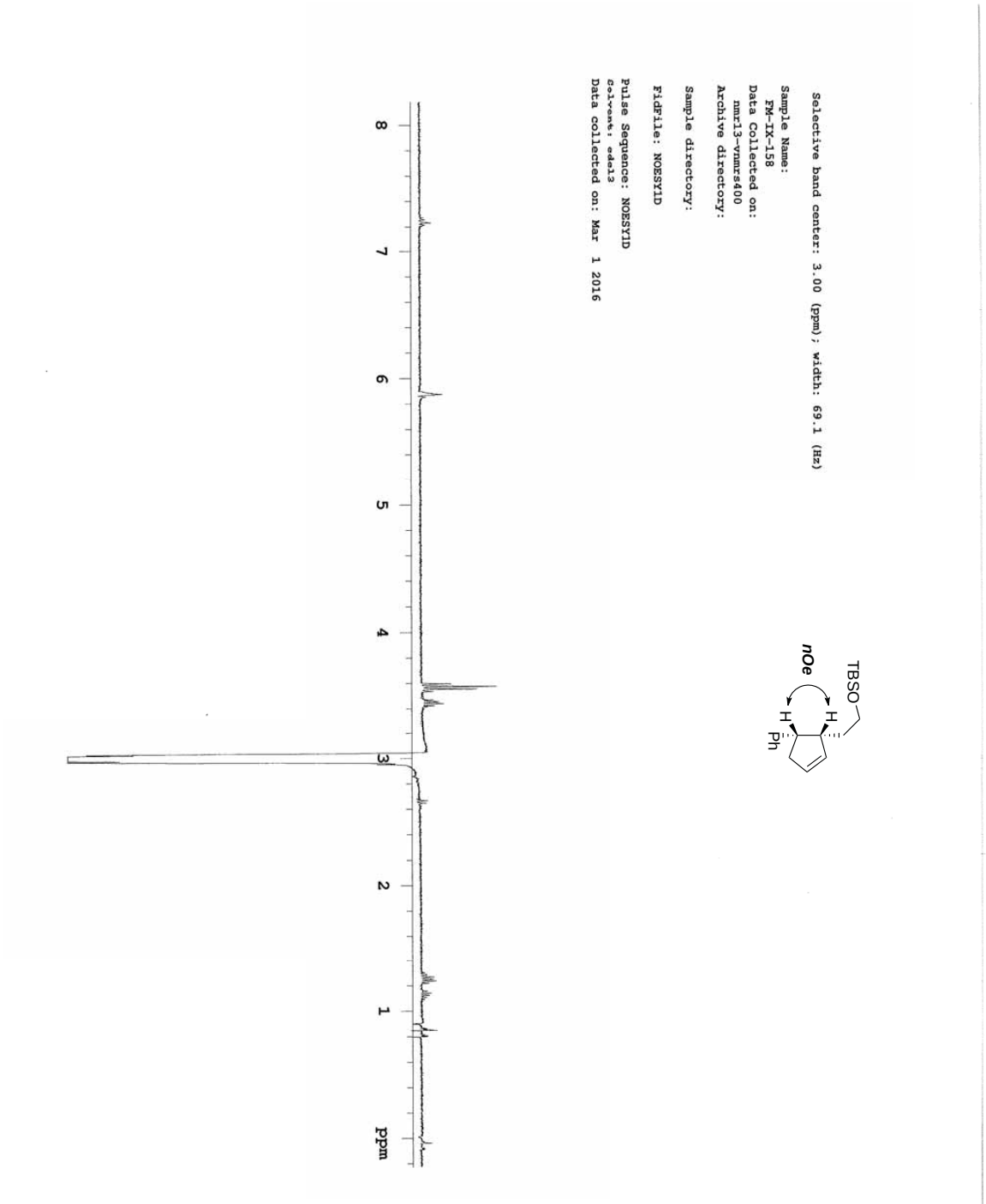


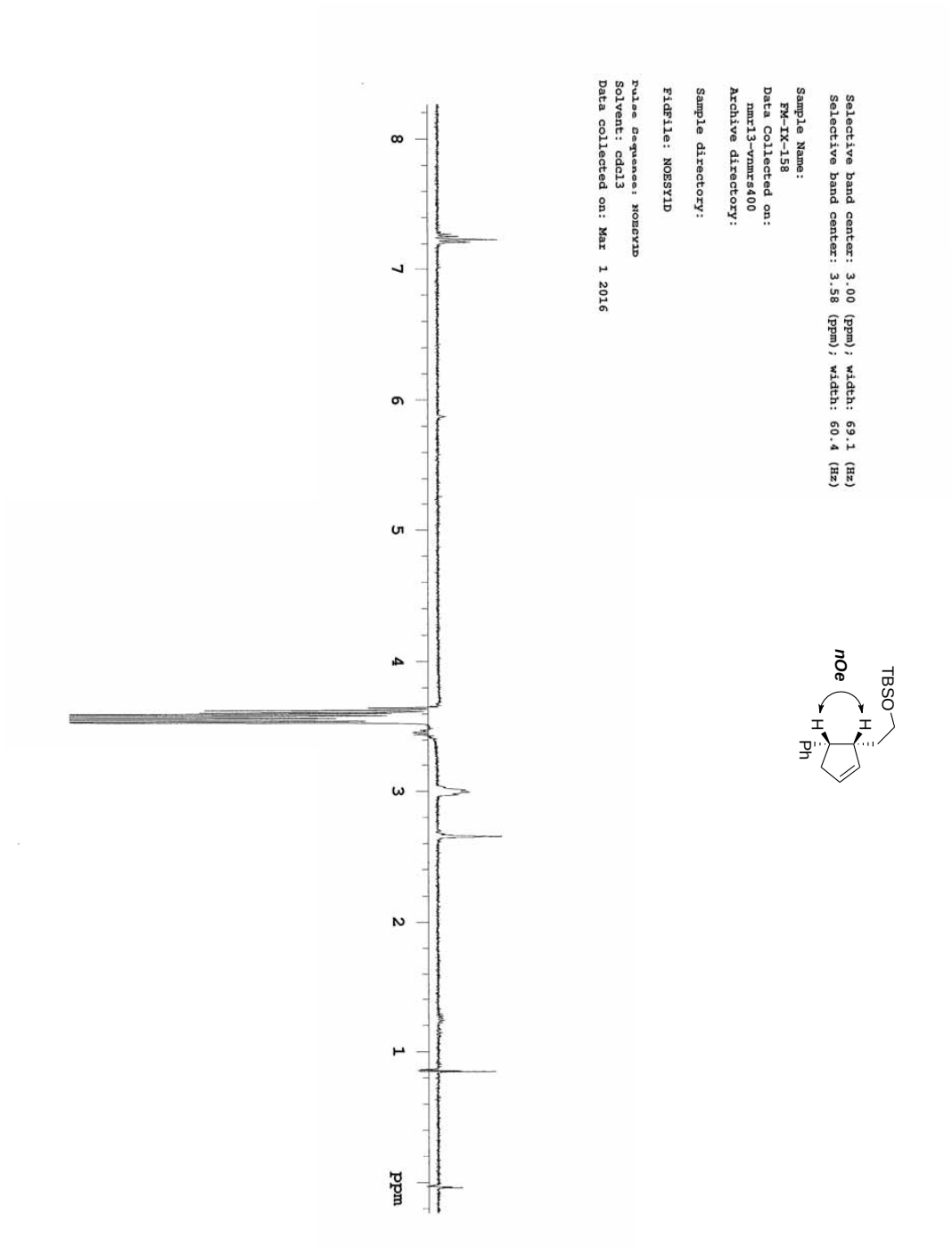

XCF-II-208-1
Sample Name:
FM-IX-157
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 29 2016
Ph
OTBS
S17
2.11
2.98
2.04
0.94
1.00
4.06
1.03
1.08
1.02
3.14
1.06
1.11
8.98
5.81
ppm

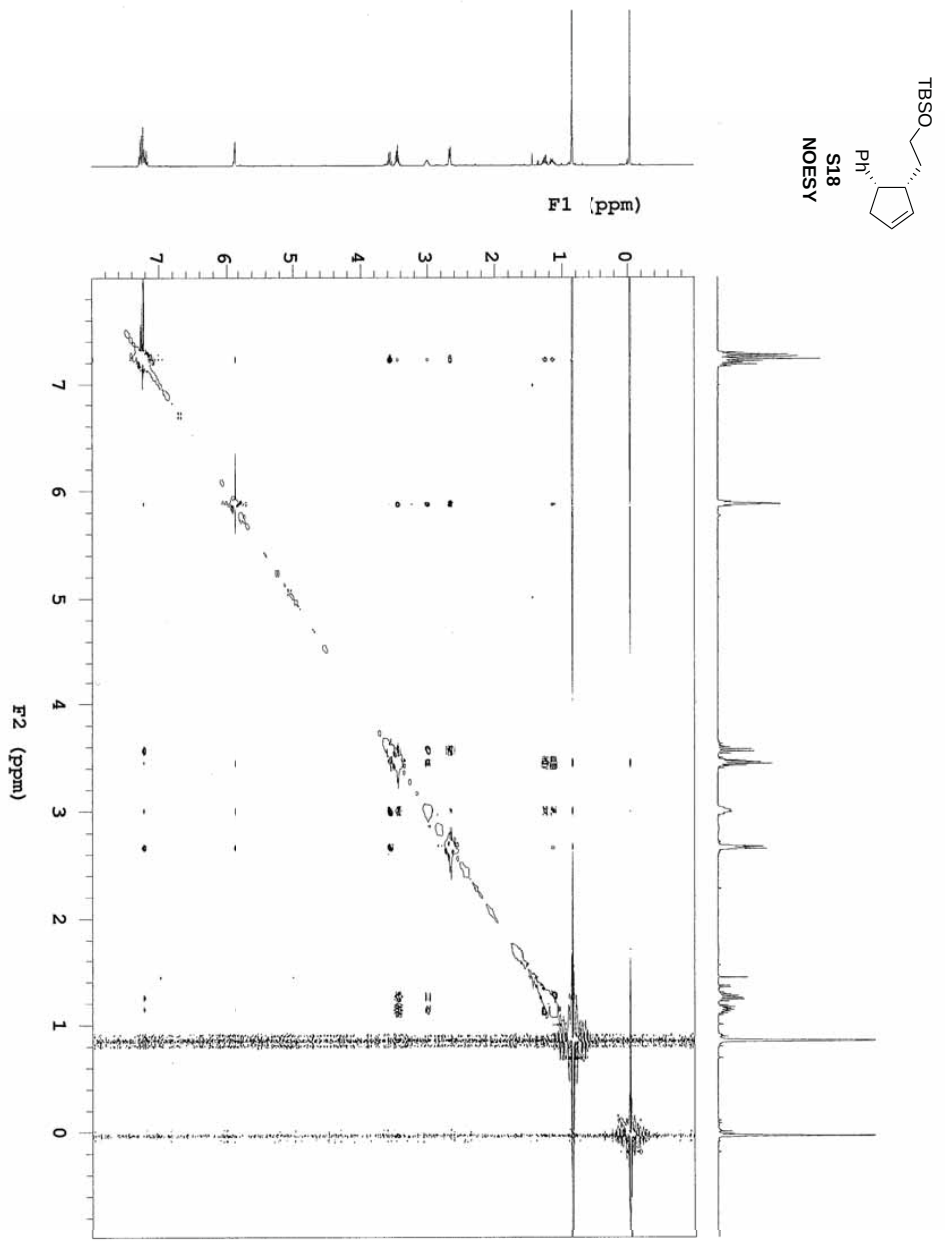

XCF-II-208-1
Sample Name:
FM-IX-157
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 29 2016
Ph
OTBS
S17
160
140
120
100
80
60
40
20
0
ppm

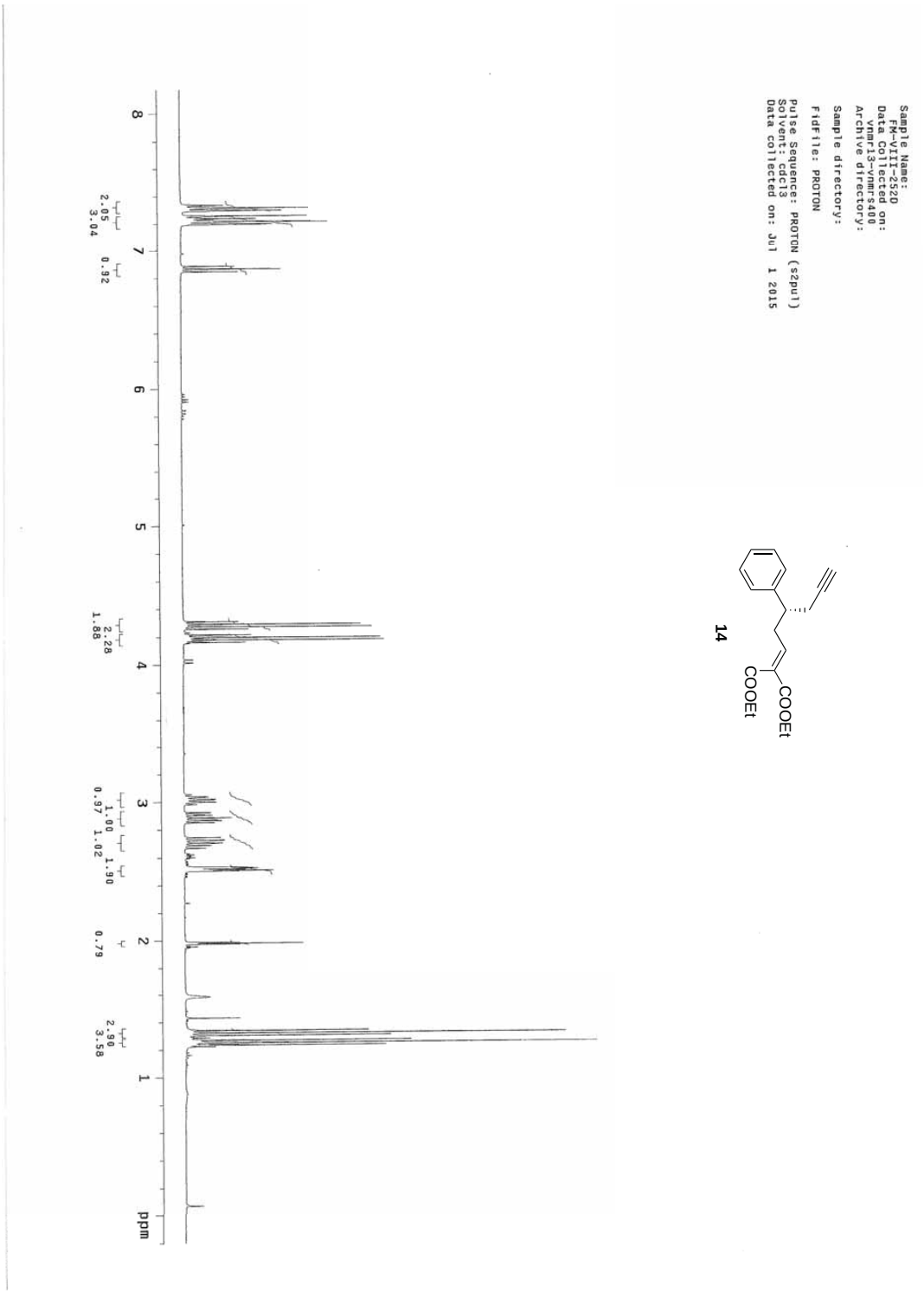

Sample Name:
FM-IX-158
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
TBSO
Ph
S18
4.90
1.82
0.98
2.00
0.99
1.85
1.13
1.01
8.91
5.46
ppm

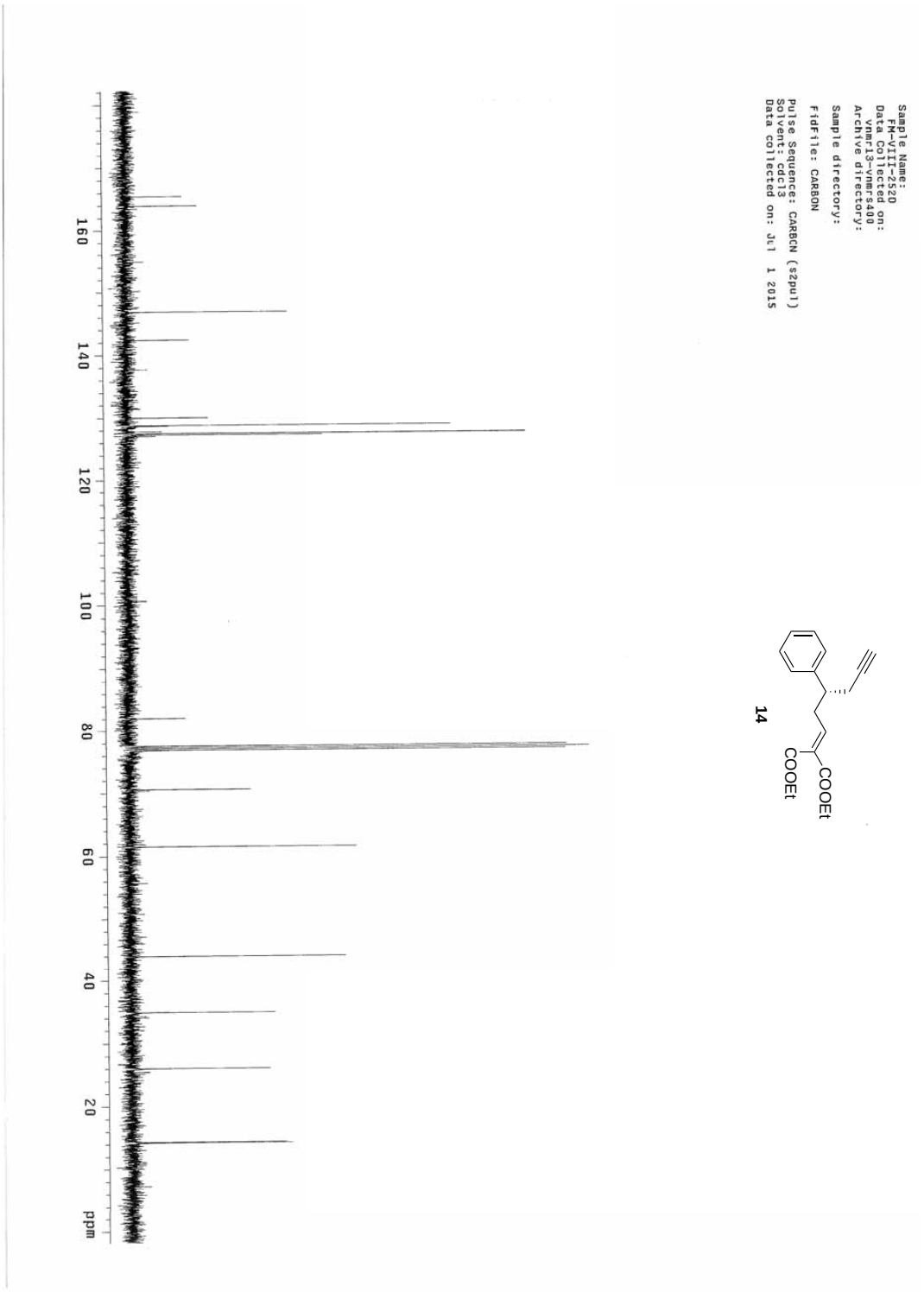

Sample Name:
FM-IX-158
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 1 2016
TBSO
Ph
S18
160
140
120
100
80
60
40
20
0 ppm

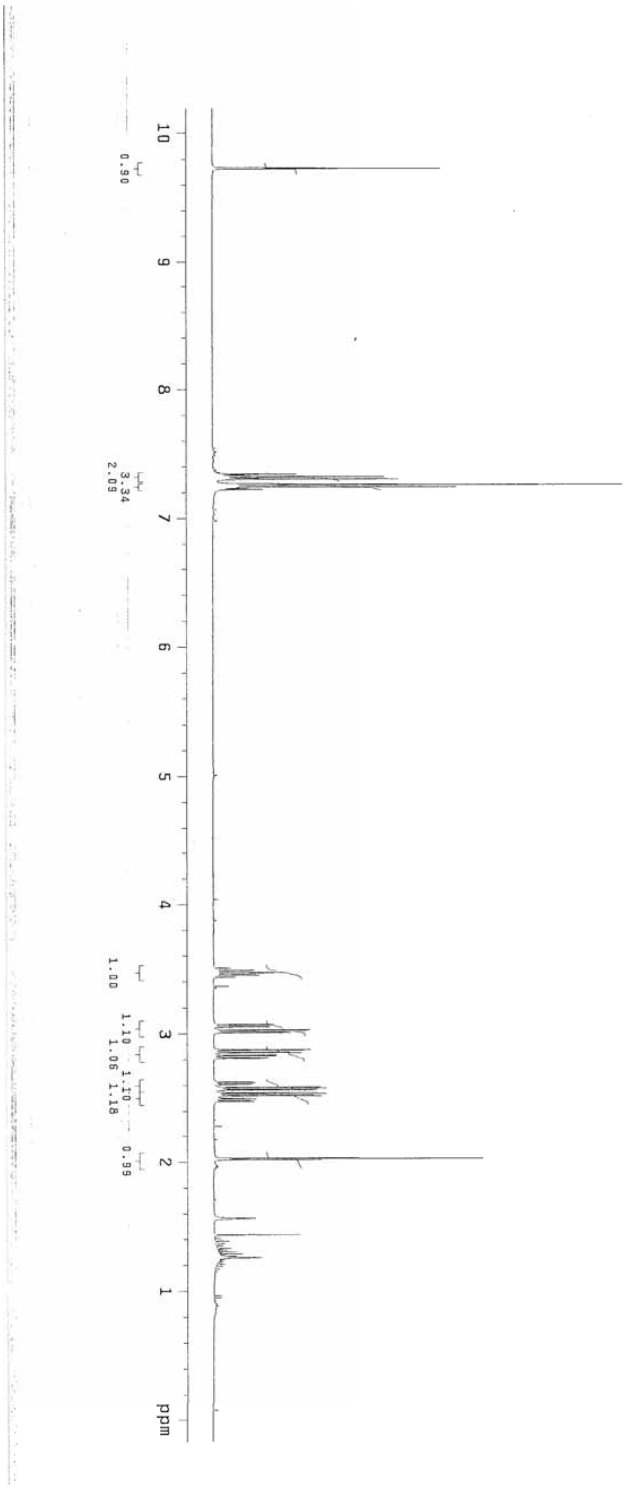

Selective band center: 3.00 (ppm); width: 69.1 (Hz)
Sample Name:
FM-IX-158
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: NOESY1D
Pulse Sequence: NOESY1D
solvents: cdcl3
Data collected on: Mar 1 2016
TBSO
nOe
H
H
Ph
8
7
6
5
4
3
2
1
ppm


Selective band center: 3.00 (ppm); width: 69.1 (Hz)
Selective band center: 3.58 (ppm); width: 60.4 (Hz)
Sample Name:
FM-IX-158
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: NOESY1D
Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Mar 1 2016
TBSO
nOe
H
H
Ph
8
7
6
5
4
3
2
1
ppm


TBSO
Ph
S18
NOESY
F1 (ppm)
F2 (ppm)
0
1
2
3
4
5
6
7


Sample Name:
FM-VIII-252D
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 1 2015
14
COOEt
COOEt
8
7
6
5
4
3
2
1
ppm
2.05
3.04
0.92
2.28
1.88
1.00
0.97
1.02
1.90
0.79
2.90
3.58


Sample Name:
FM-VIII-2520
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBCN (s2pul)
Solvent: cdcl3
Data collected on: Jul 1 2015
14
COOEt
COOEt
160
140
120
100
80
60
40
20
ppm

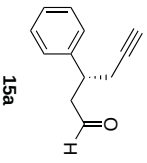


Sample Name:
FM-VIII-238
Data Collected on:
vnmr13-vnmrs400
Archive directory:

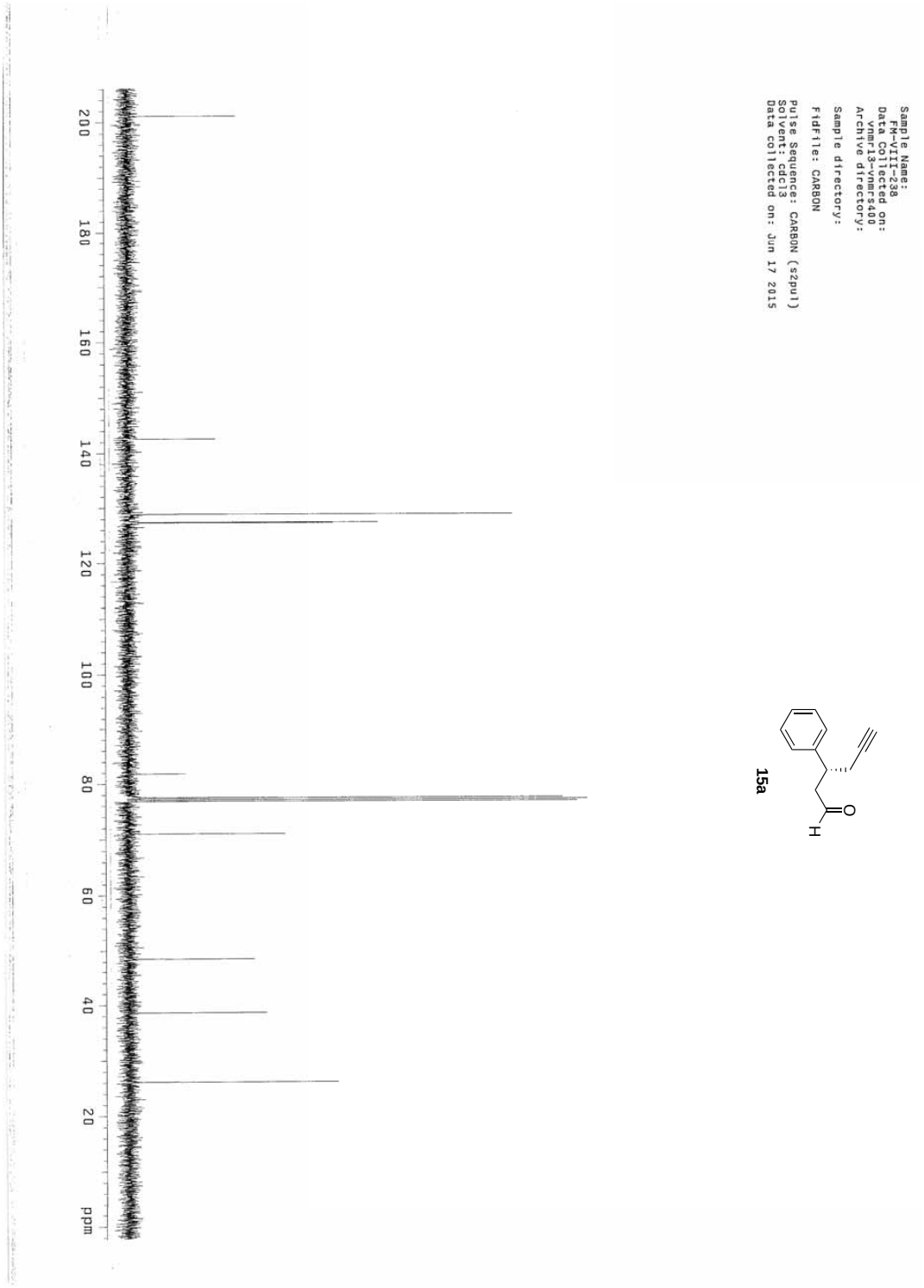
Sample directory:

FidFile: PROTON

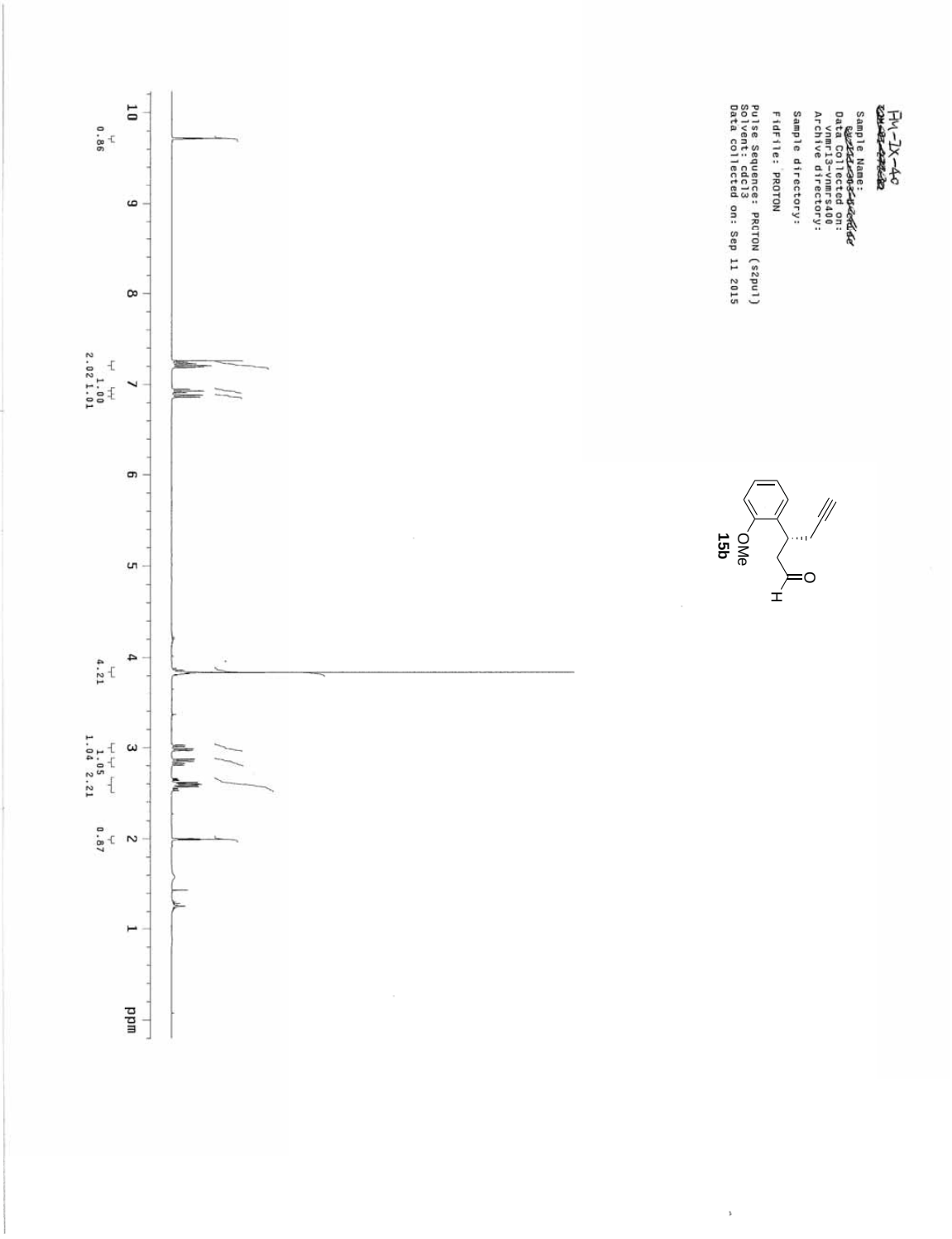
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 17 2015

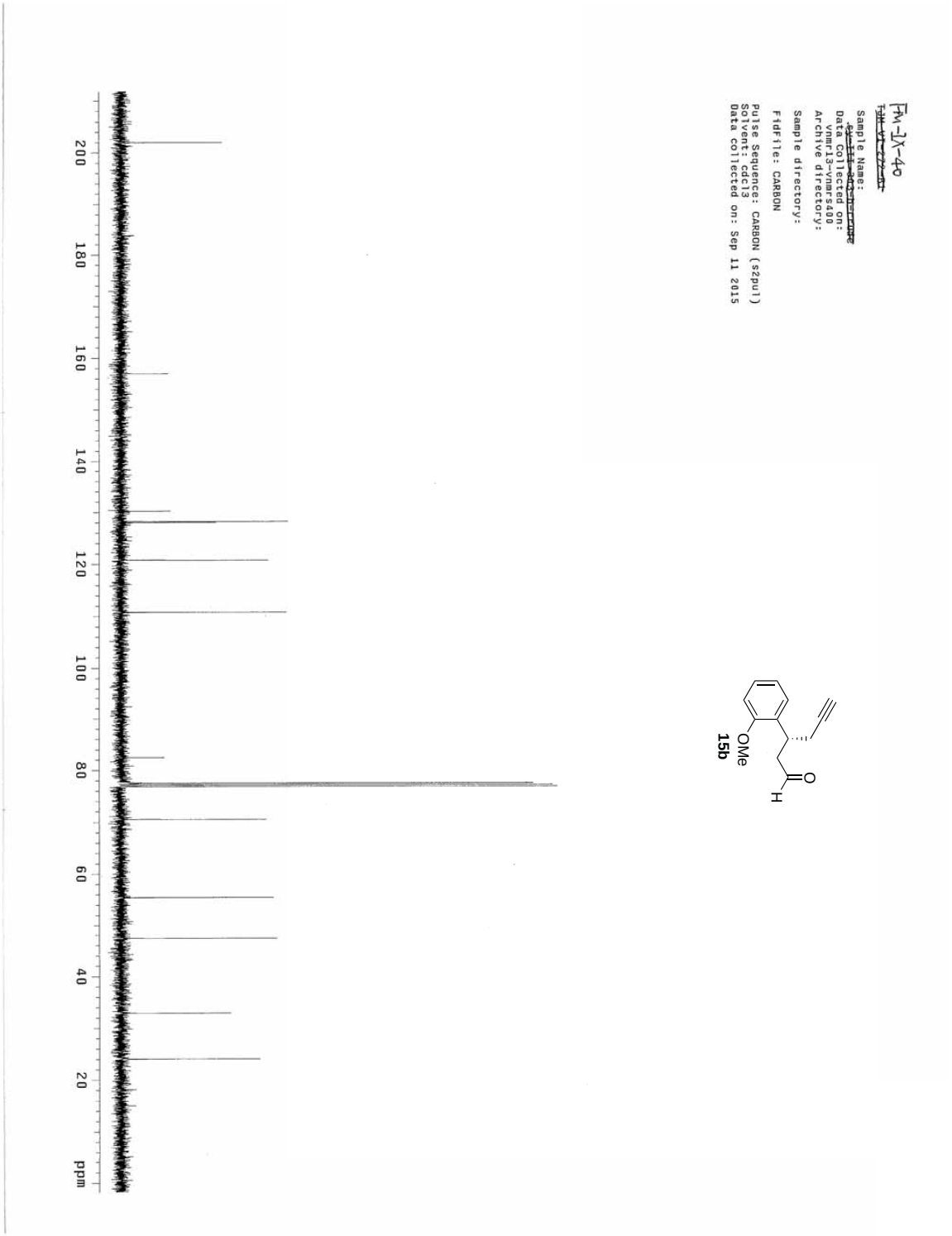


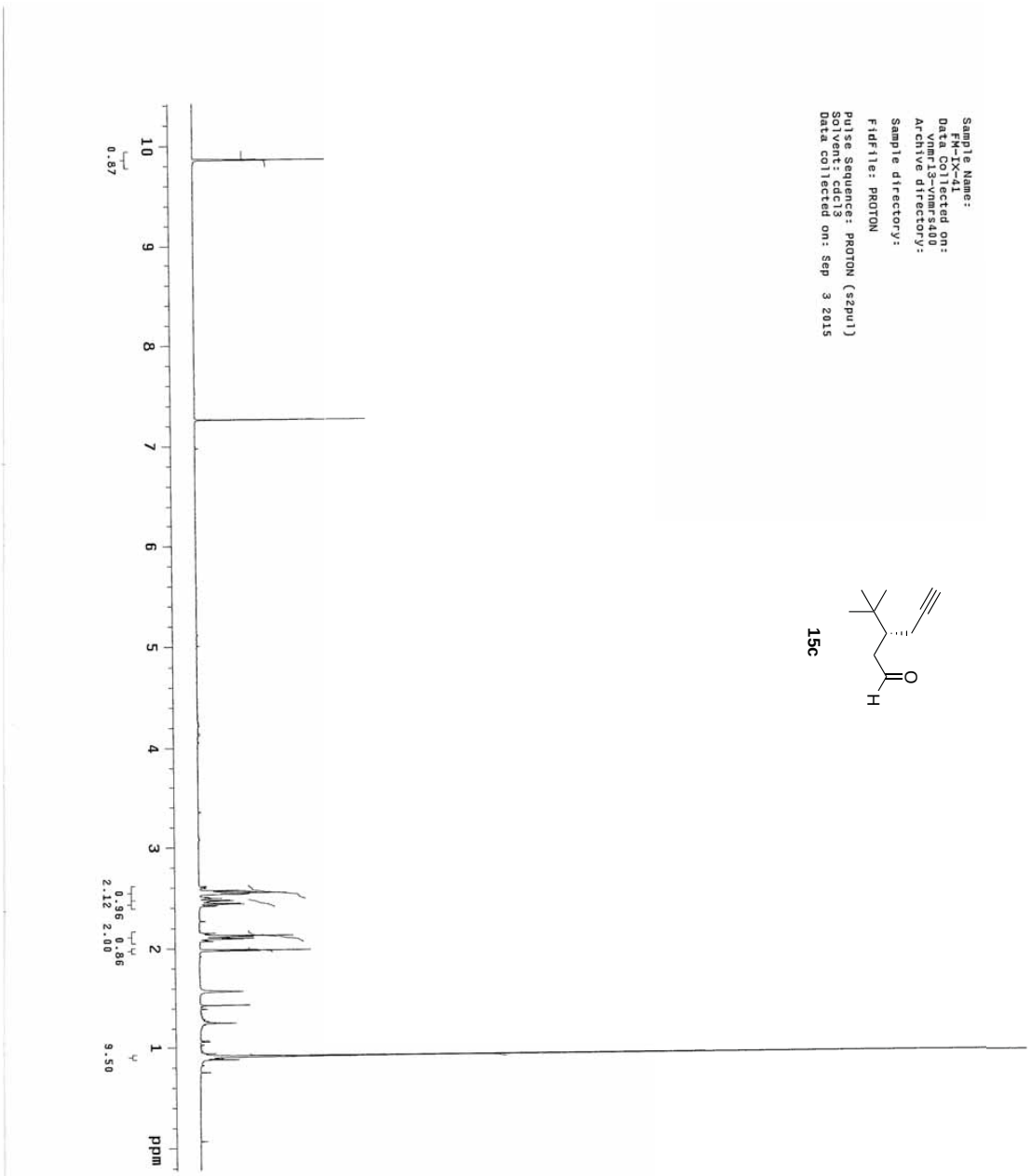
15a

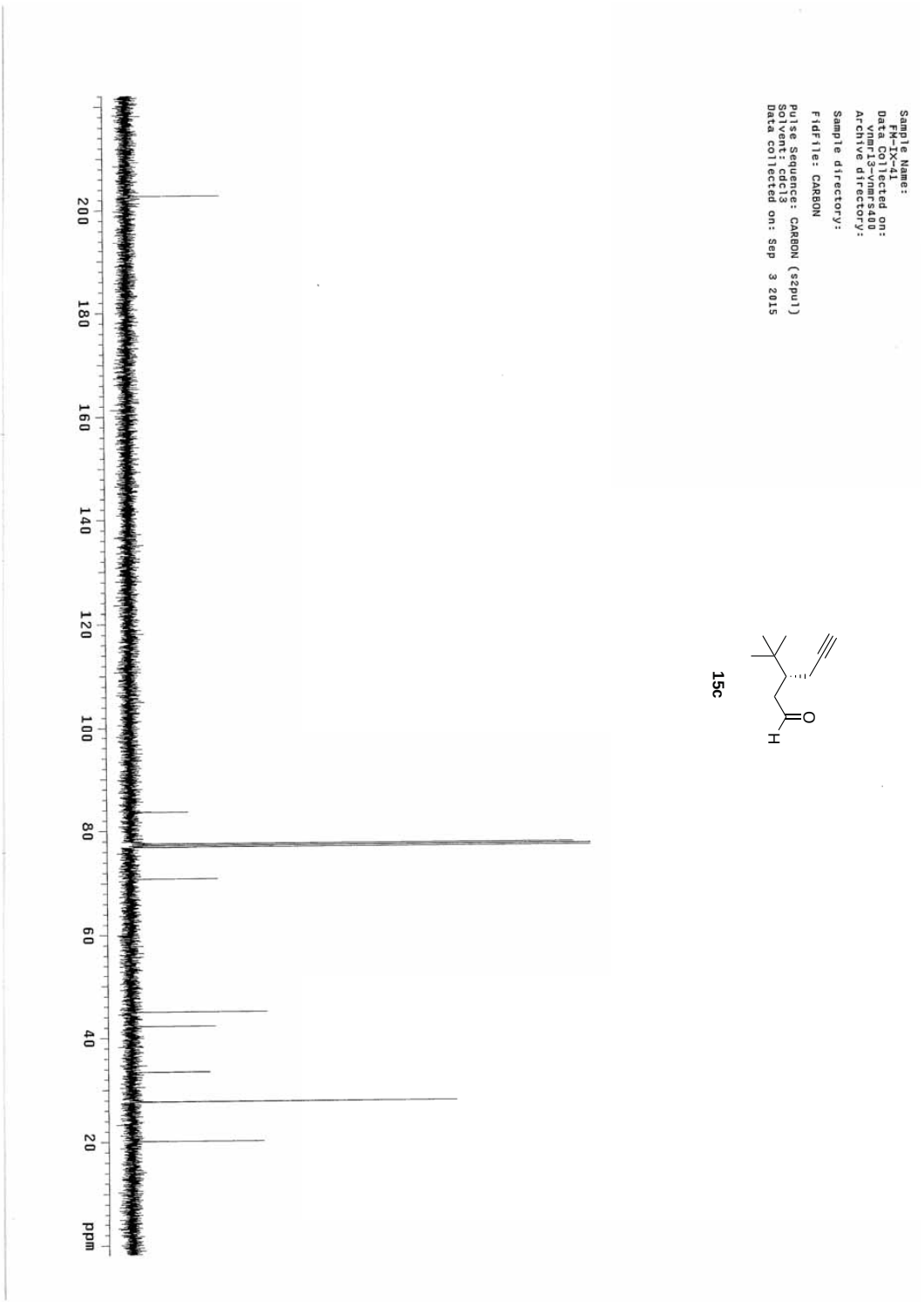

Sample Name:
FM-VIII-238
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 17 2015
200
180
160
140
120
100
80
60
40
20
ppm

15a

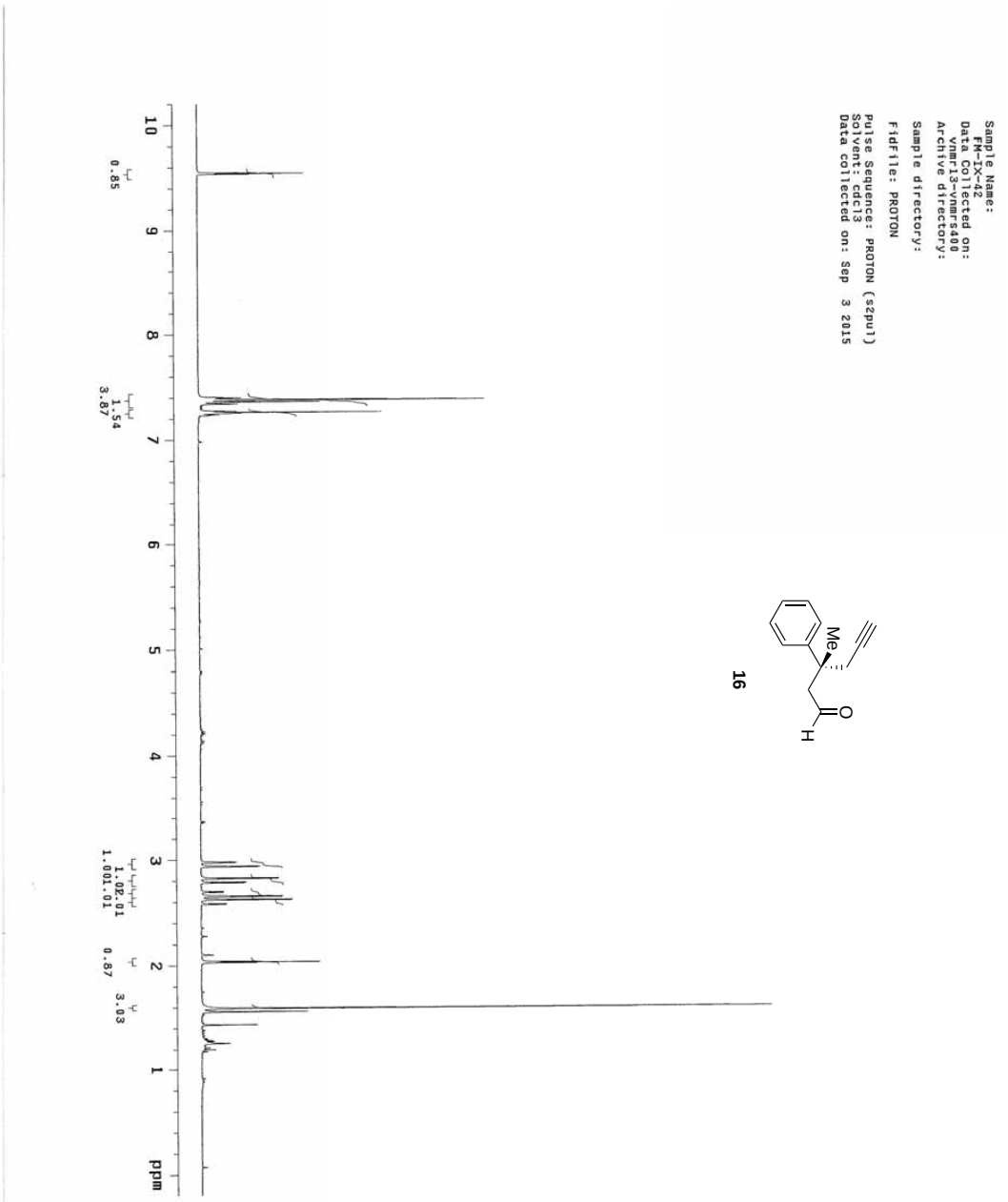

FM-IX-40
Sample Name:
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PRCTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 11 2015
OMe
15b
O
H
ppm

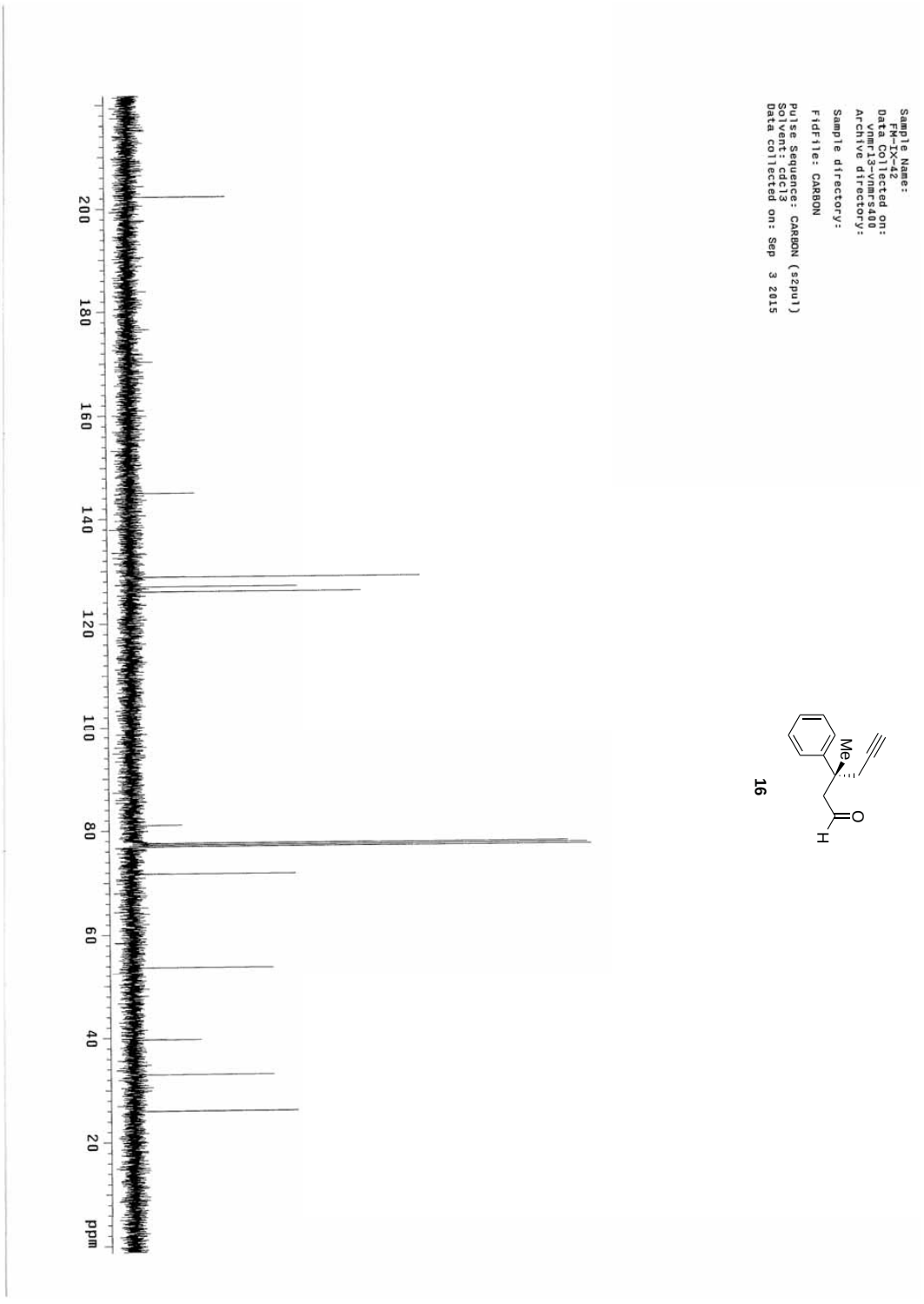

FW-JX-40
Sample Name:
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
F1dFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 11 2015
OMe
15b
O
H
200
180
160
140
120
100
80
60
40
20
ppm


Sample Name:
FM-IX-41
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 3 2015
15c
O
H
10
9
8
7
6
5
4
3
2
1
ppm
0.87
0.96
0.86
2.12
2.00
9.50


Sample Name:
FM-IX-41
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 3 2015
200
180
160
140
120
100
80
60
40
20
ppm

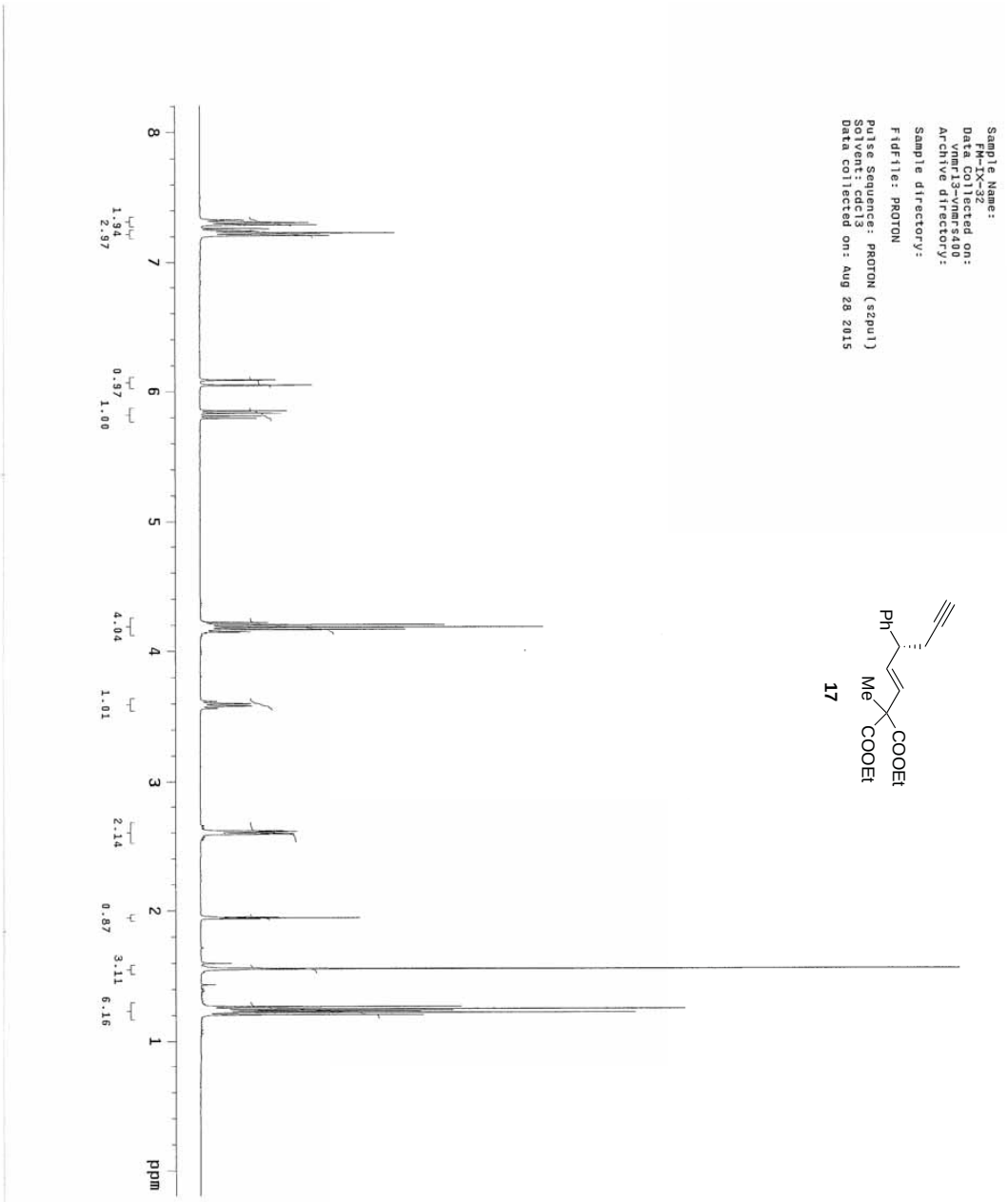
15c

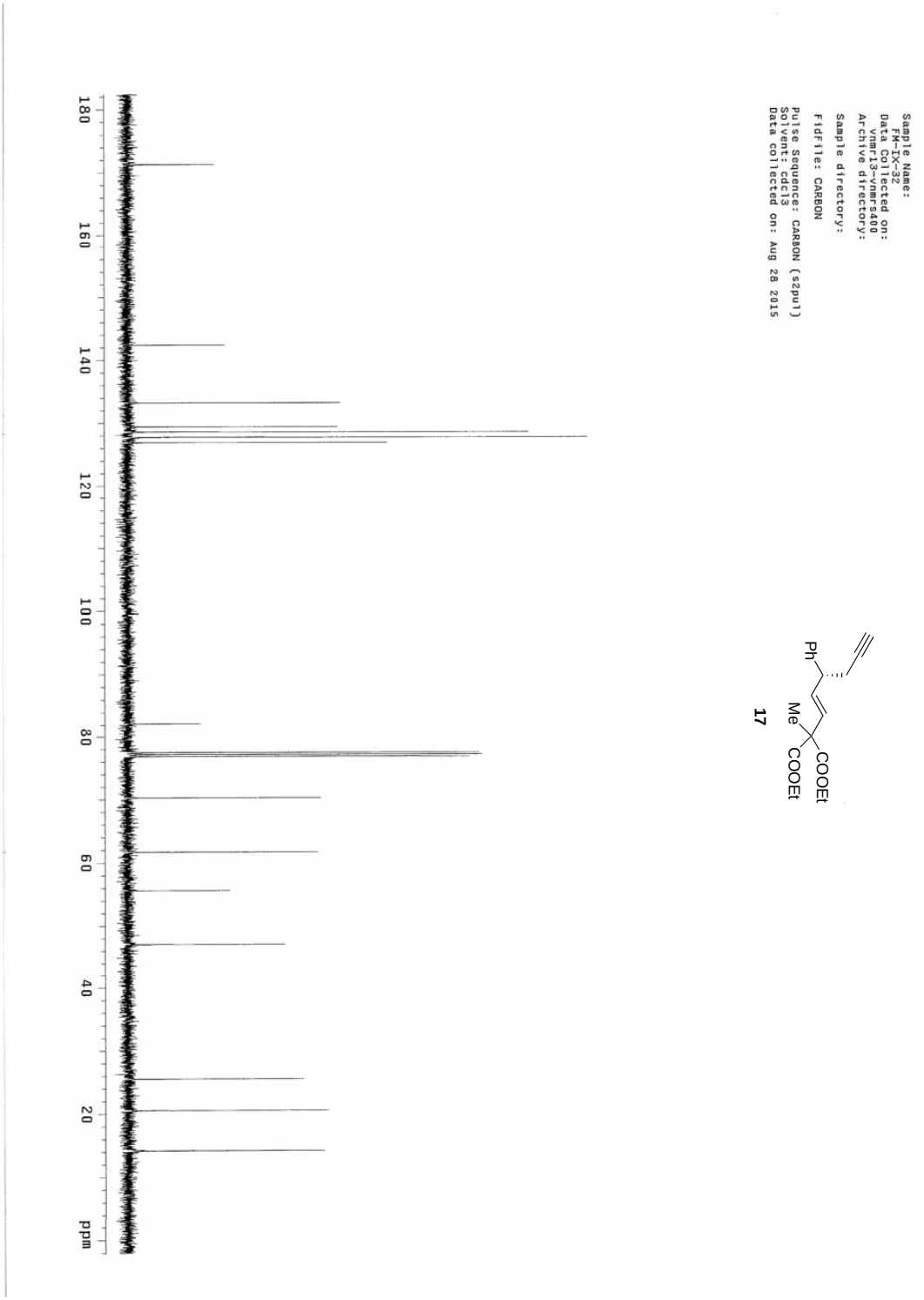

Sample Name:
FM-IX-42
Data Collected on:
vnmrj3-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 3 2015
Me
O
H
16
10
9
8
7
6
5
4
3
2
1
ppm
0.85
1.54
3.87
1.00
2.01
1.00
1.01
0.87
3.03

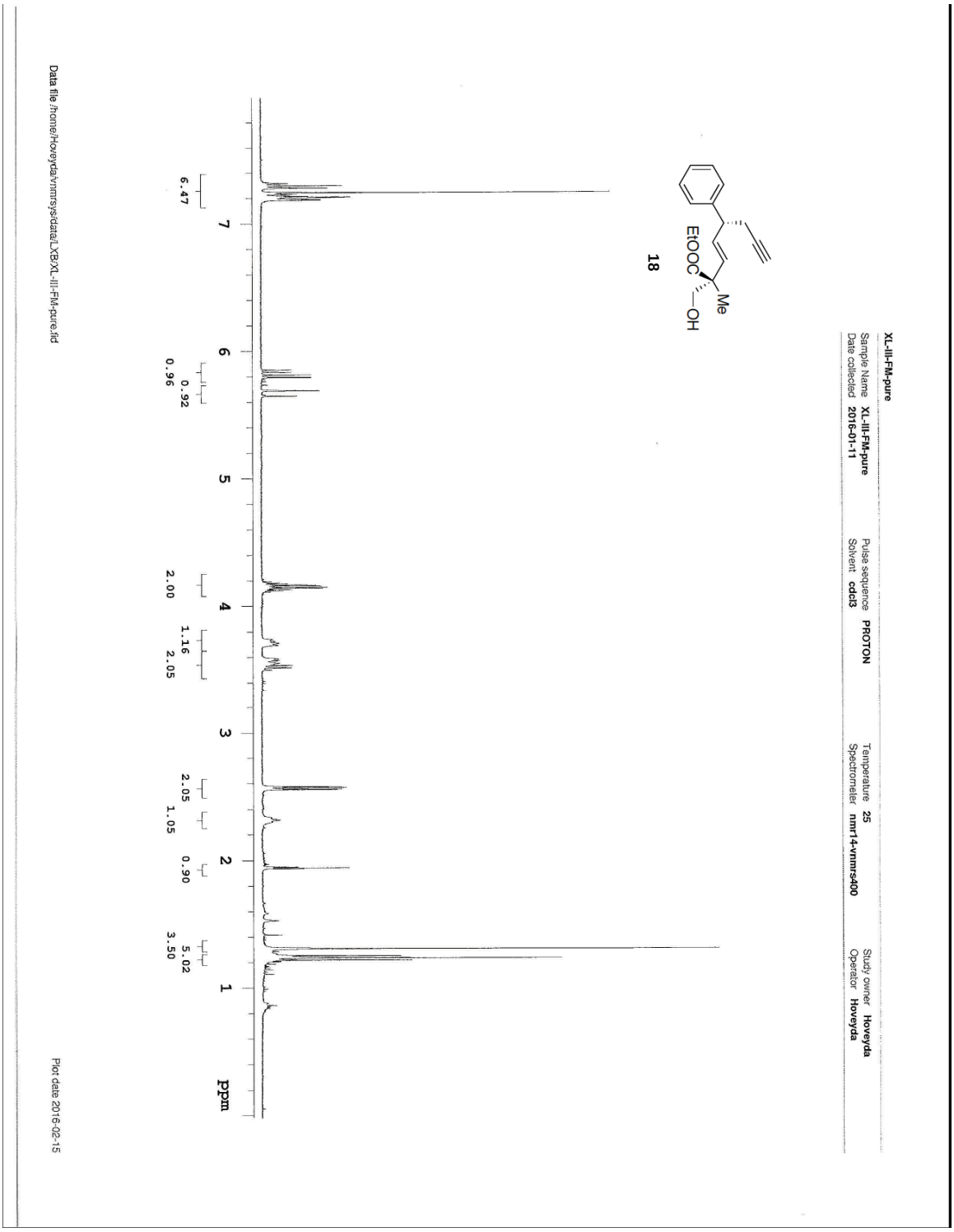

Sample Name:
FM-IX-42
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
Fidfile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 3 2015
200
180
160
140
120
100
80
60
40
20
ppm

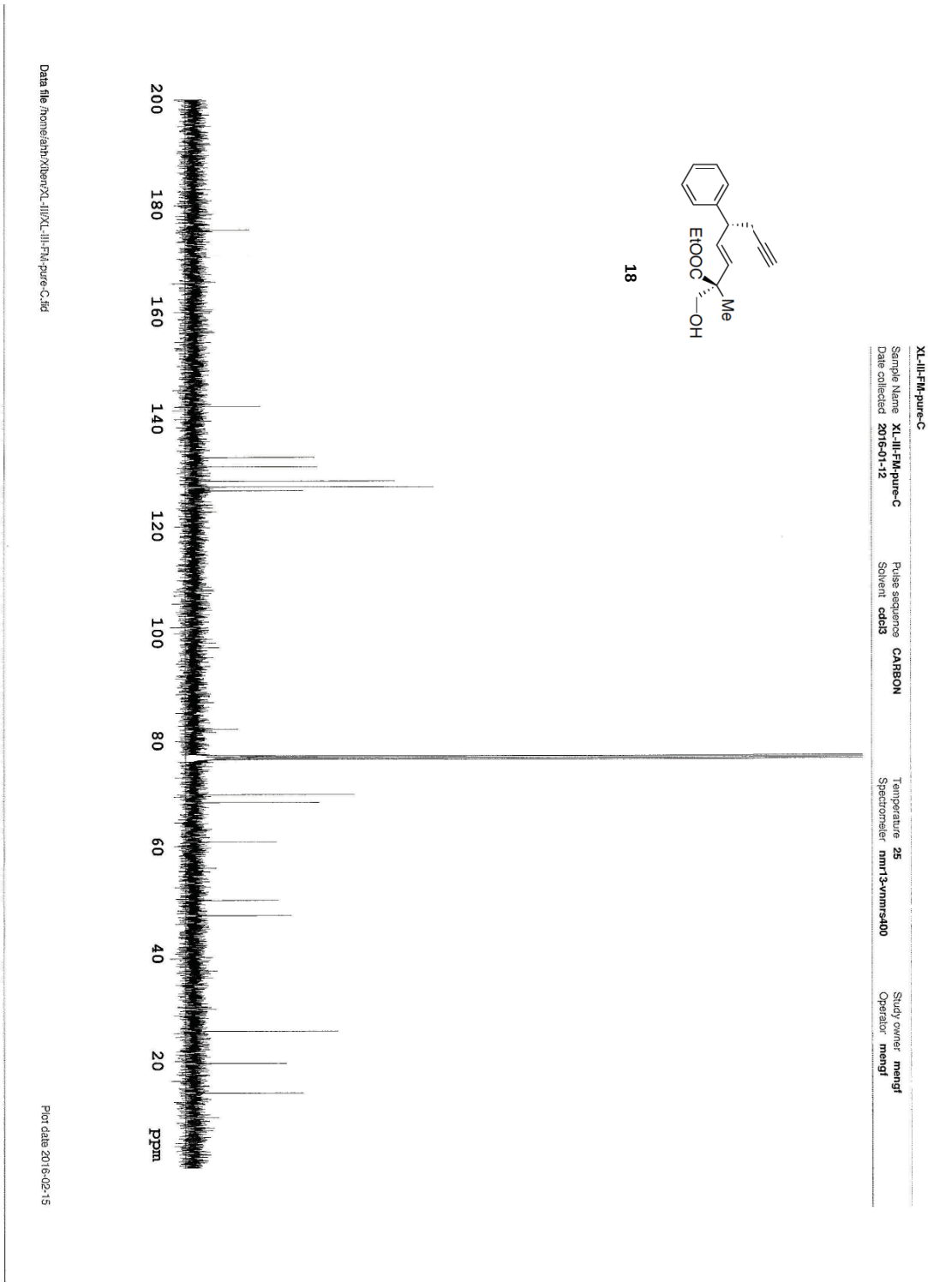
16

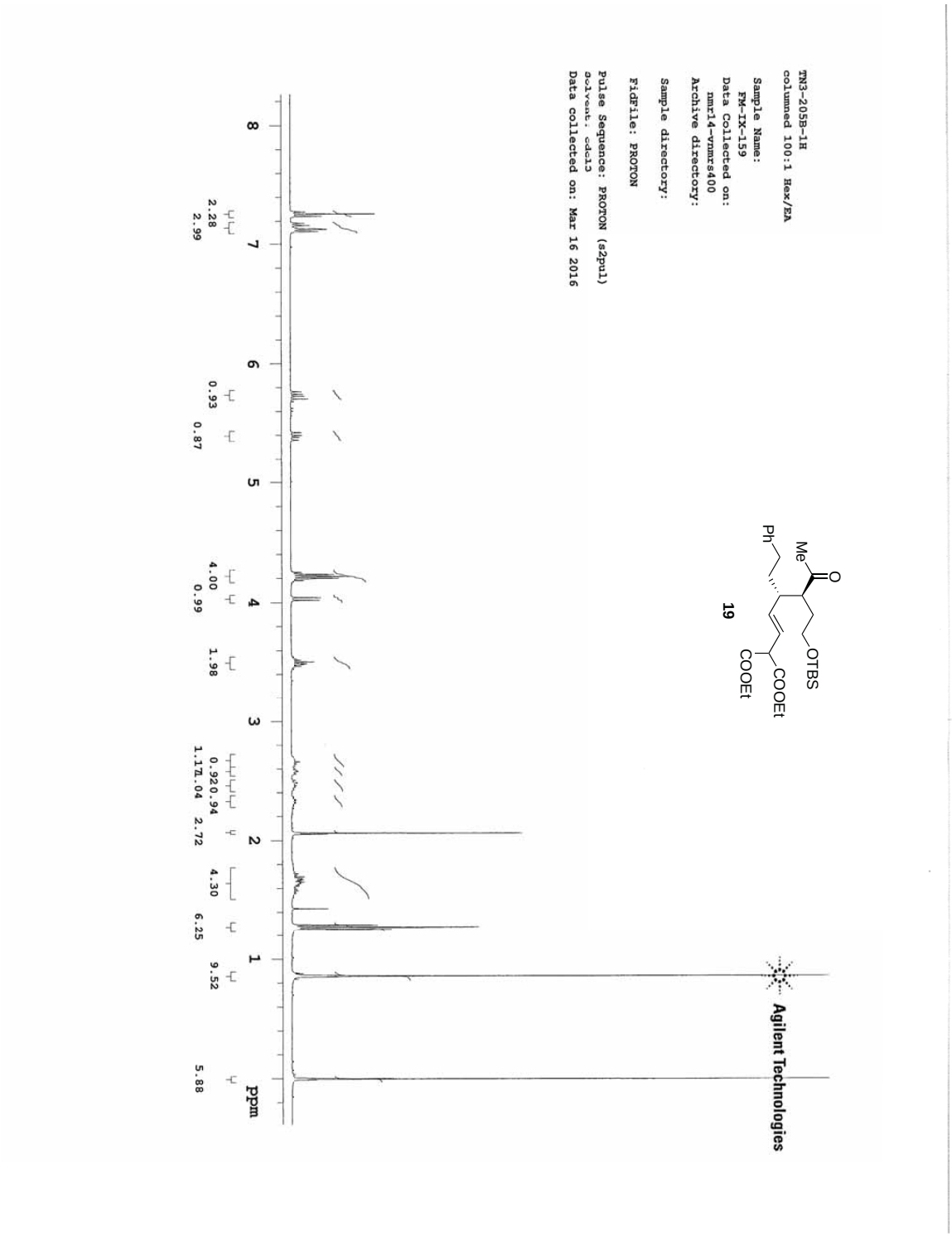
Me
O
H


Sample Name:
FM-IX-32
Data Collected on:
vnmrs3-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 28 2015
Ph
Me
COOEt
COOEt
17
8
7
6
5
4
3
2
1
ppm
1.94
2.97
0.97
1.00
4.04
1.01
2.14
0.87
3.11
6.16


Sample Name:
FM-IX-32
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (szpul)
Solvent: cdcl3
Data collected on: Aug 28 2015
Ph
Me
COOEt
COOEt
17
180
160
140
120
100
80
60
40
20
ppm


XL-III-FM-pure
Sample Name XL-III-FM-pure
Date collected 2016-01-11
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr14-vnmrs400
Study owner Hoveyda
Operator Hoveyda
EtOOC
Me
OH
18
6.47
0.92
0.96
2.00
1.16
2.05
2.05
1.05
0.90
5.02
3.50
7
6
5
4
3
2
1
ppm
Data file /home/Hoveyda/vnmrsys/data/LXB/XL-III-FM-pure.fid
Plot date 2016-02-15


XL-III-FM-pure-C
Sample Name XL-III-FM-pure-C
Date collected 2016-01-12
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
EtOOC
Me
OH
18
200
180
160
140
120
100
80
60
40
20
ppm
Data file /home/ahh/Xiben/XL-III/XL-III-FM-pure-C.fid
Plot date 2016-02-15


TM3-205B-1H
columned 100:1 Hex/EA
Sample Name:
FM-IX-159
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
solvent: cdcl3
Data collected on: Mar 16 2016
Me
O
Ph
OTBS
COOEt
COOEt
19
Agilent Technologies
ppm
8
7
6
5
4
3
2
1
2.28
2.99
0.93
0.87
4.00
0.99
1.98
0.92
0.94
1.17
1.04
2.72
4.30
6.25
9.52
5.88

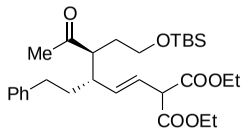
CG01-48-1H
crude

Sample Name:
FM-IX-159
Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 16 2016



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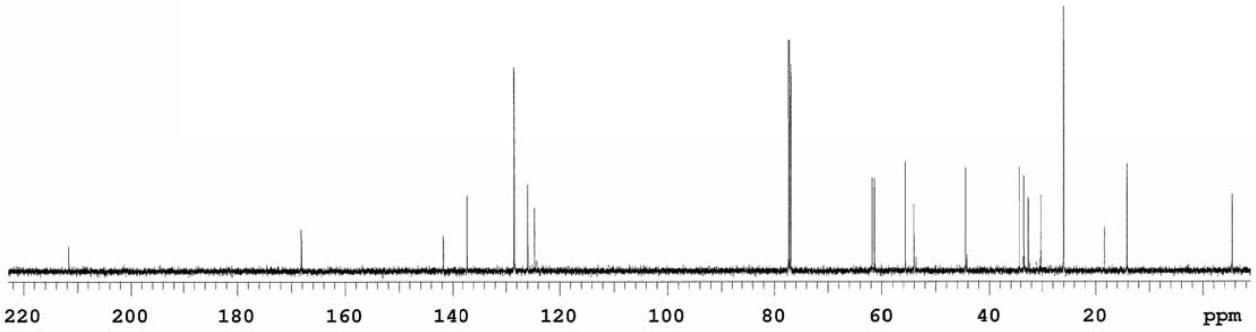
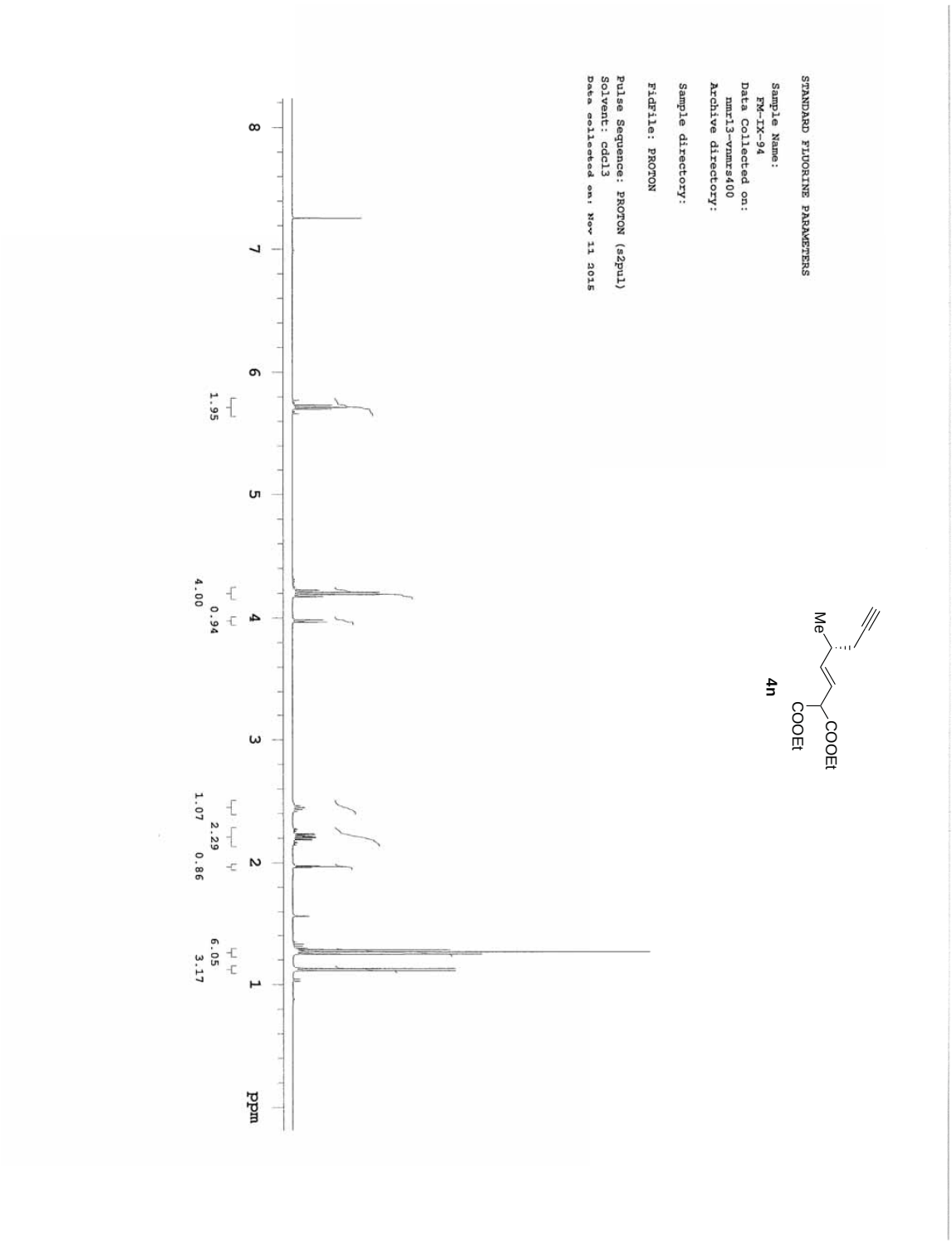
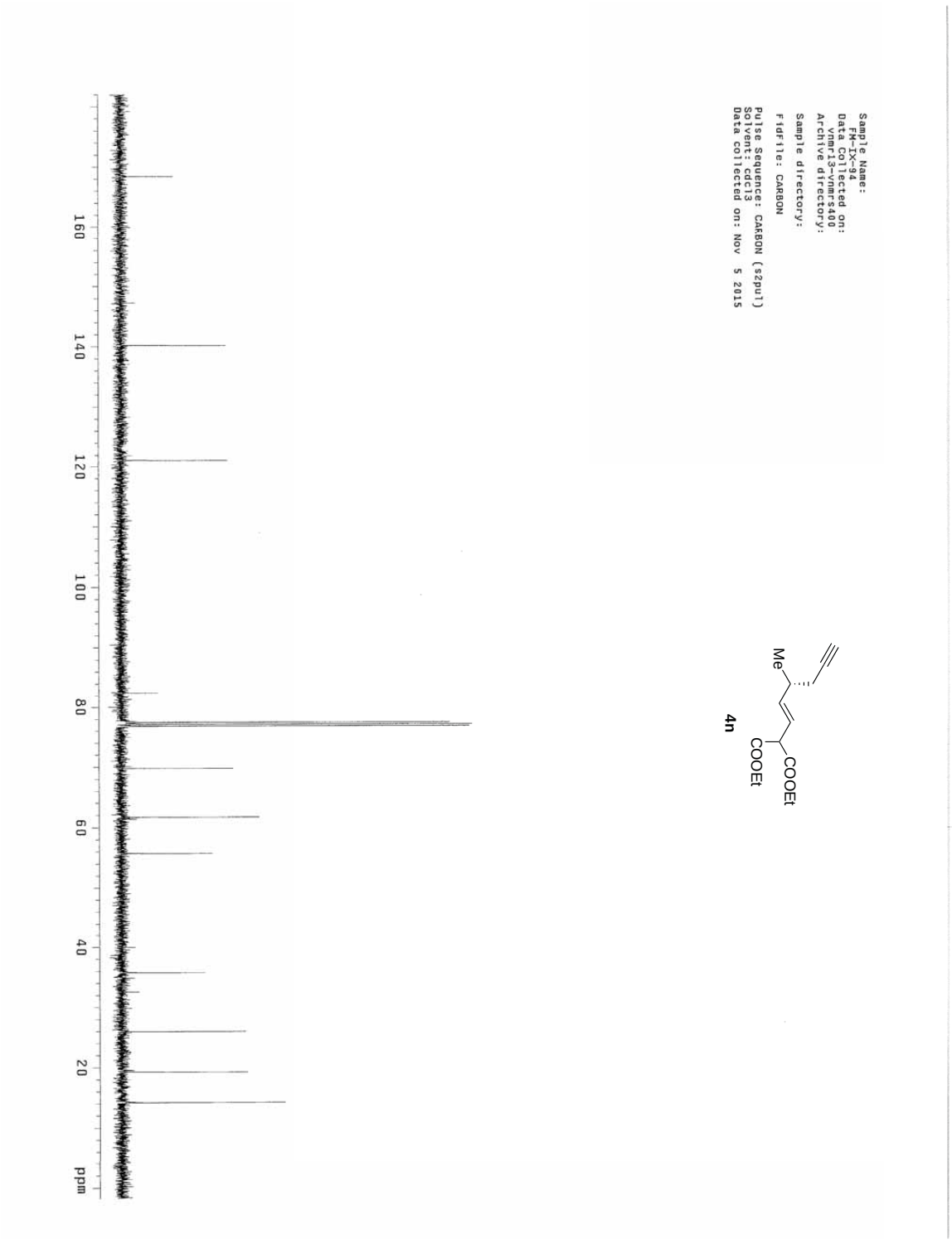
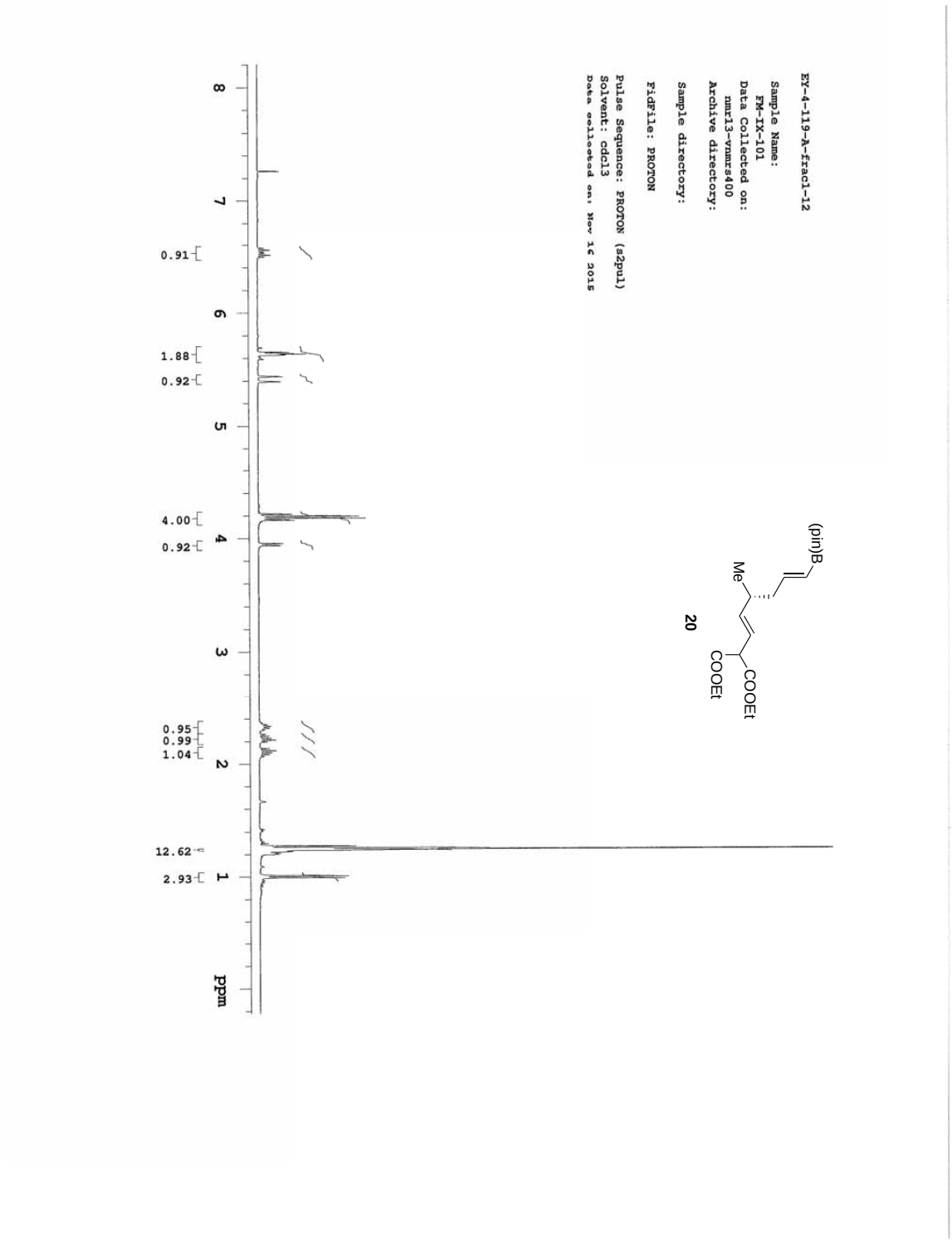
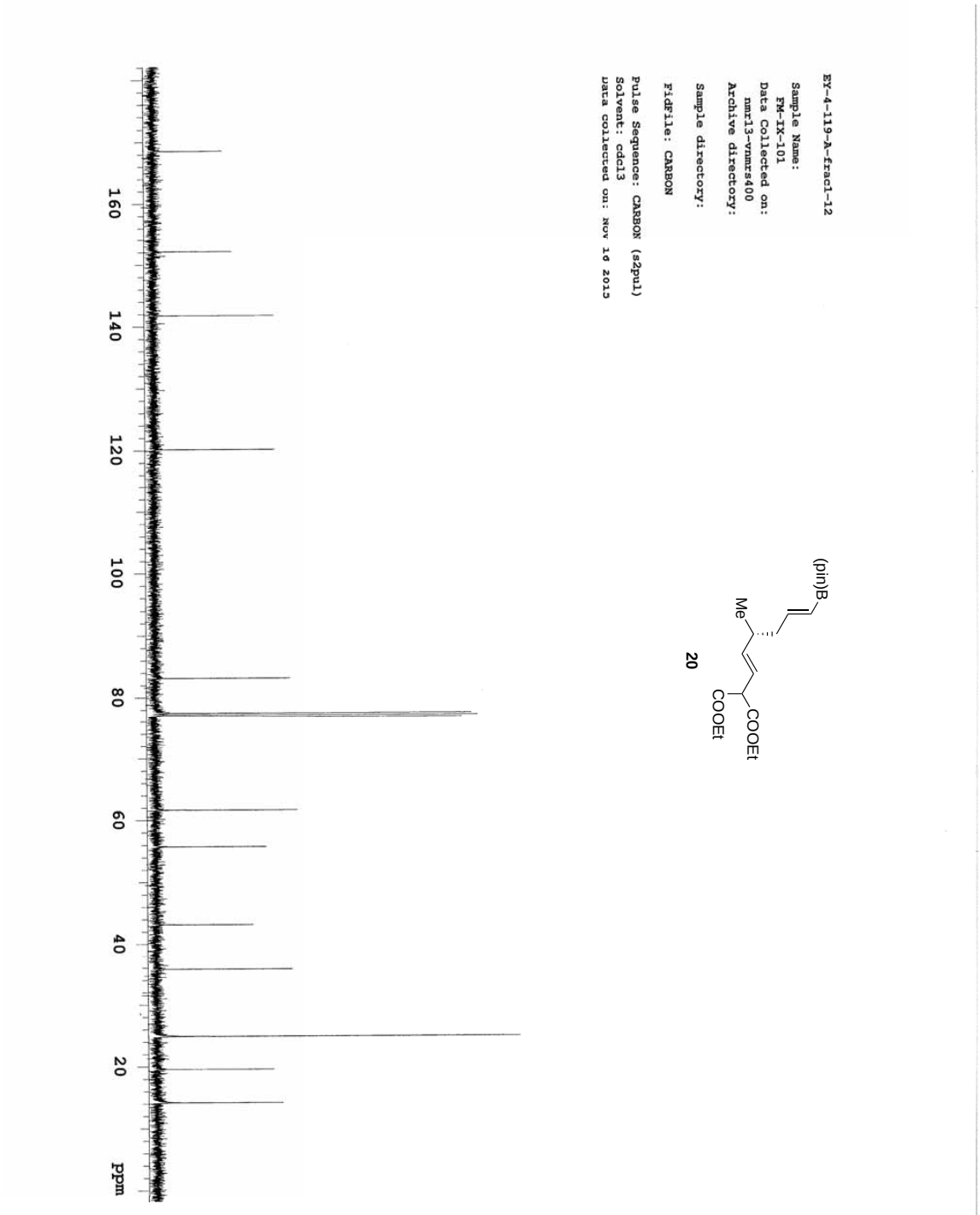
Agilent Technologies

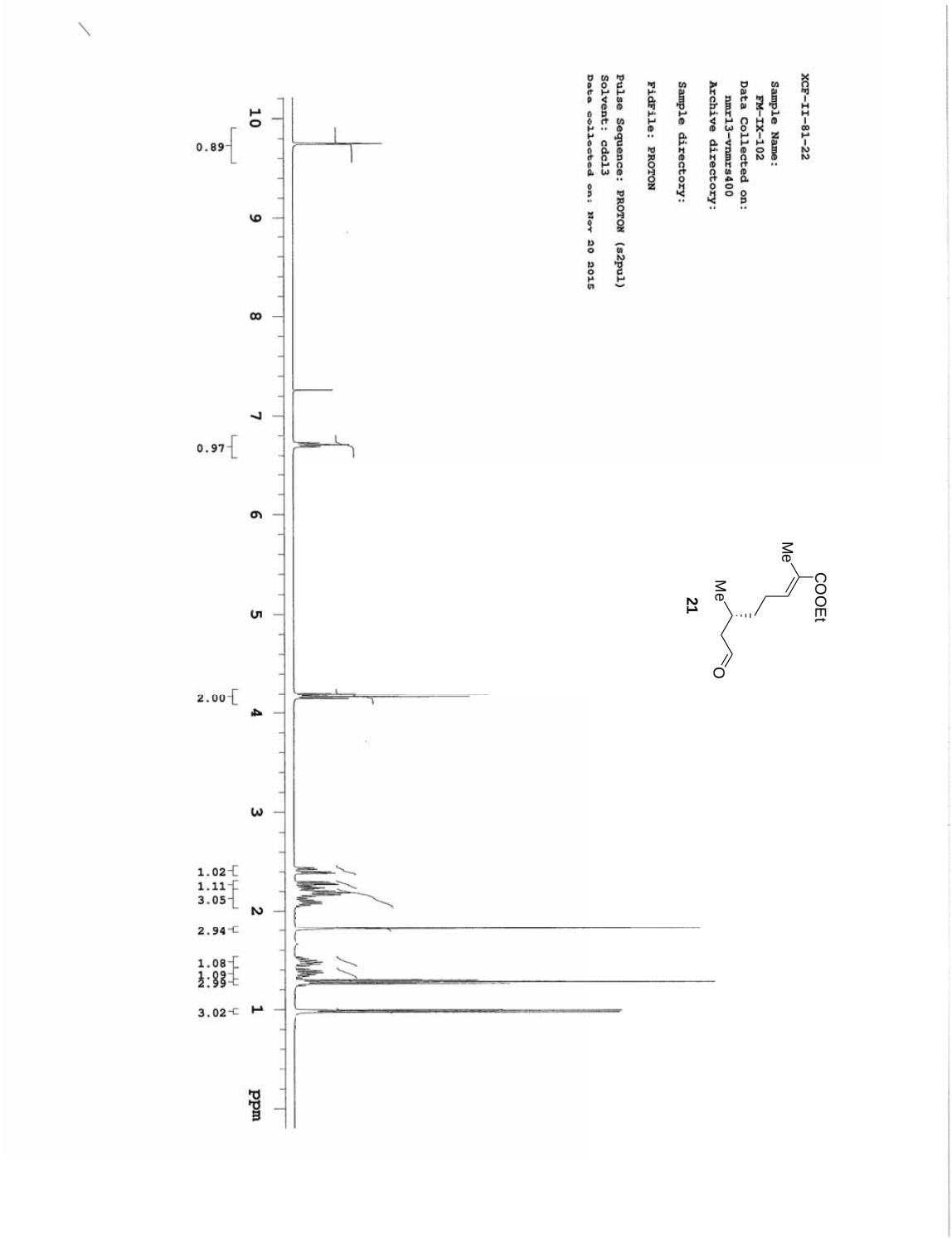


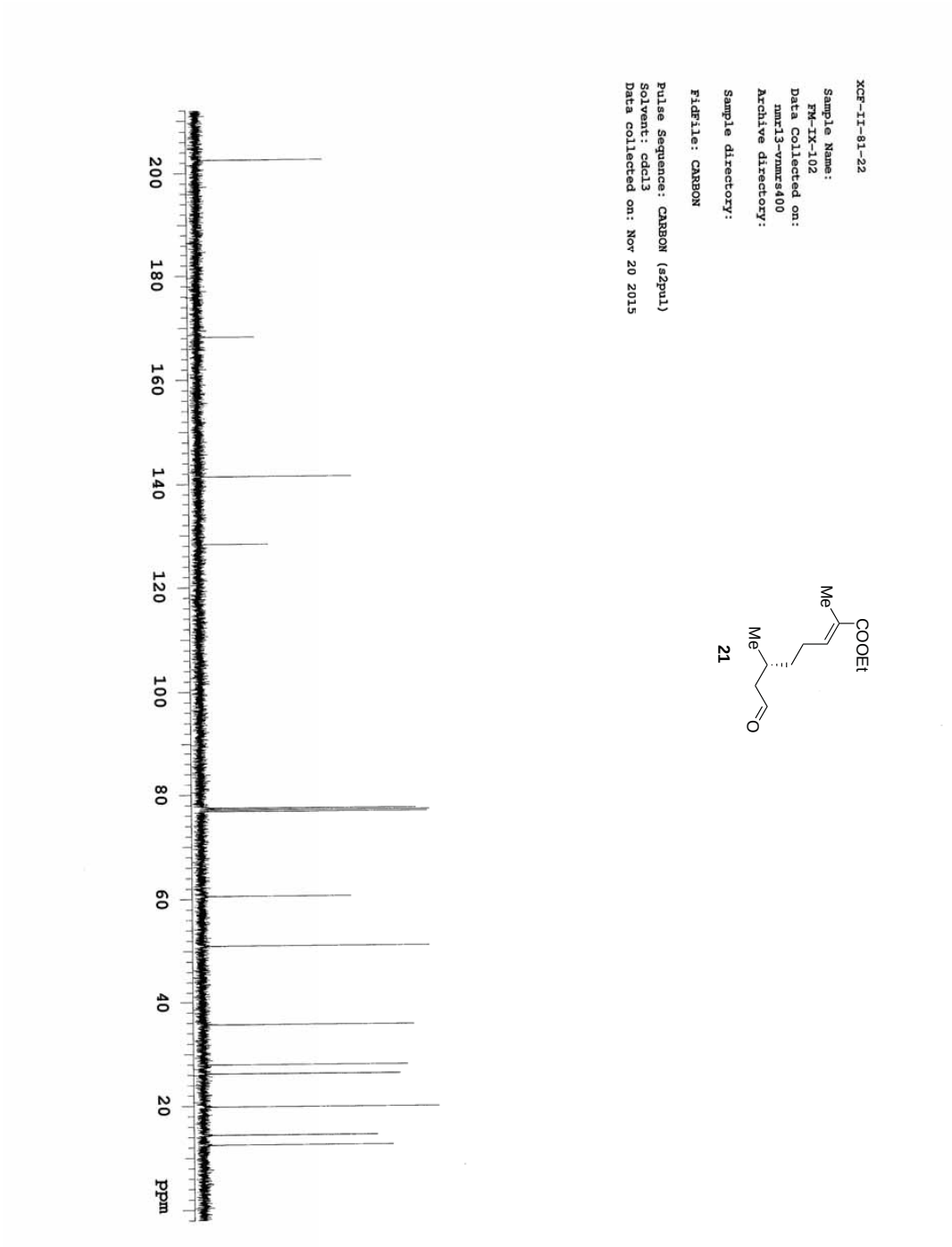

STANDARD FLUORINE PARAMETERS
Sample Name:
FM-IX-94
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 11 2015
Me
COOEt
COOEt
4n
8
7
6
5
4
3
2
1
ppm
1.95
4.00
0.94
1.07
2.29
0.86
6.05
3.17

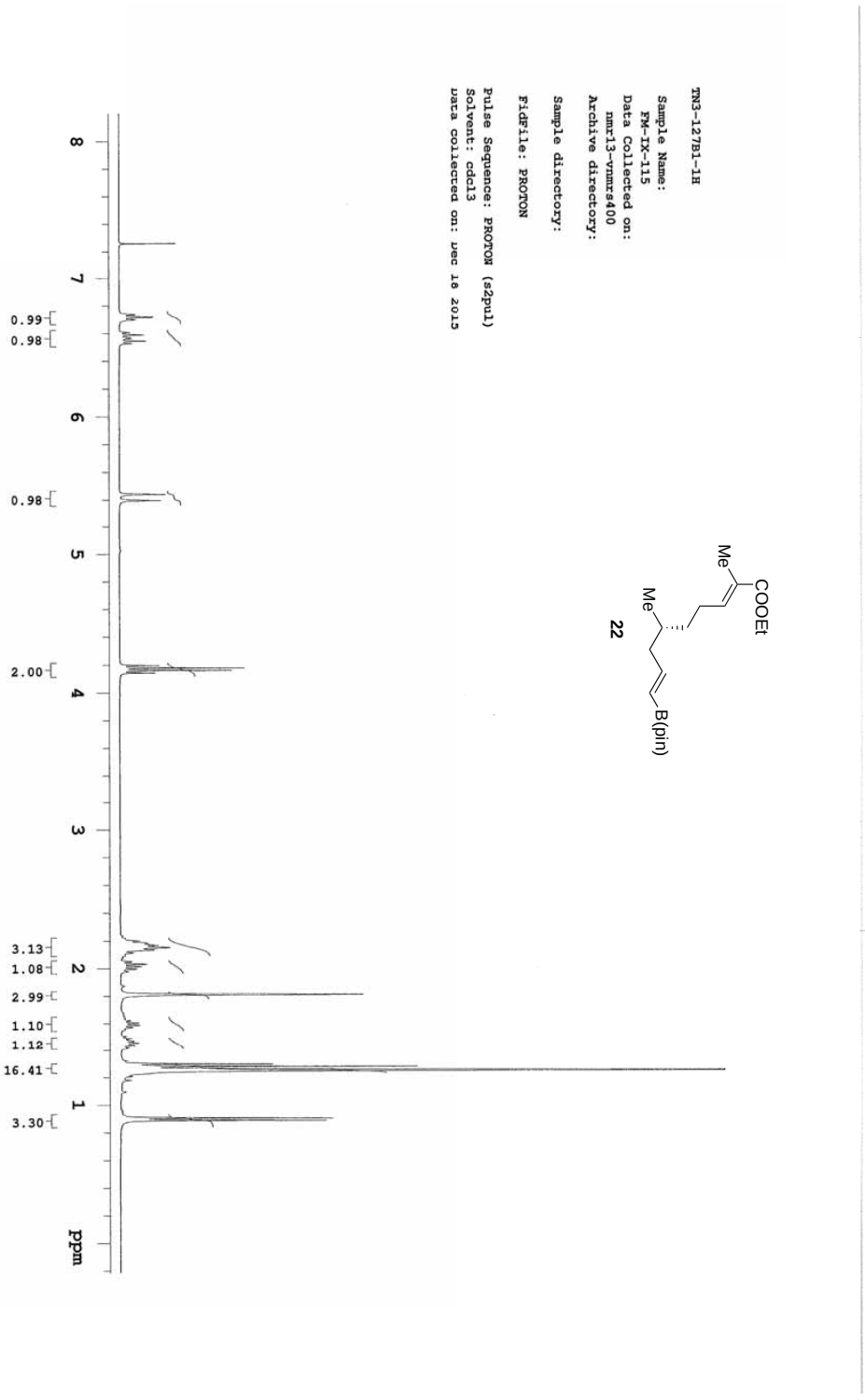

Sample Name:
FM-IX-94
Data Collected on:
vnmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 5 2015
Me
COOEt
COOEt
4n
160
140
120
100
80
60
40
20
ppm


EY-4-119-A-frac1-12
Sample Name:
FM-IX-101
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 16 2015
(pin)B
Me
COOEt
COOEt
20
0.91
1.88
0.92
4.00
0.92
0.95
0.99
1.04
12.62
2.93
ppm


EY-4-119-A-frac1-12
Sample Name:
FM-IX-101
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 16 2015
(pin)B
Me
COOEt
COOEt
20
160
140
120
100
80
60
40
20
ppm


XCF-II-81-22
Sample Name:
FM-IX-102
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 20 2015
Me
COOEt
Me
O
21
0.89
0.97
2.00
1.02
1.11
3.05
2.94
1.08
1.09
2.99
3.02
10
9
8
7
6
5
4
3
2
1
ppm


xcf-II-81-22
Sample Name:
FM-IX-102
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 20 2015
Me
COOEt
Me
O
21
200
180
160
140
120
100
80
60
40
20
ppm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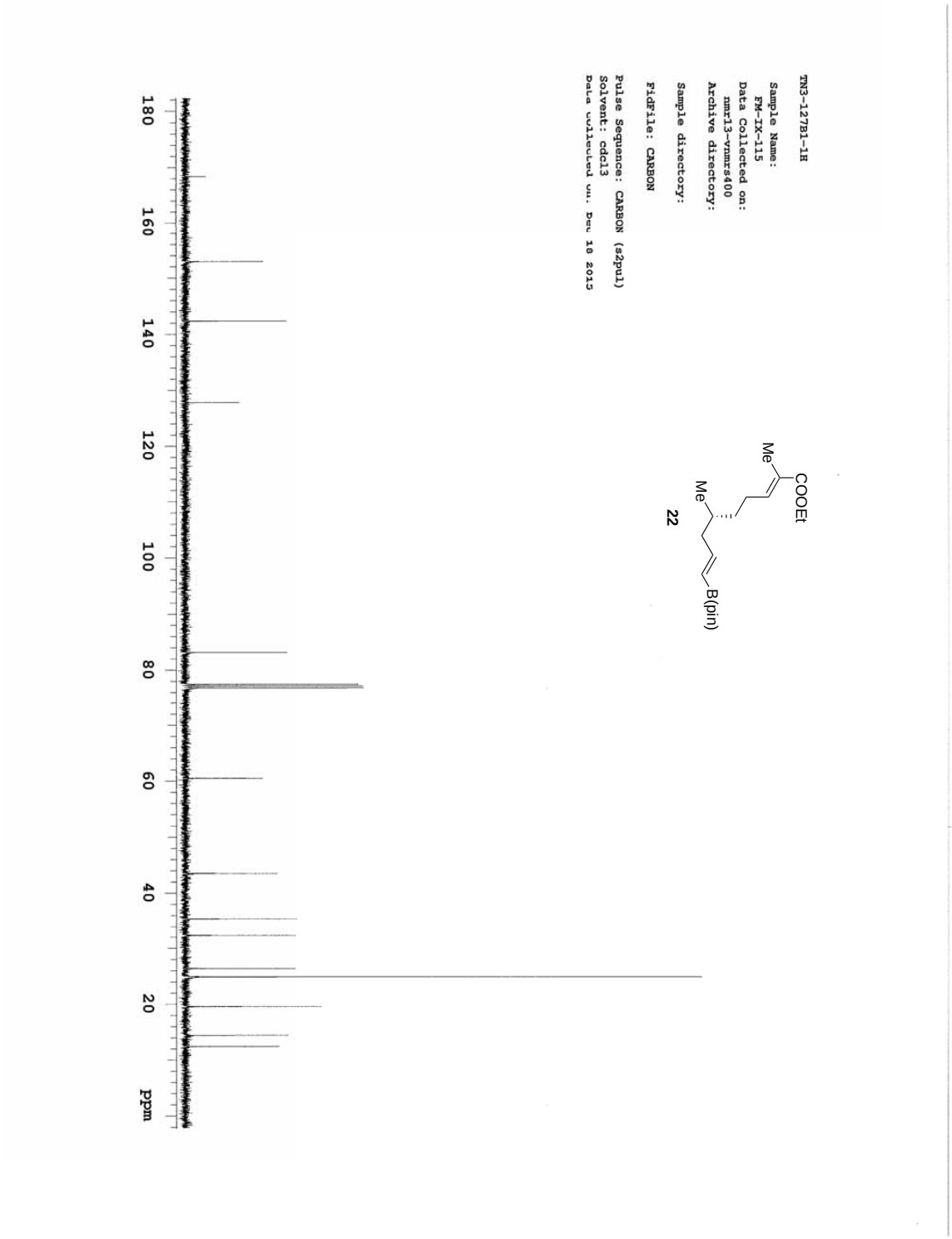
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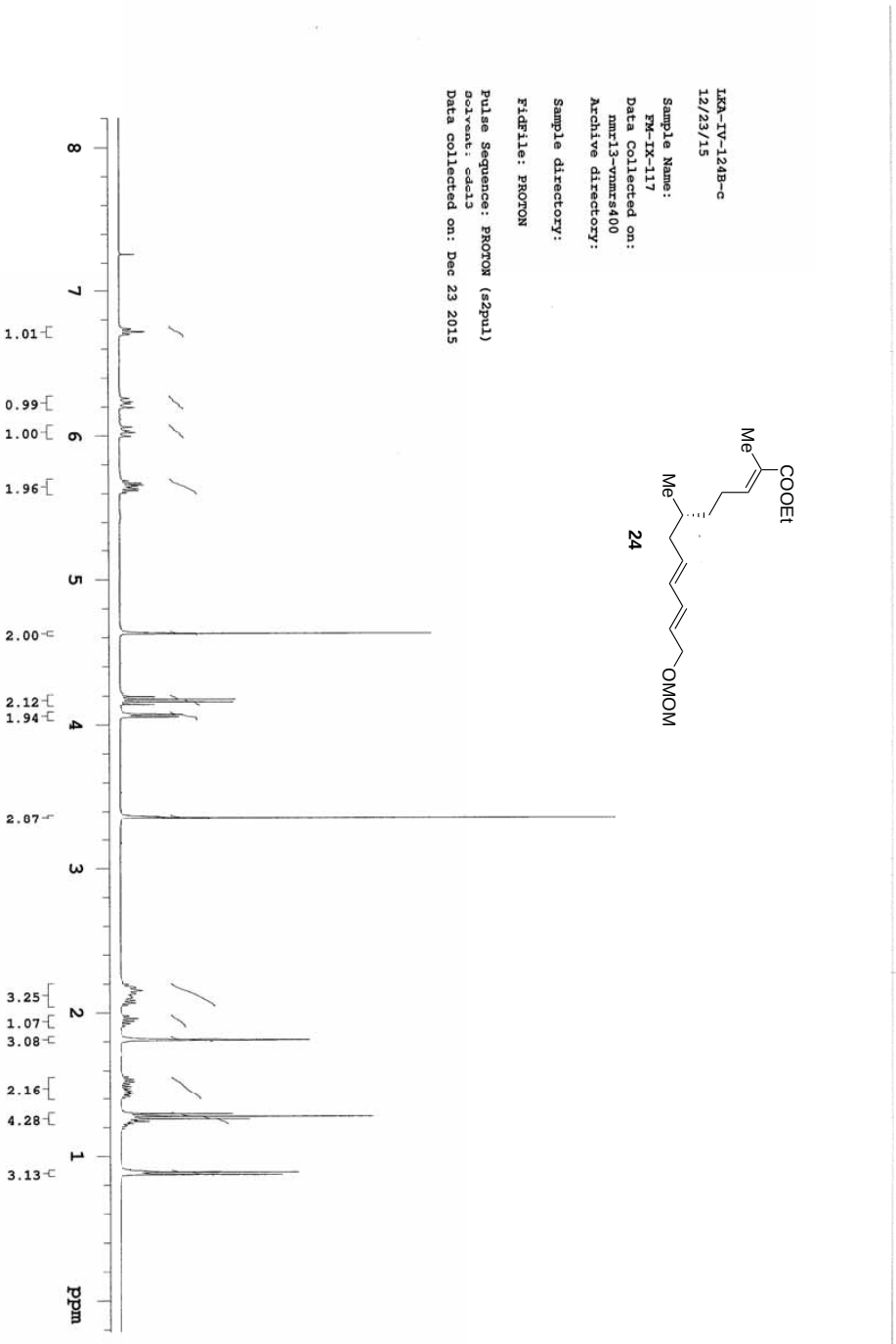
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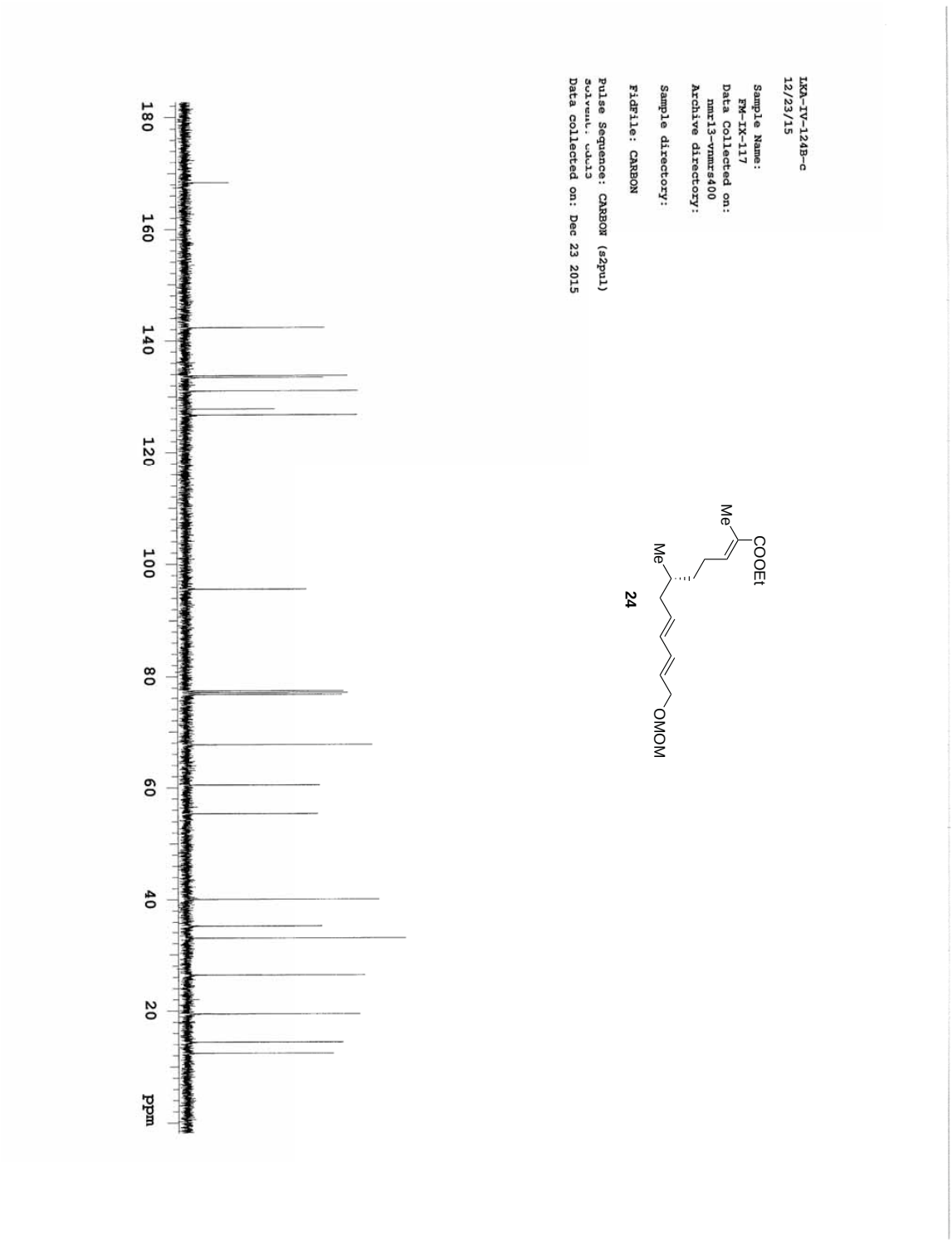
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Archive directory:
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FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 23 2015
Me
COOEt
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OMOM
24
180
160
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ppm

4. Density Functional Theory (DFT) Calculations

DFT computations[12] were performed with the Gaussian 09 suite of programs[13]. Geometries were optimized by application of the ωB97XD[14] functional. The Def2SVP basis set[15] was used for all atoms and the effect of a polar medium (THF) was modeled by means of an integral equation formalism variant of the polarizable continuum model (IEFPCM)[16]. Stationary points were probed through vibrational analysis and Gibbs free energy corrections were performed under standard conditions (298.15 K, 1.0 atm). Single point energy calculations at the geometries optimized at the ωB97XD/Def2SVP$_{THF(PCM)}$ level have been performed with a range of density functionals that account for dispersion[17] and the larger Def2TZVPP[15] basis set using the SMD solvation model[18] in THF. Since the correct density functional is not known we tested several state of the art approaches that have been developed over the past decade[12]: ωB97XD[14] and M06[19], MN12SX[20], MN12L[20], M06L[19], BP86-D3BJ[21,12b] and PBE0-D3BJ[22,12b]). Gibbs free energies are provided in Section 5 and a file for convenient

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(12) For reviews on the application of DFT calculations to transition metal chemistry, see: (a) Cramer, C. J. & Truhlar, D. G. *Phys. Chem. Chem. Phys.* **11**, 10757–10816 (2009). (b) Grimme, S., Ehrlich, S. & Goerigk, L. *J. Comp. Chem*. **32**, 1456–1465 (2011). (c) Peverati, R. & Truhlar, D. G. *Phil. Trans. R. Soc. A* **372**:20120476 (2014).

(13) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision **D.01***, Gaussian, Inc., Wallingford CT, **2009**.

(14) Chai, J.-D. & Head-Gordon, M. *Phys. Chem. Chem. Phys.*, **10**, 6615–6620 (2008).

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

(16) Scalmani, G. & Frisch, M. J. *J. Chem. Phys.* **132**, 114110 (2010).

(17) 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) Khan, R. K. M., Torker, S. & Hoveyda, A. H. *J. Am. Chem. Soc.* **136**, 14337–14340 (2014).

(18) Marenich, A. V., Cramer, C. J. & Truhlar, D. G. *J. Phys. Chem. B* **113**, 6378–6396 (2009).

(19) Zhao, Y., & Truhlar, D. G. *Acc. Chem. Res.* **41**, 157–167 (2008).

(20) Peverati, R., Truhlar, D. G. *Phys. Chem. Chem. Phys.* **14**, 16187–16191 (2012).

(21) (a) Becke, A. D. *Phys. Rev. A: At., Mol., Opt. Phys.* **38**, 3098–3100 (1988). (b) Perdew, J. P. & Yue, W. *Phys. Rev. B* **33**, 8800–8802 (1986).

(22) Adamo, C. & Barone, V. *J. Chem. Phys.* **110**, 6158–6169 (1999).

viewing of computed geometries with the program Mercury 3.3 is appended as separate "coordinates.xyz" file in Section 6[23].

Nomenclature

We have adopted the following nomenclature to label the structures investigated through DFT calculations:

i. PA and **AA** denote propargyl and allyl addition, respectively.

ii. For ground state complexes we use the sequence **ligand–Cu–nucleophile**. For example, **9d–Cu–allenyl** specifies a linear Cu complex involving ligand **9d** bound to an allenyl group.

iii. For complexes that contain a bound dienoate, we use the sequence **reaction type–ligand$_{bridge}$–structure$_{regioselectivity}$**. For example, **PA–9d$_{Na}$–ts$_{1,6major}$** denotes the transition state for 1,6-addition of a propargyl group leading to the major enantiomer promoted by a Cu complex that is derived from imidazolinium salt **9d** with a sodium bridge toward the substrate carbonyl groups.

iv. The terms **ed** (educt) and **prod** (product), denote ground states on either side of the transition state **ts**, which have been obtained through intrinsic reaction coordinate (IRC) calculations through the use of the L(ocal) Q(uadratic) A(approximation) method and subsequent optimization.[24] Unlike the transition state structures **ts**, for which extensive screening of the conformational space has been performed (Figures S15-1 to S15-9), the reported structures for **ed** and **prod** might not represent the lowest energy conformers. In cases where the educt (**ed)** is a π-complex wherein the double bond between the α and β carbon atoms of the substrate is bound to Cu, the term **pc** (π-complex) is used instead.

Investigation of different chelate geometries (Fig. S1-1)

Precise determination of the reaction barriers through DFT computations (cf. Fig. S1-1) is non-trivial. In particular, the exact ground state of the reaction mixture likely consists of a complex mixture of interconverting species involving the Na alkoxide, the dienoate substrate, the Cu salt and the free alcohol. Modeling of an enantioselective process, which reduces the number of possible reaction pathways by a factor of two, allows for formulation of a plausible stereochemical model as well as elucidation of the role of the catalyst's hydroxy group.

As a strong base, NaO*t*-Bu can deprotonate the alcohol within a complex such as **9d–Cu–allenyl** and easily establish a Na bridge with the substrate's carbonyl groups (**PA–9d$_{Na}$–ts$_{1,6major}$**) with a barrier of only 0.7 kcal/mol at the ωB97XD/Def2TZVPP$_{THF(SMD)}$//ωB97XD/Def2SVP$_{THF(PCM)}$ level (Figure S1-1a). With the less basic NaOPh the barrier to hydroxyl deprotonation is significantly higher for **PA–9d$_{Na}$–ts$_{1,6major}$** (16.0 kcal/mol; see Fig. S1-1b). However, NaOPh, can still establish a bridge giving rise to **PA-9d$_{NaOPh}$-ts$_{1,6major}$** with a readily accessible barrier of 2.8 kcal/mol relative the ground

(23) 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 6 into a text file without empty lines and changing the extension to ".xyz".

(24) (a) Page, M., McIver Jr., J. W. *J. Chem. Phys.* **88**, 922–935 (1988). (b) Page, M., Doubleday Jr., C. & McIver Jr., J. W. *J. Chem. Phys.* **93**, 5634–5642 (1990).

state **9d–Cu–allenyl** (see Fig. S1-1c). In the absence of a base formation of the aforementioned Na-based complex and conjugate addition seems to be unlikely (H-bonding transition state **PA–9d–ts$_{1,6major}$** with a barrier of 20.8 kcal/mol; see Fig. S1-1d).

Furthermore, we investigated the possibility of involvement of a sodium-borate bridge involving the alcohol on the NHC ligand (see Fig. S1-1e). Depending on the ground state [phenoxyBpin (**PhOBpin**) + NaOPh (***ground state II***) or the derived borate complex **(PhO)$_2$Bpin-Na$^+$** formed from the former two components (***ground state I***)], the barrier to the transition state (**PA–9d$_{Na\text{-}borate}$–ts$_{1,6major}$**) may vary. If a borate-containing ground state were to be involved (***ground state I***), the barrier to the transition state (1.6 kcal/mol) would be close to that obtained in Fig. S1-1c with a NaOPh bridge (2.8 kcal/mol). Although such a possibility cannot be ruled out on the basis of DFT calculations, we chose to focus on the simpler system with the NaOPh bridge in the studies detailed below.

Stereochemical model with a NaOPh bridge (Fig. S2-1 and S3-1)

The pathways leading to major and minor enantiomers for 1,6-addition of a propargyl or a (pin)B–substituted allyl group with ligands derived from **9b** and **9d** involving a bridge through an additional NaOPh molecule are shown in Fig. S2-1 and S3-1 (cf. Fig. 4 in the manuscript). Single point energy calculations with various density functionals (Fig. S2-2 and S3-2) reveal similar trends regarding the energy differences between the pathways that lead to major and minor enantiomers. Nonetheless, there are significant distinctions. For example, ωB97XD, M06, MN12SX, which are ranked among the most accurate approaches in a recent comparison of density functionals[12c], predict **AA–9d$_{NaOPh}$–ts$_{1,6major}$** for allyl addition (AA) in a close range between 4.6 and 7.7 kcal/mol (Fig. S3-2), whereas MN12L, M06L and PBE0-D3BJ estimate **AA–9d$_{NaOPh}$–ts$_{1,6major}$** at a lower energy relative to the ground state **9d$_{NaOPh}$–Cu–allyl** (−5.1, −1.4 and −1.9 kcal/mol, respectively). With BP86-D3BJ the energy of **AA–9d$_{NaOPh}$–ts$_{1,6major}$** is lower still (−11.5 kcal/mol). Similar trends were observed with propargyl additions (Fig. S2-2).

Stereochemical model involving deprotonation with NaO*t*-Bu and a Na bridge (Fig. S4-1 & S5-1)

We have investigated the energy differences between the pathways leading to the major and minor enantiomers for 1,6-addition of a propargyl or a (pin)B-substituted allyl group with ligands derived from **9b** and **9d** after hydroxyl deprotonation (Na bridge); the results of this segment of our studies are illustrated in Fig. S4-1 and S5-1. For propargyl additions, the minor pathways **PA–9d$_{Na}$–ts$_{1,6minor}$** and **PA–9b$_{Na}$–ts$_{1,6minor}$** are destabilized by 1.3 and 6.4 kcal/mol, respectively (Fig. S4-1; compared to 1.1 and 4.4 kcal/mol with a NaOPh bridge in Fig. S2-1). In the case of allyl additions, the corresponding energy differences are 3.5 and 1.7 kcal/mol, respectively (Fig. S5-1; vs. 2.4 and 0.4 kcal/mol with a NaOPh bridge in Fig. S3-1). Although the overall trends are similar there are minor differences in the magnitude of the energy values, which may either be ascribed to the alterations in the size of the bridging unit (a NaOPh bridge might provide a longer arm to establish coordination to the carbonyl groups on the substrate) or arise from the error bar in computational studies. The likelihood for the different salt bridges has been discussed in the text associated with Fig. S1-1.

Influence of the base on the background reaction (Fig. S6-1)

As was already noted (see discussion related to Fig. S1-1), determination of the precise energy barrier for the background reaction is non-trivial; this is because the exact ground state energy of the reaction mixture is unknown (Fig. S6-1). At the ωB97XD/Def2TZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{thf(PCM)}$ level of theory the ground state with a model NHC ligand ($Me_2C_3H_4N_2$, **Me_2NHC–Cu–allenyl**) is 7.6 kcal/mol lower than the corresponding ground state with a PMe_3 ligand (**PMe_3–Cu–allenyl**). Without an NHC or a phosphine ligand the ground state energy is increased to 15.7 kcal/mol (**THF–Cu–allenyl**). These values are congruent with the well-established attribute of NHC ligands regarding their higher bond dissociation energies (BDEs) than phosphine ligands[25]. In agreement with the experimental data, it is improbable that either NaO*t*-Bu or NaOPh are capable of replacing the NHC ligand from the coordination sphere of Cu (16.5 and 27.2 kcal/mol, respectively for the 1,6-propargyl addition transition states **PA–NaOPh–ts$_{1,6}$** and **PA–NaO*t*-Bu–ts$_{1,6}$** relative to ground state **Me_2NHC–Cu–allenyl**). In the case of PMe_3, these barriers are reduced to 8.9 and 19.6 kcal/mol relative to ground state **PMe_3–Cu–allenyl**. The control experiments shown in Scheme S4 (page S42) suggest that NaO*t*-Bu is better able to perform the background reaction in absence of a ligand. Nonetheless, corresponding experiments in the presence of SIMes (Fig. 1b) or PPh_3/PCy_3 (Scheme S4, page S42) rule out phosphine ligand lability as the sole reason for background reactivity since the observation of 1,4-propargyl addition products can clearly be attributed to the presence of a phosphine ligand. Furthermore, the low computed regioselectivity for the background reaction in Fig. S6-1, i.e. the transition states for 1,6-propargyl addition **PA–NaO*t*Bu–ts$_{1,6}$** (8.9 kcal/mol) and 1,4-propargyl addition **PA-NaO*t*Bu-ts$_{1,4}$** (7.4 kcal/mol) are similar in magnitude, likely suggests alternative pathways to be operative or it may be attributed to a more complex environment for the ionic salt bridge.

Analysis of the origin of diastereoselectivity for allyl addition with a model NHC ligand (Fig. S7-1)

The calculations shown in Fig. S7-1 performed with a model NHC ligand (**Me_2NHC**, $Me_2C_3H_4N_2$) without a sodium salt reveal that the minor diastereomer is generated through a boat-like transition state **AA–Me_2NHC–ts$_{1,6minor}$**; such a complex suffers from additional steric repulsion between the substrate phenyl ring and the pincacolatoboron group. These destabilizing interactions are absent in the transition state leading to the major diastereomer **AA–Me_2NHC–ts$_{1,6major}$** with energies relative to the ground state **Me_2NHC–Cu–allyl** of 20.1 and 14.2 kcal/mol, respectively (ωB97XD/Def2TZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{thf(PCM)}$ level of theory). The calculated preferred sense of diastereoselectivity is consistent with experimental data and, consequently, the minor diastereomer has not been considered in modeling studies with the chiral ligands. Comparable trends have been calculated with the other investigated density functionals (Fig. S7-2).

(25) For example, see: Dorta, R., Stevens, E. D., Scott, N. M., Costabile, C., Cavallo, L., Hoff, C. D. & Nolan, S. P. *J. Am. Chem. Soc.* **127**, 2485–2495 (2005).

Difference in selectivity with NHC and phosphine ligands – Part I (Fig. S8-1, S9-1, S10-1 & S11-1)

To probe the origin of the difference between NHC and phosphine ligands during 1,6-propargyl addition to a **dienoate** substrate, we investigated the following three competitive pathways: **i)** 1,6-addition (denoted $\mathbf{ts_{1,6}}$); **ii)** 1,4-allenyl addition (denoted $\mathbf{ts_{1,4AA}}$); **iii)** 1,4-propargyl addition (denoted $\mathbf{ts_{1,4}}$). Comparison of Cu complexes bearing an NHC ligand (SIMes) and a phosphine ligand (PPh_3) is illustrated in Fig. S8-1. Although there are minor differences between the complexes, with both ligand systems 1,6-propargyl addition (24.4 and 26.0 kcal/mol for $\mathbf{PA–SIMes–ts_{1,6}}$ and $\mathbf{PA–PPh_3–ts_{1,6}}$, respectively) is favored to a substantial degree compared to 1,4-propargyl addition (30.9 and 30.4 kcal/mol for $\mathbf{PA–SIMes–ts_{1,4}}$ and $\mathbf{PA–PPh_3–ts_{1,4}}$, respectively). Similar trends were observed with smaller model NHC and phosphine ligands in which case steric effects can largely be eliminated (Fig. S9-1). 1,6-Propargyl addition ($\mathbf{PA–Me_2NHC–ts_{1,6}}$ and $\mathbf{PA–PMe_3–ts_{1,6}}$) is favored by 6.9 and 5.8 kcal/mol over 1,4-propargyl addition ($\mathbf{PA–Me_2NHC–ts_{1,4}}$ and $\mathbf{PA–PMe_3–ts_{1,4}}$) with Me_2NHC and PMe_3 as ligands, respectively. Furthermore, selectivity does not change when the substrate is activated through a sodium borate salt (**dienoate–Na–borate**), although the barrier heights are diminished noticeably (Fig. S10-1). The calculated energy barriers for 1,6-propargyl addition are 14.3 and 14.6 kcal/mol for $\mathbf{PA–SIMes_{(Na\text{-}borate)}–ts_{1,6}}$ and $\mathbf{PA–PPh_{3(Na\text{-}borate)}–ts_{1,6}}$, respectively, whereas the magnitude of the barriers for 1,4-propargyl addition ($\mathbf{PA–SIMes_{(Na\text{-}borate)}–ts_{1,4}}$ and $\mathbf{PA–PPh_{3(Na\text{-}borate)}–ts_{1,4}}$) are 22.0 and 21.0 kcal/mol. Additionally, 1,6-propargyl addition through γ-transfer is also favored over 1,4-allenyl addition through α-transfer of the nucleophile to the β-carbon atom of the electrophile (Figs. S8-1, S9-1 & S10-1). In presence of chiral NHC ligand **9d**, modeled with a sodium bridge, 1,4-allenyl addition $\mathbf{PA–9d_{Na}–ts_{1,4AA}}$ is disfavored by 6.8 kcal/mol relative to 1,6-propargyl addition $\mathbf{PA–9d_{Na}–ts_{1,6}}$ (Fig. S11-1). It is likely that these trends are the result of the d^{10} ligand field on Cu (Fig. S9-3).[26] Natural bond orbital analysis (NBO) indicates that the allenyl nucleophile would have to move across the filled $d_{x^2-y^2}$ orbital on Cu (NBO 103) for α-addition to occur. This would engender a significant degree of filled-filled interaction with the filled sp^2 hybrid orbital on the nucleophile. Such destabilizing interaction is absent in the transition state for 1,6-propargyl addition.

Difference in selectivity with NHC and phosphine ligands – Part II (Fig. S12-1, S13-1 & S14-1)

A significant difference between phosphine (PPh_3) and NHC ligands (SIMes) is linked to their substantially different σ-donating properties. As a result, the HOMO in **SIMes–Cu–allenyl** (–7.14 eV) is about 0.29 eV (corresponds to 6.7 kcal/mol) higher in energy than in **PPh_3–Cu–allenyl** (–7.43 eV; Fig. S12-1). A more nucleophilic d_{z^2} (linear geometry, cf. Fig. 1c) or d_{xy} orbital (bent geometry, cf. Figure 1c) on Cu likely facilitates interaction with the π-acidic olefinic substrate. In contrast, a more π-acidic phosphine ligand would make the Cu center more susceptible to hard π-donor ligands (e.g. alkoxides). According to the $\omega B97XD/Def2TZVPP_{thf(SMD)}//\omega B97XD/Def2SVP_{thf(PCM)}$ energies shown in

(26) Walroth, R. C., Lukens, J. T., MacMillan, S. N., Finkelstein, K. D. & Lancaster, K. M. *J. Am. Chem. Soc.* **128**, 1922–1931 (2016).

Fig. 12-1, **PPh_3–Cu–allenyl** binds Na–O*t*Bu more tightly (–9.2 kcal/mol, red curves) relative to **SIMes–Cu–allenyl** (–5.7 kcal/mol, blue curves). Additionally we find that, in agreement with the experimental data (cf. Fig. 1b), the transition state for 1,6-propargyl addition after π-complex formation with Cu (i.e. **PA–SIMes$_{NaO\mathit{t}Bu}$–ts$_{1,6}$**;17.6 kcal/mol) is significantly favored over the transition state for 1,4-propargyl addition **PA–SIMes$_{NaO\mathit{t}Bu}$–ts$_{1,4}$** (26.5 kcal/mol); in the latter Na–O*t*Bu is coordinated to Cu. Furthermore, this scenario is able to explain the experimentally observed selectivity differences with phosphine ligands (cf. Scheme S4; page S42), wherein the order of computed energies for 1,6-propargyl addition **PA–PPh$_{3(NaO\mathit{t}Bu)}$–ts$_{1,6}$** (22.2 kcal/mol) and 1,4-propargyl addition **PA–PPh$_{3(NaO\mathit{t}Bu)}$–ts$_{1,4}$** (13.4 kcal/mol) is reversed. Similar trends are observed with sterically modified model systems: In Fig. S13-1, Na–OMe has been used as base instead of Na–O*t*Bu, whereas model ligands Me_2NHC and PMe_3 have been used in Fig. S14-1 instead of SIMes and PPh_3. Assuming that the σ-donor strength of the Lewis basic ligand (NHC or PR_3) is largely responsible for π-complexation and consequently the regioselectivity of the reaction, it is likely that the anionic and highly nucleophilic $(allenyl)_2$–Cu species may be the reason for the high 1,6-selectivity observed for the background reactions.

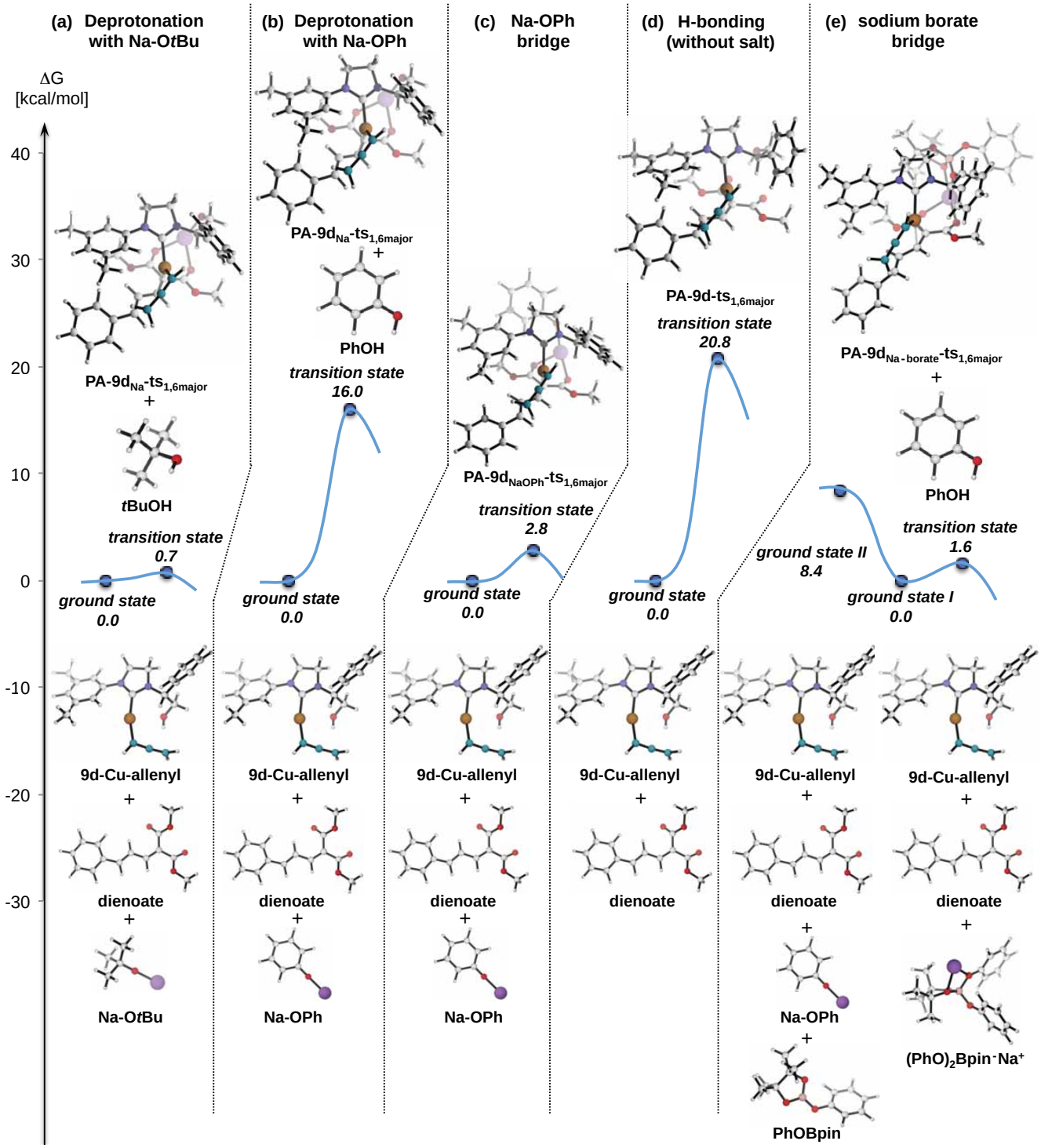

Figure S1-1. Free energy surfaces (ΔG, kcal/mol) for chelate geometries for the pathway leading to the major enantiomer for 1,6-addition of a propargyl group to a dienoate relative to the allenyl–Cu intermediate bearing the protonated NHC ligand (**9d–Cu–allenyl**) at the ωB97XD/Def2TZVPP$_{THF(SMD)}$//ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

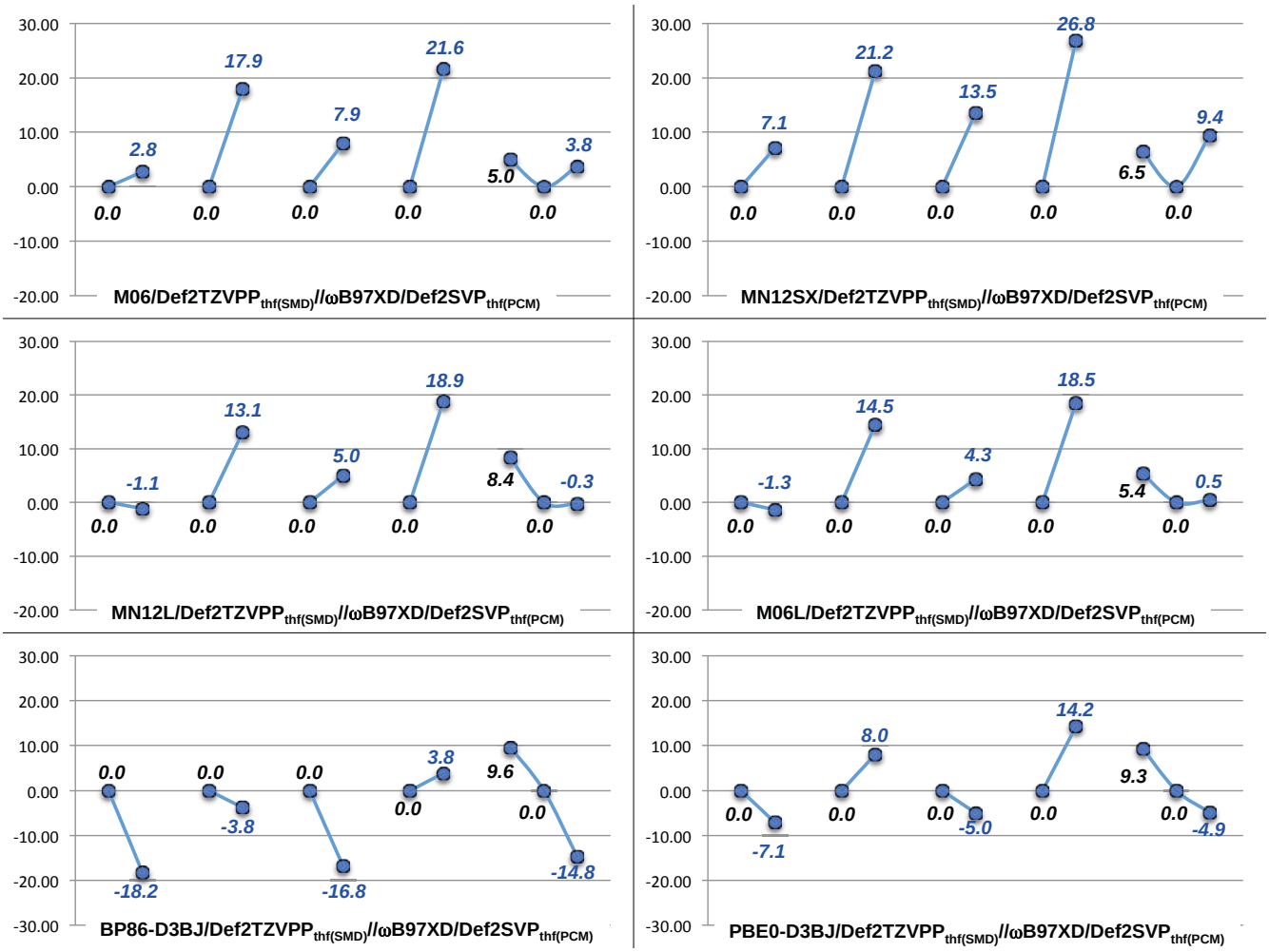

***Figure S1-2*.** Free energy surfaces (ΔG, kcal/mol) for chelate geometries for the pathway leading to the major enantiomer for 1,6-addition of a propargyl group to a dienoate relative to the allenyl–Cu intermediate bearing the protonated NHC ligand (**9d–Cu–allenyl**) with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

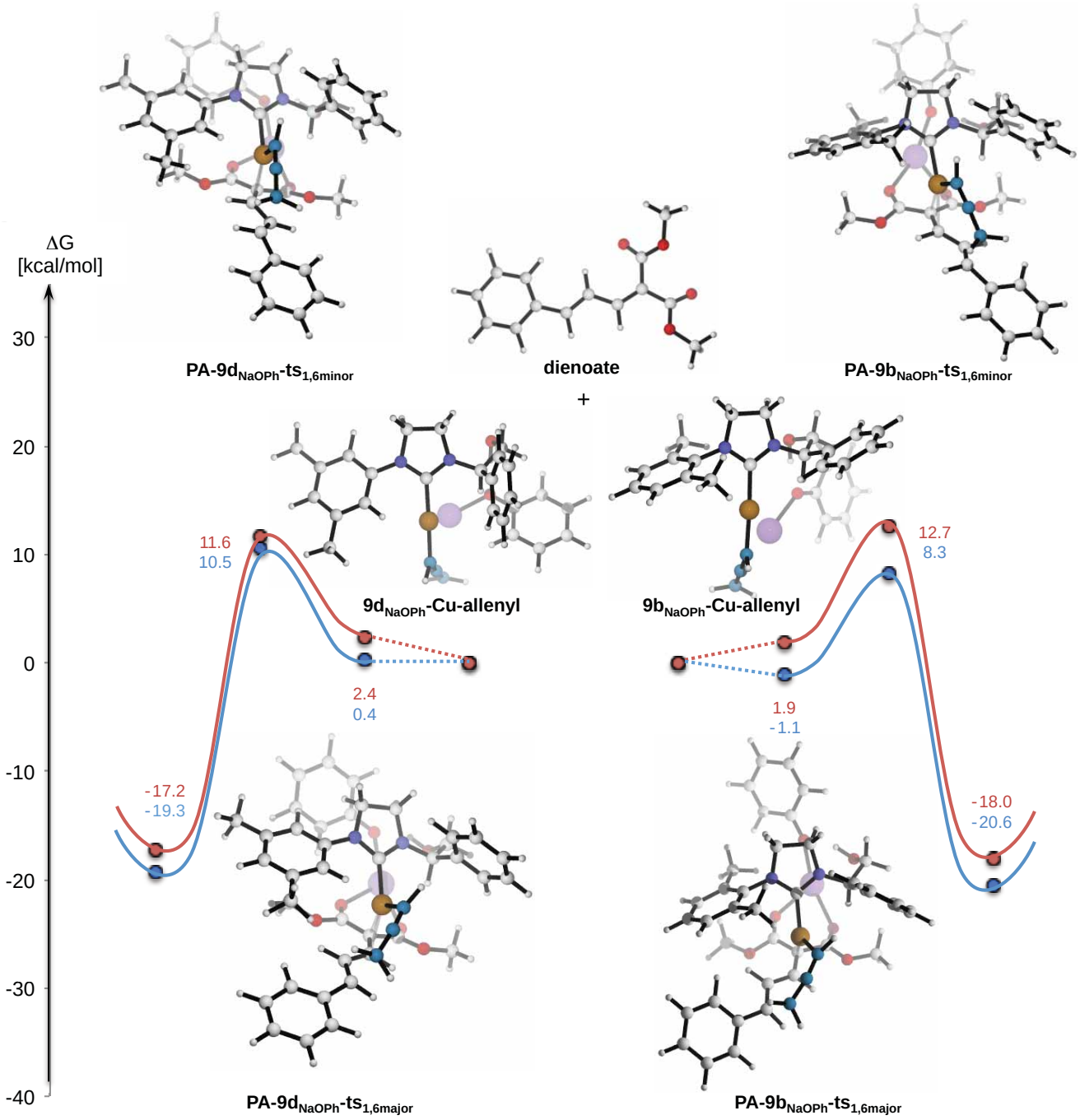

Figure S2-1. Free energy surfaces (ΔG, kcal/mol) for pathways leading to the major and minor enantiomers for 1,6-addition of a propargyl group to a dienoate with ligands **9d** (left) and **9b** (right) relative to the allenyl–Cu intermediate bearing an additional NaOPh molecule on the NHC ligand at the ωB97XD/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

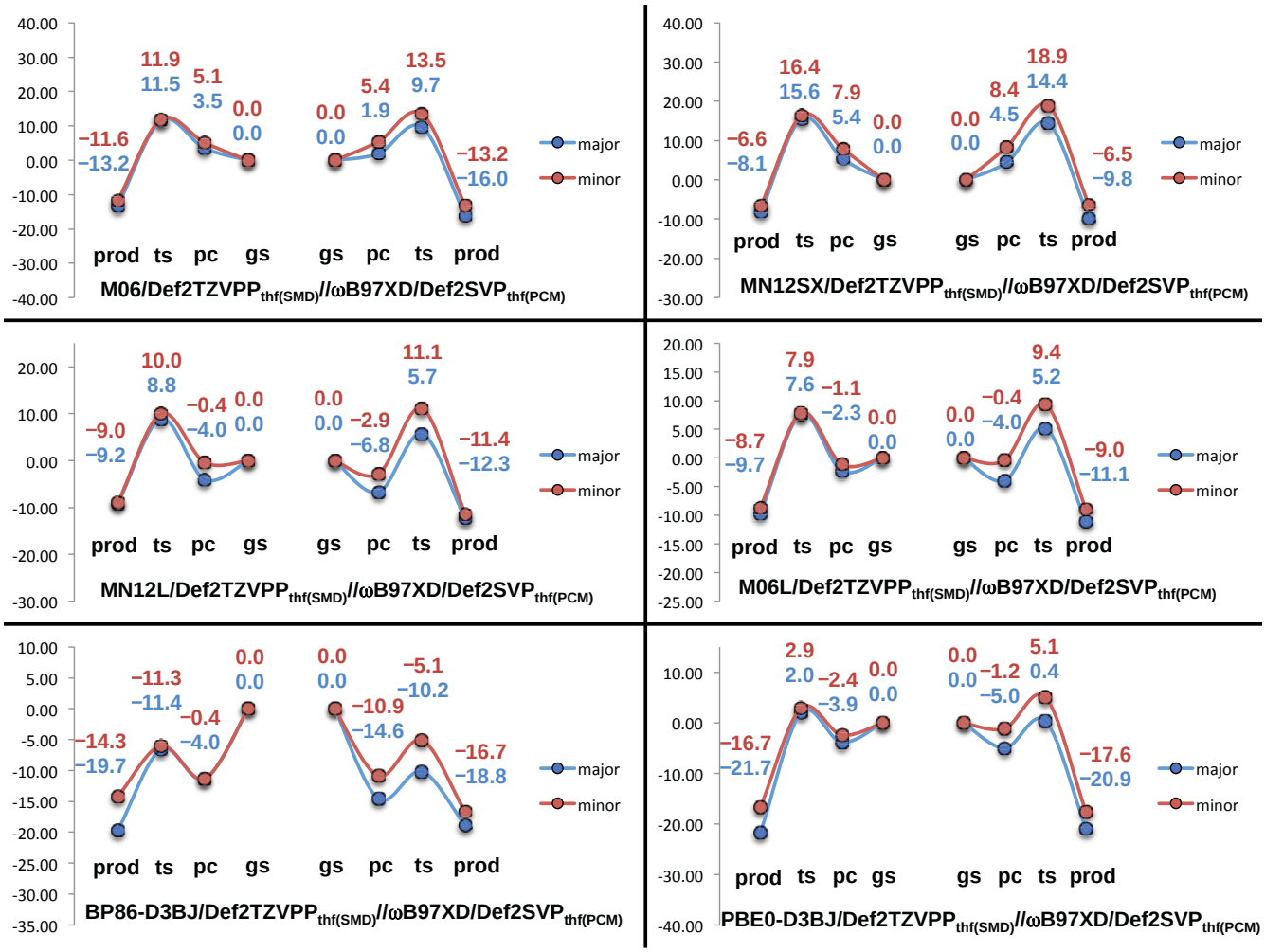

Figure S2-2. Free energy surfaces (ΔG, kcal/mol) for pathways leading to the major and minor enantiomers for 1,6-addition of a propargyl group to a dienoate with ligands **9d** (left) and **9b** (right) relative to the allenyl–Cu intermediate bearing an additional NaOPh molecule on the NHC ligand with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

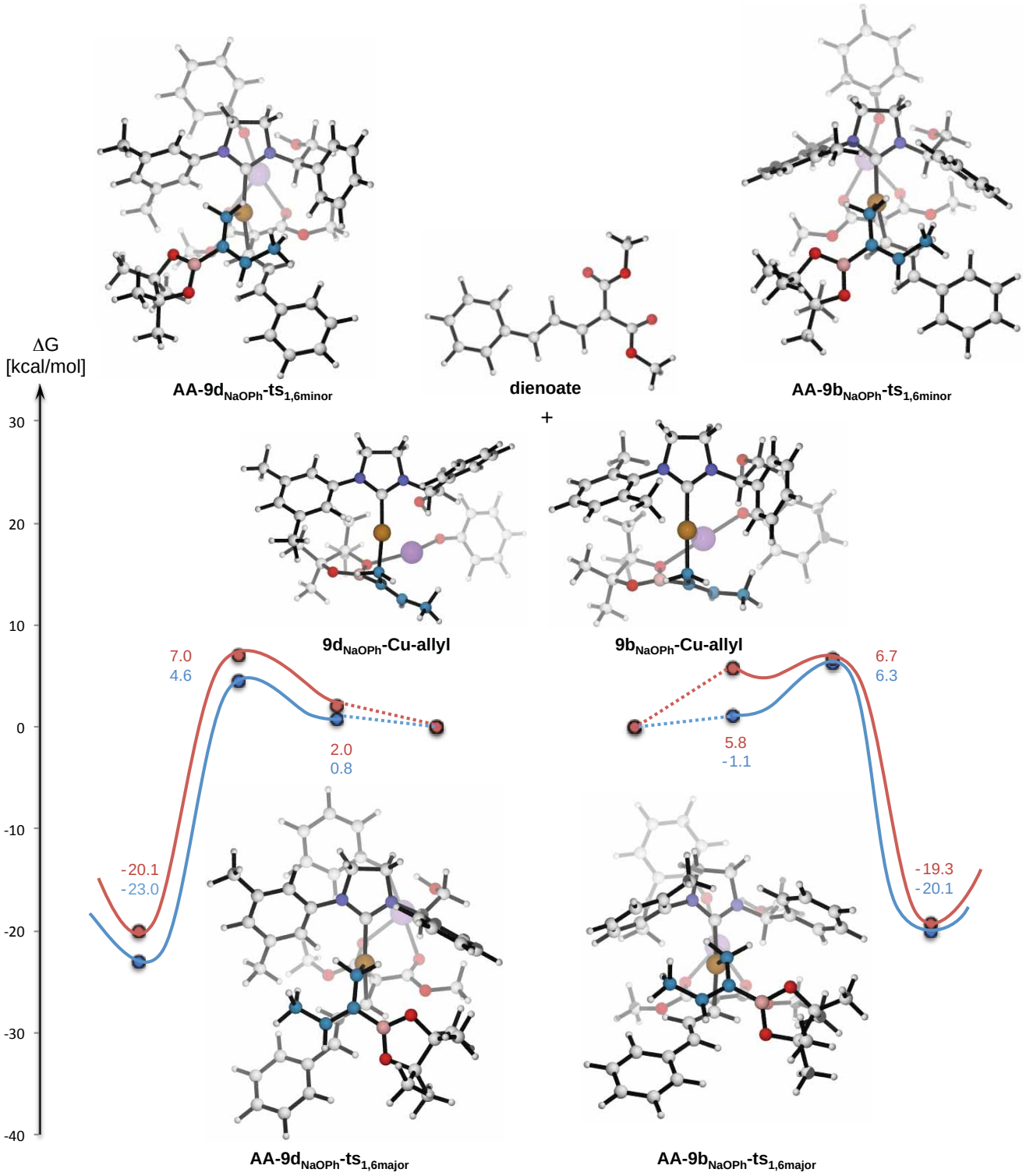

Figure S3-1. Free energy surfaces (ΔG, kcal/mol) for pathways leading to the major and minor enantiomers for 1,6-addition of a pinacolatoboron substituted allyl group to a dienoate with ligands **9d** (left) and **9b** (right) relative to the allyl–Cu intermediate bearing an additional NaOPh molecule on the NHC ligand at the ωB97XD/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

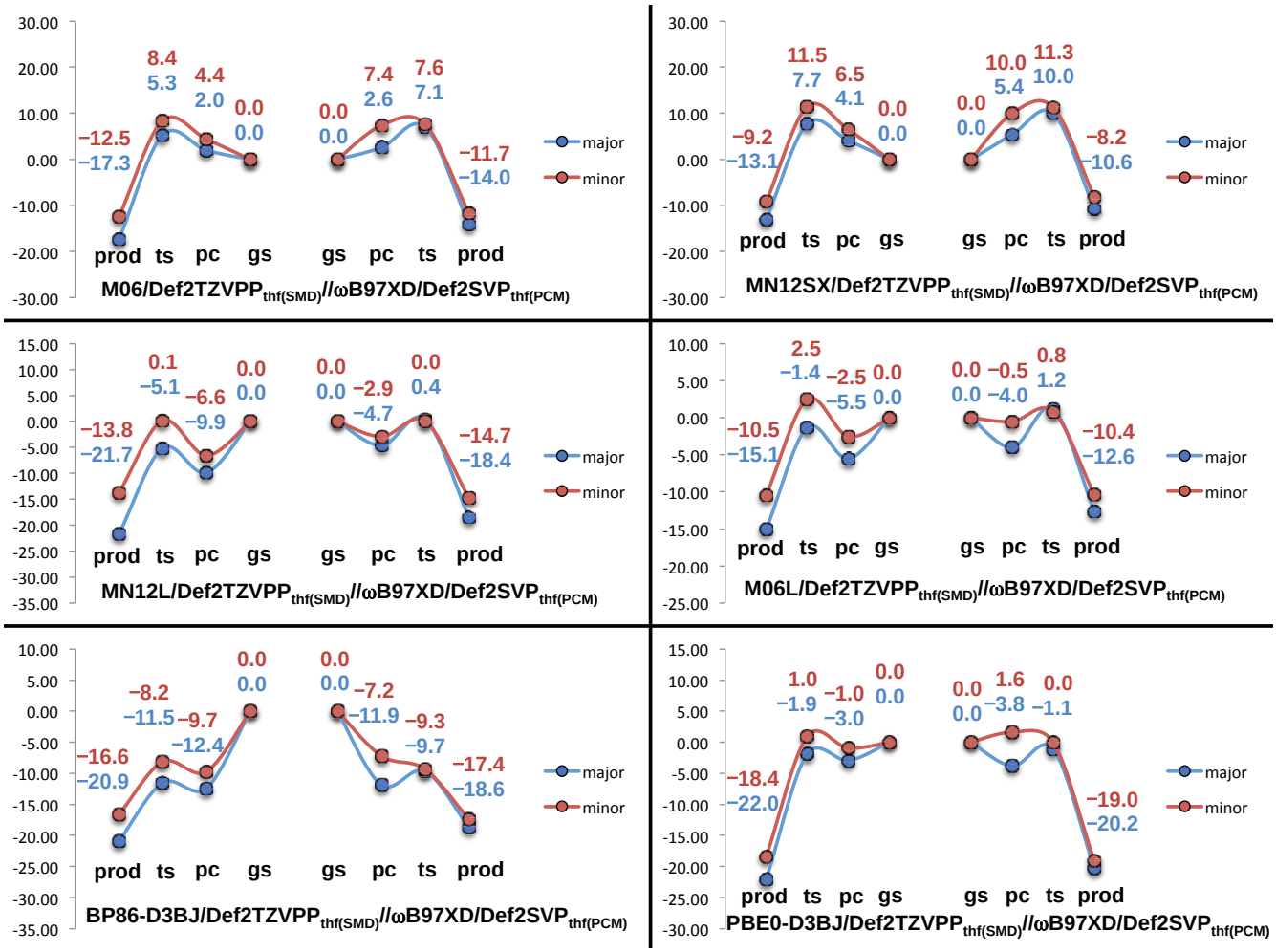

Figure S3-2. Free energy surfaces (ΔG, kcal/mol) for pathways leading to the major and minor enantiomers for 1,6-addition of a pinacolatoboron substituted allyl group to a dienoate with ligands **9d** (left) and **9b** (right) relative to the allyl–Cu intermediate bearing an additional NaOPh molecule on the NHC ligand with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

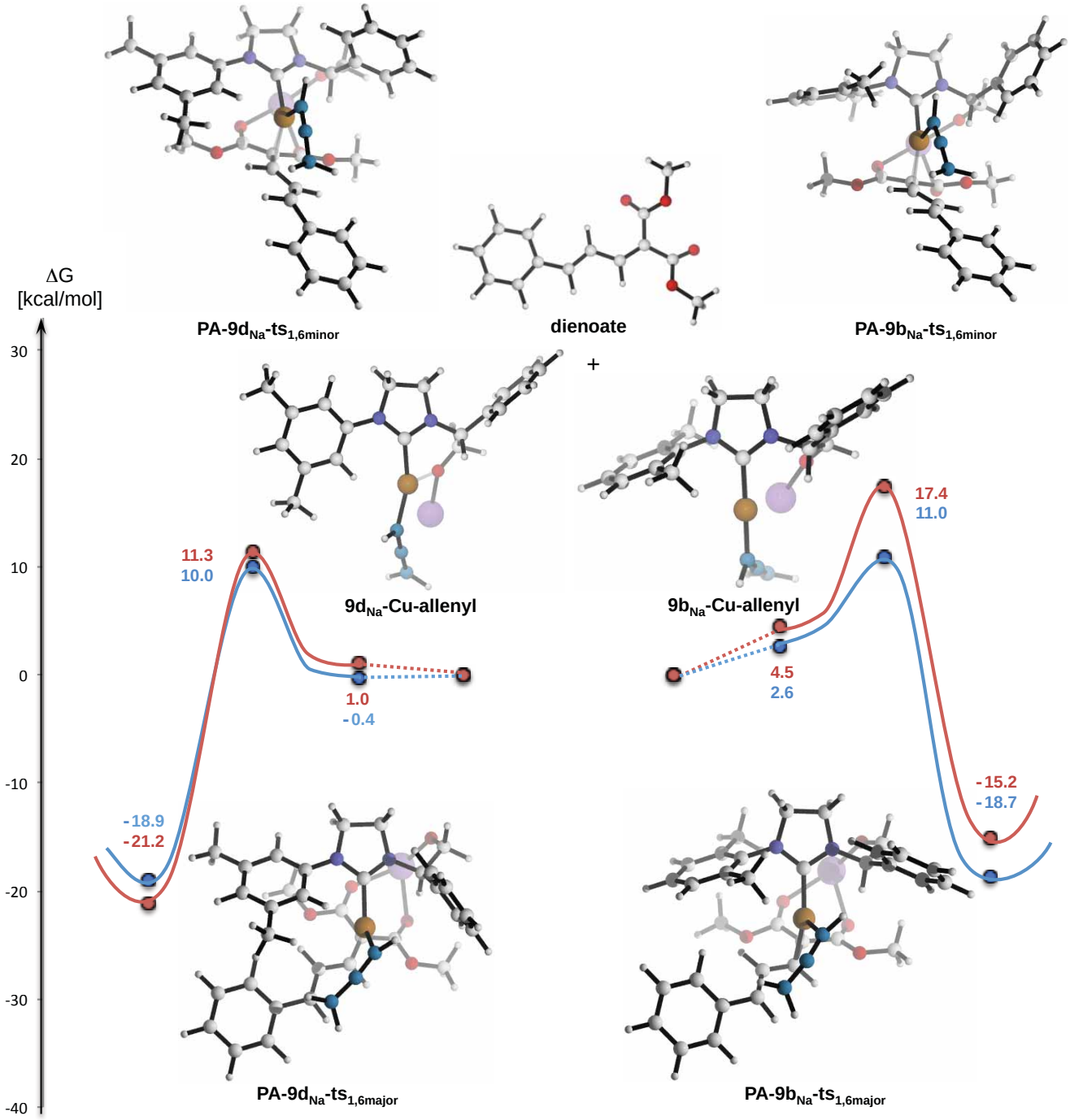

Figure S4-1. Free energy surfaces (ΔG, kcal/mol) for pathways leading to the major and minor enantiomers for 1,6-addition of a propargyl group to a dienoate with ligands **9d** (left) and **9b** (right) relative to the allenyl–Cu intermediate bearing a deprotonated NHC ligand (Na bridge) at the ωB97XD/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

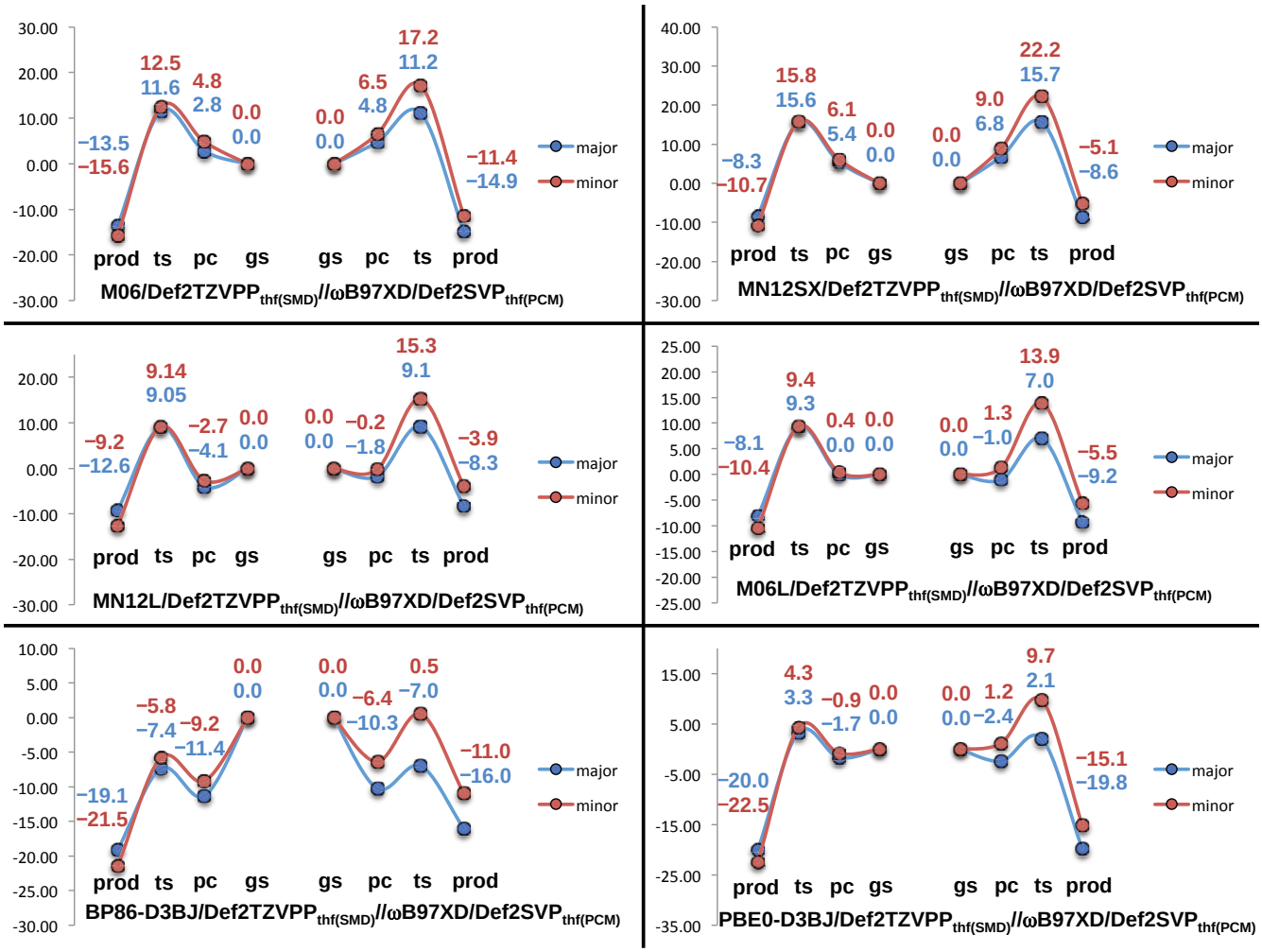

***Figure S4-2*.** Free energy surfaces (ΔG, kcal/mol) for pathways leading to the major and minor enantiomers for 1,6-addition of a propargyl group to a dienoate with ligands **9d** (left) and **9b** (right) relative to the allenyl–Cu intermediate bearing a deprotonated NHC ligand (Na bridge) with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

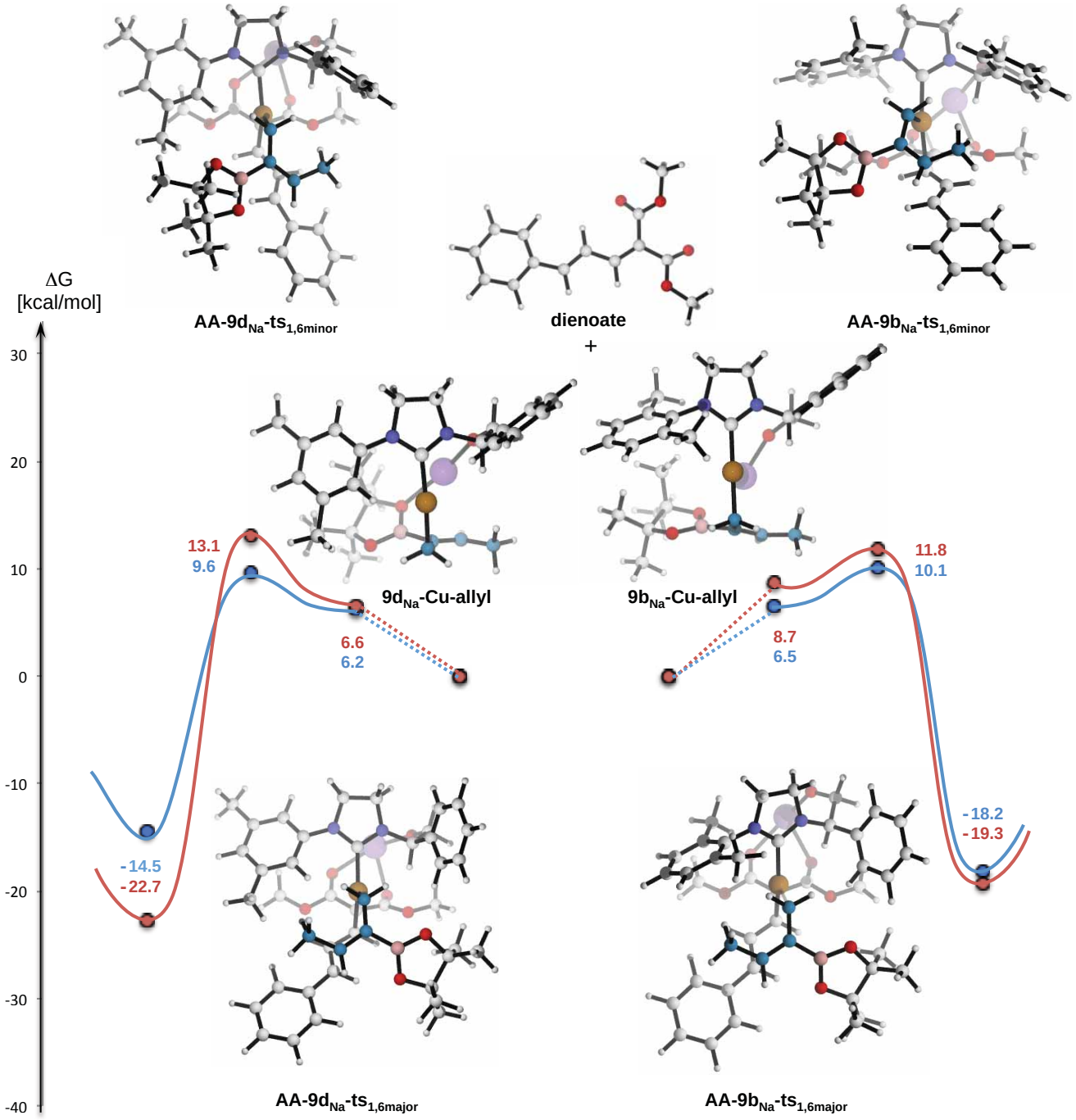

Figure S5-1. Free energy surfaces (ΔG, kcal/mol) for pathways leading to the major and minor enantiomers for 1,6-addition of a pinacolatoboron substituted allyl group to a dienoate with ligands **9d** (left) and **9b** (right) relative to the allyl–Cu intermediate bearing a deprotonated NHC ligand (Na bridge) at the ωB97XD/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{thf(PCM)}$ level of theory.

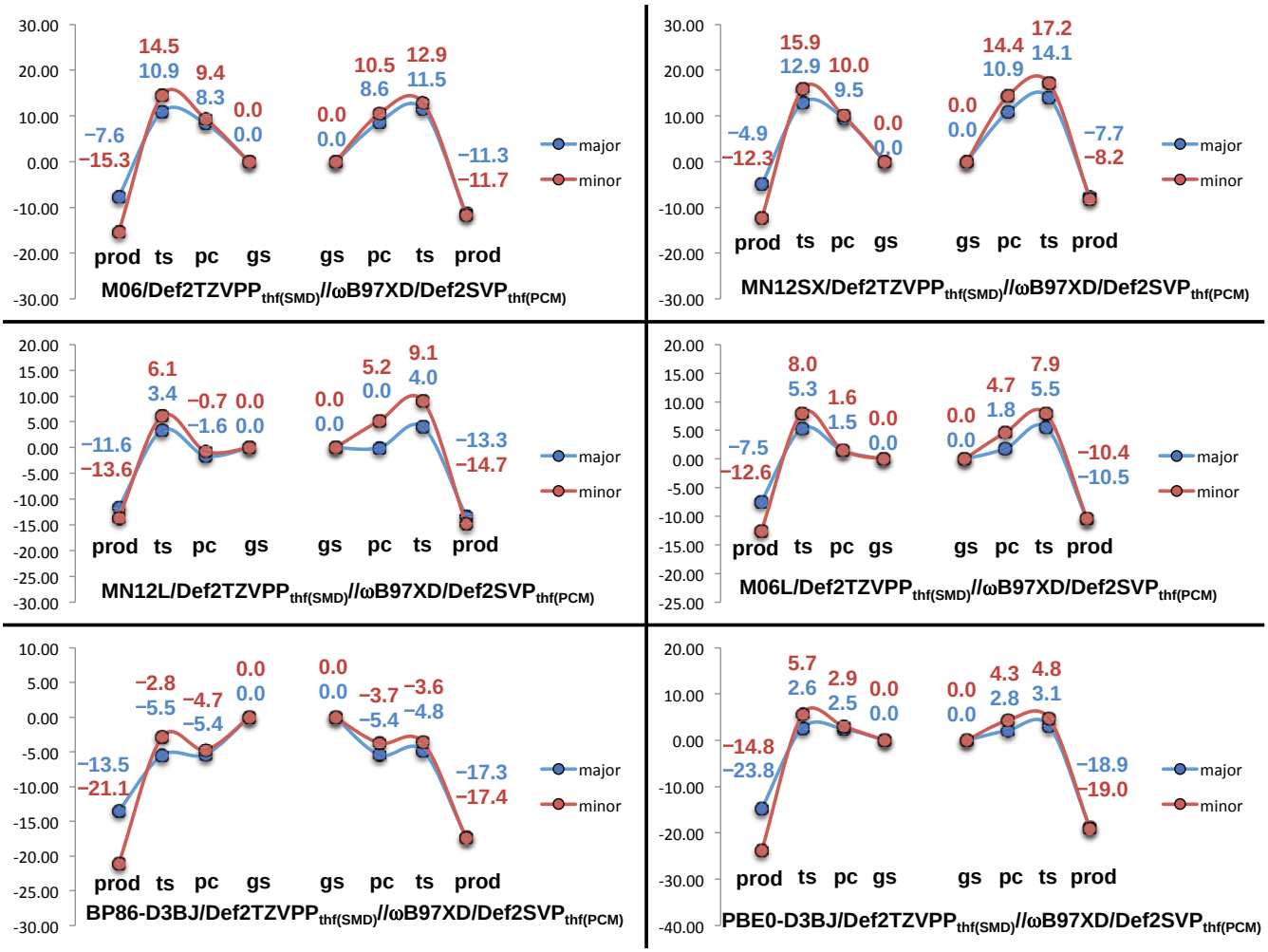

***Figure S5-2*.** Free energy surfaces (ΔG, kcal/mol) for pathways leading to the major and minor enantiomers for 1,6-addition of a pinacolatoboron substituted allyl group to a dienoate with ligands **9d** (left) and **9b** (right) relative to the allyl–Cu intermediate bearing a deprotonated NHC ligand (Na bridge) with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

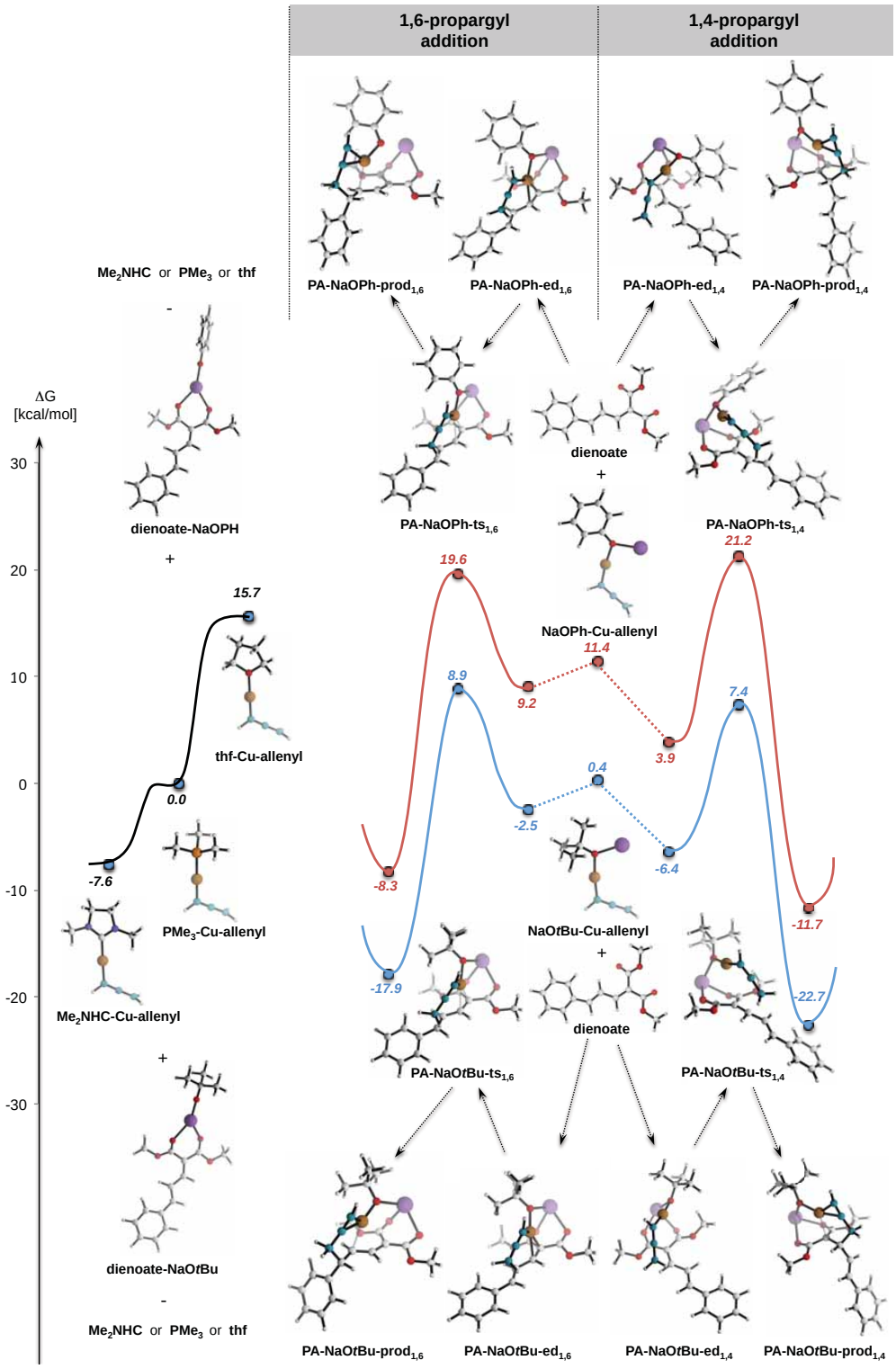

Figure S6-1. Free energy surfaces (ΔG, kcal/mol) for the background reactions promoted by NaO*t*-Bu (blue) or NaOPh (red) leading to 1,6-addition or 1,4-addition of a propargyl group to a dienoate relative to various allenyl Cu intermediates bearing either a model NHC ligand ($Me_2C_3H_4N_2$, **Me_2NHC–Cu–allenyl**), a model phosphine ligand (PMe_3, **PMe_3–Cu–allenyl**) or a THF molecule (**THF–Cu–allenyl**) at the ωB97XD/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

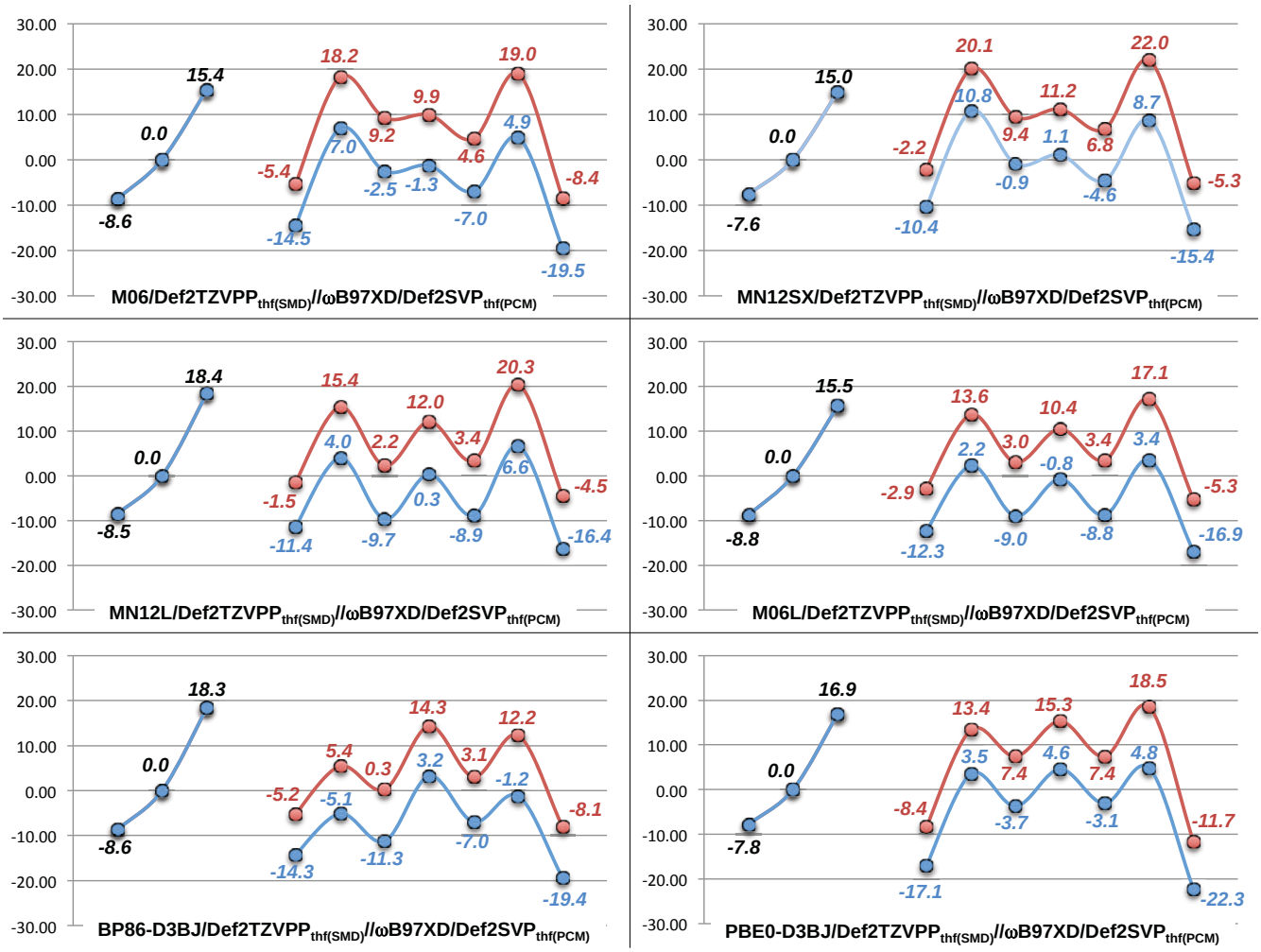

Figure S6-2. Free energy surfaces (ΔG, kcal/mol) for the background reactions promoted by NaO*t*-Bu (blue) or NaOPh (red) leading to 1,6-addition or 1,4-addition of a propargyl group to a dienoate relative to various allenyl Cu intermediates bearing either a model NHC ligand ($Me_2C_3H_4N_2$, **Me_2NHC–Cu–allenyl**), a model phosphine ligand (PMe_3, **PMe_3–Cu–allenyl**) or a THF molecule (**THF–Cu–allenyl**) with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

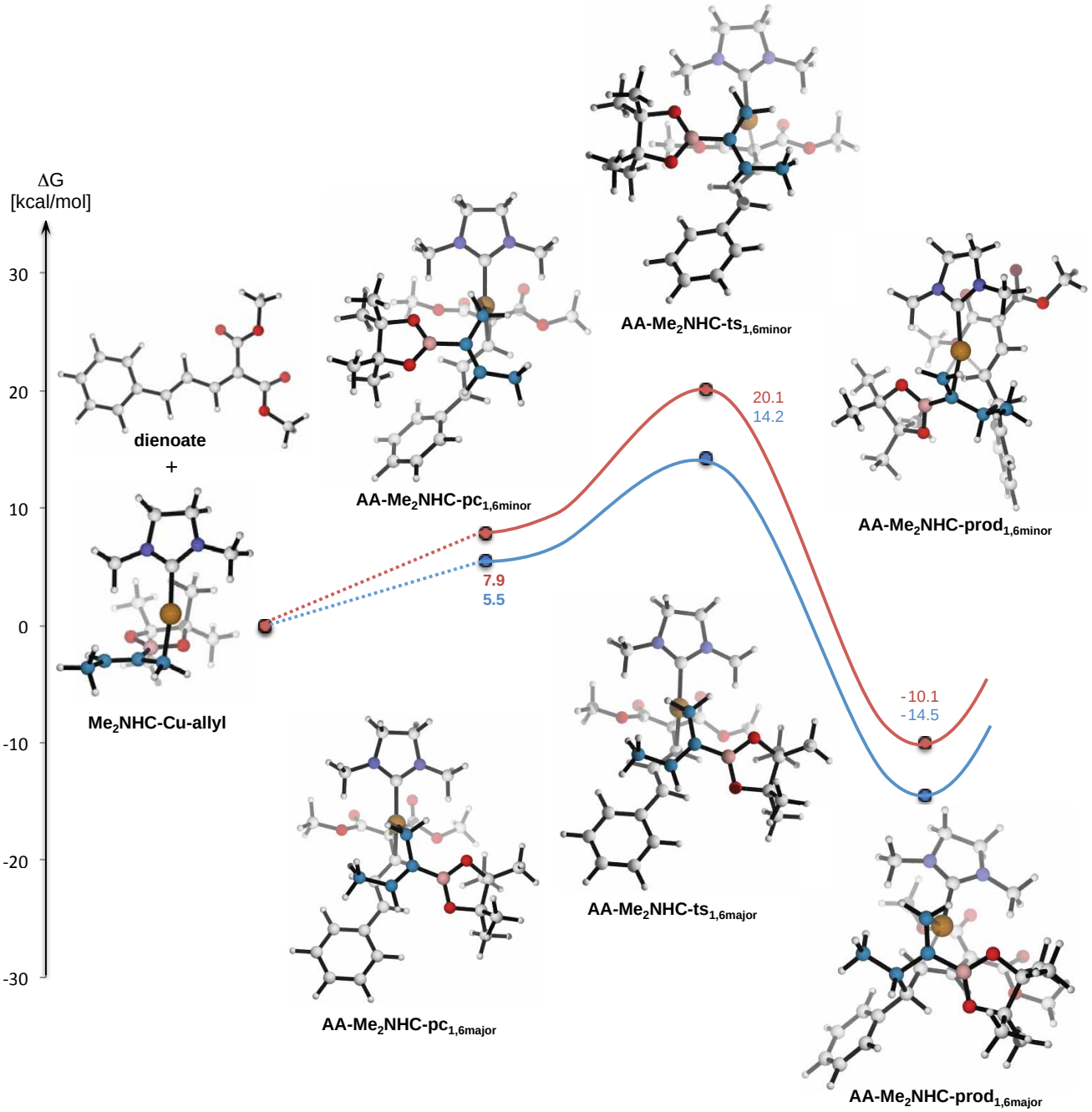

Figure S7-1. Free energy surfaces (ΔG, kcal/mol) for the pathways leading to the major and minor diastereomer of 1,6-addition of a pinacolatoboron substituted allyl group to a dienoate relative to allyl–Cu intermediate bearing a model NHC ligand ($Me_2C_3H_4N_2$, **Me_2NHC–Cu–allenyl**) at the ωB97XD/Def2TZVPP$_{thf(SMD)}$//ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

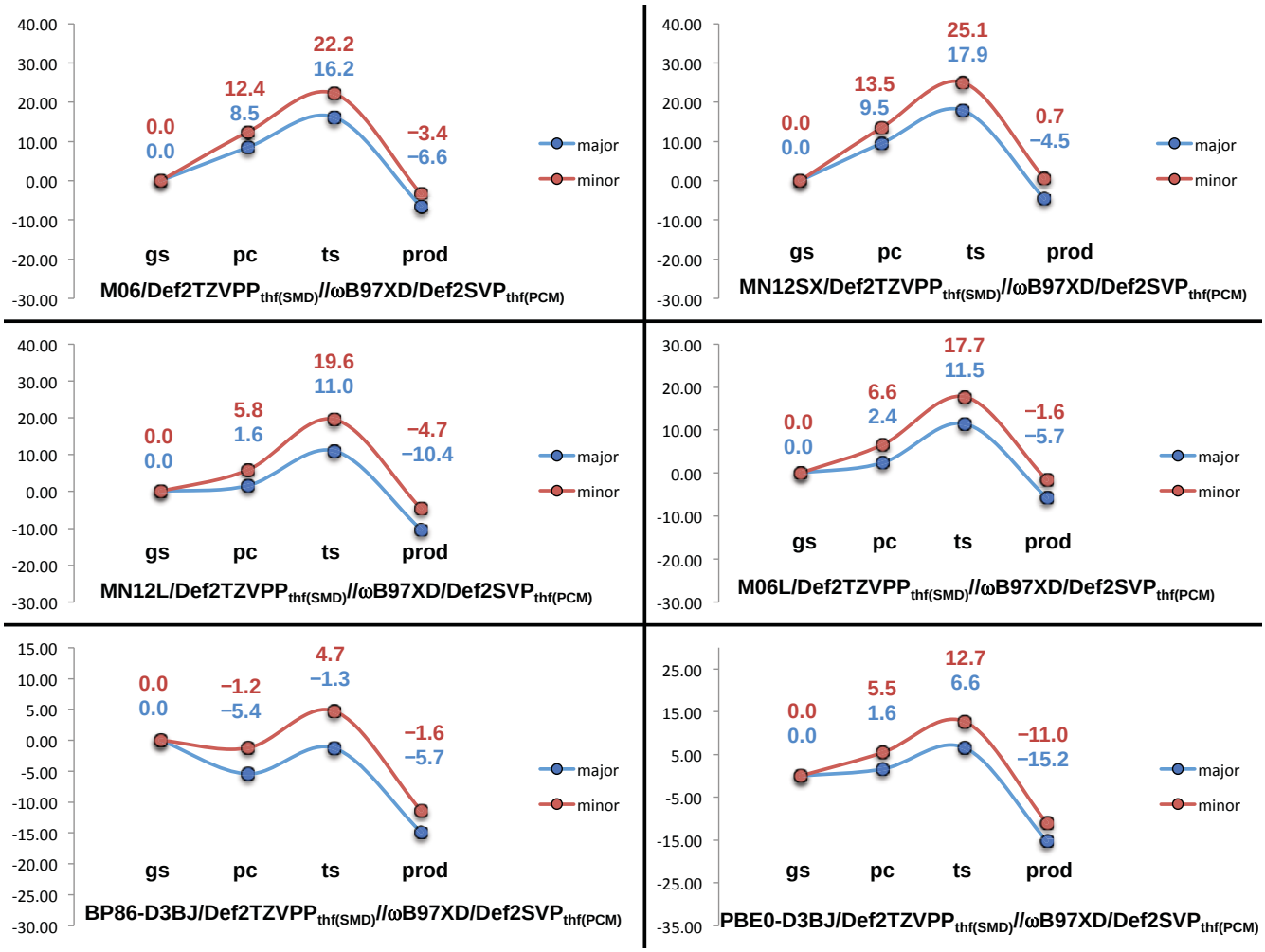

***Figure S7-2*.** Free energy surfaces (ΔG, kcal/mol) for the pathways leading to the major and minor diastereomer of 1,6-addition of a pinacolatoboron substituted allyl group to a dienoate relative to allyl–Cu intermediate bearing a model NHC ligand ($Me_2C_3H_4N_2$, **Me_2NHC–Cu–allenyl**) with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

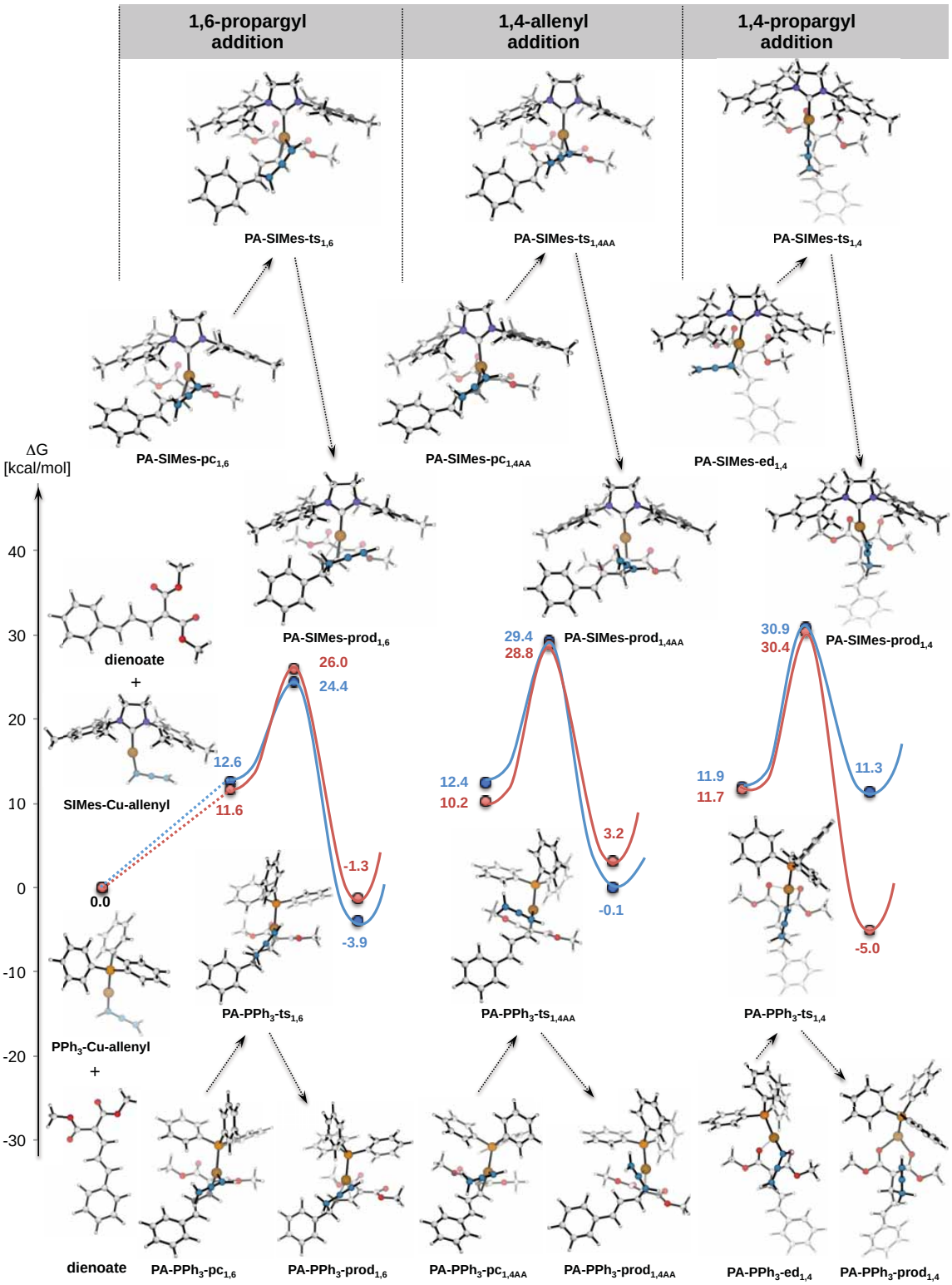

Figure S8-1. Free energy surfaces (ΔG, kcal/mol) for the pathways leading 1,6-propargyl addition, 1,4-allenyl addition and 1,4-propargyl addition to a dienoate relative to allenyl Cu intermediate bearing either an NHC ligand (SIMes, blue) or a phosphine ligand (PPh_3, red) at the ωB97XD/Def2TZVPP$_{THF(SMD)}$//ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

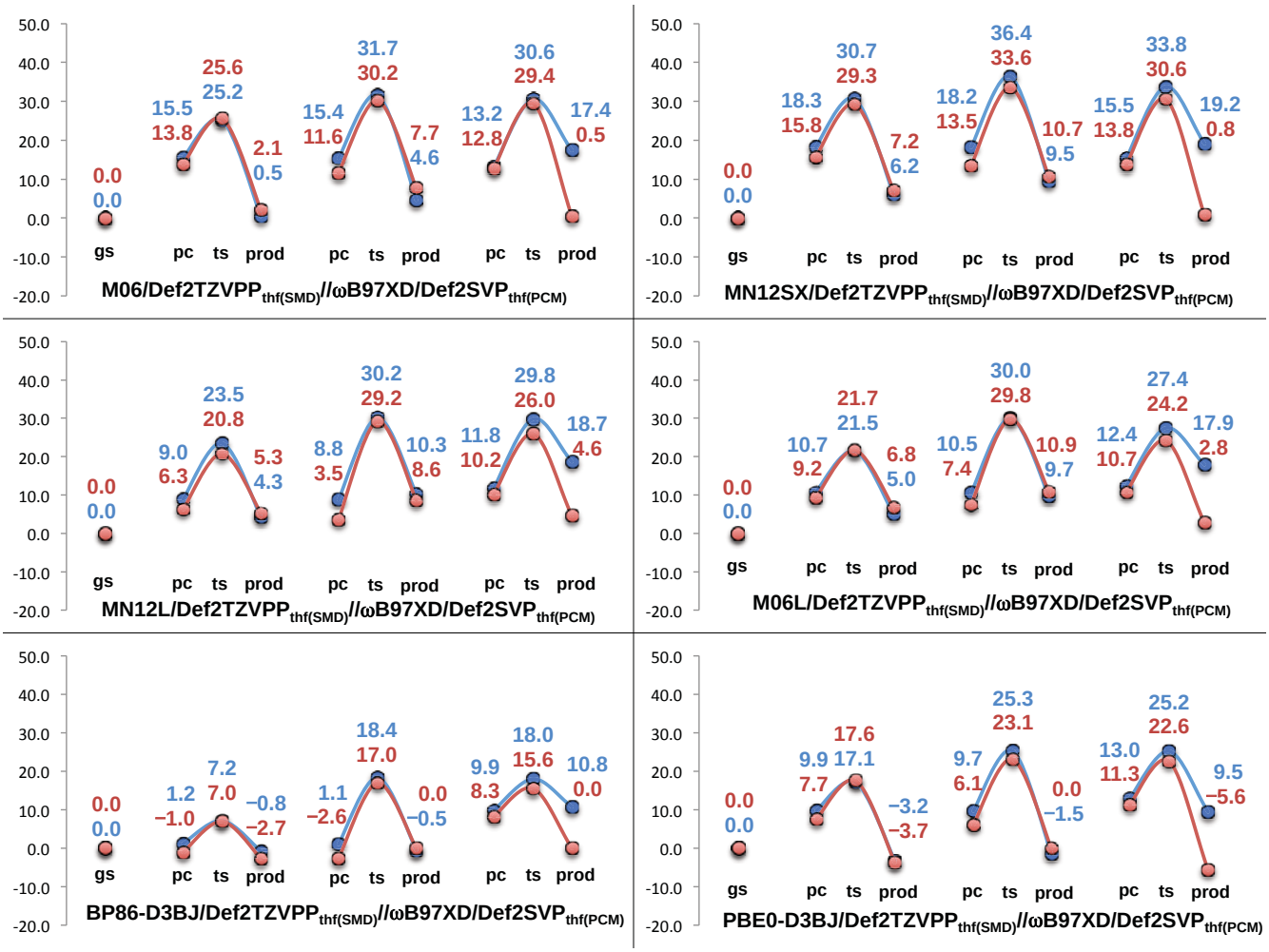

Figure S8-2. Free energy surfaces (ΔG, kcal/mol) for the pathways leading 1,6-propargyl addition, 1,4-allenyl addition and 1,4-propargyl addition to a dienoate relative to allenyl–Cu intermediate bearing either an NHC ligand (SIMes, blue) or a phosphine ligand (PPh_3, red) with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

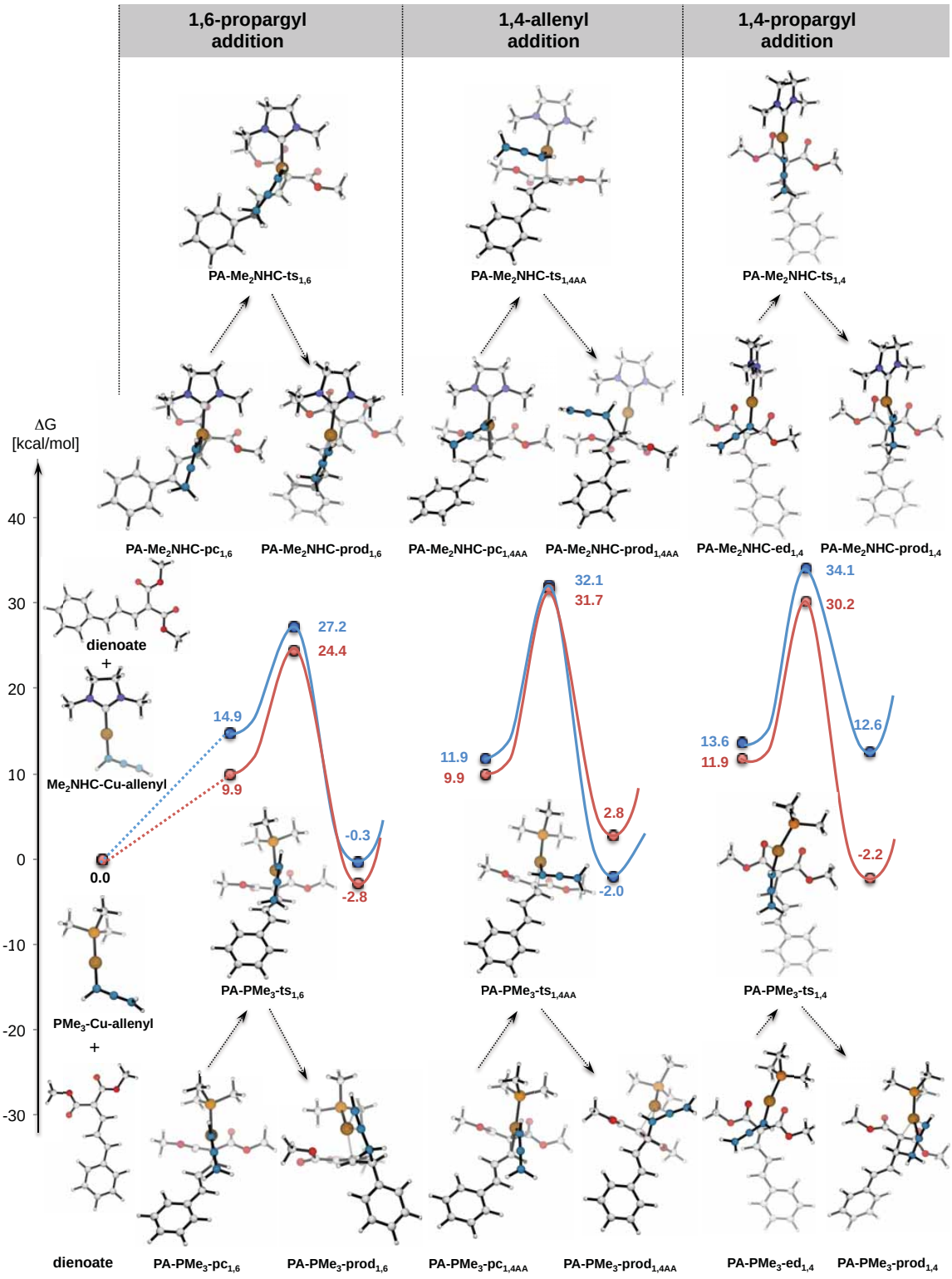

Figure S9-1. Free energy surfaces (ΔG, kcal/mol) for the pathways leading 1,6-propargyl addition, 1,4-allenyl addition and 1,4-propargyl addition to a dienoate relative to allenyl–Cu intermediate bearing either a model NHC ligand ($Me_2C_3H_4N_2$, blue) or a model phosphine ligand (PMe_3, red) at the ωB97XD/Def2TZVPP$_{THF(SMD)}$//ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

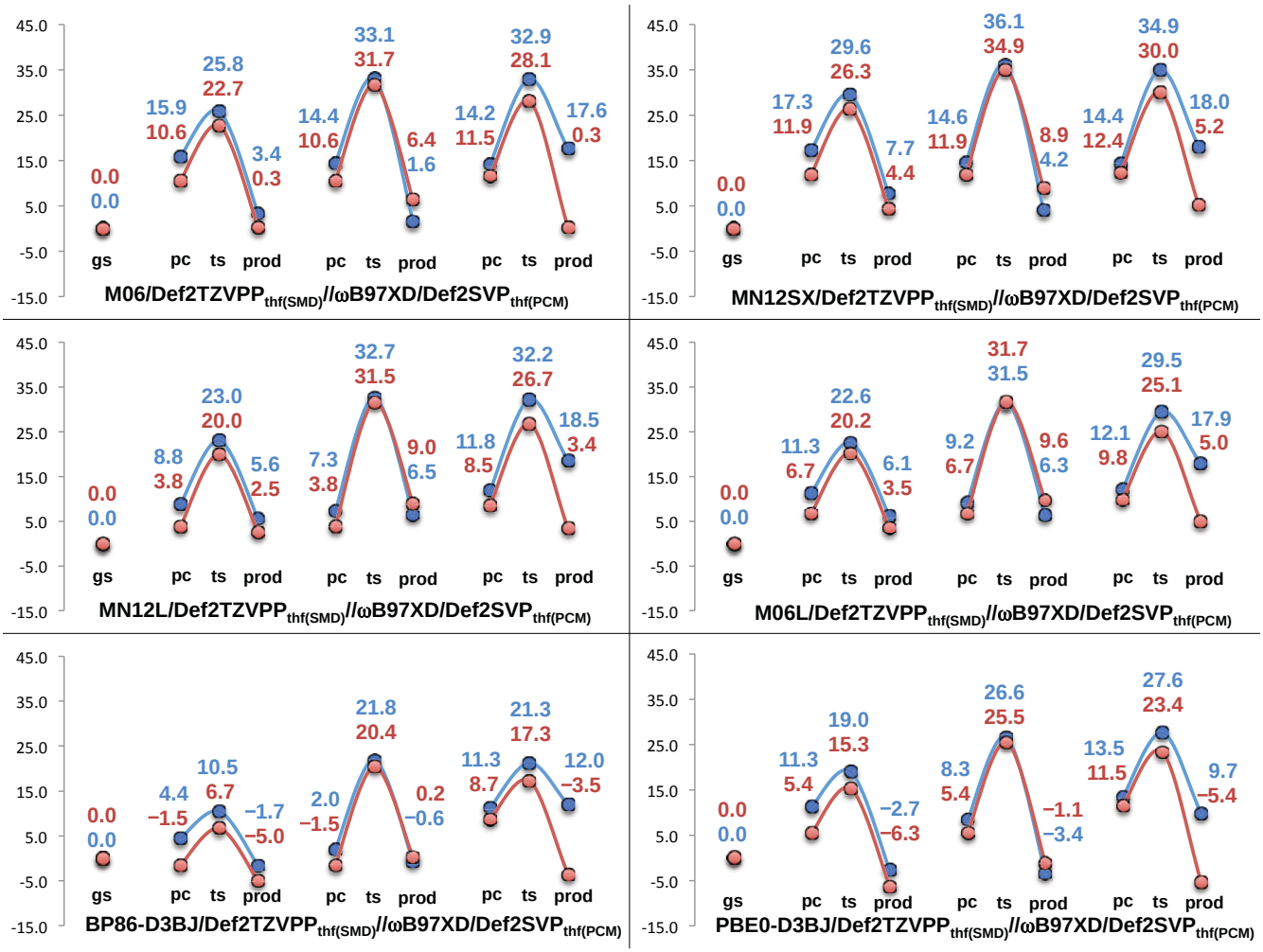

Figure S9-2. Free energy surfaces (ΔG, kcal/mol) for the pathways leading 1,6-propargyl addition, 1,4-allenyl addition and 1,4-propargyl addition to a dienoate relative to allenyl–Cu intermediate bearing either a model NHC ligand ($Me_2C_3H_4N_2$, blue) or a model phosphine ligand (PMe_3, red) with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

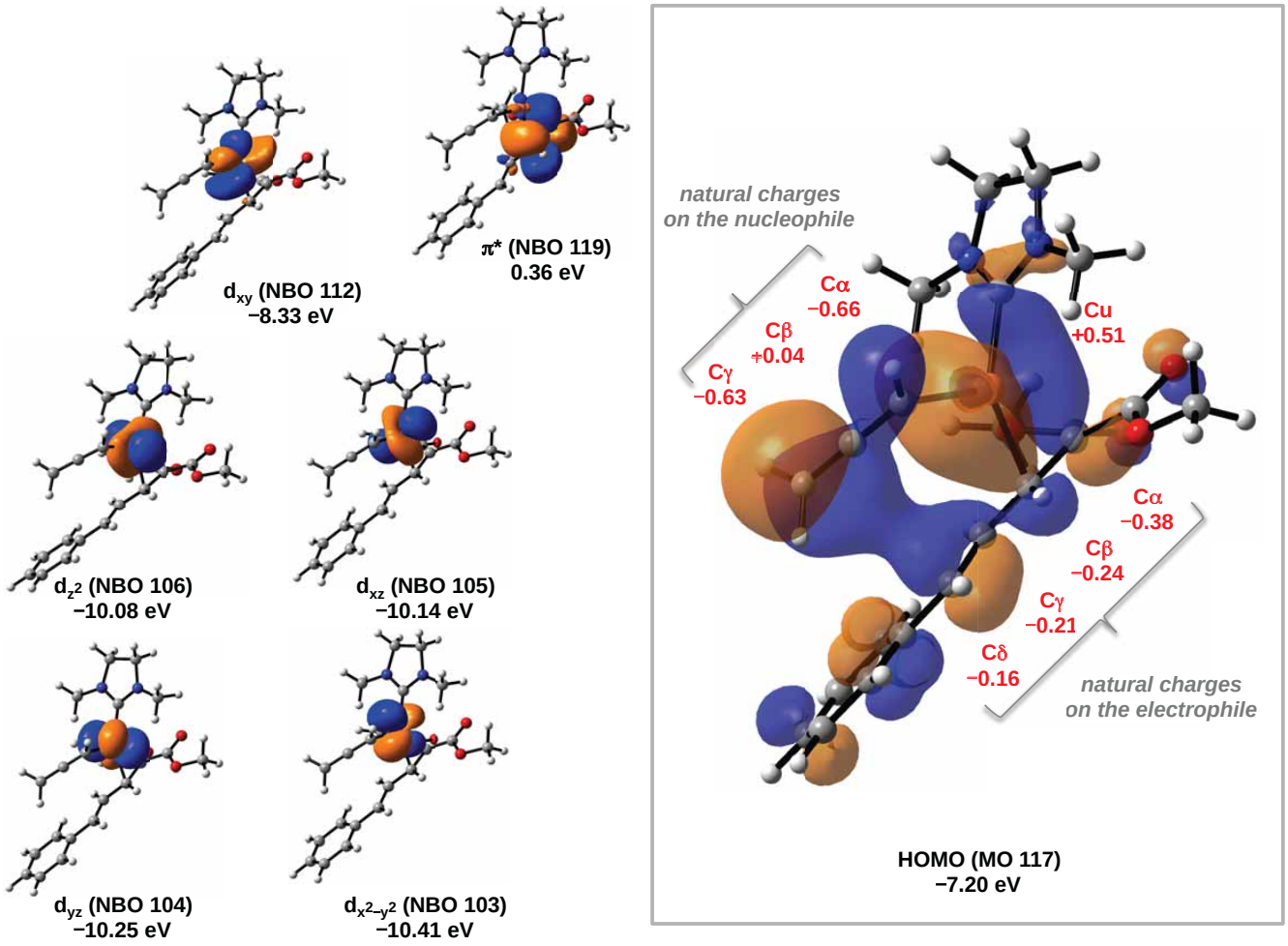

Figure S9-3. Natural bond orbital analysis (NBO; highest NBO = NBO 117) and HOMO (MO 117) for π-complex **PA–Me$_2$NHC–pc$_{1,4AA}$** at the ωB97XD/Def2TZVPP$_{THF(SMD)}$//ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

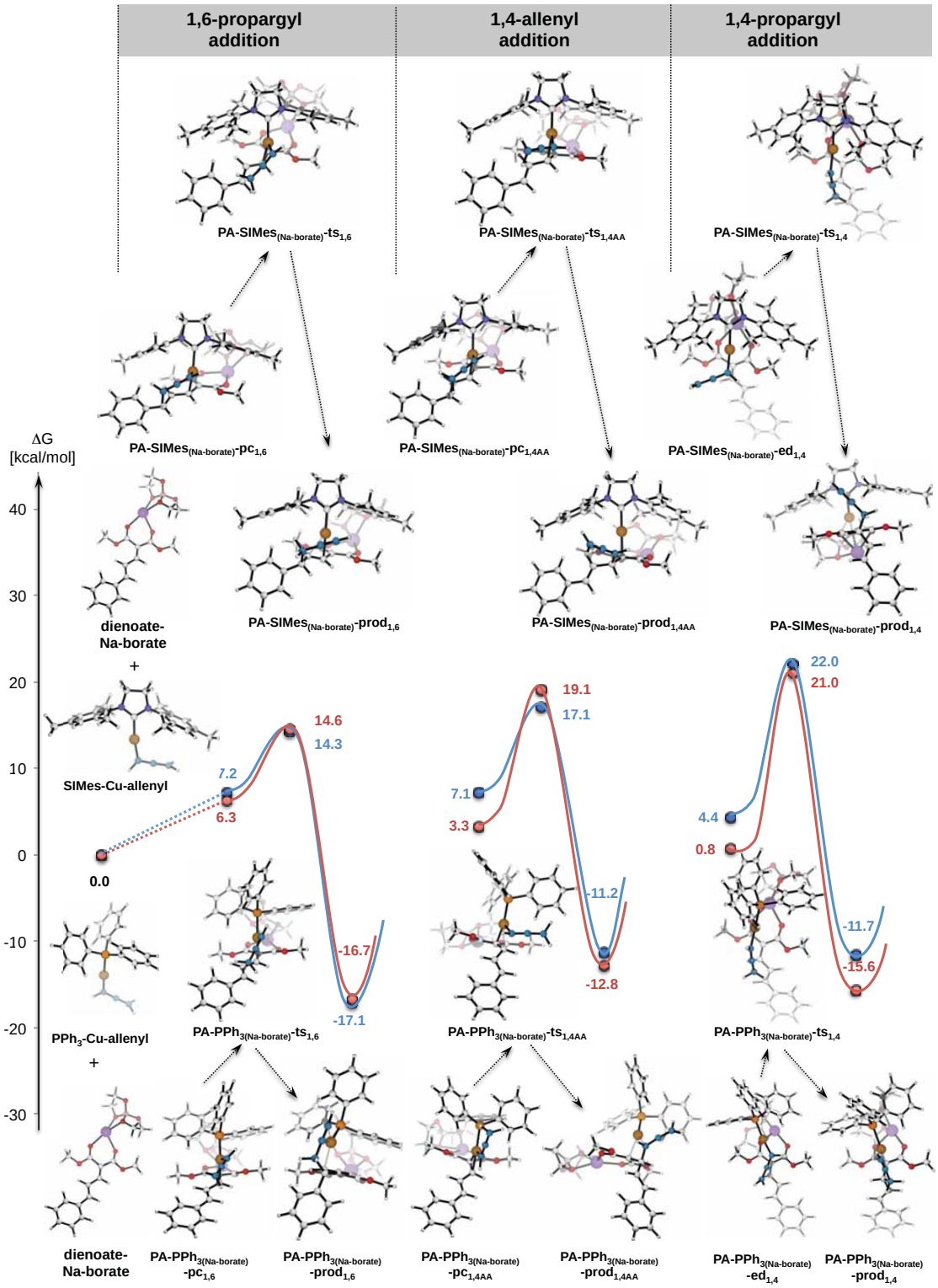

Figure S10-1. Free energy surfaces (ΔG, kcal/mol) for the pathways leading 1,6-propargyl addition, 1,4-allenyl addition and 1,4-propargyl addition to a dienoate bearing a model Na-borate relative to allenyl–Cu intermediate bearing either an NHC ligand (SIMes, blue) or a phosphine ligand (PPh_3, red) at the ωB97XD/Def2TZVPP$_{THF(SMD)}$//ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

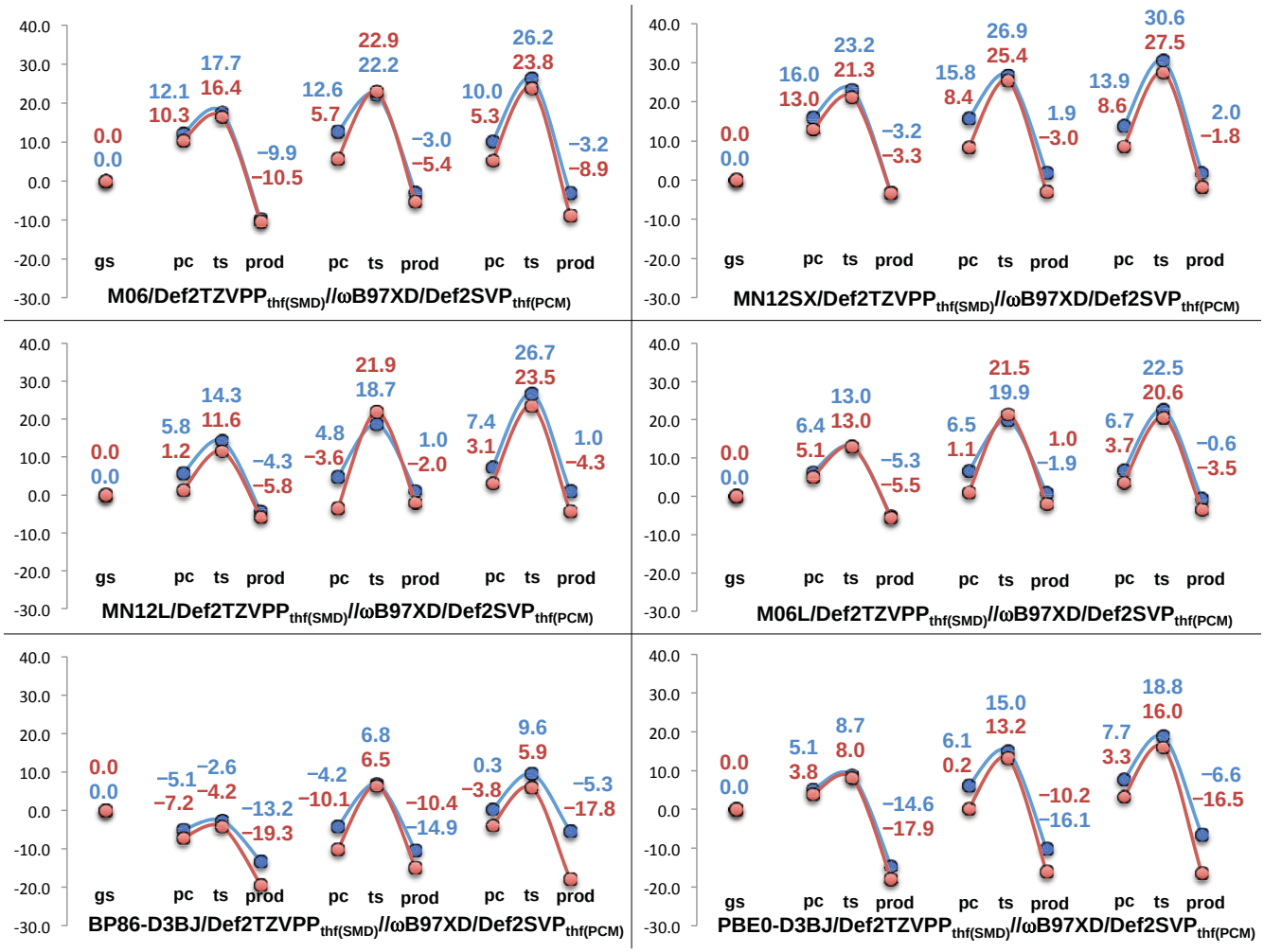

Figure S10-2. Free energy surfaces (ΔG, kcal/mol) for the pathways leading 1,6-propargyl addition, 1,4-allenyl addition and 1,4-propargyl addition to a dienoate bearing a model Na-borate relative to allenyl–Cu intermediate bearing either an NHC ligand (SIMes, blue) or a phosphine ligand (PPh_3, red) with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

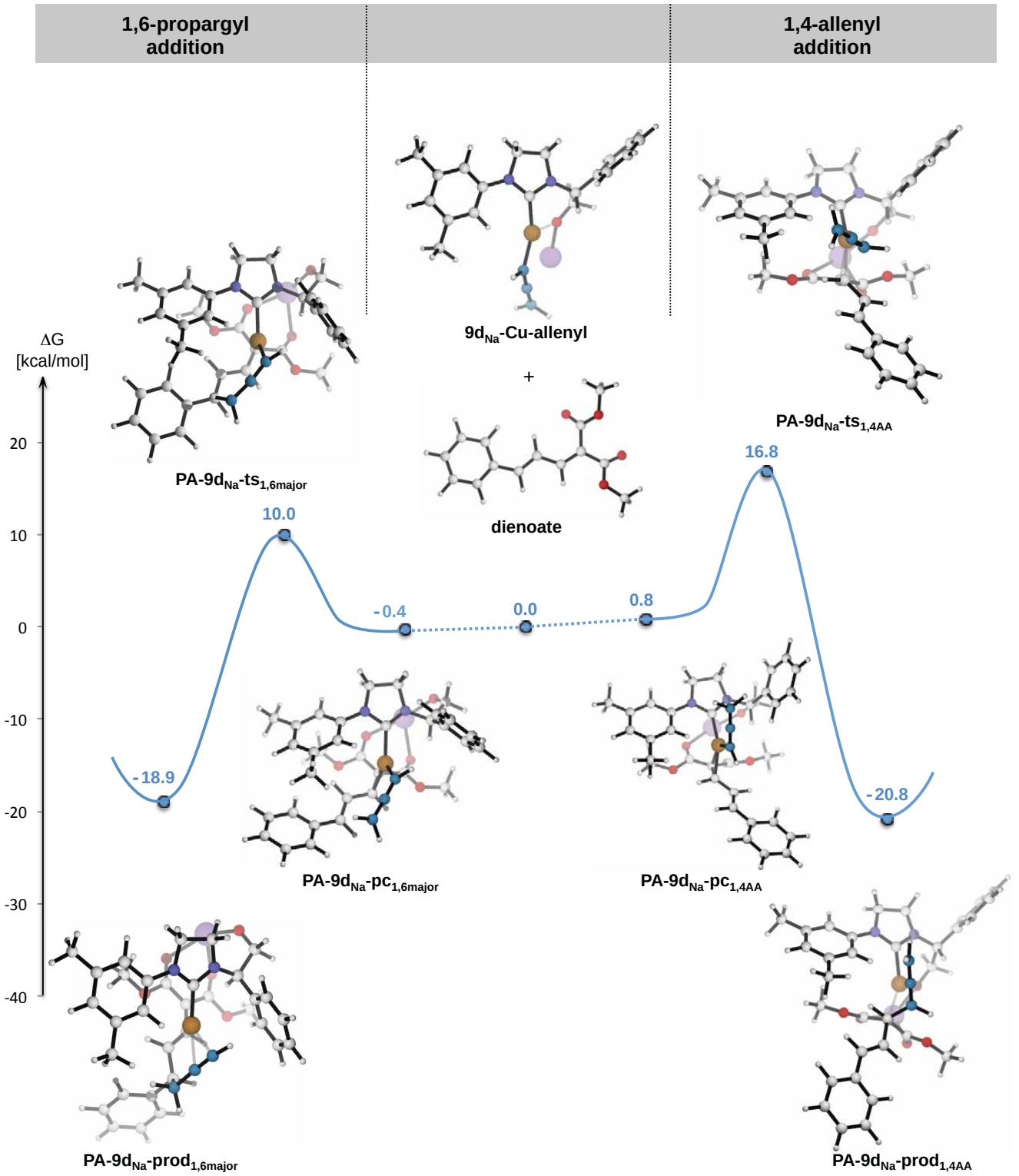

Figure S11-1. Free energy surface (ΔG, kcal/mol) for the pathways leading 1,6-propargyl addition and 1,4-allenyl addition to a dienoate relative to allenyl–Cu intermediate bearing either NHC ligand **9d** at the ωB97XD/Def2TZVPP$_{THF(SMD)}$//ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

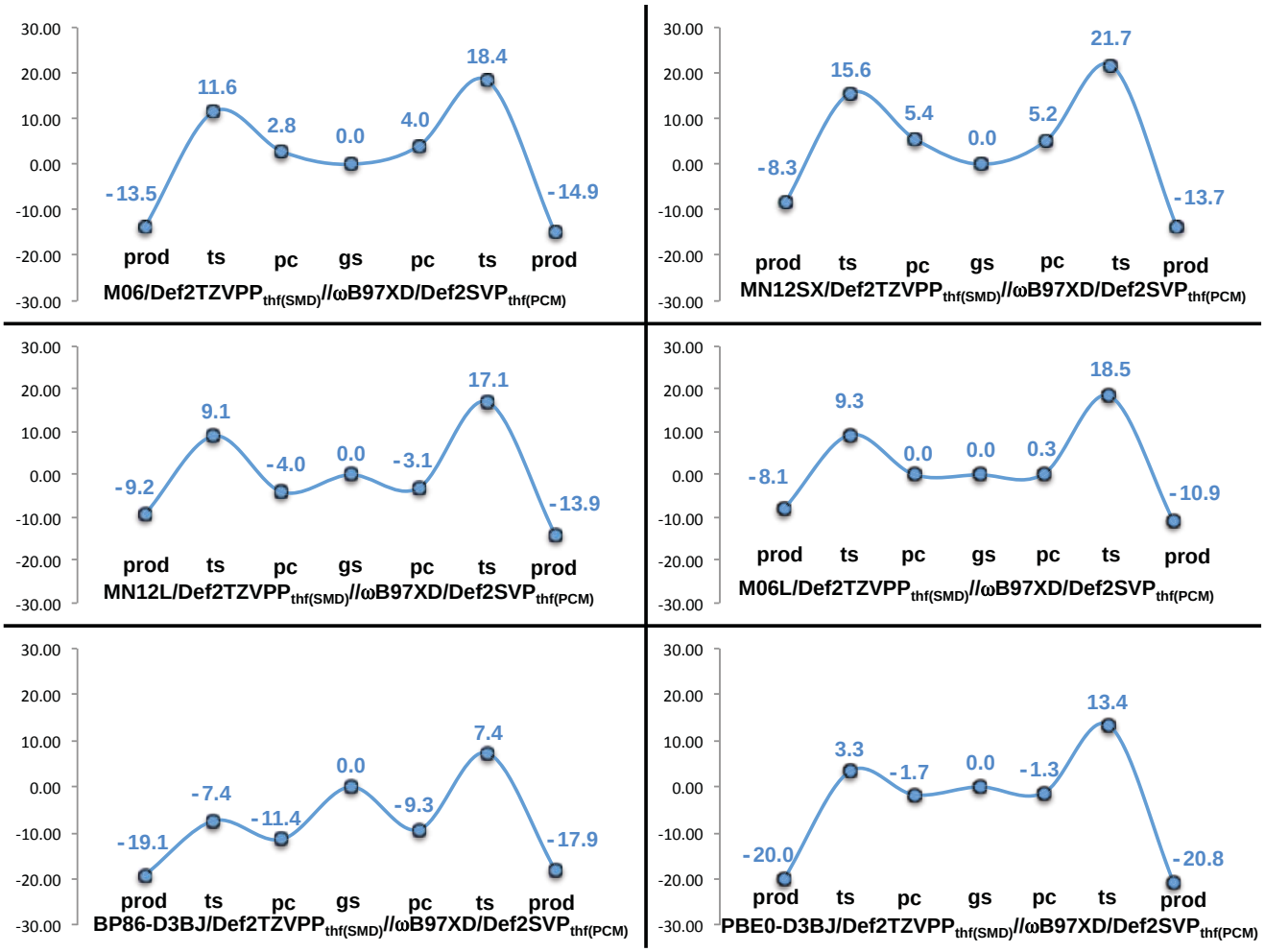

***Figure S11-2*.** Free energy surface (ΔG, kcal/mol) for the pathways leading 1,6-propargyl addition and 1,4-allenyl addition to a dienoate relative to allenyl–Cu intermediate bearing either NHC ligand **9d** with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

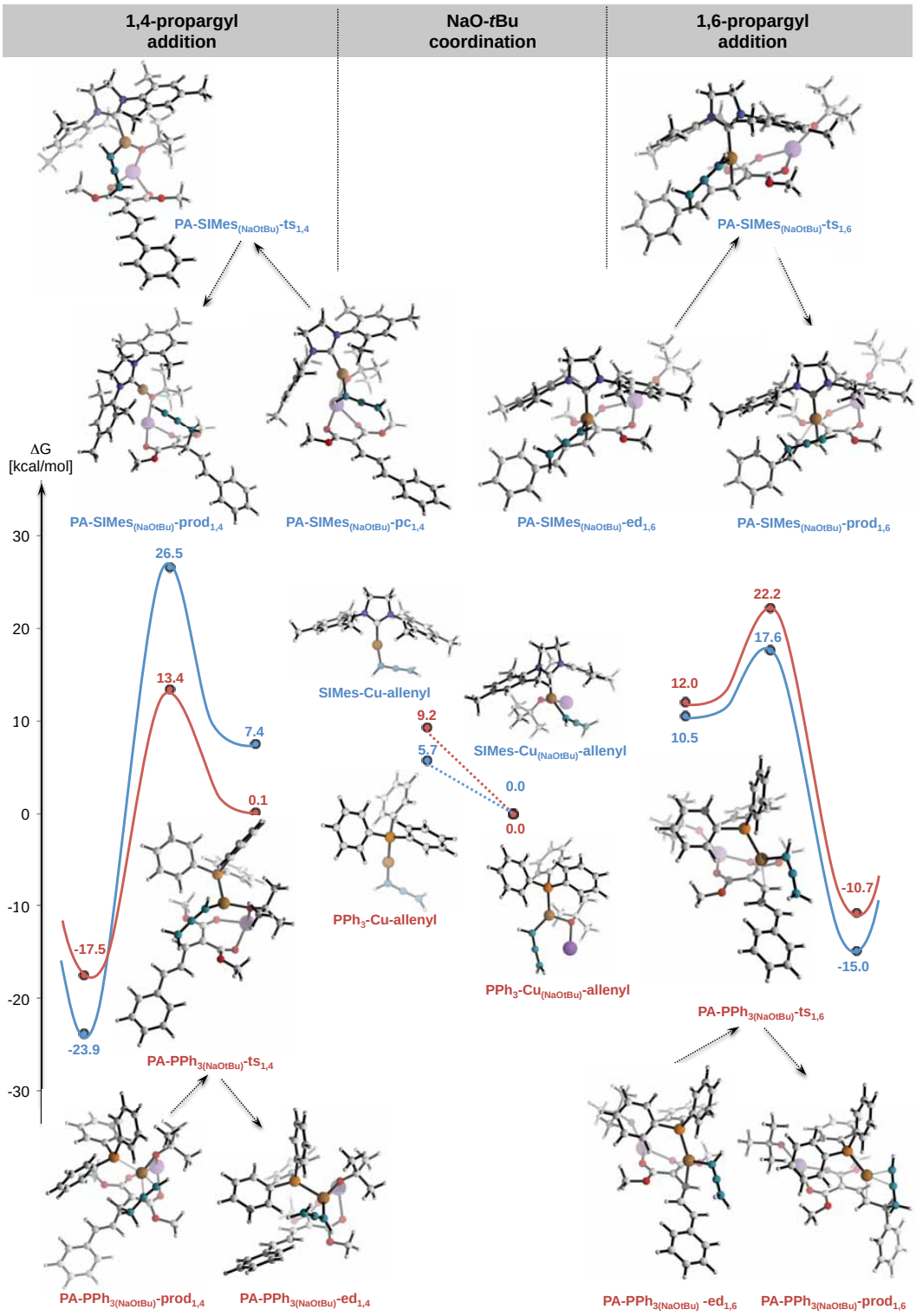

Figure S12-1. Free energy surfaces (ΔG, kcal/mol) for the pathways leading 1,4-propargyl addition and 1,6-propargyl addition to a dienoate relative to allenyl–Cu intermediate bearing a Na–O*t*Bu molecule and either an NHC ligand (SIMes, blue) or a phosphine ligand (PPh_3, red) at the ωB97XD/Def2TZVPP$_{THF(SMD)}$//ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

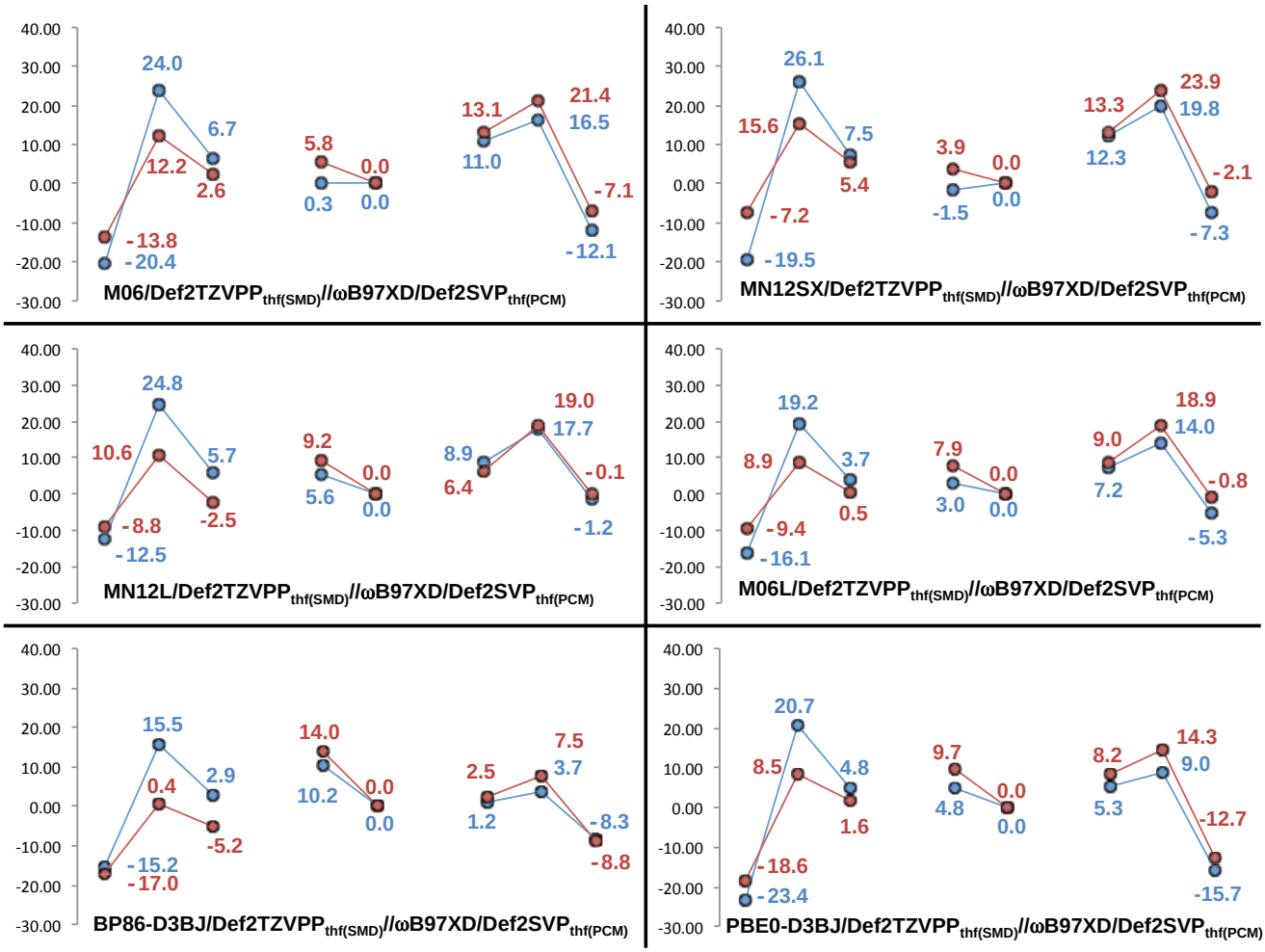

Figure S12-2. Free energy surfaces (ΔG, kcal/mol) for the pathways leading 1,4-propargyl addition and 1,6-propargyl addition to a dienoate relative to allenyl–Cu intermediate bearing a Na–O*t*Bu molecule and either an NHC ligand (SIMes, blue) or a phosphine ligand (PPh_3, red) with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

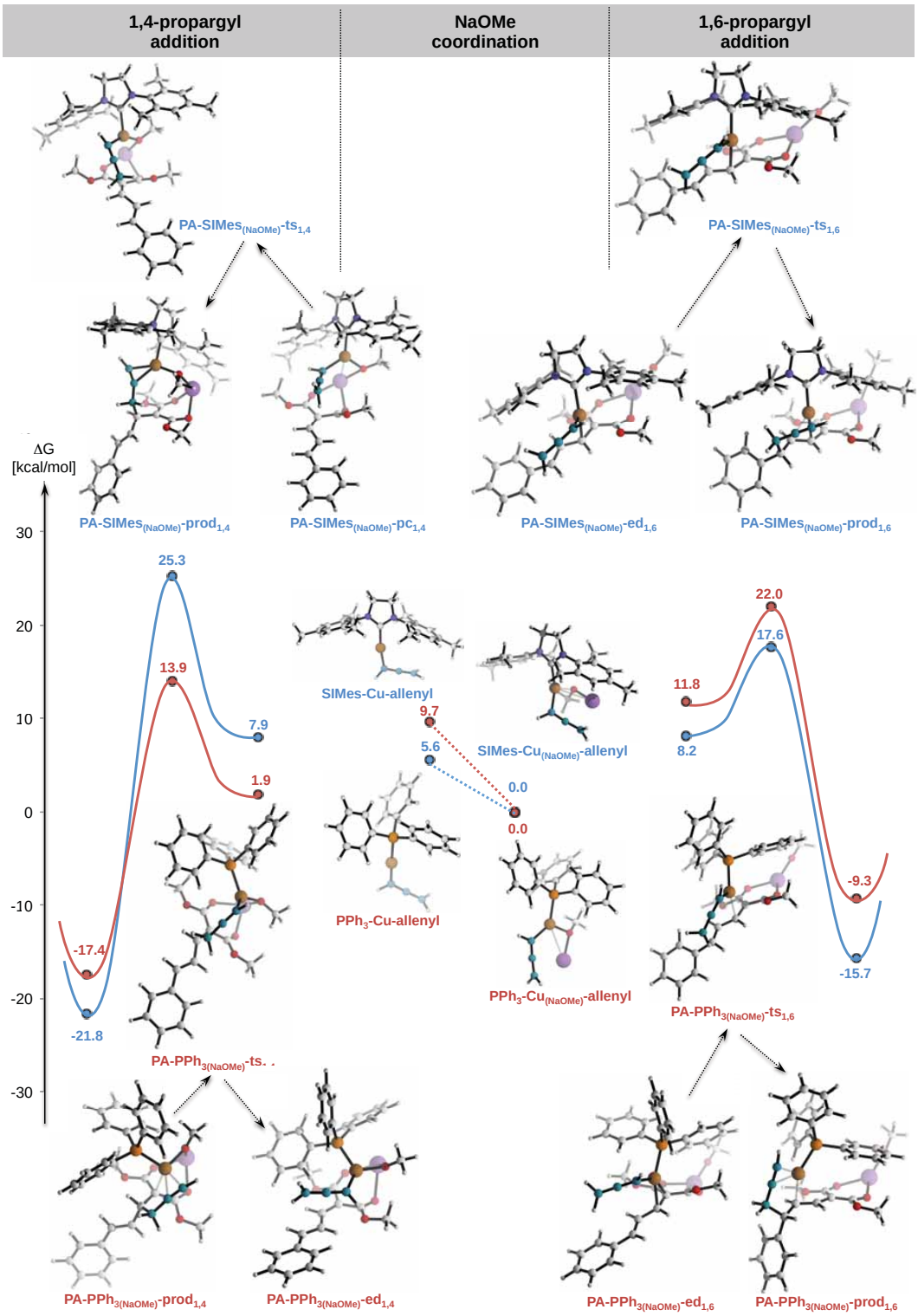

Figure S13-1. Free energy surfaces (ΔG, kcal/mol) for the pathways leading 1,4-propargyl addition and 1,6-propargyl addition to a dienoate relative to allenyl–Cu intermediate bearing a Na–OMe molecule and either an NHC ligand (SIMes, blue) or a phosphine ligand (PPh_3, red) at the ωB97XD/Def2TZVPP$_{THF(SMD)}$//ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

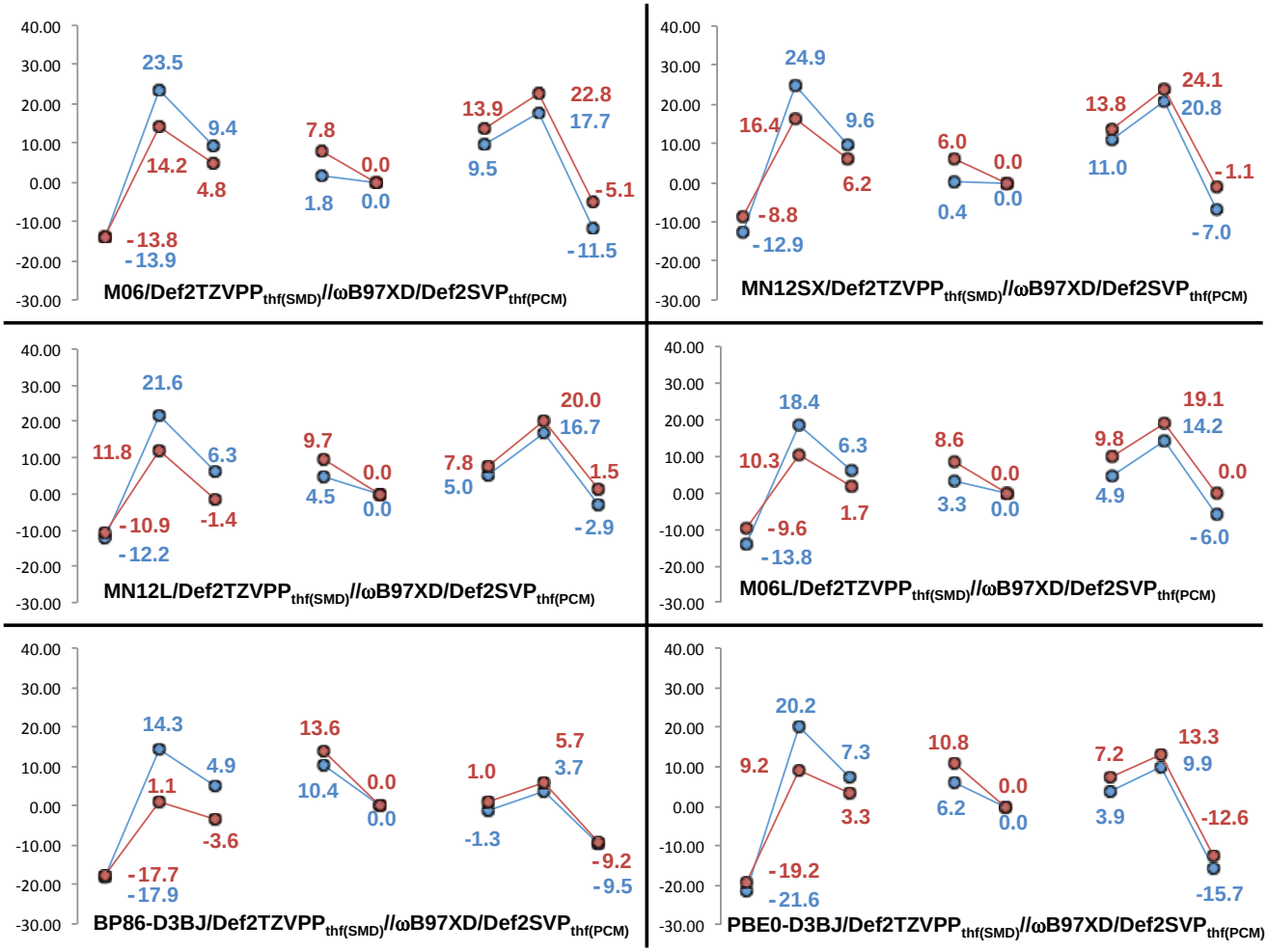

Figure S13-2. Free energy surfaces (ΔG, kcal/mol) for the pathways leading 1,4-propargyl addition and 1,6-propargyl addition to a dienoate relative to allenyl–Cu intermediate bearing a Na–OMe molecule and either an NHC ligand (SIMes, blue) or a phosphine ligand (PPh_3, red) with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

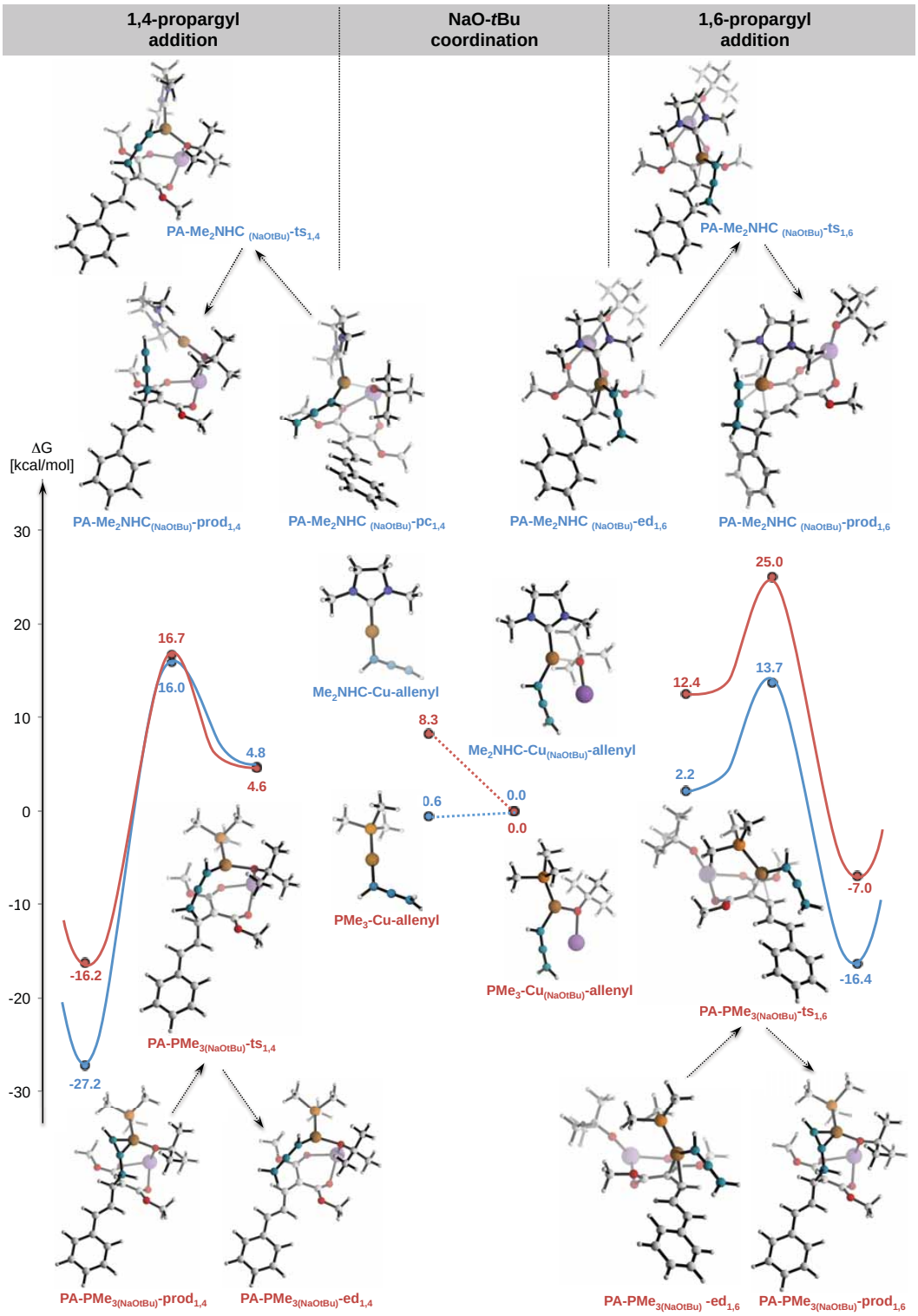

Figure S14-1. Free energy surfaces (ΔG, kcal/mol) for the pathways leading 1,4-propargyl addition and 1,6-propargyl addition to a dienoate relative to allenyl–Cu intermediate bearing a Na–O*t*Bu molecule and either a model NHC ligand (Me_2NHC, blue) or a model phosphine ligand (PMe_3, red) at the ωB97XD/Def2TZVPP$_{THF(SMD)}$//ωB97XD/Def2SVP$_{THF(PCM)}$ level of theory.

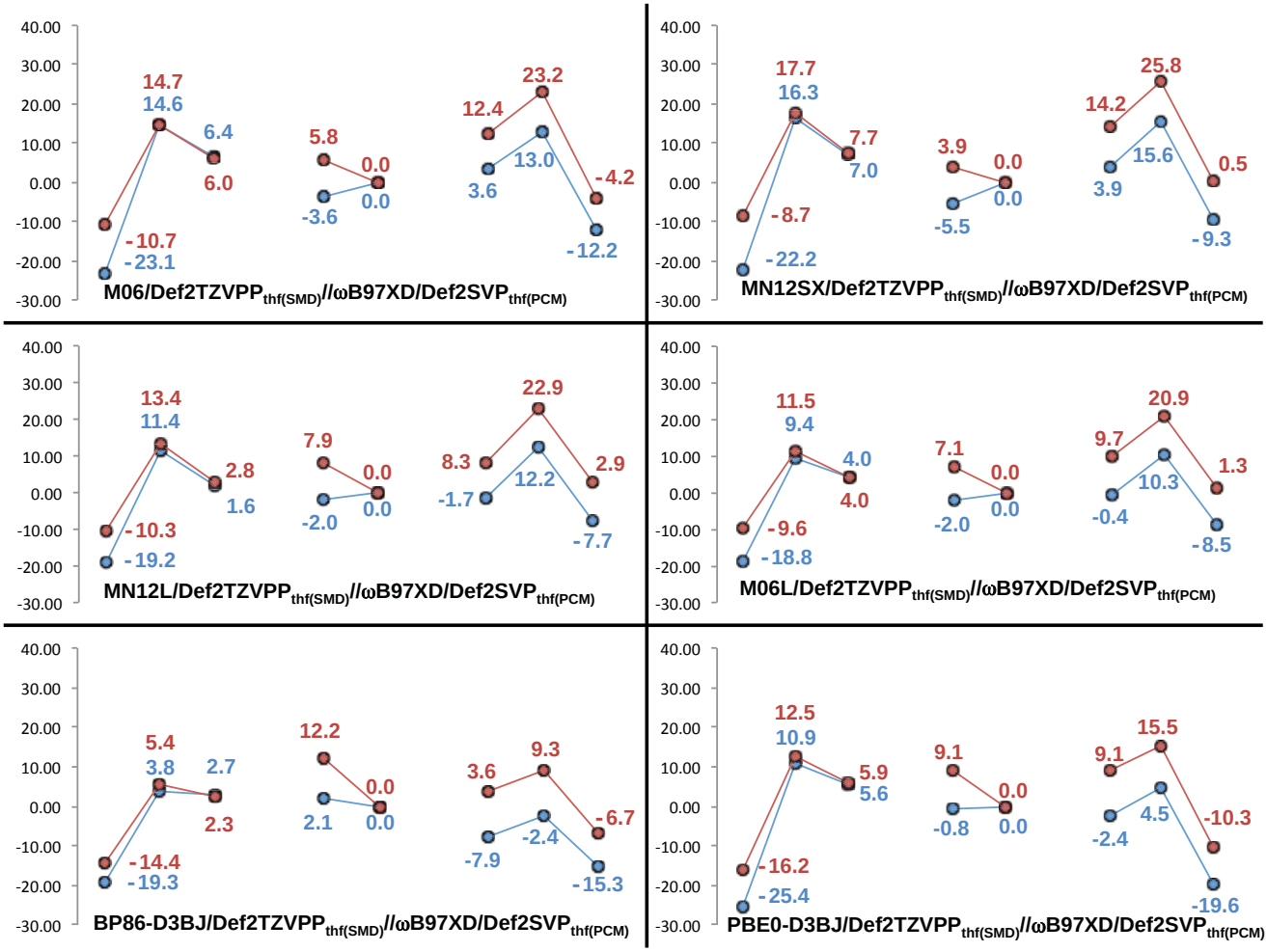

Figure S14-2. Free energy surfaces (ΔG, kcal/mol) for the pathways leading 1,4-propargyl addition and 1,6-propargyl addition to a dienoate relative to allenyl–Cu intermediate bearing a Na–O*t*Bu molecule and either a model NHC ligand (Me_2NHC, blue) or a model phosphine ligand (PMe_3, red) with various density functionals after geometry optimization with ωB97XD/Def2SVP$_{THF(PCM)}$.

Conformer distribution for transition states (Figures S15-1 to S15-9)

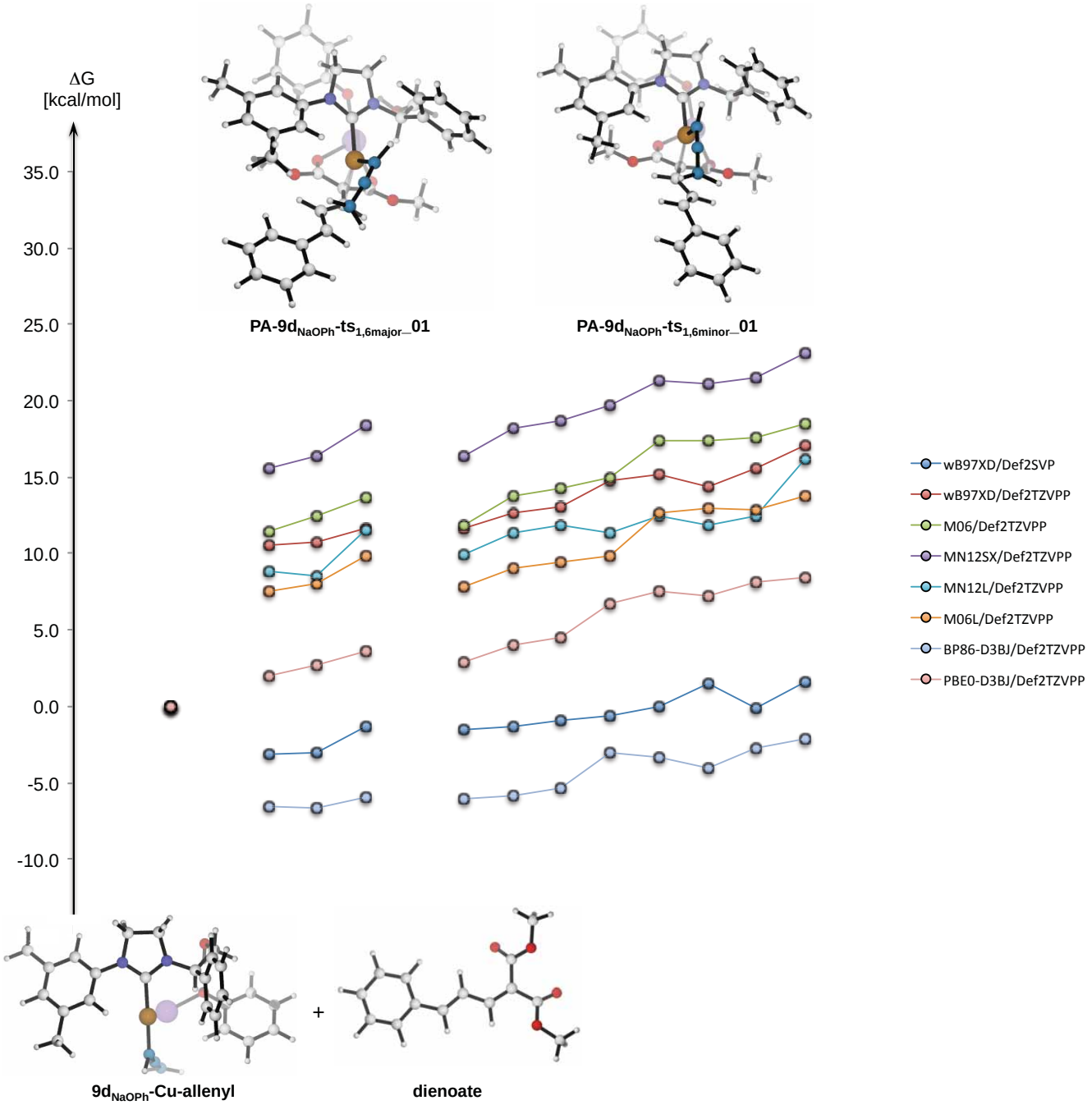

Figure S15-1. Conformer distribution (ΔG, kcal/mol) for the major (**PA–9d$_{NaOPh}$–ts$_{1,6major_}$01**) and minor (**PA–9d$_{NaOPh}$–ts$_{1,6minor_}$01**) transition states leading 1,6-propargyl addition relative to allenyl–Cu intermediate **9d$_{NaOPh}$–Cu-allenyl**; conformers are ordered from low to high energy according to the M06/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{THF(PCM)}$ energies.

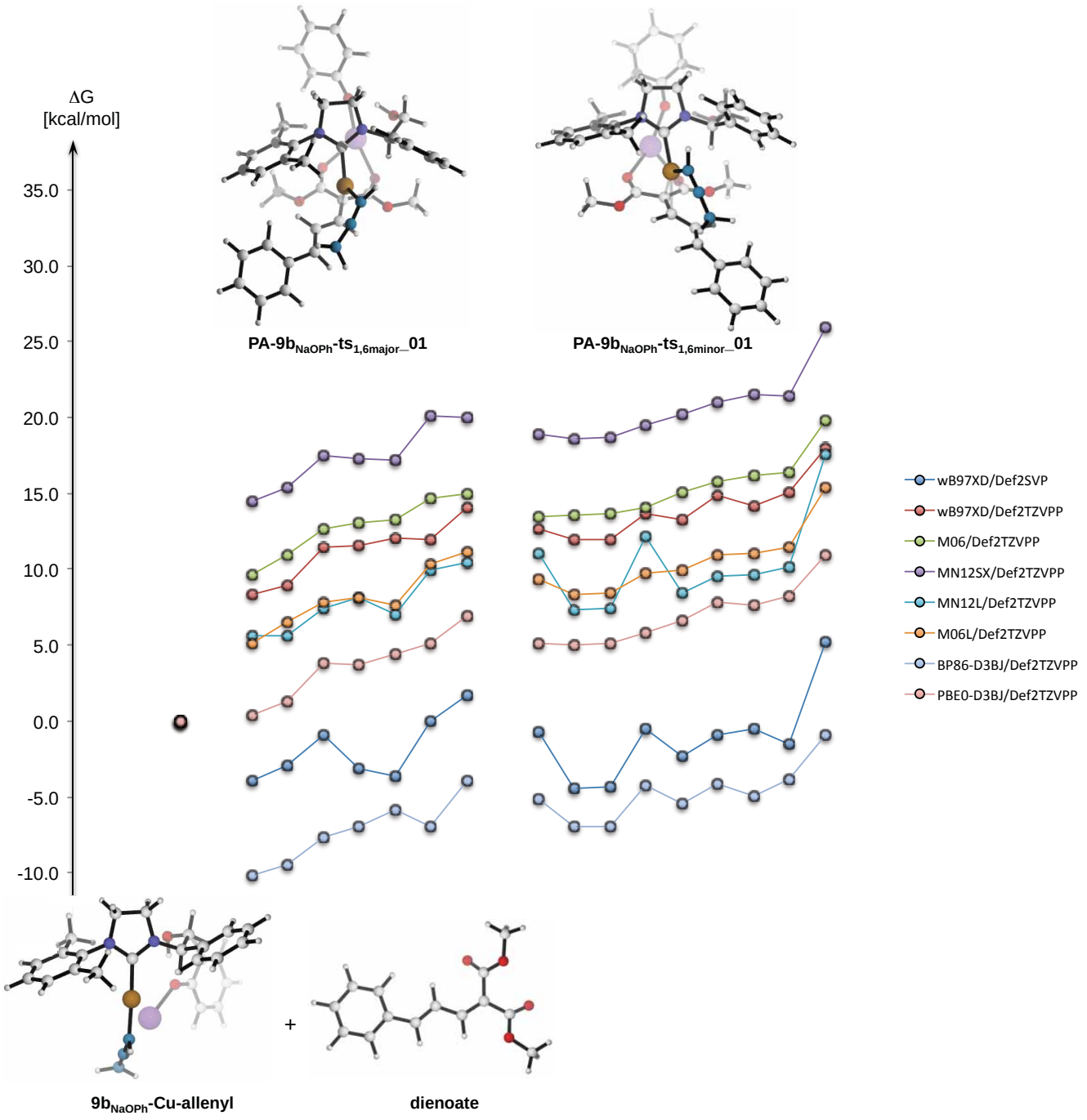

Figure S15-2. Conformer distribution (ΔG, kcal/mol) for the major (**PA–9b$_{NaOPh}$–ts$_{1,6major_}$01**) and minor (**PA–9b$_{NaOPh}$–ts$_{1,6minor_}$01**) transition states leading 1,6-propargyl addition relative to allenyl–Cu intermediate **9b$_{NaOPh}$–Cu-allenyl**; conformers are ordered from low to high energy according to the M06/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{THF(PCM)}$ energies.

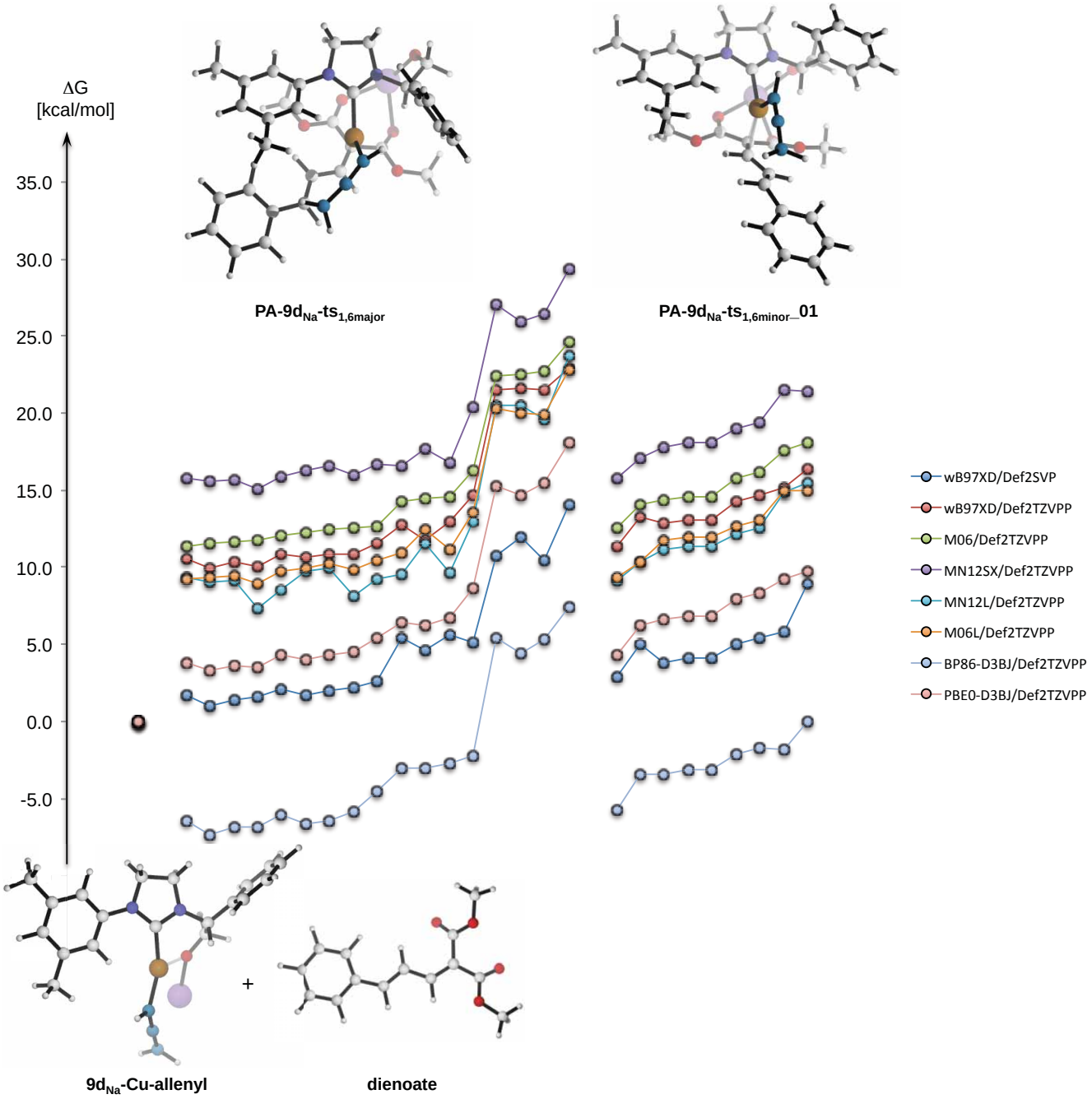

Figure S15-3. Conformer distribution (ΔG,kcal/mol) for the major (**PA-9d$_{Na}$-ts$_{1,6major}$_01**) and minor (**PA-9d$_{Na}$-ts$_{1,6minor}$_01**) transition states leading 1,6-propargyl addition relative to allenyl–Cu intermediate **9d$_{Na}$–Cu–allenyl**; conformers are ordered from low to high energy according to the M06/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{THF(PCM)}$ energies.

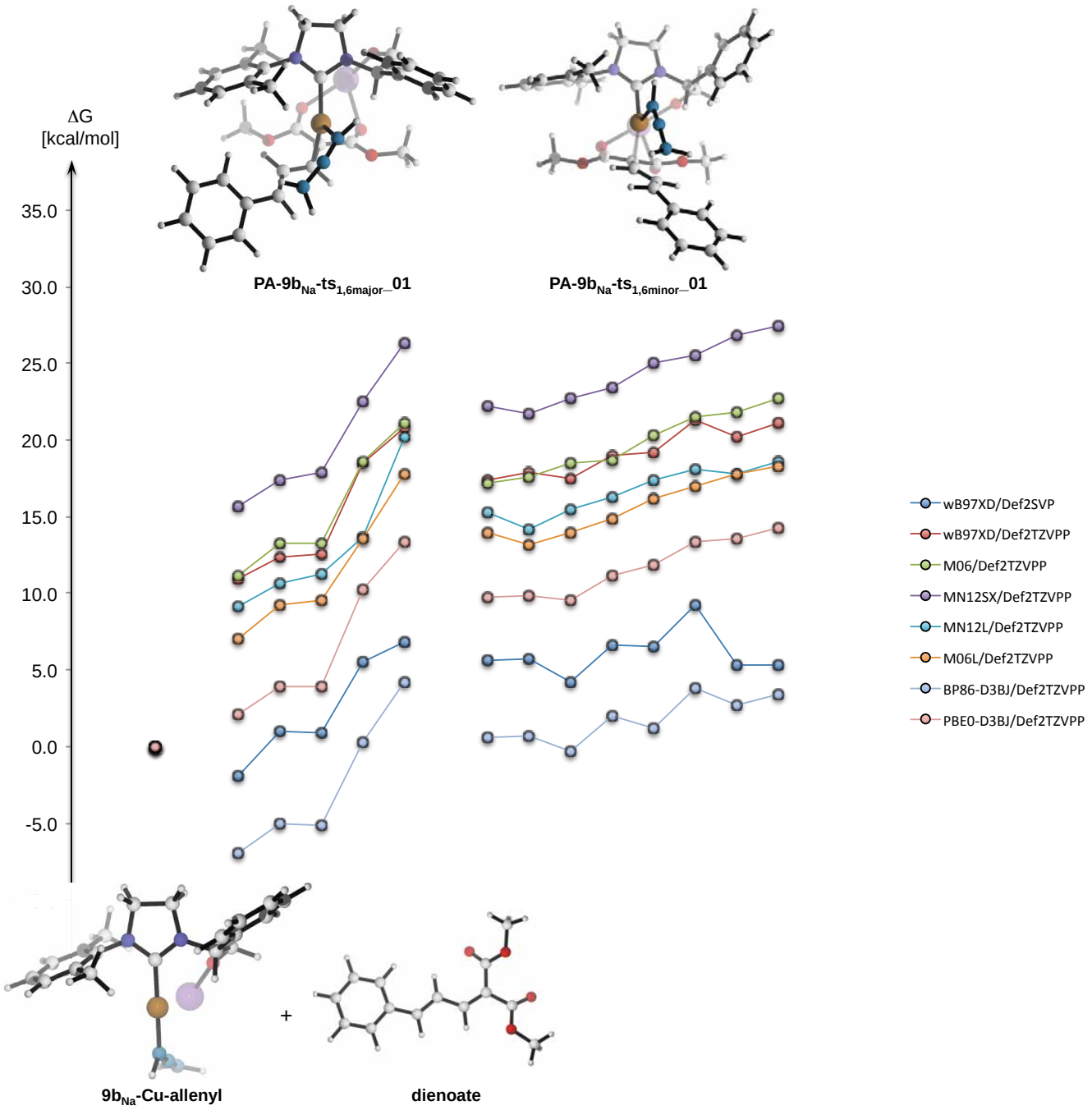

Figure S15-4. Conformer distribution (ΔG, kcal/mol) for the major (**PA–9b$_{Na}$–ts$_{1,6major}$_01**) and minor (**PA–9b$_{Na}$–ts$_{1,6minor}$_01**) transition states leading 1,6-propargyl addition relative to allenyl–Cu intermediate **9b$_{Na}$-Cu-allenyl**; conformers are ordered from low to high energy according to the M06/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{THF(PCM)}$ energies.

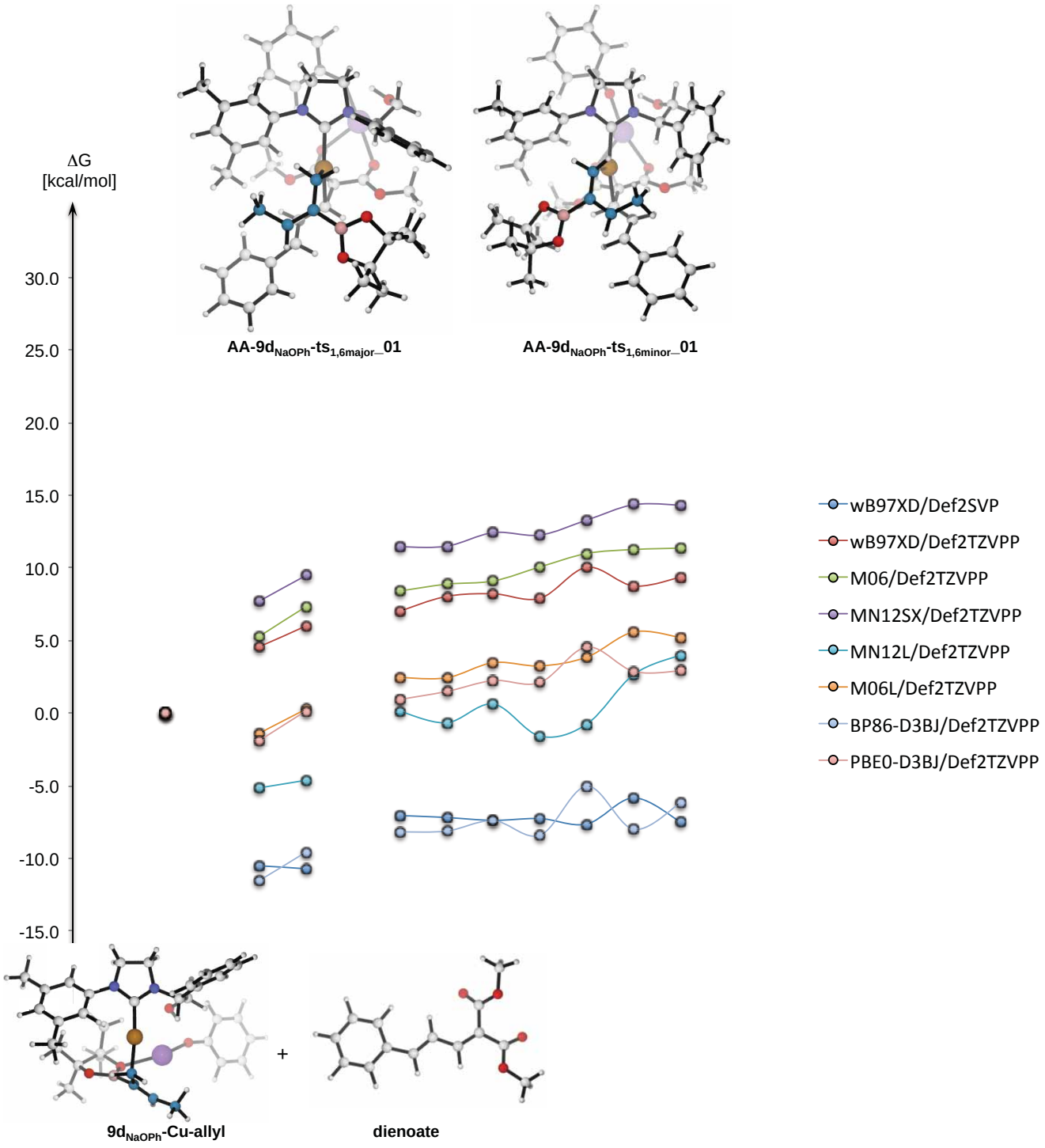

Figure S15-5. Conformer distribution (ΔG, kcal/mol) for the major (**AA-9d$_{NaOPh}$-ts$_{1,6major}$_01**) and minor (**AA–9d$_{NaOPh}$–ts$_{1,6minor}$_01**) transition states leading 1,6-propargyl addition relative to allyl–Cu intermediate **9d$_{NaOPh}$-Cu-allyl**; conformers are ordered from low to high energy according to the M06/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{THF(PCM)}$ energies.

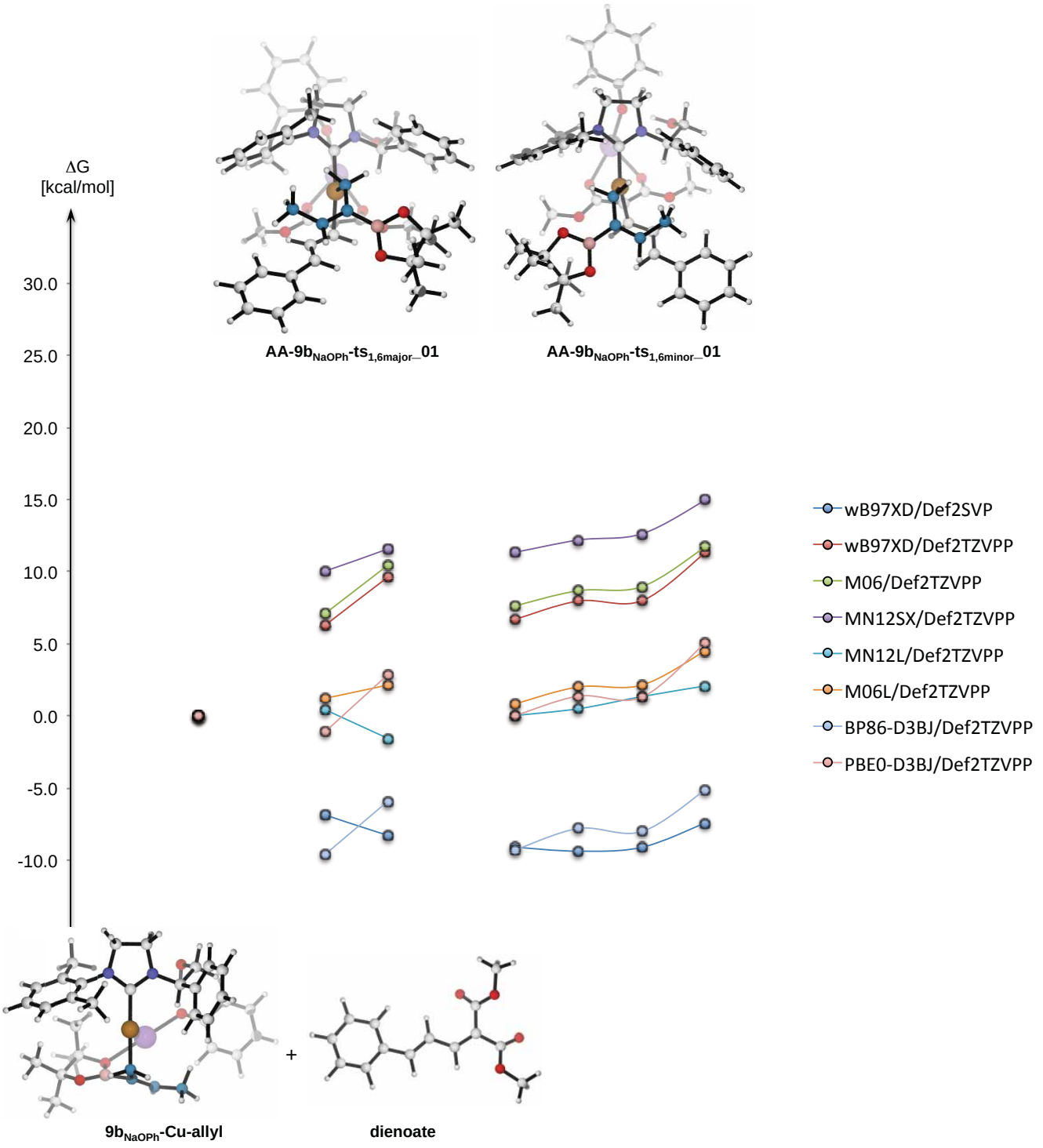

Figure S15-6. Conformer distribution (ΔG, kcal/mol) for the major (**AA-9b$_{NaOPh}$-ts$_{1,6major}$_01**) and minor (**AA–9b$_{NaOPh}$–ts$_{1,6minor}$_01**) transition states leading 1,6-propargyl addition relative to allyl–Cu intermediate **9b$_{NaOPh}$-Cu-allyl**; conformers are ordered from low to high energy according to the M06/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{THF(PCM)}$ energies.

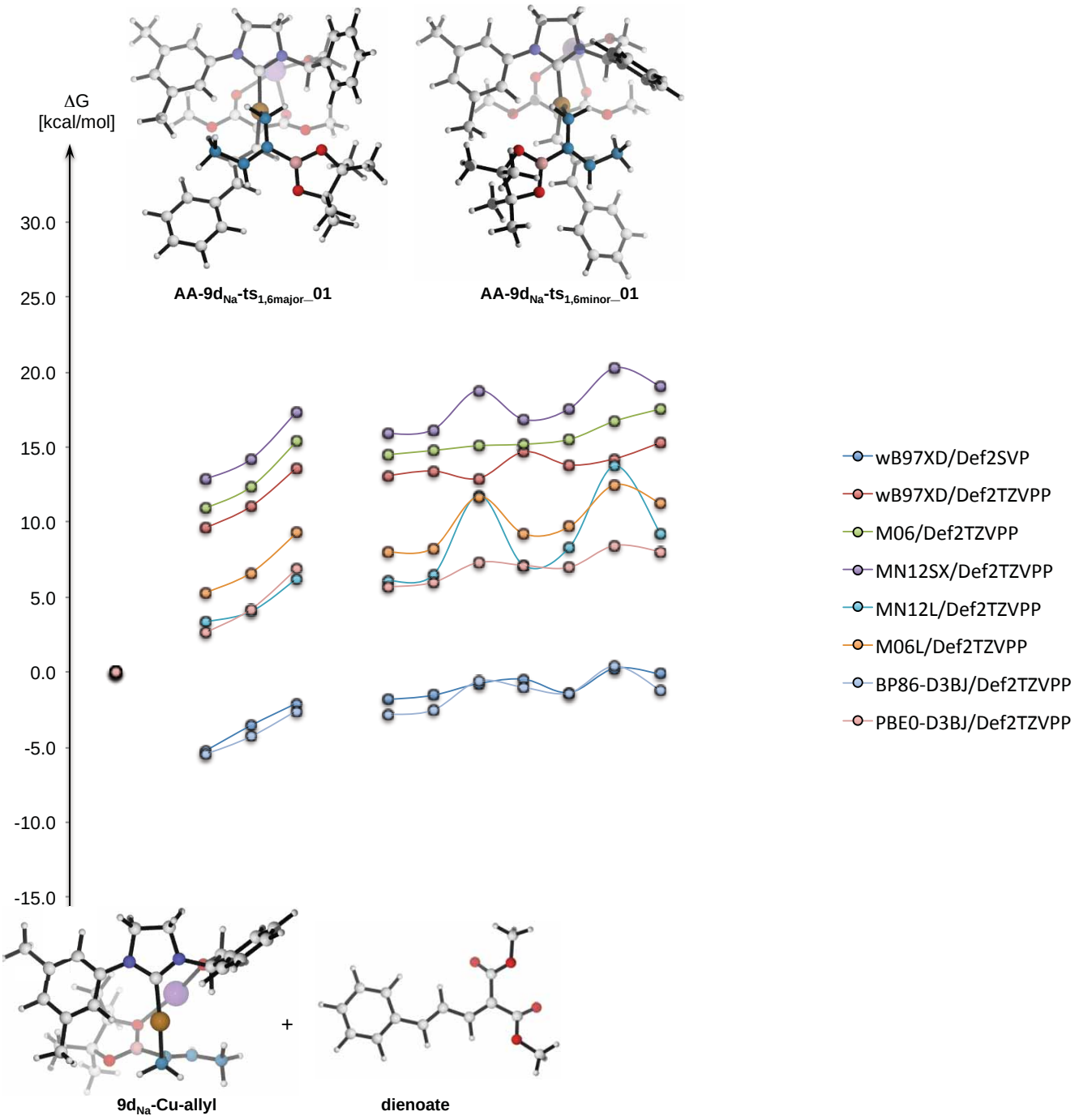

Figure S15-7. Conformer distribution (ΔG, kcal/mol) for the major (**AA-9d$_{Na}$-ts$_{1,6major}$_01**) and minor (**AA-9d$_{Na}$-ts$_{1,6minor}$_01**) transition states leading 1,6-propargyl addition relative to allyl–Cu intermediate **9d$_{Na}$-Cu-allyl**; conformers are ordered from low to high energy according to the M06/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{THF(PCM)}$ energies.

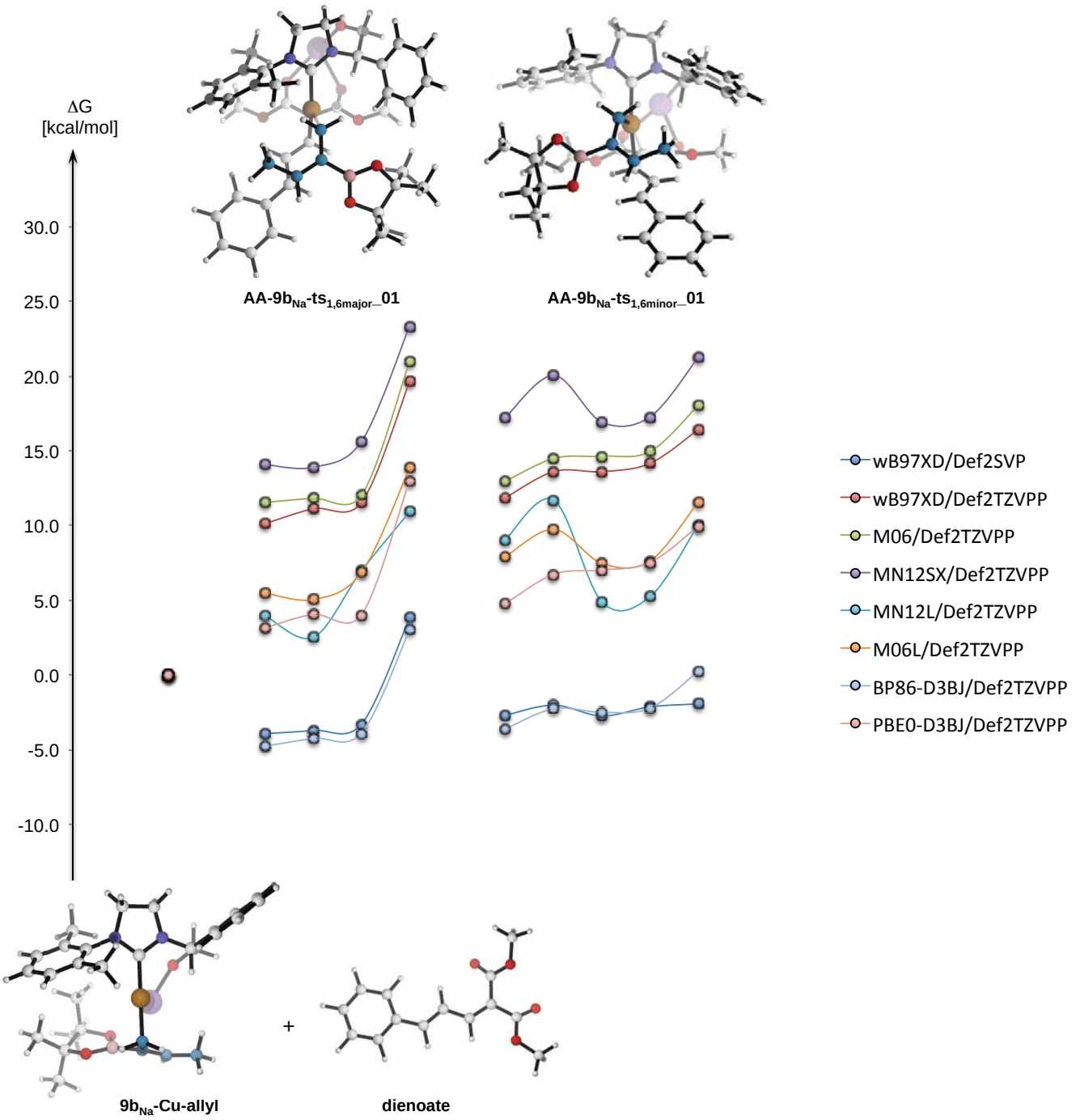

Figure S15-8. Conformer distribution (ΔG, kcal/mol) for the major (**AA–9b$_{Na}$–ts$_{1,6major}$_01**) and minor (**AA-9b$_{Na}$-ts$_{1,6minor}$_01**) transition states leading 1,6-propargyl addition relative to allyl–Cu intermediate **9b$_{Na}$–Cu–allyl**; conformers are ordered from low to high energy according to the M06/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{THF(PCM)}$ energies.

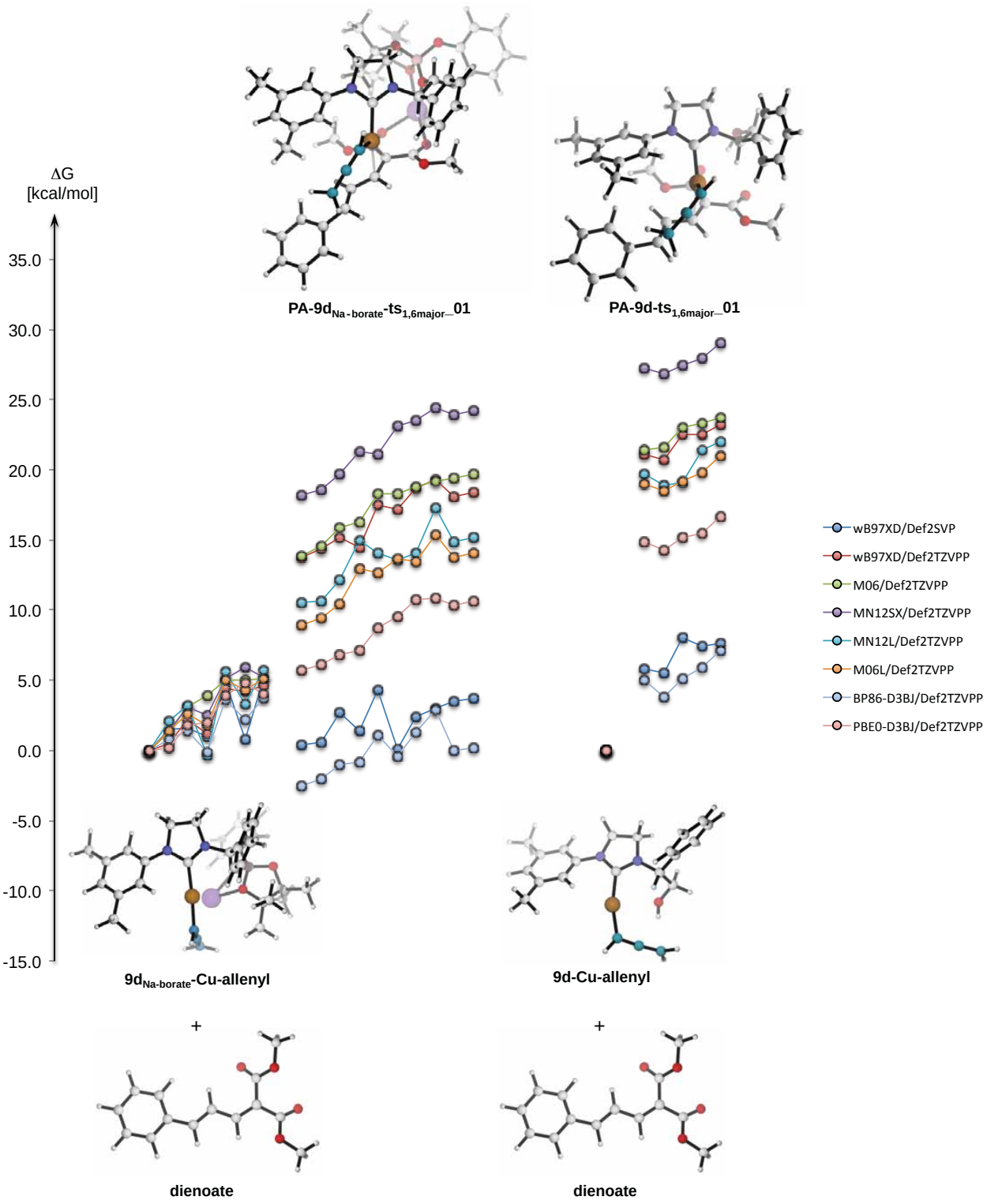

Figure S15-9. Conformer distribution (ΔG, kcal/mol) for the major transition states **PA–9d$_{Na-borate}$–ts$_{1,6major}$_01** and **PA–9d–ts$_{1,6major}$_01**) leading 1,6-propargyl addition relative to allenyl–Cu intermediates **9d$_{Na-borate}$–Cu–allenyl** and **9d-Cu-allenyl**; conformers are ordered from low to high energy according to the M06/Def2TZVPP$_{THF(SMD)}$// ωB97XD/Def2SVP$_{THF(PCM)}$ energies.

5. Energies and Gibbs Free Energies

Table S1. Optimization in Figures S1-1–S15-9 with ωB97XD/Def2SVP$_{thf(PCM)}$

structure	E [hartree]	E(sum) [hartree]	ΔE [kcal/mol]	G [hartree]	G(sum) [hartree]	ΔG [kcal/mol]	ΔG_{Corr} [kcal/mol]	FREQ [cm^{-1}]
Figure S1-1								
dienoate	-841.92707848			-841.718723				24.6
PhOH	-307.15051815			-307.073623				229.5
NaOPh	-468.85364944			-468.794061				15.7
tBuOH	-233.44101319			-233.333432				210.6
NaOtBu	-395.11737857			-395.027576				32.7
PhOBpin	-717.46665894			-717.228760				34.0
(PhO)2BpinNa	-1186.36814498			-1186.044662				14.0
9d-Cu-allenyl	-2677.36469942	-3914.40915647	0.0	-2677.000607	-3913.746906	0.0	0.0	18.9
PA-9d(Na)-ts(1,6major)	-3681.01674239	-3914.45775558	-30.5	-3680.427020	-3913.760452	-8.5	22.0	-425.8
9d-Cu-allenyl	-2677.36469942	-3988.14542734	0.0	-2677.000607	-3987.513391	0.0	0.0	18.9
PA-9d(Na)-ts(1,6major)	-3681.01674239	-3988.16726054	-13.7	-3680.427020	-3987.500643	8.0	21.7	-425.8
9d-Cu-allenyl	-2677.36469942	-3988.14542734	0.0	-2677.000607	-3987.513391	0.0	0.0	18.9
PA-9d(NaOPh)-ts(1,6major)	-3988.22213482	-3988.22213482	-48.1	-3987.529839	-3987.529839	-10.3	37.8	-455.1
9d-Cu-allenyl	-2677.36469942	-3519.29177790	0.0	-2677.000607	-3518.719330	0.0	0.0	18.9
PA-9d-ts(1,6major)	-3519.31441637	-3519.31441637	-14.2	-3518.710549	-3518.710549	5.5	19.7	-439.9
9d-Cu-allenyl	-2677.36469942	-4705.61208628	30.0	-2677.000607	-4704.742151	13.7	-16.3	18.9
9d-Cu-allenyl	-2677.36469942	-4705.65992288	0.0	-2677.000607	-4704.763992	0.0	0.0	18.9
PA-9d(Naborate)-ts(1,6major)	-4398.56325172	-4705.71376987	-33.8	-4397.705820	-4704.779443	-9.7	24.1	-433.7
Figure S2-1								
PA-9d(NaOPh)-prod(1,6major)	-3988.27463791	-3988.27463791	-57.3	-3987.579601	-3987.579601	-34.3	23.0	15.8
PA-9d(NaOPh)-ts(1,6major)	-3988.22213482	-3988.22213482	-24.4	-3987.529839	-3987.529839	-3.1	21.3	-455.1
PA-9d(NaOPh)-pc(1,6major)	-3988.23491900	-3988.23491900	-32.4	-3987.543634	-3987.543634	-11.8	20.6	15.6
9d(NaOPh)-Cu-allenyl	-3146.25617778	-3988.18325626	0.0	-3145.806149	-3987.524872	0.0	0.0	11.9
9b(NaOPh)-Cu-allenyl	-3146.25183127	-3988.17890975	0.0	-3145.801041	-3987.519764	0.0	0.0	14.5
PA-9b(NaOPh)-pc(1,6major)	-3988.22941216	-3988.22941216	-31.7	-3987.537711	-3987.537711	-11.3	20.4	14.7
PA-9b(NaOPh)-ts(1,6major)	-3988.21834759	-3988.21834759	-24.7	-3987.526031	-3987.526031	-3.9	20.8	-441.8
PA-9b(NaOPh)-prod(1,6major)	-3988.26800024	-3988.26800024	-55.9	-3987.573233	-3987.573233	-33.6	22.4	17.1

PA-9d(NaOPh)-prod(1,6minor)	-3988.26945033	-3988.26945033	-54.1	-3987.576186	-3987.576186	-32.2	21.9	17.6
PA-9d(NaOPh)-ts(1,6minor)	-3988.21792967	-3988.21792967	-21.8	-3987.527227	-3987.527227	-1.5	20.3	-450.4
PA-9d(NaOPh)-pc(1,6minor)	-3988.23046303	-3988.23046303	-29.6	-3987.540361	-3987.540361	-9.7	19.9	12.7
9d(NaOPh)-Cu-allenyl	-3146.25617778	-3988.18325626	0.0	-3145.806149	-3987.524872	0.0	0.0	11.9
9b(NaOPh)-Cu-allenyl	-3146.25183127	-3988.17890975	0.0	-3145.801041	-3987.519764	0.0	0.0	14.5
PA-9b(NaOPh)-pc(1,6minor)	-3988.23004284	-3988.23004284	-32.1	-3987.538461	-3987.538461	-11.7	20.4	13.9
PA-9b(NaOPh)-ts(1,6minor)	-3988.21330777	-3988.21330777	-21.6	-3987.520948	-3987.520948	-0.7	20.8	-465.4
PA-9b(NaOPh)-prod(1,6minor)	-3988.27007628	-3988.27007628	-57.2	-3987.574523	-3987.574523	-34.4	22.8	22.1

Figure S3-1

AA-9d(NaOPh)-prod(1,6major)	-4439.10399315	-4439.10399315	-68.1	-4438.191242	-4438.191242	-42.1	26.0	15.5
AA-9d(NaOPh)-ts(1,6major)	-4439.05034678	-4439.05034678	-34.4	-4438.140890	-4438.140890	-10.5	23.9	-323.9
AA-9d(NaOPh)-pc(1,6major)	-4439.05320939	-4439.05320939	-36.2	-4438.144765	-4438.144765	-12.9	23.3	15.8
9d(NaOPh)-Cu-allyl	-3597.06845638	-4438.99553486	0.0	-3596.405435	-4438.124158	0.0	0.0	14.7
9b(NaOPh)-Cu-allyl	-3597.06856996	-4438.99564844	0.0	-3596.404446	-4438.123169	0.0	0.0	15.3
AA-9b(NaOPh)-pc(1,6major)	-4439.04439972	-4439.04439972	-30.6	-4438.140103	-4438.140103	-10.6	20.0	11.8
AA-9b(NaOPh)-ts(1,6major)	-4439.04225300	-4439.04225300	-29.2	-4438.134169	-4438.134169	-6.9	22.3	-302.4
AA-9b(NaOPh)-prod(1,6major)	-4439.09912432	-4439.09912432	-64.9	-4438.186797	-4438.186797	-39.9	25.0	18.3
AA-9d(NaOPh)-prod(1,6minor)	-4439.09249888	-4439.09249888	-60.8	-4438.183988	-4438.183988	-37.5	23.3	11.3
AA-9d(NaOPh)-ts(1,6minor)	-4439.04244814	-4439.04244814	-29.4	-4438.135375	-4438.135375	-7.0	22.4	-345.5
AA-9d(NaOPh)-pc(1,6minor)	-4439.04673704	-4439.04673704	-32.1	-4438.141327	-4438.141327	-10.8	21.4	15.4
9d(NaOPh)-Cu-allyl	-3597.06845638	-4438.99553486	0.0	-3596.405435	-4438.124158	0.0	0.0	14.7
9b(NaOPh)-Cu-allyl	-3597.06856996	-4438.99564844	0.0	-3596.404446	-4438.123169	0.0	0.0	15.3
AA-9b(NaOPh)-pc(1,6minor)	-4439.04836588	-4439.04836588	-33.1	-4438.139826	-4438.139826	-10.5	22.6	17.7
AA-9b(NaOPh)-ts(1,6minor)	-4439.04436355	-4439.04436355	-30.6	-4438.137712	-4438.137712	-9.1	21.4	-305.4
AA-9b(NaOPh)-prod(1,6minor)	-4131.89527188	-4131.89527188	-62.2	-4131.081150	-4131.081150	-35.8	26.4	22.8

Figure S4-1

PA-9d(Na)-prod(1,6major)	-3681.07040691	-3681.07040691	-52.2	-3680.475261	-3680.475261	-29.2	22.9	16.8
PA-9d(Na)-ts(1,6major)	-3681.01674239	-3681.01674239	-18.5	-3680.427020	-3680.427020	1.0	19.5	-425.8
PA-9d(Na)-pc(1,6major)	-3681.03006649	-3681.03006649	-26.8	-3680.439972	-3680.439972	-7.1	19.8	18.4
9d(Na)-Cu-allenyl	-2839.06020575	-3680.98728423	0.0	-2838.709953	-3680.428676	0.0	0.0	14.4
9b(Na)-Cu-allenyl	-2839.05552233	-3680.98260081	0.0	-2838.703755	-3680.422478	0.0	0.0	18.5
PA-9b(Na)-pc(1,6major)	-3681.02455274	-3681.02455274	-26.3	-3680.435891	-3680.435891	-8.4	17.9	18.5
PA-9b(Na)-ts(1,6major)	-3681.01420703	-3681.01420703	-19.8	-3680.425466	-3680.425466	-1.9	18.0	-427.0
PA-9b(Na)-prod(1,6major)	-3681.06325058	-3681.06325058	-50.6	-3680.471031	-3680.471031	-30.5	20.1	-13.0

PA-9d(Na)-prod(1,6minor)	-3681.07164701	-3681.07164701	-52.9	-3680.477648	-3680.477648	-30.7	22.2	12.1
PA-9d(Na)-ts(1,6minor)	-3681.01261478	-3681.01261478	-15.9	-3680.424040	-3680.424040	2.9	18.8	-460.0
PA-9d(Na)-pc(1,6minor)	-3681.02763302	-3681.02763302	-25.3	-3680.439088	-3680.439088	-6.5	18.8	8.2
9d(Na)-Cu-allenyl	-2839.06020575	-3680.98728423	0.0	-2838.709953	-3680.428676	0.0	0.0	14.4
9b(Na)-Cu-allenyl	-2839.05552233	-3680.98260081	0.0	-2838.703755	-3680.422478	0.0	0.0	18.5
PA-9b(Na)-pc(1,6minor)	-3681.02166482	-3681.02166482	-24.5	-3680.432001	-3680.432001	-6.0	18.5	4.1
PA-9b(Na)-ts(1,6minor)	-3681.00662586	-3681.00662586	-15.1	-3680.413477	-3680.413477	5.6	20.7	-473.7
PA-9b(Na)-prod(1,6minor)	-3681.06430128	-3681.06430128	-51.3	-3680.471969	-3680.471969	-31.1	20.2	21.2

Figure S5-1

AA-9d(Na)-prod(1,6major)	-4131.89053036	-4131.89053036	-56.6	-4131.076083	-4131.076083	-30.9	25.7	23.0
AA-9d(Na)-ts(1,6major)	-4131.84208395	-4131.84208395	-26.2	-4131.035217	-4131.035217	-5.2	21.0	-388.7
AA-9d(Na)-pc(1,6major)	-4131.84678962	-4131.84678962	-29.2	-4131.038237	-4131.038237	-7.1	22.0	18.7
9d(Na)-Cu-allyl	-3289.87323919	-4131.80031767	0.0	-3289.308165	-4131.026888	0.0	0.0	20.5
9b(Na)-Cu-allyl	-3289.86902565	-4131.79610413	0.0	-3289.305371	-4131.024094	0.0	0.0	17.5
AA-9b(Na)-pc(1,6major)	-4131.84106861	-4131.84106861	-28.2	-4131.034300	-4131.034300	-6.4	21.8	14.0
AA-9b(Na)-ts(1,6major)	-4131.83854441	-4131.83854441	-26.6	-4131.030376	-4131.030376	-3.9	22.7	-314.0
AA-9b(Na)-prod(1,6major)	-4131.89305721	-4131.89305721	-60.8	-4131.080900	-4131.080900	-35.6	25.2	14.3
AA-9d(Na)-prod(1,6minor)	-4131.89461386	-4131.89461386	-59.2	-4131.087676	-4131.087676	-38.1	21.0	15.1
AA-9d(Na)-ts(1,6minor)	-4131.83826859	-4131.83826859	-23.8	-4131.029821	-4131.029821	-1.8	22.0	-396.3
AA-9d(Na)-pc(1,6minor)	-4131.84483185	-4131.84483185	-27.9	-4131.038399	-4131.038399	-7.2	20.7	-3.5
9d(Na)-Cu-allyl	-3289.87323919	-4131.80031767	0.0	-3289.308165	-4131.026888	0.0	0.0	20.5
9b(Na)-Cu-allyl	-3289.86902565	-4131.79610413	0.0	-3289.305371	-4131.024094	0.0	0.0	17.5
AA-9b(Na)-pc(1,6minor)	-4131.83917004	-4131.83917004	-27.0	-4131.031466	-4131.031466	-4.6	22.4	12.6
AA-9b(Na)-ts(1,6minor)	-4131.83618193	-4131.83618193	-25.1	-4131.028391	-4131.028391	-2.7	22.5	-326.5
AA-9b(Na)-prod(1,6minor)	-4131.89527188	-4131.89527188	-62.2	-4131.081150	-4131.081150	-35.8	26.4	22.8

Figure S6-1

thf	-232.21317836	-232.123926	60.3
PMe3	-460.86841611	-460.785102	167.4
Me2NHC	-305.69353942	-305.575630	35.8
NaOPh	-468.85364944	-468.794061	15.7
NaOtBu	-395.11737857	-395.027576	32.7
dienoate	-841.92707848	-841.718723	24.5
dienoate-NaOPh	-1310.80369108	-1310.516445	9.2
dienoate-NaOtBu	-1237.06693666	-1236.747187	12.6

Me2NHC-Cu-allenyl	-2062.03073671	-3067.14088837	-15.6	-2061.876119	-3066.816934	-14.7	0.9	16.2
PMe3-Cu-allenyl	-2217.18081038	-3067.11608535	0.0	-2217.062244	-3066.793587	0.0	0.0	11.6
thf-Cu-allenyl	-1988.50872863	-3067.09924135	10.6	-1988.383937	-3066.776456	10.7	0.2	20.9
PA-NaOPh-prod(1,6)	-3067.16986516	-3067.16986516	-33.7	-3066.832807	-3066.832807	-24.6	9.1	15.9
PA-NaOPh-ts(1,6)	-3067.12456351	-3067.12456351	-5.3	-3066.788885	-3066.788885	3.0	8.3	-446.9
PA-NaOPh-ed(1,6)	-3067.13714909	-3067.13714909	-13.2	-3066.803204	-3066.803204	-6.0	7.2	20.6
NaOPh-Cu-allenyl	-2225.17069737	-3067.09777585	11.5	-2225.073825	-3066.792548	0.7	-10.8	21.0
PA-NaOPh-ed(1,4)	-3067.14378699	-3067.14378699	-17.4	-3066.807977	-3066.807977	-9.0	8.4	20.3
PA-NaOPh-ts(1,4)	-3067.11795157	-3067.11795157	-1.2	-3066.783244	-3066.783244	6.5	7.7	-466.6
PA-NaOPh-prod(1,4)	-3067.17831935	-3067.17831935	-39.1	-3066.840874	-3066.840874	-29.7	9.4	16.9
Me2NHC-Cu-allenyl	-2062.03073671	-2993.40413395	-15.6	-2061.876119	-2993.047676	-14.7	0.9	16.2
PMe3-Cu-allenyl	-2217.18081038	-2993.37933093	0.0	-2217.062244	-2993.024329	0.0	0.0	11.6
thf-Cu-allenyl	-1988.50872863	-2993.36248693	10.6	-1988.383937	-2993.007198	10.7	0.2	20.9
PA-NaOtBu-prod(1,6)	-2993.44684250	-2993.44684250	-42.4	-2993.077409	-2993.077409	-33.3	9.1	17.6
PA-NaOtBu-ts(1,6)	-2993.40265452	-2993.40265452	-14.6	-2993.036695	-2993.036695	-7.8	6.9	-461.3
PA-NaOtBu-ed(1,6)	-2993.41544293	-2993.41544293	-22.7	-2993.051747	-2993.051747	-17.2	5.5	9.6
NaOtBu-Cu-allenyl	-2151.45184434	-2993.37892282	0.3	-2151.321355	-2993.040078	-9.9	-10.1	-9.2
PA-NaOtBu-ed(1,4)	-2993.41491749	-2993.41491749	-22.3	-2993.053280	-2993.053280	-18.2	4.2	12.1
PA-NaOtBu-ts(1,4)	-2993.39686790	-2993.39686790	-11.0	-2993.035077	-2993.035077	-6.7	4.3	-458.7
PA-NaOtBu-prod(1,4)	-2993.45855811	-2993.45855811	-49.7	-2993.089320	-2993.089320	-40.8	8.9	12.7

Figure S7-1

Me2NHC-Cu-allyl	-2512.83406354	-3354.76114202	0.0	-2512.466482	-3354.185205	0.0	0.0	19.7
AA-Me2NHC-pc(1,6major)	-3354.79756035	-3354.79756035	-22.9	-3354.192981	-3354.192981	-4.9	18.0	11.9
AA-Me2NHC-ts(1,6major)	-3354.79031886	-3354.79031886	-18.3	-3354.182580	-3354.182580	1.6	20.0	-403.7
AA-Me2NHC-prod(1,6major)	-3354.84618081	-3354.84618081	-53.4	-3354.233098	-3354.233098	-30.1	23.3	21.2
Me2NHC-Cu-allyl	-2512.83406354	-3354.76114202	0.0	-2512.466482	-3354.185205	0.0	0.0	19.7
AA-Me2NHC-pc(1,6minor)	-3354.79657990	-3354.79657990	-22.2	-3354.189771	-3354.189771	-2.9	19.4	25.2
AA-Me2NHC-ts(1,6minor)	-3354.78177396	-3354.78177396	-12.9	-3354.173882	-3354.173882	7.1	20.1	-454.8
AA-Me2NHC-prod(1,6minor)	-3354.83876879	-3354.83876879	-48.7	-3354.225997	-3354.225997	-25.6	23.1	20.3

Figure S8-1

dienoate	-841.92707848			-841.718723				24.5
SIMes-Cu-allenyl	-2680.78923765	-3522.71631613	0.0	-2680.381618	-3522.100341	0.0	0.0	16.7

PA-SIMes-ed(1,6)	-3522.75056416	-3522.75056416	-21.5	-3522.100784	-3522.100784	-0.3	21.2	18.0
PA-SIMes-ts(1,6)	-3522.73490214	-3522.73490214	-11.7	-3522.085300	-3522.085300	9.4	21.1	-466.8
PA-SIMes-prod(1,6)	-3522.78247192	-3522.78247192	-41.5	-3522.129774	-3522.129774	-18.5	23.0	12.7
PA-SIMes-ed(1,4AA)	-3522.75057238	-3522.75057238	-21.5	-3522.100973	-3522.100973	-0.4	21.1	18.1
PA-SIMes-ts(1,4AA)	-3522.72443459	-3522.72443459	-5.1	-3522.076183	-3522.076183	15.2	20.3	-348.7
PA-SIMes-prod(1,4AA)	-3522.77095735	-3522.77095735	-34.3	-3522.123860	-3522.123860	-14.8	19.5	13.5
PA-SIMes-ed(1,4)	-3522.74163171	-3522.74163171	-15.9	-3522.095775	-3522.095775	2.9	18.8	14.5
PA-SIMes-ts(1,4)	-3522.71682623	-3522.71682623	-0.3	-3522.073311	-3522.073311	17.0	17.3	-448.7
PA-SIMes-prod(1,4)	-3522.75830146	-3522.75830146	-26.3	-3522.108013	-3522.108013	-4.8	21.5	13.5
PPh3-Cu-allenyl	-2791.78064609	-3633.70772457	0.0	-2791.511938	-3633.230661	0.0	0.0	-8.5
PA-PPh3-ed(1,6)	-3633.73942416	-3633.73942416	-19.9	-3633.234471	-3633.234471	-2.4	17.5	9.9
PA-PPh3-ts(1,6)	-3633.72277720	-3633.72277720	-9.4	-3633.215506	-3633.215506	9.5	19.0	-480.0
PA-PPh3-prod(1,6)	-3633.76592730	-3633.76592730	-36.5	-3633.256846	-3633.256846	-16.4	20.1	12.3
PA-PPh3-ed(1,4AA)	-3633.73998513	-3633.73998513	-20.2	-3633.237076	-3633.237076	-4.0	16.2	13.7
PA-PPh3-ts(1,4AA)	-3633.71057140	-3633.71057140	-1.8	-3633.208386	-3633.208386	14.0	15.8	-331.1
PA-PPh3-prod(1,4AA)	-3633.75762400	-3633.75762400	-31.3	-3633.251129	-3633.251129	-12.8	18.5	9.1
PA-PPh3-ed(1,4)	-3633.73304715	-3633.73304715	-15.9	-3633.231145	-3633.231145	-0.3	15.6	9.8
PA-PPh3-ts(1,4)	-3633.70950892	-3633.70950892	-1.1	-3633.208630	-3633.208630	13.8	14.9	-430.0
PA-PPh3-prod(1,4)	-3633.77054729	-3633.77054729	-39.4	-3633.263965	-3633.263965	-20.9	18.5	12.5

Figures S9-1

Me2NHC-Cu-allenyl	-2062.03073671	-2903.95781519	0.0	-2061.876119	-2903.594842	0.0	0.0	16.2
PA-Me2NHC-ed(1,6)	-2903.98097792	-2903.98097792	-14.5	-2903.589483	-2903.589483	3.4	17.9	19.5
PA-Me2NHC-ts(1,6)	-2903.96575719	-2903.96575719	-5.0	-2903.574155	-2903.574155	13.0	18.0	-471.6
PA-Me2NHC-prod(1,6)	-2904.01565681	-2904.01565681	-36.3	-2903.617734	-2903.617734	-14.4	21.9	26.6
PA-Me2NHC-ed(1,4AA)	-2903.98119581	-2903.98119581	-14.7	-2903.592317	-2903.592317	1.6	16.3	16.1
PA-Me2NHC-ts(1,4AA)	-2903.95210289	-2903.95210289	3.6	-2903.564162	-2903.564162	19.3	15.7	-325.5
PA-Me2NHC-prod(1,4AA)	-2904.00315785	-2904.00315785	-28.5	-2903.615225	-2903.615225	-12.8	15.7	12.1
PA-Me2NHC-ed(1,4)	-2903.97461848	-2903.97461848	-10.5	-2903.587739	-2903.587739	4.5	15.0	13.6
PA-Me2NHC-ts(1,4)	-2903.94929051	-2903.94929051	5.3	-2903.560627	-2903.560627	21.5	16.1	-450.0
PA-Me2NHC-prod(1,4)	-2903.99035566	-2903.99035566	-20.4	-2903.598009	-2903.598009	-2.0	18.4	12.4
PMe3-Cu-allenyl	-2217.18081038	-3059.10788886	0.0	-2217.062244	-3058.780967	0.0	0.0	11.6
PA-PMe3-ed(1,6)	-3059.13763951	-3059.13763951	-18.7	-3058.783550	-3058.783550	-1.6	17.0	6.6

PA-PMe3-ts(1,6)	-3059.12059614	-3059.12059614	-8.0	-3058.764913	-3058.764913	10.1	18.0	-486.1
PA-PMe3-prod(1,6)	-3059.16803726	-3059.16803726	-37.7	-3058.809791	-3058.809791	-18.1	19.7	11.1
PA-PMe3-ed(1,4AA)	-3059.13763951	-3059.13763951	-18.7	-3058.783552	-3058.783552	-1.6	17.0	6.6
PA-PMe3-ts(1,4AA)	-3059.10503746	-3059.10503746	1.8	-3058.752459	-3058.752459	17.9	16.1	-349.3
PA-PMe3-prod(1,4AA)	-3059.15445792	-3059.15445792	-29.2	-3058.799771	-3058.799771	-11.8	17.4	10.1
PA-PMe3-ed(1,4)	-3059.13081436	-3059.13081436	-14.4	-3058.778278	-3058.778278	1.7	16.1	15.0
PA-PMe3-ts(1,4)	-3059.10625840	-3059.10625840	1.0	-3058.755276	-3058.755276	16.1	15.1	-463.1
PA-PMe3-prod(1,4)	-3059.16938303	-3059.16938303	-38.6	-3058.809679	-3058.809679	-18.0	20.6	24.5

Figure S10-1

dienoate	-841.92707848			-841.718723				24.5
dienoate-Naborate	-1486.89608401			-1486.563543				15.5
SIMes-Cu-allenyl	-2680.78923765	-4167.68532166	0.0	-2680.381618	-4166.945161	0.0	0.0	16.7
PA-SIMes(Naborate)-ed(1,6)	-4167.72984142	-4167.72984142	-27.9	-4166.953118	-4166.953118	-5.0	22.9	15.7
PA-SIMes(Naborate)-ts(1,6)	-4167.72041851	-4167.72041851	-22.0	-4166.944949	-4166.944949	0.1	22.2	-419.8
PA-SIMes(Naborate)-prod(1,6)	-4167.77319994	-4167.77319994	-55.1	-4166.995501	-4166.995501	-31.6	23.6	11.5
PA-SIMes(Naborate)-ed(1,4AA)	-4167.73112443	-4167.73112443	-28.7	-4166.956197	-4166.956197	-6.9	21.8	14.6
PA-SIMes(Naborate)-ts(1,4AA)	-4167.71268692	-4167.71268692	-17.2	-4166.939666	-4166.939666	3.4	20.6	-302.0
PA-SIMes(Naborate)-prod(1,4AA)	-4167.75978235	-4167.75978235	-46.7	-4166.984388	-4166.984388	-24.6	22.1	13.9
PA-SIMes(Naborate)-ed(1,4)	-4167.72594722	-4167.72594722	-25.5	-4166.951422	-4166.951422	-3.9	21.6	-12.7
PA-SIMes(Naborate)-ts(1,4)	-4167.70362749	-4167.70362749	-11.5	-4166.930624	-4166.930624	9.1	20.6	-447.0
PA-SIMes(Naborate)-prod(1,4)	-4167.77405497	-4167.77405497	-55.7	-4166.996784	-4166.996784	-32.4	23.3	15.5
dienoate	-841.92707848			-841.718723				24.5
dienoate-Naborate	-1486.89608401			-1486.563543				15.5
PPh3-Cu-allenyl	-2791.78064609	-4278.67673010	0.0	-2791.511938	-4278.075481	0.0	0.0	-8.5
PA-PPh3(Naborate)-ed(1,6)	-4278.71914908	-4278.71914908	-26.6	-4278.086340	-4278.086340	-6.8	19.8	17.8
PA-PPh3(Naborate)-ts(1,6)	-4278.70801041	-4278.70801041	-19.6	-4278.075731	-4278.075731	-0.2	19.5	-446.5
PA-PPh3(Naborate)-prod(1,6)	-4278.76045462	-4278.76045462	-52.5	-4278.123447	-4278.123447	-30.1	22.4	14.9
PA-PPh3(Naborate)-ed(1,4AA)	-4278.72067874	-4278.72067874	-27.6	-4278.091963	-4278.091963	-10.3	17.2	13.6
PA-PPh3(Naborate)-ts(1,4AA)	-4278.69171118	-4278.69171118	-9.4	-4278.066438	-4278.066438	5.7	15.1	-303.5
PA-PPh3(Naborate)-prod(1,4AA)	-4278.74542342	-4278.74542342	-43.1	-4278.117823	-4278.117823	-26.6	16.5	12.0
PA-PPh3(Naborate)-ed(1,4)	-4278.71589517	-4278.71589517	-24.6	-4278.088006	-4278.088006	-7.9	16.7	9.2
PA-PPh3(Naborate)-ts(1,4)	-4278.69317096	-4278.69317096	-10.3	-4278.063095	-4278.063095	7.8	18.1	-422.9
PA-PPh3(Naborate)-prod(1,4)	-4278.76423088	-4278.76423088	-54.9	-4278.125760	-4278.125760	-31.6	23.4	15.3

Figure S11-1

dienoate	-841.92707848			-841.718723				24.5
PA-9d(Na)-prod(1,6major)	-3681.07040691	-3681.07040691	-52.2	-3680.475261	-3680.475261	-29.2	22.9	16.8
PA-9d(Na)-ts(1,6major)	-3681.01674239	-3681.01674239	-18.5	-3680.427020	-3680.427020	1.0	19.5	-425.8
PA-9d(Na)-pc(1,6major)	-3681.03006649	-3681.03006649	-26.8	-3680.439972	-3680.439972	-7.1	19.8	18.4
9d(Na)-Cu-allenyl	-2839.06020575	-3680.98728423	0.0	-2838.709953	-3680.428676	0.0	0.0	14.4
PA-9d(Na)-pc(1,4AA)	-3681.02869646	-3681.02869646	-26.0	-3680.440268	-3680.440268	-7.3	18.7	15.3
PA-9d(Na)-ts(1,4AA)	-3681.00195136	-3681.00195136	-9.2	-3680.415510	-3680.415510	8.3	17.5	-312.4
PA-9d(Na)-prod(1,4AA)	-3681.06975124	-3681.06975124	-51.7	-3680.482101	-3680.482101	-33.5	18.2	13.2

Figure S12-1

NaOtBu	-395.11737857			-395.027576				32.7
dienoate	-841.92707848			-841.718723				24.6
PA-SIMes(NaOtBu)-prod(1,4)	-3917.95611486	-2680.91165781	-50.4	-3917.190802	-2680.444503	-31.4	19.0	10.4
PA-SIMes(NaOtBu)-ts(1,4)	-3917.87960041	-2680.83514336	-2.4	-3917.115941	-2680.369642	15.6	18.0	-420.3
PA-SIMes(NaOtBu)-ed(1,4)	-3917.90470258	-2680.86024553	-18.1	-3917.141520	-2680.395221	-0.5	17.7	9.6
SIMes-Cu-allenyl	-2680.78923765	-2680.78923765	26.4	-2680.381618	-2680.381618	8.1	-18.4	16.7
SIMes-Cu(NaOtBu)-allenyl	-3075.94872495	-2680.83134638	0.0	-3075.422058	-2680.394482	0.0	0.0	27.3
PA-SIMes(NaOtBu)-ed(1,6)	-3917.90118513	-2680.85672808	-15.9	-3917.136643	-2680.390344	2.6	18.5	13.4
PA-SIMes(NaOtBu)-ts(1,6)	-3917.89152237	-2680.84706532	-9.9	-3917.128322	-2680.382023	7.8	17.7	-424.8
PA-SIMes(NaOtBu)-prod(1,6)	-3917.94472680	-2680.90026975	-43.3	-3917.180195	-2680.433896	-24.7	18.5	14.3
PA-PPh3(NaOtBu)-prod(1,4)	-4028.96421775	-2791.91976070	-55.0	-4028.335477	-2791.589178	-31.9	23.1	14.4
PA-PPh3(NaOtBu)-ts(1,4)	-4028.89777635	-2791.85331930	-13.3	-4028.276246	-2791.529947	5.3	18.6	-353.7
PA-PPh3(NaOtBu)-ed(1,4)	-4028.91570865	-2791.87125160	-24.6	-4028.292273	-2791.545974	-4.8	19.8	15.8
PPh3-Cu-allenyl	-2791.78064609	-2791.78064609	32.3	-2791.511938	-2791.511938	16.6	-15.7	-8.5
PPh3-Cu(NaOtBu)-allenyl	-3186.94946047	-2791.83208190	0.0	-3186.565929	-2791.538353	0.0	0.0	17.5
PA-PPh3(NaOtBu)-ed(1,6)	-4028.88980074	-2791.84534369	-8.3	-4028.269434	-2791.523135	9.5	17.9	13.3
PA-PPh3(NaOtBu)-ts(1,6)	-4028.87865129	-2791.83419424	-1.3	-4028.255865	-2791.509566	18.1	19.4	-449.1
PA-PPh3(NaOtBu)-prod(1,6)	-4028.93073582	-2791.88627877	-34.0	-4028.305792	-2791.559493	-13.3	20.7	14.5

Figure S13-1

NaOMe	-277.27660539			-277.264690				96.5
dienoate	-841.92707848			-841.718723				24.6
PA-SIMes(NaOMe)-prod(1,4)	-3800.11624361	-2680.91255974	-53.8	-3799.429523	-2680.446110	-32.4	21.4	12.2
PA-SIMes(NaOMe)-ts(1,4)	-3800.03623090	-2680.83254703	-3.6	-3799.354189	-2680.370776	14.8	18.5	-400.1
PA-SIMes(NaOMe)-ed(1,4)	-3800.05869359	-2680.85500972	-17.7	-3799.376352	-2680.392939	0.9	18.7	13.8
SIMes-Cu-allenyl	-2680.78923765	-2680.78923765	23.5	-2680.381618	-2680.381618	8.0	-15.5	16.7
SIMes-Cu(NaOMe)-allenyl	-2958.10335257	-2680.82674718	0.0	-2957.659100	-2680.394410	0.0	0.0	26.9
PA-SIMes(NaOMe)-ed(1,6)	-3800.05935298	-2680.85566911	-18.1	-3799.377728	-2680.394315	0.1	18.2	16.1
PA-SIMes(NaOMe)-ts(1,6)	-3800.04969158	-2680.84600771	-12.1	-3799.365328	-2680.381915	7.8	19.9	-424.9
PA-SIMes(NaOMe)-prod(1,6)	-3800.10311238	-2680.89942851	-45.6	-3799.418625	-2680.435212	-25.6	20.0	6.4
PA-PPh3(NaOMe)-prod(1,4)	-3911.12006641	-2791.91638254	-54.5	-3910.572951	-2791.589538	-31.7	22.8	12.8
PA-PPh3(NaOMe)-ts(1,4)	-3911.05049032	-2791.84680645	-10.8	-3910.510854	-2791.527441	7.3	18.1	-356.7
PA-PPh3(NaOMe)-ed(1,4)	-3911.06860824	-2791.86492437	-22.2	-3910.526719	-2791.543306	-2.7	19.5	16.2
PPh3-Cu-allenyl	-2791.78064609	-2791.78064609	30.7	-2791.511938	-2791.511938	17.0	-13.7	-8.5
PPh3-Cu(NaOMe)-allenyl	-3069.10617160	-2791.82956621	0.0	-3068.803691	-2791.539001	0.0	0.0	20.7
PA-PPh3(NaOMe)-ed(1,6)	-3911.04850322	-2791.84481935	-9.6	-3910.510871	-2791.527458	7.2	16.8	12.8
PA-PPh3(NaOMe)-ts(1,6)	-3911.03470938	-2791.83102551	-0.9	-3910.495249	-2791.511836	17.0	18.0	-446.9
PA-PPh3(NaOMe)-prod(1,6)	-3911.08630820	-2791.88262433	-33.3	-3910.542647	-2791.559234	-12.7	20.6	-6.9

Figure S14-1

NaOtBu	-395.11737857			-395.027576				32.7
dienoate	-841.92707848			-841.718723				24.6
PA-Me2NHC(NaOtBu)-prod(1,4)	-3299.19328289	-2062.14882584	-52.8	-3298.681822	-2061.935523	-32.8	19.9	18.2
PA-Me2NHC(NaOtBu)-ts(1,4)	-3299.12254340	-2062.07808635	-8.4	-3298.616012	-2061.869713	8.5	16.9	-363.3
PA-Me2NHC(NaOtBu)-ed(1,4)	-3299.13603253	-2062.09157548	-16.8	-3298.627567	-2061.881268	1.2	18.1	19.0
Me2NHC-Cu-allenyl	-2062.03078001	-2062.03078001	21.3	-2061.876100	-2061.876100	4.5	-16.8	21.6
Me2NHC-Cu(NaOtBu)-allenyl	-2457.18214053	-2062.06476196	0.0	-2456.910822	-2061.883246	0.0	0.0	21.9
PA-Me2NHC(NaOtBu)-ed(1,6)	-3299.13575585	-2062.09129880	-16.7	-3298.631215	-2061.884916	-1.0	15.6	13.7
PA-Me2NHC(NaOtBu)-ts(1,6)	-3299.12365436	-2062.07919731	-9.1	-3298.616671	-2061.870372	8.1	17.1	-453.3
PA-Me2NHC(NaOtBu)-prod(1,6)	-3299.17749962	-2062.13304257	-42.8	-3298.666239	-2061.919940	-23.0	19.8	16.5
PA-PMe3(NaOtBu)-prod(1,4)	-3454.34900971	-2217.30455266	-49.8	-3453.871365	-2217.125066	-26.0	23.8	-2.2

PA-PMe3(NaOtBu)-ts(1,4)	-3454.28410031	-2217.23964326	-9.0	-3453.815964	-2217.069665	8.8	17.8	-357.4
PA-PMe3(NaOtBu)-ed(1,4)	-3454.29818810	-2217.25373105	-17.9	-3453.830124	-2217.083825	-0.1	17.8	18.2
PMe3-Cu-allenyl	-2217.18081039	-2217.18081039	27.9	-2217.062239	-2217.062239	13.5	-14.4	11.6
PMe3-Cu(NaOtBu)-allenyl	-2612.34261472	-2217.22523615	0.0	-2612.111268	-2217.083692	0.0	0.0	8.8
PA-PMe3(NaOtBu)-ed(1,6)	-3454.28842449	-2217.24396744	-11.8	-3453.818447	-2217.072148	7.2	19.0	19.3
PA-PMe3(NaOtBu)-ts(1,6)	-3454.27252064	-2217.22806359	-1.8	-3453.801003	-2217.054704	18.2	20.0	-463.8
PA-PMe3(NaOtBu)-prod(1,6)	-3454.32484583	-2217.28038878	-34.6	-3453.850892	-2217.104593	-13.1	21.5	17.6

Figure S15-1

NaOPh	-468.85364944			-468.794061				15.7
dienoate	-841.92707848			-841.718723				24.5
9d(NaOPh)-Cu-allenyl	-3146.25617778	-3988.18325626	0.0	-3145.806149	-3987.524872	0.0	0.0	11.9
PA-9d(NaOPh)-ts(1,6major)_01	-3988.22213482	-3988.22213482	-24.4	-3987.529839	-3987.529839	-3.1	21.3	-455.1
PA-9d(NaOPh)-ts(1,6major)_02	-3988.22242215	-3988.22242215	-24.6	-3987.529646	-3987.529646	-3.0	21.6	-444.6
PA-9d(NaOPh)-ts(1,6major)_03	-3988.21826606	-3988.21826606	-22.0	-3987.526957	-3987.526957	-1.3	20.7	-458.7
PA-9d(NaOPh)-ts(1,6minor)_01	-3988.21792967	-3988.21792967	-21.8	-3987.527227	-3987.527227	-1.5	20.3	-450.4
PA-9d(NaOPh)-ts(1,6minor)_02	-3988.21925399	-3988.21925399	-22.6	-3987.527003	-3987.527003	-1.3	21.3	-446.9
PA-9d(NaOPh)-ts(1,6minor)_03	-3988.21926870	-3988.21926870	-22.6	-3987.526287	-3987.526287	-0.9	21.7	-449.7
PA-9d(NaOPh)-ts(1,6minor)_04	-3988.21743768	-3988.21743768	-21.4	-3987.525800	-3987.525800	-0.6	20.9	-446.6
PA-9d(NaOPh)-ts(1,6minor)_05	-3988.21946363	-3988.21946363	-22.7	-3987.524868	-3987.524868	0.0	22.7	-426.0
PA-9d(NaOPh)-ts(1,6minor)_06	-3988.21636174	-3988.21636174	-20.8	-3987.522534	-3987.522534	1.5	22.2	-441.9
PA-9d(NaOPh)-ts(1,6minor)_07	-3988.21954606	-3988.21954606	-22.8	-3987.525031	-3987.525031	-0.1	22.7	-424.4
PA-9d(NaOPh)-ts(1,6minor)_08	-3988.21575574	-3988.21575574	-20.4	-3987.522283	-3987.522283	1.6	22.0	-451.9

Figure S15-2

dienoate	-841.92707848			-841.718723				24.5
9b(NaOPh)-Cu-allenyl	-3146.25183127	-3988.17890975	0.0	-3145.801041	-3987.519764	0.0	0.0	14.5
PA-9b(NaOPh)-ts(1,6major)_01	-3988.21834759	-3988.21834759	-24.7	-3987.526031	-3987.526031	-3.9	20.8	-441.8
PA-9b(NaOPh)-ts(1,6major)_02	-3988.21729738	-3988.21729738	-24.1	-3987.524378	-3987.524378	-2.9	21.2	-451.3
PA-9b(NaOPh)-ts(1,6major)_03	-3988.21368855	-3988.21368855	-21.8	-3987.521201	-3987.521201	-0.9	20.9	-436.1
PA-9b(NaOPh)-ts(1,6major)_04	-3988.21708629	-3988.21708629	-24.0	-3987.524815	-3987.524815	-3.2	20.8	-456.1
PA-9b(NaOPh)-ts(1,6major)_05	-3988.21870349	-3988.21870349	-25.0	-3987.525618	-3987.525618	-3.7	21.3	-445.3
PA-9b(NaOPh)-ts(1,6major)_06	-3988.21476261	-3988.21476261	-22.5	-3987.519765	-3987.519765	0.0	22.5	-437.7
PA-9b(NaOPh)-ts(1,6major)_07	-3988.20625665	-3988.20625665	-17.2	-3987.517045	-3987.517045	1.7	18.9	-462.5
PA-9b(NaOPh)-ts(1,6minor)_01	-3988.21330777	-3988.21330777	-21.6	-3987.520948	-3987.520948	-0.7	20.8	-465.4

PA-9b(NaOPh)-ts(1,6minor)_02	-3988.21880720	-3988.21880720	-25.0	-3987.526760	-3987.526760	-4.4	20.6	-417.0
PA-9b(NaOPh)-ts(1,6minor)_03	-3988.21880751	-3988.21880751	-25.0	-3987.526691	-3987.526691	-4.3	20.7	-417.0
PA-9b(NaOPh)-ts(1,6minor)_04	-3988.21355466	-3988.21355466	-21.7	-3987.520570	-3987.520570	-0.5	21.2	-462.6
PA-9b(NaOPh)-ts(1,6minor)_05	-3988.21868997	-3988.21868997	-25.0	-3987.523538	-3987.523538	-2.4	22.6	-417.9
PA-9b(NaOPh)-ts(1,6minor)_06	-3988.21301922	-3988.21301922	-21.4	-3987.521281	-3987.521281	-1.0	20.5	-426.0
PA-9b(NaOPh)-ts(1,6minor)_07	-3988.21538734	-3988.21538734	-22.9	-3987.520567	-3987.520567	-0.5	22.4	-421.6
PA-9b(NaOPh)-ts(1,6minor)_08	-3988.21376729	-3988.21376729	-21.9	-3987.522139	-3987.522139	-1.5	20.4	-435.9
PA-9b(NaOPh)-ts(1,6minor)_09	-3988.20604707	-3988.20604707	-17.0	-3987.511377	-3987.511377	5.3	22.3	-450.0

Figure S15-3

dienoate	-841.92707848			-841.718723				24.5
9d(Na)-Cu-allenyl	-2839.06020575	-3680.98728423	0.0	-2838.709953	-3680.428676	0.0	0.0	14.4
PA-9d(Na)-ts(1,6major)_01	-3681.01695194	-3681.01695194	-18.6	-3680.425988	-3680.425988	1.7	20.3	-446.9
PA-9d(Na)-ts(1,6major)_02	-3681.01674239	-3681.01674239	-18.5	-3680.427020	-3680.427020	1.0	19.5	-425.8
PA-9d(Na)-ts(1,6major)_03	-3681.01674622	-3681.01674622	-18.5	-3680.426398	-3680.426398	1.4	19.9	-439.7
PA-9d(Na)-ts(1,6major)_04	-3681.01671223	-3681.01671223	-18.5	-3680.426081	-3680.426081	1.6	20.1	-455.5
PA-9d(Na)-ts(1,6major)_05	-3681.01685875	-3681.01685875	-18.6	-3680.425350	-3680.425350	2.1	20.6	-455.9
PA-9d(Na)-ts(1,6major)_06	-3681.01677377	-3681.01677377	-18.5	-3680.425936	-3680.425936	1.7	20.2	-425.8
PA-9d(Na)-ts(1,6major)_07	-3681.01671535	-3681.01671535	-18.5	-3680.425560	-3680.425560	2.0	20.4	-426.2
PA-9d(Na)-ts(1,6major)_08	-3681.01672564	-3681.01672564	-18.5	-3680.425099	-3680.425099	2.2	20.7	-455.7
PA-9d(Na)-ts(1,6major)_09	-3681.01602735	-3681.01602735	-18.0	-3680.424545	-3680.424545	2.6	20.6	-466.7
PA-9d(Na)-ts(1,6major)_10	-3681.01100626	-3681.01100626	-14.9	-3680.420047	-3680.420047	5.4	20.3	-418.2
PA-9d(Na)-ts(1,6major)_11	-3681.01145389	-3681.01145389	-15.2	-3680.421377	-3680.421377	4.6	19.7	-445.8
PA-9d(Na)-ts(1,6major)_12	-3681.01103126	-3681.01103126	-14.9	-3680.419733	-3680.419733	5.6	20.5	-418.4
PA-9d(Na)-ts(1,6major)_13	-3681.01155941	-3681.01155941	-15.2	-3680.420595	-3680.420595	5.1	20.3	-461.8
PA-9d(Na)-ts(1,6major)_14	-3681.00352015	-3681.00352015	-10.2	-3680.411575	-3680.411575	10.7	20.9	-478.6
PA-9d(Na)-ts(1,6major)_15	-3680.99812292	-3680.99812292	-6.8	-3680.409627	-3680.409627	12.0	18.8	-456.2
PA-9d(Na)-ts(1,6major)_16	-3681.00337669	-3681.00337669	-10.1	-3680.412046	-3680.412046	10.4	20.5	-462.6
PA-9d(Na)-ts(1,6major)_17	-3680.99860603	-3680.99860603	-7.1	-3680.406275	-3680.406275	14.1	21.2	-447.6
PA-9d(Na)-ts(1,6minor)_01	-3681.01261478	-3681.01261478	-15.9	-3680.424040	-3680.424040	2.9	18.8	-460.0
PA-9d(Na)-ts(1,6minor)_02	-3681.01062138	-3681.01062138	-14.6	-3680.420615	-3680.420615	5.1	19.7	-444.3
PA-9d(Na)-ts(1,6minor)_03	-3681.01372521	-3681.01372521	-16.6	-3680.422611	-3680.422611	3.8	20.4	-473.8
PA-9d(Na)-ts(1,6minor)_04	-3681.01376311	-3681.01376311	-16.6	-3680.422164	-3680.422164	4.1	20.7	-473.6
PA-9d(Na)-ts(1,6minor)_05	-3681.01376311	-3681.01376311	-16.6	-3680.422162	-3680.422162	4.1	20.7	-473.6
PA-9d(Na)-ts(1,6minor)_06	-3681.01280902	-3681.01280902	-16.0	-3680.420713	-3680.420713	5.0	21.0	-467.7
PA-9d(Na)-ts(1,6minor)_07	-3681.01290228	-3681.01290228	-16.1	-3680.420054	-3680.420054	5.4	21.5	-467.7
PA-9d(Na)-ts(1,6minor)_08	-3681.00936876	-3681.00936876	-13.9	-3680.419415	-3680.419415	5.8	19.7	-472.8
PA-9d(Na)-ts(1,6minor)_09	-3681.00528804	-3681.00528804	-11.3	-3680.414418	-3680.414418	8.9	20.2	-436.3

Figure S15-4

9b(Na)-Cu-allenyl	-2839.05552233	-3680.98260081	0.0	-2838.703755	-3680.422478	0.0	0.0	18.5
PA-9b(Na)-ts(1,6major)_01	-3681.01420703	-3681.01420703	-19.8	-3680.425466	-3680.425466	-1.9	18.0	-427.0
PA-9b(Na)-ts(1,6major)_02	-3681.01281667	-3681.01281667	-19.0	-3680.420838	-3680.420838	1.0	20.0	-438.8
PA-9b(Na)-ts(1,6major)_03	-3681.01313518	-3681.01313518	-19.2	-3680.421077	-3680.421077	0.9	20.0	-434.7
PA-9b(Na)-ts(1,6major)_04	-3681.00780852	-3681.00780852	-15.8	-3680.413734	-3680.413734	5.5	21.3	-440.9
PA-9b(Na)-ts(1,6major)_05	-3681.00473590	-3681.00473590	-13.9	-3680.411641	-3680.411641	6.8	20.7	-469.7
PA-9b(Na)-ts(1,6minor)_01	-3681.00662586	-3681.00662586	-15.1	-3680.413477	-3680.413477	5.6	20.7	-473.7
PA-9b(Na)-ts(1,6minor)_02	-3681.00610479	-3681.00610479	-14.7	-3680.413346	-3680.413346	5.7	20.5	-471.4
PA-9b(Na)-ts(1,6minor)_03	-3681.00799031	-3681.00799031	-15.9	-3680.415714	-3680.415714	4.2	20.2	-409.9
PA-9b(Na)-ts(1,6minor)_04	-3681.00623136	-3681.00623136	-14.8	-3680.411941	-3680.411941	6.6	21.4	-470.1
PA-9b(Na)-ts(1,6minor)_05	-3681.00676070	-3681.00676070	-15.2	-3680.412139	-3680.412139	6.5	21.6	-408.8
PA-9b(Na)-ts(1,6minor)_06	-3681.00111925	-3681.00111925	-11.6	-3680.407699	-3680.407699	9.3	20.9	-471.1
PA-9b(Na)-ts(1,6minor)_07	-3681.00898900	-3681.00898900	-16.6	-3680.413956	-3680.413956	5.3	21.9	-435.9
PA-9b(Na)-ts(1,6minor)_08	-3681.00969248	-3681.00969248	-17.0	-3680.414055	-3680.414055	5.3	22.3	-442.2

Figure S15-5

9d(NaOPh)-Cu-allyl_01	-3597.06845638	-4438.99553486	0.0	-3596.405435	-4438.124158	0.0	0.0	14.7
AA-9d(NaOPh)-ts(1,6major)_01	-4439.05034678	-4439.05034678	-34.4	-4438.140890	-4438.140890	-10.5	23.9	-323.9
AA-9d(NaOPh)-ts(1,6major)_02	-4439.05088590	-4439.05088590	-34.7	-4438.141250	-4438.141250	-10.7	24.0	-338.7
AA-9d(NaOPh)-ts(1,6minor)_01	-4439.04244814	-4439.04244814	-29.4	-4438.135375	-4438.135375	-7.0	22.4	-345.5
AA-9d(NaOPh)-ts(1,6minor)_02	-4439.04486199	-4439.04486199	-31.0	-4438.135620	-4438.135620	-7.2	23.8	-347.7
AA-9d(NaOPh)-ts(1,6minor)_03	-4439.04473040	-4439.04473040	-30.9	-4438.135930	-4438.135930	-7.4	23.5	-309.8
AA-9d(NaOPh)-ts(1,6minor)_04	-4439.04421454	-4439.04421454	-30.5	-4438.135735	-4438.135735	-7.3	23.3	-323.7
AA-9d(NaOPh)-ts(1,6minor)_05	-4439.04612350	-4439.04612350	-31.7	-4438.136326	-4438.136326	-7.6	24.1	-325.2
AA-9d(NaOPh)-ts(1,6minor)_06	-4439.04259063	-4439.04259063	-29.5	-4438.133463	-4438.133463	-5.8	23.7	-326.3
AA-9d(NaOPh)-ts(1,6minor)_07	-4439.04642717	-4439.04642717	-31.9	-4438.136104	-4438.136104	-7.5	24.4	-374.3

Figure S15-6

9b(NaOPh)-Cu-allyl_01	-3597.06856996	-4438.99564844	0.0	-3596.404446	-4438.123169	0.0	0.0	15.3
AA-9b(NaOPh)-ts(1,6major)_01	-4439.04225300	-4439.04225300	-29.2	-4438.134169	-4438.134169	-6.9	22.3	-302.4
AA-9b(NaOPh)-ts(1,6major)_02	-4439.04481123	-4439.04481123	-30.9	-4438.136397	-4438.136397	-8.3	22.5	-334.4
AA-9b(NaOPh)-ts(1,6minor)_01	-4439.04436355	-4439.04436355	-30.6	-4438.137712	-4438.137712	-9.1	21.4	-305.4
AA-9b(NaOPh)-ts(1,6minor)_02	-4439.04584920	-4439.04584920	-31.5	-4438.138137	-4438.138137	-9.4	22.1	-309.1
AA-9b(NaOPh)-ts(1,6minor)_03	-4439.04644860	-4439.04644860	-31.9	-4438.137711	-4438.137711	-9.1	22.8	-305.4
AA-9b(NaOPh)-ts(1,6minor)_04	-4439.04525456	-4439.04525456	-31.1	-4438.135009	-4438.135009	-7.4	23.7	-267.5

Figure S15-7								
dienoate	-841.92707848			-841.718723				24.5
9d(Na)-Cu-allyl_01	-3289.87323919	-4131.80031767	0.0	-3289.308165	-4131.026888	0.0	0.0	20.5
AA-9d(Na)-ts(1,6major)_01	-4131.84208395	-4131.84208395	-26.2	-4131.035217	-4131.035217	-5.2	21.0	-388.7
AA-9d(Na)-ts(1,6major)_02	-4131.84213530	-4131.84213530	-26.2	-4131.032534	-4131.032534	-3.5	22.7	-365.1
AA-9d(Na)-ts(1,6major)_03	-4131.84066850	-4131.84066850	-25.3	-4131.030186	-4131.030186	-2.1	23.3	-367.1
AA-9d(Na)-ts(1,6minor)_01	-4131.83826859	-4131.83826859	-23.8	-4131.029821	-4131.029821	-1.8	22.0	-396.3
AA-9d(Na)-ts(1,6minor)_02	-4131.83828091	-4131.83828091	-23.8	-4131.029349	-4131.029349	-1.5	22.3	-396.5
AA-9d(Na)-ts(1,6minor)_03	-4131.83588529	-4131.83588529	-22.3	-4131.028104	-4131.028104	-0.8	21.6	-368.2
AA-9d(Na)-ts(1,6minor)_04	-4131.83709746	-4131.83709746	-23.1	-4131.027647	-4131.027647	-0.5	22.6	-406.0
AA-9d(Na)-ts(1,6minor)_05	-4131.83763873	-4131.83763873	-23.4	-4131.029058	-4131.029058	-1.4	22.1	-403.7
AA-9d(Na)-ts(1,6minor)_06	-4131.83545844	-4131.83545844	-22.1	-4131.026478	-4131.026478	0.3	22.3	-358.7
AA-9d(Na)-ts(1,6minor)_07	-4131.83586301	-4131.83586301	-22.3	-4131.027099	-4131.027099	-0.1	22.2	-394.3

Figure S15-8								
9b(Na)-Cu-allyl_01	-3289.86902565	-4131.79610413	0.0	-3289.305371	-4131.024094	0.0	0.0	17.5
AA-9b(Na)-ts(1,6major)_01	-4131.83854441	-4131.83854441	-26.6	-4131.030376	-4131.030376	-3.9	22.7	-314.0
AA-9b(Na)-ts(1,6major)_02	-4131.83936333	-4131.83936333	-27.1	-4131.030009	-4131.030009	-3.7	23.4	-320.0
AA-9b(Na)-ts(1,6major)_03	-4131.83794438	-4131.83794438	-26.3	-4131.029341	-4131.029341	-3.3	23.0	-314.9
AA-9b(Na)-ts(1,6major)_04	-4131.83111422	-4131.83111422	-22.0	-4131.018011	-4131.018011	3.8	25.8	-361.4
AA-9b(Na)-ts(1,6minor)_01	-4131.83618193	-4131.83618193	-25.1	-4131.028391	-4131.028391	-2.7	22.5	-326.5
AA-9b(Na)-ts(1,6minor)_02	-4131.83467184	-4131.83467184	-24.2	-4131.027319	-4131.027319	-2.0	22.2	-367.2
AA-9b(Na)-ts(1,6minor)_03	-4131.83689786	-4131.83689786	-25.6	-4131.028480	-4131.028480	-2.8	22.8	-278.5
AA-9b(Na)-ts(1,6minor)_04	-4131.83652085	-4131.83652085	-25.4	-4131.027501	-4131.027501	-2.1	23.2	-256.3
AA-9b(Na)-ts(1,6minor)_05	-4131.83783555	-4131.83783555	-26.2	-4131.027189	-4131.027189	-1.9	24.2	-304.4

Figure S15-9								
NaOPh	-468.85364944			-468.794061				15.7
(PhO)2BpinNa	-1186.36814498			-1186.044662				14.0
PhOBpin	-717.46665894			-717.228760				34.0
dienoate	-841.92707848			-841.718723				24.5
9d(Naborate)-Cu-allenyl_01	-3556.59972133	-4398.52679981	0.0	-3555.987651	-4397.706374	0.0	0.0	7.0
9d(Naborate)-Cu-allenyl_02	-3556.59879587	-4398.52587435	0.6	-3555.985261	-4397.703984	1.5	0.9	11.9
9d(Naborate)-Cu-allenyl_03	-3556.60003110	-4398.52710958	-0.2	-3555.985138	-4397.703861	1.6	1.8	12.6
9d(Naborate)-Cu-allenyl_04	-3556.60702129	-4398.53409977	-4.6	-3555.986104	-4397.704827	1.0	5.6	23.7

9d(Naborate)-Cu-allenyl_05	-3556.59701117	-4398.52408965	1.7	-3555.979780	-4397.698503	4.9	3.2	13.8
9d(Naborate)-Cu-allenyl_06	-3556.60439142	-4398.53146990	-2.9	-3555.986428	-4397.705151	0.8	3.7	20.0
9d(Naborate)-Cu-allenyl_07	-3556.59700883	-4398.52408731	1.7	-3555.979518	-4397.698241	5.1	3.4	14.2
PA-9b(Naborate)-ts(1,6major)_01	-4398.56325172	-4398.56325172	-22.9	-4397.705820	-4397.705820	0.3	23.2	-433.7
PA-9b(Naborate)-ts(1,6major)_02	-4398.56128250	-4398.56128250	-21.6	-4397.705461	-4397.705461	0.6	22.2	-438.4
PA-9b(Naborate)-ts(1,6major)_03	-4398.56061938	-4398.56061938	-21.2	-4397.702017	-4397.702017	2.7	24.0	-437.5
PA-9b(Naborate)-ts(1,6major)_04	-4398.56064928	-4398.56064928	-21.2	-4397.704192	-4397.704192	1.4	22.6	-431.7
PA-9b(Naborate)-ts(1,6major)_05	-4398.55507914	-4398.55507914	-17.7	-4397.699424	-4397.699424	4.4	22.1	-437.5
PA-9b(Naborate)-ts(1,6major)_06	-4398.56485118	-4398.56485118	-23.9	-4397.706188	-4397.706188	0.1	24.0	-459.0
PA-9b(Naborate)-ts(1,6major)_07	-4398.56096625	-4398.56096625	-21.4	-4397.702604	-4397.702604	2.4	23.8	-450.7
PA-9b(Naborate)-ts(1,6major)_08	-4398.56213541	-4398.56213541	-22.2	-4397.701620	-4397.701620	3.0	25.2	-466.0
PA-9b(Naborate)-ts(1,6major)_09	-4398.56071055	-4398.56071055	-21.3	-4397.700859	-4397.700859	3.5	24.7	-403.1
PA-9b(Naborate)-ts(1,6major)_10	-4398.56065632	-4398.56065632	-21.2	-4397.700390	-4397.700390	3.8	25.0	-402.8
9d-Cu-allenyl	-2677.36469942	-3519.29177790	0.0	-2677.000607	-3518.719330	0.0	0.0	18.9
PA-9b-ts(1,6major)_01	-3519.31528051	-3519.31528051	-14.7	-3518.710003	-3518.710003	5.9	20.6	-465.3
PA-9b-ts(1,6major)_02	-3519.31441637	-3519.31441637	-14.2	-3518.710549	-3518.710549	5.5	19.7	-439.9
PA-9b-ts(1,6major)_03	-3519.31189147	-3519.31189147	-12.6	-3518.706575	-3518.706575	8.0	20.6	-467.9
PA-9b-ts(1,6major)_04	-3519.31309758	-3519.31309758	-13.4	-3518.707448	-3518.707448	7.5	20.8	-455.2
PA-9b-ts(1,6major)_05	-3519.31462563	-3519.31462563	-14.3	-3518.707187	-3518.707187	7.6	22.0	-460.9

E …… electronic energy in Hartree after opt with ωB97XD/Def2SVP in thf(PCM)

E(sum) electronic energy in Hartree after opt with ωB97XD/Def2SVP in thf(PCM) after mass balance

G …… gas phase sum of electronic and thermal free energies in Hartree after opt with ωB97XD/Def2SVP in thf(PCM)

G(sum) gas phase sum of electronic and thermal free energies in Hartree after opt with ωB97XD/Def2SVP in thf(PCM) after mass balance

ΔE … relative electronic energy in kcal/mol after opt with ωB97XD/Def2SVP in thf(PCM)

ΔG … relative free energy in kcal/mol after opt with ωB97XD/Def2SVP in thf(PCM)

ΔG_{corr} thermal correction to free energy in kcal/mol obtained with ωB97XD/Def2SVP in thf(PCM) ($\Delta G = \Delta E + \Delta G_{corr}$)

Table S2. Single point energies in Figures S1-1–S15-9 with ωB97XD, M06 and MN12SX

structure	ωB97XD/Def2TZVPP$_{thf(SMD)}$			M06/Def2TZVPP$_{thf(SMD)}$			MN12SX/Def2TZVPP$_{thf(SMD)}$		
	E(sp,sum) [hartree]	ΔE(sp) [kcal/mol]	ΔG(sp) [kcal/mol]	E(sp,sum) [hartree]	ΔE(sp) [kcal/mol]	ΔG(sp) [kcal/mol]	E(sp,sum) [hartree]	ΔE(sp) [kcal/mol]	ΔG(sp) [kcal/mol]
Figure S1-1									
dienoate									
PhOH									
NaOPh									
tBuOH									
NaOtBu									
PhOBpin									
(PhO)2BpinNa									
9d-Cu-allenyl	-3917.02235026	0.0	0.0	-3916.13339022	0.0	0.0	-3915.68723465	0.0	0.0
PA-9d(Na)-ts(1,6major)	-3917.05625370	-21.3	0.7	-3916.16406749	-19.3	2.7	-3915.71092569	-14.9	7.1
9d-Cu-allenyl	-3990.83197127	0.0	0.0	-3989.92599364	0.0	0.0	-3989.50539943	0.0	0.0
PA-9d(Na)-ts(1,6major)	-3990.84100045	-5.7	16.0	-3989.93198846	-3.8	17.9	-3989.50619279	-0.5	21.2
9d-Cu-allenyl	-3990.83197127	0.0	0.0	-3989.92599364	0.0	0.0	-3989.50539943	0.0	0.0
PA-9d(NaOPh)-ts(1,6major)	-3990.88771241	-35.0	2.8	-3989.97360811	-29.9	7.9	-3989.54407839	-24.3	13.5
9d-Cu-allenyl	-3521.60502971	0.0	0.0	-3520.81022808	0.0	0.0	-3520.43853460	0.0	0.0
PA-9d-ts(1,6major)	-3521.60337835	1.0	20.8	-3520.80721035	1.9	21.6	-3520.42723261	7.1	26.8
9d-Cu-allenyl	-4709.09162998	24.7	8.4	-4707.92901238	21.3	5.0	-4707.42546453	22.8	6.4
9d-Cu-allenyl	-4709.13104909	0.0	0.0	-4707.96295860	0.0	0.0	-4707.46173526	0.0	0.0
PA-9d(Naborate)-ts(1,6major)	-4709.16683434	-22.5	1.6	-4707.99538130	-20.3	3.7	-4707.48509002	-14.7	9.4
Figure S2-1									
PA-9d(NaOPh)-prod(1,6major)	-3990.93800549	-42.3	-19.3	-3990.01574785	-36.2	-13.2	-3989.58455465	-31.1	-8.1
PA-9d(NaOPh)-ts(1,6major)	-3990.88771241	-10.7	10.5	-3989.97360811	-9.8	11.5	-3989.54407839	-5.7	15.6
PA-9d(NaOPh)-pc(1,6major)	-3990.90290388	-20.3	0.4	-3989.98535431	-17.2	3.5	-3989.55936552	-15.3	5.4
9d(NaOPh)-Cu-allenyl	-3990.87058638	0.0	0.0	-3989.95800524	0.0	0.0	-3989.53501617	0.0	0.0
9b(NaOPh)-Cu-allenyl	-3990.86589294	0.0	0.0	-3989.95169678	0.0	0.0	-3989.52840609	0.0	0.0
PA-9b(NaOPh)-pc(1,6major)	-3990.90018125	-21.5	-1.1	-3989.98116503	-18.5	1.9	-3989.55380230	-15.9	4.5
PA-9b(NaOPh)-ts(1,6major)	-3990.88583980	-12.5	8.3	-3989.96949657	-11.2	9.6	-3989.53857734	-6.4	14.4
PA-9b(NaOPh)-prod(1,6major)	-3990.93430599	-42.9	-20.6	-3990.01285705	-38.4	-16.0	-3989.57956414	-32.1	-9.7

PA-9d(NaOPh)-prod(1,6minor)	-3990.93290336	-39.1	-17.2	-3990.01143988	-33.5	-11.6	-3989.58039504	-28.5	-6.6
PA-9d(NaOPh)-ts(1,6minor)	-3990.88435999	-8.6	11.6	-3989.97142413	-8.4	11.9	-3989.54116499	-3.9	16.4
PA-9d(NaOPh)-pc(1,6minor)	-3990.89850237	-17.5	2.4	-3989.98158240	-14.8	5.1	-3989.55414047	-12.0	7.9
9d(NaOPh)-Cu-allenyl	-3990.87058638	0.0	0.0	-3989.95800524	0.0	0.0	-3989.53501617	0.0	0.0
9b(NaOPh)-Cu-allenyl	-3990.86589294	0.0	0.0	-3989.95169678	0.0	0.0	-3989.52840609	0.0	0.0
PA-9b(NaOPh)-pc(1,6minor)	-3990.89534926	-18.5	1.9	-3989.97550961	-14.9	5.4	-3989.54744118	-11.9	8.4
PA-9b(NaOPh)-ts(1,6minor)	-3990.87893790	-8.2	12.7	-3989.96342848	-7.4	13.5	-3989.53149363	-1.9	18.9
PA-9b(NaOPh)-prod(1,6minor)	-3990.93100974	-40.9	-18.0	-3990.00918140	-36.1	-13.2	-3989.57515695	-29.3	-6.5
Figure S3-1									
AA-9d(NaOPh)-prod(1,6major)	-4442.25425183	-49.0	-23.0	-4441.15464221	-43.2	-17.3	-4440.64572347	-39.1	-13.1
AA-9d(NaOPh)-ts(1,6major)	-4442.20703033	-19.3	4.6	-4441.11533859	-18.6	5.3	-4440.60922583	-16.2	7.7
AA-9d(NaOPh)-pc(1,6major)	-4442.21197294	-22.4	0.8	-4441.11965289	-21.3	2.0	-4440.61399771	-19.2	4.1
9d(NaOPh)-Cu-allyl	-4442.17621217	0.0	0.0	-4441.08572350	0.0	0.0	-4440.58346898	0.0	0.0
9b(NaOPh)-Cu-allyl	-4442.17569662	0.0	0.0	-4441.08335295	0.0	0.0	-4440.57955401	0.0	0.0
AA-9b(NaOPh)-pc(1,6major)	-4442.20571405	-18.8	1.1	-4441.11106454	-17.4	2.6	-4440.60279951	-14.6	5.4
AA-9b(NaOPh)-ts(1,6major)	-4442.20131098	-16.1	6.3	-4441.10769971	-15.3	7.1	-4440.59922567	-12.3	10.0
AA-9b(NaOPh)-prod(1,6major)	-4442.24761702	-45.1	-20.1	-4441.14554836	-39.0	-14.0	-4440.63636545	-35.6	-10.6
AA-9d(NaOPh)-prod(1,6minor)	-4442.24538245	-43.4	-20.1	-4441.14271630	-35.8	-12.5	-4440.63526265	-32.5	-9.2
AA-9d(NaOPh)-ts(1,6minor)	-4442.20068755	-15.4	7.0	-4441.10803999	-14.0	8.4	-4440.60092130	-11.0	11.4
AA-9d(NaOPh)-pc(1,6minor)	-4442.20701084	-19.3	2.0	-4441.11272163	-16.9	4.4	-4440.60717458	-14.9	6.5
9d(NaOPh)-Cu-allyl	-4442.17621217	0.0	0.0	-4441.08572350	0.0	0.0	-4440.58346898	0.0	0.0
9b(NaOPh)-Cu-allyl	-4442.17569662	0.0	0.0	-4441.08335295	0.0	0.0	-4440.57955401	0.0	0.0
AA-9b(NaOPh)-pc(1,6minor)	-4442.20252596	-16.8	5.8	-4441.10766838	-15.3	7.4	-4440.59964701	-12.6	10.0
AA-9b(NaOPh)-ts(1,6minor)	-4442.19924457	-14.8	6.7	-4441.10534786	-13.8	7.6	-4440.59570571	-10.1	11.3
AA-9b(NaOPh)-prod(1,6minor)	-4134.71087898	-45.7	-19.3	-4133.72848179	-38.1	-11.7	-4133.24493202	-34.6	-8.2
Figure S4-1									
PA-9d(Na)-prod(1,6major)	-3683.39784182	-41.9	-18.9	-3682.59738631	-36.4	-13.5	-3682.19185658	-31.2	-8.3
PA-9d(Na)-ts(1,6major)	-3683.34637627	-9.6	10.0	-3682.55204777	-8.0	11.5	-3682.14838128	-3.9	15.6
PA-9d(Na)-pc(1,6major)	-3683.36321378	-20.1	-0.4	-3682.56636861	-17.0	2.8	-3682.16499630	-14.3	5.4
9d(Na)-Cu-allenyl	-3683.33114499	0.0	0.0	-3682.53933632	0.0	0.0	-3682.14215505	0.0	0.0
9b(Na)-Cu-allenyl	-3683.33122166	0.0	0.0	-3682.53742270	0.0	0.0	-3682.13953768	0.0	0.0
PA-9b(Na)-pc(1,6major)	-3683.35560070	-15.3	2.6	-3682.55836100	-13.1	4.8	-3682.15725021	-11.1	6.8
PA-9b(Na)-ts(1,6major)	-3683.34236298	-7.0	11.0	-3682.54822576	-6.8	11.2	-3682.14321630	-2.3	15.6
PA-9b(Na)-prod(1,6major)	-3683.39313924	-38.9	-18.7	-3682.59320296	-35.0	-14.9	-3682.18528563	-28.7	-8.6

PA-9d(Na)-prod(1,6minor)	-3683.40031948	-43.4	-21.2	-3682.59965810	-37.9	-15.6	-3682.19462082	-32.9	-10.7
PA-9d(Na)-ts(1,6minor)	-3683.34306318	-7.5	11.3	-3682.54933664	-6.3	12.5	-3682.14702419	-3.1	15.7
PA-9d(Na)-pc(1,6minor)	-3683.35945929	-17.8	1.0	-3682.56156905	-14.0	4.8	-3682.16240876	-12.7	6.1
9d(Na)-Cu-allenyl	-3683.33114499	0.0	0.0	-3682.53933632	0.0	0.0	-3682.14215505	0.0	0.0
9b(Na)-Cu-allenyl	-3683.33122166	0.0	0.0	-3682.53742270	0.0	0.0	-3682.13953768	0.0	0.0
PA-9b(Na)-pc(1,6minor)	-3683.35359137	-14.0	4.5	-3682.55654715	-12.0	6.5	-3682.15477881	-9.6	9.0
PA-9b(Na)-ts(1,6minor)	-3683.33654017	-3.3	17.4	-3682.54299270	-3.5	17.2	-3682.13718221	1.5	22.2
PA-9b(Na)-prod(1,6minor)	-3683.38759741	-35.4	-15.2	-3682.58775481	-31.6	-11.4	-3682.17978765	-25.3	-5.0

Figure S5-1

AA-9d(Na)-prod(1,6major)	-4134.70550277	-40.3	-14.5	-4133.72532266	-33.4	-7.6	-4133.24320321	-30.6	-4.9
AA-9d(Na)-ts(1,6major)	-4134.65947596	-11.4	9.6	-4133.68817393	-10.1	10.9	-4133.20733197	-8.1	12.9
AA-9d(Na)-pc(1,6major)	-4134.66659548	-15.9	6.2	-4133.69397273	-13.7	8.3	-4133.21435381	-12.5	9.5
9d(Na)-Cu-allyl	-4134.64133271	0.0	0.0	-4133.67213363	0.0	0.0	-4133.19437368	0.0	0.0
9b(Na)-Cu-allyl	-4134.63799627	0.0	0.0	-4133.66778602	0.0	0.0	-4133.18981887	0.0	0.0
AA-9b(Na)-pc(1,6major)	-4134.66235872	-15.3	6.5	-4133.68882459	-13.2	8.6	-4133.20729302	-11.0	10.8
AA-9b(Na)-ts(1,6major)	-4134.65804731	-12.6	10.1	-4133.68556131	-11.2	11.5	-4133.20353635	-8.6	14.1
AA-9b(Na)-prod(1,6major)	-4134.70719414	-43.4	-18.2	-4133.72597427	-36.5	-11.3	-4133.24218952	-32.9	-7.7
AA-9d(Na)-prod(1,6minor)	-4134.71098644	-43.7	-22.7	-4133.73005127	-36.3	-15.3	-4133.24743867	-33.3	-12.3
AA-9d(Na)-ts(1,6minor)	-4134.65544875	-8.9	13.1	-4133.68404505	-7.5	14.5	-4133.20411140	-6.1	15.9
AA-9d(Na)-pc(1,6minor)	-4134.66379593	-14.1	6.6	-4133.69023515	-11.4	9.4	-4133.21148125	-10.7	10.0
9d(Na)-Cu-allyl	-4134.64133271	0.0	0.0	-4133.67213363	0.0	0.0	-4133.19437368	0.0	0.0
9b(Na)-Cu-allyl	-4134.63799627	0.0	0.0	-4133.66778602	0.0	0.0	-4133.18981887	0.0	0.0
AA-9b(Na)-pc(1,6minor)	-4134.65984054	-13.7	8.7	-4133.68675858	-11.9	10.5	-4133.20263410	-8.0	14.4
AA-9b(Na)-ts(1,6minor)	-4134.65491128	-10.6	11.8	-4133.68294647	-9.5	12.9	-4133.19814032	-5.2	17.2
AA-9b(Na)-prod(1,6minor)	-4134.71087898	-45.7	-19.3	-4133.72848179	-38.1	-11.7	-4133.24493202	-34.6	-8.2

Figure S6-1

thf

PMe3

Me2NHC

NaOPh

NaOtBu

dienoate

dienoate-NaOPh

dienoate-NaOtBu

Me2NHC-Cu-allenyl	-3068.82928331	-8.5	-7.6	-3068.30875957	-9.5	-8.6	-3067.96232859	-8.6	-7.7
PMe3-Cu-allenyl	-3068.81575877	0.0	0.0	-3068.29363839	0.0	0.0	-3067.94866008	0.0	0.0
thf-Cu-allenyl	-3068.79103206	15.5	15.7	-3068.26934047	15.2	15.4	-3067.92511116	14.8	15.0
PA-NaOPh-prod(1,6)	-3068.84357882	-17.5	-8.3	-3068.31679925	-14.5	-5.4	-3067.96676616	-11.4	-2.2
PA-NaOPh-ts(1,6)	-3068.79775941	11.3	19.6	-3068.27777257	10.0	18.2	-3067.92987275	11.8	20.1
PA-NaOPh-ed(1,6)	-3068.81261617	2.0	9.2	-3068.29038779	2.0	9.2	-3067.94511397	2.2	9.4
NaOPh-Cu-allenyl	-3068.78025160	22.3	11.4	-3068.26060579	20.7	9.9	-3067.91360817	22.0	11.2
PA-NaOPh-ed(1,4)	-3068.82290138	-4.5	3.9	-3068.29954852	-3.7	4.6	-3067.95120914	-1.6	6.8
PA-NaOPh-ts(1,4)	-3068.79414584	13.6	21.2	-3068.27565479	11.3	18.9	-3067.92589394	14.3	21.9
PA-NaOPh-prod(1,4)	-3068.84931260	-21.1	-11.7	-3068.32203973	-17.8	-8.4	-3067.97196924	-14.6	-5.2
Me2NHC-Cu-allenyl	-2995.01744986	-8.5	-7.6	-2994.51396505	-9.5	-8.6	-2994.14163588	-8.6	-7.7
PMe3-Cu-allenyl	-2995.00392532	0.0	0.0	-2994.49884387	0.0	0.0	-2994.12796737	0.0	0.0
thf-Cu-allenyl	-2994.97919861	15.5	15.7	-2994.47454595	15.2	15.4	-2994.10441845	14.8	15.0
PA-NaOtBu-prod(1,6)	-2995.04688960	-27.0	-17.9	-2994.53633318	-23.5	-14.5	-2994.15898795	-19.5	-10.4
PA-NaOtBu-ts(1,6)	-2995.00077189	2.0	8.9	-2994.49872442	0.1	7.0	-2994.12179243	3.9	10.8
PA-NaOtBu-ed(1,6)	-2995.01655294	-7.9	-2.5	-2994.51153622	-8.0	-2.5	-2994.13816262	-6.4	-0.9
NaOtBu-Cu-allenyl	-2994.98718705	10.5	0.4	-2994.48472280	8.9	-1.3	-2994.11010278	11.2	1.1
PA-NaOtBu-ed(1,4)	-2995.02081716	-10.6	-6.4	-2994.51666040	-11.2	-7.0	-2994.14196351	-8.8	-4.6
PA-NaOtBu-ts(1,4)	-2994.99895360	3.1	7.4	-2994.49779724	0.7	4.9	-2994.12084986	4.5	8.7
PA-NaOtBu-prod(1,4)	-2995.05428820	-31.6	-22.7	-2994.54421081	-28.5	-19.5	-2994.16668659	-24.3	-15.4

Figure S7-1

Me2NHC-Cu-allyl	-3356.90190046	0.0	0.0	-3356.19082586	0.0	0.0	-3355.76947919	0.0	0.0
AA-Me2NHC-pc(1,6major)	-3356.92173542	-12.4	5.5	-3356.20596661	-9.5	8.5	-3355.78294379	-8.4	9.5
AA-Me2NHC-ts(1,6major)	-3356.91107985	-5.8	14.2	-3356.19684095	-3.8	16.2	-3355.77271369	-2.0	17.9
AA-Me2NHC-prod(1,6major)	-3356.96212920	-37.8	-14.5	-3356.23841491	-29.9	-6.6	-3355.81382406	-27.8	-4.5
Me2NHC-Cu-allyl	-3356.90190046	0.0	0.0	-3356.19082586	0.0	0.0	-3355.76947919	0.0	0.0
AA-Me2NHC-pc(1,6minor)	-3356.92018482	-11.5	7.9	-3356.20198203	-7.0	12.4	-3355.77885671	-5.9	13.5
AA-Me2NHC-ts(1,6minor)	-3356.90184702	0.0	20.1	-3356.18737922	2.2	22.2	-3355.76151812	5.0	25.0
AA-Me2NHC-prod(1,6minor)	-3356.95475893	-33.2	-10.1	-3356.23307270	-26.5	-3.4	-3355.80524014	-22.4	0.7

Figure S8-1

dienoate									
SIMes-Cu-allenyl	-3525.02126270	0.0	0.0	-3524.19135955	0.0	0.0	-3523.82072108	0.0	0.0
PA-SIMes-ed(1,6)	-3525.03501217	-8.6	12.6	-3524.20038963	-5.7	15.5	-3523.82534428	-2.9	18.3

PA-SIMes-ts(1,6)	-3525.01599756	3.3	24.4	-3524.18482097	4.1	25.2	-3523.80541778	9.6	30.7
PA-SIMes-prod(1,6)	-3525.06427418	-27.0	-3.9	-3524.22735126	-22.6	0.5	-3523.84759504	-16.9	6.2
PA-SIMes-ed(1,4AA)	-3525.03504845	-8.7	12.4	-3524.20050687	-5.7	15.4	-3523.82539531	-2.9	18.2
PA-SIMes-ts(1,4AA)	-3525.00671358	9.1	29.4	-3524.17318282	11.4	31.7	-3523.79494539	16.2	36.4
PA-SIMes-prod(1,4AA)	-3525.05252178	-19.6	-0.1	-3524.21507413	-14.9	4.6	-3523.83664071	-10.0	9.5
PA-SIMes-ed(1,4)	-3525.03218345	-6.9	11.9	-3524.20020482	-5.6	13.2	-3523.82592051	-3.3	15.5
PA-SIMes-ts(1,4)	-3524.99957892	13.6	30.9	-3524.17009122	13.3	30.6	-3523.79443209	16.5	33.8
PA-SIMes-prod(1,4)	-3525.03760248	-10.3	11.3	-3524.19790947	-4.1	17.4	-3523.82447708	-2.4	19.2
PPh3-Cu-allenyl	-3635.89081165	0.0	0.0	-3635.15239600	0.0	0.0	-3634.82371919	0.0	0.0
PA-PPh3-ed(1,6)	-3635.90023076	-5.9	11.6	-3635.15826545	-3.7	13.8	-3634.82650137	-1.7	15.8
PA-PPh3-ts(1,6)	-3635.87965155	7.0	26.0	-3635.14176346	6.7	25.6	-3634.80725567	10.3	29.3
PA-PPh3-prod(1,6)	-3635.92484797	-21.4	-1.3	-3635.18101473	-18.0	2.1	-3634.84425697	-12.9	7.2
PA-PPh3-ed(1,4AA)	-3635.90033582	-6.0	10.2	-3635.15969220	-4.6	11.6	-3634.82810853	-2.8	13.5
PA-PPh3-ts(1,4AA)	-3635.87000911	13.1	28.8	-3635.12933309	14.5	30.2	-3634.79529613	17.8	33.6
PA-PPh3-prod(1,4AA)	-3635.91519247	-15.3	3.2	-3635.16950782	-10.7	7.7	-3634.83611730	-7.8	10.7
PA-PPh3-ed(1,4)	-3635.89704236	-3.9	11.7	-3635.15683178	-2.8	12.8	-3634.82662491	-1.8	13.8
PA-PPh3-ts(1,4)	-3635.86619047	15.5	30.4	-3635.12930261	14.5	29.4	-3634.79877876	15.7	30.6
PA-PPh3-prod(1,4)	-3635.92832707	-23.5	-5.0	-3635.18111023	-18.0	0.5	-3634.85193029	-17.7	0.8
Figures S9-1									
Me2NHC-Cu-allenyl	-2905.61065891	0.0	0.0	-2905.07228030	0.0	0.0	-2904.73008855	0.0	0.0
PA-Me2NHC-ed(1,6)	-2905.61551037	-3.0	14.9	-2905.07542739	-2.0	15.9	-2904.73109735	-0.6	17.3
PA-Me2NHC-ts(1,6)	-2905.59596441	9.2	27.2	-2905.05971940	7.9	25.8	-2904.71160347	11.6	29.6
PA-Me2NHC-prod(1,6)	-2905.64614630	-22.3	-0.3	-2905.10183379	-18.5	3.4	-2904.75269112	-14.2	7.7
PA-Me2NHC-ed(1,4AA)	-2905.61763066	-4.4	11.9	-2905.07519052	-1.8	14.4	-2904.73270474	-1.6	14.6
PA-Me2NHC-ts(1,4AA)	-2905.58445465	16.4	32.1	-2905.04452805	17.4	33.1	-2904.69753498	20.4	36.1
PA-Me2NHC-prod(1,4AA)	-2905.63888257	-17.7	-2.0	-2905.09464210	-14.0	1.6	-2904.74843178	-11.5	4.2
PA-Me2NHC-ed(1,4)	-2905.61283807	-1.4	13.6	-2905.07352500	-0.8	14.2	-2904.73109017	-0.6	14.4
PA-Me2NHC-ts(1,4)	-2905.58205030	18.0	34.1	-2905.04548147	16.8	32.9	-2904.70011167	18.8	34.9
PA-Me2NHC-prod(1,4)	-2905.62000587	-5.9	12.6	-2905.07362957	-0.8	17.6	-2904.73069935	-0.4	18.0
PMe3-Cu-allenyl	-3060.68423543	0.0	0.0	-3060.18986551	0.0	0.0	-3059.84008469	0.0	0.0
PA-PMe3-ed(1,6)	-3060.69567408	-7.2	9.9	-3060.20020876	-6.5	10.6	-3059.84827443	-5.1	11.9
PA-PMe3-ts(1,6)	-3060.67410433	6.4	24.4	-3060.18241140	4.7	22.7	-3059.82686972	8.3	26.3

PA-PMe3-prod(1,6)	-3060.71995989	-22.4	-2.8	-3060.22063684	-19.3	0.3	-3059.86445362	-15.3	4.4
PA-PMe3-ed(1,4AA)	-3060.69567408	-7.2	9.9	-3060.20020883	-6.5	10.6	-3059.84827450	-5.1	11.9
PA-PMe3-ts(1,4AA)	-3060.65934538	15.6	31.7	-3060.16495629	15.6	31.7	-3059.81004673	18.8	34.9
PA-PMe3-prod(1,4AA)	-3060.70755126	-14.6	2.8	-3060.20738444	-11.0	6.4	-3059.85362578	-8.5	8.9
PA-PMe3-ed(1,4)	-3060.69092142	-4.2	11.9	-3060.19712988	-4.6	11.5	-3059.84600211	-3.7	12.4
PA-PMe3-ts(1,4)	-3060.66021586	15.1	30.2	-3060.16917418	13.0	28.1	-3059.81631528	14.9	30.0
PA-PMe3-prod(1,4)	-3060.72052409	-22.8	-2.2	-3060.22224154	-20.3	0.3	-3059.86453791	-15.3	5.2

Figure S10-1

dienoate
dienoate-Naborate

SIMes-Cu-allenyl	-4170.57644708	0.0	0.0	-4169.62279097	0.0	0.0	-4169.14720784	0.0	0.0
PA-SIMes(Naborate)-ed(1,6)	-4170.60154244	-15.7	7.2	-4169.64006692	-10.8	12.1	-4169.15833641	-7.0	16.0
PA-SIMes(Naborate)-ts(1,6)	-4170.58902765	-7.9	14.3	-4169.62994310	-4.5	17.7	-4169.14555865	1.0	23.2
PA-SIMes(Naborate)-prod(1,6)	-4170.64124287	-40.7	-17.1	-4169.67605831	-33.4	-9.9	-4169.18979225	-26.7	-3.2
PA-SIMes(Naborate)-ed(1,4AA)	-4170.59982759	-14.7	7.1	-4169.63780212	-9.4	12.4	-4169.15577160	-5.4	16.4
PA-SIMes(Naborate)-ts(1,4AA)	-4170.58199140	-3.5	17.1	-4169.62031454	1.6	22.2	-4169.13725708	6.2	26.9
PA-SIMes(Naborate)-prod(1,4AA)	-4170.62959750	-33.4	-11.2	-4169.66275344	-25.1	-3.0	-4169.17942681	-20.2	1.9
PA-SIMes(Naborate)-ed(1,4)	-4170.60383364	-17.2	4.4	-4169.64114501	-11.5	10.0	-4169.15938207	-7.6	13.9
PA-SIMes(Naborate)-ts(1,4)	-4170.57418227	1.4	22.0	-4169.61385891	5.6	26.2	-4169.13131782	10.0	30.6
PA-SIMes(Naborate)-prod(1,4)	-4170.63212445	-34.9	-11.7	-4169.66493164	-26.4	-3.2	-4169.18108052	-21.3	2.0

dienoate
dienoate-Naborate

PPh3-Cu-allenyl	-4281.44599603	0.0	0.0	-4280.58382742	0.0	0.0	-4280.15020595	0.0	0.0
PA-PPh3(Naborate)-ed(1,6)	-4281.46746198	-13.5	6.3	-4280.59890883	-9.5	10.3	-4280.16102512	-6.8	13.0
PA-PPh3(Naborate)-ts(1,6)	-4281.45382085	-4.9	14.6	-4280.58875865	-3.1	16.4	-4280.14728851	1.8	21.3
PA-PPh3(Naborate)-prod(1,6)	-4281.50836163	-39.1	-16.7	-4280.63634687	-33.0	-10.5	-4280.19118616	-25.7	-3.3
PA-PPh3(Naborate)-ed(1,4AA)	-4281.46812950	-13.9	3.3	-4280.60217750	-11.5	5.7	-4280.16424940	-8.8	8.4
PA-PPh3(Naborate)-ts(1,4AA)	-4281.43958118	4.0	19.1	-4280.57140524	7.8	22.9	-4280.13367614	10.4	25.4
PA-PPh3(Naborate)-prod(1,4AA)	-4281.49279310	-29.4	-12.8	-4280.61881368	-22.0	-5.4	-4280.18126052	-19.5	-3.0
PA-PPh3(Naborate)-ed(1,4)	-4281.47138378	-15.9	0.8	-4280.60207454	-11.5	5.3	-4280.16316545	-8.1	8.6
PA-PPh3(Naborate)-ts(1,4)	-4281.44141220	2.9	21.0	-4280.57475036	5.7	23.8	-4280.13513113	9.5	27.5
PA-PPh3(Naborate)-prod(1,4)	-4281.50805388	-38.9	-15.6	-4280.63518412	-32.2	-8.9	-4280.19023961	-25.1	-1.8

Figure S11-1									
dienoate									
PA-9d(Na)-prod(1,6major)	-3683.39784182	-41.9	-18.9	-3682.59738631	-36.4	-13.5	-3682.19185658	-31.2	-8.3
PA-9d(Na)-ts(1,6major)	-3683.34637627	-9.6	10.0	-3682.55204777	-8.0	11.5	-3682.14838128	-3.9	15.6
PA-9d(Na)-pc(1,6major)	-3683.36321378	-20.1	-0.4	-3682.56636861	-17.0	2.8	-3682.16499630	-14.3	5.4
9d(Na)-Cu-allenyl	-3683.33114499	0.0	0.0	-3682.53933632	0.0	0.0	-3682.14215505	0.0	0.0
PA-9d(Na)-pc(1,4AA)	-3683.35966006	-17.9	0.8	-3682.56283640	-14.7	4.0	-3682.16370288	-13.5	5.2
PA-9d(Na)-ts(1,4AA)	-3683.33219811	-0.7	16.8	-3682.53782334	0.9	18.4	-3682.13545302	4.2	21.7
PA-9d(Na)-prod(1,4AA)	-3683.39331473	-39.0	-20.8	-3682.59217563	-33.2	-14.9	-3682.19295841	-31.9	-13.7
Figure S12-1									
NaOtBu									
dienoate									
PA-SIMes(NaOtBu)-prod(1,4)	-2682.26036288	-42.9	-23.9	-2681.68866579	-39.4	-20.4	-2681.41224991	-38.5	-19.5
PA-SIMes(NaOtBu)-ts(1,4)	-2682.17841192	8.6	26.5	-2681.61636955	6.0	24.0	-2681.33795643	8.1	26.1
PA-SIMes(NaOtBu)-ed(1,4)	-2682.20840072	-10.3	7.4	-2681.64342161	-11.0	6.7	-2681.36713021	-10.2	7.4
SIMes-Cu-allenyl	-2682.15378194	24.0	5.7	-2681.59626512	18.6	0.3	-2681.32394289	16.9	-1.5
SIMes-Cu(NaOtBu)-allenyl	-2682.19206462	0.0	0.0	-2681.62592745	0.0	0.0	-2681.35083456	0.0	0.0
PA-SIMes(NaOtBu)-ed(1,6)	-2682.20484762	-8.0	10.5	-2681.63786848	-7.5	11.0	-2681.36069832	-6.2	12.3
PA-SIMes(NaOtBu)-ts(1,6)	-2682.19215840	-0.1	17.6	-2681.62787391	-1.2	16.5	-2681.34747993	2.1	19.8
PA-SIMes(NaOtBu)-prod(1,6)	-2682.24539528	-33.5	-14.9	-2681.67467793	-30.6	-12.1	-2681.39195407	-25.8	-7.3
PA-PPh3(NaOtBu)-prod(1,4)	-2793.12770822	-40.6	-17.4	-2792.65029930	-36.9	-13.8	-2792.40656300	-30.3	-7.2
PA-PPh3(NaOtBu)-ts(1,4)	-2793.07132615	-5.2	13.4	-2792.60168576	-6.4	12.2	-2792.36294430	-3.0	15.6
PA-PPh3(NaOtBu)-ed(1,4)	-2793.09449946	-19.7	0.1	-2792.61889716	-17.2	2.6	-2792.38121552	-14.4	5.4
PPh3-Cu-allenyl	-2793.02333089	24.9	9.2	-2792.55730157	21.5	5.8	-2792.32694100	19.6	3.9
PPh3-Cu(NaOtBu)-allenyl	-2793.06304992	0.0	0.0	-2792.59153231	0.0	0.0	-2792.35821531	0.0	0.0
PA-PPh3(NaOtBu)-ed(1,6)	-2793.07243155	-5.9	12.0	-2792.59919364	-4.8	13.1	-2792.36546539	-4.5	13.3
PA-PPh3(NaOtBu)-ts(1,6)	-2793.05860435	2.8	22.2	-2792.58841354	2.0	21.3	-2792.35111405	4.5	23.8
PA-PPh3(NaOtBu)-prod(1,6)	-2793.11322554	-31.5	-10.7	-2792.63583254	-27.8	-7.1	-2792.39454951	-22.8	-2.1
Figure S13-1									

NaOMe dienoate									
PA-SIMes(NaOMe)-prod(1,4)	-2682.25617022	-43.2	-21.8	-2681.68012460	-35.3	-13.9	-2681.40394301	-34.3	-12.9
PA-SIMes(NaOMe)-ts(1,4)	-2682.17655336	6.8	25.3	-2681.61576620	5.0	23.5	-2681.33902998	6.5	24.9
PA-SIMes(NaOMe)-ed(1,4)	-2682.20446296	-10.7	7.9	-2681.63854656	-9.3	9.4	-2681.36379706	-9.1	9.6
SIMes-Cu-allenyl	-2682.15378194	21.1	5.6	-2681.59626512	17.3	1.8	-2681.32394289	15.9	0.4
SIMes-Cu(NaOMe)-allenyl	-2682.18738500	0.0	0.0	-2681.62380065	0.0	0.0	-2681.34934568	0.0	0.0
PA-SIMes(NaOMe)-ed(1,6)	-2682.20339526	-10.0	8.2	-2681.63765084	-8.7	9.5	-2681.36086340	-7.2	11.0
PA-SIMes(NaOMe)-ts(1,6)	-2682.19104064	-2.3	17.6	-2681.62733751	-2.2	17.7	-2681.34791937	0.9	20.8
PA-SIMes(NaOMe)-prod(1,6)	-2682.24424038	-35.7	-15.7	-2681.67407351	-31.5	-11.5	-2681.39231903	-27.0	-7.0
PA-PPh3(NaOMe)-prod(1,4)	-2793.12465662	-40.2	-17.4	-2792.64975877	-36.5	-13.7	-2792.40857725	-31.5	-8.8
PA-PPh3(NaOMe)-ts(1,4)	-2793.06720052	-4.1	13.9	-2792.59782985	-3.9	14.1	-2792.36105713	-1.7	16.4
PA-PPh3(NaOMe)-ed(1,4)	-2793.08865104	-17.6	1.9	-2792.61496002	-14.7	4.8	-2792.37950844	-13.3	6.2
PPh3-Cu-allenyl	-2793.02333089	23.4	9.7	-2792.55730157	21.5	7.8	-2792.32694100	19.7	6.0
PPh3-Cu(NaOMe)-allenyl	-2793.06061324	0.0	0.0	-2792.59157425	0.0	0.0	-2792.35832675	0.0	0.0
PA-PPh3(NaOMe)-ed(1,6)	-2793.06855993	-5.0	11.8	-2792.59628875	-3.0	13.9	-2792.36318959	-3.1	13.8
PA-PPh3(NaOMe)-ts(1,6)	-2793.05422433	4.0	22.0	-2792.58395105	4.8	22.7	-2792.34849634	6.2	24.1
PA-PPh3(NaOMe)-prod(1,6)	-2793.10829534	-29.9	-9.3	-2792.63255995	-25.7	-5.1	-2792.39292060	-21.7	-1.1

Figure S14-1

NaOtBu dienoate									
PA-Me2NHC(NaOtBu)-prod(1,4)	-2062.84417434	-47.2	-27.2	-2062.56695032	-43.1	-23.1	-2062.31847525	-42.1	-22.2
PA-Me2NHC(NaOtBu)-ts(1,4)	-2062.77041845	-0.9	16.0	-2062.50191206	-2.3	14.6	-2062.25229522	-0.6	16.2
PA-Me2NHC(NaOtBu)-ed(1,4)	-2062.79019327	-13.3	4.8	-2062.51687665	-11.7	6.4	-2062.26891368	-11.0	7.0
Me2NHC-Cu-allenyl	-2062.74316302	16.2	-0.6	-2062.47724548	13.2	-3.6	-2062.23330198	11.3	-5.5
Me2NHC-Cu(NaOtBu)-allenyl	-2062.76898754	0.0	0.0	-2062.49828566	0.0	0.0	-2062.25132722	0.0	0.0
PA-Me2NHC(NaOtBu)-ed(1,6)	-2062.79041117	-13.4	2.2	-2062.51735490	-12.0	3.6	-2062.26992510	-11.7	3.9
PA-Me2NHC(NaOtBu)-ts(1,6)	-2062.77449941	-3.5	13.7	-2062.50494956	-4.2	13.0	-2062.25382814	-1.6	15.6
PA-Me2NHC(NaOtBu)-prod(1,6)	-2062.82670228	-36.2	-16.4	-2062.54923506	-32.0	-12.2	-2062.29766014	-29.1	-9.3
PA-PMe3(NaOtBu)-prod(1,4)	-2217.91670257	-40.0	-16.2	-2217.68197015	-34.5	-10.7	-2217.42437067	-32.5	-8.7
PA-PMe3(NaOtBu)-ts(1,4)	-2217.85468265	-1.1	16.7	-2217.63198737	-3.1	14.7	-2217.37269734	-0.1	17.7

PA-PMe3(NaOtBu)-ed(1,4)	-2217.87387324	-13.2	4.6	-2217.64573863	-11.8	6.0	-2217.38862406	-10.1	7.7
PMe3-Cu-allenyl	-2217.81675467	22.7	8.3	-2217.59477108	20.2	5.8	-2217.34330650	18.3	3.9
PMe3-Cu(NaOtBu)-allenyl	-2217.85291100	0.0	0.0	-2217.62699871	0.0	0.0	-2217.37250196	0.0	0.0
PA-PMe3(NaOtBu)-ed(1,6)	-2217.86338221	-6.6	12.4	-2217.63748046	-6.6	12.4	-2217.38011583	-4.8	14.2
PA-PMe3(NaOtBu)-ts(1,6)	-2217.84491109	5.0	25.0	-2217.62188974	3.2	23.2	-2217.36315277	5.9	25.8
PA-PMe3(NaOtBu)-prod(1,6)	-2217.89832095	-28.5	-7.0	-2217.66795153	-25.7	-4.2	-2217.40591267	-21.0	0.5

Figure S15-1

NaOPh dienoate									
9d(NaOPh)-Cu-allenyl	-3990.87058638	0.0	0.0	-3989.95800524	0.0	0.0	-3989.53501617	0.0	0.0
PA-9d(NaOPh)-ts(1,6major)_01	-3990.88771241	-10.7	10.5	-3989.97360811	-9.8	11.5	-3989.54407839	-5.7	15.6
PA-9d(NaOPh)-ts(1,6major)_02	-3990.88781156	-10.8	10.8	-3989.97259516	-9.2	12.4	-3989.54335300	-5.2	16.3
PA-9d(NaOPh)-ts(1,6major)_03	-3990.88488307	-9.0	11.7	-3989.96914226	-7.0	13.7	-3989.53864573	-2.3	18.4
PA-9d(NaOPh)-ts(1,6minor)_01	-3990.88435999	-8.6	11.6	-3989.97142413	-8.4	11.9	-3989.54116499	-3.9	16.4
PA-9d(NaOPh)-ts(1,6minor)_02	-3990.88435393	-8.6	12.6	-3989.96992569	-7.5	13.8	-3989.53991742	-3.1	18.2
PA-9d(NaOPh)-ts(1,6minor)_03	-3990.88433659	-8.6	13.1	-3989.96989725	-7.5	14.2	-3989.53987600	-3.0	18.7
PA-9d(NaOPh)-ts(1,6minor)_04	-3990.88031711	-6.1	14.8	-3989.96747449	-5.9	14.9	-3989.53694530	-1.2	19.7
PA-9d(NaOPh)-ts(1,6minor)_05	-3990.88256361	-7.5	15.2	-3989.96654589	-5.4	17.4	-3989.53732880	-1.5	21.3
PA-9d(NaOPh)-ts(1,6minor)_06	-3990.88307144	-7.8	14.4	-3989.96574736	-4.9	17.4	-3989.53676773	-1.1	21.1
PA-9d(NaOPh)-ts(1,6minor)_07	-3990.88184561	-7.1	15.6	-3989.96609115	-5.1	17.6	-3989.53686513	-1.2	21.5
PA-9d(NaOPh)-ts(1,6minor)_08	-3990.87841703	-4.9	17.1	-3989.96356809	-3.5	18.5	-3989.53324107	1.1	23.1

Figure S15-2

dienoate									
9b(NaOPh)-Cu-allenyl	-3990.86589294	0.0	0.0	-3989.95169678	0.0	0.0	-3989.52840609	0.0	0.0
PA-9b(NaOPh)-ts(1,6major)_01	-3990.88583980	-12.5	8.3	-3989.96949657	-11.2	9.6	-3989.53857734	-6.4	14.4
PA-9b(NaOPh)-ts(1,6major)_02	-3990.88548206	-12.3	8.9	-3989.96797330	-10.2	11.0	-3989.53772754	-5.8	15.3
PA-9b(NaOPh)-ts(1,6major)_03	-3990.88101107	-9.5	11.4	-3989.96483694	-8.2	12.7	-3989.53393017	-3.5	17.5
PA-9b(NaOPh)-ts(1,6major)_04	-3990.88067273	-9.3	11.5	-3989.96399024	-7.7	13.1	-3989.53393846	-3.5	17.3
PA-9b(NaOPh)-ts(1,6major)_05	-3990.88060330	-9.2	12.1	-3989.96443848	-8.0	13.3	-3989.53493498	-4.1	17.2
PA-9b(NaOPh)-ts(1,6major)_06	-3990.88274944	-10.6	11.9	-3989.96414669	-7.8	14.7	-3989.53227581	-2.4	20.1
PA-9b(NaOPh)-ts(1,6major)_07	-3990.87353187	-4.8	14.1	-3989.95790390	-3.9	15.0	-3989.52662121	1.1	20.0
PA-9b(NaOPh)-ts(1,6minor)_01	-3990.87893790	-8.2	12.7	-3989.96342848	-7.4	13.5	-3989.53149363	-1.9	18.9
PA-9b(NaOPh)-ts(1,6minor)_02	-3990.87980368	-8.7	11.9	-3989.96294977	-7.1	13.6	-3989.53160224	-2.0	18.6

PA-9b(NaOPh)-ts(1,6minor)_03	-3990.87977702	-8.7	12.0	-3989.96290940	-7.0	13.7	-3989.53152023	-2.0	18.7
PA-9b(NaOPh)-ts(1,6minor)_04	-3990.87796356	-7.6	13.7	-3989.96311122	-7.2	14.1	-3989.53113853	-1.7	19.5
PA-9b(NaOPh)-ts(1,6minor)_05	-3990.88083576	-9.4	13.2	-3989.96368908	-7.5	15.1	-3989.53220270	-2.4	20.2
PA-9b(NaOPh)-ts(1,6minor)_06	-3990.87483398	-5.6	14.8	-3989.95921919	-4.7	15.7	-3989.52758540	0.5	21.0
PA-9b(NaOPh)-ts(1,6minor)_07	-3990.87892017	-8.2	14.2	-3989.96162398	-6.2	16.2	-3989.52977495	-0.9	21.5
PA-9b(NaOPh)-ts(1,6minor)_08	-3990.87438737	-5.3	15.1	-3989.95815071	-4.0	16.3	-3989.52673028	1.1	21.4
PA-9b(NaOPh)-ts(1,6minor)_09	-3990.87274545	-4.3	18.0	-3989.95570731	-2.5	19.8	-3989.52262616	3.6	25.9

Figure S15-3

dienoate

9d(Na)-Cu-allenyl	-3683.33114499	0.0	0.0	-3682.53933632	0.0	0.0	-3682.14215505	0.0	0.0
PA-9d(Na)-ts(1,6major)_01	-3683.34676605	-9.8	10.5	-3682.55352058	-8.9	11.4	-3682.14942046	-4.6	15.7
PA-9d(Na)-ts(1,6major)_02	-3683.34637627	-9.6	10.0	-3682.55204777	-8.0	11.5	-3682.14838128	-3.9	15.6
PA-9d(Na)-ts(1,6major)_03	-3683.34644936	-9.6	10.3	-3682.55255109	-8.3	11.6	-3682.14889117	-4.2	15.7
PA-9d(Na)-ts(1,6major)_04	-3683.34722260	-10.1	10.0	-3682.55264082	-8.3	11.7	-3682.15014079	-5.0	15.1
PA-9d(Na)-ts(1,6major)_05	-3683.34683120	-9.8	10.8	-3682.55295126	-8.5	12.1	-3682.14977259	-4.8	15.9
PA-9d(Na)-ts(1,6major)_06	-3683.34640275	-9.6	10.6	-3682.55209567	-8.0	12.2	-3682.14836230	-3.9	16.3
PA-9d(Na)-ts(1,6major)_07	-3683.34637385	-9.6	10.9	-3682.55199435	-7.9	12.5	-3682.14832436	-3.9	16.6
PA-9d(Na)-ts(1,6major)_08	-3683.34682156	-9.8	10.9	-3682.55230287	-8.1	12.6	-3682.14967668	-4.7	16.0
PA-9d(Na)-ts(1,6major)_09	-3683.34553136	-9.0	11.6	-3682.55197571	-7.9	12.7	-3682.14848853	-4.0	16.7
PA-9d(Na)-ts(1,6major)_10	-3683.34312938	-7.5	12.8	-3682.54888208	-6.0	14.3	-3682.14806647	-3.7	16.6
PA-9d(Na)-ts(1,6major)_11	-3683.34387660	-8.0	11.8	-3682.54771420	-5.3	14.5	-3682.14542620	-2.1	17.7
PA-9d(Na)-ts(1,6major)_12	-3683.34313801	-7.5	13.0	-3682.54882640	-6.0	14.6	-3682.14811013	-3.7	16.8
PA-9d(Na)-ts(1,6major)_13	-3683.34009630	-5.6	14.7	-3682.54568387	-4.0	16.3	-3682.14207228	0.1	20.4
PA-9d(Na)-ts(1,6major)_14	-3683.33012110	0.6	21.6	-3682.53688522	1.5	22.5	-3682.13239519	6.1	27.0
PA-9d(Na)-ts(1,6major)_15	-3683.32663810	2.8	21.6	-3682.53328150	3.8	22.6	-3682.13068747	7.2	26.0
PA-9d(Na)-ts(1,6major)_16	-3683.32957456	1.0	21.5	-3682.53590927	2.2	22.7	-3682.13281618	5.9	26.4
PA-9d(Na)-ts(1,6major)_17	-3683.32833666	1.8	22.9	-3682.53381764	3.5	24.6	-3682.12909659	8.2	29.4
PA-9d(Na)-ts(1,6minor)_01	-3683.34306318	-7.5	11.3	-3682.54933664	-6.3	12.5	-3682.14702419	-3.1	15.7
PA-9d(Na)-ts(1,6minor)_02	-3683.34141621	-6.4	13.3	-3682.54825054	-5.6	14.1	-3682.14629138	-2.6	17.1
PA-9d(Na)-ts(1,6minor)_03	-3683.34317285	-7.5	12.9	-3682.54896953	-6.0	14.4	-3682.14628585	-2.6	17.8
PA-9d(Na)-ts(1,6minor)_04	-3683.34325208	-7.6	13.1	-3682.54905303	-6.1	14.6	-3682.14635475	-2.6	18.1
PA-9d(Na)-ts(1,6minor)_05	-3683.34325222	-7.6	13.1	-3682.54905303	-6.1	14.6	-3682.14635466	-2.6	18.1
PA-9d(Na)-ts(1,6minor)_06	-3683.34186027	-6.7	14.3	-3682.54768087	-5.2	15.8	-3682.14531207	-2.0	19.0
PA-9d(Na)-ts(1,6minor)_07	-3683.34200029	-6.8	14.7	-3682.54786094	-5.3	16.1	-3682.14543851	-2.1	19.4
PA-9d(Na)-ts(1,6minor)_08	-3683.33832327	-4.5	15.2	-3682.54268167	-2.1	17.6	-3682.13918713	1.9	21.5
PA-9d(Na)-ts(1,6minor)_09	-3683.33735494	-3.9	16.3	-3682.54276464	-2.2	18.1	-3682.14025993	1.2	21.4

Figure S15-4

9b(Na)-Cu-allenyl	-3683.33122166	0.0	0.0	-3682.53742270	0.0	0.0	-3682.13953768	0.0	0.0

PA-9b(Na)-ts(1,6major)_01	-3683.34236298	-7.0	11.0	-3682.54822576	-6.8	11.2	-3682.14321630	-2.3	15.6
PA-9b(Na)-ts(1,6major)_02	-3683.34345568	-7.7	12.3	-3682.54821038	-6.8	13.2	-3682.14375831	-2.6	17.3
PA-9b(Na)-ts(1,6major)_03	-3683.34309562	-7.5	12.6	-3682.54820094	-6.8	13.3	-3682.14297818	-2.2	17.9
PA-9b(Na)-ts(1,6major)_04	-3683.33572722	-2.8	18.5	-3682.54178082	-2.7	18.6	-3682.13759984	1.2	22.5
PA-9b(Na)-ts(1,6major)_05	-3683.33097423	0.2	20.8	-3682.53673734	0.4	21.1	-3682.13053896	5.6	26.3
PA-9b(Na)-ts(1,6minor)_01	-3683.33654017	-3.3	17.4	-3682.54299270	-3.5	17.2	-3682.13718221	1.5	22.2
PA-9b(Na)-ts(1,6minor)_02	-3683.33542626	-2.6	17.8	-3682.54209191	-2.9	17.5	-3682.13764836	1.2	21.7
PA-9b(Na)-ts(1,6minor)_03	-3683.33554321	-2.7	17.5	-3682.54009067	-1.7	18.5	-3682.13541286	2.6	22.8
PA-9b(Na)-ts(1,6minor)_04	-3683.33510246	-2.4	19.0	-3682.54174041	-2.7	18.7	-3682.13645397	1.9	23.4
PA-9b(Na)-ts(1,6minor)_05	-3683.33505765	-2.4	19.2	-3682.53949236	-1.3	20.3	-3682.13411206	3.4	25.1
PA-9b(Na)-ts(1,6minor)_06	-3683.33048118	0.5	21.4	-3682.53643815	0.6	21.5	-3682.13209706	4.7	25.6
PA-9b(Na)-ts(1,6minor)_07	-3683.33397766	-1.7	20.2	-3682.53753509	-0.1	21.8	-3682.13165215	4.9	26.9
PA-9b(Na)-ts(1,6minor)_08	-3683.33306589	-1.2	21.1	-3682.53671447	0.4	22.7	-3682.13126212	5.2	27.5

Figure S15-5

9d(NaOPh)-Cu-allyl_01	-4442.17621217	0.0	0.0	-4441.08572350	0.0	0.0	-4440.58346898	0.0	0.0
AA-9d(NaOPh)-ts(1,6major)_01	-4442.20703033	-19.3	4.6	-4441.11533859	-18.6	5.3	-4440.60922583	-16.2	7.7
AA-9d(NaOPh)-ts(1,6major)_02	-4442.20489375	-18.0	6.0	-4441.11228523	-16.7	7.3	-4440.60661252	-14.5	9.5
AA-9d(NaOPh)-ts(1,6minor)_01	-4442.20068755	-15.4	7.0	-4441.10803999	-14.0	8.4	-4440.60092130	-11.0	11.4
AA-9d(NaOPh)-ts(1,6minor)_02	-4442.20127586	-15.7	8.0	-4441.10944341	-14.9	8.9	-4440.60302505	-12.3	11.5
AA-9d(NaOPh)-ts(1,6minor)_03	-4442.20054743	-15.3	8.2	-4441.10864789	-14.4	9.1	-4440.60108924	-11.1	12.4
AA-9d(NaOPh)-ts(1,6minor)_04	-4442.20071652	-15.4	7.9	-4441.10678225	-13.2	10.1	-4440.60103054	-11.0	12.3
AA-9d(NaOPh)-ts(1,6minor)_05	-4442.19863449	-14.1	10.0	-4441.10662814	-13.1	11.0	-4440.60070510	-10.8	13.3
AA-9d(NaOPh)-ts(1,6minor)_06	-4442.20001422	-14.9	8.8	-4441.10552521	-12.4	11.3	-4440.59835361	-9.3	14.3
AA-9d(NaOPh)-ts(1,6minor)_07	-4442.20024707	-15.1	9.4	-4441.10656890	-13.1	11.4	-4440.59959907	-10.1	14.3

Figure S15-6

9b(NaOPh)-Cu-allyl_01	-4442.17569662	0.0	0.0	-4441.08335295	0.0	0.0	-4440.57955401	0.0	0.0
AA-9b(NaOPh)-ts(1,6major)_01	-4442.20131098	-16.1	6.3	-4441.10769971	-15.3	7.1	-4440.59922567	-12.3	10.0
AA-9b(NaOPh)-ts(1,6major)_02	-4442.19628680	-12.9	9.6	-4441.10262380	-12.1	10.5	-4440.59704010	-11.0	11.6
AA-9b(NaOPh)-ts(1,6minor)_01	-4442.19924457	-14.8	6.7	-4441.10534786	-13.8	7.6	-4440.59570571	-10.1	11.3
AA-9b(NaOPh)-ts(1,6minor)_02	-4442.19823864	-14.1	8.0	-4441.10475883	-13.4	8.7	-4440.59535551	-9.9	12.2
AA-9b(NaOPh)-ts(1,6minor)_03	-4442.19924448	-14.8	8.0	-4441.10534773	-13.8	9.0	-4440.59570572	-10.1	12.6
AA-9b(NaOPh)-ts(1,6minor)_04	-4442.19542885	-12.4	11.3	-4441.10245040	-12.0	11.7	-4440.59348192	-8.7	15.0

Figure S15-7									
dienoate									
9d(Na)-Cu-allyl_01	-4134.64133271	0.0	0.0	-4133.67213363	0.0	0.0	-4133.19437368	0.0	0.0
AA-9d(Na)-ts(1,6major)_01	-4134.65947596	-11.4	9.6	-4133.68817393	-10.1	10.9	-4133.20733197	-8.1	12.9
AA-9d(Na)-ts(1,6major)_02	-4134.65987979	-11.6	11.1	-4133.68860448	-10.3	12.4	-4133.20790137	-8.5	14.2
AA-9d(Na)-ts(1,6major)_03	-4134.65667140	-9.6	13.6	-4133.68466801	-7.9	15.4	-4133.20375446	-5.9	17.4
AA-9d(Na)-ts(1,6minor)_01	-4134.65544875	-8.9	13.1	-4133.68404505	-7.5	14.5	-4133.20411140	-6.1	15.9
AA-9d(Na)-ts(1,6minor)_02	-4134.65547384	-8.9	13.4	-4133.68409382	-7.5	14.8	-4133.20412625	-6.1	16.2
AA-9d(Na)-ts(1,6minor)_03	-4134.65510410	-8.6	12.9	-4133.68243881	-6.5	15.1	-4133.19878775	-2.8	18.8
AA-9d(Na)-ts(1,6minor)_04	-4134.65396126	-7.9	14.7	-4133.68395240	-7.4	15.2	-4133.20356064	-5.8	16.8
AA-9d(Na)-ts(1,6minor)_05	-4134.65447296	-8.2	13.8	-4133.68256520	-6.5	15.5	-4133.20154738	-4.5	17.6
AA-9d(Na)-ts(1,6minor)_06	-4134.65421490	-8.1	14.2	-4133.68102125	-5.6	16.7	-4133.19761264	-2.0	20.3
AA-9d(Na)-ts(1,6minor)_07	-4134.65229900	-6.9	15.3	-4133.67952800	-4.6	17.5	-4133.19935266	-3.1	19.0

Figure S15-8									
9b(Na)-Cu-allyl_01	-4134.63799627	0.0	0.0	-4133.66778602	0.0	0.0	-4133.18981887	0.0	0.0
AA-9b(Na)-ts(1,6major)_01	-4134.65804731	-12.6	10.1	-4133.68556131	-11.2	11.5	-4133.20353635	-8.6	14.1
AA-9b(Na)-ts(1,6major)_02	-4134.65760253	-12.3	11.1	-4133.68627281	-11.6	11.8	-4133.20501553	-9.5	13.9
AA-9b(Na)-ts(1,6major)_03	-4134.65619808	-11.4	11.5	-4133.68522536	-10.9	12.0	-4133.20152430	-7.3	15.6
AA-9b(Na)-ts(1,6major)_04	-4134.64780501	-6.2	19.6	-4133.67543477	-4.8	21.0	-4133.19370891	-2.4	23.3
AA-9b(Na)-ts(1,6minor)_01	-4134.65491128	-10.6	11.8	-4133.68294647	-9.5	12.9	-4133.19814032	-5.2	17.2
AA-9b(Na)-ts(1,6minor)_02	-4134.65163752	-8.6	13.6	-4133.68002985	-7.7	14.5	-4133.19321540	-2.1	20.0
AA-9b(Na)-ts(1,6minor)_03	-4134.65271846	-9.2	13.6	-4133.68086175	-8.2	14.6	-4133.19926292	-5.9	16.9
AA-9b(Na)-ts(1,6minor)_04	-4134.65244233	-9.1	14.2	-4133.68097173	-8.3	14.9	-4133.19930310	-6.0	17.3
AA-9b(Na)-ts(1,6minor)_05	-4134.65046102	-7.8	16.4	-4133.67766334	-6.2	18.0	-4133.19458789	-3.0	21.3

Figure S15-9									
NaOPh									
(PhO)2BpinNa									
PhOBpin									
dienoate									
9d(Naborate)-Cu-allenyl_01	-4401.65709416	0.0	0.0	-4400.60052361	0.0	0.0	-4400.11923224	0.0	0.0
9d(Naborate)-Cu-allenyl_02	-4401.65772252	-0.4	0.5	-4400.59987867	0.4	1.3	-4400.11840878	0.5	1.4
9d(Naborate)-Cu-allenyl_03	-4401.65643311	0.4	2.2	-4400.59836103	1.4	3.1	-4400.11717220	1.3	3.1
9d(Naborate)-Cu-allenyl_04	-4401.66399031	-4.3	1.2	-4400.60318264	-1.7	3.9	-4400.12403966	-3.0	2.5
9d(Naborate)-Cu-allenyl_05	-4401.65519879	1.2	4.4	-4400.59775148	1.7	5.0	-4400.11628161	1.9	5.1

9d(Naborate)-Cu-allenyl_06	-4401.65626111	0.5	4.2	-4400.59841442	1.3	5.0	-4400.11560925	2.3	6.0
9d(Naborate)-Cu-allenyl_07	-4401.65519606	1.2	4.6	-4400.59776209	1.7	5.1	-4400.11630725	1.8	5.2
PA-9b(Naborate)-ts(1,6major)_01	-4401.67221016	-9.5	13.7	-4400.61544061	-9.4	13.9	-4400.12727851	-5.0	18.2
PA-9b(Naborate)-ts(1,6major)_02	-4401.66956403	-7.8	14.4	-4400.61266902	-7.6	14.6	-4400.12497118	-3.6	18.6
PA-9b(Naborate)-ts(1,6major)_03	-4401.67111750	-8.8	15.2	-4400.61344555	-8.1	15.8	-4400.12600752	-4.3	19.7
PA-9b(Naborate)-ts(1,6major)_04	-4401.67009455	-8.2	14.5	-4400.61055808	-6.3	16.3	-4400.12124566	-1.3	21.3
PA-9b(Naborate)-ts(1,6major)_05	-4401.66447263	-4.6	17.5	-4400.60662975	-3.8	18.3	-4400.12086012	-1.0	21.1
PA-9b(Naborate)-ts(1,6major)_06	-4401.66793415	-6.8	17.2	-4400.60960197	-5.7	18.3	-4400.12069989	-0.9	23.1
PA-9b(Naborate)-ts(1,6major)_07	-4401.66528390	-5.1	18.7	-4400.60854591	-5.0	18.8	-4400.11974276	-0.3	23.5
PA-9b(Naborate)-ts(1,6major)_08	-4401.66640979	-5.8	19.3	-4400.61001616	-6.0	19.2	-4400.12040084	-0.7	24.4
PA-9b(Naborate)-ts(1,6major)_09	-4401.66770692	-6.7	18.1	-4400.60900793	-5.3	19.4	-4400.12050567	-0.8	23.9
PA-9b(Naborate)-ts(1,6major)_10	-4401.66766870	-6.6	18.4	-4400.60889092	-5.3	19.7	-4400.12042179	-0.7	24.3
9d-Cu-allenyl	-3521.60502971	0.0	0.0	-3520.81022808	0.0	0.0	-3520.43853460	0.0	0.0
PA-9b-ts(1,6major)_01	-3521.60425395	0.5	21.1	-3520.80891221	0.8	21.4	-3520.42794961	6.6	27.2
PA-9b-ts(1,6major)_02	-3521.60337835	1.0	20.8	-3520.80721035	1.9	21.6	-3520.42723261	7.1	26.8
PA-9b-ts(1,6major)_03	-3521.60195548	1.9	22.6	-3520.80639970	2.4	23.0	-3520.42762763	6.8	27.5
PA-9b-ts(1,6major)_04	-3521.60232699	1.7	22.5	-3520.80620250	2.5	23.4	-3520.42720396	7.1	27.9
PA-9b-ts(1,6major)_05	-3521.60304453	1.2	23.2	-3520.80746374	1.7	23.7	-3520.42722045	7.1	29.1

E(sp,sum) ……. single point electronic energy in Hartree with Def2TZVPP basis set in thf(SMD) after mass balance

ΔE(sp) …….. relative single point electronic energy in kcal/mol with Def2TZVPP basis set in thf(SMD)

ΔG(sp) …….. relative single point free energy in kcal/mol with Def2TZVPP basis set in thf(SMD)

[ΔG(sp) = ΔE(sp)/Def2TZVPP + ΔG_{corr}/Def2SVP]

Table S3. Single point energies in Figures S1-1–S15-9 with MN12L and M06L

structure	MN12L/Def2TZVPP$_{thf(SMD)}$ E(sp,sum) [hartree]	ΔE(sp) [kcal/mol]	ΔG(sp) [kcal/mol]	M06L/Def2TZVPP$_{thf(SMD)}$ E(sp,sum) [hartree]	ΔE(sp) [kcal/mol]	ΔG(sp) [kcal/mol]	
Figure S1-1							
dienoate							
PhOH							
NaOPh							
tBuOH							
NaOtBu							
PhOBpin							
(PhO)2BpinNa							
9d-Cu-allenyl	-3915.11725962	0.0	0.0	-3917.31740791	0.0	0.0	
PA-9d(Na)-ts(1,6major)	-3915.15407417	-23.1	-1.1	-3917.35458388	-23.3	-1.3	
9d-Cu-allenyl	-3988.95524383	0.0	0.0	-3991.15796389	0.0	0.0	
PA-9d(Na)-ts(1,6major)	-3988.96900804	-8.6	13.1	-3991.16950518	-7.2	14.5	
9d-Cu-allenyl	-3988.95524383	0.0	0.0	-3991.15796389	0.0	0.0	
PA-9d(NaOPh)-ts(1,6major)	-3989.00751557	-32.8	5.0	-3991.21133486	-33.5	4.3	
9d-Cu-allenyl	-3519.91942960	0.0	0.0	-3521.86429899	0.0	0.0	
PA-9d-ts(1,6major)	-3519.92077687	-0.8	18.9	-3521.86622676	-1.2	18.5	
9d-Cu-allenyl	-4706.75067762	24.7	8.4	-4709.53787943	21.7	5.4	
9d-Cu-allenyl	-4706.79008713	0.0	0.0	-4709.57243020	0.0	0.0	
PA-9d(Naborate)-ts(1,6major)	-4706.82890327	-24.4	-0.3	-4709.61010108	-23.6	0.5	
Figure S2-1							
PA-9d(NaOPh)-prod(1,6major)	-3989.03899396	-32.2	-9.2	-3991.24151410	-32.7	-9.7	
PA-9d(NaOPh)-ts(1,6major)	-3989.00751557	-12.4	8.8	-3991.21133486	-13.7	7.6	
PA-9d(NaOPh)-pc(1,6major)	-3989.02704061	-24.7	-4.0	-3991.22605265	-22.9	-2.3	
9d(NaOPh)-Cu-allenyl	-3988.98769475	0.0	0.0	-3991.18948193	0.0	0.0	
9b(NaOPh)-Cu-allenyl	-3988.97706437	0.0	0.0	-3991.18121663	0.0	0.0	
PA-9b(NaOPh)-pc(1,6major)	-3989.02046129	-27.2	-6.8	-3991.22010569	-24.4	-4.0	
PA-9b(NaOPh)-ts(1,6major)	-3989.00122102	-15.2	5.7	-3991.20616255	-15.7	5.2	
PA-9b(NaOPh)-prod(1,6major)	-3989.03231165	-34.7	-12.3	-3991.23456944	-33.5	-11.1	

PA-9d(NaOPh)-prod(1,6minor)	-3989.03689185	-30.9	-9.0	-3991.23820115	-30.6	-8.7
PA-9d(NaOPh)-ts(1,6minor)	-3989.00412385	-10.3	10.0	-3991.20926419	-12.4	7.9
PA-9d(NaOPh)-pc(1,6minor)	-3989.02003323	-20.3	-0.4	-3991.22297882	-21.0	-1.1
9d(NaOPh)-Cu-allenyl	-3988.98769475	0.0	0.0	-3991.18948193	0.0	0.0
9b(NaOPh)-Cu-allenyl	-3988.97706437	0.0	0.0	-3991.18121663	0.0	0.0
PA-9b(NaOPh)-pc(1,6minor)	-3989.01406047	-23.2	-2.9	-3991.21426698	-20.7	-0.4
PA-9b(NaOPh)-ts(1,6minor)	-3988.99262462	-9.8	11.1	-3991.19951812	-11.5	9.4
PA-9b(NaOPh)-prod(1,6minor)	-3989.03157967	-34.2	-11.4	-3991.23193042	-31.8	-9.0

Figure S3-1

AA-9d(NaOPh)-prod(1,6major)	-4440.01413222	-47.6	-21.7	-4442.61546916	-41.0	-15.1
AA-9d(NaOPh)-ts(1,6major)	-4439.98449643	-29.0	-5.1	-4442.59032238	-25.2	-1.4
AA-9d(NaOPh)-pc(1,6major)	-4439.99106756	-33.2	-9.9	-4442.59598568	-28.8	-5.5
9d(NaOPh)-Cu-allyl	-4439.93821085	0.0	0.0	-4442.55008509	0.0	0.0
9b(NaOPh)-Cu-allyl	-4439.93428626	0.0	0.0	-4442.54510511	0.0	0.0
AA-9b(NaOPh)-pc(1,6major)	-4439.97354222	-24.6	-4.7	-4442.58330672	-24.0	-4.0
AA-9b(NaOPh)-ts(1,6major)	-4439.96919497	-21.9	0.4	-4442.57882366	-21.2	1.2
AA-9b(NaOPh)-prod(1,6major)	-4440.00348691	-43.4	-18.4	-4442.60504374	-37.6	-12.6
AA-9d(NaOPh)-prod(1,6minor)	-4439.99730270	-37.1	-13.8	-4442.60389082	-33.8	-10.5
AA-9d(NaOPh)-ts(1,6minor)	-4439.97369382	-22.3	0.1	-4442.58185530	-19.9	2.5
AA-9d(NaOPh)-pc(1,6minor)	-4439.98273893	-27.9	-6.6	-4442.58816473	-23.9	-2.5
9d(NaOPh)-Cu-allyl	-4439.93821085	0.0	0.0	-4442.55008509	0.0	0.0
9b(NaOPh)-Cu-allyl	-4439.93428626	0.0	0.0	-4442.54510511	0.0	0.0
AA-9b(NaOPh)-pc(1,6minor)	-4439.97502838	-25.6	-2.9	-4442.58198960	-23.1	-0.5
AA-9b(NaOPh)-ts(1,6minor)	-4439.96841951	-21.4	0.0	-4442.57797333	-20.6	0.8
AA-9b(NaOPh)-prod(1,6minor)	-4132.65871479	-41.1	-14.7	-4135.01532842	-36.8	-10.4

Figure S4-1

PA-9d(Na)-prod(1,6major)	-3681.69346285	-32.2	-9.2	-3683.64965008	-31.0	-8.1
PA-9d(Na)-ts(1,6major)	-3681.65890032	-10.5	9.0	-3683.61645791	-10.2	9.3
PA-9d(Na)-pc(1,6major)	-3681.68014307	-23.8	-4.0	-3683.63163457	-19.7	0.0
9d(Na)-Cu-allenyl	-3681.64220587	0.0	0.0	-3683.60017309	0.0	0.0
9b(Na)-Cu-allenyl	-3681.63854301	0.0	0.0	-3683.59431594	0.0	0.0
PA-9b(Na)-pc(1,6major)	-3681.66991213	-19.7	-1.8	-3683.62447087	-18.9	-1.0
PA-9b(Na)-ts(1,6major)	-3681.65260731	-8.8	9.1	-3683.61172700	-10.9	7.0
PA-9b(Na)-prod(1,6major)	-3681.68384053	-28.4	-8.3	-3683.64102610	-29.3	-9.2

PA-9d(Na)-prod(1,6minor)	-3681.69767573	-34.8	-12.6	-3683.65214580	-32.6	-10.4	
PA-9d(Na)-ts(1,6minor)	-3681.65761381	-9.7	9.1	-3683.61518754	-9.4	9.4	
PA-9d(Na)-pc(1,6minor)	-3681.67644378	-21.5	-2.7	-3683.62940223	-18.3	0.4	
9d(Na)-Cu-allenyl	-3681.64220587	0.0	0.0	-3683.60017309	0.0	0.0	
9b(Na)-Cu-allenyl	-3681.63854301	0.0	0.0	-3683.59431594	0.0	0.0	
PA-9b(Na)-pc(1,6minor)	-3681.66846404	-18.8	-0.2	-3683.62173223	-17.2	1.3	
PA-9b(Na)-ts(1,6minor)	-3681.64719232	-5.4	15.3	-3683.60512824	-6.8	13.9	
PA-9b(Na)-prod(1,6minor)	-3681.67698136	-24.1	-3.9	-3683.63526451	-25.7	-5.5	

Figure S5-1

AA-9d(Na)-prod(1,6major)	-4132.65875663	-37.4	-11.6	-4135.01579235	-33.2	-7.5	
AA-9d(Na)-ts(1,6major)	-4132.62729388	-17.6	3.4	-4134.98781113	-15.7	5.3	
AA-9d(Na)-pc(1,6major)	-4132.63690188	-23.7	-1.6	-4134.99564009	-20.6	1.5	
9d(Na)-Cu-allyl	-4132.59920742	0.0	0.0	-4134.96284992	0.0	0.0	
9b(Na)-Cu-allyl	-4132.59314173	0.0	0.0	-4134.95669225	0.0	0.0	
AA-9b(Na)-pc(1,6major)	-4132.62795971	-21.8	0.0	-4134.98852372	-20.0	1.8	
AA-9b(Na)-ts(1,6major)	-4132.62290671	-18.7	4.0	-4134.98408524	-17.2	5.5	
AA-9b(Na)-prod(1,6major)	-4132.65449061	-38.5	-13.3	-4135.01348828	-35.6	-10.4	
AA-9d(Na)-prod(1,6minor)	-4132.65438935	-34.6	-13.6	-4135.01646323	-33.6	-12.6	
AA-9d(Na)-ts(1,6minor)	-4132.62446762	-15.9	6.1	-4134.98513729	-14.0	8.0	
AA-9d(Na)-pc(1,6minor)	-4132.63335143	-21.4	-0.7	-4134.99337369	-19.2	1.6	
9d(Na)-Cu-allyl	-4132.59920742	0.0	0.0	-4134.96284992	0.0	0.0	
9b(Na)-Cu-allyl	-4132.59314173	0.0	0.0	-4134.95669225	0.0	0.0	
AA-9b(Na)-pc(1,6minor)	-4132.62056758	-17.2	5.2	-4134.98497847	-17.7	4.6	
AA-9b(Na)-ts(1,6minor)	-4132.61446188	-13.4	9.1	-4134.97988308	-14.6	7.9	
AA-9b(Na)-prod(1,6minor)	-4132.65871479	-41.1	-14.7	-4135.01532842	-36.8	-10.4	

Figure S6-1

thf

PMe3

Me2NHC

NaOPh

NaOtBu

dienoate

dienoate-NaOPh

dienoate-NaOtBu

Me2NHC-Cu-allenyl	-3067.57268677	-9.4	-8.5	-3068.99446394	-9.7	-8.8
PMe3-Cu-allenyl	-3067.55764389	0.0	0.0	-3068.97897207	0.0	0.0
thf-Cu-allenyl	-3067.52865966	18.2	18.4	-3068.95449265	15.4	15.5
PA-NaOPh-prod(1,6)	-3067.57451817	-10.6	-1.5	-3068.99814559	-12.0	-2.9
PA-NaOPh-ts(1,6)	-3067.54632075	7.1	15.4	-3068.97042261	5.4	13.6
PA-NaOPh-ed(1,6)	-3067.56556432	-5.0	2.2	-3068.98566931	-4.2	3.0
NaOPh-Cu-allenyl	-3067.52117963	22.9	12.0	-3068.94507477	21.3	10.4
PA-NaOPh-ed(1,4)	-3067.56557650	-5.0	3.4	-3068.98683009	-4.9	3.4
PA-NaOPh-ts(1,4)	-3067.53751321	12.6	20.3	-3068.96389522	9.5	17.1
PA-NaOPh-prod(1,4)	-3067.57977095	-13.9	-4.5	-3069.00233144	-14.7	-5.3
Me2NHC-Cu-allenyl	-2993.73206876	-9.4	-8.5	-2995.15164903	-9.7	-8.8
PMe3-Cu-allenyl	-2993.71702588	0.0	0.0	-2995.13615716	0.0	0.0
thf-Cu-allenyl	-2993.68804165	18.2	18.4	-2995.11167774	15.4	15.5
PA-NaOtBu-prod(1,6)	-2993.74967708	-20.5	-11.4	-2995.17020059	-21.4	-12.3
PA-NaOtBu-ts(1,6)	-2993.72167593	-2.9	4.0	-2995.14360482	-4.7	2.2
PA-NaOtBu-ed(1,6)	-2993.74111995	-15.1	-9.7	-2995.15925402	-14.5	-9.0
NaOtBu-Cu-allenyl	-2993.70041292	10.4	0.3	-2995.12122885	9.4	-0.8
PA-NaOtBu-ed(1,4)	-2993.73783340	-13.1	-8.9	-2995.15684426	-13.0	-8.8
PA-NaOtBu-ts(1,4)	-2993.71331891	2.3	6.6	-2995.13749247	-0.8	3.4
PA-NaOtBu-prod(1,4)	-2993.75732276	-25.3	-16.4	-2995.17738375	-25.9	-16.9

Figure S7-1

Me2NHC-Cu-allyl	-3355.24321642	0.0	0.0	-3357.10632272	0.0	0.0
AA-Me2NHC-pc(1,6major)	-3355.26935032	-16.4	1.6	-3357.13110963	-15.6	2.4
AA-Me2NHC-ts(1,6major)	-3355.25748740	-9.0	11.0	-3357.11986845	-8.5	11.5
AA-Me2NHC-prod(1,6major)	-3355.29689897	-33.7	-10.4	-3357.15255945	-29.0	-5.7
Me2NHC-Cu-allyl	-3355.24321642	0.0	0.0	-3357.10632272	0.0	0.0
AA-Me2NHC-pc(1,6minor)	-3355.26483825	-13.6	5.8	-3357.12662993	-12.7	6.6
AA-Me2NHC-ts(1,6minor)	-3355.24399525	-0.5	19.6	-3357.11002309	-2.3	17.7
AA-Me2NHC-prod(1,6minor)	-3355.28748327	-27.8	-4.7	-3357.14567474	-24.7	-1.6

Figure S8-1

dienoate						
SIMes-Cu-allenyl	-3523.29081705	0.0	0.0	-3525.27967395	0.0	0.0
PA-SIMes-ed(1,6)	-3523.31032234	-12.2	9.0	-3525.29638633	-10.5	10.7

PA-SIMes-ts(1,6)	-3523.28696552	2.4	23.5	-3525.27897181	0.4	21.5
PA-SIMes-prod(1,6)	-3523.32069688	-18.7	4.3	-3525.30840766	-18.0	5.0
PA-SIMes-ed(1,4AA)	-3523.31040061	-12.3	8.8	-3525.29649479	-10.6	10.5
PA-SIMes-ts(1,4AA)	-3523.27496891	9.9	30.2	-3525.26409812	9.8	30.0
PA-SIMes-prod(1,4AA)	-3523.30558967	-9.3	10.3	-3525.29531886	-9.8	9.7
PA-SIMes-ed(1,4)	-3523.30185942	-6.9	11.8	-3525.28980866	-6.4	12.4
PA-SIMes-ts(1,4)	-3523.27086805	12.5	29.8	-3525.26350146	10.1	27.4
PA-SIMes-prod(1,4)	-3523.29530207	-2.8	18.7	-3525.28541990	-3.6	17.9
PPh3-Cu-allenyl	-3634.37473733	0.0	0.0	-3636.12405204	0.0	0.0
PA-PPh3-ed(1,6)	-3634.39255636	-11.2	6.3	-3636.13720128	-8.3	9.2
PA-PPh3-ts(1,6)	-3634.37179150	1.8	20.8	-3636.11969411	2.7	21.7
PA-PPh3-prod(1,6)	-3634.39834254	-14.8	5.3	-3636.14527592	-13.3	6.8
PA-PPh3-ed(1,4AA)	-3634.39500421	-12.7	3.5	-3636.13810576	-8.8	7.4
PA-PPh3-ts(1,4AA)	-3634.35336214	13.4	29.2	-3636.10167173	14.0	29.8
PA-PPh3-prod(1,4AA)	-3634.39043759	-9.9	8.6	-3636.13614291	-7.6	10.9
PA-PPh3-ed(1,4)	-3634.38329604	-5.4	10.2	-3636.13177471	-4.8	10.7
PA-PPh3-ts(1,4)	-3634.35715169	11.0	26.0	-3636.10926249	9.3	24.2
PA-PPh3-prod(1,4)	-3634.39691294	-13.9	4.6	-3636.14917369	-15.8	2.8

Figures S9-1

Me2NHC-Cu-allenyl	-2904.29853208	0.0	0.0	-2905.75529300	0.0	0.0
PA-Me2NHC-ed(1,6)	-2904.31306431	-9.1	8.8	-2905.76585482	-6.6	11.3
PA-Me2NHC-ts(1,6)	-2904.29048712	5.0	23.0	-2905.74797770	4.6	22.6
PA-Me2NHC-prod(1,6)	-2904.32456865	-16.3	5.6	-2905.78046860	-15.8	6.1
PA-Me2NHC-ed(1,4AA)	-2904.31285139	-9.0	7.3	-2905.76658869	-7.1	9.2
PA-Me2NHC-ts(1,4AA)	-2904.27143391	17.0	32.7	-2905.72999526	15.9	31.5
PA-Me2NHC-prod(1,4AA)	-2904.31311535	-9.2	6.5	-2905.77014571	-9.3	6.3
PA-Me2NHC-ed(1,4)	-2904.30356875	-3.2	11.8	-2905.75996655	-2.9	12.1
PA-Me2NHC-ts(1,4)	-2904.27296027	16.0	32.2	-2905.73404811	13.3	29.5
PA-Me2NHC-prod(1,4)	-2904.29837301	0.1	18.5	-2905.75621766	-0.6	17.9
PMe3-Cu-allenyl	-3059.44142523	0.0	0.0	-3060.79278105	0.0	0.0
PA-PMe3-ed(1,6)	-3059.46255113	-13.3	3.8	-3060.80924612	-10.3	6.7
PA-PMe3-ts(1,6)	-3059.43836677	1.9	20.0	-3060.78930859	2.2	20.2

PA-PMe3-prod(1,6)	-3059.46870932	-17.1	2.5	-3060.81852370	-16.2	3.5	
PA-PMe3-ed(1,4AA)	-3059.46255120	-13.3	3.8	-3060.80924613	-10.3	6.7	
PA-PMe3-ts(1,4AA)	-3059.41687751	15.4	31.5	-3060.76799334	15.6	31.7	
PA-PMe3-prod(1,4AA)	-3059.45490062	-8.5	9.0	-3060.80517642	-7.8	9.6	
PA-PMe3-ed(1,4)	-3059.45343333	-7.5	8.5	-3060.80280537	-6.3	9.8	
PA-PMe3-ts(1,4)	-3059.42286466	11.6	26.7	-3060.77688803	10.0	25.1	
PA-PMe3-prod(1,4)	-3059.46878775	-17.2	3.4	-3060.81765335	-15.6	5.0	

Figure S10-1

dienoate
dienoate-Naborate

SIMes-Cu-allenyl	-4168.54657814	0.0	0.0	-4170.91075872	0.0	0.0	
PA-SIMes(Naborate)-ed(1,6)	-4168.57396846	-17.2	5.8	-4170.93719144	-16.6	6.4	
PA-SIMes(Naborate)-ts(1,6)	-4168.55903745	-7.8	14.3	-4170.92535650	-9.2	13.0	
PA-SIMes(Naborate)-prod(1,6)	-4168.59103323	-27.9	-4.3	-4170.95667949	-28.8	-5.3	
PA-SIMes(Naborate)-ed(1,4AA)	-4168.57255642	-16.3	5.5	-4170.93425893	-14.7	7.1	
PA-SIMes(Naborate)-ts(1,4AA)	-4168.54961643	-1.9	18.7	-4170.91184700	-0.7	19.9	
PA-SIMes(Naborate)-prod(1,4AA)	-4168.58016946	-21.1	1.0	-4170.94447426	-21.2	1.0	
PA-SIMes(Naborate)-ed(1,4)	-4168.56919756	-14.2	7.4	-4170.93447285	-14.9	6.7	
PA-SIMes(Naborate)-ts(1,4)	-4168.53682327	6.1	26.7	-4170.90769161	1.9	22.5	
PA-SIMes(Naborate)-prod(1,4)	-4168.58194312	-22.2	1.1	-4170.94875846	-23.8	-0.6	

dienoate
dienoate-Naborate

PPh3-Cu-allenyl	-4279.63049842	0.0	0.0	-4281.75513681	0.0	0.0	
PA-PPh3(Naborate)-ed(1,6)	-4279.66007306	-18.6	1.2	-4281.77850422	-14.7	5.1	
PA-PPh3(Naborate)-ts(1,6)	-4279.64307242	-7.9	11.6	-4281.76552549	-6.5	13.0	
PA-PPh3(Naborate)-prod(1,6)	-4279.67544517	-28.2	-5.8	-4281.79963842	-27.9	-5.5	
PA-PPh3(Naborate)-ed(1,4AA)	-4279.66365288	-20.8	-3.6	-4281.78092068	-16.2	1.1	
PA-PPh3(Naborate)-ts(1,4AA)	-4279.61970053	6.8	21.9	-4281.74494460	6.4	21.5	
PA-PPh3(Naborate)-prod(1,4AA)	-4279.66004136	-18.5	-2.0	-4281.78454966	-18.5	-1.9	
PA-PPh3(Naborate)-ed(1,4)	-4279.65214949	-13.6	3.1	-4281.77593959	-13.1	3.7	
PA-PPh3(Naborate)-ts(1,4)	-4279.62190142	5.4	23.5	-4281.75121016	2.5	20.6	
PA-PPh3(Naborate)-prod(1,4)	-4279.67456744	-27.7	-4.3	-4281.79794098	-26.9	-3.5	

Figure S11-1						
dienoate						
PA-9d(Na)-prod(1,6major)	-3681.69346285	-32.2	-9.2	-3683.64965008	-31.0	-8.1
PA-9d(Na)-ts(1,6major)	-3681.65890032	-10.5	9.0	-3683.61645791	-10.2	9.3
PA-9d(Na)-pc(1,6major)	-3681.68014307	-23.8	-4.0	-3683.63163457	-19.7	0.0
9d(Na)-Cu-allenyl	-3681.64220587	0.0	0.0	-3683.60017309	0.0	0.0
PA-9d(Na)-pc(1,4AA)	-3681.67695298	-21.8	-3.1	-3683.62960104	-18.5	0.2
PA-9d(Na)-ts(1,4AA)	-3681.64286191	-0.4	17.1	-3683.59859721	1.0	18.5
PA-9d(Na)-prod(1,4AA)	-3681.69337452	-32.1	-13.9	-3683.64664235	-29.2	-10.9
Figure S12-1						
NaOtBu						
dienoate						
PA-SIMes(NaOtBu)-prod(1,4)	-2681.01158198	-31.5	-12.5	-2682.33360210	-35.1	-16.1
PA-SIMes(NaOtBu)-ts(1,4)	-2680.95049607	6.8	24.8	-2682.27574713	1.2	19.2
PA-SIMes(NaOtBu)-ed(1,4)	-2680.98050930	-12.0	5.6	-2682.29988097	-13.9	3.7
SIMes-Cu-allenyl	-2680.92322911	23.9	5.6	-2682.24368403	21.3	3.0
SIMes-Cu(NaOtBu)-allenyl	-2680.96134791	0.0	0.0	-2682.27767721	0.0	0.0
PA-SIMes(NaOtBu)-ed(1,6)	-2680.97677028	-9.7	8.8	-2682.29568679	-11.3	7.2
PA-SIMes(NaOtBu)-ts(1,6)	-2680.96128513	0.0	17.7	-2682.28348059	-3.6	14.0
PA-SIMes(NaOtBu)-prod(1,6)	-2680.99281613	-19.7	-1.2	-2682.31556896	-23.8	-5.3
PA-PPh3(NaOtBu)-prod(1,4)	-2792.09786618	-32.0	-8.9	-2793.17743540	-32.5	-9.4
PA-PPh3(NaOtBu)-ts(1,4)	-2792.05966742	-8.0	10.6	-2793.14110019	-9.7	8.9
PA-PPh3(NaOtBu)-ed(1,4)	-2792.08240508	-22.3	-2.5	-2793.15636218	-19.3	0.5
PPh3-Cu-allenyl	-2792.00714939	24.9	9.2	-2793.08806212	23.6	7.9
PPh3-Cu(NaOtBu)-allenyl	-2792.04686639	0.0	0.0	-2793.12561387	0.0	0.0
PA-PPh3(NaOtBu)-ed(1,6)	-2792.06512212	-11.5	6.4	-2793.13977301	-8.9	9.0
PA-PPh3(NaOtBu)-ts(1,6)	-2792.04752033	-0.4	19.0	-2793.12642983	-0.5	18.9
PA-PPh3(NaOtBu)-prod(1,6)	-2792.08004009	-20.8	-0.1	-2793.15993175	-21.5	-0.8
Figure S13-1						

NaOMe dienoate						
PA-SIMes(NaOMe)-prod(1,4)	-2681.00869379	-33.6	-12.2	-2682.32978917	-35.2	-13.8
PA-SIMes(NaOMe)-ts(1,4)	-2680.95007529	3.2	21.7	-2682.27386062	-0.1	18.4
PA-SIMes(NaOMe)-ed(1,4)	-2680.97481086	-12.3	6.3	-2682.29342783	-12.4	6.3
SIMes-Cu-allenyl	-2680.92322911	20.0	4.5	-2682.24368403	18.8	3.3
SIMes-Cu(NaOMe)-allenyl	-2680.95517855	0.0	0.0	-2682.27370087	0.0	0.0
PA-SIMes(NaOMe)-ed(1,6)	-2680.97618321	-13.2	5.0	-2682.29498499	-13.4	4.9
PA-SIMes(NaOMe)-ts(1,6)	-2680.96034498	-3.2	16.7	-2682.28286620	-5.8	14.2
PA-SIMes(NaOMe)-prod(1,6)	-2680.99169730	-22.9	-2.9	-2682.31507181	-26.0	-6.0
PA-PPh3(NaOMe)-prod(1,4)	-2792.09813069	-33.6	-10.9	-2793.17532327	-32.4	-9.6
PA-PPh3(NaOMe)-ts(1,4)	-2792.05449013	-6.3	11.8	-2793.13614579	-7.8	10.2
PA-PPh3(NaOMe)-ed(1,4)	-2792.07786545	-20.9	-1.4	-2793.15207512	-17.8	1.7
PPh3-Cu-allenyl	-2792.00714939	23.4	9.7	-2793.08806212	22.3	8.6
PPh3-Cu(NaOMe)-allenyl	-2792.04451882	0.0	0.0	-2793.12367594	0.0	0.0
PA-PPh3(NaOMe)-ed(1,6)	-2792.05883192	-9.0	7.8	-2793.13484034	-7.0	9.8
PA-PPh3(NaOMe)-ts(1,6)	-2792.04124173	2.1	20.0	-2793.12191820	1.1	19.1
PA-PPh3(NaOMe)-prod(1,6)	-2792.07490789	-19.1	1.5	-2793.15644102	-20.6	0.0

Figure S14-1

NaOtBu dienoate						
PA-Me2NHC(NaOtBu)-prod(1,4)	-2062.01692017	-39.1	-19.1	-2062.80470147	-38.7	-18.8
PA-Me2NHC(NaOtBu)-ts(1,4)	-2061.96325074	-5.4	11.4	-2062.75487771	-7.4	9.4
PA-Me2NHC(NaOtBu)-ed(1,4)	-2061.98079241	-16.4	1.6	-2062.76543987	-14.1	4.0
Me2NHC-Cu-allenyl	-2061.93092983	14.9	-2.0	-2062.71931777	14.9	-2.0
Me2NHC-Cu(NaOtBu)-allenyl	-2061.95461986	0.0	0.0	-2062.74302749	0.0	0.0
PA-Me2NHC(NaOtBu)-ed(1,6)	-2061.98215734	-17.3	-1.7	-2062.76851811	-16.0	-0.4
PA-Me2NHC(NaOtBu)-ts(1,6)	-2061.96252871	-5.0	12.2	-2062.75400440	-6.9	10.2
PA-Me2NHC(NaOtBu)-prod(1,6)	-2061.99851021	-27.5	-7.7	-2062.78817363	-28.3	-8.5
PA-PMe3(NaOtBu)-prod(1,4)	-2217.16382074	-34.1	-10.3	-2217.84422101	-33.4	-9.5
PA-PMe3(NaOtBu)-ts(1,4)	-2217.11646275	-4.4	13.4	-2217.80110599	-6.3	11.5

PA-PMe3(NaOtBu)-ed(1,4)	-2217.13337855	-15.0	2.8	-2217.81299290	-13.8	4.0	
PMe3-Cu-allenyl	-2217.07383729	22.3	7.9	-2217.75679113	21.5	7.1	
PMe3-Cu(NaOtBu)-allenyl	-2217.10941604	0.0	0.0	-2217.79106277	0.0	0.0	
PA-PMe3(NaOtBu)-ed(1,6)	-2217.12650231	-10.7	8.3	-2217.80590894	-9.3	9.7	
PA-PMe3(NaOtBu)-ts(1,6)	-2217.10469744	3.0	22.9	-2217.78964372	0.9	20.9	
PA-PMe3(NaOtBu)-prod(1,6)	-2217.13913008	-18.6	2.8	-2217.82318067	-20.2	1.3	

Figure S15-1

NaOPh dienoate							
9d(NaOPh)-Cu-allenyl	-3988.98769475	0.0	0.0	-3991.18948193	0.0	0.0	
PA-9d(NaOPh)-ts(1,6major)_01	-3989.00751557	-12.4	8.8	-3991.21133486	-13.7	7.6	
PA-9d(NaOPh)-ts(1,6major)_02	-3989.00855577	-13.1	8.5	-3991.21106691	-13.5	8.0	
PA-9d(NaOPh)-ts(1,6major)_03	-3989.00225925	-9.1	11.5	-3991.20679575	-10.9	9.8	
PA-9d(NaOPh)-ts(1,6minor)_01	-3989.00412385	-10.3	10.0	-3991.20926419	-12.4	7.9	
PA-9d(NaOPh)-ts(1,6minor)_02	-3989.00347070	-9.9	11.4	-3991.20901727	-12.3	9.0	
PA-9d(NaOPh)-ts(1,6minor)_03	-3989.00340749	-9.9	11.9	-3991.20895959	-12.2	9.5	
PA-9d(NaOPh)-ts(1,6minor)_04	-3989.00292070	-9.6	11.3	-3991.20709310	-11.1	9.8	
PA-9d(NaOPh)-ts(1,6minor)_05	-3989.00407258	-10.3	12.4	-3991.20558884	-10.1	12.6	
PA-9d(NaOPh)-ts(1,6minor)_06	-3989.00431408	-10.4	11.8	-3991.20434352	-9.3	12.9	
PA-9d(NaOPh)-ts(1,6minor)_07	-3989.00392992	-10.2	12.5	-3991.20503805	-9.8	12.9	
PA-9d(NaOPh)-ts(1,6minor)_08	-3988.99696407	-5.8	16.2	-3991.20267596	-8.3	13.7	

Figure S15-2

dienoate							
9b(NaOPh)-Cu-allenyl	-3988.97706437	0.0	0.0	-3991.18121663	0.0	0.0	
PA-9b(NaOPh)-ts(1,6major)_01	-3989.00122102	-15.2	5.7	-3991.20616255	-15.7	5.2	
PA-9b(NaOPh)-ts(1,6major)_02	-3989.00180413	-15.5	5.7	-3991.20461588	-14.7	6.5	
PA-9b(NaOPh)-ts(1,6major)_03	-3988.99857144	-13.5	7.4	-3991.20209966	-13.1	7.8	
PA-9b(NaOPh)-ts(1,6major)_04	-3988.99723215	-12.7	8.1	-3991.20142194	-12.7	8.1	
PA-9b(NaOPh)-ts(1,6major)_05	-3988.99977113	-14.2	7.0	-3991.20292311	-13.6	7.7	
PA-9b(NaOPh)-ts(1,6major)_06	-3988.99704889	-12.5	10.0	-3991.20055918	-12.1	10.4	
PA-9b(NaOPh)-ts(1,6major)_07	-3988.99041056	-8.4	10.5	-3991.19344823	-7.7	11.2	
PA-9b(NaOPh)-ts(1,6minor)_01	-3988.99262462	-9.8	11.1	-3991.19951812	-11.5	9.4	
PA-9b(NaOPh)-ts(1,6minor)_02	-3988.99821876	-13.3	7.4	-3991.20075841	-12.3	8.4	

PA-9b(NaOPh)-ts(1,6minor)_03	-3988.99811765	-13.2	7.5	-3991.20069813	-12.2	8.5
PA-9b(NaOPh)-ts(1,6minor)_04	-3988.99154901	-9.1	12.1	-3991.19952709	-11.5	9.7
PA-9b(NaOPh)-ts(1,6minor)_05	-3988.99955797	-14.1	8.5	-3991.20142088	-12.7	9.9
PA-9b(NaOPh)-ts(1,6minor)_06	-3988.99445142	-10.9	9.5	-3991.19628328	-9.5	11.0
PA-9b(NaOPh)-ts(1,6minor)_07	-3988.99731955	-12.7	9.7	-3991.19931176	-11.4	11.0
PA-9b(NaOPh)-ts(1,6minor)_08	-3988.99342975	-10.3	10.1	-3991.19551283	-9.0	11.4
PA-9b(NaOPh)-ts(1,6minor)_09	-3988.98457282	-4.7	17.6	-3991.19226624	-6.9	15.4

Figure S15-3

dienoate

9d(Na)-Cu-allenyl	-3681.64220587	0.0	0.0	-3683.60017309	0.0	0.0
PA-9d(Na)-ts(1,6major)_01	-3681.65973748	-11.0	9.3	-3683.61772924	-11.0	9.3
PA-9d(Na)-ts(1,6major)_02	-3681.65890032	-10.5	9.0	-3683.61645791	-10.2	9.3
PA-9d(Na)-ts(1,6major)_03	-3681.65937536	-10.8	9.1	-3683.61687054	-10.5	9.4
PA-9d(Na)-ts(1,6major)_04	-3681.66260080	-12.8	7.3	-3683.61794415	-11.2	8.9
PA-9d(Na)-ts(1,6major)_05	-3681.66144561	-12.1	8.6	-3683.61750955	-10.9	9.8
PA-9d(Na)-ts(1,6major)_06	-3681.65888860	-10.5	9.8	-3683.61647690	-10.2	10.0
PA-9d(Na)-ts(1,6major)_07	-3681.65884611	-10.4	10.0	-3683.61639249	-10.2	10.2
PA-9d(Na)-ts(1,6major)_08	-3681.66223765	-12.6	8.1	-3683.61749440	-10.9	9.9
PA-9d(Na)-ts(1,6major)_09	-3681.66033409	-11.4	9.3	-3683.61641726	-10.2	10.4
PA-9d(Na)-ts(1,6major)_10	-3681.65939834	-10.8	9.5	-3683.61511300	-9.4	10.9
PA-9d(Na)-ts(1,6major)_11	-3681.65521086	-8.2	11.6	-3683.61179052	-7.3	12.5
PA-9d(Na)-ts(1,6major)_12	-3681.65946037	-10.8	9.7	-3683.61514765	-9.4	11.1
PA-9d(Na)-ts(1,6major)_13	-3681.65382618	-7.3	13.0	-3683.61096278	-6.8	13.5
PA-9d(Na)-ts(1,6major)_14	-3681.64283348	-0.4	20.5	-3683.60120102	-0.6	20.3
PA-9d(Na)-ts(1,6major)_15	-3681.63944632	1.7	20.5	-3683.59810702	1.3	20.1
PA-9d(Na)-ts(1,6major)_16	-3681.64375937	-1.0	19.6	-3683.60113754	-0.6	19.9
PA-9d(Na)-ts(1,6major)_17	-3681.63816402	2.5	23.7	-3683.59756976	1.6	22.8
PA-9d(Na)-ts(1,6minor)_01	-3681.65761381	-9.7	9.1	-3683.61518754	-9.4	9.4
PA-9d(Na)-ts(1,6minor)_02	-3681.65709706	-9.3	10.4	-3683.61505028	-9.3	10.4
PA-9d(Na)-ts(1,6minor)_03	-3681.65697203	-9.3	11.1	-3683.61400305	-8.7	11.7
PA-9d(Na)-ts(1,6minor)_04	-3681.65704203	-9.3	11.4	-3683.61408660	-8.7	12.0
PA-9d(Na)-ts(1,6minor)_05	-3681.65704203	-9.3	11.4	-3683.61408657	-8.7	12.0
PA-9d(Na)-ts(1,6minor)_06	-3681.65634115	-8.9	12.1	-3683.61353101	-8.4	12.6
PA-9d(Na)-ts(1,6minor)_07	-3681.65643037	-8.9	12.6	-3683.61364680	-8.5	13.0
PA-9d(Na)-ts(1,6minor)_08	-3681.64986214	-4.8	14.9	-3683.60761370	-4.7	15.0
PA-9d(Na)-ts(1,6minor)_09	-3681.64972412	-4.7	15.5	-3683.60862100	-5.3	14.9

Figure S15-4

9b(Na)-Cu-allenyl	-3681.63854301	0.0	0.0	-3683.59431594	0.0	0.0

PA-9b(Na)-ts(1,6major)_01	-3681.65260731	-8.8	9.1	-3683.61172700	-10.9	7.0	
PA-9b(Na)-ts(1,6major)_02	-3681.65350670	-9.4	10.6	-3683.61137773	-10.7	9.3	
PA-9b(Na)-ts(1,6major)_03	-3681.65255339	-8.8	11.2	-3683.61104870	-10.5	9.5	
PA-9b(Na)-ts(1,6major)_04	-3681.65069168	-7.6	13.7	-3683.60668217	-7.8	13.5	
PA-9b(Na)-ts(1,6major)_05	-3681.63939099	-0.5	20.2	-3683.59897771	-2.9	17.8	
PA-9b(Na)-ts(1,6minor)_01	-3681.64719232	-5.4	15.3	-3683.60512824	-6.8	13.9	
PA-9b(Na)-ts(1,6minor)_02	-3681.64857584	-6.3	14.2	-3683.60598018	-7.3	13.2	
PA-9b(Na)-ts(1,6minor)_03	-3681.64600285	-4.7	15.5	-3683.60428570	-6.3	13.9	
PA-9b(Na)-ts(1,6minor)_04	-3681.64668739	-5.1	16.3	-3683.60472536	-6.5	14.9	
PA-9b(Na)-ts(1,6minor)_05	-3681.64538389	-4.3	17.4	-3683.60301713	-5.5	16.2	
PA-9b(Na)-ts(1,6minor)_06	-3681.64305388	-2.8	18.1	-3683.60057987	-3.9	17.0	
PA-9b(Na)-ts(1,6minor)_07	-3681.64509327	-4.1	17.8	-3683.60087894	-4.1	17.8	
PA-9b(Na)-ts(1,6minor)_08	-3681.64444133	-3.7	18.6	-3683.60061722	-4.0	18.3	

Figure S15-5

9d(NaOPh)-Cu-allyl_01	-4439.93821085	0.0	0.0	-4442.55008509	0.0	0.0	
AA-9d(NaOPh)-ts(1,6major)_01	-4439.98449643	-29.0	-5.1	-4442.59032238	-25.2	-1.4	
AA-9d(NaOPh)-ts(1,6major)_02	-4439.98383773	-28.6	-4.6	-4442.58789779	-23.7	0.3	
AA-9d(NaOPh)-ts(1,6minor)_01	-4439.97369382	-22.3	0.1	-4442.58185530	-19.9	2.5	
AA-9d(NaOPh)-ts(1,6minor)_02	-4439.97714033	-24.4	-0.7	-4442.58408048	-21.3	2.4	
AA-9d(NaOPh)-ts(1,6minor)_03	-4439.97464467	-22.9	0.6	-4442.58197373	-20.0	3.5	
AA-9d(NaOPh)-ts(1,6minor)_04	-4439.97785218	-24.9	-1.6	-4442.58201364	-20.0	3.2	
AA-9d(NaOPh)-ts(1,6minor)_05	-4439.97783459	-24.9	-0.8	-4442.58236006	-20.3	3.9	
AA-9d(NaOPh)-ts(1,6minor)_06	-4439.97172787	-21.0	2.7	-4442.57893097	-18.1	5.6	
AA-9d(NaOPh)-ts(1,6minor)_07	-4439.97079085	-20.4	4.0	-4442.58073697	-19.2	5.2	

Figure S15-6

9b(NaOPh)-Cu-allyl_01	-4439.93428626	0.0	0.0	-4442.54510511	0.0	0.0	
AA-9b(NaOPh)-ts(1,6major)_01	-4439.96919497	-21.9	0.4	-4442.57882366	-21.2	1.2	
AA-9b(NaOPh)-ts(1,6major)_02	-4439.97273296	-24.1	-1.6	-4442.57763165	-20.4	2.1	
AA-9b(NaOPh)-ts(1,6minor)_01	-4439.96841951	-21.4	0.0	-4442.57797333	-20.6	0.8	
AA-9b(NaOPh)-ts(1,6minor)_02	-4439.96874244	-21.6	0.5	-4442.57714867	-20.1	2.0	
AA-9b(NaOPh)-ts(1,6minor)_03	-4439.96841962	-21.4	1.3	-4442.57797329	-20.6	2.1	
AA-9b(NaOPh)-ts(1,6minor)_04	-4439.96875104	-21.6	2.1	-4442.57568461	-19.2	4.5	

Figure S15-7						
dienoate						
9d(Na)-Cu-allyl_01	-4132.59920742	0.0	0.0	-4134.96284992	0.0	0.0
AA-9d(Na)-ts(1,6major)_01	-4132.62729388	-17.6	3.4	-4134.98781113	-15.7	5.3
AA-9d(Na)-ts(1,6major)_02	-4132.62893033	-18.7	4.0	-4134.98845938	-16.1	6.6
AA-9d(Na)-ts(1,6major)_03	-4132.62631562	-17.0	6.2	-4134.98510346	-14.0	9.3
AA-9d(Na)-ts(1,6minor)_01	-4132.62446762	-15.9	6.1	-4134.98513729	-14.0	8.0
AA-9d(Na)-ts(1,6minor)_02	-4132.62440344	-15.8	6.5	-4134.98518004	-14.0	8.3
AA-9d(Na)-ts(1,6minor)_03	-4132.61477818	-9.8	11.8	-4134.97855006	-9.9	11.7
AA-9d(Na)-ts(1,6minor)_04	-4132.62390286	-15.5	7.1	-4134.98419154	-13.4	9.2
AA-9d(Na)-ts(1,6minor)_05	-4132.62110301	-13.7	8.3	-4134.98256014	-12.4	9.7
AA-9d(Na)-ts(1,6minor)_06	-4132.61285936	-8.6	13.7	-4134.97849931	-9.8	12.5
AA-9d(Na)-ts(1,6minor)_07	-4132.61977727	-12.9	9.3	-4134.98024852	-10.9	11.3

Figure S15-8						
9b(Na)-Cu-allyl_01	-4132.59314173	0.0	0.0	-4134.95669225	0.0	0.0
AA-9b(Na)-ts(1,6major)_01	-4132.62290671	-18.7	4.0	-4134.98408524	-17.2	5.5
AA-9b(Na)-ts(1,6major)_02	-4132.62647896	-20.9	2.5	-4134.98600401	-18.4	5.0
AA-9b(Na)-ts(1,6major)_03	-4132.61861915	-16.0	7.0	-4134.98236549	-16.1	6.9
AA-9b(Na)-ts(1,6major)_04	-4132.61684962	-14.9	10.9	-4134.97573346	-11.9	13.8
AA-9b(Na)-ts(1,6minor)_01	-4132.61446188	-13.4	9.1	-4134.97988308	-14.6	7.9
AA-9b(Na)-ts(1,6minor)_02	-4132.60984167	-10.5	11.7	-4134.97650355	-12.4	9.7
AA-9b(Na)-ts(1,6minor)_03	-4132.62176638	-18.0	4.9	-4134.98120906	-15.4	7.5
AA-9b(Na)-ts(1,6minor)_04	-4132.62181060	-18.0	5.2	-4134.98154297	-15.6	7.6
AA-9b(Na)-ts(1,6minor)_05	-4132.61576881	-14.2	10.0	-4134.97687655	-12.7	11.6

Figure S15-9						
NaOPh						
(PhO)2BpinNa						
PhOBpin						
dienoate						
9d(Naborate)-Cu-allenyl_01	-4399.49862226	0.0	0.0	-4402.03434163	0.0	0.0
9d(Naborate)-Cu-allenyl_02	-4399.49675768	1.2	2.1	-4402.03365706	0.4	1.3
9d(Naborate)-Cu-allenyl_03	-4399.49629242	1.5	3.2	-4402.03302937	0.8	2.6
9d(Naborate)-Cu-allenyl_04	-4399.50796677	-5.9	-0.3	-4402.04034648	-3.8	1.8
9d(Naborate)-Cu-allenyl_05	-4399.49480647	2.4	5.6	-4402.03158165	1.7	5.0

9d(Naborate)-Cu-allenyl_06	-4399.49920993	-0.4	3.3	-4402.03341646	0.6	4.3
9d(Naborate)-Cu-allenyl_07	-4399.49486942	2.4	5.8	-4402.03162241	1.7	5.1
PA-9b(Naborate)-ts(1,6major)_01	-4399.51879555	-12.7	10.6	-4402.05705381	-14.3	9.0
PA-9b(Naborate)-ts(1,6major)_02	-4399.51710928	-11.6	10.6	-4402.05467305	-12.8	9.5
PA-9b(Naborate)-ts(1,6major)_03	-4399.51734929	-11.8	12.2	-4402.05584456	-13.5	10.5
PA-9b(Naborate)-ts(1,6major)_04	-4399.51081372	-7.7	15.0	-4402.04971516	-9.6	13.0
PA-9b(Naborate)-ts(1,6major)_05	-4399.51143249	-8.0	14.1	-4402.04943819	-9.5	12.6
PA-9b(Naborate)-ts(1,6major)_06	-4399.51521676	-10.4	13.6	-4402.05084347	-10.4	13.6
PA-9b(Naborate)-ts(1,6major)_07	-4399.51421050	-9.8	14.0	-4402.05089868	-10.4	13.4
PA-9b(Naborate)-ts(1,6major)_08	-4399.51113742	-7.9	17.3	-4402.04997309	-9.8	15.3
PA-9b(Naborate)-ts(1,6major)_09	-4399.51442068	-9.9	14.8	-4402.05176313	-10.9	13.8
PA-9b(Naborate)-ts(1,6major)_10	-4399.51430481	-9.8	15.2	-4402.05168421	-10.9	14.1
9d-Cu-allenyl	-3519.91942960	0.0	0.0	-3521.86429899	0.0	0.0
PA-9b-ts(1,6major)_01	-3519.92080559	-0.9	19.7	-3521.86686895	-1.6	19.0
PA-9b-ts(1,6major)_02	-3519.92077687	-0.8	18.9	-3521.86622676	-1.2	18.5
PA-9b-ts(1,6major)_03	-3519.92187182	-1.5	19.1	-3521.86662225	-1.5	19.2
PA-9b-ts(1,6major)_04	-3519.91844085	0.6	21.5	-3521.86587153	-1.0	19.8
PA-9b-ts(1,6major)_05	-3519.91926994	0.1	22.1	-3521.86576011	-0.9	21.0

E(sp,sum) ……. single point electronic energy in Hartree with Def2TZVPP basis set in thf(SMD) after mass balance

ΔE(sp) …….. relative single point electronic energy in kcal/mol with Def2TZVPP basis set in thf(SMD)

ΔG(sp) …….. relative single point free energy in kcal/mol with Def2TZVPP basis set in thf(SMD)

[ΔG(sp) = ΔE(sp)/Def2TZVPP + ΔG_{corr}/Def2SVP]

Table S4. Single point energies in Figures S1-1–S15-9 with BP86-D3BJ and PBE0-D3BJ

structure	BP86-D3BJ/Def2TZVPP$_{thf(SMD)}$ E(sp,sum) [hartree]	ΔE(sp) [kcal/mol]	ΔG(sp) [kcal/mol]	PBE0-D3BJ/Def2TZVPP$_{thf(SMD)}$ E(sp,sum) [hartree]	ΔE(sp) [kcal/mol]	ΔG(sp) [kcal/mol]	
Figure S1-1							
dienoate							
PhOH							
NaOPh							
tBuOH							
NaOtBu							
PhOBpin							
(PhO)2BpinNa							
9d-Cu-allenyl	-3918.11090782	0.0	0.0	-3914.94154622	0.0	0.0	
PA-9d(Na)-ts(1,6major)	-3918.17489209	-40.2	-18.2	-3914.98796143	-29.1	-7.1	
9d-Cu-allenyl	-3991.96461045	0.0	0.0	-3988.71129340	0.0	0.0	
PA-9d(Na)-ts(1,6major)	-3992.00528960	-25.5	-3.8	-3988.73314230	-13.7	8.0	
9d-Cu-allenyl	-3991.96461045	0.0	0.0	-3988.71129340	0.0	0.0	
PA-9d(NaOPh)-ts(1,6major)	-3992.05166190	-54.6	-16.8	-3988.77951579	-42.8	-5.0	
9d-Cu-allenyl	-3522.59908511	0.0	0.0	-3519.82155195	0.0	0.0	
PA-9d-ts(1,6major)	-3522.62439727	-15.9	3.8	-3519.83030742	-5.5	14.2	
9d-Cu-allenyl	-4710.48441746	25.9	9.6	-4706.38741845	25.6	9.3	
9d-Cu-allenyl	-4710.52564785	0.0	0.0	-4706.42823267	0.0	0.0	
PA-9d(Naborate)-ts(1,6major)	-4710.58756776	-38.9	-14.8	-4706.47446297	-29.0	-4.9	
Figure S2-1							
PA-9d(NaOPh)-prod(1,6major)	-3992.07530973	-42.7	-19.7	-3988.82001382	-44.7	-21.7	
PA-9d(NaOPh)-ts(1,6major)	-3992.05166190	-27.9	-6.6	-3988.77951579	-19.3	2.0	
PA-9d(NaOPh)-pc(1,6major)	-3992.05835054	-32.1	-11.4	-3988.78784260	-24.5	-3.9	
9d(NaOPh)-Cu-allenyl	-3992.00726325	0.0	0.0	-3988.74876006	0.0	0.0	
9b(NaOPh)-Cu-allenyl	-3991.99949353	0.0	0.0	-3988.74305227	0.0	0.0	
PA-9b(NaOPh)-pc(1,6major)	-3992.05529031	-35.0	-14.6	-3988.78360162	-25.4	-5.0	
PA-9b(NaOPh)-ts(1,6major)	-3992.04887398	-31.0	-10.2	-3988.77567306	-20.5	0.3	
PA-9b(NaOPh)-prod(1,6major)	-3992.06511394	-41.2	-18.8	-3988.81204048	-43.3	-20.9	

PA-9d(NaOPh)-prod(1,6minor)	-3992.06469260	-36.0	-14.1	-3988.81025471	-38.6	-16.7
PA-9d(NaOPh)-ts(1,6minor)	-3992.04916265	-26.3	-6.0	-3988.77649127	-17.4	2.9
PA-9d(NaOPh)-pc(1,6minor)	-3992.05705222	-31.2	-11.3	-3988.78432931	-22.3	-2.4
9d(NaOPh)-Cu-allenyl	-3992.00726325	0.0	0.0	-3988.74876006	0.0	0.0
9b(NaOPh)-Cu-allenyl	-3991.99949353	0.0	0.0	-3988.74305227	0.0	0.0
PA-9b(NaOPh)-pc(1,6minor)	-3992.04926967	-31.2	-10.9	-3988.77733345	-21.5	-1.2
PA-9b(NaOPh)-ts(1,6minor)	-3992.04085109	-26.0	-5.1	-3988.76818927	-15.8	5.1
PA-9b(NaOPh)-prod(1,6minor)	-3992.06245070	-39.5	-16.7	-3988.80757473	-40.5	-17.6

Figure S3-1

AA-9d(NaOPh)-prod(1,6major)	-4443.53956791	-46.9	-20.9	-4439.75052149	-48.0	-22.0
AA-9d(NaOPh)-ts(1,6major)	-4443.52133333	-35.4	-11.5	-4439.71513797	-25.8	-1.9
AA-9d(NaOPh)-pc(1,6major)	-4443.52170507	-35.7	-12.4	-4439.71589768	-26.2	-3.0
9d(NaOPh)-Cu-allyl	-4443.46486884	0.0	0.0	-4439.67409117	0.0	0.0
9b(NaOPh)-Cu-allyl	-4443.46188377	0.0	0.0	-4439.67037956	0.0	0.0
AA-9b(NaOPh)-pc(1,6major)	-4443.51261718	-31.8	-11.9	-4439.70830901	-23.8	-3.8
AA-9b(NaOPh)-ts(1,6major)	-4443.51286576	-32.0	-9.6	-4439.70780214	-23.5	-1.1
AA-9b(NaOPh)-prod(1,6major)	-4443.53141611	-43.6	-18.6	-4439.74246516	-45.2	-20.2
AA-9d(NaOPh)-prod(1,6minor)	-4443.52846650	-39.9	-16.6	-4439.74052836	-41.7	-18.4
AA-9d(NaOPh)-ts(1,6minor)	-4443.51357738	-30.6	-8.2	-4439.70826334	-21.4	1.0
AA-9d(NaOPh)-pc(1,6minor)	-4443.51439359	-31.1	-9.7	-4439.70966160	-22.3	-1.0
9d(NaOPh)-Cu-allyl	-4443.46486884	0.0	0.0	-4439.67409117	0.0	0.0
9b(NaOPh)-Cu-allyl	-4443.46188377	0.0	0.0	-4439.67037956	0.0	0.0
AA-9b(NaOPh)-pc(1,6minor)	-4443.50943727	-29.8	-7.2	-4439.70384962	-21.0	1.6
AA-9b(NaOPh)-ts(1,6minor)	-4443.51094440	-30.8	-9.3	-4439.70458757	-21.5	0.0
AA-9b(NaOPh)-prod(1,6minor)	-4135.86950359	-43.8	-17.4	-4132.44864709	-45.4	-19.0

Figure S4-1

PA-9d(Na)-prod(1,6major)	-3684.41094470	-42.0	-19.1	-3681.52395309	-42.9	-20.0
PA-9d(Na)-ts(1,6major)	-3684.38683272	-26.9	-7.4	-3681.48137249	-16.2	3.3
PA-9d(Na)-pc(1,6major)	-3684.39356949	-31.1	-11.3	-3681.48976031	-21.5	-1.7
9d(Na)-Cu-allenyl	-3684.34400351	0.0	0.0	-3681.45554823	0.0	0.0
9b(Na)-Cu-allenyl	-3684.34130309	0.0	0.0	-3681.45127568	0.0	0.0
PA-9b(Na)-pc(1,6major)	-3684.38619465	-28.2	-10.3	-3681.48365822	-20.3	-2.4
PA-9b(Na)-ts(1,6major)	-3684.38105171	-24.9	-7.0	-3681.47660469	-15.9	2.1
PA-9b(Na)-prod(1,6major)	-3684.39894208	-36.2	-16.0	-3681.51485980	-39.9	-19.8

PA-9d(Na)-prod(1,6minor)	-3684.41356914	-43.7	-21.4	-3681.52671950	-44.7	-22.5	
PA-9d(Na)-ts(1,6minor)	-3684.38319287	-24.6	-5.8	-3681.47868489	-14.5	4.3	
PA-9d(Na)-pc(1,6minor)	-3684.38857507	-28.0	-9.2	-3681.48683895	-19.6	-0.8	
9d(Na)-Cu-allenyl	-3684.34400351	0.0	0.0	-3681.45554823	0.0	0.0	
9b(Na)-Cu-allenyl	-3684.34130309	0.0	0.0	-3681.45127568	0.0	0.0	
PA-9b(Na)-pc(1,6minor)	-3684.38100480	-24.9	-6.4	-3681.47896844	-17.4	1.2	
PA-9b(Na)-ts(1,6minor)	-3684.37346564	-20.2	0.5	-3681.46878764	-11.0	9.7	
PA-9b(Na)-prod(1,6minor)	-3684.39096760	-31.2	-11.0	-3681.50752342	-35.3	-15.1	

Figure S5-1

AA-9d(Na)-prod(1,6major)	-4135.86786923	-39.2	-13.5	-4132.44595292	-40.5	-14.7	
AA-9d(Na)-ts(1,6major)	-4135.84759100	-26.5	-5.5	-4132.41066897	-18.3	2.6	
AA-9d(Na)-pc(1,6major)	-4135.84905559	-27.4	-5.4	-4132.41263431	-19.6	2.5	
9d(Na)-Cu-allyl	-4135.80539302	0.0	0.0	-4132.38143186	0.0	0.0	
9b(Na)-Cu-allyl	-4135.79970911	0.0	0.0	-4132.37621802	0.0	0.0	
AA-9b(Na)-pc(1,6major)	-4135.84311002	-27.2	-5.4	-4132.40753350	-19.7	2.2	
AA-9b(Na)-ts(1,6major)	-4135.84350716	-27.5	-4.8	-4132.40738079	-19.6	3.1	
AA-9b(Na)-prod(1,6major)	-4135.86736486	-42.5	-17.3	-4132.44644449	-44.1	-18.9	
AA-9d(Na)-prod(1,6minor)	-4135.87246735	-42.1	-21.1	-4132.45278736	-44.8	-23.7	
AA-9d(Na)-ts(1,6minor)	-4135.84493698	-24.8	-2.8	-4132.40740722	-16.3	5.7	
AA-9d(Na)-pc(1,6minor)	-4135.84589569	-25.4	-4.7	-4132.40968798	-17.7	3.0	
9d(Na)-Cu-allyl	-4135.80539302	0.0	0.0	-4132.38143186	0.0	0.0	
9b(Na)-Cu-allyl	-4135.79970911	0.0	0.0	-4132.37621802	0.0	0.0	
AA-9b(Na)-pc(1,6minor)	-4135.84133823	-26.1	-3.7	-4132.40504157	-18.1	4.3	
AA-9b(Na)-ts(1,6minor)	-4135.84124147	-26.1	-3.6	-4132.40442562	-17.7	4.8	
AA-9b(Na)-prod(1,6minor)	-4135.86950359	-43.8	-17.4	-4132.44864709	-45.4	-19.0	

Figure S6-1

thf

PMe3

Me2NHC

NaOPh

NaOtBu

dienoate

dienoate-NaOPh

dienoate-NaOtBu

Me2NHC-Cu-allenyl	-3069.59080568	-9.5	-8.6	-3067.45525044	-8.7	-7.8
PMe3-Cu-allenyl	-3069.57561019	0.0	0.0	-3067.44142451	0.0	0.0
thf-Cu-allenyl	-3069.54673409	18.1	18.3	-3067.41474895	16.7	16.9
PA-NaOPh-prod(1,6)	-3069.59842850	-14.3	-5.2	-3067.46931832	-17.5	-8.4
PA-NaOPh-ts(1,6)	-3069.58013041	-2.8	5.4	-3067.43327212	5.1	13.4
PA-NaOPh-ed(1,6)	-3069.58665011	-6.9	0.3	-3067.44103235	0.2	7.4
NaOPh-Cu-allenyl	-3069.53550015	25.2	14.3	-3067.39977608	26.1	15.3
PA-NaOPh-ed(1,4)	-3069.58403683	-5.3	3.1	-3067.44292944	-0.9	7.4
PA-NaOPh-ts(1,4)	-3069.56833146	4.6	12.2	-3067.42415694	10.8	18.5
PA-NaOPh-prod(1,4)	-3069.60344299	-17.5	-8.1	-3067.47500051	-21.1	-11.7
Me2NHC-Cu-allenyl	-2995.73461710	-9.5	-8.6	-2993.68295515	-8.7	-7.8
PMe3-Cu-allenyl	-2995.71942161	0.0	0.0	-2993.66912922	0.0	0.0
thf-Cu-allenyl	-2995.69054551	18.1	18.3	-2993.64245366	16.7	16.9
PA-NaOtBu-prod(1,6)	-2995.75655758	-23.3	-14.2	-2993.71082755	-26.2	-17.1
PA-NaOtBu-ts(1,6)	-2995.73852416	-12.0	-5.1	-2993.67448627	-3.4	3.5
PA-NaOtBu-ed(1,6)	-2995.74606412	-16.7	-11.3	-2993.68374293	-9.2	-3.7
NaOtBu-Cu-allenyl	-2995.69813227	13.4	3.2	-2993.64570406	14.7	4.6
PA-NaOtBu-ed(1,4)	-2995.73717559	-11.1	-7.0	-2993.68069354	-7.3	-3.1
PA-NaOtBu-ts(1,4)	-2995.72814855	-5.5	-1.2	-2993.66826570	0.5	4.8
PA-NaOtBu-prod(1,4)	-2995.76460604	-28.4	-19.4	-2993.71891227	-31.2	-22.3

Figure S7-1

Me2NHC-Cu-allyl	-3357.79024157	0.0	0.0	-3355.22323589	0.0	0.0
AA-Me2NHC-pc(1,6major)	-3357.82753103	-23.4	-5.4	-3355.24932609	-16.4	1.6
AA-Me2NHC-ts(1,6major)	-3357.82409254	-21.2	-1.3	-3355.24457841	-13.4	6.6
AA-Me2NHC-prod(1,6major)	-3357.85111123	-38.2	-14.9	-3355.28461943	-38.5	-15.2
Me2NHC-Cu-allyl	-3357.79024157	0.0	0.0	-3355.22323589	0.0	0.0
AA-Me2NHC-pc(1,6minor)	-3357.82309356	-20.6	-1.2	-3355.24537984	-13.9	5.5
AA-Me2NHC-ts(1,6minor)	-3357.81467574	-15.3	4.7	-3355.23498225	-7.4	12.7
AA-Me2NHC-prod(1,6minor)	-3357.84522718	-34.5	-11.4	-3355.27754178	-34.1	-11.0

Figure S8-1

dienoate

SIMes-Cu-allenyl	-3526.01532262	0.0	0.0	-3523.21633309	0.0	0.0
PA-SIMes-ed(1,6)	-3526.04718255	-20.0	1.2	-3523.23443484	-11.4	9.9

PA-SIMes-ts(1,6)	-3526.03744920	-13.9	7.2	-3523.22267278	-4.0	17.1
PA-SIMes-prod(1,6)	-3526.05330773	-23.8	-0.8	-3523.25814644	-26.2	-3.2
PA-SIMes-ed(1,4AA)	-3526.04720639	-20.0	1.1	-3523.23444703	-11.4	9.7
PA-SIMes-ts(1,4AA)	-3526.01827797	-1.9	18.4	-3523.20822531	5.1	25.3
PA-SIMes-prod(1,4AA)	-3526.04726814	-20.0	-0.5	-3523.24989283	-21.1	-1.5
PA-SIMes-ed(1,4)	-3526.02948481	-8.9	9.9	-3523.22549882	-5.8	13.0
PA-SIMes-ts(1,4)	-3526.01415047	0.7	18.0	-3523.20369474	7.9	25.2
PA-SIMes-prod(1,4)	-3526.03240781	-10.7	10.8	-3523.23557877	-12.1	9.5
PPh3-Cu-allenyl	-3636.85858267	0.0	0.0	-3634.17271872	0.0	0.0
PA-PPh3-ed(1,6)	-3636.88809120	-18.5	-1.0	-3634.18833636	-9.8	7.7
PA-PPh3-ts(1,6)	-3636.87766146	-12.0	7.0	-3634.17494190	-1.4	17.6
PA-PPh3-prod(1,6)	-3636.89484986	-22.8	-2.7	-3634.21056135	-23.7	-3.7
PA-PPh3-ed(1,4AA)	-3636.88864094	-18.9	-2.6	-3634.18879181	-10.1	6.1
PA-PPh3-ts(1,4AA)	-3636.85664773	1.2	17.0	-3634.16096722	7.4	23.1
PA-PPh3-prod(1,4AA)	-3636.88803871	-18.5	0.0	-3634.20220538	-18.5	0.0
PA-PPh3-ed(1,4)	-3636.87025735	-7.3	8.3	-3634.17954629	-4.3	11.3
PA-PPh3-ts(1,4)	-3636.85755882	0.6	15.6	-3634.16055616	7.6	22.6
PA-PPh3-prod(1,4)	-3636.88802499	-18.5	0.0	-3634.21117007	-24.1	-5.6

Figures S9-1

Me2NHC-Cu-allenyl	-2906.34676690	0.0	0.0	-2904.31244991	0.0	0.0
PA-Me2NHC-ed(1,6)	-2906.36820860	-13.5	4.4	-2904.32303022	-6.6	11.3
PA-Me2NHC-ts(1,6)	-2906.35870339	-7.5	10.5	-2904.31082060	1.0	19.0
PA-Me2NHC-prod(1,6)	-2906.38435152	-23.6	-1.7	-2904.35168171	-24.6	-2.7
PA-Me2NHC-ed(1,4AA)	-2906.36948383	-14.3	2.0	-2904.32509745	-7.9	8.3
PA-Me2NHC-ts(1,4AA)	-2906.33694241	6.2	21.8	-2904.29499524	11.0	26.6
PA-Me2NHC-prod(1,4AA)	-2906.37273337	-16.3	-0.6	-2904.34286878	-19.1	-3.4
PA-Me2NHC-ed(1,4)	-2906.35273317	-3.7	11.3	-2904.31486302	-1.5	13.5
PA-Me2NHC-ts(1,4)	-2906.33858257	5.1	21.3	-2904.29415596	11.5	27.6
PA-Me2NHC-prod(1,4)	-2906.35699837	-6.4	12.0	-2904.32628813	-8.7	9.7
PMe3-Cu-allenyl	-3061.38799261	0.0	0.0	-3059.40483824	0.0	0.0
PA-PMe3-ed(1,6)	-3061.41761518	-18.6	-1.5	-3059.42339130	-11.6	5.4
PA-PMe3-ts(1,6)	-3061.40606925	-11.3	6.7	-3059.40924084	-2.8	15.3

PA-PMe3-prod(1,6)	-3061.42733065	-24.7	-5.0	-3059.44623527	-26.0	-6.3
PA-PMe3-ed(1,4AA)	-3061.41761516	-18.6	-1.5	-3059.42339134	-11.6	5.4
PA-PMe3-ts(1,4AA)	-3061.38114455	4.3	20.4	-3059.38983225	9.4	25.5
PA-PMe3-prod(1,4AA)	-3061.41544119	-17.2	0.2	-3059.43443467	-18.6	-1.1
PA-PMe3-ed(1,4)	-3061.39972670	-7.4	8.7	-3059.41209322	-4.6	11.5
PA-PMe3-ts(1,4)	-3061.38452988	2.2	17.3	-3059.39166751	8.3	23.4
PA-PMe3-prod(1,4)	-3061.42640538	-24.1	-3.5	-3059.44623887	-26.0	-5.4

Figure S10-1

dienoate
dienoate-Naborate

SIMes-Cu-allenyl	-4171.74947715	0.0	0.0	-4168.30319348	0.0	0.0
PA-SIMes(Naborate)-ed(1,6)	-4171.79416051	-28.0	-5.1	-4168.33168234	-17.9	5.1
PA-SIMes(Naborate)-ts(1,6)	-4171.78893020	-24.8	-2.6	-4168.32460895	-13.4	8.7
PA-SIMes(Naborate)-prod(1,6)	-4171.80809714	-36.8	-13.2	-4168.36406260	-38.2	-14.6
PA-SIMes(Naborate)-ed(1,4AA)	-4171.79205581	-26.7	-4.9	-4168.32851328	-15.9	5.9
PA-SIMes(Naborate)-ts(1,4AA)	-4171.77143042	-13.8	6.8	-4168.31208485	-5.6	15.0
PA-SIMes(Naborate)-prod(1,4AA)	-4171.80126749	-32.5	-10.4	-4168.35460691	-32.3	-10.2
PA-SIMes(Naborate)-ed(1,4)	-4171.78343724	-21.3	0.3	-4168.32525125	-13.8	7.7
PA-SIMes(Naborate)-ts(1,4)	-4171.76705397	-11.0	9.6	-4168.30606016	-1.8	18.8
PA-SIMes(Naborate)-prod(1,4)	-4171.79494883	-28.5	-5.2	-4168.35069323	-29.8	-6.5

dienoate
dienoate-Naborate

PPh3-Cu-allenyl	-4282.59273720	0.0	0.0	-4279.25957911	0.0	0.0
PA-PPh3(Naborate)-ed(1,6)	-4282.63578227	-27.0	-7.2	-4279.28502263	-16.0	3.8
PA-PPh3(Naborate)-ts(1,6)	-4282.63048183	-23.7	-4.2	-4279.27784955	-11.5	8.0
PA-PPh3(Naborate)-prod(1,6)	-4282.65924778	-41.7	-19.3	-4279.32385937	-40.3	-17.9
PA-PPh3(Naborate)-ed(1,4AA)	-4282.63635133	-27.4	-10.1	-4279.28671163	-17.0	0.2
PA-PPh3(Naborate)-ts(1,4AA)	-4282.60641457	-8.6	6.5	-4279.26261681	-1.9	13.2
PA-PPh3(Naborate)-prod(1,4AA)	-4282.64279454	-31.4	-14.9	-4279.31156460	-32.6	-16.1
PA-PPh3(Naborate)-ed(1,4)	-4282.62541498	-20.5	-3.8	-4279.28103205	-13.5	3.3
PA-PPh3(Naborate)-ts(1,4)	-4282.61213512	-12.2	5.9	-4279.26285551	-2.1	16.0
PA-PPh3(Naborate)-prod(1,4)	-4282.65836135	-41.2	-17.8	-4279.32305455	-39.8	-16.5

Figure S11-1						
dienoate						
PA-9d(Na)-prod(1,6major)	-3684.41094470	-42.0	-19.1	-3681.52395309	-42.9	-20.0
PA-9d(Na)-ts(1,6major)	-3684.38683272	-26.9	-7.4	-3681.48137249	-16.2	3.3
PA-9d(Na)-pc(1,6major)	-3684.39356949	-31.1	-11.3	-3681.48976031	-21.5	-1.7
9d(Na)-Cu-allenyl	-3684.34400351	0.0	0.0	-3681.45554823	0.0	0.0
PA-9d(Na)-pc(1,4AA)	-3684.38863659	-28.0	-9.3	-3681.48735615	-20.0	-1.2
PA-9d(Na)-ts(1,4AA)	-3684.36012968	-10.1	7.3	-3681.46210495	-4.1	13.4
PA-9d(Na)-prod(1,4AA)	-3684.40161734	-36.2	-17.9	-3681.51765910	-39.0	-20.8
Figure S12-1						
NaOtBu						
dienoate						
PA-SIMes(NaOtBu)-prod(1,4)	-2682.90889554	-34.2	-15.2	-2681.10773701	-42.4	-23.4
PA-SIMes(NaOtBu)-ts(1,4)	-2682.85830968	-2.5	15.5	-2681.03581136	2.7	20.7
PA-SIMes(NaOtBu)-ed(1,4)	-2682.87787625	-14.8	2.9	-2681.06066246	-12.9	4.8
SIMes-Cu-allenyl	-2682.80893365	28.5	10.2	-2681.00330393	23.1	4.7
SIMes-Cu(NaOtBu)-allenyl	-2682.85436097	0.0	0.0	-2681.04011606	0.0	0.0
PA-SIMes(NaOtBu)-ed(1,6)	-2682.88193280	-17.3	1.2	-2681.06112264	-13.2	5.3
PA-SIMes(NaOtBu)-ts(1,6)	-2682.87672376	-14.0	3.6	-2681.05401346	-8.7	9.0
PA-SIMes(NaOtBu)-prod(1,6)	-2682.89711409	-26.8	-8.3	-2681.09466624	-34.2	-15.7
PA-PPh3(NaOtBu)-prod(1,4)	-2793.76350170	-40.1	-17.0	-2792.06662454	-41.7	-18.5
PA-PPh3(NaOtBu)-ts(1,4)	-2793.72852420	-18.2	0.4	-2792.01638134	-10.1	8.5
PA-PPh3(NaOtBu)-ed(1,4)	-2793.73938424	-25.0	-5.2	-2792.02917221	-18.2	1.6
PPh3-Cu-allenyl	-2793.65219370	29.7	14.0	-2791.95968956	25.4	9.7
PPh3-Cu(NaOtBu)-allenyl	-2793.69955220	0.0	0.0	-2792.00021385	0.0	0.0
PA-PPh3(NaOtBu)-ed(1,6)	-2793.72413310	-15.4	2.4	-2792.01563634	-9.7	8.2
PA-PPh3(NaOtBu)-ts(1,6)	-2793.71845282	-11.9	7.5	-2792.00826547	-5.1	14.3
PA-PPh3(NaOtBu)-prod(1,6)	-2793.74658168	-29.5	-8.8	-2792.05352384	-33.5	-12.7
Figure S13-1						

NaOMe dienoate						
PA-SIMes(NaOMe)-prod(1,4)	-2682.91287496	-39.3	-17.9	-2681.10638448	-43.0	-21.6
PA-SIMes(NaOMe)-ts(1,4)	-2682.85685677	-4.2	14.3	-2681.03513143	1.7	20.2
PA-SIMes(NaOMe)-ed(1,4)	-2682.87216565	-13.8	4.9	-2681.05589929	-11.3	7.3
SIMes-Cu-allenyl	-2682.80893365	25.9	10.4	-2681.00330393	21.7	6.2
SIMes-Cu(NaOMe)-allenyl	-2682.85017751	0.0	0.0	-2681.03782716	0.0	0.0
PA-SIMes(NaOMe)-ed(1,6)	-2682.88133505	-19.6	-1.3	-2681.06060139	-14.3	3.9
PA-SIMes(NaOMe)-ts(1,6)	-2682.87608789	-16.3	3.7	-2681.05385801	-10.1	9.9
PA-SIMes(NaOMe)-prod(1,6)	-2682.89718148	-29.5	-9.5	-2681.09478096	-35.7	-15.7
PA-PPh3(NaOMe)-prod(1,4)	-2793.76033632	-40.5	-17.7	-2792.06562250	-41.9	-19.2
PA-PPh3(NaOMe)-ts(1,4)	-2793.72287931	-17.0	1.1	-2792.01287647	-8.8	9.2
PA-PPh3(NaOMe)-ed(1,4)	-2793.73250696	-23.0	-3.6	-2792.02457383	-16.2	3.3
PPh3-Cu-allenyl	-2793.65219370	27.4	13.6	-2791.95968956	24.5	10.8
PPh3-Cu(NaOMe)-allenyl	-2793.69579061	0.0	0.0	-2791.99878218	0.0	0.0
PA-PPh3(NaOMe)-ed(1,6)	-2793.72105284	-15.9	1.0	-2792.01406739	-9.6	7.2
PA-PPh3(NaOMe)-ts(1,6)	-2793.71540045	-12.3	5.7	-2792.00629710	-4.7	13.2
PA-PPh3(NaOMe)-prod(1,6)	-2793.74322195	-29.8	-9.2	-2792.05165288	-33.2	-12.6

Figure S14-1

NaOtBu dienoate						
PA-Me2NHC(NaOtBu)-prod(1,4)	-2063.23294191	-39.2	-19.3	-2062.19715108	-45.3	-25.3
PA-Me2NHC(NaOtBu)-ts(1,4)	-2063.19133236	-13.1	3.8	-2062.13441643	-5.9	10.9
PA-Me2NHC(NaOtBu)-ed(1,4)	-2063.19489513	-15.3	2.7	-2062.14478092	-12.4	5.6
Me2NHC-Cu-allenyl	-2063.14035749	18.9	2.0	-2062.09940685	16.0	-0.8
Me2NHC-Cu(NaOtBu)-allenyl	-2063.17045645	0.0	0.0	-2062.12496781	0.0	0.0
PA-Me2NHC(NaOtBu)-ed(1,6)	-2063.20787397	-23.5	-7.9	-2062.15367044	-18.0	-2.4
PA-Me2NHC(NaOtBu)-ts(1,6)	-2063.20158543	-19.5	-2.4	-2062.14510942	-12.6	4.5
PA-Me2NHC(NaOtBu)-prod(1,6)	-2063.22634958	-35.1	-15.3	-2062.18783762	-39.5	-19.6
PA-PMe3(NaOtBu)-prod(1,4)	-2218.28483626	-38.2	-14.4	-2217.29311317	-40.0	-16.2
PA-PMe3(NaOtBu)-ts(1,4)	-2218.24392606	-12.5	5.4	-2217.23790528	-5.4	12.5

PA-PMe3(NaOtBu)-ed(1,4)	-2218.24869111	-15.5	2.3	-2217.24837195	-11.9	5.8	
PMe3-Cu-allenyl	-2218.18160364	26.6	12.2	-2217.19180908	23.5	9.1	
PMe3-Cu(NaOtBu)-allenyl	-2218.22402238	0.0	0.0	-2217.22932901	0.0	0.0	
PA-PMe3(NaOtBu)-ed(1,6)	-2218.24858381	-15.4	3.6	-2217.24508172	-9.9	9.1	
PA-PMe3(NaOtBu)-ts(1,6)	-2218.24108932	-10.7	9.3	-2217.23647756	-4.5	15.5	
PA-PMe3(NaOtBu)-prod(1,6)	-2218.26899956	-28.2	-6.7	-2217.28001706	-31.8	-10.3	

Figure S15-1

NaOPh dienoate							
9d(NaOPh)-Cu-allenyl	-3992.00726325	0.0	0.0	-3988.74876006	0.0	0.0	
PA-9d(NaOPh)-ts(1,6major)_01	-3992.05166190	-27.9	-6.6	-3988.77951579	-19.3	2.0	
PA-9d(NaOPh)-ts(1,6major)_02	-3992.05229106	-28.3	-6.7	-3988.77887716	-18.9	2.7	
PA-9d(NaOPh)-ts(1,6major)_03	-3992.04973850	-26.7	-6.0	-3988.77595352	-17.1	3.6	
PA-9d(NaOPh)-ts(1,6minor)_01	-3992.04916265	-26.3	-6.0	-3988.77649127	-17.4	2.9	
PA-9d(NaOPh)-ts(1,6minor)_02	-3992.05039934	-27.1	-5.8	-3988.77616753	-17.2	4.1	
PA-9d(NaOPh)-ts(1,6minor)_03	-3992.05037272	-27.1	-5.3	-3988.77615462	-17.2	4.5	
PA-9d(NaOPh)-ts(1,6minor)_04	-3992.04531892	-23.9	-3.0	-3988.77131035	-14.2	6.7	
PA-9d(NaOPh)-ts(1,6minor)_05	-3992.04877207	-26.0	-3.3	-3988.77301706	-15.2	7.5	
PA-9d(NaOPh)-ts(1,6minor)_06	-3992.04909257	-26.2	-4.0	-3988.77270768	-15.0	7.2	
PA-9d(NaOPh)-ts(1,6minor)_07	-3992.04770415	-25.4	-2.7	-3988.77190836	-14.5	8.1	
PA-9d(NaOPh)-ts(1,6minor)_08	-3992.04576110	-24.2	-2.1	-3988.77046367	-13.6	8.4	

Figure S15-2

dienoate							
9b(NaOPh)-Cu-allenyl	-3991.99949353	0.0	0.0	-3988.74305227	0.0	0.0	
PA-9b(NaOPh)-ts(1,6major)_01	-3992.04887398	-31.0	-10.2	-3988.77567306	-20.5	0.3	
PA-9b(NaOPh)-ts(1,6major)_02	-3992.04843081	-30.7	-9.5	-3988.77479986	-19.9	1.3	
PA-9b(NaOPh)-ts(1,6major)_03	-3992.04507295	-28.6	-7.7	-3988.77025003	-17.1	3.9	
PA-9b(NaOPh)-ts(1,6major)_04	-3992.04363920	-27.7	-6.9	-3988.77034078	-17.1	3.7	
PA-9b(NaOPh)-ts(1,6major)_05	-3992.04280956	-27.2	-5.9	-3988.77000815	-16.9	4.4	
PA-9b(NaOPh)-ts(1,6major)_06	-3992.04643986	-29.5	-7.0	-3988.77076548	-17.4	5.1	
PA-9b(NaOPh)-ts(1,6major)_07	-3992.03578291	-22.8	-3.9	-3988.76208918	-11.9	6.9	
PA-9b(NaOPh)-ts(1,6minor)_01	-3992.04085109	-26.0	-5.1	-3988.76818927	-15.8	5.1	
PA-9b(NaOPh)-ts(1,6minor)_02	-3992.04350985	-27.6	-7.0	-3988.76794301	-15.6	5.0	

PA-9b(NaOPh)-ts(1,6minor)_03	-3992.04347841	-27.6	-6.9	-3988.76790216	-15.6	5.1
PA-9b(NaOPh)-ts(1,6minor)_04	-3992.04011574	-25.5	-4.3	-3988.76765743	-15.4	5.8
PA-9b(NaOPh)-ts(1,6minor)_05	-3992.04422701	-28.1	-5.5	-3988.76843385	-15.9	6.7
PA-9b(NaOPh)-ts(1,6minor)_06	-3992.03865176	-24.6	-4.1	-3988.76318245	-12.6	7.8
PA-9b(NaOPh)-ts(1,6minor)_07	-3992.04303960	-27.3	-4.9	-3988.76650603	-14.7	7.7
PA-9b(NaOPh)-ts(1,6minor)_08	-3992.03806506	-24.2	-3.8	-3988.76245160	-12.2	8.2
PA-9b(NaOPh)-ts(1,6minor)_09	-3992.03647445	-23.2	-0.9	-3988.76108979	-11.3	11.0

Figure S15-3

dienoate

9d(Na)-Cu-allenyl	-3684.34400351	0.0	0.0	-3681.45554823	0.0	0.0
PA-9d(Na)-ts(1,6major)_01	-3684.38660966	-26.7	-6.4	-3681.48176740	-16.5	3.9
PA-9d(Na)-ts(1,6major)_02	-3684.38683272	-26.9	-7.4	-3681.48137249	-16.2	3.3
PA-9d(Na)-ts(1,6major)_03	-3684.38658476	-26.7	-6.8	-3681.48148343	-16.3	3.6
PA-9d(Na)-ts(1,6major)_04	-3684.38693231	-26.9	-6.8	-3681.48190108	-16.5	3.6
PA-9d(Na)-ts(1,6major)_05	-3684.38647347	-26.7	-6.0	-3681.48165160	-16.4	4.3
PA-9d(Na)-ts(1,6major)_06	-3684.38681555	-26.9	-6.6	-3681.48134397	-16.2	4.0
PA-9d(Na)-ts(1,6major)_07	-3684.38679528	-26.9	-6.4	-3681.48129932	-16.2	4.3
PA-9d(Na)-ts(1,6major)_08	-3684.38631972	-26.6	-5.8	-3681.48136535	-16.2	4.5
PA-9d(Na)-ts(1,6major)_09	-3684.38413774	-25.2	-4.6	-3681.47976004	-15.2	5.4
PA-9d(Na)-ts(1,6major)_10	-3684.38113860	-23.3	-3.0	-3681.47759166	-13.8	6.5
PA-9d(Na)-ts(1,6major)_11	-3684.38028465	-22.8	-3.0	-3681.47708945	-13.5	6.2
PA-9d(Na)-ts(1,6major)_12	-3684.38107178	-23.3	-2.7	-3681.47758296	-13.8	6.7
PA-9d(Na)-ts(1,6major)_13	-3684.37991017	-22.5	-2.2	-3681.47412585	-11.7	8.6
PA-9d(Na)-ts(1,6major)_14	-3684.36872992	-15.5	5.4	-3681.46460575	-5.7	15.2
PA-9d(Na)-ts(1,6major)_15	-3684.36689176	-14.4	4.4	-3681.46205902	-4.1	14.7
PA-9d(Na)-ts(1,6major)_16	-3684.36832752	-15.3	5.3	-3681.46357092	-5.0	15.5
PA-9d(Na)-ts(1,6major)_17	-3684.36588489	-13.7	7.4	-3681.46050726	-3.1	18.0
PA-9d(Na)-ts(1,6minor)_01	-3684.38319287	-24.6	-5.8	-3681.47868489	-14.5	4.3
PA-9d(Na)-ts(1,6minor)_02	-3684.38087463	-23.1	-3.4	-3681.47704313	-13.5	6.2
PA-9d(Na)-ts(1,6minor)_03	-3684.38190553	-23.8	-3.4	-3681.47753860	-13.8	6.6
PA-9d(Na)-ts(1,6minor)_04	-3684.38193893	-23.8	-3.1	-3681.47760104	-13.8	6.9
PA-9d(Na)-ts(1,6minor)_05	-3684.38193905	-23.8	-3.1	-3681.47760103	-13.8	6.9
PA-9d(Na)-ts(1,6minor)_06	-3684.38094847	-23.2	-2.2	-3681.47641491	-13.1	7.9
PA-9d(Na)-ts(1,6minor)_07	-3684.38106148	-23.3	-1.8	-3681.47653146	-13.2	8.3
PA-9d(Na)-ts(1,6minor)_08	-3684.37819320	-21.5	-1.8	-3681.47218785	-10.4	9.2
PA-9d(Na)-ts(1,6minor)_09	-3684.37628432	-20.3	0.0	-3681.47220305	-10.5	9.8

Figure S15-4

9b(Na)-Cu-allenyl	-3684.34130309	0.0	0.0	-3681.45127568	0.0	0.0

PA-9b(Na)-ts(1,6major)_01	-3684.38105171	-24.9	-7.0	-3681.47660469	-15.9	2.1
PA-9b(Na)-ts(1,6major)_02	-3684.38118376	-25.0	-5.0	-3681.47691186	-16.1	3.9
PA-9b(Na)-ts(1,6major)_03	-3684.38149711	-25.2	-5.2	-3681.47696215	-16.1	3.9
PA-9b(Na)-ts(1,6major)_04	-3684.37475862	-21.0	0.3	-3681.46889938	-11.1	10.2
PA-9b(Na)-ts(1,6major)_05	-3684.36763807	-16.5	4.2	-3681.46293120	-7.3	13.4
PA-9b(Na)-ts(1,6minor)_01	-3684.37346564	-20.2	0.5	-3681.46878764	-11.0	9.7
PA-9b(Na)-ts(1,6minor)_02	-3684.37277477	-19.7	0.7	-3681.46819088	-10.6	9.9
PA-9b(Na)-ts(1,6minor)_03	-3684.37402103	-20.5	-0.4	-3681.46816590	-10.6	9.6
PA-9b(Na)-ts(1,6minor)_04	-3684.37230164	-19.5	2.0	-3681.46760003	-10.2	11.2
PA-9b(Na)-ts(1,6minor)_05	-3684.37383755	-20.4	1.2	-3681.46693180	-9.8	11.8
PA-9b(Na)-ts(1,6minor)_06	-3684.36850239	-17.1	3.8	-3681.46320463	-7.5	13.4
PA-9b(Na)-ts(1,6minor)_07	-3684.37186851	-19.2	2.7	-3681.46460850	-8.4	13.5
PA-9b(Na)-ts(1,6minor)_08	-3684.37139520	-18.9	3.4	-3681.46409148	-8.0	14.2

Figure S15-5

9d(NaOPh)-Cu-allyl_01	-4443.46486884	0.0	0.0	-4439.67409117	0.0	0.0
AA-9d(NaOPh)-ts(1,6major)_01	-4443.52133333	-35.4	-11.5	-4439.71513797	-25.8	-1.9
AA-9d(NaOPh)-ts(1,6major)_02	-4443.51836120	-33.6	-9.6	-4439.71209859	-23.9	0.2
AA-9d(NaOPh)-ts(1,6minor)_01	-4443.51357738	-30.6	-8.2	-4439.70826334	-21.4	1.0
AA-9d(NaOPh)-ts(1,6minor)_02	-4443.51568277	-31.9	-8.1	-4439.70959008	-22.3	1.5
AA-9d(NaOPh)-ts(1,6minor)_03	-4443.51409093	-30.9	-7.4	-4439.70794755	-21.2	2.2
AA-9d(NaOPh)-ts(1,6minor)_04	-4443.51536893	-31.7	-8.4	-4439.70783247	-21.2	2.1
AA-9d(NaOPh)-ts(1,6minor)_05	-4443.51130761	-29.1	-5.0	-4439.70526697	-19.6	4.5
AA-9d(NaOPh)-ts(1,6minor)_06	-4443.51537683	-31.7	-8.0	-4439.70726807	-20.8	2.9
AA-9d(NaOPh)-ts(1,6minor)_07	-4443.51365954	-30.6	-6.2	-4439.70840896	-21.5	2.9

Figure S15-6

9b(NaOPh)-Cu-allyl_01	-4443.46188377	0.0	0.0	-4439.67037956	0.0	0.0
AA-9b(NaOPh)-ts(1,6major)_01	-4443.51286576	-32.0	-9.6	-4439.70780214	-23.5	-1.1
AA-9b(NaOPh)-ts(1,6major)_02	-4443.50724262	-28.5	-5.9	-4439.70174460	-19.7	2.9
AA-9b(NaOPh)-ts(1,6minor)_01	-4443.51094440	-30.8	-9.3	-4439.70458757	-21.5	0.0
AA-9b(NaOPh)-ts(1,6minor)_02	-4443.50957337	-29.9	-7.8	-4439.70343706	-20.7	1.4
AA-9b(NaOPh)-ts(1,6minor)_03	-4443.51094440	-30.8	-8.0	-4439.70458750	-21.5	1.3
AA-9b(NaOPh)-ts(1,6minor)_04	-4443.50782875	-28.8	-5.1	-4439.70006372	-18.6	5.1

Figure S15-7						
dienoate						
9d(Na)-Cu-allyl_01	-4135.80539302	0.0	0.0	-4132.38143186	0.0	0.0
AA-9d(Na)-ts(1,6major)_01	-4135.84759100	-26.5	-5.5	-4132.41066897	-18.3	2.6
AA-9d(Na)-ts(1,6major)_02	-4135.84838469	-27.0	-4.3	-4132.41090700	-18.5	4.2
AA-9d(Na)-ts(1,6major)_03	-4135.84653724	-25.8	-2.6	-4132.40749701	-16.4	6.9
AA-9d(Na)-ts(1,6minor)_01	-4135.84493698	-24.8	-2.8	-4132.40740722	-16.3	5.7
AA-9d(Na)-ts(1,6minor)_02	-4135.84493399	-24.8	-2.5	-4132.40741023	-16.3	6.0
AA-9d(Na)-ts(1,6minor)_03	-4135.84070943	-22.2	-0.6	-4132.40413683	-14.2	7.3
AA-9d(Na)-ts(1,6minor)_04	-4135.84304397	-23.6	-1.0	-4132.40612460	-15.5	7.1
AA-9d(Na)-ts(1,6minor)_05	-4135.84274336	-23.4	-1.4	-4132.40545190	-15.1	7.0
AA-9d(Na)-ts(1,6minor)_06	-4135.84030088	-21.9	0.4	-4132.40353329	-13.9	8.4
AA-9d(Na)-ts(1,6minor)_07	-4135.84266603	-23.4	-1.2	-4132.40395782	-14.1	8.0

Figure S15-8						
9b(Na)-Cu-allyl_01	-4135.79970911	0.0	0.0	-4132.37621802	0.0	0.0
AA-9b(Na)-ts(1,6major)_01	-4135.84350716	-27.5	-4.8	-4132.40738079	-19.6	3.1
AA-9b(Na)-ts(1,6major)_02	-4135.84382415	-27.7	-4.2	-4132.40709904	-19.4	4.1
AA-9b(Na)-ts(1,6major)_03	-4135.84250319	-26.9	-3.9	-4132.40641442	-18.9	4.0
AA-9b(Na)-ts(1,6major)_04	-4135.83599319	-22.8	3.0	-4132.39655676	-12.8	13.0
AA-9b(Na)-ts(1,6minor)_01	-4135.84124147	-26.1	-3.6	-4132.40442562	-17.7	4.8
AA-9b(Na)-ts(1,6minor)_02	-4135.83865109	-24.4	-2.3	-4132.40081326	-15.4	6.7
AA-9b(Na)-ts(1,6minor)_03	-4135.84011322	-25.4	-2.5	-4132.40144646	-15.8	7.0
AA-9b(Na)-ts(1,6minor)_04	-4135.84026091	-25.4	-2.2	-4132.40124112	-15.7	7.5
AA-9b(Na)-ts(1,6minor)_05	-4135.83794846	-24.0	0.2	-4132.39898592	-14.3	10.0

Figure S15-9						
NaOPh						
(PhO)2BpinNa						
PhOBpin						
dienoate						
9d(Naborate)-Cu-allenyl_01	-4402.92814227	0.0	0.0	-4399.19480498	0.0	0.0
9d(Naborate)-Cu-allenyl_02	-4402.92826395	-0.1	0.8	-4399.19590677	-0.7	0.2
9d(Naborate)-Cu-allenyl_03	-4402.92868128	-0.3	1.4	-4399.19475274	0.0	1.8
9d(Naborate)-Cu-allenyl_04	-4402.93723838	-5.7	-0.2	-4399.20053326	-3.6	2.0
9d(Naborate)-Cu-allenyl_05	-4402.92759120	0.3	3.6	-4399.19381205	0.6	3.9

9d(Naborate)-Cu-allenyl_06	-4402.93056150	-1.5	2.2	-4399.19304152	1.1	4.8
9d(Naborate)-Cu-allenyl_07	-4402.92762960	0.3	3.7	-4399.19382481	0.6	4.0
PA-9b(Naborate)-ts(1,6major)_01	-4402.96911088	-25.7	-2.5	-4399.22269316	-17.5	5.7
PA-9b(Naborate)-ts(1,6major)_02	-4402.96668490	-24.2	-2.0	-4399.22046745	-16.1	6.1
PA-9b(Naborate)-ts(1,6major)_03	-4402.96791622	-25.0	-1.0	-4399.22214847	-17.2	6.8
PA-9b(Naborate)-ts(1,6major)_04	-4402.96551321	-23.5	-0.8	-4399.21952702	-15.5	7.1
PA-9b(Naborate)-ts(1,6major)_05	-4402.96158402	-21.0	1.1	-4399.21613588	-13.4	8.7
PA-9b(Naborate)-ts(1,6major)_06	-4402.96696816	-24.4	-0.4	-4399.21790935	-14.5	9.5
PA-9b(Naborate)-ts(1,6major)_07	-4402.96399012	-22.5	1.3	-4399.21553883	-13.0	10.8
PA-9b(Naborate)-ts(1,6major)_08	-4402.96359886	-22.2	2.9	-4399.21762865	-14.3	10.8
PA-9b(Naborate)-ts(1,6major)_09	-4402.96762109	-24.8	0.0	-4399.21776256	-14.4	10.3
PA-9b(Naborate)-ts(1,6major)_10	-4402.96761066	-24.8	0.2	-4399.21773837	-14.4	10.6
9d-Cu-allenyl	-3522.59908511	0.0	0.0	-3519.82155195	0.0	0.0
PA-9b-ts(1,6major)_01	-3522.62386542	-15.5	5.1	-3519.83070138	-5.7	14.9
PA-9b-ts(1,6major)_02	-3522.62439727	-15.9	3.8	-3519.83030742	-5.5	14.2
PA-9b-ts(1,6major)_03	-3522.62375539	-15.5	5.1	-3519.83018196	-5.4	15.2
PA-9b-ts(1,6major)_04	-3522.62291835	-15.0	5.9	-3519.83006684	-5.3	15.5
PA-9b-ts(1,6major)_05	-3522.62263767	-14.8	7.2	-3519.82987664	-5.2	16.7

E(sp,sum) ……. single point electronic energy in Hartree with Def2TZVPP basis set in thf(SMD) after mass balance

ΔE(sp) …….. relative single point electronic energy in kcal/mol with Def2TZVPP basis set in thf(SMD)

ΔG(sp) …….. relative single point free energy in kcal/mol with Def2TZVPP basis set in thf(SMD)

[ΔG(sp) = ΔE(sp)/Def2TZVPP + ΔG_{corr}/Def2SVP]

6. Geometries of computed structures with ωB97XD/Def2SVP$_{thf(PCM)}$

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32
Figure_S1-1_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C   -0.660544   -0.726572    0.059153
 C   -1.860539   -0.097447    0.115996
 H   -0.691600   -1.818492   -0.004770
 C   -1.976243    1.390665    0.160143
 C   -3.120576   -0.891785    0.187355
 O   -3.041424    1.823605   -0.507466
 O   -1.182749    2.134043    0.689285
 O   -4.147702   -0.497504    0.683440
 O   -2.981802   -2.118850   -0.320932
 C   -4.097604   -2.989729   -0.195724
 H   -4.332384   -3.170881    0.862818
 H   -3.810049   -3.927003   -0.683244
 H   -4.981752   -2.562067   -0.688186
 C   -3.254671    3.228152   -0.535442
 H   -3.354009    3.627502    0.483524
 H   -4.184056    3.384216   -1.092621
 H   -2.420438    3.737793   -1.038016
 C    0.656646   -0.129211    0.062308
 H    0.725624    0.955889    0.150505
 C    1.759981   -0.902956   -0.019704
 H    1.621029   -1.988149   -0.089650
 C    3.156351   -0.453635   -0.025165
 C    4.175093   -1.416830   -0.109525
 C    3.522207    0.902114    0.053056
 C    5.517020   -1.042840   -0.114390
 H    3.907556   -2.474776   -0.172060
 C    4.861836    1.275255    0.048166
 H    2.754752    1.675486    0.118691
 C    5.863995    0.305241   -0.035401
 H    6.294080   -1.807149   -0.179427
 H    5.127957    2.332459    0.111300
 H    6.914980    0.602284   -0.038425
13
Figure_S1-1_PhOH / electronic energy: -307.150518153 a.u. / lowest freq: 229.45 cm-1
 C    1.125381   -1.219560    0.000000
 C   -0.269323   -1.196698    0.000012
 C   -0.947244    0.027670    0.000021
 C   -0.218172    1.223214    0.000014
 C    1.173552    1.186894   -0.000002
 C    1.855907   -0.031913   -0.000013
 H    1.642554   -2.181822   -0.000008
 H   -0.835464   -2.132547    0.000025
 H   -0.759892    2.171100    0.000022
 H    1.731740    2.126121   -0.000009
 H    2.947293   -0.054666   -0.000025
 O   -2.295715    0.113012   -0.000021
 H   -2.681132   -0.769923   -0.000028
13
Figure_S1-1_NaOPh / electronic energy: -468.853649444 a.u. / lowest freq: 15.68 cm-1
 C   -1.912599   -1.200838   -0.011375
 C   -0.521476   -1.206572    0.015351
 C    0.241248    0.001459    0.028090
 C   -0.524240    1.207747    0.015228
 C   -1.915348    1.198823   -0.011498
 C   -2.633248   -0.001829   -0.025828
 H   -2.448993   -2.155315   -0.021458
 H    0.025710   -2.154567    0.026010
 H    0.020847    2.156944    0.025804
 H   -2.453903    2.152085   -0.021671
 H   -3.725390   -0.003095   -0.047610
 O    1.527681    0.002959    0.048939
Na    3.632205   -0.001133   -0.037490
15
Figure_S1-1_tBuOH / electronic energy: -233.441013186 a.u. / lowest freq: 210.58 cm-1
 O    0.065052   -0.000004   -1.443660
 C   -0.006173    0.000001   -0.021758
 C    0.669714    1.259454    0.527496
 H    0.587173    1.313300    1.623543
 H    1.741269    1.269991    0.269361
 H    0.203702    2.158344    0.097210
 C    0.669615   -1.259504    0.527499
 H    0.587068   -1.313344    1.623545
 H    0.203536   -2.158359    0.097212
 H    1.741170   -1.270125    0.269365
 C   -1.494539    0.000058    0.313449
 H   -1.980331   -0.891394   -0.110366
 H   -1.650877    0.000067    1.401900
 H   -1.980266    0.891542   -0.110372
 H    0.995436   -0.000040   -1.692235
15
Figure_S1-1_NaOtBu / electronic energy: -395.117378571 a.u. / lowest freq: 32.67 cm-1
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 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
 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
33
Figure_S1-1_PhOBpin / electronic energy: -717.466658936 a.u. / lowest freq: 34.04 cm-1
 B    0.316485   -0.649497    0.152442
 O    0.547339    0.656564   -0.167517
 O    1.450352   -1.390749    0.310010
 C    1.953393    0.765407   -0.475562
 C    2.556556   -0.464329    0.303349
 C    3.750402   -1.118973   -0.372082
 H    4.110941   -1.956020    0.242581
 H    3.490766   -1.511055   -1.363342
 H    4.572751   -0.396645   -0.481985
 C    2.881450   -0.142716    1.761241
 H    3.761317    0.510734    1.842022
 H    2.033939    0.348756    2.261363
 H    3.094875   -1.080566    2.293131
 C    2.090739    0.636050   -1.991454
 H    3.132712    0.771530   -2.312966
 H    1.476060    1.410062   -2.472261
 H    1.740869   -0.345498   -2.343688
 C    2.458430    2.121802   -0.012348
 H    1.979441    2.916387   -0.602078
 H    2.232209    2.298870    1.046507
 H    3.546064    2.197566   -0.158022
 H   -2.930733   -2.174758   -0.976580
 O   -0.912560   -1.220338    0.303715
 C   -3.126356   -1.200585   -0.524893
 C   -2.103803   -0.564658    0.181286
 C   -4.371635   -0.585968   -0.642680
 C   -2.327104    0.678308    0.778803
 C   -4.601602    0.659823   -0.057725
 H   -1.522715    1.166044    1.330768
 C   -3.575625    1.285149    0.651396
 H   -5.577031    1.140857   -0.152884
 H   -3.745791    2.258600    1.116820
 H   -5.168218   -1.087052   -1.197239
46
Figure_S1-1_(PhO)2BpinNa / electronic energy: -1186.36814498 a.u. / lowest freq: 13.97 cm-1
 B   -0.563220    0.044928   -0.178943
 O    0.291267    0.926614    0.688425
 C    1.283536    1.704672    0.236971
 C    1.570313    1.877919   -1.127640
 C    2.065408    2.387362    1.183443
 C    2.618259    2.709596   -1.518355
 H    0.968476    1.357829   -1.872206
 C    3.108859    3.216376    0.779645
 H    1.838595    2.254777    2.244585
 C    3.395857    3.384044   -0.576007
 H    2.826632    2.832602   -2.584305
 H    3.704622    3.736239    1.534259
 H    4.214297    4.033139   -0.893992
Na   -0.808966    0.523795    2.687870
 O   -1.401273    0.751365   -1.110868
 O   -1.477954   -0.585186    0.786000
 C   -2.750349    0.668453   -0.700149
 C   -2.762683   -0.634075    0.179234
 C   -3.835371   -0.661639    1.260867
 C   -2.856470   -1.909073   -0.666303
 C   -3.649998    0.599972   -1.930115
 C   -3.098822    1.925515    0.107771
 H   -3.332450   -0.201151   -2.609851
 H   -3.597144    1.551134   -2.480503
 H   -4.700038    0.428292   -1.646429
 H   -2.493507    1.994151    1.022809
 H   -4.162427    1.964752    0.386050
 H   -2.867924    2.809936   -0.503853
 H   -3.713572    0.159050    1.981888
 H   -3.788318   -1.612147    1.813558
 H   -4.838966   -0.577840    0.817054
 H   -2.121263   -1.893048   -1.482449
 H   -3.861061   -2.045468   -1.092990
 H   -2.632217   -2.773934   -0.024406
 H    1.663800   -2.361720   -2.479463
 C    1.156468   -1.758231   -0.480048
 C    1.868619   -2.528543   -1.419688
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 C    1.421837   -1.970396    0.885132
 C    2.803385   -3.473353   -1.010584
 C    2.361381   -2.920725    1.284246
 H    3.340044   -4.056682   -1.763421
 C    3.059848   -3.680848    0.347231
 H    2.547156   -3.067370    2.351610
 H    3.793490   -4.423052    0.668193
 O    0.272585   -0.884037   -0.951749
 H    0.889028   -1.388098    1.633642
51
Figure_S1-1_9d-Cu-allenyl / electronic energy: -2677.36469942 a.u. / lowest freq: 18.91 cm-1
 C   -0.949725   -2.111091   -0.745708
 H   -1.456710   -2.283710   -1.705397
 C    0.561005   -2.346837   -0.831595
 H    0.890390   -3.232260   -0.270668
 C    0.165570   -0.172304   -0.062012
 C    2.489588   -0.947618   -0.009125
 C    3.411595   -1.770382   -0.661262
 C    2.949352    0.031053    0.882181
 C    4.786704   -1.603717   -0.456366
 C    4.314605    0.217353    1.092648
 C    5.223765   -0.605927    0.415840
 H    6.296282   -0.467228    0.579491
Cu    0.319303    1.720856    0.321210
 N   -1.018985   -0.701736   -0.358187
 N    1.108117   -1.120853   -0.238640
 H   -1.611031    2.294197   -1.821534
 H    0.899252   -2.452084   -1.873899
 H   -1.438768   -2.738242    0.015197
 C   -2.263181    0.059952   -0.389790
 H   -2.079760    0.941851    0.244418
 C   -3.394832   -0.734034    0.234210
 C   -4.274734   -1.509681   -0.527751
 C   -3.538962   -0.723986    1.626854
 C   -5.279826   -2.255582    0.089569
 H   -4.183468   -1.543227   -1.615414
 C   -4.540821   -1.467687    2.245898
 H   -2.855877   -0.121511    2.231908
 C   -5.415255   -2.236764    1.476429
 H   -5.958977   -2.855647   -0.519831
 H   -4.643075   -1.444096    3.332974
 H   -6.203316   -2.819047    1.958824
 C   -2.550525    0.591965   -1.802286
 H   -3.536244    1.092393   -1.782965
 H   -2.627040   -0.245072   -2.514744
 O   -1.535632    1.430876   -2.265600
 C    4.800481    1.257189    2.068770
 H    4.053326    2.049530    2.216065
 H    5.002982    0.802287    3.051711
 H    5.735078    1.721832    1.723578
 C    5.770329   -2.464765   -1.205878
 H    6.734464   -2.524069   -0.682115
 H    5.386771   -3.485941   -1.343318
 H    5.962508   -2.048637   -2.207961
 H    3.073111   -2.542835   -1.353500
 H    2.231718    0.647662    1.427342
 C    0.056509    3.624341    0.493740
 H    0.571009    4.357231    1.130573
 C   -0.918418    4.038216   -0.261867
 C   -1.925600    4.342938   -1.074928
 H   -2.962524    4.334227   -0.721718
 H   -1.744517    4.692912   -2.096941
83
Figure_S1-1_PA-9d(Na)-ts(1,6major) / electronic energy: -3681.01674239 a.u. / lowest freq: -425.84 cm-1
 C    2.866803    2.675946    1.037241
 H    3.618483    3.073400    0.344267
 C    1.496643    3.345149    0.935558
 H    1.285729    4.038149    1.760640
 C    1.246966    1.039170    0.692392
 C   -0.796962    2.290790    1.180897
 C   -1.490484    3.438376    0.798338
 C   -1.479557    1.247321    1.820637
 C   -2.874586    3.531001    0.998245
 C   -2.851518    1.327151    2.045160
 C   -3.540848    2.470137    1.614215
 H   -4.618525    2.543255    1.788127
Cu    0.443095   -0.673683    0.087133
 N    2.545629    1.293601    0.660974
 N    0.593216    2.188102    0.972750
 C   -0.520351   -1.415746   -1.646627
 C    0.525645   -0.530428   -2.098307
Na    3.541048    1.559954   -2.683597
 H    1.377226    3.887276   -0.017588
 H    3.266719    2.708454    2.064537
 H   -0.293059   -2.477742   -1.765329
 C    0.359803    0.903986   -2.362672
 C    1.798868   -1.136899   -2.511518
 O   -0.906702    1.322018   -2.270671
 O    1.249489    1.695745   -2.636288
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 O    2.729106   -0.577606   -3.070754
 O    1.883062   -2.439152   -2.201216
 C    3.067140   -3.118499   -2.585350
 H    3.157940   -3.161586   -3.680079
 H    2.981622   -4.130150   -2.174801
 H    3.957585   -2.618517   -2.178973
 C   -1.154302    2.696016   -2.515703
 H   -0.506982    3.328730   -1.895213
 H   -2.204989    2.866151   -2.256610
 H   -0.981270    2.936927   -3.574367
 C    3.541140    0.255101    0.406446
 H    3.238270   -0.254293   -0.521579
 C    3.569791   -0.776710    1.510104
 C    3.338648   -0.440898    2.848798
 C    3.833792   -2.114224    1.194831
 C    3.358980   -1.418274    3.843111
 H    3.114557    0.593821    3.117691
 C    3.857616   -3.094769    2.184782
 H    4.001163   -2.392857    0.151635
 C    3.616254   -2.750116    3.514915
 H    3.167032   -1.139253    4.881685
 H    4.052018   -4.135263    1.915236
 H    3.623372   -3.516908    4.292376
 C    4.920609    0.898773    0.075156
 H    5.615125    0.019787   -0.011122
 H    5.252989    1.400160    1.029742
 O    4.871332    1.700685   -0.997615
 C   -1.825621   -1.113976   -1.224459
 H   -2.112915   -0.072661   -1.093273
 C   -2.736375   -2.126181   -0.917369
 H   -2.504266   -3.121690   -1.302082
 C   -4.180716   -1.862138   -0.728250
 C   -5.091188   -2.927133   -0.811338
 C   -4.686171   -0.577836   -0.471120
 C   -6.457825   -2.720791   -0.638977
 H   -4.716894   -3.934837   -1.011349
 C   -6.052175   -0.370517   -0.297835
 H   -4.007551    0.273745   -0.389597
 C   -6.945620   -1.439678   -0.379347
 H   -7.147072   -3.565407   -0.707643
 H   -6.421400    0.637572   -0.095148
 H   -8.016271   -1.274778   -0.241455
 C   -3.571403    0.223601    2.775210
 H   -2.873392   -0.563606    3.091738
 H   -4.079472    0.612349    3.670806
 H   -4.340469   -0.236372    2.136249
 C   -3.621699    4.751481    0.526618
 H   -4.614503    4.821204    0.991853
 H   -3.067914    5.673798    0.755415
 H   -3.766496    4.721037   -0.565435
 H   -0.962707    4.269764    0.326130
 H   -0.924754    0.375016    2.167759
 C    0.058354   -2.071084    1.498789
 H    0.887162   -2.110107    2.209329
 C   -1.081011   -2.617436    1.438593
 C   -2.349736   -2.995465    1.131882
 H   -2.536143   -4.018874    0.794614
 H   -3.176879   -2.515024    1.662542
51
Figure_S1-1_9d-Cu-allenyl / electronic energy: -2677.36469942 a.u. / lowest freq: 18.91 cm-1
 C   -0.949725   -2.111091   -0.745708
 H   -1.456710   -2.283710   -1.705397
 C    0.561005   -2.346837   -0.831595
 H    0.890390   -3.232260   -0.270668
 C    0.165570   -0.172304   -0.062012
 C    2.489588   -0.947618   -0.009125
 C    3.411595   -1.770382   -0.661262
 C    2.949352    0.031053    0.882181
 C    4.786704   -1.603717   -0.456366
 C    4.314605    0.217353    1.092648
 C    5.223765   -0.605927    0.415840
 H    6.296282   -0.467228    0.579491
Cu    0.319303    1.720856    0.321210
 N   -1.018985   -0.701736   -0.358187
 N    1.108117   -1.120853   -0.238640
 H   -1.611031    2.294197   -1.821534
 H    0.899252   -2.452084   -1.873899
 H   -1.438768   -2.738242    0.015197
 C   -2.263181    0.059952   -0.389790
 H   -2.079760    0.941851    0.244418
 C   -3.394832   -0.734034    0.234210
 C   -4.274734   -1.509681   -0.527751
 C   -3.538962   -0.723986    1.626854
 C   -5.279826   -2.255582    0.089569
 H   -4.183468   -1.543227   -1.615414
 C   -4.540821   -1.467687    2.245898
 H   -2.855877   -0.121511    2.231908
 C   -5.415255   -2.236764    1.476429
 H   -5.958977   -2.855647   -0.519831
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 H   -4.643075   -1.444096    3.332974
 H   -6.203316   -2.819047    1.958824
 C   -2.550525    0.591965   -1.802286
 H   -3.536244    1.092393   -1.782965
 H   -2.627040   -0.245072   -2.514744
 O   -1.535632    1.430876   -2.265600
 C    4.800481    1.257189    2.068770
 H    4.053326    2.049530    2.216065
 H    5.002982    0.802287    3.051711
 H    5.735078    1.721832    1.723578
 C    5.770329   -2.464765   -1.205878
 H    6.734464   -2.524069   -0.682115
 H    5.386771   -3.485941   -1.343318
 H    5.962508   -2.048637   -2.207961
 H    3.073111   -2.542835   -1.353500
 H    2.231718    0.647662    1.427342
 C    0.056509    3.624341    0.493740
 H    0.571009    4.357231    1.130573
 C   -0.918418    4.038216   -0.261867
 C   -1.925600    4.342938   -1.074928
 H   -2.962524    4.334227   -0.721718
 H   -1.744517    4.692912   -2.096941
83
Figure_S1-1_PA-9d(Na)-ts(1,6major) / electronic energy: -3681.01674239 a.u. / lowest freq: -425.84 cm-1
 C    2.866803    2.675946    1.037241
 H    3.618483    3.073400    0.344267
 C    1.496643    3.345149    0.935558
 H    1.285729    4.038149    1.760640
 C    1.246966    1.039170    0.692392
 C   -0.796962    2.290790    1.180897
 C   -1.490484    3.438376    0.798338
 C   -1.479557    1.247321    1.820637
 C   -2.874586    3.531001    0.998245
 C   -2.851518    1.327151    2.045160
 C   -3.540848    2.470137    1.614215
 H   -4.618525    2.543255    1.788127
Cu    0.443095   -0.673683    0.087133
 N    2.545629    1.293601    0.660974
 N    0.593216    2.188102    0.972750
 C   -0.520351   -1.415746   -1.646627
 C    0.525645   -0.530428   -2.098307
Na    3.541048    1.559954   -2.683597
 H    1.377226    3.887276   -0.017588
 H    3.266719    2.708454    2.064537
 H   -0.293059   -2.477742   -1.765329
 C    0.359803    0.903986   -2.362672
 C    1.798868   -1.136899   -2.511518
 O   -0.906702    1.322018   -2.270671
 O    1.249489    1.695745   -2.636288
 O    2.729106   -0.577606   -3.070754
 O    1.883062   -2.439152   -2.201216
 C    3.067140   -3.118499   -2.585350
 H    3.157940   -3.161586   -3.680079
 H    2.981622   -4.130150   -2.174801
 H    3.957585   -2.618517   -2.178973
 C   -1.154302    2.696016   -2.515703
 H   -0.506982    3.328730   -1.895213
 H   -2.204989    2.866151   -2.256610
 H   -0.981270    2.936927   -3.574367
 C    3.541140    0.255101    0.406446
 H    3.238270   -0.254293   -0.521579
 C    3.569791   -0.776710    1.510104
 C    3.338648   -0.440898    2.848798
 C    3.833792   -2.114224    1.194831
 C    3.358980   -1.418274    3.843111
 H    3.114557    0.593821    3.117691
 C    3.857616   -3.094769    2.184782
 H    4.001163   -2.392857    0.151635
 C    3.616254   -2.750116    3.514915
 H    3.167032   -1.139253    4.881685
 H    4.052018   -4.135263    1.915236
 H    3.623372   -3.516908    4.292376
 C    4.920609    0.898773    0.075156
 H    5.615125    0.019787   -0.011122
 H    5.252989    1.400160    1.029742
 O    4.871332    1.700685   -0.997615
 C   -1.825621   -1.113976   -1.224459
 H   -2.112915   -0.072661   -1.093273
 C   -2.736375   -2.126181   -0.917369
 H   -2.504266   -3.121690   -1.302082
 C   -4.180716   -1.862138   -0.728250
 C   -5.091188   -2.927133   -0.811338
 C   -4.686171   -0.577836   -0.471120
 C   -6.457825   -2.720791   -0.638977
 H   -4.716894   -3.934837   -1.011349
 C   -6.052175   -0.370517   -0.297835
 H   -4.007551    0.273745   -0.389597
 C   -6.945620   -1.439678   -0.379347
 H   -7.147072   -3.565407   -0.707643
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 H   -6.421400    0.637572   -0.095148
 H   -8.016271   -1.274778   -0.241455
 C   -3.571403    0.223601    2.775210
 H   -2.873392   -0.563606    3.091738
 H   -4.079472    0.612349    3.670806
 H   -4.340469   -0.236372    2.136249
 C   -3.621699    4.751481    0.526618
 H   -4.614503    4.821204    0.991853
 H   -3.067914    5.673798    0.755415
 H   -3.766496    4.721037   -0.565435
 H   -0.962707    4.269764    0.326130
 H   -0.924754    0.375016    2.167759
 C    0.058354   -2.071084    1.498789
 H    0.887162   -2.110107    2.209329
 C   -1.081011   -2.617436    1.438593
 C   -2.349736   -2.995465    1.131882
 H   -2.536143   -4.018874    0.794614
 H   -3.176879   -2.515024    1.662542
51
Figure_S1-1_9d-Cu-allenyl / electronic energy: -2677.36469942 a.u. / lowest freq: 18.91 cm-1
 C   -0.949725   -2.111091   -0.745708
 H   -1.456710   -2.283710   -1.705397
 C    0.561005   -2.346837   -0.831595
 H    0.890390   -3.232260   -0.270668
 C    0.165570   -0.172304   -0.062012
 C    2.489588   -0.947618   -0.009125
 C    3.411595   -1.770382   -0.661262
 C    2.949352    0.031053    0.882181
 C    4.786704   -1.603717   -0.456366
 C    4.314605    0.217353    1.092648
 C    5.223765   -0.605927    0.415840
 H    6.296282   -0.467228    0.579491
Cu    0.319303    1.720856    0.321210
 N   -1.018985   -0.701736   -0.358187
 N    1.108117   -1.120853   -0.238640
 H   -1.611031    2.294197   -1.821534
 H    0.899252   -2.452084   -1.873899
 H   -1.438768   -2.738242    0.015197
 C   -2.263181    0.059952   -0.389790
 H   -2.079760    0.941851    0.244418
 C   -3.394832   -0.734034    0.234210
 C   -4.274734   -1.509681   -0.527751
 C   -3.538962   -0.723986    1.626854
 C   -5.279826   -2.255582    0.089569
 H   -4.183468   -1.543227   -1.615414
 C   -4.540821   -1.467687    2.245898
 H   -2.855877   -0.121511    2.231908
 C   -5.415255   -2.236764    1.476429
 H   -5.958977   -2.855647   -0.519831
 H   -4.643075   -1.444096    3.332974
 H   -6.203316   -2.819047    1.958824
 C   -2.550525    0.591965   -1.802286
 H   -3.536244    1.092393   -1.782965
 H   -2.627040   -0.245072   -2.514744
 O   -1.535632    1.430876   -2.265600
 C    4.800481    1.257189    2.068770
 H    4.053326    2.049530    2.216065
 H    5.002982    0.802287    3.051711
 H    5.735078    1.721832    1.723578
 C    5.770329   -2.464765   -1.205878
 H    6.734464   -2.524069   -0.682115
 H    5.386771   -3.485941   -1.343318
 H    5.962508   -2.048637   -2.207961
 H    3.073111   -2.542835   -1.353500
 H    2.231718    0.647662    1.427342
 C    0.056509    3.624341    0.493740
 H    0.571009    4.357231    1.130573
 C   -0.918418    4.038216   -0.261867
 C   -1.925600    4.342938   -1.074928
 H   -2.962524    4.334227   -0.721718
 H   -1.744517    4.692912   -2.096941
96
Figure_S1-1_PA-9d(NaOPh)-ts(1,6major) / electronic energy: -3988.22213482 a.u. / lowest freq: -455.12 cm-1
 C   -3.327935   -0.170787   -1.529052
 H   -4.192691   -0.031508   -0.867769
 C   -2.662458    1.167411   -1.862437
 H   -2.655559    1.391704   -2.938936
 C   -1.099710   -0.222582   -0.802762
 C   -0.307353    1.984154   -1.521281
 C   -0.693752    3.326459   -1.474443
 C    1.035198    1.654344   -1.714125
 C    0.261227    4.341403   -1.568307
 C    2.003898    2.654658   -1.817377
 C    1.606037    3.992765   -1.733262
 H    2.359633    4.782000   -1.811087
Cu    0.589861   -0.977070   -0.055773
 N   -2.252470   -0.892686   -0.840558
 N   -1.286505    0.971906   -1.385249
 C    1.965462   -1.086241    1.563534
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 C    0.662027   -0.741864    2.082639
 H   -4.346931   -0.894357    1.133336
 H   -3.149871    1.996130   -1.333085
 H   -3.658809   -0.718542   -2.424534
 H    2.207410   -2.145612    1.676566
 C    0.156130    0.624372    2.257305
 C   -0.154870   -1.838740    2.621282
 O    0.994914    1.557152    1.797065
 O   -0.924652    0.939399    2.729923
 O   -1.159894   -1.740230    3.305429
 O    0.294497   -3.051590    2.257921
 C   -0.426588   -4.176792    2.732978
 H   -0.354837   -4.256153    3.826921
 H    0.033866   -5.051897    2.262414
 H   -1.487690   -4.108639    2.454327
 C    0.542522    2.902684    1.797709
 H   -0.423369    2.988225    1.282248
 H    1.301639    3.473870    1.251265
 H    0.442156    3.281767    2.824648
 C   -2.373061   -2.267514   -0.386333
 H   -1.685211   -2.369161    0.467484
 C   -1.937462   -3.280305   -1.436109
 C   -1.683413   -4.598887   -1.038105
 C   -1.742102   -2.940560   -2.777612
 C   -1.251371   -5.553514   -1.955278
 H   -1.807979   -4.881373    0.010719
 C   -1.310564   -3.895215   -3.700081
 H   -1.897914   -1.914732   -3.115175
 C   -1.064815   -5.205010   -3.293562
 H   -1.051187   -6.573748   -1.621048
 H   -1.159109   -3.607622   -4.742649
 H   -0.721669   -5.950079   -4.014199
 C   -3.778561   -2.558934    0.165904
 H   -3.812528   -3.629966    0.416967
 H   -4.528915   -2.408374   -0.633139
 O   -4.078303   -1.835000    1.314456
 C    3.032978   -0.282111    1.136206
 H    2.890660    0.791420    1.033708
 C    4.242865   -0.875850    0.766478
 H    4.381132   -1.910989    1.088387
 C    5.509869   -0.119045    0.623319
 C    6.721975   -0.824116    0.557491
 C    5.556988    1.282101    0.564712
 C    7.937097   -0.157824    0.422689
 H    6.708202   -1.916124    0.613352
 C    6.771171    1.950494    0.426032
 H    4.636864    1.864097    0.632769
 C    7.966812    1.235301    0.350907
 H    8.866906   -0.728969    0.374719
 H    6.782858    3.041911    0.380514
 H    8.917917    1.760896    0.242826
 C    3.438840    2.280829   -2.079289
 H    3.687790    1.316241   -1.615480
 H    3.621636    2.181143   -3.161356
 H    4.135300    3.039489   -1.695484
 C   -0.150970    5.784508   -1.437302
 H    0.455210    6.436575   -2.082376
 H   -1.209991    5.926549   -1.694249
 H   -0.013809    6.131473   -0.400079
 H   -1.741173    3.589623   -1.321334
 H    1.331896    0.608822   -1.811012
 C    1.564418   -1.991444   -1.528407
 H    0.834209   -2.419130   -2.217874
 C    2.826855   -1.914298   -1.540685
 C    4.141091   -1.648662   -1.309680
 H    4.813686   -2.478652   -1.076657
 H    4.601615   -0.814920   -1.849771
 O   -4.369248    0.677629    1.574864
Na   -2.871114   -0.291780    2.919350
 C   -4.435046    1.836235    0.998837
 C   -3.478783    2.858527    1.261779
 C   -5.450364    2.153186    0.052960
 C   -3.526907    4.085453    0.607708
 H   -2.682447    2.640935    1.979065
 C   -5.478837    3.380657   -0.603153
 H   -6.208769    1.393480   -0.157842
 C   -4.517069    4.362197   -0.341689
 H   -2.765505    4.839045    0.832557
 H   -6.268084    3.577275   -1.335127
 H   -4.544731    5.324404   -0.857420
51
Figure_S1-1_9d-Cu-allenyl / electronic energy: -2677.36469942 a.u. / lowest freq: 18.91 cm-1
 C   -0.949725   -2.111091   -0.745708
 H   -1.456710   -2.283710   -1.705397
 C    0.561005   -2.346837   -0.831595
 H    0.890390   -3.232260   -0.270668
 C    0.165570   -0.172304   -0.062012
 C    2.489588   -0.947618   -0.009125
 C    3.411595   -1.770382   -0.661262
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 C    2.949352    0.031053    0.882181
 C    4.786704   -1.603717   -0.456366
 C    4.314605    0.217353    1.092648
 C    5.223765   -0.605927    0.415840
 H    6.296282   -0.467228    0.579491
Cu    0.319303    1.720856    0.321210
 N   -1.018985   -0.701736   -0.358187
 N    1.108117   -1.120853   -0.238640
 H   -1.611031    2.294197   -1.821534
 H    0.899252   -2.452084   -1.873899
 H   -1.438768   -2.738242    0.015197
 C   -2.263181    0.059952   -0.389790
 H   -2.079760    0.941851    0.244418
 C   -3.394832   -0.734034    0.234210
 C   -4.274734   -1.509681   -0.527751
 C   -3.538962   -0.723986    1.626854
 C   -5.279826   -2.255582    0.089569
 H   -4.183468   -1.543227   -1.615414
 C   -4.540821   -1.467687    2.245898
 H   -2.855877   -0.121511    2.231908
 C   -5.415255   -2.236764    1.476429
 H   -5.958977   -2.855647   -0.519831
 H   -4.643075   -1.444096    3.332974
 H   -6.203316   -2.819047    1.958824
 C   -2.550525    0.591965   -1.802286
 H   -3.536244    1.092393   -1.782965
 H   -2.627040   -0.245072   -2.514744
 O   -1.535632    1.430876   -2.265600
 C    4.800481    1.257189    2.068770
 H    4.053326    2.049530    2.216065
 H    5.002982    0.802287    3.051711
 H    5.735078    1.721832    1.723578
 C    5.770329   -2.464765   -1.205878
 H    6.734464   -2.524069   -0.682115
 H    5.386771   -3.485941   -1.343318
 H    5.962508   -2.048637   -2.207961
 H    3.073111   -2.542835   -1.353500
 H    2.231718    0.647662    1.427342
 C    0.056509    3.624341    0.493740
 H    0.571009    4.357231    1.130573
 C   -0.918418    4.038216   -0.261867
 C   -1.925600    4.342938   -1.074928
 H   -2.962524    4.334227   -0.721718
 H   -1.744517    4.692912   -2.096941
83
Figure_S1-1_PA-9d-ts(1,6major) / electronic energy: -3519.31441637 a.u. / lowest freq: -439.92 cm-1
 C   -2.736778    2.980363   -0.100816
 H   -3.290936    3.283679    0.795415
 C   -1.325690    3.576136   -0.149421
 H   -1.204588    4.344022   -0.925176
 C   -1.184069    1.246358   -0.307451
 C    0.887946    2.481105   -0.706873
 C    1.678369    3.409484   -0.031224
 C    1.463842    1.634344   -1.660251
 C    3.057121    3.474558   -0.272037
 C    2.831896    1.686408   -1.919360
 C    3.616634    2.608887   -1.213322
 H    4.691530    2.657028   -1.411590
Cu   -0.444180   -0.604290   -0.219012
 N   -2.455482    1.544289   -0.059072
 N   -0.501014    2.398433   -0.448224
 C    0.435762   -1.900086    1.218416
 C   -0.632618   -1.219439    1.898582
 H   -3.184290    0.995915    2.637551
 H   -1.037244    4.013654    0.819465
 H   -3.325204    3.232437   -0.997558
 H    0.218940   -2.945195    0.984524
 C   -0.517462    0.086993    2.556672
 C   -1.904101   -1.944340    2.087930
 O    0.733423    0.574841    2.556386
 O   -1.424964    0.733899    3.049959
 O   -2.845490   -1.597053    2.769282
 O   -1.957551   -3.086945    1.367753
 C   -3.142634   -3.855330    1.487274
 H   -3.335951   -4.122765    2.535440
 H   -2.981264   -4.760066    0.891056
 H   -4.010171   -3.301152    1.099118
 C    0.907953    1.887994    3.057037
 H    0.235117    2.591313    2.546699
 H    1.951759    2.153360    2.854963
 H    0.707939    1.929800    4.137041
 C   -3.455591    0.510997    0.186955
 H   -2.900711   -0.299747    0.670800
 C   -4.041833   -0.044591   -1.094581
 C   -4.879407    0.718366   -1.916774
 C   -3.715293   -1.347158   -1.486729
 C   -5.374389    0.189689   -3.108165
 H   -5.151130    1.737819   -1.631291
 C   -4.211455   -1.879969   -2.676226
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 H   -3.057242   -1.949712   -0.853606
 C   -5.041715   -1.110684   -3.490551
 H   -6.024979    0.796875   -3.741363
 H   -3.946926   -2.899249   -2.966012
 H   -5.432321   -1.524624   -4.422711
 C   -4.511278    0.957082    1.201807
 H   -5.131194    0.064881    1.414832
 H   -5.184746    1.708522    0.755021
 O   -3.958882    1.517221    2.349744
 C    1.739897   -1.471776    0.916535
 H    2.024453   -0.441405    1.120700
 C    2.666245   -2.339930    0.327314
 H    2.472099   -3.408456    0.441140
 C    4.097715   -1.979969    0.209306
 C    5.064789   -2.992382    0.123656
 C    4.527600   -0.644509    0.167979
 C    6.418320   -2.683106    0.003386
 H    4.748429   -4.038722    0.151984
 C    5.879017   -0.334526    0.045129
 H    3.798470    0.167014    0.209303
 C    6.831970   -1.351384   -0.037876
 H    7.155027   -3.487132   -0.058777
 H    6.188947    0.712717    0.008848
 H    7.891900   -1.107581   -0.136669
 C    3.453643    0.784503   -2.952253
 H    2.718755    0.074429   -3.356039
 H    3.862651    1.368923   -3.790931
 H    4.286178    0.210218   -2.517492
 C    3.913745    4.435523    0.510591
 H    4.889948    4.588341    0.030316
 H    3.423661    5.414093    0.618524
 H    4.098158    4.049088    1.525977
 H    1.233087    4.080990    0.705571
 H    0.832392    0.935985   -2.209739
 C   -0.075076   -1.564201   -1.970953
 H   -0.883180   -1.376076   -2.679607
 C    1.038597   -2.156753   -2.060294
 C    2.286944   -2.654392   -1.852506
 H    2.428016   -3.737762   -1.801674
 H    3.137313   -2.087412   -2.242056
51
Figure_S1-1_9d-Cu-allenyl / electronic energy: -2677.36469942 a.u. / lowest freq: 18.91 cm-1
 C   -0.949725   -2.111091   -0.745708
 H   -1.456710   -2.283710   -1.705397
 C    0.561005   -2.346837   -0.831595
 H    0.890390   -3.232260   -0.270668
 C    0.165570   -0.172304   -0.062012
 C    2.489588   -0.947618   -0.009125
 C    3.411595   -1.770382   -0.661262
 C    2.949352    0.031053    0.882181
 C    4.786704   -1.603717   -0.456366
 C    4.314605    0.217353    1.092648
 C    5.223765   -0.605927    0.415840
 H    6.296282   -0.467228    0.579491
Cu    0.319303    1.720856    0.321210
 N   -1.018985   -0.701736   -0.358187
 N    1.108117   -1.120853   -0.238640
 H   -1.611031    2.294197   -1.821534
 H    0.899252   -2.452084   -1.873899
 H   -1.438768   -2.738242    0.015197
 C   -2.263181    0.059952   -0.389790
 H   -2.079760    0.941851    0.244418
 C   -3.394832   -0.734034    0.234210
 C   -4.274734   -1.509681   -0.527751
 C   -3.538962   -0.723986    1.626854
 C   -5.279826   -2.255582    0.089569
 H   -4.183468   -1.543227   -1.615414
 C   -4.540821   -1.467687    2.245898
 H   -2.855877   -0.121511    2.231908
 C   -5.415255   -2.236764    1.476429
 H   -5.958977   -2.855647   -0.519831
 H   -4.643075   -1.444096    3.332974
 H   -6.203316   -2.819047    1.958824
 C   -2.550525    0.591965   -1.802286
 H   -3.536244    1.092393   -1.782965
 H   -2.627040   -0.245072   -2.514744
 O   -1.535632    1.430876   -2.265600
 C    4.800481    1.257189    2.068770
 H    4.053326    2.049530    2.216065
 H    5.002982    0.802287    3.051711
 H    5.735078    1.721832    1.723578
 C    5.770329   -2.464765   -1.205878
 H    6.734464   -2.524069   -0.682115
 H    5.386771   -3.485941   -1.343318
 H    5.962508   -2.048637   -2.207961
 H    3.073111   -2.542835   -1.353500
 H    2.231718    0.647662    1.427342
 C    0.056509    3.624341    0.493740
 H    0.571009    4.357231    1.130573
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 C   -0.918418    4.038216   -0.261867
 C   -1.925600    4.342938   -1.074928
 H   -2.962524    4.334227   -0.721718
 H   -1.744517    4.692912   -2.096941
51
Figure_S1-1_9d-Cu-allenyl / electronic energy: -2677.36469942 a.u. / lowest freq: 18.91 cm-1
 C   -0.949725   -2.111091   -0.745708
 H   -1.456710   -2.283710   -1.705397
 C    0.561005   -2.346837   -0.831595
 H    0.890390   -3.232260   -0.270668
 C    0.165570   -0.172304   -0.062012
 C    2.489588   -0.947618   -0.009125
 C    3.411595   -1.770382   -0.661262
 C    2.949352    0.031053    0.882181
 C    4.786704   -1.603717   -0.456366
 C    4.314605    0.217353    1.092648
 C    5.223765   -0.605927    0.415840
 H    6.296282   -0.467228    0.579491
Cu    0.319303    1.720856    0.321210
 N   -1.018985   -0.701736   -0.358187
 N    1.108117   -1.120853   -0.238640
 H   -1.611031    2.294197   -1.821534
 H    0.899252   -2.452084   -1.873899
 H   -1.438768   -2.738242    0.015197
 C   -2.263181    0.059952   -0.389790
 H   -2.079760    0.941851    0.244418
 C   -3.394832   -0.734034    0.234210
 C   -4.274734   -1.509681   -0.527751
 C   -3.538962   -0.723986    1.626854
 C   -5.279826   -2.255582    0.089569
 H   -4.183468   -1.543227   -1.615414
 C   -4.540821   -1.467687    2.245898
 H   -2.855877   -0.121511    2.231908
 C   -5.415255   -2.236764    1.476429
 H   -5.958977   -2.855647   -0.519831
 H   -4.643075   -1.444096    3.332974
 H   -6.203316   -2.819047    1.958824
 C   -2.550525    0.591965   -1.802286
 H   -3.536244    1.092393   -1.782965
 H   -2.627040   -0.245072   -2.514744
 O   -1.535632    1.430876   -2.265600
 C    4.800481    1.257189    2.068770
 H    4.053326    2.049530    2.216065
 H    5.002982    0.802287    3.051711
 H    5.735078    1.721832    1.723578
 C    5.770329   -2.464765   -1.205878
 H    6.734464   -2.524069   -0.682115
 H    5.386771   -3.485941   -1.343318
 H    5.962508   -2.048637   -2.207961
 H    3.073111   -2.542835   -1.353500
 H    2.231718    0.647662    1.427342
 C    0.056509    3.624341    0.493740
 H    0.571009    4.357231    1.130573
 C   -0.918418    4.038216   -0.261867
 C   -1.925600    4.342938   -1.074928
 H   -2.962524    4.334227   -0.721718
 H   -1.744517    4.692912   -2.096941
116
Figure_S1-1_PA-9d(Naborate)-ts(1,6major) / electronic energy: -4398.56325172 a.u. / lowest freq: -433.67 cm-1
 H    5.797940    2.532949    0.596683
 H    6.963864    3.051104   -1.899424
 H    4.704182    2.588892   -1.456197
 H    9.243414    2.365363   -2.578522
 C    7.185485    1.992191   -2.058303
 C    4.820159    1.501774   -1.468964
 C    8.469503    1.607186   -2.439232
 C    6.169159    1.042761   -1.874278
 C    8.764441    0.259393   -2.641663
 H    9.770085   -0.046006   -2.938646
 C    6.480921   -0.310027   -2.079656
 C    7.763505   -0.696598   -2.459469
 H    5.717070   -1.074501   -1.933309
 H    7.983070   -1.755376   -2.614234
 H    2.438478    2.469411   -1.445404
 C    2.401070    1.384218   -1.570359
 C    3.656844    0.768668   -1.698867
 H    3.714699   -0.294662   -1.919598
Cu    1.507608    0.800125    0.251881
 H    2.320983    1.584188    2.613719
 C    2.816334    1.503532    1.645373
 C    4.036234    1.601539    1.319164
 C    5.249099    1.594260    0.710811
 H    5.864106    0.693390    0.802860
 N   -1.026655    0.400537    1.792347
 C    0.187997   -0.034738    1.493140
 N    0.505244   -1.020444    2.363082
 C   -1.679766    1.539683    1.163268
 O   -1.098164    1.745558   -2.486599
 C   -0.002847    1.892539   -1.972662
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 C    1.067162    0.888066   -1.849207
 C    0.755689   -0.473962   -2.291986
 O   -0.325745   -0.878846   -2.688079
Na   -2.439204   -0.111997   -2.458558
 C   -1.659965   -0.334294    2.892038
 H   -2.474603   -0.953758    2.485630
 C   -0.497912   -1.172478    3.423451
 H   -0.106956   -0.783907    4.377396
 C    1.709463   -1.750512    2.359546
 C    2.216392   -2.261967    3.557834
 C    2.402592   -1.972775    1.164723
 C    3.428201   -2.959665    3.579132
 C    3.622301   -2.650087    1.169806
 C    4.126227   -3.133691    2.381732
 H    5.082603   -3.664722    2.390182
 H   -0.759283   -2.231265    3.562096
 H   -2.057864    0.362722    3.643188
 O    1.789937   -1.322322   -2.201774
 O    0.325697    3.069818   -1.413527
 C   -0.638959    4.110192   -1.475433
 H   -1.559434    3.823064   -0.946855
 H   -0.182540    4.974211   -0.981411
 H   -0.884938    4.353105   -2.518214
 C    1.538111   -2.676445   -2.555045
 H    0.794126   -3.118315   -1.877999
 H    2.495572   -3.197444   -2.453929
 H    1.173497   -2.751001   -3.588143
 H   -1.107974    1.729853    0.247704
 C   -1.567424    2.770362    2.048398
 C   -2.580522    3.161824    2.929091
 C   -0.381326    3.515127    2.011813
 C   -2.408999    4.272196    3.758101
 H   -3.518394    2.604533    2.977122
 C   -0.207111    4.621762    2.838485
 H    0.414178    3.218507    1.322020
 C   -1.223161    5.002934    3.716930
 H   -3.209278    4.565736    4.440857
 H    0.725013    5.189431    2.795241
 H   -1.090477    5.870677    4.366709
 C   -3.102147    1.195727    0.726247
 H   -3.565954    2.126491    0.344385
 H   -3.711022    0.880817    1.592180
 O   -3.071367    0.214200   -0.250899
 C    4.369762   -2.887830   -0.115225
 H    5.448935   -2.721817    0.015765
 H    4.236634   -3.924519   -0.463539
 H    4.009647   -2.218049   -0.906763
 C    3.966447   -3.521524    4.869366
 H    5.054835   -3.382583    4.941202
 H    3.500524   -3.046144    5.743557
 H    3.770177   -4.603731    4.934819
 H    1.681928   -2.101669    4.495436
 H    1.987152   -1.622060    0.218058
 B   -3.955752   -0.968938   -0.157641
 O   -3.561335   -1.948622    0.837021
 O   -3.801069   -1.636254   -1.455632
 C   -2.944746   -3.043413    0.190100
 C   -3.614876   -3.023493   -1.233659
 C   -2.741031   -3.593031   -2.346054
 H   -3.280017   -3.546882   -3.304995
 H   -1.805361   -3.026327   -2.451580
 H   -2.492660   -4.647672   -2.150344
 C   -4.985543   -3.707657   -1.243293
 H   -4.900788   -4.800419   -1.148349
 H   -5.616383   -3.327717   -0.427397
 H   -5.487906   -3.481155   -2.195588
 C   -1.430980   -2.807110    0.117846
 H   -0.903506   -3.665260   -0.325062
 H   -1.042361   -2.669058    1.135456
 H   -1.191603   -1.904243   -0.461136
 C   -3.214393   -4.312965    0.990678
 H   -2.697577   -4.255947    1.960973
 H   -4.286877   -4.439776    1.186406
 H   -2.843171   -5.203759    0.460490
 H   -4.610150    1.252894   -1.676818
 O   -5.347213   -0.579939    0.160886
 C   -5.680666    1.082496   -1.571193
 C   -6.139906    0.144820   -0.625528
 C   -6.584975    1.809712   -2.344734
 C   -7.531013   -0.022198   -0.484538
 C   -7.960883    1.633784   -2.200219
 H   -7.887528   -0.748057    0.249610
 C   -8.424465    0.712031   -1.258077
 H   -8.661643    2.208738   -2.809070
 H   -9.498682    0.558890   -1.125271
 H   -6.201335    2.532592   -3.069896
96
Figure_S2-1_PA-9d(NaOPh)-prod(1,6major) / electronic energy: -3988.27463791 a.u. / lowest freq: 15.81 cm-1
 C   -3.069461   -0.943531   -1.551036
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H	-3.830375	-1.333363	-0.864874
C	-3.096060	0.583016	-1.602848
H	-3.494752	0.978567	-2.546818
C	-0.923421	-0.131742	-1.104049
C	-1.247854	2.274913	-1.407850
C	-2.155548	3.278848	-1.054115
C	0.078928	2.612526	-1.682110
C	-1.729656	4.601019	-0.911049
C	0.527833	3.926615	-1.532938
C	-0.384391	4.910537	-1.142188
H	-0.043819	5.943558	-1.026695
Cu	1.050643	-0.162533	-0.912653
N	-1.711949	-1.205864	-1.064845
N	-1.677050	0.930042	-1.455583
C	2.026921	-0.798391	1.142905
C	0.875185	-0.980829	1.995714
H	-3.572693	-2.558814	0.828612
H	-3.682783	0.996961	-0.772566
H	-3.219795	-1.400172	-2.542618
H	2.560321	-1.738597	0.969959
C	-0.065893	0.072636	2.296850
C	0.599378	-2.310886	2.487796
O	0.293232	1.260104	1.772223
O	-1.118223	-0.018442	2.924842
O	-0.355427	-2.675082	3.169031
O	1.517063	-3.234608	2.104283
C	1.268694	-4.576251	2.478831
H	1.192092	-4.679522	3.570356
H	2.120573	-5.157848	2.107983
H	0.338182	-4.949008	2.024589
C	-0.609766	2.339958	1.927419
H	-1.592940	2.095497	1.502689
H	-0.174117	3.182642	1.376685
H	-0.735020	2.601386	2.988240
C	-1.188009	-2.525621	-0.713197
H	-0.615876	-2.390227	0.215550
C	-0.234662	-3.054547	-1.766059
C	1.028570	-3.511855	-1.378364
C	-0.586532	-3.099123	-3.120157
C	1.928988	-3.999769	-2.325490
H	1.311609	-3.469209	-0.322807
C	0.311693	-3.588247	-4.067897
H	-1.565660	-2.738644	-3.444788
C	1.573331	-4.038408	-3.672545
H	2.915926	-4.343619	-2.008449
H	0.026631	-3.616908	-5.121908
H	2.278599	-4.414594	-4.416561
C	-2.290728	-3.541020	-0.380862
H	-1.793746	-4.521120	-0.317124
H	-3.008141	-3.610998	-1.221008
O	-2.925128	-3.312492	0.835938
C	2.617945	0.294840	0.550376
H	2.268614	1.305646	0.775116
C	3.966513	0.164182	-0.136447
H	4.208887	-0.908261	-0.202199
C	5.082556	0.846193	0.634462
C	6.194940	0.118841	1.069126
C	5.028576	2.216884	0.920081
C	7.229351	0.741642	1.769076
H	6.253401	-0.952308	0.857857
C	6.059129	2.843063	1.617942
H	4.167139	2.808031	0.598007
C	7.165380	2.106488	2.044634
H	8.089591	0.155352	2.100116
H	5.996910	3.912660	1.830441
H	7.974445	2.596150	2.591060
C	1.977881	4.253765	-1.776163
H	2.587342	3.971759	-0.901929
H	2.371506	3.705056	-2.644438
H	2.129635	5.327713	-1.949677
C	-2.696194	5.664165	-0.458192
H	-2.508601	6.621372	-0.965663
H	-3.737931	5.369396	-0.646169
H	-2.591985	5.842264	0.624247
H	-3.197268	3.033709	-0.842291
H	0.770306	1.849252	-2.041298
C	1.922994	-0.497929	-2.955311
H	1.243892	-1.009372	-3.619659
C	2.812610	0.047769	-2.320097
C	3.903154	0.695679	-1.586493
H	4.857478	0.529956	-2.110037
H	3.723092	1.783093	-1.580987
O	-4.276615	-1.306631	1.619256
Na	-2.460469	-1.871603	2.835282
C	-4.778897	-0.154461	1.305155
C	-4.246843	1.061117	1.824665
C	-5.870783	-0.025492	0.400897
C	-4.747181	2.300222	1.437479
H	-3.400112	0.993438	2.513177

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 C   -6.357621    1.221398    0.017739
 H   -6.310911   -0.941561   -0.004102
 C   -5.801066    2.401631    0.522013
 H   -4.295429    3.208997    1.847678
 H   -7.187454    1.274677   -0.693600
 H   -6.186364    3.377013    0.216946
96
Figure_S2-1_PA-9d(NaOPh)-ts(1,6major) / electronic energy: -3988.22213482 a.u. / lowest freq: -455.12 cm-1
 C   -3.327935   -0.170787   -1.529052
 H   -4.192691   -0.031508   -0.867769
 C   -2.662458    1.167411   -1.862437
 H   -2.655559    1.391704   -2.938936
 C   -1.099710   -0.222582   -0.802762
 C   -0.307353    1.984154   -1.521281
 C   -0.693752    3.326459   -1.474443
 C    1.035198    1.654344   -1.714125
 C    0.261227    4.341403   -1.568307
 C    2.003898    2.654658   -1.817377
 C    1.606037    3.992765   -1.733262
 H    2.359633    4.782000   -1.811087
Cu    0.589861   -0.977070   -0.055773
 N   -2.252470   -0.892686   -0.840558
 N   -1.286505    0.971906   -1.385249
 C    1.965462   -1.086241    1.563534
 C    0.662027   -0.741864    2.082639
 H   -4.346931   -0.894357    1.133336
 H   -3.149871    1.996130   -1.333085
 H   -3.658809   -0.718542   -2.424534
 H    2.207410   -2.145612    1.676566
 C    0.156130    0.624372    2.257305
 C   -0.154870   -1.838740    2.621282
 O    0.994914    1.557152    1.797065
 O   -0.924652    0.939399    2.729923
 O   -1.159894   -1.740230    3.305429
 O    0.294497   -3.051590    2.257921
 C   -0.426588   -4.176792    2.732978
 H   -0.354837   -4.256153    3.826921
 H    0.033866   -5.051897    2.262414
 H   -1.487690   -4.108639    2.454327
 C    0.542522    2.902684    1.797709
 H   -0.423369    2.988225    1.282248
 H    1.301639    3.473870    1.251265
 H    0.442156    3.281767    2.824648
 C   -2.373061   -2.267514   -0.386333
 H   -1.685211   -2.369161    0.467484
 C   -1.937462   -3.280305   -1.436109
 C   -1.683413   -4.598887   -1.038105
 C   -1.742102   -2.940560   -2.777612
 C   -1.251371   -5.553514   -1.955278
 H   -1.807979   -4.881373    0.010719
 C   -1.310564   -3.895215   -3.700081
 H   -1.897914   -1.914732   -3.115175
 C   -1.064815   -5.205010   -3.293562
 H   -1.051187   -6.573748   -1.621048
 H   -1.159109   -3.607622   -4.742649
 H   -0.721669   -5.950079   -4.014199
 C   -3.778561   -2.558934    0.165904
 H   -3.812528   -3.629966    0.416967
 H   -4.528915   -2.408374   -0.633139
 O   -4.078303   -1.835000    1.314456
 C    3.032978   -0.282111    1.136206
 H    2.890660    0.791420    1.033708
 C    4.242865   -0.875850    0.766478
 H    4.381132   -1.910989    1.088387
 C    5.509869   -0.119045    0.623319
 C    6.721975   -0.824116    0.557491
 C    5.556988    1.282101    0.564712
 C    7.937097   -0.157824    0.422689
 H    6.708202   -1.916124    0.613352
 C    6.771171    1.950494    0.426032
 H    4.636864    1.864097    0.632769
 C    7.966812    1.235301    0.350907
 H    8.866906   -0.728969    0.374719
 H    6.782858    3.041911    0.380514
 H    8.917917    1.760896    0.242826
 C    3.438840    2.280829   -2.079289
 H    3.687790    1.316241   -1.615480
 H    3.621636    2.181143   -3.161356
 H    4.135300    3.039489   -1.695484
 C   -0.150970    5.784508   -1.437302
 H    0.455210    6.436575   -2.082376
 H   -1.209991    5.926549   -1.694249
 H   -0.013809    6.131473   -0.400079
 H   -1.741173    3.589623   -1.321334
 H    1.331896    0.608822   -1.811012
 C    1.564418   -1.991444   -1.528407
 H    0.834209   -2.419130   -2.217874
 C    2.826855   -1.914298   -1.540685
 C    4.141091   -1.648662   -1.309680
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 H    4.813686   -2.478652   -1.076657
 H    4.601615   -0.814920   -1.849771
 O   -4.369248    0.677629    1.574864
Na   -2.871114   -0.291780    2.919350
 C   -4.435046    1.836235    0.998837
 C   -3.478783    2.858527    1.261779
 C   -5.450364    2.153186    0.052960
 C   -3.526907    4.085453    0.607708
 H   -2.682447    2.640935    1.979065
 C   -5.478837    3.380657   -0.603153
 H   -6.208769    1.393480   -0.157842
 C   -4.517069    4.362197   -0.341689
 H   -2.765505    4.839045    0.832557
 H   -6.268084    3.577275   -1.335127
 H   -4.544731    5.324404   -0.857420
96
Figure_S2-1_PA-9d(NaOPh)-pc(1,6major) / electronic energy: -3988.23491900 a.u. / lowest freq: 15.62 cm-1
 C    3.293820    0.253128   -1.512928
 H    4.151525    0.027802   -0.864619
 C    2.577367   -1.027974   -1.950113
 H    2.484453   -1.123997   -3.042171
 C    1.101323    0.287583   -0.692360
 C    0.246722   -1.865855   -1.495431
 C    0.625576   -3.199910   -1.658893
 C   -1.111793   -1.528291   -1.487882
 C   -0.340303   -4.206088   -1.765463
 C   -2.089463   -2.518154   -1.588517
 C   -1.690642   -3.853931   -1.720258
 H   -2.453078   -4.634494   -1.801099
Cu   -0.570661    1.021673    0.095918
 N    2.249671    0.957485   -0.762261
 N    1.243254   -0.872684   -1.353180
 C   -1.943542    1.083455    1.609587
 C   -0.715925    0.560844    2.113002
 H    4.159726    0.614190    1.279370
 H    3.085420   -1.918180   -1.558830
 H    3.645303    0.861331   -2.359565
 H   -2.096361    2.147597    1.798133
 C   -0.339091   -0.871923    2.215584
 C    0.200863    1.525651    2.780763
 O   -1.304975   -1.708456    1.856918
 O    0.755558   -1.277586    2.556329
 O    1.069199    1.253145    3.583895
 O   -0.019287    2.785561    2.399100
 C    0.804198    3.793134    2.974664
 H    0.643620    3.852446    4.059630
 H    0.508540    4.731263    2.494582
 H    1.864726    3.581375    2.779154
 C   -0.968277   -3.087862    1.756120
 H   -0.181161   -3.232432    1.002284
 H   -1.884487   -3.596013    1.438711
 H   -0.627878   -3.477413    2.724860
 C    2.426885    2.294452   -0.226878
 H    1.646093    2.414329    0.539974
 C    2.209212    3.384011   -1.270353
 C    2.322089    4.731044   -0.899581
 C    1.838873    3.087659   -2.585489
 C    2.091585    5.749414   -1.821782
 H    2.575574    4.996749    0.129400
 C    1.609437    4.105308   -3.511813
 H    1.697712    2.050898   -2.894075
 C    1.740100    5.440285   -3.136078
 H    2.183061    6.791957   -1.509271
 H    1.319698    3.848648   -4.533021
 H    1.559112    6.236984   -3.860642
 C    3.779876    2.413761    0.496384
 H    3.868533    3.437796    0.887601
 H    4.599190    2.292766   -0.237374
 O    3.896738    1.530977    1.564363
 C   -3.150421    0.358403    1.245144
 H   -3.102329   -0.727846    1.202850
 C   -4.294723    1.010348    0.954187
 H   -4.284206    2.105783    0.959150
 C   -5.585206    0.390757    0.628110
 C   -6.625140    1.195258    0.134726
 C   -5.832603   -0.981828    0.799531
 C   -7.859501    0.646280   -0.204932
 H   -6.456198    2.267915    0.008510
 C   -7.065207   -1.531383    0.461858
 H   -5.054970   -1.628496    1.210507
 C   -8.082964   -0.721135   -0.046310
 H   -8.651181    1.290624   -0.593293
 H   -7.236739   -2.600833    0.602502
 H   -9.049897   -1.155317   -0.309240
 C   -3.549729   -2.151005   -1.591534
 H   -3.703872   -1.096015   -1.324504
 H   -3.990993   -2.311332   -2.588175
 H   -4.116836   -2.776460   -0.886251
 C    0.083776   -5.647858   -1.871009
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 H   -0.648034   -6.243816   -2.434397
 H    1.062514   -5.744206   -2.361937
 H    0.174442   -6.098686   -0.869188
 H    1.680462   -3.473858   -1.670686
 H   -1.419467   -0.481175   -1.444504
 C   -1.464180    2.201522   -1.212601
 H   -0.874660    3.065326   -1.556361
 C   -2.609389    1.964938   -1.775932
 C   -3.773819    1.642490   -2.314607
 H   -4.716711    2.032074   -1.918749
 H   -3.831726    0.980195   -3.185093
 O    4.186868   -0.990639    1.509218
Na    2.769739   -0.215890    3.036467
 C    4.261298   -2.090344    0.826979
 C    3.290727   -3.122607    0.966387
 C    5.302707   -2.327780   -0.113515
 C    3.355700   -4.288289    0.210542
 H    2.467283   -2.961812    1.667905
 C    5.345941   -3.492671   -0.874863
 H    6.071247   -1.558043   -0.231529
 C    4.373724   -4.487574   -0.728133
 H    2.582905   -5.052329    0.341252
 H    6.155753   -3.628740   -1.598099
 H    4.413365   -5.401447   -1.324824
64
Figure_S2-1_9d(NaOPh)-Cu-allenyl / electronic energy: -3146.25617778 a.u. / lowest freq: 11.92 cm-1
Cu   -0.619467   -0.796156    0.827096
 C   -0.346515   -2.401130    1.871679
 C   -0.937222    0.741398   -0.321533
 N   -2.143873    1.194277   -0.727784
 N    0.001999    1.491143   -0.883402
 C    1.428889    1.329861   -0.605320
 C    0.000505   -3.552073    1.370637
 C    0.379012   -4.681143    0.783804
 C   -0.538280    2.590848   -1.682850
 H   -0.064878    2.614677   -2.671898
 C   -2.024791    2.234507   -1.754997
 H   -2.687930    3.081346   -1.533017
 C   -3.384438    0.644678   -0.341043
 C   -4.475496    0.689404   -1.214462
 C   -3.536012    0.067039    0.924065
 C   -5.702527    0.127497   -0.846977
 C   -4.745649   -0.518589    1.301216
 C   -5.819800   -0.481859    0.406051
 H   -6.774855   -0.927927    0.697213
 H    1.928082   -0.165857   -2.634416
 H   -2.295340    1.829362   -2.742745
 H   -0.361921    3.553497   -1.177043
 H    1.548128    0.269518   -0.343982
 C    1.868628    2.158545    0.586139
 C    2.053601    3.544278    0.504275
 C    2.081183    1.523956    1.815389
 C    2.431048    4.278172    1.628804
 H    1.910466    4.065296   -0.445429
 C    2.459838    2.254661    2.940604
 H    1.953127    0.439958    1.885623
 C    2.633553    3.635791    2.850098
 H    2.572759    5.358128    1.547429
 H    2.623645    1.742288    3.891151
 H    2.931610    4.210602    3.729810
 C    2.268177    1.568157   -1.865892
 H    3.322384    1.385089   -1.581130
 H    2.205771    2.626217   -2.173769
 O    1.853004    0.780671   -2.934328
 H   -0.497865   -2.385581    2.963745
 H    1.440706   -4.937140    0.691804
 H   -0.352724   -5.417789    0.434912
 O    2.095699   -1.595484   -1.830360
 C    3.222727   -1.564585   -1.170414
 C    4.447353   -1.226071   -1.804986
 C    3.281741   -1.828571    0.224015
 C    5.640423   -1.157639   -1.091733
 H    4.422841   -1.005951   -2.875978
 C    4.482514   -1.757915    0.926085
 H    2.350068   -2.074064    0.744595
 C    5.675802   -1.422792    0.280923
 H    6.562662   -0.890149   -1.616402
 H    4.483811   -1.961209    2.001267
 H    6.614856   -1.365732    0.835649
Na    0.382018   -2.891610   -1.448261
 C   -4.878061   -1.148536    2.663108
 H   -4.770153   -0.392767    3.456561
 H   -5.854279   -1.635792    2.789687
 H   -4.092521   -1.902634    2.823354
 C   -6.862411    0.151859   -1.808539
 H   -7.814286   -0.041059   -1.295092
 H   -6.937309    1.122263   -2.320462
 H   -6.741086   -0.619441   -2.586003
 H   -2.706191    0.090239    1.634257
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 H   -4.376491    1.152925   -2.197690
64
Figure_S2-1_9b(NaOPh)-Cu-allenyl / electronic energy: -3146.25183127 a.u. / lowest freq: 14.48 cm-1
Cu   -1.159994   -0.590393    1.249005
 C   -1.116318   -1.661983    2.858319
 C   -1.308620    0.472985   -0.363800
 N   -2.371853    0.399588   -1.177453
 N   -0.493582    1.418385   -0.819509
 C    0.814281    1.723428   -0.265472
 C   -0.596166   -2.849269    2.995372
 C   -0.025278   -4.043820    3.070053
 C   -0.945998    2.002813   -2.084278
 H   -0.272077    1.686950   -2.894296
 C   -2.351352    1.408165   -2.240987
 H   -3.149298    2.149610   -2.075173
 C   -3.440408   -0.525568   -0.997211
 C   -3.475273   -1.678430   -1.799498
 C   -4.415212   -0.266257   -0.018691
 C   -4.525858   -2.580829   -1.607528
 C   -5.446875   -1.195447    0.143691
 C   -5.503845   -2.341479   -0.645832
 H   -6.315317   -3.058967   -0.505594
 H    2.120613   -0.435489   -1.301376
 H   -2.511030    0.949494   -3.226320
 H   -0.945517    3.100865   -2.029370
 H    0.971060    0.976016    0.528978
 C    0.814478    3.104087    0.377621
 C    1.750663    4.094003    0.065960
 C   -0.169357    3.389740    1.334883
 C    1.702016    5.341374    0.693971
 H    2.532536    3.907255   -0.671765
 C   -0.220119    4.630799    1.961712
 H   -0.905210    2.621803    1.589754
 C    0.718062    5.614499    1.640496
 H    2.440976    6.102966    0.435574
 H   -0.993041    4.832638    2.706634
 H    0.680478    6.590470    2.129154
 C    1.902113    1.482826   -1.323653
 H    2.887379    1.589112   -0.831044
 H    1.848654    2.269951   -2.096199
 O    1.751113    0.246580   -1.937746
 H   -1.654416   -1.288009    3.746046
 H    0.986244   -4.167031    3.474573
 H   -0.566270   -4.953493    2.789462
 O    2.821164   -1.346953   -0.192222
 C    4.108122   -1.475818   -0.364930
 C    4.777182   -0.916478   -1.488893
 C    4.920292   -2.188977    0.557579
 C    6.149052   -1.066440   -1.667172
 H    4.175796   -0.369004   -2.219089
 C    6.291874   -2.333409    0.366447
 H    4.444043   -2.630613    1.438885
 C    6.926653   -1.775348   -0.746475
 H    6.622021   -0.621629   -2.548077
 H    6.877295   -2.893512    1.101940
 H    8.002320   -1.892512   -0.894117
Na    1.484647   -2.445468    1.154493
 H   -6.214114   -1.015553    0.900660
 H   -4.568838   -3.488419   -2.214687
 C   -4.327742    0.958995    0.851507
 H   -5.265653    1.121622    1.398270
 H   -3.517629    0.850456    1.591941
 H   -4.103510    1.862442    0.265913
 C   -2.409874   -1.938363   -2.830953
 H   -2.615164   -1.387375   -3.763086
 H   -1.418478   -1.620506   -2.477586
 H   -2.364271   -3.005637   -3.085514
96
Figure_S2-1_PA-9b(NaOPh)-pc(1,6major) / electronic energy: -3988.22941216 a.u. / lowest freq: 14.70 cm-1
 C    2.918428    0.420905   -1.662170
 H    3.868123    0.174580   -1.175603
 C    2.188022   -0.844614   -2.127559
 H    2.027338   -0.875028   -3.214989
 C    0.823876    0.326661   -0.624633
 C   -0.151144   -1.693501   -1.568349
 C   -0.026804   -2.950967   -0.952124
 C   -1.280877   -1.347236   -2.333127
 C   -1.101555   -3.840942   -1.055289
 C   -2.337908   -2.260666   -2.394975
 C   -2.254990   -3.492827   -1.752097
 H   -3.088052   -4.197087   -1.812611
Cu   -0.818412    0.904441    0.336177
 N    1.972906    0.998307   -0.699274
 N    0.901340   -0.740778   -1.426914
 C   -2.216186    0.586205    1.788860
 C   -0.972387    0.080499    2.255193
 H    4.094378    0.378963    1.043728
 H    2.726526   -1.756096   -1.828935
 H    3.116477    1.127725   -2.482248
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 H   -2.529509    1.565328    2.155556
 C   -0.633725   -1.364420    2.343800
 C   -0.052182    0.992626    2.976440
 O   -1.704131   -2.142837    2.428612
 O    0.493117   -1.817149    2.389568
 O    0.990214    0.673083    3.517777
 O   -0.463559    2.260071    2.953579
 C    0.377741    3.228555    3.567641
 H    0.481631    3.029241    4.642698
 H   -0.108644    4.195357    3.404919
 H    1.374956    3.223405    3.105600
 C   -1.489458   -3.541442    2.567148
 H   -0.940096   -3.936614    1.703998
 H   -2.484399   -3.994977    2.618899
 H   -0.926466   -3.754543    3.485980
 C    2.215438    2.242045    0.006819
 H    1.535509    2.228388    0.874453
 C    1.877881    3.477514   -0.818660
 C    1.965906    4.744444   -0.226597
 C    1.423918    3.392075   -2.138230
 C    1.626122    5.892837   -0.938084
 H    2.284018    4.840808    0.814514
 C    1.084661    4.540517   -2.854334
 H    1.297849    2.418658   -2.613928
 C    1.188465    5.795592   -2.259381
 H    1.697277    6.869249   -0.454093
 H    0.726194    4.447286   -3.881703
 H    0.919198    6.694742   -2.817605
 C    3.645656    2.274462    0.575487
 H    3.781021    3.237004    1.090486
 H    4.370734    2.269878   -0.260870
 O    3.888872    1.253377    1.487439
 C   -3.219172   -0.194983    1.090178
 H   -2.906697   -1.145296    0.652479
 C   -4.485505    0.240841    0.923198
 H   -4.775220    1.188100    1.385332
 C   -5.545493   -0.457932    0.184518
 C   -6.799537    0.157406    0.042015
 C   -5.357696   -1.723623   -0.397067
 C   -7.828579   -0.462985   -0.662638
 H   -6.961932    1.142975    0.485927
 C   -6.384392   -2.343675   -1.101996
 H   -4.396894   -2.232103   -0.302053
 C   -7.624663   -1.716471   -1.239797
 H   -8.794921    0.035802   -0.763944
 H   -6.216088   -3.326458   -1.548476
 H   -8.429745   -2.204997   -1.792982
 C   -1.694890    2.434236   -0.577680
 H   -0.979370    3.170245   -0.975220
 C   -2.959005    2.632897   -0.788133
 C   -4.261424    2.745565   -0.988778
 H   -4.904106    3.287279   -0.287321
 H   -4.737617    2.313290   -1.875067
 O    4.009507   -1.210934    0.838969
Na    2.505731   -0.700231    2.387720
 C    4.823163   -1.938583    0.133651
 C    5.881605   -1.364687   -0.623012
 C    4.696463   -3.352710    0.064344
 C    6.724963   -2.146158   -1.408731
 H    6.034910   -0.282617   -0.562024
 C    5.545666   -4.122575   -0.724404
 H    3.910057   -3.828057    0.655944
 C    6.565964   -3.532453   -1.477362
 H    7.526287   -1.661890   -1.974976
 H    5.409627   -5.208005   -0.751540
 H    7.228007   -4.141900   -2.096111
 C    1.239449   -3.361412   -0.253549
 H    1.038947   -4.092819    0.540841
 H    1.928887   -3.838377   -0.968948
 H    1.771922   -2.510363    0.190167
 C   -1.348209   -0.045644   -3.084206
 H   -1.594072    0.790448   -2.411991
 H   -0.384686    0.189681   -3.559711
 H   -2.119228   -0.090813   -3.864718
 H   -3.233201   -2.002090   -2.965481
 H   -1.025566   -4.824442   -0.584623
96
Figure_S2-1_PA-9b(NaOPh)-ts(1,6major) / electronic energy: -3988.21834759 a.u. / lowest freq: -441.84 cm-1
 C    2.922414    0.429802   -1.695778
 H    3.860551    0.219443   -1.172217
 C    2.236525   -0.867157   -2.138580
 H    2.104802   -0.937626   -3.228128
 C    0.803687    0.313433   -0.707976
 C   -0.086863   -1.763320   -1.622590
 C    0.049225   -2.992460   -0.954587
 C   -1.184815   -1.485804   -2.456696
 C   -0.982581   -3.928515   -1.084987
 C   -2.190373   -2.451526   -2.562200
 C   -2.098720   -3.657111   -1.870965
```

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 H   -2.895943   -4.398509   -1.959475
Cu   -0.823872    0.859921    0.284910
 N    1.936156    1.015424   -0.780295
 N    0.930242   -0.774923   -1.474145
 C   -2.204880    0.628600    1.847805
 C   -0.921242    0.176567    2.329538
 H    4.077180    0.564705    0.992854
 H    2.790138   -1.753458   -1.795804
 H    3.132125    1.111568   -2.533749
 H   -2.507817    1.623409    2.184343
 C   -0.546841   -1.239987    2.458831
 C   -0.031665    1.156508    2.958134
 O   -1.590857   -2.066677    2.386390
 O    0.580755   -1.669343    2.644655
 O    1.032929    0.932331    3.514633
 O   -0.483842    2.417118    2.845236
 C    0.324283    3.441986    3.400822
 H    0.421573    3.320535    4.488542
 H   -0.180740    4.385652    3.169340
 H    1.329525    3.432000    2.955675
 C   -1.345345   -3.453132    2.553836
 H   -0.637956   -3.820614    1.800685
 H   -2.314315   -3.948155    2.429703
 H   -0.941082   -3.657638    3.555114
 C    2.126148    2.287406   -0.107837
 H    1.467591    2.261116    0.775679
 C    1.708036    3.483835   -0.951465
 C    1.606399    4.742155   -0.343838
 C    1.369123    3.369512   -2.302922
 C    1.188186    5.855869   -1.068067
 H    1.835467    4.854126    0.719168
 C    0.953179    4.484373   -3.032581
 H    1.395613    2.396899   -2.795903
 C    0.863325    5.731873   -2.419552
 H    1.106210    6.824933   -0.571308
 H    0.690386    4.369611   -4.086295
 H    0.532116    6.603217   -2.988264
 C    3.561746    2.419386    0.431664
 H    3.650166    3.413057    0.896434
 H    4.272621    2.414195   -0.417198
 O    3.875870    1.462009    1.388460
 C   -3.155308   -0.100368    1.114443
 H   -2.888659   -1.086867    0.731842
 C   -4.415233    0.429156    0.820228
 H   -4.778472    1.214346    1.486097
 C   -5.472465   -0.394296    0.191487
 C   -6.822089   -0.124418    0.457978
 C   -5.162555   -1.443195   -0.688304
 C   -7.832602   -0.887518   -0.125885
 H   -7.082654    0.692768    1.136063
 C   -6.170352   -2.204162   -1.272758
 H   -4.120020   -1.657003   -0.931701
 C   -7.511333   -1.931460   -0.993155
 H   -8.878393   -0.665085    0.097958
 H   -5.905855   -3.013860   -1.957192
 H   -8.302268   -2.527931   -1.452967
 C   -1.737108    2.375541   -0.741870
 H   -0.974778    3.010437   -1.195899
 C   -2.998603    2.344286   -0.821026
 C   -4.314415    2.014075   -0.751116
 H   -5.004423    2.673653   -0.218062
 H   -4.747561    1.453889   -1.585663
 O    4.000986   -1.037809    0.898803
Na    2.528816   -0.462660    2.461997
 C    4.800380   -1.840980    0.264080
 C    5.836089   -1.361067   -0.584407
 C    4.679956   -3.253978    0.369114
 C    6.660905   -2.230265   -1.294378
 H    5.986997   -0.279601   -0.659401
 C    5.511410   -4.111757   -0.343643
 H    3.909763   -3.654591    1.033348
 C    6.507407   -3.615023   -1.191084
 H    7.442598   -1.816898   -1.938860
 H    5.380576   -5.192608   -0.234208
 H    7.155322   -4.292610   -1.751099
 C    1.292224   -3.319854   -0.175094
 H    1.100874   -4.089163    0.584691
 H    2.068210   -3.721131   -0.846549
 H    1.721990   -2.439705    0.321344
 C   -1.272830   -0.195750   -3.225584
 H   -1.548916    0.639870   -2.565194
 H   -0.308796    0.061131   -3.688869
 H   -2.030718   -0.266451   -4.017047
 H   -3.052668   -2.254308   -3.203920
 H   -0.901157   -4.887259   -0.566807
96
Figure_S2-1_PA-9b(NaOPh)-prod(1,6major) / electronic energy: -3988.26800024 a.u. / lowest freq: 17.09 cm-1
 C    2.949058    0.002568   -1.826749
 H    3.857467   -0.316183   -1.302978
```

C	2.113819	-1.204432	-2.276397
H	2.059629	-1.312994	-3.368661
C	0.809114	0.174009	-0.912652
C	-0.395982	-1.613777	-2.029143
C	-0.675263	-2.808601	-1.349778
C	-1.258946	-1.090977	-3.007862
C	-1.849308	-3.494268	-1.679089
C	-2.422785	-1.805035	-3.307951
C	-2.712288	-3.000603	-2.653521
H	-3.626708	-3.545544	-2.898136
Cu	-0.680895	0.744959	0.178418
N	2.034962	0.698932	-0.914936
N	0.793108	-0.890430	-1.717944
C	-1.866432	0.979191	1.872200
C	-0.618123	0.615525	2.546984
H	4.104879	0.235568	0.868922
H	2.500918	-2.142790	-1.848309
H	3.240572	0.655952	-2.664581
H	-2.143585	2.030708	1.995847
C	-0.248671	-0.747220	2.881128
C	0.274006	1.681310	2.952570
O	-1.219305	-1.641996	2.614626
O	0.808775	-1.128491	3.371153
O	1.388769	1.570884	3.454911
O	-0.214922	2.916209	2.690618
C	0.587551	4.016807	3.071097
H	0.638224	4.111782	4.165882
H	0.111737	4.906464	2.643110
H	1.612341	3.913366	2.686997
C	-0.991287	-2.981240	3.012911
H	-0.041347	-3.362593	2.615619
H	-1.828164	-3.563540	2.610519
H	-0.972580	-3.065990	4.109426
C	2.332885	1.973165	-0.281201
H	1.756983	1.993099	0.658460
C	1.882773	3.160949	-1.122577
C	1.781049	4.421100	-0.519696
C	1.531583	3.039805	-2.469976
C	1.339400	5.528646	-1.240866
H	2.030924	4.538034	0.537358
C	1.096596	4.147669	-3.198664
H	1.568449	2.068236	-2.963331
C	0.997003	5.395989	-2.587941
H	1.255457	6.498512	-0.746183
H	0.824035	4.026876	-4.249129
H	0.647277	6.261268	-3.154549
C	3.812016	2.079503	0.123335
H	3.974881	3.104199	0.489979
H	4.442864	1.973771	-0.781511
O	4.181711	1.200852	1.132543
C	-2.676094	0.232443	1.051128
H	-2.530008	-0.845721	0.957803
C	-3.908257	0.825249	0.397273
H	-4.223706	1.703886	0.981369
C	-5.059989	-0.161420	0.369918
C	-6.288445	0.147160	0.960987
C	-4.913741	-1.403506	-0.261509
C	-7.346524	-0.762925	0.926598
H	-6.419550	1.111809	1.458641
C	-5.967233	-2.313774	-0.298956
H	-3.963024	-1.667510	-0.731776
C	-7.189351	-1.996525	0.296697
H	-8.298008	-0.505976	1.397673
H	-5.831640	-3.277930	-0.794790
H	-8.015239	-2.710773	0.271039
C	-1.679537	3.176390	-1.048667
H	-0.899622	3.919133	-1.051348
C	-2.565609	2.349108	-1.071782
C	-3.617237	1.333729	-1.043149
H	-4.539975	1.749266	-1.478249
H	-3.314276	0.486322	-1.681412
O	3.685371	-1.278610	1.095283
Na	2.805606	-0.133025	2.824130
C	4.124129	-2.348731	0.509001
C	5.215467	-2.318319	-0.403970
C	3.530359	-3.621687	0.732012
C	5.643448	-3.463687	-1.070423
H	5.726352	-1.363979	-0.566053
C	3.968854	-4.759187	0.062018
H	2.703961	-3.681273	1.445492
C	5.023657	-4.697429	-0.854947
H	6.481505	-3.392120	-1.770435
H	3.475904	-5.716460	0.257501
H	5.361924	-5.593237	-1.379981
C	0.266927	-3.326269	-0.302446
H	-0.197049	-4.131056	0.282227
H	1.186883	-3.730185	-0.751971
H	0.581136	-2.526053	0.384119
C	-0.942948	0.211020	-3.693584

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 H   -0.947626    1.044784   -2.973877
 H    0.055388    0.188745   -4.157174
 H   -1.679614    0.431304   -4.477124
 H   -3.109772   -1.417129   -4.063931
 H   -2.087484   -4.425198   -1.159149
96
Figure_S2-1_PA-9d(NaOPh)-prod(1,6minor) / electronic energy: -3988.26945033 a.u. / lowest freq: 17.61 cm-1
 C    1.821528   -2.470637    1.900618
 H    2.286359   -3.265836    1.302161
 C    2.794874   -1.311499    2.147059
 H    2.987856   -1.132684    3.214913
 C    0.947579   -0.523059    0.956204
 C    2.658570    1.127020    1.537962
 C    3.992752    1.305530    1.905923
 C    1.902423    2.245703    1.156893
 C    4.586204    2.573245    1.860451
 C    2.469592    3.516299    1.117404
 C    3.820075    3.667883    1.461134
 H    4.276837    4.660805    1.422465
Cu   -0.298913    0.516049   -0.078056
 N    0.750919   -1.822363    1.143887
 N    2.095213   -0.163445    1.557070
 C   -1.643425    1.410087   -1.323096
 C   -0.745629    0.767106   -2.293712
 H    1.189978   -3.196476   -1.156696
 H    3.753318   -1.477206    1.634590
 H    1.435569   -2.913207    2.831829
 H   -1.559246    2.501229   -1.293365
 C    0.387877    1.535541   -2.783139
 C   -0.965255   -0.555931   -2.851481
 O    0.426216    2.794361   -2.295074
 O    1.284077    1.147634   -3.524946
 O   -0.354349   -1.077466   -3.775651
 O   -1.962019   -1.237494   -2.249792
 C   -2.172952   -2.573185   -2.683550
 H   -2.316072   -2.621677   -3.771131
 H   -3.083298   -2.914558   -2.176856
 H   -1.316562   -3.204727   -2.398834
 C    1.570856    3.566654   -2.607515
 H    2.466875    3.146809   -2.125448
 H    1.378782    4.570031   -2.212577
 H    1.737148    3.616396   -3.692152
 C   -0.436092   -2.501859    0.647847
 H   -0.741692   -1.954765   -0.258018
 C   -1.599425   -2.433860    1.628522
 C   -2.880064   -2.793542    1.187213
 C   -1.450281   -1.993325    2.945621
 C   -3.977169   -2.733982    2.043035
 H   -3.024504   -3.117698    0.153832
 C   -2.547370   -1.931569    3.806776
 H   -0.473698   -1.669304    3.307991
 C   -3.813599   -2.303854    3.361182
 H   -4.965931   -3.018954    1.676670
 H   -2.408179   -1.577984    4.830504
 H   -4.671982   -2.251514    4.034037
 C   -0.124805   -3.932920    0.189866
 H   -1.091516   -4.436565    0.022039
 H    0.351594   -4.477346    1.031684
 O    0.624487   -4.007882   -0.976320
 C   -2.486799    0.842984   -0.398084
 H   -2.703614   -0.227909   -0.426791
 C   -3.372192    1.658813    0.512344
 H   -3.091259    2.719941    0.424580
 C   -4.820150    1.519388    0.069515
 C   -5.493517    2.595585   -0.516215
 C   -5.499075    0.301661    0.210350
 C   -6.813428    2.463282   -0.950178
 H   -4.977286    3.551823   -0.637031
 C   -6.817037    0.166451   -0.220745
 H   -4.992223   -0.556398    0.659432
 C   -7.479991    1.247810   -0.803342
 H   -7.321734    3.316423   -1.405298
 H   -7.329446   -0.791054   -0.101969
 H   -8.512701    1.141410   -1.142709
 C   -0.886130    1.982409    3.082735
 H    0.052103    2.276288    3.517969
 C   -1.933274    1.638379    2.581902
 C   -3.213404    1.246868    1.995186
 H   -3.327060    0.155046    2.096486
 H   -4.025232    1.701901    2.585074
 O    2.075453   -1.971902   -1.677543
Na    1.897311   -1.049740   -3.711970
 C    3.279301   -1.850287   -1.202572
 C    3.928747   -0.586350   -1.140573
 C    4.023407   -2.967094   -0.727235
 C    5.220291   -0.455002   -0.640415
 H    3.372127    0.294751   -1.476530
 C    5.311130   -2.819832   -0.220563
 H    3.548737   -3.951523   -0.772940
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 C    5.928051   -1.564830   -0.168002
 H    5.677482    0.537899   -0.601664
 H    5.846944   -3.703358    0.139553
 H    6.938953   -1.454709    0.230334
 C    1.626825    4.712109    0.758290
 H    0.699044    4.411347    0.251900
 H    1.346906    5.274083    1.663794
 H    2.174818    5.404387    0.102528
 C    6.038518    2.724772    2.231380
 H    6.205246    2.463127    3.287811
 H    6.669501    2.054247    1.627809
 H    6.389587    3.754210    2.077578
 H    0.841666    2.139449    0.922503
 H    4.604792    0.450451    2.193158
96
Figure_S2-1_PA-9d(NaOPh)-ts(1,6minor) / electronic energy: -3988.21792967 a.u. / lowest freq: -450.44 cm-1
 C    2.947852   -1.853253    1.292620
 H    3.636009   -2.242294    0.530857
 C    3.291331   -0.408970    1.667599
 H    3.492434   -0.274941    2.740739
 C    1.121921   -0.476297    0.781732
 C    1.983263    1.727379    1.434222
 C    3.147647    2.496801    1.459914
 C    0.740052    2.361285    1.548608
 C    3.078034    3.892791    1.552925
 C    0.648625    3.748597    1.620576
 C    1.827043    4.506250    1.621827
 H    1.764113    5.596357    1.686889
Cu   -0.755762    0.011850    0.301166
 N    1.591961   -1.721432    0.749736
 N    2.072511    0.323670    1.296305
 C   -2.059354    1.038188   -1.066307
 C   -0.953404    0.439594   -1.774156
 H    2.968430   -2.887236   -1.454515
 H    4.157379   -0.048443    1.098707
 H    2.962229   -2.535511    2.155470
 H   -1.835292    2.036698   -0.674990
 C    0.240514    1.251315   -2.060058
 C   -1.025600   -0.884182   -2.404348
 O    0.109489    2.526422   -1.682795
 O    1.278087    0.851598   -2.563347
 O   -0.268341   -1.330817   -3.249899
 O   -2.023718   -1.641971   -1.926776
 C   -2.160949   -2.945326   -2.472590
 H   -2.346251   -2.899492   -3.554395
 H   -3.015918   -3.398966   -1.960268
 H   -1.252544   -3.539319   -2.295974
 C    1.264349    3.348333   -1.771322
 H    2.062027    2.967890   -1.116630
 H    0.953987    4.342508   -1.432833
 H    1.632659    3.395868   -2.805279
 C    0.782273   -2.850435    0.323874
 H    0.094406   -2.459963   -0.442337
 C   -0.073497   -3.427600    1.442287
 C   -1.147768   -4.259261    1.103237
 C    0.148552   -3.141701    2.791753
 C   -1.976139   -4.796735    2.084966
 H   -1.350812   -4.476581    0.051234
 C   -0.677987   -3.680511    3.778918
 H    0.956848   -2.470961    3.087892
 C   -1.741573   -4.510077    3.430303
 H   -2.813655   -5.435884    1.797175
 H   -0.490606   -3.442499    4.828196
 H   -2.392400   -4.925014    4.202740
 C    1.633016   -3.921768   -0.378528
 H    0.968934   -4.771779   -0.597040
 H    2.397865   -4.302802    0.324972
 O    2.185070   -3.486558   -1.577706
 C   -3.411297    0.676238   -1.013817
 H   -3.740212   -0.238365   -1.504379
 C   -4.309035    1.410480   -0.240619
 H   -3.959336    2.388635    0.103806
 C   -5.779080    1.312363   -0.402577
 C   -6.581030    2.409017   -0.054926
 C   -6.408837    0.155625   -0.888536
 C   -7.966706    2.360356   -0.199429
 H   -6.108584    3.315786    0.332444
 C   -7.792624    0.105451   -1.032280
 H   -5.813989   -0.722460   -1.149303
 C   -8.578608    1.207940   -0.690469
 H   -8.570623    3.228776    0.073451
 H   -8.262977   -0.803707   -1.413509
 H   -9.663826    1.165699   -0.805359
 C   -0.700495    4.415791    1.671096
 H   -0.952933    4.846097    0.688441
 H   -1.491391    3.699156    1.933822
 H   -0.717897    5.236896    2.402316
 C    4.349549    4.700826    1.543868
 H    4.153328    5.766504    1.723904
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 H     5.051977    4.344864    2.312389
 H     4.861295    4.609640    0.572872
 H     4.125428    2.022775    1.374119
 H    -0.175029    1.770787    1.607872
 C    -1.787100   -0.179647    2.036798
 H    -1.174648   -0.659549    2.801312
 C    -2.993111    0.208894    2.062094
 C    -4.257774    0.645955    1.828583
 H    -5.037649   -0.107471    1.686176
 H    -4.587903    1.585159    2.282960
 O     3.878431   -1.599328   -1.883493
Na     2.006085   -1.285180   -3.033121
 C     4.731029   -0.761716   -1.381871
 C     4.568302    0.645878   -1.526398
 C     5.865781   -1.190932   -0.638046
 C     5.465525    1.543087   -0.957652
 H     3.691963    1.009661   -2.070241
 C     6.747784   -0.279936   -0.062416
 H     6.023561   -2.266959   -0.519254
 C     6.561258    1.098359   -0.209630
 H     5.296666    2.616652   -1.086971
 H     7.601364   -0.653082    0.511686
 H     7.257897    1.809077    0.240241
96
Figure_S2-1_PA-9d(NaOPh)-pc(1,6minor) / electronic energy: -3988.23046303 a.u. / lowest freq: 12.68 cm-1
 C     2.268623   -1.899566    1.677184
 H     2.824407   -2.651307    1.103619
 C     3.051005   -0.589999    1.790238
 H     3.355654   -0.358139    2.820466
 C     0.962742   -0.160137    0.827340
 C     2.368685    1.787113    1.311018
 C     3.690929    2.218297    1.167526
 C     1.346753    2.727572    1.466236
 C     3.995427    3.583091    1.156787
 C     1.629416    4.094280    1.450716
 C     2.956128    4.508842    1.291533
 H     3.184934    5.578361    1.274914
Cu    -0.740384    0.704546    0.248976
 N     1.053907   -1.477155    0.974348
 N     2.080682    0.404946    1.314478
 C    -2.000759    1.414301   -1.198462
 C    -0.735253    1.084199   -1.774099
 H     2.092576   -2.846280   -1.098749
 H     3.945082   -0.604093    1.151622
 H     2.020899   -2.324084    2.661648
 H    -2.121451    2.471287   -0.948040
 C     0.280313    2.170808   -1.912757
 C    -0.431596   -0.168723   -2.513327
 O    -0.230426    3.383178   -1.726735
 O     1.460660    2.012735   -2.159249
 O     0.571197   -0.370273   -3.170105
 O    -1.373137   -1.102556   -2.401014
 C    -1.139285   -2.347877   -3.063310
 H    -1.021173   -2.190093   -4.143370
 H    -2.029435   -2.954712   -2.865327
 H    -0.239914   -2.830830   -2.652998
 C     0.664455    4.484411   -1.836365
 H     1.512935    4.363120   -1.150330
 H     0.083003    5.372872   -1.569665
 H     1.038067    4.571864   -2.865944
 C     0.021595   -2.381162    0.475083
 H    -0.387931   -1.894621   -0.418326
 C    -1.141510   -2.561726    1.432110
 C    -2.441004   -2.472123    0.921596
 C    -0.972653   -2.793123    2.799850
 C    -3.550211   -2.599108    1.753424
 H    -2.582078   -2.269055   -0.143296
 C    -2.080833   -2.917292    3.638095
 H     0.028713   -2.865210    3.228462
 C    -3.371686   -2.818276    3.118834
 H    -4.555280   -2.504059    1.335645
 H    -1.932953   -3.088425    4.706634
 H    -4.236762   -2.904849    3.779806
 C     0.621716   -3.700776   -0.023153
 H    -0.223497   -4.366651   -0.260109
 H     1.175088   -4.191157    0.804339
 O     1.390190   -3.557161   -1.173038
 C    -3.238709    0.660057   -1.230254
 H    -3.195103   -0.378540   -1.548517
 C    -4.410187    1.203500   -0.838371
 H    -4.429884    2.258723   -0.549698
 C    -5.703920    0.508437   -0.784684
 C    -6.863411    1.246399   -0.498918
 C    -5.834190   -0.876348   -0.988301
 C    -8.109147    0.628167   -0.418007
 H    -6.780106    2.323165   -0.330073
 C    -7.077635   -1.495501   -0.907183
 H    -4.951958   -1.483136   -1.202425
 C    -8.221779   -0.746942   -0.620808
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 H   -8.996887    1.222914   -0.191418
 H   -7.156013   -2.573511   -1.064881
 H   -9.195869   -1.235913   -0.553043
 C   -1.740749    0.915690    1.944395
 H   -1.116159    0.831671    2.846947
 C   -3.021751    1.032632    2.109470
 C   -4.337139    1.115540    2.200561
 H   -4.953718    0.211083    2.223090
 H   -4.850866    2.080343    2.258186
 O    3.274684   -1.721869   -1.218464
Na    2.675572    0.074441   -2.346865
 C    4.473073   -2.104930   -0.890542
 C    5.555293   -1.185201   -0.800313
 C    4.769447   -3.459100   -0.569697
 C    6.829678   -1.591846   -0.413633
 H    5.365422   -0.133280   -1.039708
 C    6.047940   -3.851161   -0.184127
 H    3.959262   -4.189857   -0.645924
 C    7.094050   -2.927281   -0.098016
 H    7.631795   -0.849965   -0.356401
 H    6.233187   -4.903607    0.050976
 H    8.094825   -3.242244    0.204992
 C    0.516765    5.092770    1.634263
 H   -0.423118    4.722163    1.200340
 H    0.334254    5.278090    2.704776
 H    0.760446    6.057599    1.167839
 C    5.424433    4.041880    1.025684
 H    5.895538    4.127914    2.018108
 H    6.024212    3.332669    0.437928
 H    5.486796    5.028585    0.545789
 H    0.319143    2.393807    1.622303
 H    4.495940    1.491000    1.046379
64
Figure_S2-1_9d(NaOPh)-Cu-allenyl / electronic energy: -3146.25617778 a.u. / lowest freq: 11.92 cm-1
Cu   -0.619467   -0.796156    0.827096
 C   -0.346515   -2.401130    1.871679
 C   -0.937222    0.741398   -0.321533
 N   -2.143873    1.194277   -0.727784
 N    0.001999    1.491143   -0.883402
 C    1.428889    1.329861   -0.605320
 C    0.000505   -3.552073    1.370637
 C    0.379012   -4.681143    0.783804
 C   -0.538280    2.590848   -1.682850
 H   -0.064878    2.614677   -2.671898
 C   -2.024791    2.234507   -1.754997
 H   -2.687930    3.081346   -1.533017
 C   -3.384438    0.644678   -0.341043
 C   -4.475496    0.689404   -1.214462
 C   -3.536012    0.067039    0.924065
 C   -5.702527    0.127497   -0.846977
 C   -4.745649   -0.518589    1.301216
 C   -5.819800   -0.481859    0.406051
 H   -6.774855   -0.927927    0.697213
 H    1.928082   -0.165857   -2.634416
 H   -2.295340    1.829362   -2.742745
 H   -0.361921    3.553497   -1.177043
 H    1.548128    0.269518   -0.343982
 C    1.868628    2.158545    0.586139
 C    2.053601    3.544278    0.504275
 C    2.081183    1.523956    1.815389
 C    2.431048    4.278172    1.628804
 H    1.910466    4.065296   -0.445429
 C    2.459838    2.254661    2.940604
 H    1.953127    0.439958    1.885623
 C    2.633553    3.635791    2.850098
 H    2.572759    5.358128    1.547429
 H    2.623645    1.742288    3.891151
 H    2.931610    4.210602    3.729810
 C    2.268177    1.568157   -1.865892
 H    3.322384    1.385089   -1.581130
 H    2.205771    2.626217   -2.173769
 O    1.853004    0.780671   -2.934328
 H   -0.497865   -2.385581    2.963745
 H    1.440706   -4.937140    0.691804
 H   -0.352724   -5.417789    0.434912
 O    2.095699   -1.595484   -1.830360
 C    3.222727   -1.564585   -1.170414
 C    4.447353   -1.226071   -1.804986
 C    3.281741   -1.828571    0.224015
 C    5.640423   -1.157639   -1.091733
 H    4.422841   -1.005951   -2.875978
 C    4.482514   -1.757915    0.926085
 H    2.350068   -2.074064    0.744595
 C    5.675802   -1.422792    0.280923
 H    6.562662   -0.890149   -1.616402
 H    4.483811   -1.961209    2.001267
 H    6.614856   -1.365732    0.835649
Na    0.382018   -2.891610   -1.448261
 C   -4.878061   -1.148536    2.663108
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 H   -4.770153   -0.392767    3.456561
 H   -5.854279   -1.635792    2.789687
 H   -4.092521   -1.902634    2.823354
 C   -6.862411    0.151859   -1.808539
 H   -7.814286   -0.041059   -1.295092
 H   -6.937309    1.122263   -2.320462
 H   -6.741086   -0.619441   -2.586003
 H   -2.706191    0.090239    1.634257
 H   -4.376491    1.152925   -2.197690
64
Figure_S2-1_9b(NaOPh)-Cu-allenyl / electronic energy: -3146.25183127 a.u. / lowest freq: 14.48 cm-1
Cu   -1.159994   -0.590393    1.249005
 C   -1.116318   -1.661983    2.858319
 C   -1.308620    0.472985   -0.363800
 N   -2.371853    0.399588   -1.177453
 N   -0.493582    1.418385   -0.819509
 C    0.814281    1.723428   -0.265472
 C   -0.596166   -2.849269    2.995372
 C   -0.025278   -4.043820    3.070053
 C   -0.945998    2.002813   -2.084278
 H   -0.272077    1.686950   -2.894296
 C   -2.351352    1.408165   -2.240987
 H   -3.149298    2.149610   -2.075173
 C   -3.440408   -0.525568   -0.997211
 C   -3.475273   -1.678430   -1.799498
 C   -4.415212   -0.266257   -0.018691
 C   -4.525858   -2.580829   -1.607528
 C   -5.446875   -1.195447    0.143691
 C   -5.503845   -2.341479   -0.645832
 H   -6.315317   -3.058967   -0.505594
 H    2.120613   -0.435489   -1.301376
 H   -2.511030    0.949494   -3.226320
 H   -0.945517    3.100865   -2.029370
 H    0.971060    0.976016    0.528978
 C    0.814478    3.104087    0.377621
 C    1.750663    4.094003    0.065960
 C   -0.169357    3.389740    1.334883
 C    1.702016    5.341374    0.693971
 H    2.532536    3.907255   -0.671765
 C   -0.220119    4.630799    1.961712
 H   -0.905210    2.621803    1.589754
 C    0.718062    5.614499    1.640496
 H    2.440976    6.102966    0.435574
 H   -0.993041    4.832638    2.706634
 H    0.680478    6.590470    2.129154
 C    1.902113    1.482826   -1.323653
 H    2.887379    1.589112   -0.831044
 H    1.848654    2.269951   -2.096199
 O    1.751113    0.246580   -1.937746
 H   -1.654416   -1.288009    3.746046
 H    0.986244   -4.167031    3.474573
 H   -0.566270   -4.953493    2.789462
 O    2.821164   -1.346953   -0.192222
 C    4.108122   -1.475818   -0.364930
 C    4.777182   -0.916478   -1.488893
 C    4.920292   -2.188977    0.557579
 C    6.149052   -1.066440   -1.667172
 H    4.175796   -0.369004   -2.219089
 C    6.291874   -2.333409    0.366447
 H    4.444043   -2.630613    1.438885
 C    6.926653   -1.775348   -0.746475
 H    6.622021   -0.621629   -2.548077
 H    6.877295   -2.893512    1.101940
 H    8.002320   -1.892512   -0.894117
Na    1.484647   -2.445468    1.154493
 H   -6.214114   -1.015553    0.900660
 H   -4.568838   -3.488419   -2.214687
 C   -4.327742    0.958995    0.851507
 H   -5.265653    1.121622    1.398270
 H   -3.517629    0.850456    1.591941
 H   -4.103510    1.862442    0.265913
 C   -2.409874   -1.938363   -2.830953
 H   -2.615164   -1.387375   -3.763086
 H   -1.418478   -1.620506   -2.477586
 H   -2.364271   -3.005637   -3.085514
96
Figure_S2-1_PA-9b(NaOPh)-pc(1,6minor) / electronic energy: -3988.23004284 a.u. / lowest freq: 13.92 cm-1
 C   -2.128192   -1.673600   -1.649696
 H   -2.794970   -2.374368   -1.129738
 C   -2.840536   -0.364051   -1.996836
 H   -3.004390   -0.234152   -3.075656
 C   -0.913413    0.108280   -0.758171
 C   -2.034454    2.027139   -1.781224
 C   -2.822977    2.844724   -0.959451
 C   -1.388651    2.524497   -2.930515
 C   -2.910608    4.206930   -1.278892
 C   -1.497466    3.888000   -3.208979
 C   -2.246943    4.726474   -2.383739
 H   -2.323687    5.791348   -2.614389
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Cu    0.655581    1.049814    0.015102
 N   -1.045644   -1.217452   -0.774629
 N   -1.900077    0.639817   -1.487388
 C    1.956266    1.497100    1.523873
 C    0.694920    1.178925    2.115626
 H   -2.225082   -2.077384    1.454321
 H   -3.810307   -0.271561   -1.482193
 H   -1.706301   -2.176345   -2.535678
 H    2.157885    2.561176    1.393696
 C   -0.292376    2.286212    2.261136
 C    0.402241   -0.053257    2.894912
 O    0.189999    3.456576    1.848857
 O   -1.435508    2.179409    2.664375
 O   -0.542667   -0.191916    3.646636
 O    1.301394   -1.017660    2.735230
 C    1.116522   -2.214921    3.490548
 H    1.200549   -2.002894    4.565191
 H    1.922568   -2.886879    3.176978
 H    0.132738   -2.644489    3.262316
 C   -0.697048    4.567024    1.827262
 H   -1.473266    4.418730    1.063836
 H   -0.084754    5.436227    1.566352
 H   -1.167087    4.711559    2.808866
 C   -0.083563   -2.132371   -0.176875
 H    0.486160   -1.526842    0.540534
 C    0.900685   -2.669768   -1.201685
 C    0.641144   -3.820057   -1.955730
 C    2.105602   -1.986592   -1.412695
 C    1.568197   -4.280862   -2.891617
 H   -0.291394   -4.371492   -1.816431
 C    3.035836   -2.448386   -2.341488
 H    2.322331   -1.072222   -0.851945
 C    2.769276   -3.599646   -3.083757
 H    1.350580   -5.181858   -3.469529
 H    3.973020   -1.904544   -2.477811
 H    3.497565   -3.964543   -3.811338
 C   -0.793137   -3.211796    0.646041
 H   -0.020316   -3.902315    1.021944
 H   -1.455134   -3.816138   -0.005970
 O   -1.481924   -2.689987    1.733236
 C    3.113015    0.627330    1.380067
 H    2.981953   -0.434299    1.576433
 C    4.309537    1.092366    0.967840
 H    4.428788    2.168740    0.803849
 C    5.502733    0.272116    0.718482
 C    6.752976    0.898003    0.596117
 C    5.440415   -1.124665    0.570957
 C    7.906421    0.155679    0.348741
 H    6.819205    1.984375    0.698403
 C    6.590485   -1.865483    0.320116
 H    4.477902   -1.637682    0.623696
 C    7.829584   -1.229615    0.210133
 H    8.869598    0.662700    0.258990
 H    6.518050   -2.948451    0.197889
 H    8.731039   -1.812554    0.009389
 C    1.718668    1.948489   -1.388048
 H    1.202894    2.815015   -1.830772
 C    2.871267    1.606817   -1.875844
 C    4.044178    1.205079   -2.336045
 H    4.982481    1.590754   -1.924299
 H    4.114967    0.478855   -3.152917
Na   -2.691032    0.223828    2.905612
 O   -3.470524   -1.061131    1.284859
 C   -4.543884   -1.618698    0.802828
 C   -4.644701   -3.028137    0.630868
 C   -5.671875   -0.854205    0.397907
 C   -5.778300   -3.615304    0.076187
 H   -3.803938   -3.645377    0.960023
 C   -6.799893   -1.455185   -0.154202
 H   -5.633215    0.230197    0.526700
 C   -6.869235   -2.840354   -0.327860
 H   -5.812215   -4.702762   -0.040662
 H   -7.643451   -0.827277   -0.456838
 H   -7.755519   -3.305828   -0.764104
 H   -0.993315    4.296498   -4.088073
 H   -3.518390    4.861634   -0.648572
 C   -3.583647    2.300483    0.218989
 H   -3.423623    1.223342    0.363622
 H   -3.284465    2.812762    1.145070
 H   -4.662354    2.471597    0.080289
 C   -0.615137    1.602605   -3.834400
 H   -0.131234    2.164530   -4.644249
 H    0.164770    1.061098   -3.279691
 H   -1.276849    0.851636   -4.293955
96
Figure_S2-1_PA-9b(NaOPh)-ts(1,6minor) / electronic energy: -3988.21330777 a.u. / lowest freq: -465.41 cm-1
 C   -2.703452    1.527561    1.353933
 H   -3.342978    1.905825    0.548817
 C   -3.155336    0.143503    1.821047
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H	-3.272644	0.071523	2.913922
C	-1.014417	-0.030756	0.881243
C	-2.102740	-2.123289	1.644653
C	-2.975158	-2.920971	0.883049
C	-1.370947	-2.661514	2.721948
C	-3.092329	-4.276835	1.209117
C	-1.500112	-4.026170	2.996819
C	-2.357832	-4.829913	2.251286
H	-2.457981	-5.891270	2.488351
Cu	0.859807	-0.558380	0.410665
N	-1.350496	1.261217	0.853276
N	-2.047049	-0.720818	1.386494
C	2.331979	-1.418163	-0.920109
C	1.048918	-1.306588	-1.572761
H	-2.438726	1.975637	-1.581425
H	-4.101670	-0.162762	1.352981
H	-2.688138	2.269838	2.164430
H	2.461082	-2.357793	-0.374127
C	0.147202	-2.468699	-1.550408
C	0.692124	-0.195381	-2.465502
O	0.702653	-3.542964	-0.980137
O	-1.000453	-2.506542	-1.968308
O	-0.228000	-0.181820	-3.267190
O	1.481597	0.873607	-2.320431
C	1.192088	2.009920	-3.130770
H	1.301819	1.762723	-4.195843
H	1.929614	2.768787	-2.846745
H	0.170278	2.362424	-2.931149
C	-0.107745	-4.698383	-0.833584
H	-1.000735	-4.474812	-0.236347
H	0.513163	-5.438721	-0.317822
H	-0.416811	-5.085609	-1.814710
C	-0.482404	2.304778	0.336006
H	0.254405	1.798385	-0.307085
C	0.293606	3.040450	1.418193
C	1.348131	3.878162	1.033349
C	0.033677	2.884306	2.781895
C	2.112520	4.551342	1.982683
H	1.588681	3.991999	-0.027258
C	0.796379	3.558260	3.737016
H	-0.752112	2.204916	3.116019
C	1.836308	4.396519	3.341790
H	2.934312	5.194253	1.659717
H	0.579539	3.416732	4.798059
H	2.436228	4.920867	4.088588
C	-1.263157	3.260334	-0.584936
H	-0.578174	4.072129	-0.874175
H	-2.076458	3.740584	-0.003726
O	-1.722358	2.655935	-1.746480
C	3.502782	-0.663839	-1.072041
H	3.490791	0.224788	-1.700418
C	4.646293	-0.980088	-0.337409
H	4.657466	-1.966834	0.134946
C	5.990060	-0.461868	-0.692620
C	7.125634	-1.216212	-0.365546
C	6.173511	0.771167	-1.338108
C	8.405143	-0.761858	-0.682127
H	7.001564	-2.176422	0.142453
C	7.450542	1.226768	-1.653352
H	5.308632	1.390169	-1.586721
C	8.573059	0.462274	-1.327830
H	9.275623	-1.367996	-0.420911
H	7.572271	2.189941	-2.154033
H	9.574174	0.822709	-1.574003
C	1.952881	0.073812	2.000379
H	1.299089	0.480418	2.772223
C	3.218731	0.050390	1.946370
C	4.535742	-0.023082	1.621950
H	5.032841	0.906130	1.328877
H	5.171147	-0.754209	2.131239
O	-3.569546	0.815804	-1.575626
Na	-2.323226	-0.706554	-2.549778
C	-4.803419	1.207097	-1.425874
C	-5.131349	2.570645	-1.189136
C	-5.893282	0.296363	-1.470665
C	-6.446899	2.980098	-0.989008
H	-4.318714	3.302700	-1.187844
C	-7.204161	0.719154	-1.269195
H	-5.682421	-0.757126	-1.671689
C	-7.500188	2.062491	-1.019664
H	-6.652998	4.039557	-0.809779
H	-8.012740	-0.016900	-1.308984
H	-8.530570	2.387595	-0.860949
C	-3.783597	-2.374056	-0.261061
H	-3.538461	-2.920323	-1.184349
H	-4.859107	-2.512488	-0.073296
H	-3.611323	-1.304644	-0.435043
C	-0.473954	-1.808441	3.575976
H	0.522893	-1.709706	3.121311

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 H   -0.871488   -0.791004    3.700403
 H   -0.345925   -2.256461    4.570381
 H   -0.935187   -4.456049    3.827526
 H   -3.766485   -4.905046    0.621477
96
Figure_S2-1_PA-9b(NaOPh)-prod(1,6minor) / electronic energy: -3988.27007628 a.u. / lowest freq: 22.13 cm-1
 C   -1.838505   -1.896047   -1.756205
 H   -2.543113   -2.556009   -1.234202
 C   -2.523032   -0.610976   -2.232664
 H   -2.611068   -0.544169   -3.326279
 C   -0.704229   -0.056835   -0.872513
 C   -1.798377    1.808220   -2.007663
 C   -2.569567    2.614222   -1.158134
 C   -1.178098    2.319784   -3.162404
 C   -2.706461    3.969876   -1.486444
 C   -1.356067    3.670445   -3.465816
 C   -2.113781    4.492005   -2.631537
 H   -2.240595    5.548845   -2.876077
Cu    0.539189    0.962392    0.195761
 N   -0.811616   -1.385493   -0.842576
 N   -1.625903    0.425757   -1.711311
 C    1.773970    1.572949    1.755357
 C    0.549606    1.215626    2.479977
 H   -2.127055   -2.327875    1.252199
 H   -3.527294   -0.493834   -1.793870
 H   -1.370648   -2.462610   -2.578414
 H    1.942138    2.651634    1.688543
 C   -0.447461    2.251077    2.684755
 C    0.313927   -0.086492    3.077370
 O   -0.022005    3.477590    2.315052
 O   -1.594307    2.104219    3.100705
 O   -0.679033   -0.438659    3.703881
 O    1.332713   -0.946831    2.901028
 C    1.170746   -2.248013    3.450052
 H    1.136726   -2.204926    4.548214
 H    2.050201   -2.818380    3.128832
 H    0.245502   -2.706515    3.073978
 C   -0.962209    4.533948    2.348720
 H   -1.747603    4.386778    1.591525
 H   -0.402906    5.447546    2.117529
 H   -1.433415    4.621910    3.337086
 C    0.127955   -2.246619   -0.147964
 H    0.538170   -1.640048    0.674896
 C    1.301857   -2.661208   -1.032264
 C    2.239329   -3.597456   -0.574213
 C    1.520100   -2.069262   -2.282246
 C    3.341034   -3.950716   -1.351310
 H    2.122601   -4.056928    0.409233
 C    2.626457   -2.415263   -3.059154
 H    0.823151   -1.320283   -2.661058
 C    3.538594   -3.363208   -2.600594
 H    4.054712   -4.685283   -0.971709
 H    2.772743   -1.937309   -4.030211
 H    4.404119   -3.635906   -3.208084
 C   -0.613554   -3.417907    0.511796
 H    0.130443   -4.101590    0.945373
 H   -1.140785   -4.000985   -0.271084
 O   -1.456852   -3.014995    1.537894
 C    2.650363    0.781706    1.056011
 H    2.630216   -0.305282    1.152478
 C    3.771589    1.393463    0.239171
 H    4.067208    2.344085    0.710084
 C    4.991719    0.495417    0.185902
 C    6.228496    0.936495    0.665638
 C    4.902070   -0.796406   -0.349997
 C    7.352096    0.109737    0.615085
 H    6.314379    1.940360    1.090382
 C    6.022138   -1.623113   -0.403838
 H    3.945745   -1.169191   -0.729208
 C    7.252092   -1.172947    0.078931
 H    8.308673    0.471854    0.998922
 H    5.929329   -2.625688   -0.827033
 H    8.129425   -1.822443    0.038496
 C    1.149077    3.320716   -1.149669
 H    0.275200    3.949499   -1.123653
 C    2.134156    2.616275   -1.216295
 C    3.309348    1.745426   -1.206671
 H    4.136374    2.233237   -1.746700
 H    3.070033    0.817728   -1.753384
Na   -2.710183    0.052202    2.796363
 O   -3.326091   -1.230985    1.081231
 C   -4.413554   -1.717160    0.555333
 C   -4.571256   -3.110795    0.308828
 C   -5.504242   -0.886658    0.175782
 C   -5.721534   -3.620830   -0.286097
 H   -3.762603   -3.779347    0.617080
 C   -6.648901   -1.411212   -0.418659
 H   -5.425600    0.187508    0.360130
 C   -6.774157   -2.781625   -0.662674
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 H   -5.800162   -4.699002   -0.455601
 H   -7.461261   -0.733350   -0.697983
 H   -7.673991   -3.187596   -1.129615
 H   -0.879503    4.087415   -4.356005
 H   -3.303260    4.615928   -0.837313
 C   -3.216483    2.066199    0.082968
 H   -3.239259    0.968390    0.103479
 H   -2.673068    2.394555    0.982801
 H   -4.246183    2.441535    0.177614
 C   -0.286019    1.443407   -3.997464
 H    0.061731    1.973370   -4.893655
 H    0.599143    1.145924   -3.411703
 H   -0.791204    0.520818   -4.319326
121
Figure_S3-1_AA-9d(NaOPh)-prod(1,6major) / electronic energy: -4439.10399315 a.u. / lowest freq: 15.52 cm-1
 H    1.745022    3.046511   -3.349345
 H    0.490706    1.002296   -3.163602
 C    2.554172    2.112788   -1.557677
 C    1.134413    0.286066   -2.642912
 H    3.588725    2.241020   -1.921206
 C    2.174286    0.667160   -1.843647
 H    1.001980   -0.765112   -2.911212
 B    3.117203   -0.465489   -1.297933
 O    2.754485   -1.779265   -1.247926
 H    5.244427   -1.818743   -2.801013
 O    4.379438   -0.238108   -0.836578
 H    6.587384   -0.959100   -2.009696
 C    5.863992   -1.778520   -1.893238
 H    4.169721   -3.771597   -2.249130
 C    5.016001   -1.520610   -0.649324
 C    3.782297   -2.494736   -0.527418
 C    3.982217   -3.856479   -1.171527
 H    6.420730   -2.721849   -1.808131
 H    3.079587   -4.465761   -1.030527
 H    3.075141   -1.694212    1.383689
 H    2.359494   -3.247079    0.898002
 C    3.288972   -2.661713    0.907120
 H    6.718111   -0.742852    0.417642
 C    5.897668   -1.454624    0.587000
 H    5.334856   -1.122855    1.468555
 H    4.830229   -4.379226   -0.704738
 H    4.022043   -3.204437    1.520003
 H    6.337933   -2.440141    0.798427
 H    1.985405    4.163213   -1.986594
 C    1.676140    3.143177   -2.255827
 H    0.618183    3.026704   -1.978606
 C   -2.696149   -2.596571   -0.805801
 H   -3.321053   -2.744372    0.088315
 C   -3.245632   -1.501532   -1.718668
 H   -3.192180   -1.792130   -2.780062
 C   -1.239725   -0.767429   -0.753173
 C   -2.519639    0.892190   -2.007373
 C   -2.001824    2.025826   -1.366445
 C   -3.244913    1.037109   -3.188923
 C   -2.151111    3.289489   -1.935104
 C   -3.428767    2.302164   -3.761774
 C   -2.864772    3.412932   -3.135376
 H   -2.993135    4.403323   -3.581546
Cu    0.413935    0.311131   -0.541032
 N   -1.393159   -2.046811   -0.421643
 N   -2.326653   -0.388020   -1.453307
 C    1.125528    1.060757    1.646386
 C    0.095143    0.803376    2.617943
 H   -2.422876   -2.070384    2.112661
 H   -4.278270   -1.216510   -1.475806
 H   -2.574225   -3.561427   -1.317650
 H    2.024875    0.459185    1.820340
 C   -1.102927    1.589015    2.764070
 C    0.294744   -0.289863    3.548542
 O   -1.153732    2.681276    1.961336
 O   -2.050949    1.365924    3.513882
 O   -0.364484   -0.546739    4.549974
 O    1.358131   -1.070369    3.238681
 C    1.620705   -2.153634    4.105538
 H    1.844582   -1.807793    5.125274
 H    2.492623   -2.672678    3.690448
 H    0.761934   -2.839023    4.148879
 C   -2.289227    3.517709    2.103112
 H   -3.191067    3.035523    1.697144
 H   -2.071329    4.429281    1.536952
 H   -2.468436    3.766033    3.157531
 C   -0.405592   -2.848782    0.271975
 H    0.429203   -2.161557    0.487424
 C    0.106054   -3.973923   -0.621543
 C    0.433199   -5.237795   -0.117131
 C    0.276319   -3.744899   -1.992374
 C    0.910278   -6.243322   -0.960720
 H    0.318469   -5.460461    0.944354
 C    0.748671   -4.744967   -2.836875
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 H    0.030235   -2.764675   -2.404100
 C    1.066990   -6.002940   -2.323326
 H    1.155433   -7.222457   -0.543740
 H    0.873081   -4.540415   -3.902407
 H    1.436548   -6.790210   -2.983727
 C   -0.961482   -3.328270    1.621732
 H   -0.134251   -3.785609    2.187158
 H   -1.710790   -4.126250    1.451603
 O   -1.478034   -2.282249    2.366187
 C    1.241454    1.960772    0.607596
 H    0.434346    2.673290    0.436076
 C    2.586125    2.284334   -0.011498
 H    3.306989    1.538839    0.358517
 C    3.142384    3.641561    0.395065
 C    4.493770    3.918176    0.140980
 C    2.368172    4.636024    1.001864
 C    5.051683    5.151498    0.467492
 H    5.120488    3.145648   -0.314383
 C    2.923191    5.875169    1.329618
 H    1.319741    4.443058    1.237127
 C    4.264367    6.140023    1.061441
 H    6.108246    5.340870    0.263835
 H    2.298977    6.636698    1.803088
 H    4.698445    7.108600    1.319188
 C   -4.208387    2.437319   -5.043787
 H   -3.684165    1.945658   -5.878226
 H   -5.196207    1.960479   -4.954943
 H   -4.359873    3.491318   -5.313259
 C   -1.586238    4.515516   -1.266281
 H   -0.878724    4.252453   -0.468340
 H   -1.057436    5.151473   -1.991365
 H   -2.388388    5.125487   -0.821751
 H   -1.516713    1.919262   -0.394670
 H   -3.675642    0.164497   -3.682449
 O   -3.919748   -1.599218    2.322942
Na   -2.618894   -0.793222    4.046991
 C   -4.651103   -0.939401    1.470576
 C   -4.291409    0.354244    1.005846
 C   -5.851040   -1.485090    0.936781
 C   -5.074456    1.048413    0.089473
 H   -3.363454    0.788631    1.383904
 C   -6.625767   -0.784070    0.015578
 H   -6.151014   -2.482407    1.271699
 C   -6.250391    0.490506   -0.421251
 H   -4.749549    2.036864   -0.249373
 H   -7.540625   -1.242552   -0.372345
 H   -6.859250    1.036680   -1.144941
121
Figure_S3-1_AA-9d(NaOPh)-ts(1,6major) / electronic energy: -4439.05034678 a.u. / lowest freq: -323.92 cm-1
 H    1.531852    2.790146   -2.844247
 H    0.412404    0.668919   -2.120806
 C    2.797337    1.816802   -1.391465
 C    1.106764    0.026893   -1.562237
 H    3.863212    2.053348   -1.431478
 C    2.443015    0.473043   -1.394451
 H    0.980905   -1.042579   -1.772976
 B    3.549881   -0.575461   -1.074372
 O    3.441876   -1.912723   -1.338260
 H    5.931808   -1.231726   -2.662388
 O    4.741925   -0.257658   -0.472719
 H    7.060334   -0.324564   -1.628083
 C    6.504967   -1.268332   -1.724530
 H    5.229237   -3.418982   -2.572010
 C    5.584466   -1.424315   -0.514875
 C    4.533680   -2.583052   -0.684149
 C    5.003175   -3.742626   -1.548148
 H    7.229857   -2.091893   -1.788292
 H    4.215154   -4.506333   -1.598906
 H    3.651512   -2.278459    1.288468
 H    3.127599   -3.747121    0.434681
 C    3.993170   -3.103209    0.645751
 H    7.113959   -0.653716    0.796776
 C    6.403413   -1.492079    0.764517
 H    5.765500   -1.434395    1.655594
 H    5.903640   -4.204201   -1.116173
 H    4.745148   -3.690144    1.191751
 H    6.978935   -2.428896    0.803870
 H    2.263621    3.895688   -1.653947
 C    1.835048    2.893134   -1.787389
 H    0.911582    2.826075   -1.190317
 C   -3.316186   -2.155874   -1.398300
 H   -4.156754   -2.422195   -0.742036
 C   -3.526707   -0.799318   -2.066112
 H   -3.326121   -0.836908   -3.148082
 C   -1.704143   -0.654114   -0.602983
 C   -2.484833    1.435382   -1.641874
 C   -1.809491    2.309622   -0.779549
 C   -3.152709    1.955574   -2.751481
 C   -1.767565    3.677195   -1.042649
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 C   -3.141830    3.329489   -3.019984
 C   -2.438441    4.176874   -2.166502
 H   -2.413719    5.251094   -2.370520
Cu    0.006515   -0.027793    0.205264
 N   -2.104610   -1.925704   -0.604990
 N   -2.531322    0.048634   -1.397788
 C    1.290145    0.606135    1.703137
 C    0.072517    0.119888    2.333086
 H   -3.772351   -2.876610    1.379068
 H   -4.536850   -0.400204   -1.902121
 H   -3.165656   -2.967768   -2.123805
 H    2.089341   -0.139005    1.673567
 C   -1.064345    0.956159    2.742909
 C    0.072792   -1.253207    2.856704
 O   -0.865063    2.269668    2.563347
 O   -2.126197    0.558475    3.193476
 O   -0.778040   -1.764397    3.566541
 O    1.144058   -1.974137    2.479366
 C    1.222875   -3.294105    2.994442
 H    1.319956   -3.281337    4.088911
 H    2.111922   -3.745191    2.543777
 H    0.326134   -3.872662    2.730344
 C   -1.948725    3.133843    2.880121
 H   -2.757723    3.021644    2.142576
 H   -1.545574    4.150890    2.838491
 H   -2.341646    2.921775    3.882390
 C   -1.362628   -3.015194    0.003200
 H   -0.779124   -2.571576    0.823411
 C   -0.383693   -3.671350   -0.965527
 C    0.492411   -4.657421   -0.493098
 C   -0.310138   -3.311832   -2.314249
 C    1.403379   -5.275553   -1.345862
 H    0.475264   -4.942237    0.561573
 C    0.603113   -3.927137   -3.170944
 H   -0.954685   -2.525176   -2.709034
 C    1.461414   -4.913066   -2.691690
 H    2.078891   -6.038961   -0.953216
 H    0.646441   -3.624325   -4.219179
 H    2.179335   -5.391531   -3.361013
 C   -2.317716   -4.042085    0.638678
 H   -1.705482   -4.860969    1.043526
 H   -2.944550   -4.492864   -0.154612
 O   -3.079136   -3.526747    1.679268
 C    1.706295    1.923543    1.411283
 H    1.000152    2.739469    1.544959
 C    2.975350    2.175312    0.914239
 H    3.702124    1.361087    0.943297
 C    3.574831    3.519582    0.821940
 C    4.958519    3.630495    0.603164
 C    2.828916    4.704466    0.931775
 C    5.574376    4.874565    0.496418
 H    5.551401    2.716561    0.507877
 C    3.443320    5.949760    0.823856
 H    1.751275    4.657613    1.094795
 C    4.818571    6.042924    0.605105
 H    6.651842    4.933812    0.326072
 H    2.841462    6.857418    0.910511
 H    5.298290    7.020266    0.519104
 C   -3.895631    3.862314   -4.210348
 H   -3.611585    3.331642   -5.131537
 H   -4.979789    3.722745   -4.076124
 H   -3.708280    4.934164   -4.360492
 C   -1.017767    4.615813   -0.135240
 H   -0.476459    4.064653    0.643801
 H   -0.285848    5.209369   -0.703696
 H   -1.702311    5.323228    0.357787
 H   -1.322372    1.929538    0.118541
 H   -3.705789    1.299131   -3.423292
 O   -4.649250   -1.533846    1.626024
Na   -3.032395   -1.546919    3.183395
 C   -5.240819   -0.644347    0.889136
 C   -4.783849    0.701559    0.828275
 C   -6.367852   -0.961991    0.080743
 C   -5.390210    1.642867    0.004416
 H   -3.911075    0.968243    1.431189
 C   -6.970611   -0.008573   -0.737110
 H   -6.749076   -1.987051    0.114924
 C   -6.489206    1.303127   -0.792408
 H   -4.982268    2.657726   -0.034847
 H   -7.831630   -0.296643   -1.348353
 H   -6.957778    2.044331   -1.443532
121
Figure_S3-1_AA-9d(NaOPh)-pc(1,6major) / electronic energy: -4439.05320939 a.u. / lowest freq: 15.82 cm-1
 H    1.390491    2.785442   -2.863349
 H    0.409655    0.632363   -2.139803
 C    2.835911    1.760402   -1.613248
 C    1.074808    0.019306   -1.511761
 H    3.900389    2.007841   -1.566204
 C    2.462249    0.460232   -1.462828
```

H	0.967804	-1.047222	-1.757973
B	3.560676	-0.586697	-1.121141
O	3.429147	-1.932566	-1.337439
H	5.930928	-1.338963	-2.690321
O	4.762612	-0.275037	-0.530712
H	7.077683	-0.421658	-1.685970
C	6.504453	-1.357436	-1.752147
H	5.176995	-3.507458	-2.536221
C	5.582029	-1.456909	-0.537553
C	4.510409	-2.601697	-0.669333
C	4.957194	-3.794590	-1.500213
H	7.213822	-2.196029	-1.790792
H	4.159168	-4.549248	-1.519940
H	3.640175	-2.231335	1.299213
H	3.086364	-3.709277	0.481428
C	3.965019	-3.077524	0.675833
H	7.130603	-0.677657	0.747443
C	6.402029	-1.501079	0.742554
H	5.767267	-1.400576	1.632147
H	5.855790	-4.254424	-1.062328
H	4.706760	-3.665386	1.234807
H	6.957160	-2.448367	0.812356
H	2.350737	3.859298	-1.810208
C	1.870121	2.873060	-1.872144
H	1.051268	2.838353	-1.133804
C	-3.328147	-2.121585	-1.401213
H	-4.173647	-2.387390	-0.750976
C	-3.527649	-0.758643	-2.058652
H	-3.316460	-0.785894	-3.139026
C	-1.716813	-0.634036	-0.580540
C	-2.475018	1.466814	-1.616099
C	-1.757698	2.329535	-0.776203
C	-3.166603	2.000206	-2.704922
C	-1.698621	3.696056	-1.040113
C	-3.139200	3.373922	-2.973497
C	-2.395221	4.208609	-2.142403
H	-2.357160	5.282214	-2.347540
Cu	0.010053	-0.023118	0.208961
N	-2.119417	-1.904584	-0.600458
N	-2.535764	0.080373	-1.373849
C	1.280773	0.559578	1.674581
C	0.055213	0.109678	2.300669
H	-3.802723	-2.834264	1.375639
H	-4.538337	-0.358817	-1.900557
H	-3.179595	-2.929006	-2.132004
H	2.068281	-0.197882	1.662262
C	-1.072272	0.972114	2.709892
C	0.027748	-1.265260	2.842661
O	-0.849375	2.278782	2.534114
O	-2.139783	0.586671	3.151211
O	-0.824816	-1.741433	3.570312
O	1.076828	-2.007934	2.461765
C	1.141639	-3.324496	2.990289
H	1.249288	-3.299563	4.083361
H	2.020302	-3.791352	2.535541
H	0.233542	-3.891035	2.739793
C	-1.924818	3.162374	2.830515
H	-2.720898	3.059440	2.077967
H	-1.503767	4.172022	2.792639
H	-2.337364	2.958650	3.826447
C	-1.388864	-3.002226	0.005926
H	-0.797982	-2.564401	0.823102
C	-0.417299	-3.670123	-0.962109
C	0.445448	-4.667696	-0.488932
C	-0.334452	-3.307887	-2.309302
C	1.352677	-5.294015	-1.339600
H	0.420807	-4.955899	0.564598
C	0.574206	-3.932293	-3.164203
H	-0.966023	-2.510541	-2.703358
C	1.419463	-4.929124	-2.684405
H	2.017817	-6.066086	-0.946184
H	0.625514	-3.626794	-4.211278
H	2.134518	-5.413931	-3.352203
C	-2.355748	-4.015288	0.645262
H	-1.754346	-4.839597	1.055403
H	-2.987645	-4.462329	-0.146030
O	-3.111746	-3.483774	1.682041
C	1.768568	1.906314	1.500928
H	1.068719	2.727809	1.635274
C	3.056066	2.149317	1.151844
H	3.743506	1.304894	1.055075
C	3.662006	3.473044	0.957628
C	5.036724	3.553394	0.678044
C	2.930276	4.671069	1.022242
C	5.659167	4.781971	0.472087
H	5.615458	2.628385	0.609476
C	3.551056	5.899582	0.816075
H	1.858589	4.646425	1.226410
C	4.918539	5.962594	0.540312

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 H    6.729177    4.818812    0.255084
 H    2.961952    6.818126    0.868798
 H    5.403262    6.927725    0.378017
 C   -3.918729    3.919587   -4.141329
 H   -3.656371    3.396917   -5.073543
 H   -4.999931    3.780708   -3.984660
 H   -3.732116    4.992302   -4.286118
 C   -0.899827    4.619236   -0.158830
 H   -0.361885    4.059913    0.616869
 H   -0.157831    5.178602   -0.748479
 H   -1.549559    5.357042    0.336733
 H   -1.246848    1.942797    0.105082
 H   -3.752729    1.355761   -3.359848
 O   -4.680751   -1.488834    1.616306
Na   -3.086338   -1.506647    3.188851
 C   -5.271307   -0.604057    0.872641
 C   -4.822321    0.744637    0.813825
 C   -6.388866   -0.930161    0.054685
 C   -5.426217    1.680361   -0.018135
 H   -3.956597    1.017984    1.423741
 C   -6.989217    0.017685   -0.771410
 H   -6.764178   -1.957425    0.087388
 C   -6.515093    1.332074   -0.825118
 H   -5.024725    2.697796   -0.055697
 H   -7.842244   -0.277009   -1.390592
 H   -6.981458    2.068929   -1.482741
89
Figure_S3-1_9d(NaOPh)-Cu-allyl / electronic energy: -3597.06845638 a.u. / lowest freq: 14.75 cm-1
Na    1.466278   -1.713895    0.568774
 H    4.895602   -3.588713    0.817161
 H    4.692117   -0.895972   -2.541156
 O    3.335573   -2.007938   -0.584046
 C    5.271052   -1.564621   -1.896670
 C    4.600612   -2.207337   -0.820863
 H    7.102470   -1.262094   -2.980981
 C    6.625148   -1.776136   -2.141098
 C    5.384324   -3.077572   -0.017672
 C    7.377630   -2.634567   -1.334758
 C    6.737508   -3.280572   -0.272517
 H    8.439672   -2.798024   -1.529682
 H    7.306712   -3.957090    0.372185
 H    1.822369   -0.807067    3.943134
 H   -2.251641   -0.329887    3.139589
 C    0.449649   -2.296353    3.162582
 C   -1.148749   -0.342683    3.068826
 H    0.743177   -3.269591    2.747587
 C   -0.656265   -1.681110    2.668089
 H   -0.722254    0.025625    4.016197
 B   -1.373536   -2.298457    1.423828
 O   -2.713492   -2.319048    1.179742
 H   -1.727987   -0.728011   -0.976153
 O   -0.646091   -2.774963    0.347830
 H   -0.369549   -1.436810   -1.877879
 C   -1.416767   -1.592283   -1.578998
 H   -3.924597   -1.288533   -0.925882
 C   -1.545189   -2.887384   -0.779148
 C   -2.937112   -3.023746   -0.060716
 C   -4.089317   -2.364956   -0.799421
 H   -2.035120   -1.618693   -2.487150
 H   -5.022038   -2.500680   -0.233511
 H   -2.452907   -4.961768    0.822840
 H   -4.156010   -4.465844    0.969667
 C   -3.284310   -4.466581    0.300122
 H   -0.161528   -3.891634   -2.091822
 C   -1.138452   -4.082032   -1.624394
 H   -1.058778   -4.996627   -1.023531
 H   -4.221693   -2.822726   -1.791255
 H   -3.534901   -5.053460   -0.594647
 H   -1.873021   -4.249881   -2.425820
 H    2.084171   -2.447422    4.577693
 C    1.310104   -1.734587    4.260318
 H    0.715848   -1.463962    5.150374
 C    0.319514    2.875268   -1.993392
 H    1.033917    2.506723   -2.740473
 C   -1.127654    2.540540   -2.354801
 H   -1.705390    3.414017   -2.684987
 C   -0.661312    1.729692   -0.210974
 C   -3.004911    1.645974   -0.933491
 C   -3.559642    1.488554    0.340873
 C   -3.804764    1.434619   -2.061581
 C   -4.882144    1.072030    0.498446
 C   -5.140732    1.044490   -1.923628
 C   -5.665477    0.864801   -0.641218
 H   -6.706703    0.550845   -0.526471
Cu   -0.836713    0.775737    1.479326
 N    0.481016    2.176611   -0.718861
 N   -1.650734    2.012129   -1.089715
 H    2.605203   -0.823585   -1.253202
 H   -1.180566    1.768453   -3.138589
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 H    0.488311    3.954711   -1.852253
 C    1.783728    1.989569   -0.103034
 H    1.577644    1.419376    0.818373
 C    2.387717    3.326050    0.305028
 C    3.684660    3.715190   -0.041325
 C    1.611056    4.193427    1.085504
 C    4.194290    4.943729    0.386120
 H    4.319736    3.066305   -0.646305
 C    2.116435    5.418098    1.511249
 H    0.594881    3.899472    1.363203
 C    3.414073    5.797630    1.161301
 H    5.210992    5.230395    0.108577
 H    1.496950    6.078282    2.122170
 H    3.815380    6.756940    1.495184
 C    2.667582    1.110708   -0.990647
 H    3.584280    0.863576   -0.424765
 H    2.991597    1.684656   -1.881421
 O    1.975771   -0.040827   -1.362266
 C   -5.977773    0.764471   -3.144325
 H   -5.678591    1.395447   -3.993282
 H   -5.860945   -0.286000   -3.456591
 H   -7.045661    0.932149   -2.946707
 C   -5.429241    0.820029    1.877761
 H   -6.526964    0.864113    1.893808
 H   -5.127045   -0.182053    2.222954
 H   -5.039940    1.546746    2.605212
 H   -2.959357    1.704718    1.226933
 H   -3.392248    1.559302   -3.063750
89
Figure_S3-1_9b(NaOPh)-Cu-allyl / electronic energy: -3597.06856996 a.u. / lowest freq: 15.34 cm-1
Na    0.148120   -2.350929   -0.661887
 H    2.438637   -3.886514    0.418400
 H    4.437536   -1.625816   -2.657585
 O    2.188175   -1.934213   -1.331976
 C    4.457113   -2.409826   -1.896029
 C    3.271723   -2.638718   -1.144621
 H    6.503884   -2.941304   -2.274753
 C    5.611926   -3.155530   -1.678013
 C    3.330703   -3.680261   -0.180384
 C    5.648755   -4.168717   -0.715703
 C    4.491286   -4.420599    0.026190
 H    6.559206   -4.747918   -0.547636
 H    4.492260   -5.208637    0.785191
 H    2.110038   -1.789209    2.251941
 H   -1.683682   -0.084569    3.012140
 C    0.177417   -2.763996    2.184032
 C   -0.716422   -0.448477    2.624984
 H    0.009685   -3.753268    1.738460
 C   -0.814296   -1.836152    2.123482
 H    0.060429   -0.307140    3.395789
 B   -2.112989   -2.153360    1.318568
 O   -3.369101   -1.737541    1.633548
 H   -2.845676   -0.482203   -0.927861
 O   -2.073350   -2.793843    0.089938
 H   -2.386052   -1.604043   -2.238318
 C   -3.158779   -1.375665   -1.489089
 H   -4.906254   -0.251131    0.103283
 C   -3.345234   -2.575300   -0.562814
 C   -4.288875   -2.263960    0.657935
 C   -5.353692   -1.214414    0.379956
 H   -4.085231   -1.134855   -2.028538
 H   -5.962317   -1.060989    1.282259
 H   -4.158934   -4.286914    1.470992
 H   -5.400718   -3.251670    2.212692
 C   -4.917121   -3.518031    1.262489
 H   -3.003759   -3.952870   -2.186413
 C   -3.717784   -3.812772   -1.361912
 H   -3.704627   -4.717295   -0.741233
 H   -6.020495   -1.543104   -0.431111
 H   -5.677701   -3.946520    0.595013
 H   -4.721339   -3.698819   -1.797645
 H    2.106807   -3.437236    2.912827
 C    1.510733   -2.517409    2.830805
 H    1.401035   -2.091228    3.843076
 C    1.280515    3.069545   -2.003442
 H    1.565108    2.605156   -2.959047
 C   -0.172818    3.561404   -1.995315
 H   -0.276419    4.578520   -1.584882
 C    0.060095    1.792810   -0.476656
 C   -2.217588    2.610963   -0.829080
 C   -2.678385    3.129778    0.395038
 C   -3.100884    2.109301   -1.801083
 C   -4.054535    3.111730    0.641038
 C   -4.470186    2.122037   -1.519756
 C   -4.944329    2.613849   -0.307033
 H   -6.016384    2.608530   -0.098720
Cu   -0.341132    0.639697    1.032050
 N    1.273784    2.050851   -0.951347
 N   -0.819266    2.595349   -1.099937
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 H    2.443780   -0.610758   -2.213460
 H   -0.629024    3.549352   -2.994037
 H    1.996706    3.870578   -1.771134
 C    2.484707    1.372525   -0.497575
 H    2.139125    0.425669   -0.056505
 C    3.187276    2.170139    0.586692
 C    4.053990    3.229208    0.291404
 C    2.928357    1.870261    1.929919
 C    4.643739    3.972204    1.314760
 H    4.282158    3.482129   -0.746497
 C    3.515716    2.610503    2.954124
 H    2.250016    1.047192    2.174293
 C    4.375475    3.666125    2.648300
 H    5.320155    4.793092    1.066340
 H    3.303057    2.360630    3.995928
 H    4.838980    4.246461    3.449152
 C    3.374358    0.994741   -1.687423
 H    4.246875    0.448944   -1.277619
 H    3.774104    1.901226   -2.172724
 O    2.681605    0.261974   -2.643836
 H   -4.432045    3.504641    1.588162
 H   -5.170862    1.726395   -2.259259
 C   -2.592705    1.563034   -3.108381
 H   -2.423060    2.369586   -3.840006
 H   -1.639450    1.031325   -2.978681
 H   -3.320420    0.870396   -3.551477
 C   -1.723572    3.682246    1.419703
 H   -1.210134    2.868739    1.959856
 H   -0.940363    4.298843    0.955650
 H   -2.256508    4.292551    2.160509
121
Figure_S3-1_AA-9b(NaOPh)-pc(1,6major) / electronic energy: -4439.04439972 a.u. / lowest freq: 11.81 cm-1
 C    0.935802    0.662649    4.096427
 H    0.864348   -0.263644    3.511863
 H    1.774421    0.549899    4.802740
 H    0.016164    0.760804    4.688880
 H   -2.186641    2.294116    3.131806
 H   -0.824239    0.494303    2.195976
 C   -3.343592    1.255678    1.625382
 C   -1.320480   -0.152220    1.462427
 H   -4.429308    1.342863    1.524385
 C   -2.754492    0.059071    1.351389
 H   -1.041122   -1.206015    1.607606
 B   -3.640387   -1.106185    0.827404
 O   -3.319076   -2.428574    0.980336
 H   -5.999906   -2.321888    2.086345
 O   -4.815730   -0.937629    0.134991
 H   -7.190220   -1.542828    1.017057
 C   -6.469790   -2.369821    1.093195
 H   -4.913804   -4.344408    1.873129
 C   -5.430907   -2.229282   -0.018341
 C   -4.205742   -3.202801    0.157521
 C   -4.524700   -4.512495    0.861112
 H   -7.020801   -3.317290    1.011525
 H   -3.608805   -5.114896    0.943618
 H   -3.224170   -2.540841   -1.674324
 H   -2.515442   -3.978184   -0.905258
 C   -3.463342   -3.476829   -1.148551
 H   -6.942428   -1.588843   -1.417452
 C   -6.104192   -2.299544   -1.380336
 H   -5.406396   -2.044820   -2.188021
 H   -5.266537   -5.089106    0.288687
 H   -4.044421   -4.123403   -1.821250
 H   -6.503026   -3.308476   -1.563180
 H   -3.219095    3.354563    2.137021
 C   -2.591065    2.453015    2.116391
 H   -1.715261    2.656255    1.473318
 C    3.520175   -1.470835    1.434027
 H    4.429499   -1.679494    0.859947
 C    3.564871   -0.069324    2.048333
 H    3.584512   -0.079463    3.147198
 C    1.673850   -0.248777    0.673083
 C    1.846144    1.792755    2.007961
 C    1.139981    1.869738    3.219537
 C    2.129107    2.932216    1.237629
 C    0.650881    3.119347    3.614239
 C    1.613123    4.159904    1.660479
 C    0.869581    4.250915    2.835200
 H    0.468412    5.215698    3.153137
Cu   -0.108214    0.185874   -0.130214
 N    2.349269   -1.396078    0.551049
 N    2.316873    0.523946    1.556278
 C   -1.407678    0.718872   -1.594307
 C   -0.109584    0.540838   -2.206971
 H    4.309558   -1.924046   -1.343211
 H    4.431739    0.508302    1.690350
 H    3.389260   -2.264822    2.186114
 H   -2.074733   -0.140457   -1.699392
 C    0.808072    1.636435   -2.583034
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 C    0.194735   -0.765315   -2.821302
 O    0.274305    2.851114   -2.466395
 O    1.954345    1.500121   -2.977503
 O    1.188576   -1.047433   -3.468839
 O   -0.753022   -1.690423   -2.611853
 C   -0.547059   -2.949997   -3.235108
 H   -0.561045   -2.846983   -4.328867
 H   -1.368705   -3.592371   -2.905353
 H    0.418269   -3.382313   -2.937647
 C    1.061338    3.958218   -2.883186
 H    2.030912    3.969576   -2.371169
 H    0.484167    4.852409   -2.624705
 H    1.231005    3.920222   -3.968208
 C    1.848957   -2.554923   -0.167944
 H    1.246918   -2.160791   -0.999020
 C    0.939627   -3.440316    0.678929
 C    0.294178   -4.532599    0.083524
 C    0.694025   -3.186428    2.031108
 C   -0.559232   -5.350447    0.820149
 H    0.446798   -4.746057   -0.976860
 C   -0.161408   -4.001677    2.772297
 H    1.155670   -2.327973    2.520056
 C   -0.788590   -5.089798    2.171145
 H   -1.052885   -6.194075    0.332336
 H   -0.341136   -3.777035    3.825588
 H   -1.460374   -5.727062    2.749833
 C    3.006411   -3.348921   -0.801707
 H    2.573647   -4.227693   -1.301826
 H    3.655231   -3.745191    0.003201
 O    3.723883   -2.627575   -1.747453
 C   -2.087135    1.953321   -1.287873
 H   -1.498398    2.865397   -1.223821
 C   -3.420814    1.981716   -1.045481
 H   -3.991614    1.054306   -1.141280
 C   -4.214289    3.179807   -0.738899
 C   -5.602262    3.047185   -0.566347
 C   -3.649636    4.458368   -0.592132
 C   -6.398276    4.146848   -0.255517
 H   -6.054556    2.056994   -0.666573
 C   -4.444375    5.558454   -0.282306
 H   -2.573857    4.598421   -0.714263
 C   -5.822169    5.409381   -0.111061
 H   -7.474500    4.016612   -0.121376
 H   -3.983390    6.542509   -0.169871
 H   -6.442738    6.273848    0.135193
 H    1.811761    5.056454    1.068158
 H    0.084734    3.199451    4.545330
 C    3.011452    2.823961    0.027591
 O    4.924136   -0.442226   -1.264187
Na    3.292187   -0.360410   -2.790196
 C    5.947197    0.029438   -0.621908
 C    6.287664    1.410149   -0.667365
 C    6.784574   -0.795229    0.180192
 C    7.355374    1.924095    0.062036
 H    5.683596    2.065593   -1.300869
 C    7.849334   -0.268169    0.906644
 H    6.582117   -1.870528    0.205643
 C    8.145853    1.096950    0.866164
 H    7.576312    2.994016    0.000056
 H    8.464012   -0.938846    1.514702
 H    8.981496    1.505500    1.438206
 H    3.162910    3.806432   -0.438491
 H    2.605867    2.137149   -0.727132
 H    4.000990    2.427732    0.301084
121
Figure_S3-1_AA-9b(NaOPh)-ts(1,6major) / electronic energy: -4439.04225300 a.u. / lowest freq: -302.37 cm-1
 C    0.994657    0.629022    4.152905
 H    0.816261   -0.280969    3.564092
 H    1.904888    0.462704    4.751414
 H    0.157717    0.752953    4.852850
 H   -2.218728    2.280131    3.090642
 H   -0.785160    0.492325    2.170977
 C   -3.262119    1.334340    1.456737
 C   -1.329610   -0.183510    1.503823
 H   -4.351476    1.420712    1.443181
 C   -2.712988    0.068601    1.315025
 H   -1.039590   -1.237116    1.603453
 B   -3.618360   -1.095557    0.817808
 O   -3.314717   -2.417207    0.995351
 H   -5.983990   -2.257156    2.112316
 O   -4.794050   -0.917791    0.132915
 H   -7.170777   -1.476924    1.039672
 C   -6.461358   -2.312633    1.123140
 H   -4.926709   -4.301788    1.919199
 C   -5.428985   -2.204076    0.002360
 C   -4.215837   -3.191005    0.184963
 C   -4.548176   -4.487256    0.906230
 H   -7.026107   -3.253291    1.059066
 H   -3.640887   -5.102642    0.987943
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H	-3.234633	-2.560337	-1.657250
H	-2.540355	-3.998836	-0.877860
C	-3.482985	-3.487878	-1.120908
H	-6.941358	-1.564349	-1.395553
C	-6.111421	-2.284360	-1.354170
H	-5.415593	-2.048775	-2.169261
H	-5.303295	-5.058697	0.346199
H	-4.075709	-4.133714	-1.784018
H	-6.523173	-3.290888	-1.520711
H	-3.047810	3.418039	2.000905
C	-2.484748	2.475578	2.036996
H	-1.530048	2.621600	1.501572
C	3.525684	-1.464785	1.445159
H	4.439255	-1.676503	0.879275
C	3.563752	-0.059402	2.049284
H	3.613945	-0.062732	3.146650
C	1.665140	-0.263362	0.689854
C	1.807661	1.771641	2.036639
C	1.146095	1.841934	3.273955
C	2.021140	2.908436	1.241402
C	0.645184	3.082615	3.680133
C	1.492873	4.127062	1.676007
C	0.803203	4.212254	2.883192
H	0.392937	5.170019	3.210406
Cu	-0.099482	0.161163	-0.143852
N	2.358950	-1.398161	0.556361
N	2.294812	0.510423	1.582081
C	-1.421790	0.716156	-1.636072
C	-0.126193	0.505968	-2.260099
H	4.317977	-1.911589	-1.328775
H	4.410994	0.529868	1.663904
H	3.391423	-2.253427	2.202690
H	-2.099185	-0.138345	-1.715683
C	0.782572	1.583898	-2.679487
C	0.163637	-0.813798	-2.832815
O	0.261455	2.807221	-2.553427
O	1.913349	1.442254	-3.120644
O	1.175626	-1.140518	-3.433698
O	-0.814574	-1.716183	-2.640531
C	-0.612902	-2.988096	-3.236977
H	-0.576527	-2.902059	-4.331834
H	-1.463020	-3.607051	-2.935388
H	0.327652	-3.439978	-2.893055
C	1.038131	3.899272	-3.021440
H	2.026087	3.916713	-2.544798
H	0.475833	4.802864	-2.762013
H	1.170927	3.838726	-4.110699
C	1.868628	-2.559587	-0.166404
H	1.278385	-2.168860	-1.008231
C	0.950653	-3.442312	0.674230
C	0.299804	-4.527999	0.072922
C	0.702516	-3.192569	2.027029
C	-0.563666	-5.341404	0.802888
H	0.456067	-4.739028	-0.987382
C	-0.163054	-4.003211	2.761591
H	1.170684	-2.341249	2.522359
C	-0.797802	-5.083012	2.153454
H	-1.061797	-6.179498	0.310090
H	-0.344391	-3.781576	3.815261
H	-1.477473	-5.716615	2.726922
C	3.033926	-3.354156	-0.784286
H	2.607026	-4.236832	-1.282740
H	3.676342	-3.743843	0.029176
O	3.757611	-2.637747	-1.728897
C	-2.033507	1.924162	-1.230037
H	-1.437210	2.833493	-1.208038
C	-3.353814	1.956174	-0.820294
H	-3.963969	1.067412	-0.993847
C	-4.121858	3.197283	-0.612268
C	-5.519929	3.118415	-0.496253
C	-3.523054	4.464126	-0.513055
C	-6.292343	4.258448	-0.289256
H	-6.000857	2.138745	-0.564629
C	-4.294551	5.605130	-0.305701
H	-2.438676	4.564035	-0.590710
C	-5.682500	5.509794	-0.191774
H	-7.377515	4.168661	-0.200933
H	-3.806282	6.579452	-0.229348
H	-6.284090	6.406448	-0.027802
H	1.638670	5.021331	1.065270
H	0.114459	3.157263	4.632228
C	2.834696	2.805511	-0.016249
O	4.891885	-0.411924	-1.258193
Na	3.260473	-0.381258	-2.788678
C	5.909448	0.069296	-0.614765
C	6.224501	1.456656	-0.640249
C	6.765668	-0.752305	0.170791
C	7.285932	1.978492	0.092906
H	5.607582	2.110668	-1.262807

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 C    7.823504   -0.217304    0.901258
 H    6.582471   -1.831360    0.179632
 C    8.094641    1.153607    0.881006
 H    7.487648    3.052991    0.046521
 H    8.452672   -0.885961    1.496591
 H    8.925115    1.568487    1.456025
 H    2.967128    3.790755   -0.481698
 H    2.375484    2.130399   -0.750216
 H    3.832566    2.393282    0.194920
121
Figure_S3-1_AA-9b(NaOPh)-prod(1,6major) / electronic energy: -4439.09912432 a.u. / lowest freq: 18.30 cm-1
 C    1.121741   -0.022225    4.690419
 H    1.086055   -0.854656    3.974262
 H    2.113809   -0.044683    5.169536
 H    0.374702   -0.203594    5.475245
 H   -3.208936    1.459593    3.533476
 H   -1.332732    0.065433    3.278220
 C   -3.456389    0.657980    1.520609
 C   -1.563101   -0.706616    2.538937
 H   -4.481397    0.321057    1.752509
 C   -2.568926   -0.572727    1.626881
 H   -1.051757   -1.665203    2.659133
 B   -2.889821   -1.835167    0.747804
 O   -2.023517   -2.882297    0.634448
 H   -4.488387   -4.205682    1.471043
 O   -4.032286   -2.003535    0.024553
 H   -5.905957   -3.731561    0.504386
 C   -4.905409   -4.183741    0.453728
 H   -2.637557   -5.439728    0.938072
 C   -4.033691   -3.355219   -0.487147
 C   -2.507594   -3.740976   -0.419571
 C   -2.230215   -5.187990   -0.049029
 H   -5.009098   -5.217567    0.095982
 H   -1.145043   -5.357642   -0.022726
 H   -1.871295   -2.309271   -1.947182
 H   -0.663689   -3.531243   -1.492380
 C   -1.733611   -3.366819   -1.680103
 H   -5.685644   -3.066333   -1.841231
 C   -4.623317   -3.344984   -1.887926
 H   -4.107913   -2.624875   -2.535880
 H   -2.669100   -5.866161   -0.795901
 H   -2.031802   -3.989565   -2.535121
 H   -4.550960   -4.343461   -2.343710
 H   -3.761353    2.645358    2.331633
 C   -3.098412    1.782114    2.487667
 H   -2.060078    2.127812    2.356291
 C    3.388225   -1.126704    1.167169
 H    4.226614   -1.034790    0.463883
 C    3.284596    0.090642    2.087462
 H    3.529802   -0.138373    3.133728
 C    1.245811   -0.213897    0.967479
 C    1.274208    1.518262    2.680895
 C    0.881523    1.299993    4.011904
 C    1.087801    2.755464    2.042260
 C    0.255038    2.348969    4.692925
 C    0.452829    3.776399    2.755395
 C    0.036262    3.574341    4.068881
 H   -0.461553    4.380646    4.612037
Cu   -0.691844    0.042937    0.618147
 N    2.098689   -1.108193    0.467231
 N    1.871548    0.454683    1.947099
 C   -1.448489    0.946872   -1.527184
 C   -0.346757    1.423951   -2.328493
 H    3.328754   -0.187232   -1.616525
 H    3.925692    0.919509    1.749359
 H    3.499273   -2.074025    1.719669
 H   -1.943249    0.056263   -1.934875
 C    0.096140    2.800278   -2.337942
 C    0.254010    0.522120   -3.282086
 O   -0.758211    3.660860   -1.739348
 O    1.131080    3.240510   -2.833274
 O    1.108702    0.789301   -4.122038
 O   -0.230163   -0.741905   -3.203282
 C    0.288298   -1.669262   -4.136944
 H   -0.025921   -1.420784   -5.161834
 H   -0.119229   -2.647476   -3.855969
 H    1.385317   -1.685029   -4.096501
 C   -0.400062    5.028083   -1.732062
 H    0.586412    5.181690   -1.272697
 H   -1.170027    5.540430   -1.142713
 H   -0.377455    5.439942   -2.751563
 C    1.760258   -2.116272   -0.519414
 H    0.806433   -1.786637   -0.965780
 C    1.567198   -3.485839    0.132427
 C    1.837412   -4.680368   -0.546988
 C    1.085461   -3.572912    1.444197
 C    1.644469   -5.917085    0.070736
 H    2.206831   -4.666191   -1.573088
 C    0.893846   -4.803579    2.065623
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 H    0.857013   -2.656742    1.990116
 C    1.177372   -5.985082    1.381393
 H    1.866619   -6.833755   -0.479954
 H    0.515708   -4.838617    3.089630
 H    1.030106   -6.952836    1.865316
 C    2.803891   -2.118973   -1.647266
 H    2.465813   -2.820652   -2.423928
 H    3.760472   -2.524299   -1.256873
 O    2.960536   -0.878523   -2.242498
 C   -2.023345    1.472023   -0.392653
 H   -1.609388    2.395841    0.022089
 C   -3.431003    1.110623    0.035848
 H   -3.740115    0.235213   -0.556679
 C   -4.454863    2.199099   -0.264956
 C   -5.810353    1.962062    0.009892
 C   -4.102953    3.428248   -0.833134
 C   -6.779321    2.926616   -0.254253
 H   -6.115796    0.999513    0.429105
 C   -5.072642    4.398098   -1.098707
 H   -3.061225    3.624760   -1.092058
 C   -6.412641    4.155577   -0.806633
 H   -7.828690    2.716567   -0.033959
 H   -4.773428    5.349837   -1.544510
 H   -7.170201    4.914370   -1.015187
 H    0.289564    4.742771    2.272124
 H   -0.071396    2.195783    5.724496
 C    1.538562    2.950401    0.624423
 O    3.893795    1.206610   -1.056986
Na    2.896780    1.781163   -3.013738
 C    5.135827    1.181190   -0.670939
 C    5.673417    2.178828    0.187562
 C    6.023191    0.138667   -1.060890
 C    6.993931    2.126742    0.625477
 H    5.016408    2.996030    0.499078
 C    7.341385    0.099454   -0.615307
 H    5.639172   -0.636656   -1.730788
 C    7.845198    1.088706    0.234052
 H    7.367110    2.912753    1.289086
 H    7.990373   -0.719920   -0.939189
 H    8.879620    1.052622    0.582480
 H    1.566587    4.015940    0.363351
 H    0.843227    2.446811   -0.060730
 H    2.520876    2.499780    0.419449
121
Figure_S3-1_AA-9d(NaOPh)-prod(1,6minor) / electronic energy: -4439.09249888 a.u. / lowest freq: 11.32 cm-1
 H   -5.295853   -3.015072   -2.549329
 H   -6.703674   -2.031675   -2.081627
 C   -6.041133   -2.846888   -1.758166
 H   -6.643478   -3.759076   -1.645693
 H   -4.422769   -4.910564   -1.606698
 B   -3.359980   -1.530207   -0.943810
 O   -4.666810   -1.220665   -0.682133
 C   -4.368367   -4.858694   -0.512131
 C   -5.374540   -2.452573   -0.441058
 O   -3.066183   -2.837957   -0.669922
 H   -5.278031   -5.312247   -0.091537
 H   -3.505617   -5.456775   -0.185033
 C   -4.210352   -3.427809   -0.021764
 H   -7.187873   -1.519471    0.254646
 C   -6.426374   -2.217307    0.631253
 H   -6.927488   -3.160716    0.893543
 H   -5.988638   -1.785353    1.539954
 C   -3.934205   -3.417136    1.479404
 H   -3.022659   -3.996999    1.677313
 H   -3.773464   -2.396784    1.857017
 H   -4.758368   -3.876391    2.042915
 C   -2.335445   -0.503845   -1.531586
 C   -2.690473    0.970605   -1.510769
 H   -3.690151    1.053291   -1.974025
 H   -1.612410    1.505441   -3.324272
 H   -0.730181    1.861927   -1.822110
 C   -1.727120    1.855440   -2.287597
 H   -2.079425    2.895167   -2.326294
 H   -1.008923   -2.070338   -2.076446
 C   -1.212714   -0.995728   -2.081910
 H   -0.466896   -0.366858   -2.576833
 C    3.718753    1.240765   -1.726168
 H    4.619650    1.281111   -1.099664
 C    3.492995   -0.163298   -2.291076
 H    3.220068   -0.138516   -3.357941
 C    1.805684    0.333231   -0.747243
 C    1.878412   -1.959970   -1.548944
 C    1.968489   -2.685499   -2.737550
 C    1.271075   -2.533616   -0.429168
 C    1.406195   -3.962849   -2.831555
 C    0.678236   -3.792604   -0.510686
 C    0.749278   -4.495334   -1.717793
 H    0.287667   -5.484018   -1.789974
Cu    0.184783    0.174975    0.311288
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 N    2.521110    1.443363   -0.905977
 N    2.366793   -0.641632   -1.484140
 C   -1.402936    0.345936    1.652467
 C   -0.257955    0.065524    2.522379
 H    4.033332    1.550779    1.308303
 H    4.365627   -0.818464   -2.158263
 H    3.804399    2.008163   -2.507809
 H   -2.119882   -0.480877    1.606772
 C   -0.167841   -1.261056    3.129333
 C    0.643421    1.071608    3.052695
 O   -1.347965   -1.901969    3.195233
 O    0.844535   -1.792259    3.570098
 O    1.593097    0.878410    3.804858
 O    0.339514    2.328273    2.673102
 C    1.167614    3.361704    3.190575
 H    1.107962    3.398636    4.287358
 H    0.773772    4.295262    2.772024
 H    2.213237    3.205803    2.887082
 C   -1.380163   -3.132603    3.898148
 H   -0.854924   -3.925150    3.347640
 H   -2.438468   -3.394537    4.003317
 H   -0.920718   -3.026802    4.890240
 C    2.229900    2.691149   -0.223627
 H    1.560588    2.428925    0.608962
 C    1.486233    3.687323   -1.102135
 C    0.917180    4.821151   -0.506764
 C    1.304415    3.497670   -2.473995
 C    0.190140    5.739353   -1.260150
 H    1.030748    4.982239    0.568047
 C    0.578811    4.416458   -3.233143
 H    1.700738    2.604851   -2.959941
 C    0.017489    5.539595   -2.630480
 H   -0.252073    6.610742   -0.772239
 H    0.440876    4.242396   -4.302389
 H   -0.558992    6.252995   -3.222937
 C    3.503295    3.279391    0.405984
 H    3.251958    4.282897    0.784388
 H    4.254502    3.439977   -0.395000
 O    4.003420    2.538343    1.467318
 C   -1.658522    1.410932    0.823697
 H   -1.047641    2.312421    0.890493
 C   -2.905112    1.450001   -0.030032
 H   -3.618489    0.731061    0.399343
 C   -3.597705    2.801584   -0.000590
 C   -4.996706    2.851721    0.045711
 C   -2.895250    4.012091   -0.064486
 C   -5.675846    4.069581    0.033230
 H   -5.559954    1.915007    0.090268
 C   -3.570014    5.232109   -0.081073
 H   -1.804379    4.013485   -0.117376
 C   -4.963540    5.267180   -0.029760
 H   -6.767537    4.082677    0.076312
 H   -3.000102    6.162802   -0.135957
 H   -5.491557    6.223319   -0.038462
 C   -0.055433   -4.342199    0.679933
 H   -1.046384   -3.866172    0.746016
 H   -0.203845   -5.428298    0.606540
 H    0.487367   -4.121788    1.610692
 C    1.518112   -4.747206   -4.112668
 H    0.746277   -5.526606   -4.175105
 H    1.422715   -4.094454   -4.992277
 H    2.499514   -5.243809   -4.178918
 H    2.453858   -2.248658   -3.612097
 H    1.266871   -1.993193    0.521404
 O    4.079296   -0.082018    1.404883
Na    2.928510   -0.850287    3.138066
 C    4.936537   -0.774202    0.716039
 C    4.716621   -2.144428    0.405563
 C    6.139219   -0.203133    0.213155
 C    5.603740   -2.866575   -0.386123
 H    3.804835   -2.619498    0.777659
 C    7.017045   -0.934273   -0.581845
 H    6.349647    0.841637    0.461102
 C    6.760196   -2.271800   -0.900441
 H    5.383960   -3.914264   -0.612654
 H    7.923017   -0.451037   -0.960149
 H    7.450640   -2.840858   -1.526540
121
Figure_S3-1_AA-9d(NaOPh)-ts(1,6minor) / electronic energy: -4439.04244814 a.u. / lowest freq: -345.54 cm-1
 H    3.639728    4.266447   -2.509121
 H    5.388690    3.936274   -2.539873
 C    4.570082    4.339701   -1.927262
 H    4.776222    5.400836   -1.728982
 H    2.364214    5.468895   -1.006152
 B    2.946946    1.894371   -0.984115
 O    4.293598    2.156885   -1.001008
 C    2.635293    5.247525    0.033642
 C    4.477675    3.534750   -0.631232
 O    2.228194    2.907443   -0.407684
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H	3.388991	5.976410	0.366474
H	1.738813	5.376955	0.653905
C	3.165161	3.830546	0.181425
H	6.626681	3.451917	-0.482954
C	5.765733	3.668006	0.165820
H	5.877723	4.691673	0.552952
H	5.792510	2.967929	1.010573
C	3.287985	3.458197	1.657553
H	2.289341	3.473404	2.113079
H	3.696833	2.444975	1.785362
H	3.930670	4.164046	2.201901
C	2.344424	0.558122	-1.513129
C	3.244296	-0.471752	-1.760560
H	4.297714	-0.202782	-1.866445
H	2.376696	-1.689252	-3.316210
H	2.021748	-2.231701	-1.672481
C	2.809661	-1.795115	-2.305954
H	3.640762	-2.510413	-2.366520
H	0.349399	1.306102	-1.583391
C	0.940349	0.383521	-1.566859
H	0.547632	-0.401635	-2.226292
C	-3.614220	-1.436651	-1.707166
H	-4.558500	-1.603409	-1.169716
C	-3.475933	0.016005	-2.162540
H	-3.158367	0.086578	-3.214195
C	-1.815917	-0.459907	-0.576082
C	-2.076995	1.881767	-1.217845
C	-2.179560	2.678147	-2.359662
C	-1.637515	2.439404	-0.015250
C	-1.811119	4.026238	-2.319131
C	-1.257322	3.780004	0.042553
C	-1.345121	4.560160	-1.114540
H	-1.054752	5.613692	-1.071678
Cu	0.021547	-0.275248	0.211713
N	-2.471127	-1.596063	-0.805778
N	-2.420161	0.516994	-1.277159
C	1.619020	-0.416432	1.536495
C	0.388120	-0.614149	2.281369
H	-4.254887	-1.851371	1.232830
H	-4.400194	0.594738	-2.026733
H	-3.551685	-2.148288	-2.542100
H	1.990119	0.612563	1.576943
C	-0.154234	0.525396	3.047909
C	-0.166797	-1.917443	2.653295
O	0.746251	1.487446	3.282294
O	-1.293425	0.625514	3.473233
O	-1.125458	-2.114787	3.383925
O	0.481878	-2.958188	2.105610
C	0.028763	-4.260130	2.446375
H	0.169204	-4.451895	3.518867
H	0.636610	-4.953092	1.854504
H	-1.034509	-4.386019	2.200285
C	0.350759	2.533149	4.158963
H	-0.601945	2.977477	3.847655
H	1.149643	3.281838	4.124912
H	0.245316	2.147352	5.183117
C	-2.145968	-2.875864	-0.191980
H	-1.433247	-2.633400	0.604049
C	-1.450638	-3.815921	-1.160249
C	-2.151766	-4.579109	-2.102145
C	-0.055575	-3.918105	-1.118897
C	-1.469672	-5.416331	-2.985435
H	-3.241900	-4.530999	-2.153245
C	0.628323	-4.755514	-1.998085
H	0.498624	-3.331243	-0.381614
C	-0.078822	-5.507119	-2.936148
H	-2.031277	-6.004778	-3.714209
H	1.717787	-4.819200	-1.949024
H	0.453548	-6.164963	-3.626338
C	-3.373630	-3.498926	0.487793
H	-3.059163	-4.474046	0.893392
H	-4.154179	-3.719565	-0.265879
O	-3.872841	-2.729916	1.530714
C	2.534770	-1.365870	1.032272
H	2.267257	-2.418633	1.073708
C	3.740545	-0.992813	0.458348
H	4.077791	0.036735	0.598278
C	4.826988	-1.945844	0.159574
C	6.120854	-1.451193	-0.074036
C	4.627918	-3.334162	0.081078
C	7.177623	-2.307834	-0.371284
H	6.291329	-0.371991	-0.026902
C	5.684061	-4.191939	-0.217170
H	3.633555	-3.754841	0.244418
C	6.964399	-3.684816	-0.444924
H	8.174285	-1.896599	-0.547198
H	5.504742	-5.268034	-0.275536
H	7.790074	-4.359898	-0.680124
C	-0.776633	4.361166	1.342263

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 H    0.153973    3.863921    1.652413
 H   -0.582673    5.439156    1.259246
 H   -1.519812    4.209758    2.139606
 C   -1.892147    4.867174   -3.566459
 H   -1.725800    5.930771   -3.347882
 H   -1.133156    4.551414   -4.299404
 H   -2.874483    4.764445   -4.051188
 H   -2.532390    2.248215   -3.298760
 H   -1.625997    1.825902    0.889153
 O   -4.504684   -0.277146    1.383540
Na   -3.012642   -0.835028    2.941519
 C   -5.288857    0.439548    0.638436
 C   -5.075086    1.830932    0.443259
 C   -6.396510   -0.128864   -0.050101
 C   -5.871997    2.577126   -0.418438
 H   -4.236909    2.300536    0.963436
 C   -7.188017    0.628250   -0.909648
 H   -6.607399   -1.191597    0.105874
 C   -6.933041    1.987567   -1.114437
 H   -5.655926    3.640806   -0.556725
 H   -8.022943    0.147865   -1.429036
 H   -7.554034    2.577573   -1.791891
121
Figure_S3-1_AA-9d(NaOPh)-pc(1,6minor) / electronic energy: -4439.04673704 a.u. / lowest freq: 15.40 cm-1
 H    3.541034    4.119440   -2.668949
 H    5.300121    3.851487   -2.706432
 C    4.470010    4.224608   -2.089911
 H    4.639563    5.291983   -1.890142
 H    2.226451    5.265610   -1.170611
 B    2.934886    1.714420   -1.138813
 O    4.272742    2.031683   -1.167114
 C    2.505869    5.059043   -0.130078
 C    4.409814    3.412629   -0.796076
 O    2.188440    2.704983   -0.553582
 H    3.228823    5.819074    0.201548
 H    1.602534    5.152727    0.486790
 C    3.090801    3.664093    0.023303
 H    6.561426    3.399370   -0.654413
 C    5.695890    3.589398   -0.003505
 H    5.776701    4.616785    0.381728
 H    5.747729    2.892395    0.842888
 C    3.233781    3.310942    1.503302
 H    2.235150    3.272154    1.959415
 H    3.698107    2.323384    1.640226
 H    3.837521    4.054109    2.042682
 C    2.357343    0.356880   -1.633457
 C    3.264586   -0.591883   -1.986421
 H    4.322353   -0.314622   -2.007503
 H    2.141952   -2.074354   -3.101730
 H    2.508454   -2.514341   -1.430379
 C    2.920198   -2.007786   -2.322628
 H    3.796492   -2.579845   -2.657044
 H    0.333553    1.024402   -1.743773
 C    0.918951    0.113434   -1.550175
 H    0.559821   -0.710835   -2.187653
 C   -3.619641   -1.358941   -1.719565
 H   -4.580923   -1.512560   -1.209166
 C   -3.434890    0.097942   -2.142167
 H   -3.090229    0.180275   -3.184236
 C   -1.826193   -0.448518   -0.525685
 C   -2.011962    1.910899   -1.135359
 C   -2.060546    2.721266   -2.271180
 C   -1.614033    2.449296    0.090116
 C   -1.689639    4.066900   -2.199313
 C   -1.240984    3.790655    0.181398
 C   -1.279374    4.585463   -0.968336
 H   -0.994597    5.639036   -0.898707
Cu    0.037502   -0.323007    0.223108
 N   -2.505281   -1.562128   -0.792556
 N   -2.388269    0.555905   -1.222277
 C    1.584366   -0.384810    1.521539
 C    0.363981   -0.606761    2.259730
 H   -4.295339   -1.814575    1.249402
 H   -4.347550    0.697121   -2.016499
 H   -3.550734   -2.060461   -2.563280
 H    1.925599    0.654610    1.550371
 C   -0.190925    0.514120    3.058383
 C   -0.183271   -1.930161    2.599754
 O    0.716482    1.447226    3.350257
 O   -1.337578    0.605545    3.457677
 O   -1.104917   -2.147381    3.366771
 O    0.423524   -2.940064    1.960980
 C   -0.000478   -4.260677    2.273094
 H    0.190270   -4.487246    3.330800
 H    0.587126   -4.923356    1.629064
 H   -1.072382   -4.389469    2.070419
 C    0.326659    2.466755    4.262176
 H   -0.631628    2.914557    3.974928
 H    1.122995    3.218298    4.239899
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 H    0.235774    2.047078    5.274157
 C   -2.218721   -2.869426   -0.223132
 H   -1.481174   -2.677081    0.563404
 C   -1.576432   -3.793960   -1.242911
 C   -2.325418   -4.628072   -2.080669
 C   -0.181905   -3.790273   -1.369544
 C   -1.693068   -5.439532   -3.023688
 H   -3.414450   -4.655549   -2.004578
 C    0.451700   -4.601852   -2.307644
 H    0.411463   -3.138963   -0.721171
 C   -0.304131   -5.429647   -3.138707
 H   -2.292476   -6.084233   -3.670108
 H    1.540515   -4.589178   -2.390195
 H    0.190546   -6.067447   -3.874363
 C   -3.456652   -3.461417    0.464485
 H   -3.177763   -4.459072    0.840598
 H   -4.262621   -3.626833   -0.275580
 O   -3.901760   -2.693965    1.533284
 C    2.628860   -1.334102    1.201119
 H    2.394601   -2.394635    1.267923
 C    3.857834   -0.931273    0.805384
 H    4.076963    0.139354    0.770859
 C    4.987026   -1.801346    0.452018
 C    6.220813   -1.211453    0.130447
 C    4.889700   -3.202253    0.400912
 C    7.319277   -1.989250   -0.227030
 H    6.306986   -0.121602    0.148343
 C    5.986903   -3.980423    0.042757
 H    3.943471   -3.694176    0.635243
 C    7.207185   -3.379333   -0.272416
 H    8.267694   -1.507189   -0.474490
 H    5.887885   -5.067762    0.005992
 H    8.065753   -3.992615   -0.554797
 C   -0.828188    4.365102    1.507917
 H    0.099157    3.888802    1.858109
 H   -0.653896    5.447945    1.445636
 H   -1.600568    4.188221    2.271730
 C   -1.716935    4.923095   -3.438537
 H   -1.538062    5.980993   -3.202702
 H   -0.942639    4.601107   -4.152429
 H   -2.686333    4.844398   -3.953013
 H   -2.376463    2.304833   -3.229249
 H   -1.643679    1.823008    0.985120
 O   -4.541189   -0.247302    1.415231
Na   -3.045272   -0.861869    2.950214
 C   -5.299307    0.483158    0.656570
 C   -5.064087    1.872739    0.472850
 C   -6.398766   -0.067809   -0.058533
 C   -5.834618    2.633044   -0.400374
 H   -4.230754    2.329435    1.012041
 C   -7.163599    0.703267   -0.929584
 H   -6.625078   -1.128940    0.086531
 C   -6.888648    2.060610   -1.120853
 H   -5.602950    3.694734   -0.528399
 H   -7.993131    0.235506   -1.468699
 H   -7.489087    2.661880   -1.806855
89
Figure_S3-1_9d(NaOPh)-Cu-allyl / electronic energy: -3597.06845638 a.u. / lowest freq: 14.75 cm-1
Na    1.466278   -1.713895    0.568774
 H    4.895602   -3.588713    0.817161
 H    4.692117   -0.895972   -2.541156
 O    3.335573   -2.007938   -0.584046
 C    5.271052   -1.564621   -1.896670
 C    4.600612   -2.207337   -0.820863
 H    7.102470   -1.262094   -2.980981
 C    6.625148   -1.776136   -2.141098
 C    5.384324   -3.077572   -0.017672
 C    7.377630   -2.634567   -1.334758
 C    6.737508   -3.280572   -0.272517
 H    8.439672   -2.798024   -1.529682
 H    7.306712   -3.957090    0.372185
 H    1.822369   -0.807067    3.943134
 H   -2.251641   -0.329887    3.139589
 C    0.449649   -2.296353    3.162582
 C   -1.148749   -0.342683    3.068826
 H    0.743177   -3.269591    2.747587
 C   -0.656265   -1.681110    2.668089
 H   -0.722254    0.025625    4.016197
 B   -1.373536   -2.298457    1.423828
 O   -2.713492   -2.319048    1.179742
 H   -1.727987   -0.728011   -0.976153
 O   -0.646091   -2.774963    0.347830
 H   -0.369549   -1.436810   -1.877879
 C   -1.416767   -1.592283   -1.578998
 H   -3.924597   -1.288533   -0.925882
 C   -1.545189   -2.887384   -0.779148
 C   -2.937112   -3.023746   -0.060716
 C   -4.089317   -2.364956   -0.799421
 H   -2.035120   -1.618693   -2.487150
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 H   -5.022038   -2.500680   -0.233511
 H   -2.452907   -4.961768    0.822840
 H   -4.156010   -4.465844    0.969667
 C   -3.284310   -4.466581    0.300122
 H   -0.161528   -3.891634   -2.091822
 C   -1.138452   -4.082032   -1.624394
 H   -1.058778   -4.996627   -1.023531
 H   -4.221693   -2.822726   -1.791255
 H   -3.534901   -5.053460   -0.594647
 H   -1.873021   -4.249881   -2.425820
 H    2.084171   -2.447422    4.577693
 C    1.310104   -1.734587    4.260318
 H    0.715848   -1.463962    5.150374
 C    0.319514    2.875268   -1.993392
 H    1.033917    2.506723   -2.740473
 C   -1.127654    2.540540   -2.354801
 H   -1.705390    3.414017   -2.684987
 C   -0.661312    1.729692   -0.210974
 C   -3.004911    1.645974   -0.933491
 C   -3.559642    1.488554    0.340873
 C   -3.804764    1.434619   -2.061581
 C   -4.882144    1.072030    0.498446
 C   -5.140732    1.044490   -1.923628
 C   -5.665477    0.864801   -0.641218
 H   -6.706703    0.550845   -0.526471
Cu   -0.836713    0.775737    1.479326
 N    0.481016    2.176611   -0.718861
 N   -1.650734    2.012129   -1.089715
 H    2.605203   -0.823585   -1.253202
 H   -1.180566    1.768453   -3.138589
 H    0.488311    3.954711   -1.852253
 C    1.783728    1.989569   -0.103034
 H    1.577644    1.419376    0.818373
 C    2.387717    3.326050    0.305028
 C    3.684660    3.715190   -0.041325
 C    1.611056    4.193427    1.085504
 C    4.194290    4.943729    0.386120
 H    4.319736    3.066305   -0.646305
 C    2.116435    5.418098    1.511249
 H    0.594881    3.899472    1.363203
 C    3.414073    5.797630    1.161301
 H    5.210992    5.230395    0.108577
 H    1.496950    6.078282    2.122170
 H    3.815380    6.756940    1.495184
 C    2.667582    1.110708   -0.990647
 H    3.584280    0.863576   -0.424765
 H    2.991597    1.684656   -1.881421
 O    1.975771   -0.040827   -1.362266
 C   -5.977773    0.764471   -3.144325
 H   -5.678591    1.395447   -3.993282
 H   -5.860945   -0.286000   -3.456591
 H   -7.045661    0.932149   -2.946707
 C   -5.429241    0.820029    1.877761
 H   -6.526964    0.864113    1.893808
 H   -5.127045   -0.182053    2.222954
 H   -5.039940    1.546746    2.605212
 H   -2.959357    1.704718    1.226933
 H   -3.392248    1.559302   -3.063750
89
Figure_S3-1_9b(NaOPh)-Cu-allyl / electronic energy: -3597.06856996 a.u. / lowest freq: 15.34 cm-1
Na    0.148120   -2.350929   -0.661887
 H    2.438637   -3.886514    0.418400
 H    4.437536   -1.625816   -2.657585
 O    2.188175   -1.934213   -1.331976
 C    4.457113   -2.409826   -1.896029
 C    3.271723   -2.638718   -1.144621
 H    6.503884   -2.941304   -2.274753
 C    5.611926   -3.155530   -1.678013
 C    3.330703   -3.680261   -0.180384
 C    5.648755   -4.168717   -0.715703
 C    4.491286   -4.420599    0.026190
 H    6.559206   -4.747918   -0.547636
 H    4.492260   -5.208637    0.785191
 H    2.110038   -1.789209    2.251941
 H   -1.683682   -0.084569    3.012140
 C    0.177417   -2.763996    2.184032
 C   -0.716422   -0.448477    2.624984
 H    0.009685   -3.753268    1.738460
 C   -0.814296   -1.836152    2.123482
 H    0.060429   -0.307140    3.395789
 B   -2.112989   -2.153360    1.318568
 O   -3.369101   -1.737541    1.633548
 H   -2.845676   -0.482203   -0.927861
 O   -2.073350   -2.793843    0.089938
 H   -2.386052   -1.604043   -2.238318
 C   -3.158779   -1.375665   -1.489089
 H   -4.906254   -0.251131    0.103283
 C   -3.345234   -2.575300   -0.562814
 C   -4.288875   -2.263960    0.657935
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 C   -5.353692   -1.214414    0.379956
 H   -4.085231   -1.134855   -2.028538
 H   -5.962317   -1.060989    1.282259
 H   -4.158934   -4.286914    1.470992
 H   -5.400718   -3.251670    2.212692
 C   -4.917121   -3.518031    1.262489
 H   -3.003759   -3.952870   -2.186413
 C   -3.717784   -3.812772   -1.361912
 H   -3.704627   -4.717295   -0.741233
 H   -6.020495   -1.543104   -0.431111
 H   -5.677701   -3.946520    0.595013
 H   -4.721339   -3.698819   -1.797645
 H    2.106807   -3.437236    2.912827
 C    1.510733   -2.517409    2.830805
 H    1.401035   -2.091228    3.843076
 C    1.280515    3.069545   -2.003442
 H    1.565108    2.605156   -2.959047
 C   -0.172818    3.561404   -1.995315
 H   -0.276419    4.578520   -1.584882
 C    0.060095    1.792810   -0.476656
 C   -2.217588    2.610963   -0.829080
 C   -2.678385    3.129778    0.395038
 C   -3.100884    2.109301   -1.801083
 C   -4.054535    3.111730    0.641038
 C   -4.470186    2.122037   -1.519756
 C   -4.944329    2.613849   -0.307033
 H   -6.016384    2.608530   -0.098720
Cu   -0.341132    0.639697    1.032050
 N    1.273784    2.050851   -0.951347
 N   -0.819266    2.595349   -1.099937
 H    2.443780   -0.610758   -2.213460
 H   -0.629024    3.549352   -2.994037
 H    1.996706    3.870578   -1.771134
 C    2.484707    1.372525   -0.497575
 H    2.139125    0.425669   -0.056505
 C    3.187276    2.170139    0.586692
 C    4.053990    3.229208    0.291404
 C    2.928357    1.870261    1.929919
 C    4.643739    3.972204    1.314760
 H    4.282158    3.482129   -0.746497
 C    3.515716    2.610503    2.954124
 H    2.250016    1.047192    2.174293
 C    4.375475    3.666125    2.648300
 H    5.320155    4.793092    1.066340
 H    3.303057    2.360630    3.995928
 H    4.838980    4.246461    3.449152
 C    3.374358    0.994741   -1.687423
 H    4.246875    0.448944   -1.277619
 H    3.774104    1.901226   -2.172724
 O    2.681605    0.261974   -2.643836
 H   -4.432045    3.504641    1.588162
 H   -5.170862    1.726395   -2.259259
 C   -2.592705    1.563034   -3.108381
 H   -2.423060    2.369586   -3.840006
 H   -1.639450    1.031325   -2.978681
 H   -3.320420    0.870396   -3.551477
 C   -1.723572    3.682246    1.419703
 H   -1.210134    2.868739    1.959856
 H   -0.940363    4.298843    0.955650
 H   -2.256508    4.292551    2.160509
121
Figure_S3-1_AA-9b(NaOPh)-pc(1,6minor) / electronic energy: -4439.04836588 a.u. / lowest freq: 17.74 cm-1
 H    5.006221   -3.838273    2.000642
 H    6.968080   -3.117877    1.002714
 C    4.701490   -4.467820    1.151939
 H    3.820060   -5.049255    1.458295
 B    3.676188   -1.588518    0.714762
 O    5.014836   -1.439220    0.432725
 H    5.517082   -5.168421    0.923706
 C    6.844125   -2.928421   -0.070954
 O    3.202868   -2.811196    0.308844
 C    4.333102   -3.620057   -0.065458
 C    5.414911   -2.532865   -0.407154
 H    7.135384   -3.833500   -0.624648
 C    3.956037   -4.517430   -1.233190
 H    5.955000   -1.147801   -1.966205
 C    5.328834   -2.044576   -1.854079
 H    4.840903   -5.054843   -1.605284
 H    4.296885   -1.775206   -2.124597
 H    3.523322   -3.942074   -2.061247
 H    5.685629   -2.805294   -2.562558
 H    3.219080   -5.265699   -0.906883
 H    7.530982   -2.118548   -0.355846
 C    2.814277   -0.468212    1.365602
 C    1.375729   -0.625444    1.507095
 H    0.930908   -0.015461    2.305213
 H    1.046796   -1.673625    1.586337
 C    3.452356    0.695262    1.675816
 H    4.536244    0.746507    1.538561
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H	2.316915	1.714736	3.211653
H	1.924964	2.204122	1.564217
C	2.763164	1.904801	2.219763
H	3.443618	2.762303	2.311548
C	-3.562824	1.000128	1.681941
H	-4.436180	1.308947	1.094710
C	-3.622094	-0.491062	2.030093
H	-3.657282	-0.679790	3.113049
C	-1.676524	-0.069231	0.796944
C	-1.941852	-2.343136	1.669104
C	-2.310087	-3.335200	0.746894
C	-1.188784	-2.642071	2.820002
C	-1.848797	-4.639386	0.962924
C	-0.739873	-3.953638	2.992052
C	-1.057934	-4.944017	2.065679
H	-0.696824	-5.964156	2.213749
Cu	0.133698	-0.180063	-0.029561
N	-2.332961	1.088858	0.887173
N	-2.368977	-0.999307	1.461482
C	1.458571	0.104685	-1.523984
C	0.169066	-0.106014	-2.149090
H	-3.925911	1.630106	-1.207787
H	-4.484316	-0.990377	1.560405
H	-3.500858	1.645563	2.571614
H	2.111225	-0.771618	-1.514158
C	-0.247589	-1.502297	-2.398207
C	-0.616331	0.937371	-2.834808
O	0.656603	-2.387036	-1.969685
O	-1.299890	-1.875090	-2.894208
O	-1.599862	0.744144	-3.528825
O	-0.155230	2.176520	-2.652861
C	-0.884990	3.229818	-3.276633
H	-0.847835	3.128571	-4.369961
H	-0.386675	4.157023	-2.972052
H	-1.930423	3.211408	-2.938499
C	0.326309	-3.764029	-2.049311
H	-0.539614	-3.992502	-1.414081
H	1.202511	-4.299759	-1.674559
H	0.109510	-4.056769	-3.085686
C	-1.834500	2.325221	0.314218
H	-1.194357	2.031873	-0.529580
C	-0.965324	3.136984	1.262517
C	-0.222412	4.203439	0.738057
C	-0.846199	2.849752	2.624124
C	0.598259	4.975983	1.554904
H	-0.278862	4.424685	-0.331451
C	-0.028628	3.626087	3.447042
H	-1.379461	2.000518	3.054376
C	0.692510	4.693439	2.918089
H	1.173015	5.798520	1.123775
H	0.052378	3.384532	4.509035
H	1.337326	5.295824	3.561138
C	-2.981127	3.145192	-0.296986
H	-2.565852	4.112330	-0.619382
H	-3.722707	3.380390	0.493425
O	-3.554682	2.538426	-1.406280
C	2.121958	1.363526	-1.284667
H	1.517807	2.268652	-1.268275
C	3.450927	1.435539	-1.024366
H	4.054621	0.528412	-1.100176
C	4.199418	2.660112	-0.713614
C	5.594629	2.585333	-0.567903
C	3.581051	3.907452	-0.523348
C	6.346863	3.712176	-0.245786
H	6.088947	1.618614	-0.696528
C	4.332054	5.034810	-0.203658
H	2.496573	3.998424	-0.606827
C	5.718424	4.944389	-0.062504
H	7.429905	3.626512	-0.132208
H	3.830162	5.994069	-0.056516
H	6.304384	5.830080	0.192881
Na	-3.276992	-0.605920	-2.784464
O	-4.574046	0.129637	-1.167031
C	-5.798743	0.076411	-0.726141
C	-6.536218	1.255061	-0.422413
C	-6.464595	-1.158489	-0.497386
C	-7.830997	1.194034	0.085039
H	-6.058118	2.220397	-0.611553
C	-7.760606	-1.204374	0.009512
H	-5.933405	-2.085157	-0.728413
C	-8.460676	-0.032899	0.311747
H	-8.360460	2.126022	0.304934
H	-8.234718	-2.177026	0.172184
H	-9.475820	-0.075864	0.712096
H	-0.135263	-4.199936	3.868382
H	-2.121876	-5.423731	0.252125
C	-3.181397	-3.031692	-0.441291
H	-3.619383	-2.025434	-0.394692
H	-2.601817	-3.096453	-1.374525

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 H   -3.998205   -3.765365   -0.510444
 C   -0.904705   -1.599752    3.868615
 H    0.061951   -1.785841    4.355593
 H   -0.884611   -0.587029    3.448063
 H   -1.681598   -1.622630    4.650065
121
Figure_S3-1_AA-9b(NaOPh)-ts(1,6minor) / electronic energy: -4439.04644858 a.u. / lowest freq: -305.39 cm-1
 C   -0.816448   -1.703765    3.816329
 H   -0.728413   -0.673569    3.448528
 H   -1.666631   -1.735577    4.517117
 H    0.091652   -1.941629    4.386280
 H    2.074218    2.369535    1.540851
 H    0.950529   -1.411559    1.694922
 C    3.524345    0.779378    1.365728
 C    1.381267   -0.413942    1.547875
 H    4.608238    0.688334    1.255940
 C    2.769530   -0.379659    1.265206
 H    0.968521    0.353206    2.214848
 B    3.424432   -1.675624    0.704774
 O    2.857177   -2.918157    0.817555
 H    3.200795   -2.699393   -1.995908
 O    4.622117   -1.708923    0.036700
 H    4.830442   -2.198008   -2.504259
 C    4.266496   -2.968298   -1.958796
 H    2.506423   -4.721656   -1.074730
 C    4.773777   -3.029879   -0.518678
 C    3.845678   -3.884588    0.418373
 C    3.155100   -5.056594   -0.258178
 H    4.405402   -3.928372   -2.476126
 H    2.529591   -5.589692    0.471891
 H    5.076151   -3.522360    2.185854
 H    3.805632   -4.752332    2.387812
 C    4.554868   -4.353765    1.688973
 H    6.811134   -2.780521   -1.180317
 C    6.242541   -3.420207   -0.490186
 H    6.673107   -3.304490    0.512493
 H    3.895432   -5.764387   -0.659584
 H    5.285605   -5.145917    1.473306
 H    6.369746   -4.465260   -0.809826
 H    3.724035    2.832893    2.022770
 C    2.995015    2.012256    2.032719
 H    2.726907    1.811601    3.084803
 C   -3.479536    0.945164    1.791081
 H   -4.379440    1.279805    1.260737
 C   -3.505537   -0.567237    2.040728
 H   -3.527530   -0.825400    3.109342
 C   -1.603055   -0.027984    0.788840
 C   -1.765246   -2.345269    1.548648
 C   -1.018260   -2.686169    2.693241
 C   -2.045253   -3.281805    0.542198
 C   -0.481337   -3.972446    2.772567
 C   -1.493040   -4.563534    0.664399
 C   -0.705282   -4.901618    1.758944
 H   -0.271876   -5.901512    1.832403
Cu    0.173531   -0.071472   -0.102109
 N   -2.281709    1.106271    0.959659
 N   -2.249146   -1.009691    1.426484
 C    1.510555    0.262642   -1.637265
 C    0.199135    0.078909   -2.238643
 H   -3.918781    1.755908   -1.047723
 H   -4.361291   -1.052381    1.545017
 H   -3.390830    1.529430    2.720223
 H    2.148130   -0.624004   -1.674116
 C   -0.200935   -1.282629   -2.620828
 C   -0.622124    1.165440   -2.791431
 O    0.750782   -2.201225   -2.393177
 O   -1.281106   -1.617871   -3.084909
 O   -1.647963    1.034203   -3.440127
 O   -0.147827    2.390296   -2.535136
 C   -0.911502    3.485330   -3.031403
 H   -0.918545    3.485577   -4.130249
 H   -0.410460    4.388504   -2.664936
 H   -1.943447    3.424536   -2.657846
 C    0.431483   -3.558414   -2.655994
 H   -0.114583   -3.990292   -1.804582
 H    1.387029   -4.078921   -2.782999
 H   -0.170023   -3.653369   -3.568132
 C   -1.817523    2.381965    0.445817
 H   -1.216891    2.149096   -0.444559
 C   -0.904519    3.135009    1.402194
 C   -0.179411    4.228848    0.909791
 C   -0.730005    2.770350    2.739244
 C    0.673847    4.955221    1.735747
 H   -0.276523    4.509527   -0.142393
 C    0.122470    3.498324    3.571276
 H   -1.249582    1.899692    3.142546
 C    0.821624    4.596156    3.076014
 H    1.233051    5.800485    1.328765
 H    0.245424    3.196231    4.613569
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 H    1.491845    5.162006    3.726171
 C   -2.996249    3.230709   -0.053494
 H   -2.604122    4.224328   -0.319732
 H   -3.705897    3.397413    0.782453
 O   -3.610683    2.699079   -1.179774
 C    2.177976    1.457440   -1.284976
 H    1.617997    2.389837   -1.275160
 C    3.509629    1.450840   -0.906315
 H    4.092111    0.547897   -1.101925
 C    4.301308    2.677439   -0.707037
 C    5.702030    2.588135   -0.650833
 C    3.715013    3.943891   -0.543025
 C    6.488907    3.717610   -0.438540
 H    6.176128    1.609801   -0.769603
 C    4.500363    5.073709   -0.330733
 H    2.628625    4.049561   -0.558719
 C    5.891366    4.968166   -0.276233
 H    7.576247    3.619935   -0.396899
 H    4.020547    6.046625   -0.200064
 H    6.504986    5.855581   -0.106527
 H   -1.696383   -5.305960   -0.112022
 H    0.123932   -4.246189    3.640069
 C   -2.927916   -2.949561   -0.629403
 O   -4.497508    0.218862   -1.094721
Na   -3.261915   -0.435559   -2.798175
 C   -5.707532    0.088882   -0.631162
 C   -6.312957   -1.184783   -0.449796
 C   -6.489739    1.216901   -0.253941
 C   -7.594528   -1.314066    0.079291
 H   -5.744827   -2.073802   -0.735687
 C   -7.768831    1.072374    0.275279
 H   -6.057364    2.210276   -0.403628
 C   -8.338969   -0.191462    0.452734
 H   -8.021847   -2.313708    0.203976
 H   -8.334125    1.967478    0.552392
 H   -9.342193   -0.299671    0.870459
 H   -3.729193   -3.698486   -0.721093
 H   -2.356256   -2.963210   -1.568712
 H   -3.391512   -1.958153   -0.532641
108
Figure_S3-1_AA-9b(NaOPh)-prod(1,6minor) / electronic energy: -4131.89527188 a.u. / lowest freq: 22.82 cm-1
 C    1.394849    1.937125   -2.756669
 H    0.098919    3.479501   -2.023850
 C    0.403146    2.460198   -1.725160
 H    2.276582    2.590122   -2.814258
 H    2.835519    6.862365    0.027038
 H    0.949715    5.251263    0.002083
 C    3.035070    5.794957   -0.093054
 C    1.976159    4.888315   -0.106089
 H    5.179490    6.045863   -0.211312
 C    4.347049    5.338780   -0.224387
 C    2.200852    3.513268   -0.250438
 C    4.585361    3.972419   -0.368789
 C    1.006247    2.574450   -0.296031
 H    0.227332    3.037721    0.324728
 C    3.522571    3.069059   -0.381051
 H    5.608416    3.602622   -0.471805
 H    3.730423    2.003386   -0.492244
 C    1.305535    1.214640    0.299028
 H    2.165386    0.678749   -0.107748
 C   -0.873629    1.635922   -1.612724
 H   -0.050099    1.384209    1.894011
 C    0.793943    0.801166    1.502190
 H   -0.451378    0.152244   -3.133567
 C   -1.139181    0.524942   -2.367790
 H   -2.130485    0.064643   -2.335220
Cu   -0.265367   -0.147889   -0.490389
 C   -0.373151   -2.131976   -0.576681
 N   -1.454394   -2.893173   -0.824203
 H    2.052802   -1.588560   -5.026692
 N    0.691732   -2.923423   -0.543858
 C    2.672023   -0.592548    2.503149
 O    3.490063    0.110819    1.684107
 C    1.275920   -0.246977    2.385060
 O    0.539931   -1.819604    4.042015
 C    0.356056   -0.840918    3.321447
 C    2.053324   -2.438263   -0.388952
 C    0.385192   -4.327213   -0.841301
 H    0.830267   -4.956333   -0.060098
 C   -1.144511   -4.328313   -0.854337
 H   -1.569395   -4.805029   -1.748504
 C   -2.790689   -2.419570   -0.939222
 C   -3.521966   -2.147158    0.226763
 C   -3.351741   -2.275131   -2.219248
 C   -4.846473   -1.723381    0.091259
 C   -4.674700   -1.832057   -2.313876
 C   -5.418360   -1.563830   -1.167809
 H   -6.452618   -1.224310   -1.257949
Na    2.065336   -3.409897    3.298196
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 H   -1.576343   -4.823520    0.031012
 H    0.812017   -4.610335   -1.817384
 O   -0.847687   -0.209803    3.364734
 O    3.171221   -1.405471    3.278461
 C    4.877000   -0.118117    1.826358
 H    5.220855    0.112632    2.845035
 H    5.370391    0.550740    1.110404
 H    5.133436   -1.164435    1.600810
 C   -1.763565   -0.658320    4.344082
 H   -1.943645   -1.738807    4.260678
 H   -2.696323   -0.110031    4.167227
 H   -1.392540   -0.443283    5.357414
 H    2.012972   -1.659040    0.383381
 C    2.596607   -1.821979   -1.661062
 C    3.755741   -1.035769   -1.595913
 C    1.996846   -2.006054   -2.912371
 C    4.302820   -0.460944   -2.740789
 H    4.224675   -0.863034   -0.626131
 C    2.541588   -1.432344   -4.062178
 H    1.081086   -2.594902   -2.994985
 C    3.698377   -0.659025   -3.982906
 H    5.202579    0.153597   -2.660804
 H    4.121879   -0.204938   -4.881213
 C    2.957536   -3.573742    0.194591
 H    3.965003   -3.087322    0.303566
 H    3.108389   -4.300012   -0.656149
 O    2.463421   -4.118494    1.312350
 H    1.747427    0.923332   -2.510735
 H    0.942578    1.898845   -3.758543
 B   -2.036995    2.166233   -0.699805
 O   -2.003634    3.364042   -0.047238
 O   -3.189384    1.470049   -0.479010
 C   -3.306537    3.590572    0.529271
 C   -3.900484    2.132857    0.587714
 C   -3.548929    1.392221    1.875231
 H   -2.467620    1.412049    2.076206
 H   -4.076960    1.814547    2.741522
 H   -3.846389    0.341439    1.764972
 C   -5.394244    2.048226    0.320405
 H   -5.951696    2.639600    1.061794
 H   -5.646693    2.412860   -0.683047
 H   -5.722799    1.003006    0.395437
 C   -4.062145    4.510907   -0.426956
 H   -3.485507    5.436621   -0.563659
 H   -4.195537    4.042207   -1.412820
 H   -5.051192    4.776083   -0.028433
 C   -3.132247    4.259133    1.883322
 H   -4.104101    4.368767    2.386819
 H   -2.461278    3.683904    2.533577
 H   -2.701593    5.261608    1.748498
 C   -2.546941   -2.586937   -3.452679
 H   -1.520329   -2.202737   -3.367683
 H   -2.472417   -3.674011   -3.616177
 H   -3.010541   -2.149095   -4.346581
 C   -2.875707   -2.284296    1.576075
 H   -2.377669   -3.257826    1.696466
 H   -2.104026   -1.511204    1.715661
 H   -3.616558   -2.175461    2.379290
 H   -5.125896   -1.700201   -3.300329
 H   -5.435043   -1.515514    0.988624
83
Figure_S4-1_PA-9d(Na)-prod(1,6major) / electronic energy: -3681.07040691 a.u. / lowest freq: 16.84 cm-1
 C    3.359716    2.192561    0.186378
 H    4.084937    2.045474   -0.623987
 C    2.301682    3.253634   -0.084287
 H    2.487627    4.197878    0.443917
 C    1.252797    1.255216    0.519749
 C   -0.154011    3.268993    0.464251
 C   -0.319177    4.494082   -0.187628
 C   -1.234976    2.721506    1.168563
 C   -1.560009    5.142558   -0.190544
 C   -2.481791    3.342500    1.164703
 C   -2.635440    4.552248    0.475124
 H   -3.608401    5.051384    0.474548
Cu   -0.121667   -0.113799    0.916922
 N    2.533441    0.987727    0.317927
 N    1.081772    2.599858    0.407618
 C   -0.564338   -1.667253   -0.868412
 C    0.339764   -1.258115   -1.914799
Na    3.394344   -0.054629   -3.260847
 H    2.204253    3.468661   -1.162679
 H    3.895673    2.382327    1.131622
 H   -0.320887   -2.664768   -0.488597
 C    0.330184    0.057031   -2.510178
 C    1.379788   -2.181028   -2.311050
 O   -0.739871    0.790831   -2.142238
 O    1.175437    0.555265   -3.250797
 O    2.232930   -2.017594   -3.178391
 O    1.379155   -3.338978   -1.604480
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 C    2.407538   -4.265605   -1.896842
 H    2.351645   -4.607837   -2.940246
 H    2.254729   -5.113124   -1.218654
 H    3.399527   -3.823111   -1.723251
 C   -0.815652    2.115161   -2.630712
 H    0.107083    2.670519   -2.414192
 H   -1.657088    2.587839   -2.110041
 H   -0.986911    2.126332   -3.717459
 C    3.068782   -0.375270    0.295079
 H    2.466909   -0.929703   -0.436890
 C    2.913517   -1.055084    1.632471
 C    3.331851   -0.440029    2.819155
 C    2.353206   -2.335772    1.700930
 C    3.189746   -1.088835    4.045036
 H    3.762730    0.563840    2.785479
 C    2.209549   -2.987696    2.926046
 H    2.009673   -2.814301    0.779042
 C    2.626782   -2.366278    4.102388
 H    3.519665   -0.595379    4.962203
 H    1.758775   -3.981983    2.962468
 H    2.509601   -2.871378    5.063609
 C    4.523399   -0.386753   -0.259662
 H    4.841665   -1.457743   -0.141037
 H    5.143480    0.155563    0.512282
 O    4.619823    0.106165   -1.502499
 C   -1.673705   -1.103385   -0.279100
 H   -2.108769   -0.183596   -0.678769
 C   -2.533340   -1.923593    0.669128
 H   -1.995303   -2.860483    0.883000
 C   -3.870211   -2.293151    0.052170
 C   -4.201326   -3.633394   -0.170953
 C   -4.792318   -1.306787   -0.322316
 C   -5.420834   -3.983663   -0.751757
 H   -3.491248   -4.415155    0.111738
 C   -6.012090   -1.651995   -0.900811
 H   -4.555115   -0.250350   -0.169659
 C   -6.330977   -2.993550   -1.117888
 H   -5.658039   -5.036680   -0.919528
 H   -6.717437   -0.868909   -1.187771
 H   -7.285637   -3.264252   -1.574113
 C   -3.642936    2.709122    1.886248
 H   -3.302719    2.104875    2.739717
 H   -4.349242    3.464481    2.258237
 H   -4.204892    2.044533    1.209744
 C   -1.716402    6.449919   -0.923143
 H   -2.717092    6.878335   -0.776058
 H   -0.974363    7.186701   -0.580138
 H   -1.561701    6.313378   -2.004789
 H    0.512466    4.951260   -0.725950
 H   -1.094165    1.812936    1.754301
 C   -0.345908   -0.525533    3.086856
 H    0.549898   -0.328070    3.656043
 C   -1.418580   -0.828411    2.582812
 C   -2.721248   -1.202714    2.022067
 H   -3.270254   -1.835958    2.736222
 H   -3.314996   -0.284862    1.882176
83
Figure_S4-1_PA-9d(Na)-ts(1,6major) / electronic energy: -3681.01674239 a.u. / lowest freq: -425.84 cm-1
 C    2.866803    2.675946    1.037241
 H    3.618483    3.073400    0.344267
 C    1.496643    3.345149    0.935558
 H    1.285729    4.038149    1.760640
 C    1.246966    1.039170    0.692392
 C   -0.796962    2.290790    1.180897
 C   -1.490484    3.438376    0.798338
 C   -1.479557    1.247321    1.820637
 C   -2.874586    3.531001    0.998245
 C   -2.851518    1.327151    2.045160
 C   -3.540848    2.470137    1.614215
 H   -4.618525    2.543255    1.788127
Cu    0.443095   -0.673683    0.087133
 N    2.545629    1.293601    0.660974
 N    0.593216    2.188102    0.972750
 C   -0.520351   -1.415746   -1.646627
 C    0.525645   -0.530428   -2.098307
Na    3.541048    1.559954   -2.683597
 H    1.377226    3.887276   -0.017588
 H    3.266719    2.708454    2.064537
 H   -0.293059   -2.477742   -1.765329
 C    0.359803    0.903986   -2.362672
 C    1.798868   -1.136899   -2.511518
 O   -0.906702    1.322018   -2.270671
 O    1.249489    1.695745   -2.636288
 O    2.729106   -0.577606   -3.070754
 O    1.883062   -2.439152   -2.201216
 C    3.067140   -3.118499   -2.585350
 H    3.157940   -3.161586   -3.680079
 H    2.981622   -4.130150   -2.174801
 H    3.957585   -2.618517   -2.178973
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 C   -1.154302    2.696016   -2.515703
 H   -0.506982    3.328730   -1.895213
 H   -2.204989    2.866151   -2.256610
 H   -0.981270    2.936927   -3.574367
 C    3.541140    0.255101    0.406446
 H    3.238270   -0.254293   -0.521579
 C    3.569791   -0.776710    1.510104
 C    3.338648   -0.440898    2.848798
 C    3.833792   -2.114224    1.194831
 C    3.358980   -1.418274    3.843111
 H    3.114557    0.593821    3.117691
 C    3.857616   -3.094769    2.184782
 H    4.001163   -2.392857    0.151635
 C    3.616254   -2.750116    3.514915
 H    3.167032   -1.139253    4.881685
 H    4.052018   -4.135263    1.915236
 H    3.623372   -3.516908    4.292376
 C    4.920609    0.898773    0.075156
 H    5.615125    0.019787   -0.011122
 H    5.252989    1.400160    1.029742
 O    4.871332    1.700685   -0.997615
 C   -1.825621   -1.113976   -1.224459
 H   -2.112915   -0.072661   -1.093273
 C   -2.736375   -2.126181   -0.917369
 H   -2.504266   -3.121690   -1.302082
 C   -4.180716   -1.862138   -0.728250
 C   -5.091188   -2.927133   -0.811338
 C   -4.686171   -0.577836   -0.471120
 C   -6.457825   -2.720791   -0.638977
 H   -4.716894   -3.934837   -1.011349
 C   -6.052175   -0.370517   -0.297835
 H   -4.007551    0.273745   -0.389597
 C   -6.945620   -1.439678   -0.379347
 H   -7.147072   -3.565407   -0.707643
 H   -6.421400    0.637572   -0.095148
 H   -8.016271   -1.274778   -0.241455
 C   -3.571403    0.223601    2.775210
 H   -2.873392   -0.563606    3.091738
 H   -4.079472    0.612349    3.670806
 H   -4.340469   -0.236372    2.136249
 C   -3.621699    4.751481    0.526618
 H   -4.614503    4.821204    0.991853
 H   -3.067914    5.673798    0.755415
 H   -3.766496    4.721037   -0.565435
 H   -0.962707    4.269764    0.326130
 H   -0.924754    0.375016    2.167759
 C    0.058354   -2.071084    1.498789
 H    0.887162   -2.110107    2.209329
 C   -1.081011   -2.617436    1.438593
 C   -2.349736   -2.995465    1.131882
 H   -2.536143   -4.018874    0.794614
 H   -3.176879   -2.515024    1.662542
83
Figure_S4-1_PA-9d(Na)-pc(1,6major) / electronic energy: -3681.03006649 a.u. / lowest freq: 18.39 cm-1
 C   -3.023393    1.926663   -1.975684
 H   -3.734352    2.631185   -1.527316
 C   -1.644732    2.532563   -2.247739
 H   -1.460479    2.735628   -3.310896
 C   -1.402412    0.617317   -0.940675
 C    0.652603    1.501882   -1.882637
 C    1.359014    2.709201   -1.868560
 C    1.339277    0.294672   -2.012511
 C    2.754866    2.706409   -1.925556
 C    2.736594    0.269001   -2.064975
 C    3.429058    1.480180   -2.007548
 H    4.522556    1.472153   -2.038805
Cu   -0.443186   -0.653845    0.252837
 N   -2.699485    0.874906   -1.002373
 N   -0.752993    1.482267   -1.747403
 C    0.760117   -0.627317    1.919256
 C   -0.135673    0.472048    1.979585
Na   -2.935225    2.839754    1.562535
 H   -1.490409    3.465715   -1.680749
 H   -3.469084    1.485925   -2.882489
 H    0.498041   -1.513492    2.501012
 C    0.207989    1.890904    1.671427
 C   -1.433009    0.294213    2.680471
 O    1.493583    2.169302    1.832244
 O   -0.595730    2.739101    1.334695
 O   -2.173521    1.191039    3.035081
 O   -1.735423   -0.985506    2.885773
 C   -2.968272   -1.264192    3.539023
 H   -2.954150   -0.882689    4.569069
 H   -3.070482   -2.353768    3.537429
 H   -3.805816   -0.801485    2.998386
 C    1.914143    3.504478    1.577594
 H    1.653824    3.801238    0.554086
 H    3.001317    3.507010    1.706997
 H    1.445484    4.196091    2.290993
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 C   -3.700064    0.104960   -0.274107
 H   -3.278032   -0.077292    0.727101
 C   -3.981229   -1.240056   -0.906391
 C   -3.683604   -1.525988   -2.242664
 C   -4.571875   -2.243679   -0.127525
 C   -3.970192   -2.778103   -2.787385
 H   -3.199125   -0.773480   -2.867716
 C   -4.859570   -3.495455   -0.667201
 H   -4.794098   -2.045174    0.924454
 C   -4.560659   -3.767787   -2.002909
 H   -3.725232   -2.981151   -3.832436
 H   -5.311379   -4.266157   -0.038477
 H   -4.778748   -4.749920   -2.427927
 C   -4.966335    0.987140   -0.041987
 H   -5.669686    0.316865    0.520821
 H   -5.450089    1.080375   -1.056977
 O   -4.682120    2.151527    0.554778
 C    2.115488   -0.564051    1.404286
 H    2.390812    0.312596    0.816910
 C    3.021022   -1.546790    1.581871
 H    2.733256   -2.447012    2.132268
 C    4.396575   -1.501236    1.064643
 C    5.099492   -2.697931    0.854882
 C    5.033063   -0.289850    0.747261
 C    6.380136   -2.688708    0.307980
 H    4.618139   -3.647511    1.100718
 C    6.315497   -0.279590    0.206101
 H    4.521311    0.657534    0.929358
 C    6.991629   -1.478918   -0.024015
 H    6.903693   -3.632149    0.138402
 H    6.793165    0.672861   -0.034727
 H    7.995958   -1.470087   -0.452964
 C    3.446063   -1.050686   -2.204236
 H    3.261668   -1.486079   -3.199144
 H    4.530878   -0.945210   -2.068617
 H    3.074793   -1.767014   -1.456599
 C    3.532102    3.996742   -1.888974
 H    4.034947    4.178828   -2.851532
 H    2.881034    4.857467   -1.681796
 H    4.313956    3.964250   -1.115311
 H    0.822078    3.656540   -1.786138
 H    0.780604   -0.641757   -2.065925
 C   -0.303029   -2.519919   -0.382309
 H   -1.202178   -2.890478   -0.900205
 C    0.724707   -3.306767   -0.288710
 C    1.813396   -4.049150   -0.162957
 H    1.955701   -4.710844    0.698034
 H    2.600336   -4.042421   -0.924324
51
Figure_S4-1_9d(Na)-Cu-allenyl / electronic energy: -2839.06020575 a.u. / lowest freq: 14.37 cm-1
 C    1.401449   -2.075087    0.781893
 H    1.679476   -1.881296    1.831858
 C   -0.006213   -2.648365    0.652932
 H   -0.062301   -3.424044   -0.128912
 C    0.006182   -0.440008   -0.139162
 C   -2.189160   -1.531257    0.133738
 C   -2.845361   -2.761728    0.235329
 C   -2.951250   -0.369985   -0.075492
 C   -4.240763   -2.845245    0.119017
 C   -4.334525   -0.435941   -0.206321
 C   -4.972785   -1.681355   -0.104919
 H   -6.061043   -1.738645   -0.201130
Cu   -0.329372    1.490047   -0.372686
 N    1.273764   -0.812875    0.054580
 N   -0.787308   -1.470553    0.258845
Na    0.498306    3.958728    1.355621
 H   -0.381218   -3.078008    1.591814
 H    2.168593   -2.723176    0.339289
 C    2.372398    0.146754   -0.035438
 H    2.178954    0.736216   -0.947149
 C    3.689483   -0.579021   -0.225630
 C    4.620192   -0.739015    0.805951
 C    3.975802   -1.139609   -1.477409
 C    5.810682   -1.435686    0.589342
 H    4.421442   -0.318405    1.793568
 C    5.159152   -1.840488   -1.696033
 H    3.252345   -1.025120   -2.289480
 C    6.083241   -1.989386   -0.660216
 H    6.529017   -1.546552    1.404836
 H    5.363247   -2.270600   -2.679186
 H    7.015148   -2.533630   -0.828612
 C    2.308388    1.165951    1.128058
 H    3.266929    1.737018    1.072498
 H    2.373701    0.583431    2.082237
 O    1.207712    1.962082    1.066314
 C   -5.135842    0.816899   -0.451875
 H   -5.658483    0.763844   -1.419613
 H   -5.904556    0.954837    0.324125
 H   -4.492476    1.707881   -0.461773
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 C   -4.919272   -4.186120    0.236349
 H   -6.004229   -4.101088    0.086278
 H   -4.527345   -4.895642   -0.508698
 H   -4.747592   -4.631017    1.228910
 H   -2.283360   -3.682514    0.397907
 H   -2.449009    0.596199   -0.147487
 C   -1.307163    3.029167   -1.145241
 H   -1.961130    2.829821   -2.012024
 C   -1.311845    4.265224   -0.742674
 C   -1.248636    5.503922   -0.256051
 H   -0.536999    6.236564   -0.653695
 H   -1.960491    5.856163    0.499142
51
Figure_S4-1_9b(Na)-Cu-allenyl / electronic energy: -2839.05552233 a.u. / lowest freq: 18.49 cm-1
 C   -1.403505   -1.447218   -1.463778
 H   -1.518968   -0.926587   -2.428424
 C   -0.102320   -2.249278   -1.398621
 H   -0.227521   -3.213821   -0.877881
 C    0.053653   -0.375990   -0.006245
 C    2.115590   -1.646329   -0.323692
 C    2.447529   -2.278240    0.886897
 C    3.093354   -1.289872   -1.267445
 C    3.794134   -2.560894    1.135970
 C    4.427961   -1.594447   -0.983886
 C    4.776145   -2.227614    0.206801
 H    5.823692   -2.456465    0.414766
Cu    0.843286    1.028000    1.058904
 N   -1.218234   -0.464888   -0.392885
 N    0.750379   -1.356185   -0.608944
Na    0.955612    3.102468   -1.264571
 H    0.329842   -2.451327   -2.388040
 H   -2.298582   -2.059781   -1.291665
 C   -2.190235    0.595041   -0.173375
 H   -1.850072    1.110871    0.740288
 C   -3.556987   -0.008997    0.105143
 C   -4.706885    0.356784   -0.601576
 C   -3.677253   -0.973578    1.116074
 C   -5.942423   -0.224050   -0.305173
 H   -4.649878    1.103012   -1.395225
 C   -4.905862   -1.557315    1.412344
 H   -2.783955   -1.272241    1.671962
 C   -6.047178   -1.182627    0.699889
 H   -6.828698    0.076027   -0.869206
 H   -4.975116   -2.307462    2.203595
 H   -7.013189   -1.638603    0.927875
 C   -2.105561    1.652949   -1.307432
 H   -2.876323    2.421016   -1.032266
 H   -2.526837    1.167141   -2.231630
 O   -0.866029    2.140611   -1.461517
 C    1.722811    2.492968    1.972660
 H    1.936525    2.461721    3.053521
 C    2.118112    3.566313    1.350898
 C    2.487290    4.627547    0.641169
 H    1.831345    5.500129    0.544963
 H    3.482307    4.692597    0.187595
 H    5.202845   -1.322373   -1.704686
 H    4.072439   -3.050469    2.072400
 C    1.385066   -2.604535    1.901717
 H    0.998593   -1.681347    2.362588
 H    0.524948   -3.114869    1.443881
 H    1.783860   -3.245588    2.698815
 C    2.712511   -0.567453   -2.531971
 H    2.063535   -1.181523   -3.174815
 H    2.155428    0.354222   -2.305548
 H    3.604292   -0.299794   -3.114044
83
Figure_S4-1_PA-9b(Na)-pc(1,6major) / electronic energy: -3681.02455274 a.u. / lowest freq: 18.51 cm-1
 C   -3.233150    1.556543    1.456457
 H   -2.978288    2.346281    2.167852
 C   -1.078272    0.492669    1.955666
 H   -0.820455    1.360498    2.566626
 C   -2.372349    0.528797    1.300406
 H   -2.621831   -0.293876    0.627314
 C   -0.255688   -0.661270    2.091840
 C   -0.679628   -2.056343    1.808114
 O    0.079235   -2.990575    1.632177
 C    1.005529   -0.539406    2.866248
 O    1.641716   -1.459886    3.339753
 O    1.408451    0.726354    2.988212
 C   -4.524102    1.709208    0.772878
 C   -4.972433    0.816890   -0.216806
 C   -6.202214    1.004256   -0.840254
 C   -7.013938    2.086079   -0.490981
 C   -6.581865    2.980879    0.487815
 C   -5.350056    2.793245    1.110780
 C   -1.787039    4.045388    0.189792
 H   -1.906285    4.644943    1.098124
 H   -2.553221    4.148624   -0.585659
 C   -0.750861    3.239140    0.025612
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 C    0.201043    2.371603   -0.120736
 H    1.142116    2.686577   -0.597937
Cu    0.184867    0.447050    0.371961
 C    1.241334   -0.555655   -0.967831
 N    2.556161   -0.447351   -1.107013
 N    0.768825   -1.352332   -1.942673
 C    3.419006    0.205999   -0.139204
 C    3.084645   -1.332582   -2.150166
 H    3.578607   -2.185069   -1.659723
 C    1.813127   -1.737242   -2.899132
 H    1.678890   -1.182285   -3.842980
 C   -0.608205   -1.667330   -2.123536
 C   -1.493137   -0.678631   -2.591401
 C   -1.042339   -2.977426   -1.846890
 C   -2.847575   -1.009705   -2.710831
 C   -2.401712   -3.268651   -1.995029
 C   -3.301903   -2.289438   -2.406872
 H   -4.362310   -2.530162   -2.510055
Na    2.416192   -3.039939    1.763542
 H    1.776064   -2.810338   -3.127402
 H    3.812265   -0.814136   -2.789082
 O   -1.997050   -2.215168    1.802573
 C    2.648060    0.949287    3.649158
 H    2.593351    0.627278    4.698005
 H    2.828910    2.027200    3.590217
 H    3.454549    0.399142    3.143448
 C   -2.501269   -3.526131    1.586226
 H   -2.109684   -3.945019    0.651655
 H   -3.589605   -3.423758    1.526425
 H   -2.226347   -4.184156    2.422284
 H    2.774531    0.437247    0.724340
 C    3.986805    1.512409   -0.658439
 C    4.814131    2.286476    0.168555
 C    3.690166    2.002093   -1.935562
 C    5.340623    3.498320   -0.274146
 H    5.038857    1.943645    1.181225
 C    4.216084    3.214885   -2.382458
 H    3.018854    1.438822   -2.586402
 C    5.047896    3.967048   -1.555586
 H    5.979449    4.085321    0.389896
 H    3.966952    3.575631   -3.383158
 H    5.459405    4.917223   -1.903178
 C    4.485742   -0.817867    0.370388
 H    5.067605   -0.262753    1.152650
 H    5.223862   -0.924578   -0.475465
 O    3.938334   -1.965277    0.786661
 H   -5.013687    3.502012    1.871930
 H   -4.350274   -0.029882   -0.513774
 H   -7.207335    3.831730    0.767130
 H   -6.530058    0.299597   -1.608069
 H   -7.978369    2.231133   -0.982495
 C   -1.013146    0.695735   -2.969237
 H   -0.933334    1.346879   -2.085063
 H   -0.016121    0.663007   -3.431205
 H   -1.709667    1.165922   -3.676405
 C   -0.069034   -4.048072   -1.433553
 H   -0.577969   -4.862251   -0.900028
 H    0.418661   -4.493105   -2.315898
 H    0.715156   -3.644621   -0.780483
 H   -3.550695   -0.251077   -3.063353
 H   -2.757840   -4.279775   -1.782065
83
Figure_S4-1_PA-9b(Na)-ts(1,6major) / electronic energy: -3681.01420703 a.u. / lowest freq: -427.03 cm-1
 C    2.979277   -1.816363    1.363890
 H    2.832953   -2.499901    2.202407
 C    0.983754   -0.583498    2.061507
 H    0.687994   -1.482945    2.607573
 C    2.204575   -0.653459    1.365698
 H    2.532869    0.207846    0.781962
 C    0.132807    0.567981    2.261009
 C    0.555516    1.959815    2.064348
 O   -0.178914    2.937010    2.048099
 C   -1.162905    0.359582    2.919903
 O   -1.901175    1.216398    3.376497
 O   -1.517300   -0.936671    2.962522
 C    4.329569   -1.851716    0.760541
 C    4.682883   -1.022138   -0.315747
 C    5.957777   -1.080815   -0.871037
 C    6.907086   -1.972887   -0.367128
 C    6.566688   -2.806274    0.698073
 C    5.289634   -2.746887    1.253825
 C    2.069231   -3.442207    0.102650
 H    2.261290   -4.216338    0.850501
 H    2.774336   -3.409537   -0.733773
 C    0.793982   -3.030186   -0.121012
 C   -0.269149   -2.357956   -0.241579
 H   -1.246278   -2.540213   -0.691663
Cu   -0.175462   -0.401482    0.359787
 C   -1.144033    0.599950   -1.032719
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 N   -2.457990    0.509661   -1.204986
 N   -0.638672    1.394818   -1.990384
 C   -3.354623   -0.132049   -0.259882
 C   -2.947832    1.409435   -2.255697
 H   -3.435672    2.267963   -1.769538
 C   -1.652843    1.791478   -2.974419
 H   -1.504971    1.230046   -3.912538
 C    0.743914    1.707881   -2.131227
 C    1.624394    0.753087   -2.667616
 C    1.181826    2.986763   -1.742460
 C    2.976709    1.094986   -2.779816
 C    2.540838    3.287647   -1.871490
 C    3.433983    2.346862   -2.378552
 H    4.493435    2.594870   -2.472863
Na   -2.500038    2.928818    1.919630
 H   -1.592203    2.862329   -3.208512
 H   -3.670790    0.907902   -2.913030
 O    1.874268    2.097145    1.908907
 C   -2.790716   -1.234933    3.511430
 H   -2.834690   -0.969064    4.576959
 H   -2.929437   -2.313857    3.385119
 H   -3.580634   -0.687293    2.976474
 C    2.385404    3.411637    1.760938
 H    1.910161    3.929061    0.918794
 H    3.458436    3.298031    1.573259
 H    2.222644    3.994940    2.678345
 H   -2.747429   -0.342183    0.636144
 C   -3.895854   -1.450235   -0.775982
 C   -4.702645   -2.239439    0.057043
 C   -3.597217   -1.935173   -2.054595
 C   -5.205944   -3.462897   -0.379836
 H   -4.928757   -1.898010    1.069876
 C   -4.099393   -3.160548   -2.495451
 H   -2.943062   -1.358256   -2.711137
 C   -4.909721   -3.928399   -1.661848
 H   -5.829184   -4.061357    0.288699
 H   -3.849280   -3.517918   -3.497085
 H   -5.302642   -4.888063   -2.004790
 C   -4.448169    0.891868    0.192062
 H   -5.064236    0.335170    0.947141
 H   -5.144368    0.989581   -0.689936
 O   -3.925874    2.043648    0.626926
 H    5.029497   -3.405910    2.086631
 H    3.948303   -0.331158   -0.735039
 H    7.300106   -3.509664    1.099012
 H    6.211953   -0.425913   -1.708111
 H    7.905710   -2.020504   -0.806658
 C    1.138435   -0.602947   -3.100184
 H    0.985301   -1.258390   -2.229315
 H    0.174446   -0.541526   -3.625366
 H    1.866664   -1.084682   -3.766166
 C    0.208212    3.998497   -1.199623
 H    0.728806    4.910812   -0.878466
 H   -0.532200    4.294608   -1.957945
 H   -0.343607    3.594945   -0.338235
 H    3.677310    0.366478   -3.195724
 H    2.901920    4.273721   -1.568872
83
Figure_S4-1_PA-9b(Na)-prod(1,6major) / electronic energy: -3681.06325058 a.u. / lowest freq: -12.96 cm-1
 C   -2.521540   -1.968860   -1.057975
 H   -2.297148   -2.585707   -1.942263
 C   -0.832825   -0.415687   -2.108395
 H   -0.448278   -1.313793   -2.601455
 C   -1.894029   -0.603276   -1.255327
 H   -2.406042    0.252293   -0.809724
 C   -0.051633    0.789928   -2.389487
 C   -0.528407    2.135540   -2.125147
 O    0.134563    3.168381   -2.108413
 C    1.255304    0.634329   -2.995665
 O    2.029307    1.522388   -3.336054
 O    1.614616   -0.660983   -3.157826
 C   -4.029541   -1.881781   -0.913334
 C   -4.601267   -1.077472    0.081651
 C   -5.983869   -1.005395    0.234848
 C   -6.821785   -1.739755   -0.606356
 C   -6.264091   -2.543834   -1.599149
 C   -4.877757   -2.613614   -1.749313
 C   -1.929997   -2.720173    0.168541
 H   -2.415230   -3.704923    0.260790
 H   -2.168557   -2.160710    1.088545
 C   -0.480193   -2.897162    0.089124
 C    0.724496   -3.006992    0.007418
 H    1.795982   -3.105633   -0.046957
Cu    0.055140   -0.167273   -0.254507
 C    1.043175    0.526788    1.250276
 N    2.364814    0.538423    1.357015
 N    0.514340    1.139506    2.319292
 C    3.257591    0.062661    0.314657
 C    2.824130    1.342838    2.495838
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 H     3.234693    2.283179    2.097907
 C     1.530664    1.540375    3.296378
 H     1.480365    0.892303    4.187215
 C    -0.891066    1.244986    2.519028
 C    -1.594307    0.145410    3.037877
 C    -1.532177    2.436887    2.149040
 C    -2.980704    0.261465    3.178075
 C    -2.920167    2.513646    2.301817
 C    -3.638148    1.434443    2.811693
 H    -4.722096    1.507633    2.924543
Na     2.422215    3.149641   -1.730964
 H     1.384829    2.578815    3.624227
 H     3.605408    0.825190    3.068702
 O    -1.849233    2.184790   -1.874476
 C     2.882109   -0.901903   -3.737914
 H     2.910695   -0.570006   -4.786190
 H     3.041098   -1.984997   -3.685668
 H     3.675584   -0.376787   -3.186147
 C    -2.429272    3.457487   -1.658869
 H    -1.933451    3.990490   -0.837753
 H    -3.479511    3.273136   -1.405887
 H    -2.368250    4.075050   -2.566893
 H     2.641174   -0.016990   -0.596334
 C     3.816310   -1.312558    0.612765
 C     4.486302   -2.009509   -0.402889
 C     3.658900   -1.942710    1.852323
 C     4.984581   -3.292866   -0.187730
 H     4.602410   -1.546028   -1.385028
 C     4.159676   -3.226661    2.073250
 H     3.111031   -1.439771    2.651189
 C     4.824211   -3.907917    1.054990
 H     5.494456   -3.818432   -0.998436
 H     4.019000   -3.700264    3.047554
 H     5.210702   -4.915071    1.225317
 C     4.327892    1.157225    0.001665
 H     4.958651    0.709508   -0.812751
 H     5.019008    1.161320    0.893441
 O     3.775774    2.340915   -0.288451
 H    -4.448980   -3.246147   -2.531312
 H    -3.959434   -0.494635    0.747729
 H    -6.910385   -3.122394   -2.263137
 H    -6.408722   -0.370347    1.015893
 H    -7.906096   -1.682987   -0.487939
 C    -0.868866   -1.118871    3.414293
 H    -0.333258   -1.542164    2.550179
 H    -0.116324   -0.932544    4.195928
 H    -1.568820   -1.876139    3.791658
 C    -0.734209    3.582102    1.587382
 H    -1.377937    4.448355    1.384760
 H     0.052853    3.906353    2.284339
 H    -0.232212    3.295098    0.649758
 H    -3.550771   -0.581966    3.575413
 H    -3.441091    3.430469    2.015433
83
Figure_S4-1_PA-9d(Na)-prod(1,6minor) / electronic energy: -3681.071647O1 a.u. / lowest freq: 12.05 cm-1
 C     3.415065   -1.884314   -0.298570
 H     4.009658   -1.921787    0.623011
 C     2.325014   -2.945123   -0.397477
 H     2.578600   -3.762686   -1.084867
 C     1.377747   -0.836544   -0.715723
 C    -0.050722   -2.768048   -1.208278
 C    -0.287716   -4.100791   -0.869700
 C    -1.055506   -2.045670   -1.871504
 C    -1.529999   -4.696919   -1.125748
 C    -2.300931   -2.614233   -2.120797
 C    -2.531388   -3.942465   -1.734671
 H    -3.506499   -4.397669   -1.929244
Cu     0.043245    0.610509   -0.873840
 N     2.621837   -0.650351   -0.308314
 N     1.181538   -2.167863   -0.893321
 C    -1.123470    0.227509    1.068154
 C    -0.155054   -0.010880    2.121942
Na     3.030411   -0.741580    3.477587
 H     2.084735   -3.376263    0.589365
 H     4.089487   -1.906196   -1.170934
 H    -1.661109   -0.680854    0.773938
 C     0.077202   -1.378565    2.526209
 C     0.671169    1.009553    2.707125
 O    -0.853282   -2.241997    2.057316
 O     1.006244   -1.813995    3.205319
 O     1.453477    0.896317    3.648906
 O     0.546330    2.219432    2.106144
 C     1.349025    3.267792    2.612535
 H     1.154137    3.444225    3.679730
 H     1.085378    4.160738    2.032945
 H     2.419011    3.042867    2.485368
 C    -0.717137   -3.599663    2.416923
 H     0.252633   -4.008815    2.099107
 H    -1.524571   -4.132696    1.901723
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 H   -0.813199   -3.734151    3.504692
 C    3.148917    0.667970    0.042753
 H    2.435468    1.111366    0.754665
 C    3.235467    1.571998   -1.163502
 C    3.665717    1.096706   -2.408200
 C    2.899547    2.924799   -1.045520
 C    3.746927    1.949919   -3.508455
 H    3.919166    0.040730   -2.527151
 C    2.980462    3.782592   -2.142070
 H    2.549101    3.305556   -0.082783
 C    3.403126    3.297143   -3.379324
 H    4.080249    1.559849   -4.472991
 H    2.704011    4.833372   -2.030653
 H    3.461020    3.964895   -4.241652
 C    4.496039    0.528507    0.815727
 H    4.827593    1.591866    0.962282
 H    5.229253    0.129916    0.055401
 O    4.395684   -0.199030    1.934417
 C   -1.522075    1.379864    0.428390
 H   -1.125979    2.342377    0.758151
 C   -2.705227    1.433720   -0.521939
 H   -2.897374    0.417069   -0.901189
 C   -3.983865    1.926971    0.131800
 C   -5.160929    1.177259    0.045903
 C   -4.016099    3.143227    0.827001
 C   -6.342639    1.627276    0.636849
 H   -5.152497    0.224021   -0.489394
 C   -5.193397    3.596710    1.417667
 H   -3.107163    3.744330    0.915853
 C   -6.362658    2.839418    1.324522
 H   -7.251266    1.025843    0.559768
 H   -5.198173    4.546891    1.956553
 H   -7.285341    3.194301    1.788777
 C   -3.386931   -1.814320   -2.792131
 H   -2.998741   -0.871411   -3.202568
 H   -3.852415   -2.379594   -3.612979
 H   -4.186596   -1.568225   -2.075501
 C   -1.759852   -6.134068   -0.736362
 H   -1.528075   -6.298560    0.327196
 H   -2.801590   -6.436336   -0.909219
 H   -1.109864   -6.806460   -1.317618
 H    0.484361   -4.692488   -0.376330
 H   -0.854278   -1.033615   -2.224209
 C    0.084280    1.653061   -2.760185
 H    0.986501    1.537817   -3.343113
 C   -0.996623    1.928358   -2.248005
 C   -2.319701    2.317222   -1.731567
 H   -3.070848    2.254211   -2.533809
 H   -2.267385    3.374027   -1.422421
83
Figure_S4-1_PA-9d(Na)-ts(1,6minor) / electronic energy: -3681.01261478 a.u. / lowest freq: -459.96 cm-1
 C    3.659544    2.047246   -0.366906
 H    4.051864    2.555127    0.522168
 C    4.175987    0.617260   -0.516602
 H    4.864432    0.492678   -1.363392
 C    1.838989    0.587570   -0.437054
 C    2.960065   -1.534459   -0.968542
 C    4.149817   -2.254209   -0.824326
 C    1.799290   -2.212280   -1.368197
 C    4.182549   -3.637772   -1.048592
 C    1.805568   -3.589583   -1.566834
 C    3.006223   -4.294472   -1.407170
 H    3.021482   -5.375544   -1.571763
Cu   -0.052747   -0.026957   -0.282358
 N    2.219273    1.832147   -0.200960
 N    2.940741   -0.148649   -0.723460
 C   -1.406247   -1.192830    0.925565
 C   -0.363215   -0.625273    1.741140
Na    2.414098    1.220797    3.079838
 H    4.685482    0.268478    0.396785
 H    3.857266    2.662778   -1.258609
 H   -1.143551   -2.164928    0.493393
 C    0.833419   -1.426176    2.052715
 C   -0.517378    0.625019    2.497523
 O    0.702309   -2.713141    1.723429
 O    1.872805   -1.002170    2.535225
 O    0.139354    0.959898    3.467674
 O   -1.461712    1.436263    2.000773
 C   -1.624071    2.695875    2.639351
 H   -1.915876    2.567285    3.690473
 H   -2.414555    3.214145    2.086305
 H   -0.687394    3.271175    2.597527
 C    1.842622   -3.542856    1.887734
 H    2.707214   -3.128827    1.351460
 H    1.573747   -4.516342    1.464302
 H    2.090698   -3.650111    2.953172
 C    1.303488    2.899082    0.174318
 H    0.479763    2.409590    0.715767
 C    0.707716    3.616456   -1.017868
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 C    1.158006    3.418929   -2.327548
 C   -0.347302    4.515648   -0.808469
 C    0.580953    4.107297   -3.395645
 H    1.956395    2.701785   -2.527988
 C   -0.925803    5.204561   -1.872244
 H   -0.731667    4.667426    0.203412
 C   -0.460821    5.005697   -3.172922
 H    0.947875    3.934180   -4.409995
 H   -1.749346    5.897443   -1.684748
 H   -0.915430    5.540997   -4.009344
 C    2.011379    3.838889    1.205697
 H    1.223260    4.586326    1.490204
 H    2.737771    4.449566    0.595178
 O    2.556483    3.168668    2.226204
 C   -2.750928   -0.825870    0.784339
 H   -3.117401    0.064702    1.293180
 C   -3.585026   -1.513435   -0.096893
 H   -3.216921   -2.481294   -0.451129
 C   -5.062979   -1.407082   -0.042764
 C   -5.846104   -2.486908   -0.474925
 C   -5.717896   -0.255163    0.421237
 C   -7.238474   -2.427136   -0.433246
 H   -5.353980   -3.389598   -0.846991
 C   -7.108018   -0.193642    0.462069
 H   -5.135871    0.610796    0.744256
 C   -7.875891   -1.280064    0.037321
 H   -7.827715   -3.282881   -0.770557
 H   -7.597389    0.712199    0.827015
 H   -8.966327   -1.228993    0.070852
 C    0.528144   -4.306465   -1.915511
 H   -0.224144   -3.611830   -2.315294
 H    0.698584   -5.101549   -2.655583
 H    0.098276   -4.779192   -1.017398
 C    5.480189   -4.387041   -0.891376
 H    5.911320   -4.227961    0.108759
 H    5.340563   -5.466963   -1.035210
 H    6.224967   -4.040376   -1.624467
 H    5.071431   -1.751542   -0.528467
 H    0.876097   -1.659899   -1.549673
 C   -0.904423    0.218537   -2.097521
 H   -0.241045    0.749398   -2.781396
 C   -2.093103   -0.199342   -2.230770
 C   -3.362822   -0.671765   -2.113501
 H   -3.634098   -1.595490   -2.633831
 H   -4.165872    0.064162   -2.015214
83
Figure_S4-1_PA-9d(Na)-pc(1,6minor) / electronic energy: -3681.02763302 a.u. / lowest freq: 8.16 cm-1
 C    3.283430    2.432864   -0.167670
 H    3.550518    2.897574    0.790005
 C    3.997739    1.097056   -0.392375
 H    4.652012    1.098760   -1.276078
 C    1.682210    0.743791   -0.347367
 C    3.091100   -1.193730   -0.896784
 C    4.357694   -1.769390   -0.732595
 C    2.047530   -1.977377   -1.402378
 C    4.576485   -3.115641   -1.044982
 C    2.238643   -3.328673   -1.688100
 C    3.508123   -3.887591   -1.510230
 H    3.669281   -4.944912   -1.739455
Cu   -0.106559   -0.138747   -0.253299
 N    1.875396    2.033145   -0.132411
 N    2.883576    0.160900   -0.575885
 C   -1.307549   -1.381515    0.855694
 C   -0.299121   -0.823990    1.682302
Na    2.241492    1.142203    3.234214
 H    4.603404    0.807209    0.480249
 H    3.463599    3.158516   -0.975065
 H   -1.059303   -2.358851    0.428473
 C    0.959501   -1.571041    1.950493
 C   -0.546288    0.320303    2.606187
 O    0.905960   -2.839818    1.570037
 O    1.958066   -1.085128    2.449578
 O   -0.032602    0.435237    3.698614
 O   -1.388255    1.221910    2.116827
 C   -1.578263    2.405039    2.898087
 H   -2.065104    2.160633    3.851967
 H   -2.225287    3.052492    2.297013
 H   -0.594432    2.868183    3.071700
 C    2.090587   -3.613219    1.721894
 H    2.939606   -3.121647    1.229463
 H    1.886582   -4.577131    1.244960
 H    2.315223   -3.757275    2.787871
 C    0.816131    2.977513    0.181516
 H   -0.045153    2.363561    0.485631
 C    0.401074    3.807353   -1.019143
 C    0.944473    3.611072   -2.294208
 C   -0.592703    4.786382   -0.870530
 C    0.527149    4.380066   -3.381544
 H    1.693314    2.832826   -2.453286
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 C   -1.012372    5.554907   -1.954242
 H   -1.058076    4.941328    0.105412
 C   -0.449657    5.359599   -3.216064
 H    0.968215    4.205856   -4.365700
 H   -1.790043    6.309141   -1.812681
 H   -0.778812    5.960932   -4.066363
 C    1.235869    3.800090    1.440229
 H    0.353348    4.451262    1.669972
 H    2.014747    4.531435    1.084938
 O    1.620053    3.010699    2.452923
 C   -2.721438   -1.047817    0.816490
 H   -3.031184   -0.093774    1.243289
 C   -3.615784   -1.875050    0.240212
 H   -3.251913   -2.817213   -0.180417
 C   -5.058032   -1.637211    0.094729
 C   -5.838262   -2.589258   -0.581970
 C   -5.699545   -0.490502    0.595214
 C   -7.208242   -2.404946   -0.757136
 H   -5.356708   -3.485571   -0.981688
 C   -7.067781   -0.307017    0.423215
 H   -5.124548    0.270584    1.126364
 C   -7.829128   -1.262197   -0.254360
 H   -7.793290   -3.157643   -1.290224
 H   -7.545739    0.591022    0.820820
 H   -8.902392   -1.113443   -0.390641
 C    1.073363   -4.166717   -2.143860
 H    0.288826   -3.546352   -2.600150
 H    1.382640   -4.933756   -2.867872
 H    0.620122   -4.686449   -1.283850
 C    5.946586   -3.723682   -0.890026
 H    6.598467   -3.100181   -0.262663
 H    5.887948   -4.724552   -0.438186
 H    6.434968   -3.837088   -1.870996
 H    5.191189   -1.177428   -0.352493
 H    1.073348   -1.529360   -1.606668
 C   -1.031479   -0.008244   -1.993800
 H   -0.774107    0.861007   -2.618160
 C   -1.839622   -0.898592   -2.486115
 C   -2.669042   -1.833454   -2.920223
 H   -2.308361   -2.707240   -3.473510
 H   -3.747959   -1.749604   -2.751795
51
Figure_S4-1_9d(Na)-Cu-allenyl / electronic energy: -2839.06020575 a.u. / lowest freq: 14.37 cm-1
 C    1.401449   -2.075087    0.781893
 H    1.679476   -1.881296    1.831858
 C   -0.006213   -2.648365    0.652932
 H   -0.062301   -3.424044   -0.128912
 C    0.006182   -0.440008   -0.139162
 C   -2.189160   -1.531257    0.133738
 C   -2.845361   -2.761728    0.235329
 C   -2.951250   -0.369985   -0.075492
 C   -4.240763   -2.845245    0.119017
 C   -4.334525   -0.435941   -0.206321
 C   -4.972785   -1.681355   -0.104919
 H   -6.061043   -1.738645   -0.201130
Cu   -0.329372    1.490047   -0.372686
 N    1.273764   -0.812875    0.054580
 N   -0.787308   -1.470553    0.258845
Na    0.498306    3.958728    1.355621
 H   -0.381218   -3.078008    1.591814
 H    2.168593   -2.723176    0.339289
 C    2.372398    0.146754   -0.035438
 H    2.178954    0.736216   -0.947149
 C    3.689483   -0.579021   -0.225630
 C    4.620192   -0.739015    0.805951
 C    3.975802   -1.139609   -1.477409
 C    5.810682   -1.435686    0.589342
 H    4.421442   -0.318405    1.793568
 C    5.159152   -1.840488   -1.696033
 H    3.252345   -1.025120   -2.289480
 C    6.083241   -1.989386   -0.660216
 H    6.529017   -1.546552    1.404836
 H    5.363247   -2.270600   -2.679186
 H    7.015148   -2.533630   -0.828612
 C    2.308388    1.165951    1.128058
 H    3.266929    1.737018    1.072498
 H    2.373701    0.583431    2.082237
 O    1.207712    1.962082    1.066314
 C   -5.135842    0.816899   -0.451875
 H   -5.658483    0.763844   -1.419613
 H   -5.904556    0.954837    0.324125
 H   -4.492476    1.707881   -0.461773
 C   -4.919272   -4.186120    0.236349
 H   -6.004229   -4.101088    0.086278
 H   -4.527345   -4.895642   -0.508698
 H   -4.747592   -4.631017    1.228910
 H   -2.283360   -3.682514    0.397907
 H   -2.449009    0.596199   -0.147487
 C   -1.307163    3.029167   -1.145241
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 H   -1.961130    2.829821   -2.012024
 C   -1.311845    4.265224   -0.742674
 C   -1.248636    5.503922   -0.256051
 H   -0.536999    6.236564   -0.653695
 H   -1.960491    5.856163    0.499142
51
Figure_S4-1_9b(Na)-Cu-allenyl / electronic energy: -2839.05552233 a.u. / lowest freq: 18.49 cm-1
 C   -1.403505   -1.447218   -1.463778
 H   -1.518968   -0.926587   -2.428424
 C   -0.102320   -2.249278   -1.398621
 H   -0.227521   -3.213821   -0.877881
 C    0.053653   -0.375990   -0.006245
 C    2.115590   -1.646329   -0.323692
 C    2.447529   -2.278240    0.886897
 C    3.093354   -1.289872   -1.267445
 C    3.794134   -2.560894    1.135970
 C    4.427961   -1.594447   -0.983886
 C    4.776145   -2.227614    0.206801
 H    5.823692   -2.456465    0.414766
Cu    0.843286    1.028000    1.058904
 N   -1.218234   -0.464888   -0.392885
 N    0.750379   -1.356185   -0.608944
Na    0.955612    3.102468   -1.264571
 H    0.329842   -2.451327   -2.388040
 H   -2.298582   -2.059781   -1.291665
 C   -2.190235    0.595041   -0.173375
 H   -1.850072    1.110871    0.740288
 C   -3.556987   -0.008997    0.105143
 C   -4.706885    0.356784   -0.601576
 C   -3.677253   -0.973578    1.116074
 C   -5.942423   -0.224050   -0.305173
 H   -4.649878    1.103012   -1.395225
 C   -4.905862   -1.557315    1.412344
 H   -2.783955   -1.272241    1.671962
 C   -6.047178   -1.182627    0.699889
 H   -6.828698    0.076027   -0.869206
 H   -4.975116   -2.307462    2.203595
 H   -7.013189   -1.638603    0.927875
 C   -2.105561    1.652949   -1.307432
 H   -2.876323    2.421016   -1.032266
 H   -2.526837    1.167141   -2.231630
 O   -0.866029    2.140611   -1.461517
 C    1.722811    2.492968    1.972660
 H    1.936525    2.461721    3.053521
 C    2.118112    3.566313    1.350898
 C    2.487290    4.627547    0.641169
 H    1.831345    5.500129    0.544963
 H    3.482307    4.692597    0.187595
 H    5.202845   -1.322373   -1.704686
 H    4.072439   -3.050469    2.072400
 C    1.385066   -2.604535    1.901717
 H    0.998593   -1.681347    2.362588
 H    0.524948   -3.114869    1.443881
 H    1.783860   -3.245588    2.698815
 C    2.712511   -0.567453   -2.531971
 H    2.063535   -1.181523   -3.174815
 H    2.155428    0.354222   -2.305548
 H    3.604292   -0.299794   -3.114044
83
Figure_S4-1_PA-9b(Na)-pc(1,6minor) / electronic energy: -3681.02166482 a.u. / lowest freq: 4.07 cm-1
 C    2.892491    2.672219   -0.559859
 H    3.338014    2.967650    0.403230
 C    3.696536    1.576655   -1.253095
 H    3.744769    1.714396   -2.346290
 C    1.679758    0.686200   -0.476223
 C    3.447436   -0.910188   -1.210973
 C    4.458660   -1.397745   -0.362500
 C    3.054572   -1.613731   -2.365361
 C    5.077533   -2.608674   -0.690970
 C    3.681590   -2.832627   -2.642833
 C    4.692752   -3.323126   -1.820397
 H    5.181415   -4.269721   -2.061152
Cu   -0.001155   -0.388816   -0.338393
 N    1.610345    2.008238   -0.324133
 N    2.906806    0.379665   -0.940386
 C   -1.244655   -1.760666    0.529609
 C   -0.197357   -1.423350    1.430429
Na    2.355710    0.117136    3.203400
 H    4.724266    1.489708   -0.875574
 H    2.771522    3.568033   -1.182866
 H   -1.049448   -2.646495   -0.083016
 C    1.037462   -2.246912    1.469019
 C   -0.404029   -0.519403    2.596185
 O    0.951250   -3.335397    0.711469
 O    2.044412   -1.973183    2.096327
 O    0.141340   -0.658774    3.671625
 O   -1.273608    0.454666    2.363209
 C   -1.459923    1.401536    3.413113
 H   -1.886098    0.914780    4.301012
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 H   -2.156173    2.149425    3.019258
 H   -0.486233    1.852331    3.649631
 C    2.096345   -4.173536    0.633608
 H    2.972061   -3.603398    0.301922
 H    1.852157   -4.950819   -0.097723
 H    2.304971   -4.628450    1.612091
 C    0.559803    2.654857    0.454174
 H   -0.198095    1.875233    0.614871
 C   -0.098953    3.792501   -0.295620
 C    0.497675    5.055008   -0.414648
 C   -1.355389    3.593679   -0.883404
 C   -0.138359    6.084038   -1.109936
 H    1.469557    5.244045    0.046952
 C   -1.994863    4.619865   -1.577186
 H   -1.831910    2.612630   -0.801611
 C   -1.386273    5.869887   -1.694573
 H    0.344230    7.060674   -1.192834
 H   -2.973097    4.441904   -2.029805
 H   -1.884498    6.676383   -2.237478
 C    1.093947    3.017260    1.869398
 H    0.210712    3.496801    2.372659
 H    1.814120    3.870573    1.743180
 O    1.607062    1.957969    2.511084
 C   -2.646169   -1.381305    0.603507
 H   -2.907154   -0.508974    1.201401
 C   -3.594050   -2.067304   -0.064900
 H   -3.292742   -2.948650   -0.639196
 C   -5.030168   -1.756702   -0.097631
 C   -5.907068   -2.658576   -0.722293
 C   -5.572171   -0.585510    0.460193
 C   -7.276454   -2.409060   -0.780332
 H   -5.502389   -3.569718   -1.170757
 C   -6.939882   -0.335518    0.402958
 H   -4.917442    0.146684    0.936981
 C   -7.799451   -1.245960   -0.215971
 H   -7.938569   -3.125788   -1.271220
 H   -7.340026    0.581437    0.841462
 H   -8.872110   -1.045921   -0.262237
 C   -0.997033    0.108031   -1.978001
 H   -0.617101    1.017183   -2.469335
 C   -1.981643   -0.516419   -2.551519
 C   -2.986257   -1.191639   -3.082564
 H   -2.814614   -1.995104   -3.806788
 H   -4.024078   -0.960788   -2.821084
 C    4.901763   -0.648180    0.865674
 H    5.006893   -1.336511    1.715910
 H    5.882048   -0.172541    0.703274
 H    4.191160    0.140685    1.139199
 C    2.006838   -1.062701   -3.291664
 H    0.998408   -1.161698   -2.861908
 H    2.159558    0.010925   -3.475919
 H    2.022005   -1.587475   -4.255984
 H    3.385987   -3.390320   -3.534884
 H    5.864794   -2.996936   -0.039925
83
Figure_S4-1_PA-9b(Na)-ts(1,6minor) / electronic energy: -3681.00662586 a.u. / lowest freq: -473.73 cm-1
 C    3.186998    2.460131   -0.440560
 H    3.647008    2.672480    0.537318
 C    3.879383    1.307115   -1.162490
 H    3.958625    1.473301   -2.250094
 C    1.766979    0.614601   -0.437847
 C    3.340236   -1.134927   -1.249282
 C    4.272016   -1.803179   -0.433424
 C    2.869931   -1.709438   -2.445763
 C    4.732775   -3.060109   -0.840604
 C    3.334204   -2.979947   -2.799618
 C    4.266660   -3.648033   -2.011241
 H    4.632013   -4.632387   -2.312038
Cu    0.005988   -0.317213   -0.311251
 N    1.837946    1.930352   -0.237902
 N    2.960739    0.192986   -0.898364
 C   -1.406904   -1.719397    0.496445
 C   -0.338186   -1.474598    1.431045
Na    2.341076   -0.067471    3.032442
 H    4.886791    1.097454   -0.777504
 H    3.170785    3.383701   -1.034047
 H   -1.200541   -2.531888   -0.208867
 C    0.813034   -2.386857    1.470565
 C   -0.466059   -0.542969    2.564299
 O    0.639655   -3.476778    0.715868
 O    1.851190   -2.204395    2.089225
 O    0.131983   -0.633268    3.621496
 O   -1.312435    0.465320    2.332683
 C   -1.369839    1.478520    3.332246
 H   -1.776586    1.076378    4.270802
 H   -2.035574    2.252660    2.934780
 H   -0.356385    1.872741    3.495396
 C    1.717096   -4.396078    0.640149
 H    2.625415   -3.905373    0.270039
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 H     1.401022   -5.176326   -0.060710
 H     1.919875   -4.837944    1.626102
 C     0.844982    2.670435    0.535769
 H     0.035196    1.949400    0.719185
 C     0.262938    3.838181   -0.231649
 C     0.955183    5.044749   -0.404170
 C    -1.021970    3.726903   -0.779375
 C     0.384259    6.100928   -1.115569
 H     1.949721    5.171299    0.029685
 C    -1.595640    4.779306   -1.490778
 H    -1.573371    2.791475   -0.653319
 C    -0.891689    5.971171   -1.663722
 H     0.939063    7.034003   -1.238620
 H    -2.596754    4.666556   -1.913580
 H    -1.337755    6.798924   -2.219723
 C     1.417019    3.020451    1.939439
 H     0.572881    3.569196    2.440717
 H     2.192472    3.820797    1.789144
 O     1.860067    1.939278    2.594087
 C    -2.731472   -1.262023    0.507844
 H    -3.036623   -0.538517    1.262916
 C    -3.620363   -1.624213   -0.506240
 H    -3.318081   -2.475297   -1.124353
 C    -5.090644   -1.472624   -0.366693
 C    -5.940889   -2.321331   -1.089755
 C    -5.671629   -0.494421    0.455571
 C    -7.326841   -2.207031   -0.988907
 H    -5.506790   -3.084553   -1.741503
 C    -7.055394   -0.378967    0.557214
 H    -5.036689    0.192861    1.018626
 C    -7.890623   -1.234940   -0.163654
 H    -7.968862   -2.881076   -1.560515
 H    -7.486341    0.388587    1.204128
 H    -8.975644   -1.141062   -0.082307
 C    -0.895449    0.434790   -1.979520
 H    -0.217607    1.113147   -2.497991
 C    -2.104730    0.136683   -2.208382
 C    -3.399554   -0.282023   -2.185872
 H    -3.737853   -0.995740   -2.943565
 H    -4.151942    0.443970   -1.863978
 C     4.778701   -1.220415    0.859287
 H     4.533305   -1.895982    1.691826
 H     5.872084   -1.099274    0.835471
 H     4.332969   -0.241959    1.073633
 C     1.898989   -0.988383   -3.339136
 H     0.863420   -1.133116   -2.995777
 H     2.080238    0.095521   -3.350399
 H     1.967479   -1.364020   -4.368824
 H     2.973754   -3.438463   -3.723688
 H     5.458275   -3.587110   -0.215691
83
Figure_S4-1_PA-9b(Na)-prod(1,6minor) / electronic energy: -3681.06430128 a.u. / lowest freq: 21.21 cm-1
 C     3.226157    2.141462   -1.115406
 H     3.943756    1.730487   -1.844991
 C     1.981494    2.723116   -1.797822
 H     1.688978    3.692407   -1.364389
 C     1.391008    0.782632   -0.624078
 C    -0.298759    1.641830   -2.154522
 C    -0.513121    0.638893   -3.118299
 C    -1.297637    2.575156   -1.829407
 C    -1.768487    0.561614   -3.726573
 C    -2.538511    2.465131   -2.466118
 C    -2.778369    1.461819   -3.399903
 H    -3.755507    1.385035   -3.881485
Cu     0.727416   -0.992562   -0.169907
 N     2.657275    1.064482   -0.297718
 N     0.969858    1.699739   -1.510828
 C    -1.832112   -0.930816    0.325892
 C    -1.007297   -2.154727    0.207894
Na     1.722544   -4.072152   -0.364496
 H     2.110097    2.856500   -2.881147
 H     3.758336    2.878133   -0.499223
 H    -1.978565   -0.430436   -0.637937
 C    -1.026691   -2.860215   -1.072021
 C    -0.459206   -2.885928    1.343647
 O    -1.945656   -2.371570   -1.926840
 O    -0.315058   -3.798815   -1.422414
 O     0.164962   -3.944930    1.312347
 O    -0.666072   -2.280433    2.528386
 C    -0.062042   -2.869405    3.663606
 H    -0.423501   -3.895259    3.822619
 H    -0.340791   -2.239227    4.516116
 H     1.032967   -2.892798    3.561061
 C    -1.995492   -2.955462   -3.213147
 H    -1.046635   -2.813036   -3.750952
 H    -2.807559   -2.448853   -3.746901
 H    -2.204184   -4.032903   -3.151169
 C     3.467274    0.113806    0.477977
 H     2.892873   -0.106924    1.392953
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 C     4.777656    0.746094    0.896361
 C     5.903650    0.725237    0.063418
 C     4.879234    1.384680    2.137464
 C     7.095318    1.330880    0.459253
 H     5.851430    0.231706   -0.909704
 C     6.068752    1.993048    2.537302
 H     4.012983    1.400747    2.804840
 C     7.181330    1.969093    1.696754
 H     7.962506    1.304350   -0.204532
 H     6.127590    2.484714    3.510828
 H     8.114788    2.444019    2.006567
 C     3.622840   -1.255723   -0.242825
 H     4.473482   -1.761433    0.270156
 H     3.991107   -1.034868   -1.276301
 O     2.490694   -2.019847   -0.236841
 C    -2.359744   -0.313360    1.396369
 H    -2.271147   -0.746939    2.393636
 C    -2.967105    1.063827    1.304523
 H    -2.717889    1.480979    0.316702
 C    -4.480645    1.074848    1.433977
 C    -5.271727    1.678986    0.451536
 C    -5.119626    0.491838    2.536722
 C    -6.662841    1.706451    0.565075
 H    -4.788117    2.129077   -0.419676
 C    -6.507655    0.517726    2.655519
 H    -4.523516    0.003363    3.312454
 C    -7.285909    1.127196    1.669209
 H    -7.261519    2.182200   -0.215373
 H    -6.986267    0.056915    3.522892
 H    -8.374130    1.147637    1.762034
 C     0.325043    2.048681    2.283820
 H     1.396509    2.054139    2.202301
 C    -0.883914    2.037046    2.340177
 C    -2.346797    2.000976    2.374523
 H    -2.742993    3.021919    2.247473
 H    -2.666728    1.668513    3.376652
 C     0.580645   -0.324556   -3.494071
 H     0.338216   -0.846002   -4.429804
 H     1.543446    0.191514   -3.622838
 H     0.739795   -1.082851   -2.709355
 C    -1.053489    3.665547   -0.822685
 H    -0.428978    3.308217    0.006673
 H    -0.544233    4.526410   -1.286111
 H    -2.002005    4.033138   -0.406428
 H    -3.327043    3.180343   -2.217631
 H    -1.950815   -0.212290   -4.475386
108
Figure_S5-1_AA-9d(Na)-prod(1,6major) / electronic energy: -4131.89053036 a.u. / lowest freq: 23.01 cm-1
 C     1.412694   -3.982468   -0.477634
 H     1.932082   -4.393047    0.397398
 C    -0.077024   -4.291398   -0.475407
 H    -0.361500   -5.015731   -1.250216
 C     0.237305   -1.971147   -0.611470
 C    -2.052778   -2.864936   -0.985002
 C    -2.884293   -3.967813   -0.744251
 C    -2.619191   -1.691529   -1.494510
 C    -4.259116   -3.899775   -0.987148
 C    -3.994015   -1.593622   -1.717744
 C    -4.802202   -2.707448   -1.467068
 H    -5.878454   -2.639691   -1.647541
Cu    -0.021678    0.013066   -0.656219
 N     1.433164   -2.521871   -0.446746
 N    -0.671724   -2.977894   -0.740783
 C    -0.797907    1.094405    1.406915
 C    -0.841372    0.042940    2.381899
Na     0.392136   -2.831366    3.318224
 H    -0.421336   -4.674529    0.499060
 H     1.911517   -4.347530   -1.387892
 H    -0.048062    1.861720    1.629521
 C    -1.858276   -0.989630    2.389275
 C     0.161364   -0.002041    3.418949
 O    -2.998258   -0.630022    1.768234
 O    -1.773402   -2.107151    2.893727
 O     0.207868   -0.791452    4.358783
 O     1.106489    0.965204    3.322379
 C     2.195019    0.847642    4.220049
 H     1.857435    0.853751    5.265889
 H     2.841066    1.714124    4.035754
 H     2.741223   -0.085648    4.017711
 C    -4.056441   -1.568410    1.764836
 H    -3.735728   -2.526887    1.336107
 H    -4.848191   -1.133522    1.144380
 H    -4.431618   -1.739082    2.784993
 C     2.651646   -1.801782   -0.090881
 H     2.357407   -0.742276   -0.062150
 C     3.757830   -1.966968   -1.117480
 C     4.420905   -3.189301   -1.307445
 C     4.182505   -0.866505   -1.873486
 C     5.451152   -3.311068   -2.239894
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 H    4.145570   -4.064047   -0.715996
 C    5.217069   -0.983172   -2.802195
 H    3.705954    0.103687   -1.720208
 C    5.852499   -2.208938   -2.994194
 H    5.947516   -4.275240   -2.372199
 H    5.527198   -0.106719   -3.376374
 H    6.659970   -2.304627   -3.723637
 C    3.097173   -2.199094    1.356599
 H    3.945515   -1.491537    1.569046
 H    3.616024   -3.193663    1.253880
 O    2.104531   -2.186212    2.245485
 C    0.698238    0.713011   -2.592305
 H   -0.003328    0.299564   -3.323226
 H    1.710743    0.302913   -2.623406
 C    0.406237    1.811045   -1.825015
 C   -0.921583    2.560631   -1.889178
 H   -0.669709    3.587150   -2.209331
 C   -1.903837    1.996682   -2.907280
 H   -1.476545    2.005154   -3.920556
 H   -2.184832    0.961368   -2.672402
 H   -2.828571    2.589344   -2.926091
 C   -1.531256    1.315976    0.259607
 H   -2.358221    0.641956    0.028121
 C   -1.504096    2.659714   -0.444949
 H   -0.799228    3.293712    0.111390
 C   -2.844951    3.384293   -0.403115
 C   -2.966501    4.659217   -0.978039
 C   -3.976958    2.834894    0.210273
 C   -4.176084    5.348737   -0.961923
 H   -2.095691    5.124663   -1.447159
 C   -5.192756    3.522712    0.227813
 H   -3.910304    1.860457    0.697231
 C   -5.301190    4.779192   -0.362166
 H   -4.241611    6.338794   -1.419369
 H   -6.060465    3.068326    0.712064
 H   -6.252321    5.316038   -0.349942
 C   -4.595699   -0.309759   -2.227004
 H   -4.241082   -0.078232   -3.243020
 H   -5.691837   -0.370503   -2.260100
 H   -4.321781    0.541837   -1.585153
 C   -5.134298   -5.087570   -0.682778
 H   -6.123700   -4.987467   -1.149623
 H   -4.677516   -6.022723   -1.038405
 H   -5.285732   -5.190629    0.403680
 H   -2.474528   -4.896760   -0.347685
 H   -1.972061   -0.846760   -1.729125
 B    1.574300    2.417592   -0.964465
 O    1.425713    3.418652   -0.054397
 O    2.861846    1.974043   -1.053448
 C    2.731465    3.794223    0.433354
 C    3.613634    2.546099    0.038839
 C    5.011226    2.883758   -0.457011
 H    4.985863    3.524808   -1.346987
 H    5.585327    3.394926    0.329653
 H    5.541090    1.956146   -0.717345
 C    3.687298    1.482920    1.130090
 H    2.688466    1.174753    1.473388
 H    4.200166    0.596942    0.730964
 H    4.260729    1.840072    1.996444
 C    2.623476    4.044706    1.929136
 H    2.009845    4.938375    2.111309
 H    2.148228    3.195893    2.437129
 H    3.616595    4.217190    2.369324
 C    3.125160    5.072976   -0.301258
 H    4.087873    5.461347    0.059618
 H    3.197762    4.908026   -1.385887
 H    2.355644    5.837419   -0.123020
108
Figure_S5-1_AA-9d(Na)-ts(1,6major) / electronic energy: -4131.84208395 a.u. / lowest freq: -388.75 cm-1
 C   -2.711428   -3.560318   -1.132305
 H   -2.940555   -4.392337   -0.455983
 C   -3.822044   -2.516706   -1.175235
 H   -4.381319   -2.522257   -2.120455
 C   -1.802443   -1.482480   -0.602707
 C   -3.716520   -0.015060   -1.150647
 C   -5.117856    0.045520   -1.100061
 C   -2.992944    1.160810   -1.370541
 C   -5.791194    1.256658   -1.264968
 C   -3.650939    2.385091   -1.527585
 C   -5.045495    2.420104   -1.479188
 H   -5.563011    3.375465   -1.603033
Cu   -0.439091   -0.167115    0.015113
 N   -1.575823   -2.788080   -0.629088
 N   -3.077685   -1.262639   -1.013789
 C    0.291728    1.125930    1.468171
 C   -0.772780    0.338840    2.044785
Na   -2.895378   -2.343495    2.760611
 H   -4.538826   -2.645827   -0.347872
 H   -2.482812   -3.963920   -2.130610
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H     1.292282    0.740652    1.688668
C    -2.190886    0.724592    2.110135
C    -0.403830   -0.808671    2.891926
O    -2.423783    2.007660    1.827688
O    -3.113091   -0.033989    2.371073
O    -1.084498   -1.260615    3.795464
O     0.788673   -1.342336    2.595678
C     1.119918   -2.532643    3.306770
H     1.273412   -2.319422    4.374091
H     2.050045   -2.899797    2.862028
H     0.306457   -3.262190    3.179765
C    -3.779397    2.430074    1.825288
H    -4.391841    1.778338    1.188916
H    -3.778538    3.450142    1.425814
H    -4.185106    2.425348    2.847135
C    -0.396587   -3.433138   -0.055809
H     0.156777   -2.619573    0.435653
C     0.509425   -4.065965   -1.088689
C     0.113697   -5.164826   -1.865135
C     1.810875   -3.577008   -1.249803
C     0.986779   -5.735439   -2.792025
H    -0.883258   -5.593867   -1.743935
C     2.685025   -4.142105   -2.176962
H     2.152393   -2.725057   -0.658608
C     2.274613   -5.223836   -2.955281
H     0.657605   -6.588742   -3.389761
H     3.687218   -3.722584   -2.291455
H     2.954823   -5.668397   -3.685396
C    -0.830002   -4.414434    1.075110
H     0.150020   -4.780473    1.489969
H    -1.246107   -5.326425    0.561704
O    -1.652875   -3.853165    1.964925
C     0.822483   -0.011040   -1.639409
H     0.077293    0.283313   -2.390232
H     1.052317   -1.082375   -1.669123
C     1.910067    0.867157   -1.402852
C     1.836518    2.242102   -1.627255
H     2.777802    2.795811   -1.600745
C     0.705249    2.854033   -2.395762
H     0.645384    2.446417   -3.420227
H    -0.257424    2.632002   -1.909175
H     0.801225    3.945902   -2.469218
C     0.264652    2.415375    0.896415
H    -0.697708    2.904028    0.755150
C     1.439172    3.026760    0.473743
H     2.379378    2.570306    0.790077
C     1.545697    4.467074    0.162051
C     2.820178    5.032955   -0.010463
C     0.430656    5.309280    0.027744
C     2.976406    6.382773   -0.313412
H     3.700017    4.391303    0.091286
C     0.584028    6.659849   -0.277325
H    -0.574727    4.909557    0.169458
C     1.856624    7.204735   -0.451628
H     3.978803    6.797776   -0.442119
H    -0.300443    7.293606   -0.375782
H     1.976010    8.264327   -0.687734
C    -2.859170    3.645640   -1.749864
H    -2.328461    3.618546   -2.713672
H    -3.505951    4.533297   -1.743514
H    -2.096966    3.771127   -0.967396
C    -7.296253    1.311504   -1.225679
H    -7.646217    2.167711   -0.630719
H    -7.708889    1.430530   -2.240169
H    -7.724662    0.395764   -0.795613
H    -5.702509   -0.857679   -0.923482
H    -1.904206    1.124885   -1.436150
B     3.212845    0.333471   -0.734838
O     4.088291    1.142500   -0.055571
O     3.621695   -0.974140   -0.739793
C     5.269041    0.376300    0.243014
C     4.731333   -1.101132    0.169044
C     5.720025   -2.112219   -0.390335
H     6.009007   -1.869222   -1.420635
H     6.626905   -2.150982    0.231366
H     5.264774   -3.113121   -0.389931
C     4.163126   -1.602277    1.494787
H     3.416057   -0.905582    1.902650
H     3.666328   -2.567336    1.319421
H     4.952744   -1.754517    2.243763
C     5.795395    0.793317    1.607106
H     6.150585    1.833027    1.565445
H     5.015138    0.729706    2.376080
H     6.640080    0.155805    1.907801
C     6.295329    0.694273   -0.843383
H     7.252426    0.187867   -0.655677
H     5.929881    0.396781   -1.837088
H     6.474539    1.778812   -0.857786
108
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Figure_S5-1_AA-9d(Na)-pc(1,6major) / electronic energy: -4131.84678962 a.u. / lowest freq: 18.68 cm-1

C	-1.371062	-4.174545	-1.111776
H	-1.381890	-4.969934	-0.356999
C	-2.752660	-3.544859	-1.306379
H	-3.156029	-3.684950	-2.319340
C	-1.244812	-1.906117	-0.585995
C	-3.504150	-1.148953	-1.206812
C	-4.846589	-1.546155	-1.259604
C	-3.188798	0.207606	-1.348457
C	-5.866461	-0.606949	-1.437478
C	-4.195381	1.160716	-1.516695
C	-5.528258	0.742800	-1.565188
H	-6.319245	1.485279	-1.702461
Cu	-0.386966	-0.231643	0.043240
N	-0.575582	-3.046781	-0.624751
N	-2.499639	-2.123097	-1.043193
C	-0.069760	1.123871	1.513162
C	-0.859499	0.043654	2.036771
Na	-2.069776	-3.200260	2.701714
H	-3.485363	-3.943913	-0.587932
H	-0.944895	-4.574440	-2.044540
H	0.995992	1.052733	1.752528
C	-2.339226	-0.030211	2.079578
C	-0.185378	-0.949916	2.909672
O	-2.956987	1.124733	1.846459
O	-2.971077	-1.052944	2.282443
O	-0.734733	-1.565120	3.802637
O	1.115081	-1.099766	2.660412
C	1.774127	-2.108849	3.424634
H	1.801292	-1.832585	4.487801
H	2.791387	-2.170956	3.025715
H	1.237356	-3.059418	3.291301
C	-4.378782	1.098534	1.816484
H	-4.738374	0.317666	1.133993
H	-4.691949	2.084940	1.457967
H	-4.778671	0.917661	2.824117
C	0.747544	-3.241138	-0.051603
H	0.980965	-2.301510	0.475384
C	1.815846	-3.461031	-1.107443
C	3.094749	-3.901868	-0.736393
C	1.587606	-3.177560	-2.459013
C	4.107279	-4.049720	-1.682657
H	3.311432	-4.122011	0.310536
C	2.598771	-3.322851	-3.408511
H	0.607619	-2.814586	-2.775575
C	3.865111	-3.759092	-3.025045
H	5.095284	-4.392270	-1.365533
H	2.394045	-3.086985	-4.455274
H	4.659236	-3.869284	-3.766701
C	0.656499	-4.348264	1.048093
H	1.666143	-4.356166	1.533471
H	0.623884	-5.329506	0.495462
O	-0.357003	-4.142986	1.897574
C	0.643519	0.332020	-1.601657
H	-0.129969	0.427660	-2.380763
H	1.199415	-0.606050	-1.745366
C	1.522087	1.489073	-1.455484
C	1.168824	2.760551	-1.778585
H	1.892653	3.564612	-1.614498
C	-0.154408	3.125818	-2.377537
H	-0.312398	2.648137	-3.361148
H	-0.974786	2.776651	-1.726748
H	-0.267623	4.211643	-2.503263
C	-0.495804	2.445986	1.111403
H	-1.561904	2.618180	0.969224
C	0.403676	3.432994	0.889354
H	1.463514	3.219348	1.054705
C	0.092561	4.808730	0.480949
C	1.149137	5.710125	0.268709
C	-1.218226	5.270212	0.271881
C	0.910014	7.017116	-0.147887
H	2.175656	5.366184	0.422024
C	-1.459465	6.576342	-0.144122
H	-2.065329	4.601354	0.435775
C	-0.397396	7.456813	-0.359350
H	1.749189	7.697268	-0.310895
H	-2.487251	6.910975	-0.302784
H	-0.588480	8.480758	-0.687694
C	-3.834761	2.616249	-1.650488
H	-3.313724	2.809964	-2.600656
H	-4.725359	3.258253	-1.615099
H	-3.154374	2.925429	-0.843415
C	-7.307270	-1.047527	-1.452573
H	-7.941821	-0.325551	-1.984943
H	-7.422634	-2.029379	-1.933649
H	-7.697646	-1.137793	-0.426046
H	-5.113882	-2.598609	-1.156454
H	-2.146235	0.530467	-1.347328
B	2.910368	1.234439	-0.804242

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 O     3.573427    2.124989    0.005157
 O     3.597167    0.058059   -0.947385
 C     4.886342    1.595472    0.265743
 C     4.687357    0.058113   -0.014330
 C     5.881992   -0.639049   -0.646380
 H     6.148559   -0.189046   -1.610889
 H     6.756086   -0.592651    0.020366
 H     5.635313   -1.696163   -0.822214
 C     4.212286   -0.718985    1.211065
 H     3.336486   -0.239026    1.670895
 H     3.909333   -1.725000    0.885873
 H     5.003247   -0.817809    1.968137
 C     5.280858    1.931888    1.695513
 H     5.400780    3.019536    1.803747
 H     4.519201    1.599683    2.412292
 H     6.238528    1.455627    1.953308
 C     5.844943    2.264163   -0.718529
 H     6.884963    1.954921   -0.542503
 H     5.580207    2.026782   -1.759254
 H     5.781404    3.354381   -0.591285
76
Figure_S5-1_9d(Na)-Cu-allyl / electronic energy: -3289.87323919 a.u. / lowest freq: 20.48 cm-1
 C     2.890494    1.919481   -1.277302
 H     3.212834    1.619009   -2.282905
 C     1.580347    2.708660   -1.287786
 H     1.715166    3.773396   -1.053559
 C     1.361334    0.845889    0.116302
 C    -0.476920    2.468998    0.143962
 C    -1.201053    3.344915   -0.672658
 C    -1.049124    2.021662    1.341390
 C    -2.500751    3.731098   -0.327753
 C    -2.353152    2.373080    1.688914
 C    -3.068439    3.232389    0.847613
 H    -4.088296    3.522016    1.116164
Cu     0.549243   -0.521771    1.237838
 N     2.543033    0.749000   -0.472014
 N     0.804179    2.032970   -0.243867
 H     1.066715    2.629079   -2.259433
 H     3.717911    2.468759   -0.801157
 C     3.344698   -0.463934   -0.515154
 H     2.901187   -1.123898    0.249271
 C     4.775968   -0.154327   -0.107352
 C     5.877692   -0.460143   -0.912213
 C     5.005969    0.459152    1.132365
 C     7.175180   -0.164497   -0.487241
 H     5.732823   -0.936167   -1.883022
 C     6.297285    0.758235    1.558327
 H     4.151927    0.706681    1.769782
 C     7.389916    0.445116    0.746743
 H     8.022928   -0.413557   -1.129804
 H     6.453595    1.234919    2.528793
 H     8.405182    0.675575    1.077400
 C     3.137215   -1.190296   -1.873781
 H     3.774689   -2.111853   -1.794461
 H     3.662176   -0.569468   -2.653477
 O     1.845948   -1.423998   -2.140698
 C    -0.451569   -1.910882    2.208955
 H    -1.214664   -1.404047    2.822373
 H     0.177713   -2.546649    2.852851
 C    -1.044927   -2.620703    1.056533
 C    -0.492142   -3.711033    0.455359
 H    -0.988980   -4.153163   -0.417369
 C     0.787250   -4.340968    0.920790
 H     1.118695   -5.149002    0.253404
 H     1.593059   -3.583472    0.969365
 H     0.701537   -4.758930    1.940091
 B    -2.306527   -1.993764    0.382957
 O    -3.373025   -1.412180    1.004517
 O    -2.415671   -1.921873   -0.995612
 C    -4.386992   -1.159047    0.008097
 C    -3.540932   -1.073394   -1.313835
 C    -5.133677    0.116193    0.360060
 C    -5.338535   -2.354768    0.029500
 C    -4.233816   -1.613380   -2.553791
 C    -2.982138    0.323768   -1.572158
 H    -4.479589   -2.677383   -2.447888
 H    -3.576969   -1.498793   -3.428337
 H    -5.161058   -1.055202   -2.750289
 H    -4.818196   -3.287688   -0.232540
 H    -6.175828   -2.213317   -0.667972
 H    -5.748118   -2.466329    1.043327
 H    -2.476565    0.722952   -0.681484
 H    -3.773968    1.028313   -1.862331
 H    -2.252056    0.281035   -2.394600
 H    -4.449481    0.965059    0.476018
 H    -5.678059   -0.021758    1.305057
 H    -5.865158    0.358733   -0.425131
Na    -0.132379   -1.871828   -1.732083
 C    -3.288355    4.628767   -1.246136
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 H   -4.131202    5.101149   -0.723105
 H   -2.656663    5.421816   -1.671818
 H   -3.701543    4.052122   -2.089506
 C   -2.973914    1.790798    2.930585
 H   -2.277050    1.825374    3.780685
 H   -3.894667    2.320460    3.211548
 H   -3.228022    0.732756    2.756237
 H   -0.769050    3.721967   -1.600967
 H   -0.472166    1.385437    2.015110
76
Figure_S5-1_9b(Na)-Cu-allyl / electronic energy: -3289.86902565 a.u. / lowest freq: 17.54 cm-1
 C   -2.892697    1.596089    1.460941
 H   -2.743197    1.250407    2.497136
 C   -1.975473    2.766074    1.108473
 H   -2.463374    3.496160    0.440338
 C   -1.249374    0.839069    0.001489
 C    0.301145    2.736026   -0.016190
 C    1.264409    3.038492    0.964267
 C    0.499150    3.065316   -1.370203
 C    2.449274    3.661177    0.561084
 C    1.705816    3.672713   -1.732198
 C    2.674483    3.968356   -0.777657
 H    3.610370    4.443824   -1.078925
Cu   -0.251244   -0.335231   -1.174432
 N   -2.441060    0.564339    0.526560
 N   -0.895934    2.082234    0.388527
 H   -1.606803    3.302977    1.991271
 H   -3.958000    1.822171    1.319187
 C   -3.044007   -0.760576    0.519412
 H   -2.554189   -1.289301   -0.315468
 C   -4.525217   -0.639770    0.199869
 C   -5.531197   -1.041691    1.083724
 C   -4.902867   -0.081480   -1.029569
 C   -6.878729   -0.890279    0.747507
 H   -5.271410   -1.477151    2.049741
 C   -6.244395    0.073098   -1.368072
 H   -4.124350    0.241321   -1.727003
 C   -7.240224   -0.331892   -0.476378
 H   -7.649523   -1.209649    1.452726
 H   -6.515806    0.510614   -2.331627
 H   -8.294305   -0.210547   -0.735919
 C   -2.663657   -1.551289    1.799213
 H   -3.213957   -2.525298    1.696342
 H   -3.180113   -1.041428    2.659897
 O   -1.336986   -1.673655    1.957204
 C    0.761487   -1.541323   -2.354457
 H    1.475351   -0.912042   -2.911363
 H    0.108200   -2.075043   -3.064880
 C    1.441426   -2.424103   -1.385089
 C    0.988711   -3.644270   -0.986354
 H    1.556486   -4.204231   -0.232322
 C   -0.265528   -4.273060   -1.519961
 H   -0.471331   -5.246949   -1.053546
 H   -1.139388   -3.618105   -1.339556
 H   -0.221274   -4.425144   -2.613314
 B    2.674857   -1.814147   -0.650999
 O    3.578781   -0.949566   -1.188422
 O    2.893022   -2.014555    0.702220
 C    4.592362   -0.671470   -0.204792
 C    3.868051   -1.044195    1.142553
 C    4.996463    0.790230   -0.319960
 C    5.781401   -1.578686   -0.516488
 C    4.764620   -1.674238    2.195354
 C    3.081412    0.121336    1.736282
 H    5.219611   -2.605750    1.836445
 H    4.178808   -1.903760    3.097250
 H    5.566555   -0.977538    2.480470
 H    5.509876   -2.641027   -0.432057
 H    6.626269   -1.378286    0.157165
 H    6.109124   -1.392230   -1.548824
 H    2.392039    0.553077    0.995092
 H    3.746843    0.918937    2.094387
 H    2.489884   -0.230057    2.595248
 H    4.125398    1.455965   -0.267177
 H    5.494789    0.958336   -1.285293
 H    5.701406    1.061643    0.480029
Na    0.603802   -2.265300    1.509716
 H    1.879983    3.924594   -2.781112
 H    3.211577    3.891914    1.309483
 C   -0.547128    2.775810   -2.413076
 H   -0.507148    1.718738   -2.725077
 H   -1.561952    2.956715   -2.031076
 H   -0.390961    3.397087   -3.304993
 C    1.037472    2.696278    2.412516
 H    0.431839    3.466996    2.916158
 H    0.508160    1.738685    2.519469
 H    1.991775    2.629837    2.951304
108
Figure_S5-1_AA-9b(Na)-pc(1,6major) / electronic energy: -4131.84106861 a.u. / lowest freq: 14.01 cm-1
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C	4.426624	-0.599879	-1.594332
H	5.233006	-0.953550	-0.935369
C	3.746449	-1.740194	-2.363359
H	3.618848	-1.515235	-3.433921
C	2.250518	-0.839589	-0.796342
C	1.501349	-2.860306	-1.938086
C	1.446861	-3.924376	-1.019720
C	0.670233	-2.813539	-3.068032
C	0.464773	-4.901569	-1.194914
C	-0.293998	-3.817530	-3.214690
C	-0.411611	-4.838848	-2.277434
H	-1.179878	-5.605363	-2.400958
Cu	0.497995	-0.449048	0.084791
N	3.339933	-0.086400	-0.757895
N	2.443465	-1.821591	-1.697421
C	-0.895977	-0.361032	1.541517
C	0.349372	-0.749297	2.171439
Na	3.793395	-1.367060	3.007562
H	4.287745	-2.693815	-2.279660
H	4.817706	0.184999	-2.257265
H	-1.143828	0.697374	1.655822
C	0.705312	-2.125874	2.565811
C	1.171799	0.316752	2.778999
O	-0.260090	-3.018269	2.342537
O	1.768196	-2.478511	3.050992
O	2.103476	0.165910	3.547389
O	0.804740	1.551722	2.397882
C	1.578457	2.624164	2.920243
H	1.494758	2.668696	4.014681
H	1.172126	3.535584	2.473267
H	2.636649	2.509989	2.645089
C	-0.024959	-4.359702	2.741282
H	0.868964	-4.767448	2.253602
H	-0.912653	-4.923394	2.434680
H	0.103770	-4.423572	3.830743
C	3.536777	1.041995	0.145299
H	2.724212	0.955091	0.876443
C	3.359737	2.360207	-0.583855
C	4.402271	2.973361	-1.290574
C	2.100258	2.974782	-0.592799
C	4.189726	4.164925	-1.986099
H	5.395291	2.519168	-1.299602
C	1.879822	4.154155	-1.300588
H	1.268808	2.514624	-0.051878
C	2.927421	4.757182	-1.997494
H	5.017616	4.629808	-2.526772
H	0.876758	4.583195	-1.315549
H	2.759366	5.684473	-2.549971
C	4.858113	0.868261	0.941466
H	4.890468	1.774249	1.610433
H	5.698728	1.055143	0.215897
O	4.932456	-0.315292	1.564102
C	-0.448679	0.427885	-1.487838
H	-0.289232	-0.352610	-2.241244
H	0.263980	1.252683	-1.633423
C	-1.834068	0.856875	-1.363244
C	-2.877791	0.037673	-1.670791
H	-3.895944	0.418275	-1.549099
C	-2.713915	-1.347171	-2.215096
H	-2.253919	-1.339508	-3.219125
H	-2.036160	-1.942397	-1.576681
H	-3.673508	-1.877453	-2.285643
C	-2.025402	-1.200881	1.218838
H	-1.858481	-2.270752	1.122849
C	-3.256824	-0.682446	0.993912
H	-3.410623	0.392054	1.122675
C	-4.460441	-1.454324	0.654693
C	-5.684847	-0.778954	0.518649
C	-4.446017	-2.843081	0.437754
C	-6.850919	-1.460681	0.178937
H	-5.710778	0.303280	0.671715
C	-5.610723	-3.525607	0.099159
H	-3.510393	-3.399170	0.523507
C	-6.819684	-2.839470	-0.032817
H	-7.790315	-0.912676	0.075948
H	-5.574133	-4.604777	-0.067181
H	-7.732056	-3.376959	-0.300424
B	-2.181686	2.256833	-0.778713
O	-3.346125	2.509204	-0.093621
O	-1.391573	3.375930	-0.869645
C	-3.462971	3.927898	0.093292
C	-1.969291	4.405512	-0.045318
C	-1.805121	5.754931	-0.729155
H	-2.181719	5.734183	-1.759441
H	-2.344695	6.535391	-0.172349
H	-0.742977	6.037324	-0.758328
C	-1.204139	4.391750	1.275720
H	-1.284703	3.415021	1.775100
H	-0.141731	4.579074	1.063021

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 H   -1.559744    5.172242    1.962771
 C   -4.092439    4.197454    1.451408
 H   -5.128996    3.830544    1.457912
 H   -3.547108    3.690103    2.257425
 H   -4.111051    5.277000    1.662596
 C   -4.368212    4.452850   -1.021053
 H   -4.559280    5.529724   -0.913671
 H   -3.927965    4.271452   -2.012334
 H   -5.331065    3.924466   -0.974366
 H    0.397206   -5.727974   -0.482866
 H   -0.968417   -3.787386   -4.074025
 C    0.828630   -1.746848   -4.118624
 H   -0.131621   -1.524172   -4.603497
 H    1.228941   -0.814017   -3.700646
 H    1.524158   -2.085248   -4.904011
 C    2.463165   -4.017744    0.086141
 H    3.484660   -3.933092   -0.314037
 H    2.351071   -3.214977    0.827817
 H    2.387124   -4.981425    0.607048
108
Figure_S5-1_AA-9b(Na)-ts(1,6major) / electronic energy: -4131.83854441 a.u. / lowest freq: -314.01 cm-1
 C    4.409202   -0.678859   -1.598345
 H    5.207548   -1.054404   -0.941860
 C    3.706139   -1.798193   -2.378042
 H    3.596282   -1.568039   -3.449415
 C    2.223515   -0.871689   -0.812396
 C    1.434987   -2.867925   -1.971666
 C    1.347184   -3.924553   -1.046921
 C    0.621524   -2.813495   -3.113970
 C    0.355907   -4.889661   -1.235793
 C   -0.350795   -3.807478   -3.275246
 C   -0.497135   -4.823552   -2.336606
 H   -1.271345   -5.582115   -2.471515
Cu    0.496181   -0.459771    0.096214
 N    3.333055   -0.149647   -0.757910
 N    2.394188   -1.846363   -1.725962
 C   -0.926695   -0.354216    1.585449
 C    0.319930   -0.747922    2.224491
Na    3.736675   -1.410196    3.015045
 H    4.220373   -2.766437   -2.290448
 H    4.816547    0.103718   -2.254261
 H   -1.153101    0.711394    1.678048
 C    0.654958   -2.121833    2.619202
 C    1.157029    0.309056    2.806858
 O   -0.321657   -3.003783    2.381993
 O    1.707722   -2.496944    3.115524
 O    2.109282    0.160055    3.554073
 O    0.792913    1.550462    2.428543
 C    1.585552    2.615027    2.935263
 H    1.531681    2.656479    4.031831
 H    1.173512    3.531428    2.503325
 H    2.636148    2.498108    2.632803
 C   -0.108171   -4.346218    2.785163
 H    0.789218   -4.765425    2.313326
 H   -0.996803   -4.901057    2.464708
 H    0.002286   -4.412473    3.876704
 C    3.554110    0.965420    0.156830
 H    2.742115    0.886894    0.890514
 C    3.402118    2.292883   -0.561064
 C    4.453546    2.886630   -1.271342
 C    2.157175    2.936280   -0.558273
 C    4.263440    4.086288   -1.959333
 H    5.436350    2.411024   -1.288785
 C    1.958755    4.123771   -1.259006
 H    1.320349    2.493633   -0.010863
 C    3.014766    4.706662   -1.960045
 H    5.098247    4.535450   -2.502571
 H    0.965982    4.575798   -1.265411
 H    2.863814    5.640228   -2.506772
 C    4.874971    0.758450    0.946498
 H    4.925505    1.656483    1.624995
 H    5.716095    0.938007    0.219524
 O    4.930325   -0.433057    1.556033
 C   -0.446441    0.476821   -1.530405
 H   -0.272218   -0.355557   -2.218822
 H    0.296764    1.278015   -1.622207
 C   -1.792693    0.871003   -1.322151
 C   -2.848236   -0.018189   -1.484198
 H   -3.861083    0.390666   -1.460661
 C   -2.658429   -1.367670   -2.105762
 H   -2.287646   -1.280162   -3.142345
 H   -1.900389   -1.953703   -1.557194
 H   -3.591840   -1.945689   -2.128204
 C   -2.009583   -1.159127    1.163043
 H   -1.875852   -2.237122    1.121905
 C   -3.208743   -0.599180    0.759351
 H   -3.373906    0.460289    0.963227
 C   -4.441509   -1.376310    0.533011
 C   -5.667315   -0.694506    0.451684
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 C   -4.454014   -2.773184    0.382699
 C   -6.860582   -1.377878    0.232453
 H   -5.673321    0.393835    0.558437
 C   -5.646781   -3.457753    0.162519
 H   -3.519068   -3.335233    0.426778
 C   -6.856599   -2.765797    0.086217
 H   -7.800575   -0.824145    0.174457
 H   -5.630839   -4.544012    0.046024
 H   -7.790818   -3.304488   -0.086565
 B   -2.128721    2.290733   -0.774518
 O   -3.293047    2.563854   -0.101912
 O   -1.330156    3.398645   -0.892786
 C   -3.397117    3.988156    0.060249
 C   -1.898486    4.448267   -0.084685
 C   -1.720120    5.784224   -0.790331
 H   -2.097458    5.750960   -1.819982
 H   -2.250998    6.579176   -0.245895
 H   -0.655135    6.054910   -0.824320
 C   -1.135774    4.445992    1.237735
 H   -1.227012    3.476967    1.750165
 H   -0.070979    4.621263    1.026726
 H   -1.486740    5.238808    1.912808
 C   -4.025296    4.286900    1.412530
 H   -5.066480    3.933666    1.423106
 H   -3.487559    3.785641    2.227322
 H   -4.030070    5.369807    1.606196
 C   -4.295604    4.500327   -1.065041
 H   -4.477524    5.580422   -0.976214
 H   -3.855182    4.298549   -2.052234
 H   -5.263025    3.981206   -1.010802
 H    0.262632   -5.709887   -0.519615
 H   -1.010160   -3.771735   -4.146018
 C    0.800958   -1.744126   -4.158673
 H   -0.153909   -1.505369   -4.646711
 H    1.213103   -0.819367   -3.733760
 H    1.495772   -2.086658   -4.942798
 C    2.334580   -4.022077    0.084239
 H    3.366807   -3.937008   -0.287161
 H    2.203278   -3.220744    0.824604
 H    2.242445   -4.986516    0.600994
108
Figure_S5-1_AA-9b(Na)-prod(1,6major) / electronic energy: -4131.89305721 a.u. / lowest freq: 14.34 cm-1
 C    4.164748   -1.377524   -0.543902
 H    4.765624   -1.547913    0.357421
 C    3.465744   -2.621183   -1.090048
 H    3.905476   -2.992066   -2.026268
 C    1.883536   -0.931945   -0.720680
 C    1.191082   -2.767922   -2.193631
 C    0.438424   -3.867209   -1.754598
 C    1.108434   -2.290243   -3.514752
 C   -0.430061   -4.479860   -2.664284
 C    0.215949   -2.917077   -4.388192
 C   -0.547539   -4.004162   -3.966517
 H   -1.239629   -4.484668   -4.661403
Cu    0.081514   -0.100108   -0.556349
 N    3.030727   -0.511664   -0.202549
 N    2.100743   -2.126510   -1.308257
 C   -0.700145   -0.142677    1.746611
 C    0.432926   -0.379741    2.614873
Na    3.706184   -0.667200    3.934341
 H    3.455734   -3.448687   -0.361690
 H    4.790981   -0.890339   -1.309914
 H   -1.124043    0.864317    1.846324
 C    0.876419   -1.693342    3.016038
 C    1.096609    0.758205    3.201470
 O    0.076226   -2.698758    2.590948
 O    1.862908   -1.973577    3.693199
 O    1.937602    0.762802    4.095287
 O    0.724682    1.947860    2.652792
 C    1.418854    3.087352    3.126865
 H    1.283935    3.219079    4.209577
 H    1.001757    3.947763    2.593568
 H    2.494798    3.004492    2.912082
 C    0.399875   -4.001220    3.035382
 H    1.395772   -4.309916    2.685275
 H   -0.363352   -4.665388    2.613027
 H    0.379228   -4.064053    4.133069
 C    3.218623    0.819089    0.381528
 H    2.396377    0.954303    1.095369
 C    3.091427    1.875991   -0.695682
 C    4.070406    2.037596   -1.686887
 C    1.944838    2.675087   -0.758687
 C    3.906019    2.971968   -2.708372
 H    4.974687    1.425411   -1.665629
 C    1.773849    3.607251   -1.782656
 H    1.167084    2.556102    0.002445
 C    2.755312    3.759866   -2.760467
 H    4.680433    3.082309   -3.471265
 H    0.853142    4.189987   -1.824439
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 H     2.622590    4.487886   -3.564078
 C     4.543196    0.884218    1.192332
 H     4.567059    1.946526    1.565141
 H     5.373240    0.863580    0.430304
 O     4.650151   -0.058861    2.136759
 C    -0.715831    0.625880   -2.420159
 H    -0.598255   -0.262280   -3.047300
 H    -0.111834    1.498119   -2.689349
 C    -1.720272    0.736635   -1.492541
 C    -2.730295   -0.373056   -1.202476
 H    -3.724444    0.036035   -1.457252
 C    -2.520778   -1.644419   -2.013099
 H    -2.567653   -1.445090   -3.093502
 H    -1.544808   -2.107507   -1.804456
 H    -3.296236   -2.386447   -1.777909
 C    -1.369194   -0.973451    0.881372
 H    -1.033135   -2.005519    0.778009
 C    -2.738887   -0.616377    0.337055
 H    -3.015569    0.347716    0.782997
 C    -3.829423   -1.592900    0.744684
 C    -5.139507   -1.115274    0.885192
 C    -3.599479   -2.958274    0.951329
 C    -6.188038   -1.969978    1.219989
 H    -5.334678   -0.049954    0.731001
 C    -4.645765   -3.818340    1.287584
 H    -2.591144   -3.364450    0.851609
 C    -5.944107   -3.328690    1.423441
 H    -7.199451   -1.571423    1.329424
 H    -4.442675   -4.879981    1.446825
 H    -6.761413   -4.002220    1.690813
 B    -2.043895    2.161145   -0.908801
 O    -3.126900    2.406078   -0.113258
 O    -1.346077    3.294723   -1.207152
 C    -3.305475    3.834273   -0.028764
 C    -1.868416    4.364447   -0.389521
 C    -1.850153    5.655653   -1.191658
 H    -2.355841    5.539685   -2.158455
 H    -2.342658    6.463305   -0.630221
 H    -0.811631    5.962060   -1.382610
 C    -0.955244    4.477051    0.826738
 H    -0.931029    3.534126    1.392860
 H     0.067568    4.695791    0.488173
 H    -1.273652    5.285981    1.498763
 C    -3.783889    4.186734    1.370170
 H    -4.787238    3.768003    1.532870
 H    -3.116064    3.780476    2.140042
 H    -3.844667    5.277854    1.494669
 C    -4.362214    4.211995   -1.064673
 H    -4.594836    5.285254   -1.025095
 H    -4.032308    3.962693   -2.083696
 H    -5.283958    3.650446   -0.856657
 H    -1.033025   -5.330282   -2.336880
 H     0.126334   -2.553146   -5.414674
 C     1.977388   -1.147369   -3.970893
 H     1.806180   -0.924162   -5.032133
 H     1.789076   -0.231491   -3.390987
 H     3.044354   -1.385831   -3.840010
 C     0.562452   -4.357373   -0.340231
 H     1.489459   -4.936015   -0.198718
 H     0.594227   -3.517374    0.366705
 H    -0.279768   -5.009538   -0.072037
108
Figure_S5-1_AA-9d(Na)-prod(1,6minor) / electronic energy: -4131.89461386 a.u. / lowest freq: 15.14 cm-1
 C     1.527565    3.959244    1.128272
 H     2.402038    4.398648    0.630256
 C     0.183036    4.296853    0.481273
 H    -0.445321    4.917142    1.133522
 C     0.460338    1.969951    0.523869
 C    -1.602611    2.835008   -0.490365
 C    -2.638710    3.755604   -0.310066
 C    -1.722008    1.846550   -1.471418
 C    -3.785425    3.703744   -1.107678
 C    -2.850087    1.788961   -2.291760
 C    -3.874204    2.722207   -2.099620
 H    -4.761234    2.684591   -2.738902
Cu     0.217120    0.006197    0.452826
 N     1.585501    2.501684    0.980010
 N    -0.412104    2.968201    0.260010
 C     1.159167   -0.868446   -1.511022
 C     2.347865   -0.119169   -1.889128
Na     4.774227    2.446377   -1.738403
 H     0.290446    4.813584   -0.486170
 H     1.548789    4.232726    2.194926
 H     0.310289   -0.732629   -2.191893
 C     2.177155    1.052204   -2.713897
 C     3.685286   -0.469530   -1.484919
 O     0.895500    1.240322   -3.113881
 O     3.029016    1.866019   -3.064576
 O     4.720843    0.158750   -1.697077
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 O     3.770611   -1.642108   -0.805522
 C     5.062185   -2.059780   -0.408811
 H     5.718481   -2.212996   -1.277601
 H     4.922718   -3.008448    0.123031
 H     5.533027   -1.322804    0.258688
 C     0.625352    2.411302   -3.857115
 H     0.906778    3.312795   -3.293302
 H    -0.455620    2.416284   -4.037653
 H     1.165305    2.411682   -4.815022
 C     2.775794    1.710476    1.288780
 H     2.924825    1.029866    0.437491
 C     2.619234    0.882484    2.539475
 C     2.012578    1.389961    3.694165
 C     3.149610   -0.412598    2.577296
 C     1.933908    0.620275    4.854074
 H     1.578612    2.392484    3.682589
 C     3.077963   -1.184107    3.736444
 H     3.605977   -0.824903    1.674110
 C     2.466527   -0.669747    4.880356
 H     1.450778    1.029682    5.744135
 H     3.492840   -2.194568    3.743179
 H     2.401774   -1.272607    5.788692
 C     4.048620    2.614416    1.335450
 H     4.855619    1.903288    1.662171
 H     3.905325    3.277127    2.238366
 O     4.289887    3.266534    0.191655
 C    -0.475841   -0.725742    2.474875
 H    -0.969078    0.166253    2.870384
 H     0.485444   -0.988300    2.926647
 C    -1.121877   -1.534474    1.592333
 C    -0.601912   -2.879408    1.107298
 H    -1.463960   -3.565249    1.128593
 C     0.490312   -3.485742    1.984120
 H     1.386662   -2.851840    2.044440
 H     0.121647   -3.629721    3.010537
 H     0.798501   -4.465606    1.591055
 C     0.973841   -1.764138   -0.485689
 H     1.834180   -1.992672    0.145251
 C    -0.182946   -2.731221   -0.386490
 H    -1.052299   -2.306335   -0.919665
 C     0.098673   -4.084035   -1.026438
 C    -0.956123   -4.990472   -1.202245
 C     1.380163   -4.465050   -1.437498
 C    -0.737115   -6.246529   -1.762926
 H    -1.967075   -4.701085   -0.899335
 C     1.602896   -5.724287   -1.998576
 H     2.211669   -3.764611   -1.329868
 C     0.548160   -6.620334   -2.161166
 H    -1.573436   -6.937289   -1.894007
 H     2.611226   -6.002955   -2.314219
 H     0.722877   -7.603744   -2.603368
 C    -2.919750    0.783887   -3.412885
 H    -2.352821   -0.127471   -3.175169
 H    -3.958006    0.499075   -3.634338
 H    -2.491679    1.204636   -4.337334
 C    -4.923425    4.661111   -0.870139
 H    -5.463520    4.882128   -1.801569
 H    -5.649371    4.227028   -0.162992
 H    -4.570817    5.608717   -0.439306
 H    -2.559267    4.523296    0.462028
 H    -0.889866    1.165570   -1.646998
 B    -2.607564   -1.171924    1.232826
 O    -3.462573   -2.079566    0.681338
 O    -3.205489    0.012274    1.545801
 C    -4.723743   -1.411776    0.455280
 C    -4.632143   -0.188556    1.442648
 C    -5.278005    1.088423    0.933969
 H    -4.808714    1.434966    0.005803
 H    -6.351992    0.930159    0.755483
 H    -5.169587    1.882824    1.686449
 C    -5.135773   -0.516484    2.847224
 H    -4.684067   -1.442546    3.232308
 H    -4.861541    0.303788    3.525533
 H    -6.228919   -0.628463    2.862924
 C    -5.855743   -2.383813    0.745316
 H    -5.850387   -3.191021   -0.000852
 H    -5.757145   -2.837443    1.739521
 H    -6.826923   -1.870812    0.685871
 C    -4.739060   -0.989983   -1.009226
 H    -5.692664   -0.518619   -1.285269
 H    -3.929450   -0.278221   -1.212942
 H    -4.590735   -1.876066   -1.642537
108
Figure_S5-1_AA-9d(Na)-ts(1,6minor) / electronic energy: -4131.83826859 a.u. / lowest freq: -396.29 cm-1
 C     4.469926   -0.443997    1.672550
 H     5.247146   -1.041689    1.180404
 C     4.499512    1.026998    1.249706
 H     4.746261    1.708953    2.075439
 C     2.421749    0.104477    0.696218
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C	2.694159	2.516174	0.328613
C	3.622554	3.539170	0.105580
C	1.335007	2.773658	0.113683
C	3.206557	4.798635	-0.343625
C	0.906044	4.009041	-0.365093
C	1.849125	5.019335	-0.583949
H	1.518011	5.994382	-0.952441
Cu	0.651461	-0.233012	-0.145874
N	3.153417	-0.876718	1.197255
N	3.129732	1.255260	0.775787
C	-0.449819	-0.377166	-1.908705
C	0.950711	-0.574103	-2.219945
Na	4.395784	-1.267744	-1.911966
H	5.218917	1.203147	0.434085
H	4.556865	-0.574590	2.761710
H	-0.771980	0.671056	-1.906903
C	1.796754	0.554814	-2.631366
C	1.557204	-1.901068	-2.399781
O	1.102828	1.647176	-2.967186
O	3.019774	0.554075	-2.655052
O	2.551044	-2.139089	-3.064543
O	0.935241	-2.881995	-1.730970
C	1.568065	-4.158285	-1.755685
H	1.565912	-4.575960	-2.772163
H	0.975953	-4.795886	-1.089555
H	2.604387	-4.059483	-1.397996
C	1.854176	2.797963	-3.322961
H	2.591949	3.042654	-2.547584
H	1.131407	3.614819	-3.423296
H	2.372569	2.636210	-4.279059
C	2.729288	-2.269726	1.190057
H	2.000328	-2.350750	0.369887
C	2.030512	-2.693264	2.462173
C	1.303811	-3.891954	2.458310
C	2.047587	-1.933595	3.636297
C	0.623887	-4.324069	3.594496
H	1.253762	-4.484814	1.541294
C	1.367489	-2.362807	4.776761
H	2.573226	-0.977399	3.661215
C	0.654963	-3.560385	4.762348
H	0.058466	-5.258332	3.564838
H	1.389462	-1.749953	5.680903
H	0.118708	-3.893730	5.653464
C	3.933789	-3.167413	0.769042
H	3.517506	-4.210119	0.766053
H	4.635625	-3.170081	1.651187
O	4.476100	-2.768885	-0.387895
C	-0.617585	-0.227119	1.499638
H	-0.259743	0.665067	2.027138
H	-0.161570	-1.154496	1.875175
C	-1.998087	-0.258720	1.179527
C	-2.643875	-1.418897	0.748472
H	-3.735269	-1.406444	0.754760
C	-1.975880	-2.758440	0.801979
H	-0.987700	-2.727335	0.312538
H	-1.801482	-3.073755	1.845746
H	-2.581871	-3.532649	0.308588
C	-1.483318	-1.333013	-1.904628
H	-1.228083	-2.367889	-2.130937
C	-2.769548	-1.031796	-1.482698
H	-3.013770	0.022045	-1.329599
C	-3.949462	-1.881475	-1.751590
C	-5.230206	-1.355439	-1.509259
C	-3.856110	-3.195219	-2.237390
C	-6.375288	-2.109163	-1.751358
H	-5.312610	-0.345042	-1.099853
C	-5.002510	-3.951400	-2.476432
H	-2.878385	-3.637161	-2.438538
C	-6.267312	-3.412922	-2.238427
H	-7.359429	-1.676133	-1.557402
H	-4.905044	-4.970339	-2.858533
H	-7.164255	-4.005613	-2.431296
C	-0.550857	4.210838	-0.677788
H	-1.177033	3.580697	-0.030806
H	-0.854242	5.259895	-0.551482
H	-0.760119	3.927434	-1.722701
C	4.218891	5.896659	-0.543801
H	3.849068	6.661840	-1.240298
H	4.442114	6.397217	0.412094
H	5.166978	5.501689	-0.936412
H	4.686341	3.368745	0.274961
H	0.589000	2.008960	0.331241
B	-2.867154	1.034726	1.243105
O	-4.168686	1.066803	0.807004
O	-2.470203	2.243035	1.761486
C	-4.632911	2.425335	0.884714
C	-3.662798	3.033453	1.958791
C	-3.349024	4.508225	1.772070
H	-2.917498	4.718525	0.787415

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 H   -4.266143    5.105093    1.885539
 H   -2.630433    4.835287    2.537093
 C   -4.129722    2.778140    3.392489
 H   -4.379700    1.718700    3.550281
 H   -3.317260    3.042675    4.083975
 H   -5.009866    3.386284    3.644266
 C   -6.101976    2.428584    1.276122
 H   -6.702526    1.988364    0.467061
 H   -6.278214    1.844425    2.188036
 H   -6.455168    3.457239    1.442197
 C   -4.450664    3.041417   -0.502266
 H   -4.848405    4.065103   -0.546035
 H   -3.389948    3.064525   -0.792358
 H   -4.992125    2.429854   -1.238270
108
Figure_S5-1_AA-9d(Na)-pc(1,6minor) / electronic energy: -4131.84483185 a.u. / lowest freq: -3.52 cm-1
 C    4.461293   -0.848137    1.538673
 H    5.155156   -1.475896    0.965822
 C    4.620877    0.641259    1.222724
 H    4.903144    1.242189    2.099305
 C    2.459543   -0.049804    0.638933
 C    2.964918    2.347645    0.415199
 C    3.983563    3.287367    0.226634
 C    1.631137    2.756810    0.295017
 C    3.680683    4.618154   -0.090949
 C    1.311070    4.069192   -0.041105
 C    2.344108    4.995932   -0.226834
 H    2.100443    6.031941   -0.478494
Cu    0.617532   -0.171293   -0.124209
 N    3.092223   -1.117929    1.095045
 N    3.284205    1.018244    0.749042
 C   -0.521406   -0.159234   -1.804631
 C    0.845351   -0.414703   -2.164728
Na    4.237793   -1.401879   -2.173051
 H    5.370360    0.813916    0.434864
 H    4.578740   -1.072907    2.609278
 H   -0.810692    0.897383   -1.820307
 C    1.758191    0.680073   -2.561708
 C    1.342449   -1.774038   -2.492192
 O    1.134759    1.832561   -2.795642
 O    2.970591    0.578530   -2.654591
 O    2.220045   -2.013961   -3.298411
 O    0.740062   -2.745564   -1.808463
 C    1.243925   -4.067164   -2.002437
 H    1.084154   -4.391561   -3.039981
 H    0.673163   -4.702996   -1.317033
 H    2.317847   -4.075526   -1.760490
 C    1.951982    2.946679   -3.131024
 H    2.731359    3.101426   -2.373219
 H    1.284164    3.813709   -3.165782
 H    2.422474    2.792422   -4.112390
 C    2.547092   -2.465134    1.039809
 H    1.732241   -2.423635    0.302040
 C    1.952589   -2.923918    2.354758
 C    1.980956   -2.143857    3.515629
 C    1.297424   -4.162674    2.407203
 C    1.384726   -2.590068    4.695919
 H    2.449250   -1.158088    3.498307
 C    0.701371   -4.611603    3.583302
 H    1.232501   -4.776341    1.505467
 C    0.744204   -3.826749    4.736640
 H    1.414378   -1.958730    5.587046
 H    0.190152   -5.576913    3.596330
 H    0.272585   -4.174654    5.658221
 C    3.624082   -3.418911    0.433500
 H    3.120093   -4.418353    0.371639
 H    4.395257   -3.565461    1.241174
 O    4.103805   -2.961572   -0.731255
 C   -0.561739   -0.037531    1.507573
 H   -0.257776    0.910981    1.975829
 H   -0.111088   -0.873333    2.068443
 C   -2.015237   -0.157795    1.354703
 C   -2.622090   -1.361552    1.179660
 H   -3.708902   -1.395615    1.065769
 C   -1.870570   -2.652362    1.107164
 H   -1.059309   -2.575428    0.357734
 H   -1.371362   -2.898945    2.061539
 H   -2.519233   -3.496200    0.831971
 C   -1.620225   -1.097291   -1.926325
 H   -1.373555   -2.130106   -2.172676
 C   -2.905785   -0.763488   -1.689820
 H   -3.139123    0.260737   -1.386787
 C   -4.064653   -1.661253   -1.813800
 C   -5.292821   -1.267875   -1.255667
 C   -3.999865   -2.904885   -2.464432
 C   -6.414005   -2.090010   -1.336018
 H   -5.343142   -0.318852   -0.716739
 C   -5.121163   -3.727141   -2.544120
 H   -3.065759   -3.231894   -2.926140
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 C   -6.333710   -3.324684   -1.981214
 H   -7.355624   -1.766732   -0.886156
 H   -5.048806   -4.689813   -3.055512
 H   -7.211550   -3.971450   -2.046053
 C   -0.131639    4.450427   -0.226850
 H   -0.787884    3.817848    0.386362
 H   -0.312636    5.503877    0.030294
 H   -0.431491    4.311235   -1.279053
 C    4.795154    5.616417   -0.270547
 H    4.417539    6.575401   -0.650660
 H    5.305857    5.808813    0.686024
 H    5.553704    5.243378   -0.975012
 H    5.030786    2.998023    0.326050
 H    0.823543    2.049698    0.482911
 B   -2.920015    1.106743    1.309435
 O   -4.262975    1.069952    1.005916
 O   -2.496973    2.394962    1.552749
 C   -4.724119    2.419588    0.844901
 C   -3.669939    3.222133    1.684717
 C   -3.387108    4.623172    1.167040
 H   -3.013914    4.613980    0.135927
 H   -4.305108    5.229031    1.200334
 H   -2.632262    5.111930    1.799544
 C   -4.012188    3.276552    3.173973
 H   -4.248614    2.277319    3.567893
 H   -3.141849    3.662179    3.723683
 H   -4.866179    3.940833    3.367623
 C   -6.155306    2.522239    1.348122
 H   -6.820577    1.938255    0.695564
 H   -6.252173    2.130962    2.368748
 H   -6.497123    3.567963    1.336079
 C   -4.661753    2.748334   -0.647540
 H   -5.067941    3.747746   -0.857869
 H   -3.628222    2.705387   -1.023098
 H   -5.258795    2.013185   -1.206049
76
Figure_S5-1_9d(Na)-Cu-allyl / electronic energy: -3289.87323919 a.u. / lowest freq: 20.48 cm-1
 C    2.890494    1.919481   -1.277302
 H    3.212834    1.619009   -2.282905
 C    1.580347    2.708660   -1.287786
 H    1.715166    3.773396   -1.053559
 C    1.361334    0.845889    0.116302
 C   -0.476920    2.468998    0.143962
 C   -1.201053    3.344915   -0.672658
 C   -1.049124    2.021662    1.341390
 C   -2.500751    3.731098   -0.327753
 C   -2.353152    2.373080    1.688914
 C   -3.068439    3.232389    0.847613
 H   -4.088296    3.522016    1.116164
Cu    0.549243   -0.521771    1.237838
 N    2.543033    0.749000   -0.472014
 N    0.804179    2.032970   -0.243867
 H    1.066715    2.629079   -2.259433
 H    3.717911    2.468759   -0.801157
 C    3.344698   -0.463934   -0.515154
 H    2.901187   -1.123898    0.249271
 C    4.775968   -0.154327   -0.107352
 C    5.877692   -0.460143   -0.912213
 C    5.005969    0.459152    1.132365
 C    7.175180   -0.164497   -0.487241
 H    5.732823   -0.936167   -1.883022
 C    6.297285    0.758235    1.558327
 H    4.151927    0.706681    1.769782
 C    7.389916    0.445116    0.746743
 H    8.022928   -0.413557   -1.129804
 H    6.453595    1.234919    2.528793
 H    8.405182    0.675575    1.077400
 C    3.137215   -1.190296   -1.873781
 H    3.774689   -2.111853   -1.794461
 H    3.662176   -0.569468   -2.653477
 O    1.845948   -1.423998   -2.140698
 C   -0.451569   -1.910882    2.208955
 H   -1.214664   -1.404047    2.822373
 H    0.177713   -2.546649    2.852851
 C   -1.044927   -2.620703    1.056533
 C   -0.492142   -3.711033    0.455359
 H   -0.988980   -4.153163   -0.417369
 C    0.787250   -4.340968    0.920790
 H    1.118695   -5.149002    0.253404
 H    1.593059   -3.583472    0.969365
 H    0.701537   -4.758930    1.940091
 B   -2.306527   -1.993764    0.382957
 O   -3.373025   -1.412180    1.004517
 O   -2.415671   -1.921873   -0.995612
 C   -4.386992   -1.159047    0.008097
 C   -3.540932   -1.073394   -1.313835
 C   -5.133677    0.116193    0.360060
 C   -5.338535   -2.354768    0.029500
 C   -4.233816   -1.613380   -2.553791
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 C   -2.982138    0.323768   -1.572158
 H   -4.479589   -2.677383   -2.447888
 H   -3.576969   -1.498793   -3.428337
 H   -5.161058   -1.055202   -2.750289
 H   -4.818196   -3.287688   -0.232540
 H   -6.175828   -2.213317   -0.667972
 H   -5.748118   -2.466329    1.043327
 H   -2.476565    0.722952   -0.681484
 H   -3.773968    1.028313   -1.862331
 H   -2.252056    0.281035   -2.394600
 H   -4.449481    0.965059    0.476018
 H   -5.678059   -0.021758    1.305057
 H   -5.865158    0.358733   -0.425131
Na   -0.132379   -1.871828   -1.732083
 C   -3.288355    4.628767   -1.246136
 H   -4.131202    5.101149   -0.723105
 H   -2.656663    5.421816   -1.671818
 H   -3.701543    4.052122   -2.089506
 C   -2.973914    1.790798    2.930585
 H   -2.277050    1.825374    3.780685
 H   -3.894667    2.320460    3.211548
 H   -3.228022    0.732756    2.756237
 H   -0.769050    3.721967   -1.600967
 H   -0.472166    1.385437    2.015110
76
Figure_S5-1_9b(Na)-Cu-allyl / electronic energy: -3289.86902565 a.u. / lowest freq: 17.54 cm-1
 C   -2.892697    1.596089    1.460941
 H   -2.743197    1.250407    2.497136
 C   -1.975473    2.766074    1.108473
 H   -2.463374    3.496160    0.440338
 C   -1.249374    0.839069    0.001489
 C    0.301145    2.736026   -0.016190
 C    1.264409    3.038492    0.964267
 C    0.499150    3.065316   -1.370203
 C    2.449274    3.661177    0.561084
 C    1.705816    3.672713   -1.732198
 C    2.674483    3.968356   -0.777657
 H    3.610370    4.443824   -1.078925
Cu   -0.251244   -0.335231   -1.174432
 N   -2.441060    0.564339    0.526560
 N   -0.895934    2.082234    0.388527
 H   -1.606803    3.302977    1.991271
 H   -3.958000    1.822171    1.319187
 C   -3.044007   -0.760576    0.519412
 H   -2.554189   -1.289301   -0.315468
 C   -4.525217   -0.639770    0.199869
 C   -5.531197   -1.041691    1.083724
 C   -4.902867   -0.081480   -1.029569
 C   -6.878729   -0.890279    0.747507
 H   -5.271410   -1.477151    2.049741
 C   -6.244395    0.073098   -1.368072
 H   -4.124350    0.241321   -1.727003
 C   -7.240224   -0.331892   -0.476378
 H   -7.649523   -1.209649    1.452726
 H   -6.515806    0.510614   -2.331627
 H   -8.294305   -0.210547   -0.735919
 C   -2.663657   -1.551289    1.799213
 H   -3.213957   -2.525298    1.696342
 H   -3.180113   -1.041428    2.659897
 O   -1.336986   -1.673655    1.957204
 C    0.761487   -1.541323   -2.354457
 H    1.475351   -0.912042   -2.911363
 H    0.108200   -2.075043   -3.064880
 C    1.441426   -2.424103   -1.385089
 C    0.988711   -3.644270   -0.986354
 H    1.556486   -4.204231   -0.232322
 C   -0.265528   -4.273060   -1.519961
 H   -0.471331   -5.246949   -1.053546
 H   -1.139388   -3.618105   -1.339556
 H   -0.221274   -4.425144   -2.613314
 B    2.674857   -1.814147   -0.650999
 O    3.578781   -0.949566   -1.188422
 O    2.893022   -2.014555    0.702220
 C    4.592362   -0.671470   -0.204792
 C    3.868051   -1.044195    1.142553
 C    4.996463    0.790230   -0.319960
 C    5.781401   -1.578686   -0.516488
 C    4.764620   -1.674238    2.195354
 C    3.081412    0.121336    1.736282
 H    5.219611   -2.605750    1.836445
 H    4.178808   -1.903760    3.097250
 H    5.566555   -0.977538    2.480470
 H    5.509876   -2.641027   -0.432057
 H    6.626269   -1.378286    0.157165
 H    6.109124   -1.392230   -1.548824
 H    2.392039    0.553077    0.995092
 H    3.746843    0.918937    2.094387
 H    2.489884   -0.230057    2.595248
 H    4.125398    1.455965   -0.267177
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 H    5.494789    0.958336   -1.285293
 H    5.701406    1.061643    0.480029
Na    0.603802   -2.265300    1.509716
 H    1.879983    3.924594   -2.781112
 H    3.211577    3.891914    1.309483
 C   -0.547128    2.775810   -2.413076
 H   -0.507148    1.718738   -2.725077
 H   -1.561952    2.956715   -2.031076
 H   -0.390961    3.397087   -3.304993
 C    1.037472    2.696278    2.412516
 H    0.431839    3.466996    2.916158
 H    0.508160    1.738685    2.519469
 H    1.991775    2.629837    2.951304
108
Figure_S5-1_AA-9b(Na)-pc(1,6minor) / electronic energy: -4131.83917004 a.u. / lowest freq: 12.63 cm-1
 C   -1.744589    2.568290   -2.024714
 H   -3.616915    1.410138   -1.669354
 C   -2.526686    1.328656   -1.713314
 H   -2.375547    3.468081   -2.009502
 H   -7.009362    3.589678    0.160410
 H   -5.475048    1.687490    0.591559
 C   -5.946837    3.776867    0.331773
 C   -5.086953    2.709525    0.579410
 H   -6.122965    5.920004    0.101560
 C   -5.451977    5.080953    0.298385
 C   -3.715009    2.916881    0.800438
 C   -4.090525    5.303744    0.515089
 C   -2.853905    1.750731    1.041101
 H   -3.360402    0.782929    1.000514
 C   -3.232051    4.236312    0.762602
 H   -3.691943    6.320567    0.486526
 H   -2.169592    4.433144    0.918377
 C   -1.537243    1.785444    1.354389
 H   -1.010660    2.735383    1.411591
 C   -1.947815    0.115944   -1.507552
 H   -1.404906   -0.323137    1.643927
 C   -0.782977    0.574537    1.581561
 H    0.069863    0.593115   -2.169673
 C   -0.508451   -0.099169   -1.537898
 H   -0.253765   -1.141127   -1.759216
Cu    0.555630   -0.007680    0.176082
 C    2.320411   -0.588887   -0.575361
 N    2.713780   -1.786548   -1.048589
 H    1.717240    2.580046   -4.848949
 N    3.257573    0.302445   -0.872224
 C    1.341169    1.589176    2.623630
 O    1.060659    2.710782    1.950983
 C    0.503158    0.439358    2.230271
 O    1.958756   -1.148851    3.297740
 C    0.862383   -0.849624    2.850964
 C    3.216116    1.695196   -0.472701
 C    4.450799   -0.290522   -1.481450
 H    5.268927   -0.247924   -0.747530
 C    3.986397   -1.718662   -1.777503
 H    3.819411   -1.897458   -2.852046
 C    1.961401   -2.995186   -0.985754
 C    2.113800   -3.816227    0.146978
 C    1.148924   -3.371882   -2.067504
 C    1.366682   -4.994156    0.217225
 C    0.413182   -4.557322   -1.955584
 C    0.510252   -5.355271   -0.821912
 H   -0.071454   -6.277270   -0.751492
Na    3.951537    0.112907    2.829841
 H    4.688269   -2.482346   -1.413202
 H    4.750846    0.258825   -2.384953
 O   -0.151134   -1.720640    2.868010
 O    2.217455    1.577656    3.468723
 C    1.811151    3.868469    2.290935
 H    1.670691    4.127614    3.349036
 H    1.429495    4.671186    1.650968
 H    2.880915    3.702248    2.100541
 C    0.097051   -3.018619    3.384645
 H    0.721704   -3.599019    2.692373
 H   -0.882845   -3.497824    3.482572
 H    0.592423   -2.962258    4.362785
 H    2.438294    1.758654    0.301001
 C    2.786616    2.610624   -1.603602
 C    2.654977    3.986712   -1.366897
 C    2.443077    2.127044   -2.871279
 C    2.196119    4.847952   -2.361391
 H    2.900877    4.390953   -0.383020
 C    1.984309    2.986271   -3.870604
 H    2.512394    1.057851   -3.079264
 C    1.857295    4.351072   -3.620647
 H    2.094723    5.914766   -2.148989
 H    1.492269    5.024436   -4.399217
 C    4.557787    2.055498    0.240770
 H    4.446495    3.128515    0.550339
 H    5.332541    2.103945   -0.576990
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 O    4.840571    1.204797    1.235141
 H   -0.930291    2.704682   -1.288861
 H   -1.254731    2.511496   -3.013177
 B   -2.802727   -1.110514   -1.076364
 O   -3.992410   -1.040718   -0.393198
 O   -2.388318   -2.406203   -1.252005
 C   -4.497293   -2.379301   -0.233115
 C   -3.195843   -3.246737   -0.414203
 C   -2.417612   -3.444984    0.886330
 H   -2.252986   -2.489748    1.405557
 H   -2.936321   -4.131832    1.570286
 H   -1.431174   -3.866908    0.644687
 C   -3.413579   -4.585593   -1.101052
 H   -4.100145   -5.213436   -0.513764
 H   -3.825883   -4.461778   -2.110537
 H   -2.453036   -5.112602   -1.185561
 C   -5.528458   -2.607704   -1.336904
 H   -6.307840   -1.836001   -1.261861
 H   -5.068911   -2.532195   -2.333133
 H   -6.006593   -3.593076   -1.244127
 C   -5.151405   -2.501065    1.134546
 H   -5.453260   -3.541532    1.326316
 H   -4.472565   -2.179265    1.934570
 H   -6.051732   -1.870936    1.175455
 C    1.097898   -2.577259   -3.345812
 H    1.365902   -1.524574   -3.193848
 H    1.797540   -3.001473   -4.084559
 H    0.091477   -2.611214   -3.785129
 C    3.095196   -3.445668    1.225508
 H    4.103181   -3.302450    0.806639
 H    2.814535   -2.510439    1.728017
 H    3.154383   -4.233196    1.988894
 H   -0.245320   -4.852294   -2.775984
 H    1.469479   -5.643503    1.090369
108
Figure_S5-1_AA-9b(Na)-ts(1,6minor) / electronic energy: -4131.83618193 a.u. / lowest freq: -326.46 cm-1
 C   -1.872866   -2.485834    1.943345
 H   -3.682318   -1.248251    1.557371
 C   -2.590814   -1.244543    1.504419
 H   -2.504522   -3.379663    1.847701
 H   -7.139356   -3.354432   -0.162828
 H   -5.508330   -1.500600   -0.404607
 C   -6.080164   -3.578616   -0.308969
 C   -5.165290   -2.538189   -0.448183
 H   -6.360964   -5.722656   -0.246685
 C   -5.645900   -4.904180   -0.354799
 C   -3.796232   -2.791738   -0.637635
 C   -4.289133   -5.172954   -0.541623
 C   -2.874373   -1.647983   -0.777482
 H   -3.370248   -0.678964   -0.860874
 C   -3.374907   -4.131158   -0.680865
 H   -3.937195   -6.206648   -0.579779
 H   -2.318287   -4.366154   -0.822215
 C   -1.578968   -1.753302   -1.251353
 H   -1.096330   -2.726140   -1.299673
 C   -1.952603   -0.012615    1.452936
 H   -1.419263    0.313860   -1.668529
 C   -0.833975   -0.608723   -1.609773
 H    0.013062   -0.620903    2.154341
 C   -0.550254    0.139212    1.595973
 H   -0.213310    1.162878    1.776427
Cu    0.538394   -0.006112   -0.169540
 C    2.296908    0.501133    0.632387
 N    2.728418    1.674274    1.131238
 H    1.521526   -2.744920    4.838770
 N    3.188913   -0.433178    0.936565
 C    1.274829   -1.685682   -2.623746
 O    0.922131   -2.809443   -1.982830
 C    0.468171   -0.516230   -2.250968
 O    1.974215    1.020360   -3.319210
 C    0.869907    0.754838   -2.864994
 C    3.102081   -1.813526    0.501731
 C    4.396154    0.103404    1.570869
 H    5.221329    0.038573    0.846562
 C    3.984469    1.545151    1.880428
 H    3.805711    1.717167    2.954421
 C    2.076330    2.932948    0.989169
 C    2.334380    3.683683   -0.173858
 C    1.266117    3.428202    2.022814
 C    1.702140    4.919963   -0.319039
 C    0.647384    4.670689    1.836241
 C    0.853329    5.405479    0.675099
 H    0.360794    6.371927    0.546188
Na    3.926490   -0.280615   -2.810055
 H    4.721795    2.285207    1.537966
 H    4.661603   -0.468610    2.471063
 O   -0.108164    1.672802   -2.870446
 O    2.190636   -1.704440   -3.429634
 C    1.638282   -3.988206   -2.317519
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 H    1.514608   -4.232343   -3.381536
 H    1.213755   -4.784699   -1.696647
 H    2.709197   -3.864794   -2.102245
 C    0.203059    2.964261   -3.366504
 H    0.849921    3.505807   -2.662245
 H   -0.752987    3.490203   -3.461819
 H    0.700222    2.901428   -4.343285
 H    2.333833   -1.829739   -0.285084
 C    2.624327   -2.739051    1.604218
 C    2.446167   -4.103657    1.334013
 C    2.284506   -2.272462    2.879543
 C    1.946249   -4.970482    2.303461
 H    2.689463   -4.493748    0.343960
 C    1.784085   -3.137463    3.853619
 H    2.391464   -1.211332    3.112471
 C    1.611209   -4.490732    3.570444
 H    1.810484   -6.028084    2.065739
 H    1.214880   -5.168436    4.329713
 C    4.440836   -2.207565   -0.201187
 H    4.289894   -3.265528   -0.544441
 H    5.198318   -2.312251    0.627751
 O    4.777240   -1.341632   -1.165210
 H   -0.956900   -2.644730    1.347521
 H   -1.551054   -2.410658    2.997038
 B   -2.733112    1.269766    1.037463
 O   -3.901094    1.270715    0.319105
 O   -2.264562    2.537078    1.267299
 C   -4.334316    2.637798    0.176316
 C   -2.996139    3.430662    0.410843
 C   -2.162765    3.591536   -0.859779
 H   -2.042431    2.632254   -1.383703
 H   -2.611021    4.317881   -1.552855
 H   -1.160024    3.945880   -0.579723
 C   -3.167293    4.773039    1.102854
 H   -3.812319    5.433583    0.504410
 H   -3.608868    4.660849    2.101368
 H   -2.187169    5.257525    1.212695
 C   -5.379538    2.892948    1.260575
 H   -6.189041    2.156641    1.155032
 H   -4.946149    2.782302    2.265236
 H   -5.812806    3.899308    1.173446
 C   -4.944626    2.820521   -1.204221
 H   -5.181214    3.879860   -1.383576
 H   -4.263954    2.474545   -1.992489
 H   -5.877992    2.244348   -1.279717
 C    1.094366    2.697262    3.328219
 H    1.341399    1.631704    3.244781
 H    1.750150    3.135731    4.097711
 H    0.059200    2.780918    3.687374
 C    3.296492    3.172175   -1.210887
 H    4.266346    2.913318   -0.759677
 H    2.912881    2.269728   -1.705397
 H    3.473029    3.928770   -1.987535
 H   -0.003765    5.060678    2.622224
 H    1.889426    5.515325   -1.216154
108
Figure_S5-1_AA-9b(Na)-prod(1,6minor) / electronic energy: -4131.89527188 a.u. / lowest freq: 22.82 cm-1
 C    1.394849    1.937125   -2.756669
 H    0.098919    3.479501   -2.023850
 C    0.403146    2.460198   -1.725160
 H    2.276582    2.590122   -2.814258
 H    2.835519    6.862365    0.027038
 H    0.949715    5.251263    0.002083
 C    3.035070    5.794957   -0.093054
 C    1.976159    4.888315   -0.106089
 H    5.179490    6.045863   -0.211312
 C    4.347049    5.338780   -0.224387
 C    2.200852    3.513268   -0.250438
 C    4.585361    3.972419   -0.368789
 C    1.006247    2.574450   -0.296031
 H    0.227332    3.037721    0.324728
 C    3.522571    3.069059   -0.381051
 H    5.608416    3.602622   -0.471805
 H    3.730423    2.003386   -0.492244
 C    1.305535    1.214640    0.299028
 H    2.165386    0.678749   -0.107748
 C   -0.873629    1.635922   -1.612724
 H   -0.050099    1.384209    1.894011
 C    0.793943    0.801166    1.502190
 H   -0.451378    0.152244   -3.133567
 C   -1.139181    0.524942   -2.367790
 H   -2.130485    0.064643   -2.335220
Cu   -0.265367   -0.147889   -0.490389
 C   -0.373151   -2.131976   -0.576681
 N   -1.454394   -2.893173   -0.824203
 H    2.052802   -1.588560   -5.026692
 N    0.691732   -2.923423   -0.543858
 C    2.672023   -0.592548    2.503149
 O    3.490063    0.110819    1.684107
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 C    1.275920   -0.246977    2.385060
 O    0.539931   -1.819604    4.042015
 C    0.356056   -0.840918    3.321447
 C    2.053324   -2.438263   -0.388952
 C    0.385192   -4.327213   -0.841301
 H    0.830267   -4.956333   -0.060098
 C   -1.144511   -4.328313   -0.854337
 H   -1.569395   -4.805029   -1.748504
 C   -2.790689   -2.419570   -0.939222
 C   -3.521966   -2.147158    0.226763
 C   -3.351741   -2.275131   -2.219248
 C   -4.846473   -1.723381    0.091259
 C   -4.674700   -1.832057   -2.313876
 C   -5.418360   -1.563830   -1.167809
 H   -6.452618   -1.224310   -1.257949
Na    2.065336   -3.409897    3.298196
 H   -1.576343   -4.823520    0.031012
 H    0.812017   -4.610335   -1.817384
 O   -0.847687   -0.209803    3.364734
 O    3.171221   -1.405471    3.278461
 C    4.877000   -0.118117    1.826358
 H    5.220855    0.112632    2.845035
 H    5.370391    0.550740    1.110404
 H    5.133436   -1.164435    1.600810
 C   -1.763565   -0.658320    4.344082
 H   -1.943645   -1.738807    4.260678
 H   -2.696323   -0.110031    4.167227
 H   -1.392540   -0.443283    5.357414
 H    2.012972   -1.659040    0.383381
 C    2.596607   -1.821979   -1.661062
 C    3.755741   -1.035769   -1.595913
 C    1.996846   -2.006054   -2.912371
 C    4.302820   -0.460944   -2.740789
 H    4.224675   -0.863034   -0.626131
 C    2.541588   -1.432344   -4.062178
 H    1.081086   -2.594902   -2.994985
 C    3.698377   -0.659025   -3.982906
 H    5.202579    0.153597   -2.660804
 H    4.121879   -0.204938   -4.881213
 C    2.957536   -3.573742    0.194591
 H    3.965003   -3.087322    0.303566
 H    3.108389   -4.300012   -0.656149
 O    2.463421   -4.118494    1.312350
 H    1.747427    0.923332   -2.510735
 H    0.942578    1.898845   -3.758543
 B   -2.036995    2.166233   -0.699805
 O   -2.003634    3.364042   -0.047238
 O   -3.189384    1.470049   -0.479010
 C   -3.306537    3.590572    0.529271
 C   -3.900484    2.132857    0.587714
 C   -3.548929    1.392221    1.875231
 H   -2.467620    1.412049    2.076206
 H   -4.076960    1.814547    2.741522
 H   -3.846389    0.341439    1.764972
 C   -5.394244    2.048226    0.320405
 H   -5.951696    2.639600    1.061794
 H   -5.646693    2.412860   -0.683047
 H   -5.722799    1.003006    0.395437
 C   -4.062145    4.510907   -0.426956
 H   -3.485507    5.436621   -0.563659
 H   -4.195537    4.042207   -1.412820
 H   -5.051192    4.776083   -0.028433
 C   -3.132247    4.259133    1.883322
 H   -4.104101    4.368767    2.386819
 H   -2.461278    3.683904    2.533577
 H   -2.701593    5.261608    1.748498
 C   -2.546941   -2.586937   -3.452679
 H   -1.520329   -2.202737   -3.367683
 H   -2.472417   -3.674011   -3.616177
 H   -3.010541   -2.149095   -4.346581
 C   -2.875707   -2.284296    1.576075
 H   -2.377669   -3.257826    1.696466
 H   -2.104026   -1.511204    1.715661
 H   -3.616558   -2.175461    2.379290
 H   -5.125896   -1.700201   -3.300329
 H   -5.435043   -1.515514    0.988624
13
Figure_S6-1_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
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 H     1.950011   -0.820432    0.528064
 H     1.532897   -0.480344   -1.171814
13
Figure_S6-1_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
17
Figure_S6-1_Me2NHC / electronic energy: -305.693539420 a.u. / lowest freq: 35.85 cm-1
 C    -0.766605    1.222492   -0.000015
 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
Figure_S6-1_NaOPh / electronic energy: -468.853649444 a.u. / lowest freq: 15.68 cm-1
 C    -1.912599   -1.200838   -0.011375
 C    -0.521476   -1.206572    0.015351
 C     0.241248    0.001459    0.028090
 C    -0.524240    1.207747    0.015228
 C    -1.915348    1.198823   -0.011498
 C    -2.633248   -0.001829   -0.025828
 H    -2.448993   -2.155315   -0.021458
 H     0.025710   -2.154567    0.026010
 H     0.020847    2.156944    0.025804
 H    -2.453903    2.152085   -0.021671
 H    -3.725390   -0.003095   -0.047610
 O     1.527681    0.002959    0.048939
Na     3.632205   -0.001133   -0.037490
15
Figure_S6-1_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
 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
32
Figure_S6-1_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C    -0.660544   -0.726572    0.059153
 C    -1.860539   -0.097447    0.115996
 H    -0.691600   -1.818492   -0.004770
 C    -1.976243    1.390665    0.160143
 C    -3.120576   -0.891785    0.187355
 O    -3.041424    1.823605   -0.507466
 O    -1.182749    2.134043    0.689285
 O    -4.147702   -0.497504    0.683440
 O    -2.981802   -2.118850   -0.320932
 C    -4.097604   -2.989729   -0.195724
 H    -4.332384   -3.170881    0.862818
 H    -3.810049   -3.927003   -0.683244
 H    -4.981752   -2.562067   -0.688186
 C    -3.254671    3.228152   -0.535442
 H    -3.354009    3.627502    0.483524
 H    -4.184056    3.384216   -1.092621
 H    -2.420438    3.737793   -1.038016
 C     0.656646   -0.129211    0.062308
 H     0.725624    0.955889    0.150505
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 C    1.759981   -0.902956   -0.019704
 H    1.621029   -1.988149   -0.089650
 C    3.156351   -0.453635   -0.025165
 C    4.175093   -1.416830   -0.109525
 C    3.522207    0.902114    0.053056
 C    5.517020   -1.042840   -0.114390
 H    3.907556   -2.474776   -0.172060
 C    4.861836    1.275255    0.048166
 H    2.754752    1.675486    0.118691
 C    5.863995    0.305241   -0.035401
 H    6.294080   -1.807149   -0.179427
 H    5.127957    2.332459    0.111300
 H    6.914980    0.602284   -0.038425
45
Figure_S6-1_dienoate-NaOPh / electronic energy: -1310.80369108 a.u. / lowest freq: 9.19 cm-1
 C   -2.280519    1.058943    0.160955
 C   -0.972791    0.759991    0.397373
 H   -2.492523    2.119446   -0.001289
 C   -0.449006   -0.621179    0.591424
 C    0.034942    1.854588    0.429173
 O   -1.307158   -1.423887    1.202354
 O    0.646618   -0.999504    0.232290
 O    1.218110    1.702543    0.660167
 O   -0.486789    3.050717    0.197601
 C    0.399785    4.164684    0.223112
 H    0.869579    4.262632    1.211018
 H   -0.215078    5.043918    0.006843
 H    1.182278    4.051912   -0.539539
 C   -0.910718   -2.780849    1.389975
 H   -0.714707   -3.262803    0.422790
 H   -1.748148   -3.270133    1.896938
 H   -0.006253   -2.832517    2.010602
 C   -3.420673    0.183443    0.055930
 H   -3.280468   -0.886532    0.204274
 C   -4.639325    0.700315   -0.221969
 H   -4.716524    1.785054   -0.358230
 C   -5.898377   -0.031874   -0.369534
 C   -7.056616    0.686856   -0.709372
 C   -6.000293   -1.422727   -0.185598
 C   -8.279798    0.040129   -0.865398
 H   -6.991102    1.768074   -0.854475
 C   -7.222154   -2.067509   -0.339616
 H   -5.118701   -2.007872    0.083159
 C   -8.365160   -1.339218   -0.680480
 H   -9.169555    0.614400   -1.131301
 H   -7.287414   -3.147303   -0.191668
 H   -9.322983   -1.849627   -0.800919
Na    2.738314    0.026362    0.134785
 O    4.811878   -0.257394   -0.155918
 C    6.075973   -0.434498   -0.306247
 C    6.673664   -0.633931   -1.589140
 C    6.983127   -0.445127    0.798458
 C    8.042909   -0.825632   -1.743864
 H    6.013305   -0.631839   -2.462224
 C    8.350312   -0.637983    0.629176
 H    6.565220   -0.294828    1.798886
 C    8.904515   -0.831336   -0.641129
 H    8.450868   -0.974195   -2.749146
 H    9.001992   -0.637470    1.509288
 H    9.978696   -0.982607   -0.768985
47
Figure_S6-1_dienoate-NaOtBu / electronic energy: -1237.06693666 a.u. / lowest freq: 12.59 cm-1
 H   -1.833753    3.949419    0.466471
 O   -5.266810   -0.478539    0.274763
Na   -3.268083   -0.157523   -0.088732
 H   -0.477334    4.974139   -0.121701
 C   -1.058689    4.064810   -0.303343
 O   -1.787584    1.561143   -0.649152
 O   -0.130709    2.986648   -0.243762
 H   -1.535994    4.110015   -1.291520
 C   -0.609982    1.765070   -0.433881
 O   -1.117181   -1.090407   -0.102401
 C    0.437762    0.709610   -0.379476
 H    1.920066    2.132359   -0.065433
 C   -0.044675   -0.694245   -0.506624
 C    1.738758    1.060428   -0.184093
 H    0.313227   -3.318985   -0.244448
 C    2.907971    0.223838   -0.074619
 H    4.165933    1.873551    0.259781
 C    4.116740    0.783254    0.159071
 H    2.795234   -0.854035   -0.184540
 O    0.822337   -1.493562   -1.110812
 C    0.463373   -2.867964   -1.234622
 H   -0.458715   -2.971303   -1.821887
 C    5.398314    0.089747    0.303403
 H    6.449599    1.928958    0.729623
 H    4.666962   -1.916703   -0.093657
 C    6.541807    0.846716    0.608606
 C    5.535447   -1.301777    0.149935
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 H    1.299218   -3.350955   -1.750211
 C    7.783935    0.236166    0.761809
 C    6.776094   -1.910378    0.300800
 H    8.661494    0.840021    1.001486
 C    7.903842   -1.144447    0.608224
 H    6.868119   -2.991150    0.176104
 H    8.876380   -1.626726    0.726827
 C   -6.596121   -0.664280    0.500805
 C   -7.079392    0.200319    1.690602
 C   -6.895972   -2.145868    0.832143
 C   -7.426772   -0.272008   -0.745113
 H   -6.515052   -0.070295    2.598204
 H   -8.155809    0.081985    1.905079
 H   -6.884012    1.264390    1.478210
 H   -6.329065   -2.444940    1.729225
 H   -6.564123   -2.785005   -0.002637
 H   -7.966194   -2.343740    1.016964
 H   -8.512903   -0.413042   -0.606972
 H   -7.105775   -0.878370   -1.608349
 H   -7.243655    0.786952   -0.991410
24
Figure_S6-1_Me2NHC-Cu-allenyl / electronic energy: -2062.03073671 a.u. / lowest freq: 16.19 cm-1
 C    2.918206    1.315894    0.091326
 H    3.172197    1.838768    1.027814
 C    3.315499   -0.166410    0.114484
 H    3.900547   -0.463518   -0.771327
 C    0.986753    0.001938   -0.023023
Cu   -0.888943   -0.488741   -0.126170
 N    1.467261    1.248504   -0.070934
 N    2.017665   -0.838526    0.111392
 H    3.894306   -0.441143    1.009295
 H    3.378330    1.869933   -0.740626
 C   -2.762590   -0.927759   -0.229714
 H   -3.145854   -1.915697   -0.535398
 C   -3.673890   -0.041198    0.066597
 C   -4.559952    0.891767    0.375842
 H   -4.957585    1.574386   -0.383123
 H   -4.930838    1.010617    1.399723
 C    0.676712    2.451280   -0.144453
 H   -0.378542    2.179900   -0.275011
 H    0.779042    3.047038    0.777227
 H    0.992071    3.072048   -0.997685
 C    1.929271   -2.276075    0.147590
 H    2.401143   -2.673321    1.059948
 H    0.871323   -2.567362    0.139575
 H    2.428683   -2.724632   -0.726592
20
Figure_S6-1_PMe3-Cu-allenyl / electronic energy: -2217.18081038 a.u. / lowest freq: 11.56 cm-1
Cu   -0.560515   -0.423375   -0.001720
 C   -2.432841   -0.885632    0.001582
 H   -2.795334   -1.927022    0.005243
 C   -3.361235    0.031770    0.000489
 C   -4.267218    0.995319   -0.000581
 H   -4.662553    1.405817   -0.936021
 H   -4.659265    1.410908    0.933996
 P    1.600036    0.123265   -0.000003
 C    2.748935   -1.283966   -0.218460
 H    2.546754   -1.774384   -1.181161
 H    3.795305   -0.944626   -0.195816
 H    2.586607   -2.016869    0.584369
 C    2.107021    1.292052   -1.312942
 H    1.880617    0.855999   -2.296084
 H    1.540405    2.228072   -1.209306
 H    3.183775    1.509070   -1.250167
 C    2.192732    0.921893    1.535582
 H    2.020015    0.248277    2.386749
 H    3.265620    1.155807    1.467496
 H    1.628085    1.849223    1.706612
20
Figure_S6-1_thf-Cu-allenyl / electronic energy: -1988.50872863 a.u. / lowest freq: 20.89 cm-1
Cu    0.714206   -0.401034    0.113501
 H    4.783325    1.122457   -1.372535
 C    2.567809   -0.755972    0.263593
 H    2.949020   -1.725690    0.624440
 C    3.479970    0.127268   -0.042341
 C    4.376686    1.045342   -0.358341
 H    4.747372    1.759129    0.385423
 O   -1.182423   -0.029646   -0.034374
 C   -1.760853    1.282128    0.097494
 C   -3.242015    1.026509    0.327848
 H   -1.575036    1.839437   -0.834212
 H   -1.263521    1.798561    0.929444
 C   -3.475433   -0.262949   -0.460272
 H   -3.864528    1.863690   -0.013772
 H   -3.440759    0.864720    1.398220
 C   -2.195155   -1.039884   -0.192530
 H   -2.253447   -1.624989    0.739048
 H   -1.896049   -1.704311   -1.014265
 H   -3.576986   -0.046651   -1.534605
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 H   -4.368039   -0.813840   -0.136436
52
Figure_S6-1_PA-NaOPh-prod(1,6) / electronic energy: -3067.16986516 a.u. / lowest freq: 15.87 cm-1
 H    0.512950   -1.374642    3.438628
 H    1.133220    0.187671    4.072802
 H    2.037448   -0.678257    2.793846
 C    1.034029   -0.445327    3.179759
 H   -5.821882   -1.768640    2.501479
 C   -5.610786   -1.300114    1.537564
 H   -3.541000   -1.881806    1.565169
 O    0.244724    0.182880    2.187660
 H   -7.631835   -0.581736    1.263511
 C   -4.325207   -1.365036    1.005076
 C   -6.624638   -0.636248    0.844603
 O    1.732901    1.839664    2.157541
 H   -1.447678   -0.689578    1.093263
 C    0.712317    1.343750    1.679812
 C   -4.026682   -0.768988   -0.227661
 C   -1.586934   -0.210529    0.121835
 C   -6.340465   -0.040028   -0.382733
 H   -2.340770   -2.924065   -0.255211
 C   -0.070167    1.835947    0.575473
 C   -2.621962   -0.828394   -0.801515
 C   -5.050919   -0.108158   -0.912866
 H   -7.125971    0.483371   -0.932742
Cu    0.361801   -0.774874   -0.782683
 C   -1.032864    1.020787   -0.133173
 C   -2.213468   -2.280247   -1.141012
 C   -0.795582   -2.339713   -1.535210
 O    1.406646    3.662846    0.075201
 C    0.363201   -2.526833   -1.911092
 C    0.339623    3.065830   -0.065729
 H    1.283127   -2.892339   -2.342036
 H   -2.619222   -0.261312   -1.746060
 H   -4.836085    0.364763   -1.874976
 H   -1.372471    1.487456   -1.064578
 H   -2.846446   -2.701003   -1.937472
 O   -0.579893    3.553327   -0.928596
 C   -0.203996    4.679835   -1.696232
 H    0.037197    5.538212   -1.053164
 H    0.670292    4.459218   -2.327124
 H   -1.065512    4.920794   -2.329749
Na    3.060017    2.045602    0.286194
 O    2.165964   -0.029935   -0.586293
 C    3.188784   -0.833254   -0.385416
 C    4.474425   -0.500856   -0.878247
 C    3.079176   -2.038793    0.350932
 C    5.579858   -1.312346   -0.628786
 H    4.581350    0.404967   -1.483220
 C    4.187888   -2.845336    0.588794
 H    2.097839   -2.320612    0.744782
 C    5.451437   -2.492124    0.106363
 H    6.556131   -1.021784   -1.026790
 H    4.063103   -3.767073    1.163868
 H    6.318644   -3.127094    0.298127
52
Figure_S6-1_PA-NaOPh-ts(1,6) / electronic energy: -3067.12456351 a.u. / lowest freq: -446.87 cm-1
 H   -1.009210    0.171150    4.148180
 H    0.157209    1.523688    4.354905
 H    0.737307   -0.076555    3.802747
 C   -0.097686    0.637104    3.758541
 H   -5.810106   -1.959850    2.385206
 C   -5.722000   -1.455491    1.420269
 H   -3.603175   -1.162056    1.625675
 O   -0.383920    0.993800    2.414939
 H   -7.827193   -1.637035    0.957458
 C   -4.478451   -0.998102    0.993383
 C   -6.852892   -1.276094    0.620808
 O    1.644286    1.889001    2.270153
 H   -2.030868    0.247457    1.180188
 C    0.587150    1.603763    1.726768
 C   -4.337673   -0.346989   -0.242468
 C   -2.018255    0.567885    0.140581
 C   -6.726018   -0.637150   -0.611909
 H   -2.953051   -2.387368   -1.125598
 C    0.242541    1.838683    0.320098
 C   -3.030534    0.155140   -0.730566
 C   -5.479938   -0.180397   -1.038718
 H   -7.602753   -0.492286   -1.247160
Cu    0.715863   -0.027687   -0.541097
 C   -0.929098    1.307653   -0.342858
 C   -2.456756   -1.680035   -1.796640
 C   -1.097096   -1.709490   -1.844744
 O    2.235345    3.111834   -0.136679
 C    0.149666   -1.547370   -1.694597
 C    1.105399    2.758479   -0.439308
 H    1.016769   -2.131115   -2.013389
 H   -3.081180    0.678534   -1.689392
 H   -5.388196    0.318282   -2.007436
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 H   -1.043257    1.672591   -1.367716
 H   -3.013493   -1.428354   -2.704367
 O    0.540278    3.191485   -1.573072
 C    1.338172    3.999971   -2.423122
 H    1.635492    4.927724   -1.915227
 H    2.242692    3.461934   -2.740738
 H    0.715363    4.232083   -3.293657
Na    3.524980    1.538235    0.959353
 O    2.606034   -0.271406   -0.079037
 C    3.236524   -1.427299   -0.087430
 C    4.578290   -1.514608   -0.528127
 C    2.625453   -2.623245    0.357591
 C    5.266413   -2.725675   -0.514135
 H    5.065853   -0.603694   -0.888188
 C    3.320490   -3.829619    0.363006
 H    1.588780   -2.578032    0.703095
 C    4.647086   -3.896540   -0.070567
 H    6.302907   -2.756358   -0.862085
 H    2.816876   -4.734190    0.715380
 H    5.187512   -4.845371   -0.064520
52
Figure_S6-1_PA-NaOPh-ed(1,6) / electronic energy: -3067.13714909 a.u. / lowest freq: 20.63 cm-1
 H   -0.042410    1.880291    3.250955
 H   -1.076882    0.631661    4.031767
 H   -1.719871    1.607342    2.667279
 C   -0.822939    1.130083    3.087123
 H    5.452829    2.708352    2.073243
 C    5.472971    1.874880    1.367623
 H    3.386517    1.443766    1.628848
 O   -0.280737    0.202508    2.154337
 H    7.576753    2.101223    0.918384
 C    4.307502    1.156911    1.117672
 C    6.663458    1.535921    0.720744
 O   -2.131433   -1.015606    2.330396
 H    1.717479    0.170343    1.262965
 C   -1.049094   -0.828463    1.807018
 C    4.306260    0.079166    0.215240
 C    1.894396   -0.581895    0.496819
 C    6.677348    0.472154   -0.181117
 H    3.416531    1.222422   -2.518255
 C   -0.474350   -1.645260    0.713330
 C    3.106629   -0.713796   -0.083166
 C    5.510529   -0.246315   -0.430014
 H    7.602132    0.201670   -0.695399
Cu   -0.665350   -0.307696   -0.836085
 C    0.787347   -1.426273    0.089546
 C    2.701056    0.524089   -2.964301
 C    1.410265    0.597533   -2.685813
 O   -2.464988   -2.976802    0.416585
 C    0.159538    0.635765   -2.338618
 C   -1.264741   -2.831251    0.279986
 H   -0.523455    1.273432   -2.921629
 H    3.238583   -1.492845   -0.839911
 H    5.525611   -1.074556   -1.143146
 H    1.065829   -2.199018   -0.631449
 H    3.094626   -0.227431   -3.656775
 O   -0.519764   -3.749084   -0.327761
 C   -1.195659   -4.869421   -0.885360
 H   -1.711399   -5.439794   -0.101108
 H   -1.928816   -4.544375   -1.636351
 H   -0.422141   -5.485782   -1.354311
Na   -3.859988   -1.157383    0.725841
 O   -2.565087    0.203756   -0.603925
 C   -2.927924    1.467433   -0.539854
 C   -4.261378    1.846717   -0.825554
 C   -2.033680    2.496413   -0.157886
 C   -4.675698    3.172206   -0.716070
 H   -4.964164    1.071974   -1.146669
 C   -2.457422    3.818772   -0.056908
 H   -0.993752    2.232797    0.057476
 C   -3.781189    4.172973   -0.329794
 H   -5.715097    3.427036   -0.941593
 H   -1.738528    4.586410    0.242578
 H   -4.108635    5.211246   -0.245642
20
Figure_S6-1_NaOPh-Cu-allenyl / electronic energy: -2225.17069737 a.u. / lowest freq: 21.00 cm-1
Na   -0.543228    2.682910   -0.151317
 H   -5.637693    0.533880    0.687349
Cu   -1.190970   -0.381703    0.098178
 C   -5.108920    0.108731   -0.172968
 C   -3.998197   -0.594685   -0.020276
 C   -2.879058   -1.251261    0.127397
 H   -2.984863   -2.338988    0.274272
 H   -5.548657    0.276120   -1.162462
 O    0.376205    0.672359    0.069915
 C    1.610478    0.209227    0.025946
 C    2.711077    1.089336    0.141522
 C    1.899177   -1.164982   -0.139905
 H    2.517436    2.156672    0.281638
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 C    4.020774    0.618886    0.088209
 C    4.288220   -0.741651   -0.080072
 H    4.846610    1.329753    0.181337
 C    3.212311   -1.625296   -0.191601
 H    5.316216   -1.107429   -0.121989
 H    1.063450   -1.866243   -0.228401
 H    3.396335   -2.695089   -0.323239
52
Figure_S6-1_PA-NaOPh-ed(1,4) / electronic energy: -3067.14378699 a.u. / lowest freq: 20.30 cm-1
Cu   -1.598182   -0.706478    1.726427
 C   -0.002839   -1.047713   -1.210307
 C   -1.165737   -0.392401   -1.488490
 H   -0.117051   -2.102972   -0.942865
 C   -1.276404    1.056876   -1.792867
 C   -2.431778   -1.161831   -1.332219
 O   -0.159581    1.567889   -2.289556
 O   -2.274135    1.730491   -1.627030
 O   -3.504445   -0.693421   -0.999907
 O   -2.271142   -2.453639   -1.572196
 C   -3.350291   -3.316281   -1.232448
 H   -3.540738   -3.263032   -0.151554
 H   -3.027364   -4.325710   -1.506604
 H   -4.257940   -3.042659   -1.786998
 C   -0.113254    2.981493   -2.461302
 H   -0.896196    3.312764   -3.156441
 H    0.876651    3.199427   -2.874987
 H   -0.240206    3.480963   -1.490702
 C    1.345934   -0.550222   -1.112366
 H    1.550308    0.485311   -1.375975
 C    2.314107   -1.364087   -0.635076
 H    2.034308   -2.390302   -0.369796
 C    3.715673   -1.009696   -0.400948
 C    4.584351   -1.989296    0.107256
 C    4.229536    0.275130   -0.654811
 C    5.924171   -1.699796    0.354183
 H    4.197371   -2.990969    0.310831
 C    5.566547    0.564270   -0.406437
 H    3.578716    1.058666   -1.047478
 C    6.418870   -0.421571    0.098104
 H    6.584740   -2.474673    0.748435
 H    5.950231    1.566819   -0.606657
 H    7.468850   -0.191492    0.290887
 C   -1.532412   -2.590842    2.006736
 H   -2.168228   -3.061535    2.776168
 C   -0.779245   -3.421281    1.339676
 C   -0.010419   -4.230735    0.627836
 H   -0.373163   -4.684659   -0.300924
 H    1.005186   -4.486184    0.949644
Na   -3.707120    1.299771    0.180567
 O   -1.841596    1.160087    1.479850
 C   -0.874874    2.042839    1.342776
 C    0.488111    1.673154    1.267389
 C   -1.170340    3.423678    1.245470
 C    1.488894    2.625567    1.094330
 H    0.743842    0.612968    1.349090
 C   -0.162156    4.369313    1.078189
 H   -2.215060    3.740838    1.310165
 C    1.178714    3.983920    0.995807
 H    2.530644    2.296181    1.040639
 H   -0.428888    5.427523    1.007403
 H    1.965804    4.728921    0.862926
52
Figure_S6-1_PA-NaOPh-ts(1,4) / electronic energy: -3067.11795157 a.u. / lowest freq: -466.55 cm-1
Cu    2.171039    1.051917    1.059732
 C   -1.446970    1.226914    0.005306
 C   -0.196301    1.092740   -0.647068
 H   -1.827694    2.246558   -0.032024
 C    0.341457   -0.189827   -1.106791
 C    0.527351    2.308046   -1.004739
 O   -0.047526   -1.229635   -0.358526
 O    1.062157   -0.358313   -2.079345
 O    1.581451    2.385207   -1.629747
 O   -0.070055    3.423573   -0.561138
 C    0.634104    4.640452   -0.726756
 H    1.591938    4.609229   -0.186498
 H   -0.006268    5.422651   -0.304684
 H    0.829767    4.846510   -1.788269
 C    0.321876   -2.526812   -0.808689
 H   -0.107294   -2.729256   -1.800573
 H   -0.086221   -3.227946   -0.072504
 H    1.414343   -2.630462   -0.854587
 C   -2.508308    0.212951   -0.019370
 H   -2.203855   -0.833048   -0.045904
 C   -3.808531    0.555445   -0.014606
 H   -4.063707    1.620820    0.036998
 C   -4.959099   -0.359855   -0.065128
 C   -6.254080    0.171938    0.043959
 C   -4.824738   -1.751035   -0.219322
 C   -7.377049   -0.652798    0.008769
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 H   -6.379932    1.251345    0.162167
 C   -5.945279   -2.574852   -0.256371
 H   -3.833538   -2.198281   -0.318162
 C   -7.226764   -2.030514   -0.141309
 H   -8.373756   -0.215380    0.099205
 H   -5.818335   -3.652632   -0.379589
 H   -8.104004   -2.680496   -0.170846
 C    1.208719    1.884271    2.501669
 H    1.806950    2.236712    3.347376
 C   -0.047087    1.699753    2.450777
 C   -1.351767    1.438518    2.167954
 H   -2.052101    2.277656    2.147925
 H   -1.769196    0.487991    2.514802
Na    3.067127    0.769491   -2.188009
 O    3.373502    0.054103   -0.038812
 C    3.545852   -1.235048    0.172784
 C    3.075560   -1.884803    1.338773
 C    4.206255   -2.039325   -0.785343
 C    3.232312   -3.255724    1.516542
 H    2.565355   -1.285575    2.099933
 C    4.356029   -3.411520   -0.599795
 H    4.595118   -1.566310   -1.691766
 C    3.868330   -4.037720    0.549301
 H    2.845415   -3.721880    2.426867
 H    4.863851   -4.001196   -1.368077
 H    3.987183   -5.113657    0.691349
52
Figure_S6-1_PA-NaOPh-prod(1,4) / electronic energy: -3067.17831935 a.u. / lowest freq: 16.86 cm-1
Cu   -1.598615   -0.354991   -0.780455
 C    1.331513   -0.405435   -0.961682
 C    0.349308    0.042758    0.138381
 H    1.338389    0.407317   -1.697590
 C    0.094780   -0.814104    1.286416
 C    0.216836    1.478096    0.360051
 O    0.659901   -2.034870    1.165551
 O   -0.575688   -0.558553    2.283496
 O   -0.354704    2.043128    1.288325
 O    0.792474    2.217481   -0.608631
 C    0.654171    3.622433   -0.513192
 H   -0.404887    3.918248   -0.533014
 H    1.171983    4.039271   -1.384476
 H    1.110405    4.006038    0.410318
 C    0.386519   -2.975947    2.187753
 H    0.762650   -2.625604    3.159341
 H    0.903227   -3.898116    1.898843
 H   -0.693307   -3.163882    2.274584
 C    2.740514   -0.572016   -0.458155
 H    2.887657   -1.361758    0.285916
 C    3.762940    0.200013   -0.848058
 H    3.561805    0.983953   -1.587804
 C    5.161330    0.128605   -0.382362
 C    6.095502    1.039270   -0.900301
 C    5.611347   -0.811116    0.561159
 C    7.429092    1.017139   -0.494650
 H    5.766570    1.778995   -1.635120
 C    6.942268   -0.835090    0.967300
 H    4.913136   -1.535874    0.985181
 C    7.859031    0.078860    0.442219
 H    8.135646    1.738083   -0.912371
 H    7.268810   -1.574684    1.701970
 H    8.902855    0.057211    0.763052
 C   -1.741928   -1.480610   -2.499290
 H   -2.641875   -1.620582   -3.079501
 C   -0.577249   -1.513413   -2.082934
 C    0.845515   -1.657019   -1.726522
 H    1.442395   -1.806842   -2.639786
 H    0.953475   -2.557590   -1.105637
Na   -2.188885    1.071936    2.212987
 O   -3.033548    0.527371    0.166161
 C   -4.326650    0.325454    0.031790
 C   -4.865826   -0.855223   -0.530867
 C   -5.248291    1.300755    0.483555
 C   -6.241725   -1.040541   -0.639331
 H   -4.174748   -1.631035   -0.871890
 C   -6.622424    1.104648    0.372484
 H   -4.852596    2.224769    0.915457
 C   -7.136633   -0.065948   -0.191144
 H   -6.622163   -1.966542   -1.079837
 H   -7.304491    1.881933    0.728595
 H   -8.214472   -0.215742   -0.280845
24
Figure_S6-1_Me2NHC-Cu-allenyl / electronic energy: -2062.03073671 a.u. / lowest freq: 16.19 cm-1
 C    2.918206    1.315894    0.091326
 H    3.172197    1.838768    1.027814
 C    3.315499   -0.166410    0.114484
 H    3.900547   -0.463518   -0.771327
 C    0.986753    0.001938   -0.023023
Cu   -0.888943   -0.488741   -0.126170
 N    1.467261    1.248504   -0.070934
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 N     2.017665   -0.838526    0.111392
 H     3.894306   -0.441143    1.009295
 H     3.378330    1.869933   -0.740626
 C    -2.762590   -0.927759   -0.229714
 H    -3.145854   -1.915697   -0.535398
 C    -3.673890   -0.041198    0.066597
 C    -4.559952    0.891767    0.375842
 H    -4.957585    1.574386   -0.383123
 H    -4.930838    1.010617    1.399723
 C     0.676712    2.451280   -0.144453
 H    -0.378542    2.179900   -0.275011
 H     0.779042    3.047038    0.777227
 H     0.992071    3.072048   -0.997685
 C     1.929271   -2.276075    0.147590
 H     2.401143   -2.673321    1.059948
 H     0.871323   -2.567362    0.139575
 H     2.428683   -2.724632   -0.726592
20
Figure_S6-1_PMe3-Cu-allenyl / electronic energy: -2217.18081038 a.u. / lowest freq: 11.56 cm-1
Cu   -0.560515   -0.423375   -0.001720
 C    -2.432841   -0.885632    0.001582
 H    -2.795334   -1.927022    0.005243
 C    -3.361235    0.031770    0.000489
 C    -4.267218    0.995319   -0.000581
 H    -4.662553    1.405817   -0.936021
 H    -4.659265    1.410908    0.933996
 P     1.600036    0.123265   -0.000003
 C     2.748935   -1.283966   -0.218460
 H     2.546754   -1.774384   -1.181161
 H     3.795305   -0.944626   -0.195816
 H     2.586607   -2.016869    0.584369
 C     2.107021    1.292052   -1.312942
 H     1.880617    0.855999   -2.296084
 H     1.540405    2.228072   -1.209306
 H     3.183775    1.509070   -1.250167
 C     2.192732    0.921893    1.535582
 H     2.020015    0.248277    2.386749
 H     3.265620    1.155807    1.467496
 H     1.628085    1.849223    1.706612
20
Figure_S6-1_thf-Cu-allenyl / electronic energy: -1988.50872863 a.u. / lowest freq: 20.89 cm-1
Cu    0.714206   -0.401034    0.113501
 H     4.783325    1.122457   -1.372535
 C     2.567809   -0.755972    0.263593
 H     2.949020   -1.725690    0.624440
 C     3.479970    0.127268   -0.042341
 C     4.376686    1.045342   -0.358341
 H     4.747372    1.759129    0.385423
 O    -1.182423   -0.029646   -0.034374
 C    -1.760853    1.282128    0.097494
 C    -3.242015    1.026509    0.327848
 H    -1.575036    1.839437   -0.834212
 H    -1.263521    1.798561    0.929444
 C    -3.475433   -0.262949   -0.460272
 H    -3.864528    1.863690   -0.013772
 H    -3.440759    0.864720    1.398220
 C    -2.195155   -1.039884   -0.192530
 H    -2.253447   -1.624989    0.739048
 H    -1.896049   -1.704311   -1.014265
 H    -3.576986   -0.046651   -1.534605
 H    -4.368039   -0.813840   -0.136436
54
Figure_S6-1_PA-NaOtBu-prod(1,6) / electronic energy: -2993.44684250 a.u. / lowest freq: 17.57 cm-1
 H     0.082203   -0.887277    3.872751
 H     0.980305    0.614273    4.280520
 H     1.796925   -0.689235    3.375486
 C     0.837822   -0.172771    3.525431
 H    -5.548494   -1.354786    2.538401
 C    -5.327171   -0.788078    1.631024
 H    -3.369673   -1.652515    1.413990
 O     0.345672    0.362948    2.313948
 H    -7.231339    0.237211    1.617441
 C    -4.099659   -0.955327    0.993250
 C    -6.269743    0.104118    1.116900
 O     2.248774    1.506203    2.134204
 H    -1.187265   -0.538661    0.983925
 C     1.149952    1.225376    1.657958
 C    -3.790145   -0.236341   -0.169160
 C    -1.281495   -0.019049    0.027894
 C    -5.973557    0.825258   -0.038528
 H    -2.371251   -2.568445   -0.588522
 C     0.570319    1.730606    0.435639
 C    -2.449280   -0.403181   -0.861385
 C    -4.743220    0.653881   -0.674321
 H    -6.702862    1.528118   -0.447952
Cu    0.578107   -0.972567   -0.983199
 C    -0.538108    1.100384   -0.238462
 C    -2.270915   -1.836345   -1.406643
 C    -0.931608   -1.994471   -1.992452
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 O    2.414465    3.165998   -0.113621
 C    0.128374   -2.232368   -2.575962
 C    1.251616    2.792240   -0.270355
 H    0.886645   -2.592689   -3.254235
 H   -2.440646    0.270512   -1.733112
 H   -4.517307    1.224730   -1.579170
 H   -0.806529    1.614958   -1.167407
 H   -3.041410   -2.080693   -2.154773
 O    0.490714    3.387735   -1.217406
 C    1.124226    4.351602   -2.034531
 H    1.480675    5.206292   -1.441720
 H    1.981047    3.919034   -2.572514
 H    0.368330    4.689161   -2.753026
Na    3.501731    1.122640    0.183268
 O    2.381523   -0.786411   -0.309723
 C    3.022149   -1.952858    0.118867
 C    2.041547   -2.850750    0.893520
 H    1.227710   -3.183907    0.227083
 H    2.526380   -3.748942    1.308292
 H    1.592067   -2.279249    1.719140
 C    3.587029   -2.731482   -1.080023
 H    4.133879   -3.636482   -0.769550
 H    2.770197   -3.040566   -1.749420
 H    4.273765   -2.091481   -1.656351
 C    4.184138   -1.573063    1.055824
 H    4.681165   -2.458177    1.481317
 H    4.957100   -1.004624    0.509492
 H    3.811430   -0.957230    1.890603
54
Figure_S6-1_PA-NaOtBu-ts(1,6) / electronic energy: -2993.40265452 a.u. / lowest freq: -461.31 cm-1
 H    0.389511    1.672320    3.661517
 H   -0.929355    0.640242    4.316437
 H   -1.304073    1.899287    3.103526
 C   -0.552780    1.164920    3.427513
 H    5.446222    2.458933    1.556763
 C    5.382473    1.494258    1.048171
 H    3.237129    1.562866    0.912298
 O   -0.255539    0.251342    2.384838
 H    7.523531    1.185947    1.031387
 C    4.137268    0.984681    0.691243
 C    6.547523    0.782859    0.752728
 O   -2.387856   -0.374292    2.397420
 H    1.532994    0.205727    1.118582
 C   -1.272012   -0.481135    1.909539
 C    4.028235   -0.251214    0.033941
 C    1.559227   -0.600515    0.388291
 C    6.453736   -0.442287    0.093887
 H    3.206826    1.021603   -2.119645
 C   -0.889358   -1.353978    0.797742
 C    2.718698   -0.821861   -0.363448
 C    5.206024   -0.951188   -0.264071
 H    7.358215   -1.006641   -0.144615
Cu   -0.874790    0.022965   -0.845375
 C    0.402331   -1.358716    0.148796
 C    2.614558    0.126999   -2.335849
 C    1.293695    0.302605   -2.614682
 O   -3.082502   -2.320680    0.561528
 C    0.034051    0.424626   -2.584691
 C   -1.877745   -2.348253    0.352965
 H   -0.689871    0.774191   -3.321789
 H    2.786077   -1.791075   -0.864321
 H    5.140272   -1.912275   -0.781253
 H    0.531801   -2.184283   -0.555840
 H    3.157635   -0.681597   -2.833852
 O   -1.340492   -3.337241   -0.374261
 C   -2.235205   -4.275343   -0.949118
 H   -2.785185   -4.822498   -0.170849
 H   -2.957266   -3.775141   -1.610245
 H   -1.616166   -4.968459   -1.528778
Na   -3.948796   -0.165152    0.662584
 O   -2.515194    1.017405   -0.575691
 C   -2.572593    2.407171   -0.672180
 C   -1.266411    3.038899   -0.160551
 H   -0.420243    2.728182   -0.795067
 H   -1.305707    4.140232   -0.155923
 H   -1.066000    2.692337    0.865444
 C   -2.813473    2.836538   -2.128282
 H   -2.912003    3.929520   -2.229455
 H   -1.976618    2.511239   -2.763661
 H   -3.734513    2.369472   -2.511254
 C   -3.738368    2.907916    0.199221
 H   -3.852497    4.002675    0.159883
 H   -4.687913    2.461542   -0.140817
 H   -3.573730    2.622155    1.251309
54
Figure_S6-1_PA-NaOtBu-ed(1,6) / electronic energy: -2993.41544293 a.u. / lowest freq: 9.58 cm-1
 H   -0.235368   -1.766587    3.627129
 H    1.028179   -0.665747    4.280757
 H    1.467518   -1.906946    3.067358
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 C    0.680383   -1.213087    3.394243
 H   -5.528973   -2.400294    1.759176
 C   -5.457747   -1.465490    1.198614
 H   -3.315459   -1.399408    1.338811
 O    0.337442   -0.316144    2.347500
 H   -7.592957   -1.305450    0.893672
 C   -4.209524   -0.896698    0.964609
 C   -6.615323   -0.853650    0.712375
 O    2.417473    0.461599    2.380931
 H   -1.534701   -0.196663    1.238740
 C    1.304766    0.477020    1.887601
 C   -4.090019    0.300895    0.238735
 C   -1.607323    0.605649    0.507380
 C   -6.512678    0.333141   -0.013016
 H   -3.392248   -1.050294   -2.608263
 C    0.883162    1.321034    0.748775
 C   -2.795882    0.937323   -0.040106
 C   -5.262609    0.901098   -0.247860
 H   -7.410937    0.817478   -0.402295
Cu    0.855051   -0.047667   -0.813921
 C   -0.392243    1.293837    0.113003
 C   -2.686875   -0.264527   -2.897302
 C   -1.385311   -0.408017   -2.712865
 O    3.058435    2.321759    0.442719
 C   -0.118312   -0.532445   -2.456490
 C    1.851175    2.352142    0.287481
 H    0.508644   -0.984316   -3.240861
 H   -2.829113    1.774080   -0.744097
 H   -5.187394    1.828584   -0.821649
 H   -0.555073    2.107017   -0.597724
 H   -3.104185    0.643371   -3.345059
 O    1.266633    3.351616   -0.369242
 C    2.117461    4.330413   -0.950583
 H    2.691116    4.856016   -0.175071
 H    2.815522    3.866254   -1.661143
 H    1.458520    5.031135   -1.473240
Na    4.031173    0.226041    0.663799
 O    2.531437   -0.972392   -0.470891
 C    2.680226   -2.345622   -0.669658
 C    1.407949   -3.096331   -0.241159
 H    0.555233   -2.786485   -0.865996
 H    1.520078   -4.189141   -0.327164
 H    1.169330   -2.851653    0.806159
 C    2.983545   -2.647748   -2.145440
 H    3.141284   -3.723587   -2.324815
 H    2.150604   -2.313129   -2.780046
 H    3.890759   -2.108264   -2.460900
 C    3.855932   -2.839970    0.192736
 H    4.012866   -3.925993    0.099270
 H    4.794341   -2.345808   -0.110287
 H    3.667127   -2.613580    1.254882
22
Figure_S6-1_NaOtBu-Cu-allenyl / electronic energy: -2151.45184434 a.u. / lowest freq: -9.22 cm-1
 H    4.987078    0.961943   -0.906549
Cu    0.711587   -0.397172   -0.003208
 C    4.546878    0.574839    0.019375
 C    3.528174   -0.271277    0.000018
 C    2.493597   -1.067705   -0.018893
 H    2.727964   -2.145100   -0.052502
 H    4.996617    0.907908    0.961539
Na   -0.436856    2.561157   -0.009909
 O   -0.950325    0.448873   -0.002369
 C   -2.159353   -0.248036    0.005002
 C   -3.304506    0.770563   -0.099412
 C   -2.299522   -1.045802    1.310931
 C   -2.224548   -1.210900   -1.191136
 H   -3.267243    1.473008    0.749496
 H   -4.294272    0.287592   -0.097003
 H   -3.209583    1.349685   -1.032359
 H   -2.227265   -0.367285    2.175425
 H   -1.481916   -1.780952    1.387314
 H   -3.258338   -1.585723    1.370608
 H   -1.414456   -1.954868   -1.116945
 H   -2.085989   -0.653157   -2.130574
 H   -3.184920   -1.748887   -1.242772
54
Figure_S6-1_PA-NaOtBu-ed(1,4) / electronic energy: -2993.41491749 a.u. / lowest freq: 12.10 cm-1
Cu    2.126522    0.205303    1.156487
 C   -1.509619    1.127227   -0.744661
 C   -0.225062    0.926429   -1.140475
 H   -1.777254    2.160790   -0.519016
 C    0.333304   -0.395030   -1.537576
 C    0.717156    2.073336   -1.191729
 O   -0.135473   -1.400189   -0.816000
 O    1.140001   -0.549741   -2.432472
 O    1.898412    1.993665   -1.475153
 O    0.152764    3.226802   -0.868103
 C    1.011096    4.350092   -0.723545
 H    1.755134    4.158091    0.062101
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 H     0.366857    5.187306   -0.436540
 H     1.525671    4.572557   -1.668240
 C     0.466174   -2.674798   -1.033559
 H     0.318310   -3.006128   -2.070345
 H    -0.028036   -3.361717   -0.339001
 H     1.537445   -2.589040   -0.804271
 C    -2.578172    0.165388   -0.615091
 H    -2.370589   -0.882188   -0.834168
 C    -3.801374    0.567197   -0.207064
 H    -3.941242    1.631550    0.013345
 C    -4.989257   -0.269064   -0.012646
 C    -6.183187    0.342752    0.403329
 C    -4.987492   -1.659851   -0.221970
 C    -7.340566   -0.405927    0.603247
 H    -6.200086    1.422496    0.572248
 C    -6.142908   -2.407140   -0.022055
 H    -4.074568   -2.165942   -0.541158
 C    -7.323351   -1.783777    0.390590
 H    -8.258729    0.088269    0.927224
 H    -6.124033   -3.486331   -0.187706
 H    -8.228903   -2.373710    0.547145
 C     1.253349    1.428993    2.336240
 H     1.848699    1.803242    3.189475
 C     0.039225    1.905198    2.300323
 C    -1.194899    2.379316    2.241811
 H    -1.420340    3.301128    1.694366
 H    -2.031446    1.868106    2.730663
Na     3.305033    0.197411   -1.867400
 O     3.112610   -0.934012    0.031214
 C     4.063610   -1.806500    0.565595
 C     3.418214   -2.728038    1.614051
 H     4.140075   -3.443242    2.040582
 H     3.003109   -2.122040    2.436072
 H     2.590340   -3.297321    1.164394
 C     5.203494   -1.014773    1.229019
 H     5.985564   -1.672883    1.641321
 H     5.672625   -0.337681    0.496832
 H     4.800912   -0.398321    2.049249
 C     4.636888   -2.661926   -0.576205
 H     5.376046   -3.394852   -0.216010
 H     3.826745   -3.210141   -1.082527
 H     5.136946   -2.024131   -1.324411
54
Figure_S6-1_PA-NaOtBu-ts(1,4) / electronic energy: -2993.396867900 a.u. / lowest freq: -458.66 cm-1
Cu     2.316292    0.318045    0.979296
 C    -1.448085    1.022464    0.007992
 C    -0.255097    0.700903   -0.682286
 H    -1.675654    2.087309   -0.026179
 C     0.137913   -0.666861   -1.009917
 C     0.606422    1.789610   -1.126485
 O    -0.367251   -1.574571   -0.159896
 O     0.847789   -1.019276   -1.940408
 O     1.596038    1.705022   -1.845317
 O     0.217990    2.986588   -0.658082
 C     1.047398    4.094081   -0.956997
 H     2.049116    3.957219   -0.523605
 H     0.564330    4.967573   -0.505415
 H     1.146298    4.238339   -2.042005
 C    -0.010018   -2.928207   -0.381936
 H    -0.298258   -3.257525   -1.390043
 H    -0.546645   -3.512441    0.373571
 H     1.074226   -3.062409   -0.257815
 C    -2.646470    0.172418    0.007278
 H    -2.495108   -0.906029   -0.039729
 C    -3.883879    0.696040    0.047869
 H    -3.985985    1.785797    0.115994
 C    -5.152862   -0.048104    0.015172
 C    -6.358634    0.660356    0.141133
 C    -5.218479   -1.444357   -0.139432
 C    -7.587018    0.002636    0.117989
 H    -6.328540    1.746474    0.261977
 C    -6.444203   -2.101587   -0.164070
 H    -4.300626   -2.025773   -0.247284
 C    -7.634841   -1.382188   -0.035207
 H    -8.511838    0.574743    0.219577
 H    -6.472903   -3.186445   -0.288217
 H    -8.595522   -1.901099   -0.056402
 C     1.336889    1.049874    2.463961
 H     1.960520    1.218619    3.349683
 C     0.070140    1.142965    2.419698
 C    -1.264327    1.180683    2.162870
 H    -1.768761    2.150667    2.187304
 H    -1.869232    0.327780    2.485254
Na     2.916599   -0.094468   -2.282150
 O     3.520158   -0.490386   -0.206313
 C     4.577516   -1.258325    0.281346
 C     4.056101   -2.342888    1.238445
 H     4.863038   -2.989107    1.619959
 H     3.553677   -1.873058    2.100542
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 H    3.318874   -2.976072    0.720638
 C    5.580866   -0.362567    1.025653
 H    6.448274   -0.926145    1.405693
 H    5.946223    0.429359    0.353128
 H    5.082238    0.123206    1.880753
 C    5.277364   -1.932374   -0.909312
 H    6.118505   -2.569778   -0.594216
 H    4.559174   -2.561462   -1.459902
 H    5.671556   -1.170336   -1.601638
54
Figure_S6-1_PA-NaOtBu-prod(1,4) / electronic energy: -2993.45855811 a.u. / lowest freq: 12.67 cm-1
Cu    1.967797   -0.204010    0.840379
 C   -0.996444   -0.186244    1.064888
 C   -0.026017    0.039421   -0.111673
 H   -1.007048    0.757627    1.622229
 C    0.200905   -1.019323   -1.081847
 C    0.114368    1.406512   -0.595198
 O   -0.333698   -2.201898   -0.699452
 O    0.821943   -0.958542   -2.139841
 O    0.665659    1.786780   -1.624577
 O   -0.427488    2.321398    0.236181
 C   -0.282284    3.681291   -0.125369
 H    0.778667    3.966393   -0.179080
 H   -0.783576    4.260046    0.658899
 H   -0.751440    3.886177   -1.098160
 C   -0.077684   -3.321245   -1.526378
 H   -0.502704   -3.179302   -2.530254
 H   -0.556623   -4.177517   -1.037838
 H    1.002412   -3.503209   -1.623586
 C   -2.404647   -0.461943    0.610196
 H   -2.555377   -1.416832    0.095971
 C   -3.422680    0.393754    0.768266
 H   -3.226608    1.341948    1.282548
 C   -4.813493    0.205677    0.311685
 C   -5.769556    1.187427    0.615382
 C   -5.234843   -0.919408   -0.418227
 C   -7.097782    1.052457    0.213165
 H   -5.462933    2.072832    1.179031
 C   -6.559986   -1.056373   -0.820260
 H   -4.516942   -1.699363   -0.680220
 C   -7.499848   -0.071883   -0.506127
 H   -7.822273    1.830430    0.464456
 H   -6.863377   -1.940315   -1.386178
 H   -8.539374   -0.182542   -0.822384
 C    2.101560   -0.952704    2.748802
 H    2.992433   -1.000777    3.357232
 C    0.933444   -1.048457    2.348844
 C   -0.495390   -1.257042    2.056780
 H   -1.076472   -1.222585    2.992022
 H   -0.611984   -2.262710    1.628488
Na    2.476244    0.622318   -2.338585
 O    3.360118    0.350457   -0.331008
 C    4.717390    0.200585   -0.059071
 C    5.048148   -1.270210    0.244257
 H    6.124488   -1.431212    0.417709
 H    4.501951   -1.605138    1.140377
 H    4.732472   -1.905186   -0.598963
 C    5.119048    1.074989    1.139181
 H    6.191954    0.993482    1.377169
 H    4.887609    2.130764    0.927710
 H    4.542400    0.774633    2.028579
 C    5.512656    0.643837   -1.299228
 H    6.601184    0.577920   -1.145008
 H    5.258293    0.005743   -2.162547
 H    5.264597    1.687212   -1.553602
49
Figure_S7-1_Me2NHC-Cu-allyl / electronic energy: -2512.83406354 a.u. / lowest freq: 19.73 cm-1
 C   -3.482876   -2.154351    0.497924
 H   -3.031361   -3.105658    0.169087
 C   -2.890517   -1.648131    1.818672
 H   -3.664022   -1.323800    2.534491
 C   -2.285225   -0.188955    0.095336
Cu   -1.299425    1.213859   -0.808543
 N   -3.125028   -1.085167   -0.432091
 N   -2.094356   -0.503054    1.383204
 H   -2.257578   -2.395107    2.320683
 H   -4.573034   -2.293576    0.540620
 C    0.093634    2.448930   -1.440640
 H   -0.161586    3.513200   -1.565844
 H    0.491208    2.048089   -2.387871
 C    0.991123    2.164253   -0.292353
 C    1.122960    2.962609    0.801653
 H    1.742935    2.613981    1.634700
 C    0.405499    4.269536    0.963238
 H    0.654871    4.982764    0.157201
 H   -0.691152    4.124336    0.904199
 H    0.630949    4.755112    1.923544
 B    1.659797    0.755181   -0.229879
 O    2.270114    0.226920    0.883648
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 O    1.627375   -0.148678   -1.265630
 C    2.852606   -1.034292    0.517526
 C    2.002671   -1.431975   -0.743358
 C    2.762879   -2.206364   -1.808696
 H    3.604863   -1.625471   -2.205723
 H    3.149242   -3.151373   -1.397973
 H    2.089282   -2.446533   -2.643924
 C    0.709487   -2.164766   -0.380019
 H    0.163542   -1.638361    0.416038
 H    0.058075   -2.198111   -1.265655
 H    0.906321   -3.195051   -0.050819
 C    2.737813   -1.996580    1.690086
 H    3.362946   -1.643963    2.523077
 H    1.703980   -2.073857    2.050172
 H    3.086497   -2.999797    1.402493
 C    4.323302   -0.778601    0.188296
 H    4.853801   -1.713054   -0.043494
 H    4.427017   -0.094369   -0.666395
 H    4.806657   -0.312365    1.058680
 C   -3.487406   -1.163884   -1.824387
 H   -4.580734   -1.221320   -1.939862
 H   -3.120365   -0.265679   -2.336487
 H   -3.039560   -2.052430   -2.299717
 C   -1.295324    0.241755    2.325129
 H   -0.571169   -0.422818    2.822224
 H   -0.737917    1.024815    1.793283
 H   -1.927347    0.709105    3.098033
81
Figure_S7-1_AA-Me2NHC-pc(1,6major) / electronic energy: -3354.79756035 a.u. / lowest freq: 11.94 cm-1
 C    5.170756    1.188874   -1.531180
 H    5.892606    1.295312   -0.704546
 C    5.212640   -0.205047   -2.169969
 H    5.219996   -0.165310   -3.272253
 C    3.170143    0.077897   -1.078579
Cu    1.322807   -0.211888   -0.407027
 N    3.804090    1.250799   -1.015916
 N    3.961985   -0.798942   -1.698661
 C    0.111070   -0.589852    1.176798
 C    1.480040   -0.723122    1.575136
 H    6.078189   -0.800690   -1.845233
 H    5.356686    1.997929   -2.252678
 H   -0.327074    0.387743    1.396680
 C    2.179647   -2.031485    1.636725
 C    2.169658    0.405908    2.248180
 O    1.773480   -2.863816    0.654934
 O    3.013062   -2.363579    2.442484
 O    3.353636    0.475894    2.484777
 O    1.324764    1.405484    2.560603
 C    1.884803    2.541038    3.195755
 H    2.472766    2.248756    4.076580
 H    1.040898    3.170694    3.498441
 H    2.534815    3.099867    2.506698
 C    2.333746   -4.167155    0.650129
 H    3.424542   -4.122198    0.522667
 H    1.877079   -4.691327   -0.196665
 H    2.107900   -4.694187    1.587798
 C    0.213058    0.294427   -2.003905
 H    0.526075   -0.430570   -2.773130
 H    0.665438    1.274698   -2.222942
 C   -1.233489    0.371824   -1.787283
 C   -2.081332   -0.667774   -2.004322
 H   -3.144870   -0.531488   -1.788655
 C   -1.635538   -2.009130   -2.498992
 H   -1.204882   -1.956225   -3.514824
 H   -0.836365   -2.406738   -1.844538
 H   -2.457336   -2.738785   -2.514159
 C   -0.856737   -1.643667    0.952305
 H   -0.485241   -2.665109    0.866396
 C   -2.172284   -1.375228    0.800869
 H   -2.505688   -0.336675    0.884294
 C   -3.240077   -2.351046    0.546852
 C   -4.561390   -1.888590    0.424854
 C   -3.006909   -3.728769    0.396639
 C   -5.610706   -2.765022    0.159817
 H   -4.756649   -0.817741    0.526295
 C   -4.055181   -4.605969    0.132791
 H   -1.992693   -4.124331    0.480858
 C   -5.362490   -4.129833    0.011594
 H   -6.628129   -2.378794    0.063782
 H   -3.850653   -5.672804    0.016432
 H   -6.181860   -4.820621   -0.199041
 B   -1.807057    1.646641   -1.107380
 O   -3.076939    1.745232   -0.587785
 O   -1.079768    2.792564   -0.892924
 C   -3.294971    3.108893   -0.192441
 C   -1.825029    3.636000    0.000865
 C   -1.612410    5.090469   -0.389962
 H   -1.838526    5.261321   -1.449912
 H   -2.248002    5.750962    0.218386
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 H   -0.563339    5.370211   -0.215737
 C   -1.278164    3.387356    1.405723
 H   -1.438247    2.346628    1.722332
 H   -0.195350    3.572933    1.397963
 H   -1.742199    4.053246    2.146960
 C   -4.147681    3.129920    1.067209
 H   -5.153396    2.747352    0.840841
 H   -3.716560    2.502769    1.857905
 H   -4.251075    4.156435    1.449485
 C   -4.031367    3.801307   -1.339090
 H   -4.279956    4.842628   -1.089828
 H   -3.431079    3.796144   -2.260750
 H   -4.967249    3.260693   -1.540172
 C    3.313914    2.426406   -0.342866
 H    3.420637    3.311284   -0.988437
 H    2.248024    2.291809   -0.114042
 H    3.862265    2.602068    0.596546
 C    3.580443   -2.132538   -2.087546
 H    4.310468   -2.869925   -1.719117
 H    2.598290   -2.359289   -1.656356
 H    3.520252   -2.220880   -3.184946
81
Figure_S7-1_AA-Me2NHC-ts(1,6major) / electronic energy: -3354.79031886 a.u. / lowest freq: -403.73 cm-1
 C    5.146740    0.915997   -1.482397
 H    5.839347    0.967818   -0.625786
 C    5.131152   -0.469708   -2.138883
 H    5.156926   -0.415473   -3.240450
 C    3.080147   -0.091943   -1.096490
Cu    1.241206   -0.313784   -0.397441
 N    3.766626    1.050757   -1.018256
 N    3.845842   -1.006712   -1.693539
 C   -0.012473   -0.690668    1.225525
 C    1.364155   -0.828191    1.635108
 H    5.961127   -1.111331   -1.809743
 H    5.409008    1.721445   -2.183416
 H   -0.434885    0.297027    1.433892
 C    2.082068   -2.117354    1.662544
 C    2.041868    0.302841    2.295739
 O    1.607000   -2.983247    0.734313
 O    2.993711   -2.429960    2.391904
 O    3.225695    0.391073    2.539582
 O    1.194713    1.314670    2.593710
 C    1.765770    2.457696    3.201664
 H    2.330108    2.184195    4.104020
 H    0.930727    3.115986    3.466213
 H    2.442491    2.980822    2.509749
 C    2.190347   -4.273889    0.714438
 H    3.269946   -4.214640    0.515671
 H    1.689379   -4.823443   -0.090844
 H    2.037530   -4.789353    1.673411
 C    0.146705    0.241826   -2.059329
 H    0.415950   -0.572185   -2.745664
 H    0.702043    1.167908   -2.251578
 C   -1.208886    0.392782   -1.673364
 C   -2.131961   -0.656741   -1.689612
 H   -3.186617   -0.385618   -1.601080
 C   -1.810236   -1.952095   -2.375479
 H   -1.586741   -1.796405   -3.445617
 H   -0.913693   -2.416147   -1.926196
 H   -2.636863   -2.671903   -2.304231
 C   -0.953954   -1.661101    0.828582
 H   -0.634242   -2.697144    0.724001
 C   -2.244522   -1.283840    0.470746
 H   -2.552866   -0.269230    0.733961
 C   -3.367939   -2.235304    0.342944
 C   -4.681170   -1.736073    0.326070
 C   -3.192060   -3.623692    0.225955
 C   -5.776638   -2.586222    0.196977
 H   -4.836983   -0.657073    0.413151
 C   -4.286658   -4.475778    0.095322
 H   -2.186389   -4.048415    0.231428
 C   -5.584840   -3.963350    0.079154
 H   -6.786796   -2.170022    0.188075
 H   -4.123628   -5.552202    0.003350
 H   -6.440785   -4.634162   -0.022626
 B   -1.630938    1.753702   -1.046830
 O   -2.765246    1.930627   -0.296194
 O   -0.887584    2.902255   -1.140466
 C   -2.908531    3.337381   -0.028687
 C   -1.436377    3.862525   -0.219990
 C   -1.329120    5.252583   -0.827238
 H   -1.794723    5.299531   -1.819528
 H   -1.811900    5.996133   -0.175812
 H   -0.269933    5.527330   -0.933950
 C   -0.601288    3.779545    1.055940
 H   -0.652198    2.777263    1.504808
 H    0.450835    3.980945    0.807263
 H   -0.925451    4.518114    1.802666
 C   -3.471231    3.518927    1.372428
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 H   -4.493042    3.115388    1.416336
 H   -2.865656    2.993309    2.121559
 H   -3.513200    4.586143    1.636474
 C   -3.883072    3.894091   -1.065775
 H   -4.086374    4.960620   -0.895357
 H   -3.493355    3.769712   -2.086653
 H   -4.832764    3.345107   -0.994114
 C    3.327173    2.234766   -0.323556
 H    3.504781    3.129924   -0.938332
 H    2.249297    2.155720   -0.126648
 H    3.854111    2.347667    0.637415
 C    3.413428   -2.324679   -2.082729
 H    4.126033   -3.085349   -1.728664
 H    2.433248   -2.521961   -1.631959
 H    3.330724   -2.408464   -3.179121
81
Figure_S7-1_AA-Me2NHC-prod(1,6major) / electronic energy: -3354.84618081 a.u. / lowest freq: 21.17 cm-1
 C   -4.748833   -0.770351   -0.821798
 H   -5.064742   -0.474129    0.192830
 C   -4.786780    0.396826   -1.809043
 H   -5.132360    0.093782   -2.812965
 C   -2.567185   -0.128783   -1.317654
Cu   -0.601813    0.040249   -1.178469
 N   -3.322597   -1.093774   -0.792621
 N   -3.379807    0.788791   -1.858961
 C   -0.090848    0.390534    1.240805
 C   -1.312517    0.071242    1.919940
 H   -5.420416    1.229592   -1.470481
 H   -5.347154   -1.633267   -1.145787
 H    0.726181   -0.284000    1.518300
 C   -2.548501    0.811973    1.756327
 C   -1.336207   -1.082574    2.799724
 O   -2.366790    1.972487    1.062930
 O   -3.665133    0.516599    2.146609
 O   -2.288362   -1.545600    3.401738
 O   -0.112932   -1.688131    2.926576
 C   -0.071657   -2.837598    3.743266
 H   -0.330621   -2.600748    4.786023
 H    0.957467   -3.214869    3.696750
 H   -0.765819   -3.611515    3.382675
 C   -3.509234    2.772370    0.861947
 H   -4.293962    2.225467    0.319290
 H   -3.181627    3.634960    0.268501
 H   -3.931387    3.120231    1.816673
 C    0.439944   -0.148901   -3.044105
 H    0.111860    0.679553   -3.679344
 H    0.176498   -1.151423   -3.392094
 C    1.331966    0.015049   -2.008844
 C    1.930661    1.362314   -1.603414
 H    3.016153    1.287389   -1.793149
 C    1.403555    2.549679   -2.403124
 H    1.572411    2.419355   -3.481849
 H    0.323325    2.700440   -2.244465
 H    1.911947    3.473350   -2.093893
 C    0.275003    1.355696    0.321622
 H   -0.430131    2.151735    0.074371
 C    1.729930    1.543509   -0.067153
 H    2.296816    0.728543    0.405418
 C    2.351913    2.837262    0.441322
 C    3.732787    3.038907    0.292084
 C    1.606276    3.844227    1.062740
 C    4.344347    4.209757    0.732580
 H    4.342270    2.258888   -0.172993
 C    2.215140    5.020065    1.507636
 H    0.534437    3.707127    1.215336
 C    3.584746    5.211055    1.341175
 H    5.421425    4.341003    0.604347
 H    1.609984    5.790519    1.991527
 H    4.060975    6.130201    1.689710
 B    1.842540   -1.305311   -1.323258
 O    2.787244   -1.355765   -0.343009
 O    1.343289   -2.535973   -1.645472
 C    3.080332   -2.741122   -0.066089
 C    1.821000   -3.480447   -0.665139
 C    2.129786   -4.798409   -1.357699
 H    2.828870   -4.668152   -2.193052
 H    2.563796   -5.513409   -0.643242
 H    1.201118   -5.233508   -1.753589
 C    0.696938   -3.671437    0.349480
 H    0.441568   -2.729599    0.855835
 H   -0.196473   -4.039417   -0.174774
 H    0.969598   -4.409896    1.116094
 C    3.252663   -2.904626    1.435995
 H    4.154051   -2.369216    1.766251
 H    2.392961   -2.493944    1.980544
 H    3.369506   -3.966322    1.698733
 C    4.380698   -3.071518   -0.794794
 H    4.702996   -4.102445   -0.592849
 H    4.274103   -2.943304   -1.881707
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 H     5.167471   -2.387512   -0.446585
 C    -2.847020   -2.203650   -0.005034
 H    -3.263405   -3.148797   -0.386756
 H    -1.753567   -2.244637   -0.071620
 H    -3.130534   -2.078663    1.051543
 C    -2.954961    1.938119   -2.612697
 H    -3.486279    2.839647   -2.271568
 H    -1.879605    2.089958   -2.459092
 H    -3.145178    1.807318   -3.691234
49
Figure_S7-1_Me2NHC-Cu-allyl / electronic energy: -2512.83406354 a.u. / lowest freq: 19.73 cm-1
 C    -3.482876   -2.154351    0.497924
 H    -3.031361   -3.105658    0.169087
 C    -2.890517   -1.648131    1.818672
 H    -3.664022   -1.323800    2.534491
 C    -2.285225   -0.188955    0.095336
Cu    -1.299425    1.213859   -0.808543
 N    -3.125028   -1.085167   -0.432091
 N    -2.094356   -0.503054    1.383204
 H    -2.257578   -2.395107    2.320683
 H    -4.573034   -2.293576    0.540620
 C     0.093634    2.448930   -1.440640
 H    -0.161586    3.513200   -1.565844
 H     0.491208    2.048089   -2.387871
 C     0.991123    2.164253   -0.292353
 C     1.122960    2.962609    0.801653
 H     1.742935    2.613981    1.634700
 C     0.405499    4.269536    0.963238
 H     0.654871    4.982764    0.157201
 H    -0.691152    4.124336    0.904199
 H     0.630949    4.755112    1.923544
 B     1.659797    0.755181   -0.229879
 O     2.270114    0.226920    0.883648
 O     1.627375   -0.148678   -1.265630
 C     2.852606   -1.034292    0.517526
 C     2.002671   -1.431975   -0.743358
 C     2.762879   -2.206364   -1.808696
 H     3.604863   -1.625471   -2.205723
 H     3.149242   -3.151373   -1.397973
 H     2.089282   -2.446533   -2.643924
 C     0.709487   -2.164766   -0.380019
 H     0.163542   -1.638361    0.416038
 H     0.058075   -2.198111   -1.265655
 H     0.906321   -3.195051   -0.050819
 C     2.737813   -1.996580    1.690086
 H     3.362946   -1.643963    2.523077
 H     1.703980   -2.073857    2.050172
 H     3.086497   -2.999797    1.402493
 C     4.323302   -0.778601    0.188296
 H     4.853801   -1.713054   -0.043494
 H     4.427017   -0.094369   -0.666395
 H     4.806657   -0.312365    1.058680
 C    -3.487406   -1.163884   -1.824387
 H    -4.580734   -1.221320   -1.939862
 H    -3.120365   -0.265679   -2.336487
 H    -3.039560   -2.052430   -2.299717
 C    -1.295324    0.241755    2.325129
 H    -0.571169   -0.422818    2.822224
 H    -0.737917    1.024815    1.793283
 H    -1.927347    0.709105    3.098033
81
Figure_S7-1_AA-Me2NHC-pc(1,6minor) / electronic energy: -3354.79657990 a.u. / lowest freq: 25.23 cm-1
 H     4.534853    3.537635   -1.622966
 H     2.269243    4.015018   -1.716426
 H     5.649275    2.283394   -1.033391
 C     0.893992    0.243336   -2.211221
 O     3.157413    1.289545   -1.451504
 C     4.794906    2.917458   -0.755516
 B     1.796497    1.158627   -1.335716
 C     2.161458    4.151645   -0.630538
 H     2.890623    4.904300   -0.298742
 H     5.111552    3.576005    0.067156
 C     3.629986    2.042308   -0.320623
 H     1.150987    4.538078   -0.434325
 O     1.293695    1.949950   -0.328123
 C     2.339468    2.828454    0.114233
 H     4.826140    0.354433    0.289734
 C     4.086477    1.036889    0.732432
 H     3.245214    0.423343    1.082155
 H     4.543894    1.534660    1.599434
 C     2.205879    3.051219    1.613005
 H     3.047645    3.649224    1.992502
 H     1.275525    3.597603    1.827206
 H     2.179784    2.099477    2.158183
 H     2.570547   -0.897012   -2.785793
 C     1.482411   -0.796300   -2.851046
 C     0.731441   -1.847112   -3.614898
 H     1.377900   -2.687586   -3.906233
 H     0.276427   -1.442310   -4.536707
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 H   -0.104275   -2.248698   -3.013882
 C   -0.556418    0.489100   -2.179745
 H   -1.107554    0.027554   -3.017068
 H   -0.785465    1.565837   -2.150906
 C   -5.128541    2.202209   -0.403626
 H   -5.920514    1.861679    0.282675
 C   -4.137214    3.161057    0.268597
 H   -3.986519    4.090915   -0.303946
 C   -3.019140    1.198981   -0.329410
Cu   -1.546887   -0.126039   -0.544941
 N   -4.270513    1.079922   -0.779197
 N   -2.903595    2.376290    0.288656
 C   -0.703045   -1.848511    0.095212
 C   -1.847327   -1.544816    0.902255
 H   -4.437386    3.438902    1.290247
 H   -5.612322    2.637010   -1.291446
 H   -0.890920   -2.564440   -0.708915
 C   -1.728839   -0.892901    2.234071
 C   -3.154286   -2.179467    0.608589
 O   -0.822139    0.102961    2.219412
 O   -2.338773   -1.183423    3.232464
 O   -4.186533   -1.995493    1.211044
 O   -3.095170   -2.990857   -0.465060
 C   -4.289391   -3.663653   -0.825314
 H   -4.656046   -4.282443    0.005630
 H   -4.035847   -4.297206   -1.682221
 H   -5.077080   -2.951305   -1.107859
 C   -0.581713    0.766506    3.448826
 H   -1.503393    1.228336    3.830266
 H    0.165793    1.537840    3.236337
 H   -0.198564    0.065216    4.203940
 C    0.686160   -1.770003    0.520020
 H    0.915694   -1.174545    1.406137
 C    1.684035   -2.383617   -0.146442
 H    1.446237   -2.932006   -1.062822
 C    3.097778   -2.386379    0.262609
 C    4.105254   -2.540900   -0.702779
 C    3.483423   -2.248133    1.606289
 C    5.451318   -2.521271   -0.344698
 H    3.824479   -2.664706   -1.751599
 C    4.828251   -2.231721    1.966151
 H    2.717977   -2.163405    2.381099
 C    5.819066   -2.361738    0.991940
 H    6.218511   -2.630828   -1.114511
 H    5.104982   -2.121532    3.017154
 H    6.874124   -2.347853    1.274168
 C   -4.806961   -0.053238   -1.485829
 H   -3.989369   -0.743135   -1.731989
 H   -5.549490   -0.587514   -0.872170
 H   -5.286960    0.268980   -2.423088
 C   -1.687101    2.934647    0.823762
 H   -0.844332    2.266282    0.608561
 H   -1.481845    3.910871    0.354379
 H   -1.769427    3.086660    1.911990
81
Figure_S7-1_AA-Me2NHC-ts(1,6minor) / electronic energy: -3354.78177396 a.u. / lowest freq: -454.83 cm-1
 H    4.969168    2.906226   -1.220530
 H    3.028697    3.515922   -2.290741
 H    5.542754    1.949949    0.163293
 C    1.031409    0.050570   -1.848484
 O    3.120423    1.093828   -0.701498
 C    4.818096    2.714624   -0.150847
 B    1.806352    1.161996   -1.075236
 C    2.637426    4.116117   -1.456499
 H    3.391031    4.867350   -1.181861
 H    5.030655    3.639047    0.406512
 C    3.406408    2.228286    0.137754
 H    1.736671    4.639850   -1.806945
 O    1.223460    2.348246   -0.702323
 C    2.265309    3.235491   -0.263804
 H    4.028960    0.959346    1.759083
 C    3.299111    1.761510    1.588021
 H    2.296015    1.362946    1.800181
 H    3.512970    2.577278    2.292449
 C    1.742308    4.095251    0.876510
 H    2.550416    4.710266    1.299376
 H    0.959835    4.771876    0.504065
 H    1.309724    3.484608    1.679201
 H    2.770242   -1.138790   -2.062194
 C    1.679792   -1.163937   -2.117749
 C    1.074807   -2.151678   -3.079218
 H    1.692895   -3.055260   -3.183911
 H    0.955546   -1.708788   -4.083563
 H    0.069841   -2.467522   -2.749946
 C   -0.323430    0.308566   -2.140174
 H   -0.846091   -0.316045   -2.877987
 H   -0.629457    1.358822   -2.151915
 C   -5.014280    2.092417   -1.024360
 H   -5.978857    1.851379   -0.553935
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 C   -4.173463    3.070750   -0.194627
 H   -4.042493    4.047762   -0.683307
 C   -2.939612    1.122223   -0.558914
Cu   -1.471554   -0.214325   -0.466804
 N   -4.152367    0.912814   -1.077634
 N   -2.895241    2.369506   -0.085525
 C   -0.724219   -2.023284    0.363821
 C   -1.863500   -1.560123    1.125199
 H   -4.597076    3.246035    0.807966
 H   -5.215047    2.463133   -2.043336
 H   -0.980708   -2.761880   -0.401682
 C   -1.741637   -0.690925    2.308029
 C   -3.182499   -2.164081    0.885696
 O   -0.678509    0.151701    2.207189
 O   -2.463605   -0.655154    3.276527
 O   -4.227692   -1.876578    1.427889
 O   -3.147681   -3.106971   -0.090504
 C   -4.369089   -3.755695   -0.386011
 H   -4.775649   -4.258017    0.503535
 H   -4.143611   -4.495794   -1.162234
 H   -5.121524   -3.044541   -0.756693
 C   -0.444419    1.006081    3.310199
 H   -1.327471    1.622798    3.529013
 H    0.398895    1.647372    3.029490
 H   -0.189270    0.428682    4.210864
 C    0.646475   -1.862349    0.597432
 H    0.964219   -1.190138    1.394612
 C    1.598969   -2.396605   -0.272769
 H    1.250798   -3.207874   -0.916539
 C    3.037980   -2.484566    0.065396
 C    3.877617   -3.299285   -0.712199
 C    3.614029   -1.788627    1.137710
 C    5.239351   -3.404419   -0.440487
 H    3.450597   -3.856417   -1.550735
 C    4.975351   -1.892600    1.413810
 H    2.991537   -1.154124    1.768796
 C    5.797918   -2.697959    0.625290
 H    5.868466   -4.044005   -1.064033
 H    5.398207   -1.340622    2.257023
 H    6.865214   -2.779065    0.842360
 C   -4.577199   -0.281198   -1.759614
 H   -3.787384   -1.039717   -1.683903
 H   -5.495816   -0.681682   -1.303868
 H   -4.773411   -0.080105   -2.825732
 C   -1.777080    2.973405    0.592980
 H   -0.892269    2.335075    0.481749
 H   -1.549397    3.954054    0.147145
 H   -1.993970    3.121447    1.663684
81
Figure_S7-1_AA-Me2NHC-prod(1,6minor) / electronic energy: -3354.83876879 a.u. / lowest freq: 20.29 cm-1
 H   -5.443728   -2.159872   -0.784545
 H   -3.773335   -3.292443   -1.864949
 H   -5.705650   -0.909352    0.452639
 C   -1.201085   -0.134941   -2.166192
 O   -3.281466   -0.633151   -0.714627
 C   -5.154046   -1.831575    0.221484
 B   -2.057288   -0.999038   -1.176703
 C   -3.389201   -3.800975   -0.968755
 H   -4.217026   -4.346813   -0.495059
 H   -5.456236   -2.602275    0.945683
 C   -3.660565   -1.566790    0.320463
 H   -2.631516   -4.530211   -1.288451
 O   -1.635931   -2.207242   -0.694881
 C   -2.746835   -2.812214    0.001518
 H   -3.857293    0.060678    1.712753
 C   -3.330364   -0.901297    1.652762
 H   -2.254615   -0.694357    1.738435
 H   -3.638079   -1.527021    2.502409
 C   -2.215873   -3.539257    1.226031
 H   -3.044747   -3.927543    1.835886
 H   -1.594314   -4.390126    0.912135
 H   -1.599534   -2.879125    1.848187
 H   -2.523025    1.493466   -2.323888
 C   -1.438199    1.371947   -2.177573
 C   -0.730464    2.099448   -3.317962
 H   -0.988806    3.168736   -3.303343
 H   -1.012462    1.697766   -4.302270
 H    0.365930    2.025230   -3.218516
 C   -0.426772   -0.814343   -3.080108
 H    0.080422   -0.314114   -3.911145
 H   -0.449558   -1.906836   -3.124228
 C    4.786151   -1.173875   -0.733983
 H    5.384323   -0.387850   -0.250193
 C    4.132971   -2.106611    0.292335
 H    4.542448   -3.127228    0.273509
 C    2.468883   -1.146157   -1.025499
Cu    0.686449   -0.379197   -1.320767
 N    3.623792   -0.593220   -1.404442
 N    2.729017   -2.092190   -0.122337
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 C    1.145243    1.426423    0.376895
 C    2.091943    0.918163    1.324416
 H    4.205091   -1.701709    1.314995
 H    5.421783   -1.706081   -1.461632
 H    1.551022    2.255719   -0.212015
 C    1.786546   -0.066977    2.340295
 C    3.470318    1.369615    1.222261
 O    0.446295   -0.327322    2.443401
 O    2.557136   -0.642287    3.089980
 O    4.447765    0.950483    1.817230
 O    3.626969    2.395097    0.328909
 C    4.924922    2.933973    0.214156
 H    5.285837    3.329087    1.175659
 H    4.857294    3.748017   -0.517971
 H    5.648343    2.182883   -0.139659
 C    0.059715   -1.176003    3.503201
 H    0.386589   -2.213688    3.333414
 H   -1.035535   -1.141844    3.545574
 H    0.477545   -0.837365    4.461720
 C   -0.154318    1.083117    0.049500
 H   -0.666310    0.349283    0.675624
 C   -1.033980    1.999326   -0.793271
 H   -0.415026    2.879698   -1.038805
 C   -2.211777    2.557224    0.007386
 C   -3.257124    3.240374   -0.631671
 C   -2.254265    2.465672    1.403913
 C   -4.316718    3.784822    0.090904
 H   -3.247912    3.360446   -1.717807
 C   -3.313157    3.009177    2.132623
 H   -1.449838    1.954269    1.935388
 C   -4.354564    3.665690    1.480669
 H   -5.118554    4.307293   -0.436397
 H   -3.321858    2.912582    3.221049
 H   -5.186468    4.087644    2.048942
 C    3.768643    0.438899   -2.396639
 H    2.785905    0.652252   -2.836542
 H    4.160767    1.364060   -1.949393
 H    4.450208    0.114034   -3.199269
 C    1.749338   -2.886230    0.576130
 H    0.739780   -2.603779    0.247925
 H    1.901745   -3.958960    0.375120
 H    1.837792   -2.719171    1.660417
32
Figure_S8-1_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C   -0.660544   -0.726572    0.059153
 C   -1.860539   -0.097447    0.115996
 H   -0.691600   -1.818492   -0.004770
 C   -1.976243    1.390665    0.160143
 C   -3.120576   -0.891785    0.187355
 O   -3.041424    1.823605   -0.507466
 O   -1.182749    2.134043    0.689285
 O   -4.147702   -0.497504    0.683440
 O   -2.981802   -2.118850   -0.320932
 C   -4.097604   -2.989729   -0.195724
 H   -4.332384   -3.170881    0.862818
 H   -3.810049   -3.927003   -0.683244
 H   -4.981752   -2.562067   -0.688186
 C   -3.254671    3.228152   -0.535442
 H   -3.354009    3.627502    0.483524
 H   -4.184056    3.384216   -1.092621
 H   -2.420438    3.737793   -1.038016
 C    0.656646   -0.129211    0.062308
 H    0.725624    0.955889    0.150505
 C    1.759981   -0.902956   -0.019704
 H    1.621029   -1.988149   -0.089650
 C    3.156351   -0.453635   -0.025165
 C    4.175093   -1.416830   -0.109525
 C    3.522207    0.902114    0.053056
 C    5.517020   -1.042840   -0.114390
 H    3.907556   -2.474776   -0.172060
 C    4.861836    1.275255    0.048166
 H    2.754752    1.675486    0.118691
 C    5.863995    0.305241   -0.035401
 H    6.294080   -1.807149   -0.179427
 H    5.127957    2.332459    0.111300
 H    6.914980    0.602284   -0.038425
56
Figure_S8-1_SIMes-Cu-allenyl / electronic energy: -2680.78923765 a.u. / lowest freq: 16.67 cm-1
 C    0.255100   -2.802091    0.505112
 H    0.668208   -3.196427    1.444813
 C   -1.270500   -2.619391    0.554864
 H   -1.800083   -3.253354   -0.170485
 C   -0.267703   -0.553149    0.091367
 C   -2.705673   -0.570588    0.110299
 C   -3.379878   -0.614762   -1.117966
 C   -3.248840    0.082482    1.227243
 C   -4.637370   -0.011781   -1.202344
 C   -4.506955    0.673704    1.096602
 C   -5.220520    0.629249   -0.105733
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Cu     0.110016    1.307604   -0.228361
 N     0.723169   -1.433012    0.264097
 N    -1.429749   -1.197347    0.221108
 H    -1.690544   -2.824163    1.551562
 H     0.576639   -3.468534   -0.309931
 C     0.774672    3.096038   -0.486998
 H     0.208773    4.016056   -0.700711
 C     2.071525    3.214162   -0.388898
 C     3.389142    3.271273   -0.276397
 H     4.042154    3.124597   -1.143427
 H     3.872005    3.450329    0.690170
 H    -4.940744    1.189169    1.958286
 H    -5.171125   -0.034945   -2.156636
 C    -2.739174   -1.258856   -2.318184
 H    -1.764393   -0.794441   -2.533026
 H    -2.557008   -2.332599   -2.157552
 H    -3.373859   -1.155030   -3.207828
 C    -2.466468    0.177007    2.509466
 H    -2.161688   -0.814837    2.876499
 H    -1.543922    0.758395    2.352392
 H    -3.052793    0.668434    3.296712
 C     2.100609   -1.074402    0.152530
 C     2.710868   -1.089540   -1.109969
 C     2.796150   -0.676303    1.303159
 C     4.054490   -0.718966   -1.196317
 C     4.137867   -0.315360    1.170431
 C     4.783410   -0.329256   -0.069282
 H     4.541691   -0.721123   -2.175444
 H     4.690272    0.002663    2.059240
 C     1.914463   -1.435151   -2.339256
 H     1.411113   -2.409070   -2.245646
 H     1.129881   -0.679297   -2.505515
 H     2.554756   -1.464444   -3.230551
 C     2.087510   -0.585650    2.627443
 H     1.295980    0.179314    2.581836
 H     1.603679   -1.535221    2.901538
 H     2.783525   -0.310564    3.430477
 C    -6.591070    1.245868   -0.208877
 H    -6.854724    1.465524   -1.252764
 H    -7.356052    0.560144    0.189860
 H    -6.655115    2.179427    0.368353
 C     6.214528    0.121736   -0.194929
 H     6.791322   -0.109785    0.711774
 H     6.712484   -0.348829   -1.054371
 H     6.258068    1.212948   -0.343793
88
Figure_S8-1_PA-SIMes-ed(1,6) / electronic energy: -3522.75056416 a.u. / lowest freq: 17.96 cm-1
 C    -2.527994    2.419306   -2.302324
 H    -3.146331    3.157018   -1.766728
 C    -1.073498    2.875473   -2.462589
 H    -0.682842    2.695235   -3.476988
 C    -1.140079    1.029772   -1.023287
 C     1.019789    2.165991   -1.215969
 C     1.428317    3.203427   -0.359770
 C     1.950519    1.300238   -1.813307
 C     3.739907    2.455086   -0.616591
Cu    -0.554544   -0.564931   -0.009037
 N    -2.376841    1.203276   -1.496088
 N    -0.369497    2.015628   -1.501145
 C     0.457253   -1.333672    1.592197
 C    -0.344656   -0.278074    2.074776
 H    -0.931822    3.938255   -2.228226
 H    -3.015261    2.198652   -3.261870
 H     0.081762   -2.349144    1.729000
 C     0.140120    1.080083    2.456405
 C    -1.684050   -0.627642    2.633482
 O     1.425003    1.086897    2.821456
 O    -0.548016    2.072804    2.486238
 O    -2.257021   -0.035195    3.515072
 O    -2.189877   -1.722053    2.048285
 C    -3.411059   -2.227162    2.563449
 H    -3.260590   -2.647732    3.568502
 H    -3.731247   -3.012421    1.870353
 H    -4.169814   -1.436003    2.611432
 C     1.961306    2.323071    3.267969
 H     1.836994    3.102615    2.506421
 H     3.026077    2.144219    3.451885
 H     1.465925    2.644402    4.195054
 C     1.839678   -1.207156    1.154918
 H     2.242450   -0.199482    1.031894
 C     2.601154   -2.282621    0.869808
 H     2.156098   -3.276276    0.983412
 C     4.000181   -2.258631    0.422662
 C     4.611821   -3.457300    0.021751
 C     4.764812   -1.080112    0.384719
 C     5.932707   -3.478369   -0.419928
 H     4.036397   -4.386058    0.051573
 C     6.084368   -1.099552   -0.055973
 H     4.323588   -0.135467    0.706977
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 C    6.674150   -2.297756   -0.464108
 H    6.385889   -4.421941   -0.731589
 H    6.659378   -0.171089   -0.077404
 H    7.710139   -2.310789   -0.809683
 C   -0.610406   -2.268425   -1.044647
 H   -1.635485   -2.647512   -1.187705
 C    0.365234   -2.968038   -1.537848
 C    1.415914   -3.610512   -2.024130
 H    1.936427   -4.378823   -1.442979
 H    1.797474   -3.403341   -3.030081
 C    2.790321    3.327725   -0.077595
 H    3.120144    4.131138    0.587548
 C    3.301137    1.456769   -1.488657
 H    4.031575    0.779266   -1.939167
 C    0.432950    4.171307    0.221496
 H    0.118767    4.914825   -0.528443
 H   -0.462629    3.650747    0.585659
 H    0.869972    4.725432    1.063066
 C    1.519617    0.233395   -2.781284
 H    1.071318   -0.623260   -2.256759
 H    0.761942    0.608500   -3.485117
 H    2.377662   -0.135717   -3.358308
 C   -3.476807    0.380451   -1.114729
 C   -3.845370   -0.688784   -1.942660
 C   -4.155635    0.661387    0.081405
 C   -4.913770   -1.494793   -1.539565
 C   -5.227837   -0.160418    0.433810
 C   -5.614499   -1.247904   -0.355759
 H   -5.772793    0.051449    1.358458
 C   -3.096840   -0.959557   -3.219765
 H   -3.471370   -1.868324   -3.709155
 H   -3.201258   -0.125487   -3.931406
 H   -2.022278   -1.091341   -3.021900
 C   -3.733539    1.810599    0.956901
 H   -2.689716    1.708863    1.291718
 H   -3.810903    2.770961    0.423484
 H   -4.365423    1.871039    1.852508
 C    5.195344    2.584307   -0.251464
 H    5.485539    3.637154   -0.125658
 H    5.403976    2.074941    0.704186
 H    5.844294    2.134992   -1.016132
 C   -6.739114   -2.148604    0.082804
 H   -7.169794   -2.699584   -0.764710
 H   -6.377111   -2.891533    0.812197
 H   -7.543230   -1.578957    0.570583
 H   -5.207135   -2.338193   -2.171232
88
Figure_S8-1_PA-SIMes-ts(1,6) / electronic energy: -3522.73490214 a.u. / lowest freq: -466.76 cm-1
 C   -2.553548    2.985525   -1.600766
 H   -3.213290    3.548654   -0.921923
 C   -1.111046    3.508690   -1.595894
 H   -0.715171    3.667104   -2.611016
 C   -1.139970    1.334777   -0.716326
 C    0.993149    2.515192   -0.582576
 C    1.324290    3.057087    0.668755
 C    1.977514    2.098832   -1.490729
 C    3.683925    2.717653    0.144488
Cu   -0.493297   -0.447854   -0.165785
 N   -2.385408    1.610072   -1.117371
 N   -0.384849    2.415469   -0.936688
 C    0.472784   -1.841175    1.034531
 C   -0.405921   -1.083058    1.889616
 H   -0.998001    4.449766   -1.039720
 H   -3.007325    2.995428   -2.601600
 H    0.102458   -2.832952    0.762725
 C    0.032009   -0.001807    2.785056
 C   -1.739502   -1.663357    2.155230
 O    1.370558    0.147299    2.812346
 O   -0.689461    0.706749    3.457566
 O   -2.451704   -1.467359    3.113308
 O   -2.118303   -2.501773    1.160538
 C   -3.324584   -3.216368    1.348849
 H   -3.216548   -3.963471    2.149824
 H   -3.534861   -3.718641    0.397629
 H   -4.147446   -2.536316    1.603938
 C    1.895564    1.087908    3.729115
 H    1.422433    2.070951    3.611917
 H    2.968213    1.159513    3.515897
 H    1.742689    0.747498    4.764188
 C    1.783578   -1.547287    0.613975
 H    2.210801   -0.568223    0.833659
 C    2.525055   -2.482838   -0.117044
 H    2.205245   -3.522814   -0.019130
 C    3.976728   -2.314661   -0.362307
 C    4.792226   -3.445430   -0.512259
 C    4.571170   -1.047870   -0.466391
 C    6.160613   -3.316970   -0.747481
 H    4.345464   -4.440745   -0.438521
 C    5.936267   -0.918000   -0.705435
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 H     3.954777   -0.151810   -0.375467
 C     6.739519   -2.052194   -0.845544
 H     6.777406   -4.212140   -0.855101
 H     6.377881    0.078121   -0.788031
 H     7.810535   -1.948383   -1.032162
 C    -0.423878   -1.472821   -1.954503
 H    -1.342671   -1.263822   -2.500109
 C     0.641195   -2.090153   -2.236641
 C     1.904023   -2.599588   -2.225006
 H     2.044406   -3.683320   -2.261627
 H     2.692050   -2.013040   -2.709771
 C     2.675336    3.145065    1.012277
 H     2.947531    3.561336    1.986070
 C     3.315524    2.214538   -1.106595
 H     4.093021    1.895402   -1.806483
 C     0.246761    3.521278    1.611518
 H    -0.436514    4.234703    1.127379
 H    -0.364025    2.678320    1.970034
 H     0.681582    4.019819    2.488147
 C     1.603343    1.523150   -2.828803
 H     1.063337    0.572624   -2.702687
 H     0.946568    2.200378   -3.395389
 H     2.498065    1.330626   -3.435518
 C    -3.483553    0.721166   -0.931855
 C    -3.989154    0.008540   -2.027802
 C    -4.042900    0.596991    0.352359
 C    -5.050021   -0.875799   -1.807424
 C    -5.107384   -0.288670    0.519986
 C    -5.616989   -1.042703   -0.542939
 H    -5.552171   -0.394539    1.513746
 C    -3.431922    0.199340   -3.414045
 H    -3.508854   -0.726775   -4.000411
 H    -3.994338    0.976918   -3.956413
 H    -2.379270    0.513758   -3.393203
 C    -3.506340    1.390306    1.512722
 H    -2.547657    0.988282    1.874144
 H    -3.335331    2.442308    1.239968
 H    -4.207465    1.363670    2.356991
 C     5.130302    2.758699    0.560928
 H     5.320883    3.563213    1.284990
 H     5.415365    1.808650    1.042549
 H     5.795703    2.902398   -0.302312
 C    -6.725851   -2.034965   -0.312888
 H    -7.242690   -2.289021   -1.248565
 H    -6.322790   -2.969923    0.109559
 H    -7.467843   -1.649656    0.401348
 H    -5.443326   -1.448353   -2.652348
88
Figure_S8-1_PA-SIMes-prod(1,6) / electronic energy: -3522.78247192 a.u. / lowest freq: 12.71 cm-1
 C    -2.343354    3.489735   -0.587000
 H    -2.977800    3.835895    0.244118
 C    -0.884877    3.953618   -0.454347
 H    -0.503604    4.414974   -1.377822
 C    -0.972881    1.618208   -0.259313
 C     1.201057    2.615953    0.140870
 C     1.564122    2.497314    1.491759
 C     2.158150    2.642698   -0.882234
 C     3.903937    2.387813    0.806662
Cu    -0.416406   -0.207418   -0.001060
 N    -2.213883    2.028268   -0.538453
 N    -0.183217    2.693705   -0.184539
 C     0.323312   -2.112501    0.324824
 C    -0.504972   -1.842421    1.503513
 H    -0.735181    4.666315    0.369264
 H    -2.808073    3.815022   -1.527687
 H    -0.120464   -2.845171   -0.355951
 C     0.007472   -1.246736    2.731602
 C    -1.846777   -2.423201    1.534759
 O     1.342688   -0.999985    2.665569
 O    -0.616897   -0.962286    3.736187
 O    -2.611411   -2.486839    2.475892
 O    -2.213973   -2.926864    0.320950
 C    -3.462829   -3.580983    0.261761
 H    -3.451869   -4.516238    0.842822
 H    -3.644153   -3.806233   -0.796206
 H    -4.264816   -2.937999    0.648925
 C     1.960799   -0.519270    3.839866
 H     1.472444    0.392200    4.210688
 H     3.002729   -0.304651    3.573544
 H     1.932280   -1.275451    4.639092
 C     1.483310   -1.527598   -0.116257
 H     2.051629   -0.843365    0.518104
 C     2.106017   -1.931752   -1.435431
 H     1.708991   -2.919649   -1.716817
 C     3.615361   -2.050368   -1.340040
 C     4.256075   -3.267408   -1.591367
 C     4.400486   -0.940946   -0.999834
 C     5.644953   -3.377883   -1.504918
 H     3.659204   -4.144690   -1.855723
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 C    5.787612   -1.045416   -0.917646
 H    3.921367    0.018957   -0.792445
 C    6.416011   -2.266287   -1.168700
 H    6.125450   -4.339292   -1.700290
 H    6.381670   -0.167054   -0.654126
 H    7.502779   -2.350944   -1.099679
 C   -0.932038   -0.993178   -2.957833
 H   -1.999740   -1.036654   -3.077480
 C    0.270482   -0.948199   -2.818193
 C    1.713330   -0.958812   -2.582084
 H    2.234279   -1.248056   -3.508973
 H    2.047188    0.060063   -2.329539
 C    2.919656    2.378615    1.800205
 H    3.216768    2.277321    2.847700
 C    3.505412    2.534453   -0.524765
 H    4.263657    2.548744   -1.312772
 C    0.512377    2.484362    2.567458
 H   -0.222475    3.290191    2.424323
 H   -0.049702    1.537115    2.566403
 H    0.964861    2.608470    3.559941
 C    1.746187    2.782417   -2.323514
 H    0.851579    2.180939   -2.544400
 H    1.506284    3.829817   -2.568107
 H    2.553637    2.466308   -2.997637
 C   -3.335573    1.150961   -0.597060
 C   -3.908741    0.860661   -1.845023
 C   -3.844319    0.605193    0.594366
 C   -4.992947   -0.019753   -1.885286
 C   -4.930892   -0.267340    0.501769
 C   -5.515218   -0.596388   -0.724558
 H   -5.335317   -0.699396    1.421584
 C   -3.383122    1.490546   -3.108071
 H   -3.648070    0.889902   -3.989223
 H   -3.815951    2.493230   -3.257612
 H   -2.289949    1.603150   -3.078407
 C   -3.241861    0.924436    1.936387
 H   -2.436382    0.217439    2.189638
 H   -2.814781    1.936202    1.965906
 H   -4.000274    0.844121    2.726610
 C    5.353495    2.200443    1.168130
 H    5.619137    2.768842    2.071214
 H    5.559776    1.138541    1.379188
 H    6.019367    2.514934    0.352438
 C   -6.664776   -1.567100   -0.788847
 H   -7.186919   -1.511425   -1.753878
 H   -6.305798   -2.601204   -0.662410
 H   -7.394336   -1.377038    0.011753
 H   -5.443825   -0.258384   -2.852834
88
Figure_S8-1_PA-SIMes-ed(1,4AA) / electronic energy: -3522.75057238 a.u. / lowest freq: 18.06 cm-1
 C   -2.527572    2.419661   -2.303532
 H   -3.146476    3.157352   -1.768564
 C   -1.073069    2.876220   -2.462915
 H   -0.681822    2.696314   -3.477143
 C   -1.139997    1.030399   -1.023766
 C    1.019980    2.166419   -1.216062
 C    1.428789    3.203841   -0.359980
 C    1.950477    1.300314   -1.813251
 C    3.740170    2.454796   -0.616642
Cu   -0.554831   -0.564305   -0.009155
 N   -2.376614    1.203855   -1.496980
 N   -0.369328    2.016360   -1.501281
 C    0.456472   -1.332927    1.592596
 C   -0.345634   -0.277382    2.074907
 H   -0.931794    3.938989   -2.228246
 H   -3.014115    2.198620   -3.263362
 H    0.080924   -2.348380    1.729360
 C    0.138898    1.080894    2.456373
 C   -1.685075   -0.627138    2.633385
 O    1.423793    1.087941    2.821398
 O   -0.549381    2.073525    2.486077
 O   -2.258356   -0.034562    3.514700
 O   -2.190524   -1.721831    2.048369
 C   -3.411425   -2.227402    2.563720
 H   -3.259918   -2.650575    3.567537
 H   -3.733421   -3.010475    1.868975
 H   -4.169395   -1.435639    2.614804
 C    1.959961    2.324216    3.267782
 H    1.835586    3.103675    2.506159
 H    3.024748    2.145489    3.451725
 H    1.464543    2.645593    4.194832
 C    1.839035   -1.206598    1.155668
 H    2.242086   -0.199012    1.032859
 C    2.600220   -2.282287    0.870618
 H    2.154740   -3.275781    0.984020
 C    3.999325   -2.258855    0.423720
 C    4.610734   -3.457882    0.023529
 C    4.764234   -1.080536    0.385260
 C    5.931678   -3.479501   -0.417951
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 H     4.035107   -4.386503    0.053786
 C     6.083843   -1.100520   -0.055234
 H     4.323151   -0.135616    0.706894
 C     6.673400   -2.299085   -0.462647
 H     6.384685   -4.423348   -0.729035
 H     6.659071   -0.172202   -0.077097
 H     7.709433   -2.312551   -0.808075
 C    -0.610124   -2.268833   -1.043121
 H    -1.635044   -2.649290   -1.183682
 C     0.365423   -2.967796   -1.537406
 C     1.415951   -3.609567   -2.024963
 H     1.795289   -3.403115   -3.031904
 H     1.938633   -4.376448   -1.443869
 C     2.790818    3.327771   -0.077766
 H     3.120851    4.131145    0.587318
 C     3.301133    1.456503   -1.488595
 H     4.031385    0.778728   -1.939000
 C     0.433648    4.172018    0.221176
 H     0.119263    4.915246   -0.528963
 H    -0.461848    3.651633    0.585805
 H     0.870948    4.726488    1.062379
 C     1.519316    0.233412   -2.781047
 H     1.071292   -0.623259   -2.256310
 H     0.761385    0.608420   -3.484650
 H     2.377193   -0.135686   -3.358328
 C    -3.476187    0.380039   -1.116637
 C    -3.841124   -0.690637   -1.942781
 C    -4.155910    0.660149    0.080283
 C    -4.906989   -1.500674   -1.537793
 C    -5.224385   -0.164389    0.433776
 C    -5.608291   -1.254306   -0.355378
 H    -5.195877   -2.347378   -2.166939
 H    -5.768497    0.044646    1.359699
 C     5.195641    2.583630   -0.251506
 H     5.486203    3.636412   -0.126004
 H     5.404074    2.074473    0.704299
 H     5.844451    2.133865   -1.016027
 C    -3.734815    1.810115    0.955262
 H    -2.691216    1.708894    1.290975
 H    -3.811947    2.770016    0.421010
 H    -4.367459    1.871070    1.850301
 C    -3.091384   -0.962133   -3.219021
 H    -3.196710   -0.129164   -3.931810
 H    -2.016726   -1.092232   -3.020535
 H    -3.464399   -1.872064   -3.707406
 C    -6.745203   -2.141374    0.079386
 H    -6.503713   -2.650103    1.025954
 H    -7.661721   -1.557120    0.252061
 H    -6.967262   -2.911803   -0.671484
88
Figure_S8-1_PA-SIMes-ts(1,4AA) / electronic energy: -3522.72443459 a.u. / lowest freq: -348.68 cm-1
 C    -2.858551    3.214128   -1.054087
 H    -3.513762    3.609003   -0.261924
 C    -1.442902    3.818587   -1.011000
 H    -1.118716    4.203247   -1.990185
 C    -1.317023    1.527041   -0.561999
 C     0.772673    2.716438   -0.332342
 C     1.182323    3.033917    0.972607
 C     1.692774    2.391356   -1.337692
 C     3.499542    2.721916    0.269886
Cu    -0.604794   -0.213176   -0.187831
 N    -2.595926    1.787448   -0.832148
 N    -0.623295    2.665110   -0.620019
 C     0.500491   -1.920165    0.355640
 C    -0.327331   -1.415504    1.487368
 H    -1.350768    4.634631   -0.280373
 H    -3.359012    3.375692   -2.019225
 H     0.304810   -2.974505    0.150543
 C     0.140048   -0.520941    2.549529
 C    -1.612384   -2.088984    1.711366
 O     1.473756   -0.296613    2.516192
 O    -0.545135   -0.006930    3.413358
 O    -2.331069   -2.036474    2.686374
 O    -1.955089   -2.860149    0.643521
 C    -3.132503   -3.631998    0.770775
 H    -3.013882   -4.410416    1.539822
 H    -3.301685   -4.099193   -0.206535
 H    -3.990256   -3.000586    1.037260
 C     2.018621    0.500450    3.547037
 H     1.511123    1.471462    3.618173
 H     3.074765    0.649885    3.293304
 H     1.937786   -0.006582    4.520298
 C     1.930230   -1.562542    0.214483
 H     2.194942   -0.510063    0.331116
 C     2.866628   -2.464778   -0.106274
 H     2.563266   -3.510931   -0.229379
 C     4.296700   -2.193209   -0.328733
 C     5.142201   -3.250676   -0.698046
 C     4.859962   -0.912127   -0.194373
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 C    6.501086   -3.041235   -0.928656
 H    4.722776   -4.254309   -0.808407
 C    6.216182   -0.702470   -0.422192
 H    4.228463   -0.067021    0.087388
 C    7.044845   -1.765326   -0.790934
 H    7.138119   -3.880545   -1.216955
 H    6.634005    0.300364   -0.309343
 H    8.109092   -1.596839   -0.968762
 C   -0.170783   -1.661775   -1.552322
 H   -1.124808   -2.185638   -1.690670
 C    0.722397   -1.621728   -2.498537
 C    1.703287   -1.602376   -3.374143
 H    1.818871   -0.783161   -4.090810
 H    2.435214   -2.416566   -3.410423
 C    2.550225    3.042570    1.246385
 H    2.886622    3.293604    2.256279
 C    3.052695    2.392936   -1.012388
 H    3.781189    2.130459   -1.784428
 C    0.166339    3.301236    2.050316
 H   -0.581983    4.044213    1.739215
 H   -0.377911    2.378140    2.309034
 H    0.650307    3.674575    2.962733
 C    1.216078    2.016900   -2.714616
 H    0.650758    1.072619   -2.679178
 H    0.544689    2.782421   -3.131510
 H    2.060283    1.886688   -3.404034
 C   -3.611974    0.794072   -0.706108
 C   -4.037929    0.108089   -1.853252
 C   -4.112159    0.489400    0.569133
 C   -5.015540   -0.877675   -1.706356
 C   -5.094747   -0.499316    0.665566
 C   -5.563609   -1.186187   -0.456974
 H   -5.351987   -1.426177   -2.590819
 H   -5.490973   -0.751257    1.653140
 C    4.966669    2.719762    0.611269
 H    5.265006    3.667049    1.084504
 H    5.203500    1.914088    1.324697
 H    5.587477    2.574492   -0.283510
 C   -3.556656    1.142865    1.805693
 H   -2.623196    0.645064    2.119089
 H   -3.327747    2.206110    1.647218
 H   -4.265466    1.062449    2.640600
 C   -3.403672    0.393259   -3.188155
 H   -3.525259    1.447057   -3.481410
 H   -2.321472    0.190268   -3.150317
 H   -3.843661   -0.231731   -3.976262
 C   -6.636143   -2.235142   -0.322705
 H   -6.597802   -2.724113    0.661181
 H   -7.636308   -1.784464   -0.427304
 H   -6.541096   -3.008555   -1.098123
88
Figure_S8-1_PA-SIMes-prod(1,4AA) / electronic energy: -3522.77095735 a.u. / lowest freq: 13.52 cm-1
 C    2.640161    3.389805    1.250127
 H    3.381230    3.881550    0.601628
 C    1.214778    3.941474    1.045695
 H    0.749850    4.270098    1.986821
 C    1.271493    1.693527    0.409752
 C   -0.850639    2.784192    0.047269
 C   -1.114466    2.938982   -1.321971
 C   -1.878971    2.565875    0.977101
 C   -3.497246    2.685109   -0.846982
Cu    0.766794    0.021256   -0.357702
 N    2.490182    1.980860    0.865707
 N    0.505261    2.779808    0.494322
 C   -0.486412   -2.483952   -0.166209
 C    0.225407   -1.673997   -1.283098
 H    1.182296    4.782397    0.337937
 H    2.984858    3.481921    2.289720
 H   -0.596337   -3.545425   -0.453579
 C   -0.558683   -1.069547   -2.385321
 C    1.559201   -2.131788   -1.729722
 O   -1.863538   -1.400275   -2.341889
 O   -0.140826   -0.332201   -3.259086
 O    2.276443   -1.617223   -2.565809
 O    1.959950   -3.258922   -1.093495
 C    3.289642   -3.680887   -1.333835
 H    3.456596   -3.885010   -2.400655
 H    3.431307   -4.598404   -0.751022
 H    4.007992   -2.914172   -1.005731
 C   -2.738630   -0.684138   -3.189796
 H   -2.645456    0.398845   -3.019791
 H   -3.752048   -1.016211   -2.934224
 H   -2.532379   -0.893866   -4.249301
 C   -1.843030   -1.933202    0.186607
 H   -1.886973   -0.841284    0.287422
 C   -2.927734   -2.665633    0.453801
 H   -2.858786   -3.757493    0.383437
 C   -4.243942   -2.127082    0.843554
 C   -5.210181   -2.981474    1.396820
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 C   -4.582652   -0.773266    0.673037
 C   -6.460701   -2.501902    1.785683
 H   -4.973094   -4.040596    1.529317
 C   -5.829493   -0.292942    1.062773
 H   -3.863262   -0.085674    0.222328
 C   -6.776049   -1.153499    1.623422
 H   -7.193718   -3.188223    2.216237
 H   -6.069572    0.763129    0.917319
 H   -7.755110   -0.774444    1.924557
 C    0.374117   -2.446764    1.103269
 H    1.396385   -2.822709    1.006424
 C   -0.008058   -1.986252    2.270138
 C   -0.370110   -1.533806    3.444492
 H   -0.239226   -0.480614    3.713732
 H   -0.822319   -2.192785    4.192795
 C   -2.446139    2.890956   -1.743989
 H   -2.664934    3.012458   -2.808689
 C   -3.194075    2.531220    0.509741
 H   -4.002568    2.359704    1.225968
 C    0.005667    3.077558   -2.316753
 H    0.793477    3.756669   -1.960766
 H    0.469378    2.093613   -2.497251
 H   -0.368223    3.451025   -3.279170
 C   -1.561886    2.319818    2.426850
 H   -0.826932    1.506590    2.525195
 H   -1.130492    3.210281    2.909685
 H   -2.463723    2.036161    2.984749
 C    3.549020    1.023460    0.828640
 C    3.880944    0.330855    2.004042
 C    4.172088    0.738334   -0.395958
 C    4.874375   -0.646986    1.936091
 C    5.158590   -0.251644   -0.415353
 C    5.526362   -0.950942    0.736123
 H    5.134254   -1.199971    2.843227
 H    5.642758   -0.490672   -1.366343
 C   -4.917002    2.570536   -1.335331
 H   -5.061831    3.101202   -2.286522
 H   -5.177768    1.512572   -1.504715
 H   -5.630893    2.971375   -0.601338
 C    3.745187    1.409835   -1.673191
 H    2.898616    0.860241   -2.117239
 H    3.425063    2.448453   -1.512856
 H    4.560251    1.404634   -2.409123
 C    3.137809    0.599242    3.284784
 H    3.304653    1.624535    3.649457
 H    2.054189    0.477784    3.134735
 H    3.452961   -0.094311    4.075126
 C    6.608839   -1.997072    0.688525
 H    6.647976   -2.490160   -0.293236
 H    7.596609   -1.541890    0.866191
 H    6.458094   -2.767494    1.457982
88
Figure_S8-1_PA-SIMes-ed(1,4) / electronic energy: -3522.74163171 a.u. / lowest freq: 14.52 cm-1
 H   -5.734861    0.740948    0.551066
 H   -4.821706    2.942395    0.388308
 C   -4.990928    0.835159   -0.254647
 C   -4.389217    2.245808   -0.345432
 H   -5.468395    0.515876   -1.192566
 N   -3.811562    0.014791    0.039224
 N   -2.970420    2.007124   -0.047659
 H   -4.504381    2.695120   -1.343251
 H   -4.372332   -0.917869   -2.512992
 H   -2.684275    2.622907   -2.689801
 C   -3.599007   -1.662236   -2.272764
 C   -1.616516    2.752666   -2.458199
 H   -2.620177   -1.162387   -2.347426
 H   -1.163179    1.752051   -2.382864
 H   -3.641156   -2.451173   -3.035906
 H   -0.541364   -4.452530    2.049773
 H    5.240316   -2.602385   -0.620373
 C    5.358322   -1.540034   -0.378400
 C    6.674230   -1.161767    0.150459
 C    7.004731    0.159238    0.501717
 H    7.409493   -3.191159    0.048458
 C    7.649755   -2.158574    0.314732
 C    8.266563    0.466516    0.998778
 H    8.505055    1.498448    1.265127
 C    8.913814   -1.851063    0.813323
 C    9.226243   -0.536450    1.156783
 H    9.657864   -2.641295    0.933553
 H   10.215690   -0.291762    1.548920
 H   -4.201360   -1.544123    3.641174
 H   -4.746418   -0.200901    2.603973
 C   -3.990481   -0.992447    2.715751
 H   -3.014133   -0.493439    2.829281
 H   -4.032678   -3.715837    2.699181
 C   -3.960075   -1.914725    1.527273
 C   -3.967724   -3.301365    1.689152
 H    1.307231   -0.952864    1.814171
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 C   -3.862135   -1.399273    0.225843
 C   -2.683201    0.722615    0.173110
 C   -3.879812   -4.169366    0.597768
 C    0.346581   -1.300744    1.404411
Cu   -1.052478   -0.167261    0.700822
 C   -3.776298   -2.238956   -0.894549
 C   -3.793300   -3.619690   -0.684187
 H   -1.076764   -3.142790   -1.536620
 H   -3.721443   -4.286440   -1.548636
 C   -0.338350   -3.233415   -2.346957
 O   -0.339444   -0.609497   -2.102168
 H   -0.028471   -4.278202   -2.455331
 C    0.696617   -1.191358   -1.865462
 H   -0.777421   -2.868857   -3.285953
 O    0.836115   -2.504369   -2.019043
 C    1.923876   -0.532726   -1.346562
 H   -2.160876    3.793273    3.367979
 H   -3.515235    3.126406    2.422182
 C   -2.418183    3.171234    2.500635
 H   -2.070146    2.144146    2.694619
 H   -0.723185    5.296236    2.218871
 C   -1.788708    3.704308    1.241773
 C   -0.921990    4.798437    1.265385
 C   -2.031981    3.078602    0.008916
 C   -0.299636    5.266697    0.102552
 C    0.169038   -2.591659    1.341079
 C   -1.406573    3.502163   -1.171735
 C   -0.548494    4.603131   -1.100904
 C   -0.055780   -3.893319    1.242670
 H    0.236409   -4.453027    0.347796
 H   -0.049469    4.940817   -2.013250
 H    0.886915    2.796259    0.649508
 H   -1.142974    3.276397   -3.298823
 H    2.452131    2.708726    1.529809
 C    1.964449    2.602457    0.555140
 O    2.177320    1.257465    0.148326
 C    1.785570    0.933922   -1.084056
 C    3.053698   -1.235593   -1.108652
 H    3.026447   -2.302830   -1.345123
 O    1.368771    1.735653   -1.880960
 H    2.391692    3.309524   -0.169018
 C    4.302895   -0.725717   -0.584390
 H    4.362845    0.337750   -0.345201
 H    6.269554    0.958011    0.386974
 C    0.662463    6.424263    0.163681
 C   -3.825352   -5.659969    0.801953
 H   -2.780789   -5.985971    0.934232
 H   -4.234403   -6.201663   -0.062564
 H   -4.381598   -5.965657    1.699467
 H    0.765832    6.915289   -0.813954
 H    1.664287    6.078822    0.467141
 H    0.340454    7.176316    0.898128
88
Figure_S8-1_PA-SIMes-ts(1,4) / electronic energy: -3522.71682623 a.u. / lowest freq: -448.70 cm-1
 H   -5.838684    0.244181    0.656601
 H   -5.196545    2.540081    0.477949
 C   -5.184200    0.440290   -0.207288
 C   -4.709409    1.899611   -0.271190
 H   -5.719970    0.124714   -1.114178
 N   -3.920004   -0.292959   -0.062866
 N   -3.273765    1.769598    0.004387
 H   -4.869275    2.355214   -1.261086
 H   -4.420802   -0.971587   -2.664659
 H   -2.945536    2.240509   -2.624667
 C   -3.654910   -1.746301   -2.512279
 C   -1.888302    2.451392   -2.405846
 H   -2.670246   -1.252615   -2.542436
 H   -1.363929    1.488881   -2.297133
 H   -3.715566   -2.457151   -3.347170
 H    2.832391   -1.767425    2.419991
 H    4.960104   -2.598100    0.356185
 C    5.216779   -1.551407    0.153633
 C    6.658211   -1.256844    0.138344
 C    7.176459    0.033819   -0.069703
 H    7.184618   -3.318354    0.505775
 C    7.567580   -2.307542    0.341815
 C    8.549319    0.258834   -0.074994
 H    8.930241    1.269535   -0.238228
 C    8.942936   -2.083222    0.337031
 C    9.440431   -0.797796    0.127938
 H    9.629823   -2.917253    0.497436
 H   10.517583   -0.617556    0.123162
 H   -3.997737   -2.168381    3.403180
 H   -4.659967   -0.769833    2.519258
 C   -3.865589   -1.530843    2.519264
 H   -2.908068   -0.996148    2.619303
 H   -3.823515   -4.245533    2.262478
 C   -3.872649   -2.346668    1.254446
 C   -3.832830   -3.742050    1.291562
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 H   -0.684576    0.202434    2.998290
 C   -3.869005   -1.715824    0.000777
 C   -2.856570    0.502993    0.087090
 C   -3.804763   -4.508187    0.121443
 C   -0.038864   -0.100331    2.168777
Cu   -0.994871   -0.056969    0.412918
 C   -3.806317   -2.449642   -1.191993
 C   -3.790311   -3.844373   -1.107929
 H   -1.179101   -3.032310   -0.120051
 H   -3.737251   -4.427493   -2.031907
 C   -0.458834   -3.368672   -0.882676
 O   -0.466116   -0.836872   -1.550263
 H   -0.157739   -4.401571   -0.674997
 C    0.599658   -1.277528   -1.096730
 H   -0.940762   -3.306278   -1.867558
 O    0.724327   -2.591407   -0.835734
 C    1.784022   -0.501267   -0.792970
 H   -2.527445    3.674034    3.370672
 H   -3.960716    3.209356    2.427270
 C   -2.867206    3.099956    2.498612
 H   -2.661308    2.034381    2.681566
 H   -1.129672    5.183790    2.187043
 C   -2.181892    3.564989    1.241919
 C   -1.306846    4.651041    1.248184
 C   -2.386638    2.885281    0.030626
 C   -0.643534    5.065966    0.086938
 C    1.180791   -0.447167    2.249907
 C   -1.724789    3.256817   -1.146753
 C   -0.862910    4.356930   -1.095449
 C    2.493253   -0.775362    2.106916
 H    3.222939    0.032110    2.213759
 H   -0.334762    4.653074   -2.005908
 H    1.622403    3.514627   -0.435779
 H   -1.452032    2.975104   -3.266270
 H    3.315093    3.457442    0.168538
 C    2.609319    3.047716   -0.563238
 O    2.539874    1.656462   -0.309561
 C    1.770511    0.925827   -1.144949
 C    2.808994   -1.103838   -0.040124
 H    2.682389   -2.179753    0.083052
 O    1.162971    1.446515   -2.055600
 H    2.966156    3.249515   -1.583805
 C    4.214001   -0.680569   -0.055602
 H    4.415517    0.372474   -0.255851
 H    6.499266    0.875416   -0.228669
 C    0.296590    6.242682    0.126878
 C   -3.798609   -6.012963    0.189616
 H   -3.370769   -6.455394   -0.720849
 H   -4.823584   -6.403187    0.297363
 H   -3.220684   -6.371675    1.053388
 H    0.799708    6.388846   -0.838937
 H    1.069977    6.103996    0.898051
 H   -0.242018    7.171421    0.371804
88
Figure_S8-1_PA-SIMes-prod(1,4) / electronic energy: -3522.75830146 a.u. / lowest freq: 13.48 cm-1
 H   -5.825429   -0.316642    0.724633
 H   -5.442728    2.036732    0.553516
 C   -5.197072   -0.046795   -0.138265
 C   -4.891780    1.458377   -0.201541
 H   -5.690574   -0.422785   -1.045848
 N   -3.856879   -0.633342    0.005499
 N   -3.448954    1.492093    0.061409
 H   -5.105744    1.895632   -1.189305
 H   -4.168207   -1.229079   -2.606573
 H   -2.997228    1.700739   -2.472762
 C   -3.350149   -1.953510   -2.482597
 C   -2.016724    2.179435   -2.341527
 H   -2.401680   -1.391872   -2.489470
 H   -1.249155    1.390415   -2.283695
 H   -3.359366   -2.634089   -3.344365
 H    2.543988   -0.214696    2.575835
 H    4.769661   -2.269795    0.727551
 C    5.115470   -1.254995    0.494539
 C    6.581005   -1.105541    0.401263
 C    7.214866    0.132813    0.199761
 H    6.919153   -3.219736    0.677120
 C    7.391037   -2.246176    0.518541
 C    8.601186    0.221529    0.113567
 H    9.070838    1.195408   -0.043285
 C    8.779977   -2.159723    0.431914
 C    9.392246   -0.924188    0.228012
 H    9.385697   -3.064279    0.523622
 H   10.479795   -0.850910    0.158490
 H   -3.714392   -2.630294    3.408967
 H   -4.679253   -1.385950    2.579590
 C   -3.736004   -1.952243    2.545893
 H   -2.918532   -1.223604    2.659726
 H   -3.334271   -4.627275    2.200232
 C   -3.592286   -2.713541    1.255268
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 C   -3.379762   -4.093211    1.246821
 H   -1.243596    0.780417    2.936262
 C   -3.633263   -2.041659    0.023759
 C   -2.894409    0.279713    0.135764
 C   -3.225353   -4.806000    0.052466
 C   -0.455290    0.499033    2.253504
Cu   -0.947355    0.016443    0.371864
 C   -3.448319   -2.715899   -1.190722
 C   -3.261835   -4.100667   -1.152352
 H   -0.753835   -2.982409   -0.104202
 H   -3.114004   -4.637851   -2.093500
 C   -0.006724   -3.278594   -0.857666
 O   -0.338979   -0.769185   -1.443739
 H    0.401548   -4.263917   -0.603376
 C    0.832985   -1.081894   -1.105230
 H   -0.507860   -3.325692   -1.834419
 O    1.093186   -2.389004   -0.879955
 C    1.898260   -0.193008   -0.825177
 H   -2.924338    3.511731    3.362689
 H   -4.410174    3.446368    2.397269
 C   -3.373267    3.077594    2.459276
 H   -3.428468    1.986304    2.583711
 H   -1.687448    5.185627    2.133159
 C   -2.591907    3.457972    1.229629
 C   -1.770068    4.584416    1.222862
 C   -2.669549    2.686509    0.057587
 C   -1.039334    4.954854    0.087136
 C    0.666880    0.267823    1.781001
 C   -1.963342    3.032080   -1.103531
 C   -1.153795    4.172560   -1.062276
 C    2.139173    0.218960    1.646952
 H    2.473018    1.267286    1.603596
 H   -0.588592    4.444693   -1.957556
 H    1.660936    3.824827   -0.898200
 H   -1.799200    2.781603   -3.234085
 H    3.418306    3.870227   -0.533784
 C    2.634735    3.353863   -1.102445
 O    2.651198    2.010211   -0.676490
 C    1.807469    1.147990   -1.331279
 C    2.712456   -0.533965    0.411179
 H    2.570220   -1.606366    0.594724
 O    1.117661    1.570314   -2.248160
 H    2.839642    3.441361   -2.179740
 C    4.195700   -0.299517    0.308420
 H    4.495387    0.723286    0.060734
 H    6.618107    1.043063    0.111617
 C   -0.142417    6.164922    0.120462
 C   -3.034097   -6.299872    0.072676
 H   -2.594655   -6.663110   -0.866657
 H   -3.999357   -6.813365    0.209304
 H   -2.380522   -6.607646    0.901704
 H    0.341200    6.334454   -0.851386
 H    0.648454    6.045565    0.877394
 H   -0.707932    7.072155    0.383217
41
Figure_S8-1_PPh3-Cu-allenyl / electronic energy: -2791.78064609 a.u. / lowest freq: -8.52 cm-1
Cu    1.925957    0.441034   -0.969324
 C    3.695423    0.782212   -1.650311
 H    3.901621    1.250294   -2.626132
 C    4.739409    0.464057   -0.934464
 C    5.764894    0.124180   -0.171645
 H    6.228054   -0.865398   -0.246897
 H    6.190086    0.825011    0.554818
 P   -0.093017    0.040978   -0.106258
 C   -0.713342    1.391986    0.957863
 C   -1.380331    1.168166    2.166791
 C   -0.511650    2.705927    0.513218
 C   -1.849259    2.247854    2.915852
 H   -1.535294    0.149778    2.529631
 C   -0.989950    3.780817    1.258089
 H    0.022539    2.889678   -0.423318
 C   -1.658731    3.552160    2.461671
 H   -2.365753    2.066564    3.860640
 H   -0.832329    4.800736    0.901689
 H   -2.027713    4.394962    3.049984
 C   -0.164393   -1.456811    0.937848
 C   -1.315396   -2.246691    1.042854
 C    0.979917   -1.802657    1.668371
 C   -1.322993   -3.362695    1.878346
 H   -2.210179   -1.992779    0.469631
 C    0.967011   -2.915256    2.507351
 H    1.889455   -1.202122    1.577400
 C   -0.184532   -3.695898    2.612619
 H   -2.223689   -3.975283    1.954422
 H    1.863220   -3.177711    3.073131
 H   -0.192646   -4.571265    3.265682
 C   -1.410845   -0.201190   -1.350523
 C   -2.710237    0.290159   -1.183020
 C   -1.089521   -0.925749   -2.506174
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 C   -3.679067    0.050420   -2.157376
 H   -2.969562    0.864064   -0.290291
 C   -2.061407   -1.169847   -3.473746
 H   -0.072030   -1.299724   -2.651497
 C   -3.357069   -0.680980   -3.300219
 H   -4.690190    0.439664   -2.021497
 H   -1.803574   -1.735870   -4.371205
 H   -4.117079   -0.866243   -4.062285
73
Figure_S8-1_PA-PPh3-ed(1,6) / electronic energy: -3633.73942416 a.u. / lowest freq: 9.87 cm-1
Cu    0.281127   -0.053503   -0.846773
 C    1.747391   -1.529250   -0.714753
 C    0.588836   -1.999669   -0.061364
 H    1.829657   -1.802584   -1.771198
 C    0.354197   -2.059542    1.408843
 C   -0.330828   -2.849508   -0.890855
 O    1.297654   -1.450834    2.127796
 O   -0.611159   -2.575542    1.922721
 O   -0.783960   -3.919929   -0.585523
 O   -0.577977   -2.256524   -2.069090
 C   -1.446301   -2.931626   -2.970623
 H   -1.072482   -3.941750   -3.186193
 H   -1.463328   -2.329014   -3.884459
 H   -2.456144   -2.999963   -2.541418
 C    1.128780   -1.461170    3.540320
 H    0.130316   -1.096654    3.813124
 H    1.898791   -0.793655    3.941403
 H    1.265534   -2.477818    3.934981
 C    2.975644   -1.008685   -0.134204
 H    2.994699   -0.824010    0.937799
 C    4.043126   -0.734499   -0.908877
 H    3.958501   -0.914167   -1.986156
 C    5.329075   -0.183872   -0.465301
 C    6.312127    0.097342   -1.427631
 C    5.618499    0.093866    0.882159
 C    7.540548    0.644594   -1.061819
 H    6.103793   -0.110187   -2.480445
 C    6.844840    0.637835    1.248002
 H    4.875942   -0.113132    1.655156
 C    7.811133    0.917413    0.278113
 H    8.288975    0.859668   -1.827509
 H    7.050019    0.847539    2.300061
 H    8.771785    1.347966    0.568665
 C    1.181260    1.180925   -2.096157
 H    0.783134    1.282091   -3.119083
 C    2.198582    1.929553   -1.782244
 C    3.231333    2.660663   -1.398166
 H    4.259098    2.302851   -1.522261
 H    3.092728    3.648631   -0.945463
 P   -1.778404    0.578573   -0.009958
 C   -3.138581   -0.558840   -0.463907
 C   -4.029872   -0.222041   -1.491377
 C   -3.219543   -1.829374    0.123235
 C   -4.994673   -1.135348   -1.914128
 H   -3.974848    0.758743   -1.968050
 C   -4.192331   -2.734640   -0.297046
 H   -2.510615   -2.129396    0.898656
 C   -5.082294   -2.391295   -1.314762
 H   -5.683842   -0.859482   -2.714981
 H   -4.243175   -3.720411    0.169216
 H   -5.840238   -3.104928   -1.644543
 C   -2.406943    2.227048   -0.501712
 C   -3.559876    2.760352    0.093635
 C   -1.733894    2.961667   -1.481188
 C   -4.036701    4.007177   -0.298070
 H   -4.088590    2.197203    0.867266
 C   -2.214590    4.213526   -1.871669
 H   -0.822358    2.560169   -1.928151
 C   -3.364492    4.734849   -1.284186
 H   -4.935343    4.416275    0.168252
 H   -1.681839    4.782276   -2.636636
 H   -3.740287    5.713899   -1.589671
 C   -1.751071    0.711623    1.815504
 C   -0.640075    1.373630    2.357923
 C   -2.764618    0.260964    2.666165
 C   -0.554820    1.598959    3.729062
 H    0.162880    1.721615    1.701128
 C   -2.667046    0.471611    4.041953
 H   -3.636680   -0.255642    2.260443
 C   -1.567675    1.143874    4.574476
 H    0.312566    2.119024    4.140417
 H   -3.460024    0.111725    4.700695
 H   -1.496606    1.310090    5.651383
73
Figure_S8-1_PA-PPh3-ts(1,6) / electronic energy: -3633.72277720 a.u. / lowest freq: -479.99 cm-1
Cu    0.198749   -0.236268   -0.925173
 C    1.749466   -1.599978   -0.430970
 C    0.588754   -1.994086    0.318775
 H    1.871922   -2.120579   -1.386937
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 C    0.404037   -1.821507    1.768486
 C   -0.323579   -2.962495   -0.335634
 O    1.433657   -1.202567    2.369883
 O   -0.568884   -2.177646    2.401963
 O   -0.899563   -3.896650    0.163170
 O   -0.469787   -2.657958   -1.649806
 C   -1.369692   -3.457994   -2.399270
 H   -1.089009   -4.519221   -2.349202
 H   -1.309646   -3.099107   -3.432499
 H   -2.394173   -3.339246   -2.016569
 C    1.341079   -1.039608    3.775320
 H    0.395855   -0.556018    4.054868
 H    2.188926   -0.409032    4.066392
 H    1.408575   -2.013033    4.282673
 C    2.811533   -0.754461   -0.073616
 H    2.767885   -0.213880    0.870706
 C    3.894421   -0.560689   -0.942301
 H    4.032021   -1.332866   -1.703710
 C    5.160858    0.055805   -0.473096
 C    6.378094   -0.357303   -1.032020
 C    5.185904    1.051609    0.515827
 C    7.586681    0.192652   -0.606226
 H    6.376836   -1.127071   -1.808343
 C    6.391647    1.602785    0.940475
 H    4.250392    1.410349    0.951153
 C    7.598668    1.174336    0.383483
 H    8.523691   -0.149889   -1.051028
 H    6.390162    2.376659    1.711313
 H    8.543190    1.608075    0.718851
 C    0.868564    0.694030   -2.598198
 H    0.042284    1.044823   -3.218624
 C    2.121484    0.839148   -2.698043
 C    3.472303    0.856223   -2.512279
 H    4.105545    0.335045   -3.235909
 H    3.909716    1.766571   -2.089430
 P   -1.765948    0.627807   -0.141156
 C   -3.110822   -0.590768   -0.356080
 C   -3.963397   -0.528133   -1.467265
 C   -3.193107   -1.687008    0.512354
 C   -4.905470   -1.531620   -1.686546
 H   -3.898390    0.307333   -2.167986
 C   -4.139884   -2.685325    0.289351
 H   -2.494798   -1.787833    1.347756
 C   -5.000810   -2.608732   -0.804544
 H   -5.568261   -1.470413   -2.552342
 H   -4.188505   -3.536397    0.971214
 H   -5.741320   -3.392843   -0.976700
 C   -2.416546    2.201755   -0.815496
 C   -3.732324    2.619499   -0.569437
 C   -1.548319    3.045371   -1.515942
 C   -4.175013    3.853657   -1.035935
 H   -4.416939    1.976659   -0.010682
 C   -1.993003    4.285270   -1.978811
 H   -0.516072    2.736391   -1.695677
 C   -3.305925    4.687420   -1.743909
 H   -5.202749    4.168809   -0.844121
 H   -1.308760    4.935905   -2.527150
 H   -3.656041    5.654844   -2.110628
 C   -1.665616    1.019437    1.644300
 C   -0.457639    1.566347    2.094510
 C   -2.737827    0.893232    2.533759
 C   -0.327593    1.996007    3.413446
 H    0.389074    1.658731    1.408093
 C   -2.598585    1.304976    3.857854
 H   -3.685017    0.465936    2.197223
 C   -1.397054    1.861483    4.298220
 H    0.617029    2.424515    3.754491
 H   -3.436092    1.194956    4.549832
 H   -1.292968    2.187083    5.335388
73
Figure_S8-1_PA-PPh3-prod(1,6) / electronic energy: -3633.765927300 a.u. / lowest freq: 12.35 cm-1
Cu   0.380581   -0.033322   -0.934002
 C    1.722035   -1.651233   -0.267801
 C    0.758340   -2.302529    0.577495
 H    1.912496   -2.212134   -1.189678
 C    0.468502   -1.910106    1.944347
 C    0.043786   -3.452469    0.036169
 O    1.281315   -0.918595    2.389753
 O   -0.405154   -2.353534    2.671051
 O   -0.609621   -4.279093    0.641526
 O    0.150269   -3.535241   -1.322793
 C   -0.511432   -4.621488   -1.935364
 H   -0.146549   -5.585804   -1.551308
 H   -0.300961   -4.545475   -3.008942
 H   -1.597721   -4.568301   -1.766108
 C    1.084511   -0.500781    3.725312
 H    0.029082   -0.266140    3.917810
 H    1.697647    0.397875    3.862546
 H    1.406361   -1.280274    4.433113
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 C    2.419020   -0.460760   -0.171625
 H    2.414616    0.112586    0.756736
 C    3.447047   -0.096191   -1.233516
 H    3.693466   -1.011006   -1.794585
 C    4.733583    0.433678   -0.629578
 C    5.950445   -0.219543   -0.847939
 C    4.729320    1.588224    0.164868
 C    7.133866    0.264717   -0.288459
 H    5.972143   -1.124249   -1.461584
 C    5.908266    2.075666    0.724609
 H    3.788986    2.112906    0.356822
 C    7.116802    1.414565    0.499214
 H    8.074041   -0.261324   -0.469000
 H    5.883808    2.976370    1.342342
 H    8.041445    1.795086    0.938645
 C    0.543639    0.073596   -3.273270
 H   -0.354332   -0.246818   -3.774943
 C    1.609210    0.463876   -2.827257
 C    2.890988    0.912802   -2.277362
 H    3.612399    1.053092   -3.098074
 H    2.741414    1.899275   -1.808749
 P   -1.590451    0.691422   -0.132096
 C   -2.886314   -0.572473   -0.398310
 C   -3.896905   -0.393138   -1.350853
 C   -2.781294   -1.799953    0.272419
 C   -4.795299   -1.425328   -1.622669
 H   -3.988598    0.553906   -1.886403
 C   -3.683173   -2.825318   -0.001825
 H   -2.002846   -1.972458    1.020499
 C   -4.690042   -2.642226   -0.950657
 H   -5.579839   -1.274950   -2.367459
 H   -3.579534   -3.775950    0.524036
 H   -5.393323   -3.449186   -1.167704
 C   -2.268644    2.216720   -0.883710
 C   -3.394159    2.847089   -0.334264
 C   -1.659625    2.763137   -2.017426
 C   -3.907661    3.999858   -0.920076
 H   -3.871859    2.434324    0.557894
 C   -2.175880    3.920538   -2.603571
 H   -0.774378    2.286181   -2.444535
 C   -3.299060    4.537403   -2.056972
 H   -4.785411    4.483903   -0.487182
 H   -1.694000    4.341295   -3.488399
 H   -3.702135    5.443400   -2.514561
 C   -1.610302    1.113478    1.649203
 C   -0.631348    2.018531    2.082268
 C   -2.571431    0.655514    2.553495
 C   -0.635356    2.485176    3.392938
 H    0.134999    2.368056    1.384240
 C   -2.561523    1.110957    3.873051
 H   -3.335625   -0.055390    2.234204
 C   -1.603062    2.031811    4.291392
 H    0.125644    3.197263    3.718435
 H   -3.313890    0.745982    4.575051
 H   -1.603232    2.391871    5.322367
73
Figure_S8-1_PA-PPh3-ed(1,4AA) / electronic energy: -3633.73998513 a.u. / lowest freq: 13.71 cm-1
Cu   0.292922   -0.071940   -0.703950
 C    1.771622   -1.519561   -0.625235
 C    0.659620   -1.944994    0.135255
 H    1.781977   -1.871104   -1.663031
 C    0.519576   -1.767996    1.608451
 C   -0.274684   -2.923126   -0.512045
 O    1.232688   -0.732024    2.063933
 O   -0.207431   -2.412977    2.325549
 O   -0.656747   -3.960664   -0.040039
 O   -0.638800   -2.492515   -1.729032
 C   -1.558466   -3.302307   -2.450277
 H   -1.155579   -4.313612   -2.598304
 H   -1.706180   -2.807923   -3.415887
 H   -2.512960   -3.366267   -1.907389
 C    1.088781   -0.417295    3.443753
 H    0.034369   -0.220284    3.682984
 H    1.685694    0.484997    3.610725
 H    1.456421   -1.242140    4.069729
 C    3.052969   -1.021547   -0.147416
 H    3.138046   -0.770362    0.908528
 C    4.089727   -0.847430   -0.988099
 H    3.942646   -1.085371   -2.047581
 C    5.420638   -0.334486   -0.640798
 C    6.371929   -0.169537   -1.659894
 C    5.786369    0.014946    0.671434
 C    7.643996    0.329336   -1.383936
 H    6.105630   -0.432872   -2.686926
 C    7.055260    0.511113    0.947811
 H    5.068980   -0.095218    1.486675
 C    7.990631    0.671561   -0.078014
 H    8.367309    0.450976   -2.193179
 H    7.318501    0.777216    1.973955
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 H     8.985546    1.064495    0.142059
 C     1.130899    1.451259   -1.622282
 H     0.687183    1.913707   -2.516722
 C     2.150738    2.053340   -1.080258
 C     3.187517    2.610615   -0.478063
 H     3.053800    3.360034    0.309780
 H     4.214257    2.339508   -0.746788
 P    -1.856790    0.500452   -0.077187
 C    -2.532005    1.865053   -1.085743
 C    -2.253482    1.871561   -2.457945
 C    -3.341211    2.868464   -0.540837
 C    -2.787134    2.863364   -3.278585
 H    -1.615371    1.094423   -2.886476
 C    -3.865483    3.865511   -1.361930
 H    -3.560769    2.874546    0.529464
 C    -3.591441    3.862565   -2.730015
 H    -2.568137    2.859991   -4.348267
 H    -4.492948    4.648239   -0.930632
 H    -4.003124    4.644878   -3.371261
 C    -1.794821    1.179669    1.617735
 C    -2.707312    0.865091    2.628939
 C    -0.744746    2.071822    1.885332
 C    -2.570152    1.436518    3.895212
 H    -3.528005    0.171698    2.434488
 C    -0.623074    2.652655    3.144057
 H    -0.016721    2.309100    1.103231
 C    -1.533675    2.332528    4.152693
 H    -3.283792    1.181941    4.681370
 H     0.193458    3.349946    3.342183
 H    -1.431645    2.780946    5.143197
 C    -3.182638   -0.761732   -0.106981
 C    -4.257484   -0.676245   -1.001346
 C    -3.066930   -1.893536    0.713197
 C    -5.196235   -1.704960   -1.075261
 H    -4.367967    0.194415   -1.650260
 C    -4.011839   -2.914304    0.641664
 H    -2.233658   -1.997528    1.411607
 C    -5.076697   -2.825721   -0.255052
 H    -6.026044   -1.626392   -1.780776
 H    -3.903049   -3.790276    1.283855
 H    -5.812993   -3.629961   -0.314415
73
Figure_S8-1_PA-PPh3-ts(1,4AA) / electronic energy: -3633.71057140 a.u. / lowest freq: -331.12 cm-1
Cu   -0.060758   -0.351513   -0.685955
 C    1.948711   -1.078823   -0.753740
 C    1.111078   -1.825647    0.210038
 H    2.172365   -1.707043   -1.617088
 C    0.949156   -1.426880    1.611178
 C    0.541622   -3.107630   -0.215073
 O    1.225976   -0.104853    1.786875
 O    0.570723   -2.106913    2.538919
 O    0.001699   -3.944107    0.476928
 O    0.639665   -3.278805   -1.559884
 C    0.099282   -4.477185   -2.083569
 H    0.598866   -5.358609   -1.656317
 H    0.267351   -4.441917   -3.165968
 H   -0.977923   -4.550431   -1.874554
 C    1.063731    0.410156    3.096276
 H    0.002434    0.406294    3.387569
 H    1.431310    1.441854    3.066641
 H    1.638642   -0.177696    3.825302
 C    3.141995   -0.330136   -0.290307
 H    2.983680    0.420456    0.483157
 C    4.363623   -0.581554   -0.779883
 H    4.470743   -1.354065   -1.550378
 C    5.617541    0.080237   -0.378389
 C    6.828754   -0.368767   -0.927286
 C    5.660637    1.150097    0.532565
 C    8.041971    0.222681   -0.578520
 H    6.816655   -1.197335   -1.640346
 C    6.870858    1.741261    0.881612
 H    4.736776    1.530957    0.972941
 C    8.068322    1.280512    0.328785
 H    8.970933   -0.146398   -1.018903
 H    6.880983    2.570589    1.592468
 H    9.016488    1.747365    0.603981
 C    1.233107    0.360787   -2.059009
 H    1.225046   -0.072780   -3.065247
 C    1.473138    1.628108   -1.869594
 C    1.758373    2.882105   -1.594225
 H    0.974981    3.643752   -1.527878
 H    2.796359    3.198381   -1.446792
 P   -2.103989    0.363645   -0.157475
 C   -2.923582    1.422403   -1.397135
 C   -2.647020    1.187286   -2.749281
 C   -3.810382    2.446272   -1.040545
 C   -3.266973    1.952959   -3.735356
 H   -1.934775    0.407367   -3.031882
 C   -4.424990    3.213404   -2.028300
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 H   -4.017723    2.648349    0.013268
 C   -4.156387    2.965197   -3.375111
 H   -3.047897    1.764186   -4.788171
 H   -5.115963    4.009762   -1.744506
 H   -4.637631    3.569037   -4.147435
 C   -1.964208    1.430194    1.321732
 C   -2.715501    1.232024    2.483238
 C   -1.026280    2.471610    1.272941
 C   -2.535204    2.073932    3.582600
 H   -3.442264    0.418692    2.537372
 C   -0.859423    3.316248    2.365565
 H   -0.413941    2.617687    0.378434
 C   -1.612997    3.116973    3.524158
 H   -3.121111    1.910679    4.489354
 H   -0.127093    4.124782    2.318492
 H   -1.475593    3.774221    4.385326
 C   -3.317053   -0.924484    0.288970
 C   -4.692018   -0.780648    0.068213
 C   -2.830378   -2.091514    0.893694
 C   -5.570803   -1.790853    0.456599
 H   -5.082836    0.119493   -0.410934
 C   -3.713898   -3.096056    1.284117
 H   -1.760360   -2.230081    1.067406
 C   -5.083546   -2.947611    1.065818
 H   -6.641852   -1.672441    0.280189
 H   -3.322113   -4.000918    1.752444
 H   -5.774756   -3.737527    1.367515
73
Figure_S8-1_PA-PPh3-prod(1,4AA) / electronic energy: -3633.75762400 a.u. / lowest freq: 9.15 cm-1
Cu   -0.328106    0.746986    0.828306
 C    2.133387    1.571345    1.011669
 C    1.156139    1.920957   -0.151987
 H    2.681108    2.489291    1.264505
 C    1.149075    1.201104   -1.424216
 C    0.606846    3.271711   -0.154731
 O    1.556070   -0.092184   -1.285143
 O    0.798032    1.611597   -2.512247
 O   -0.126523    3.786713   -0.979138
 O    0.962073    3.965342    0.965190
 C    0.399619    5.252938    1.113332
 H    0.687826    5.914470    0.283492
 H    0.788437    5.653242    2.057210
 H   -0.698989    5.205590    1.153308
 C    1.652766   -0.854103   -2.470889
 H    0.665297   -0.994627   -2.935506
 H    2.060863   -1.828627   -2.178731
 H    2.321756   -0.372486   -3.198994
 C    3.147500    0.494457    0.752679
 H    2.783190   -0.535388    0.768502
 C    4.442598    0.738083    0.523306
 H    4.798770    1.775139    0.544191
 C    5.467274   -0.285165    0.240255
 C    6.825804    0.031025    0.395871
 C    5.135041   -1.579815   -0.193842
 C    7.818211   -0.917002    0.151601
 H    7.105497    1.037356    0.719303
 C    6.125010   -2.527653   -0.438042
 H    4.087736   -1.840890   -0.360886
 C    7.471833   -2.202743   -0.262987
 H    8.868920   -0.649702    0.285450
 H    5.844386   -3.527279   -0.778200
 H    8.247148   -2.946776   -0.458402
 C    1.242950    1.244467    2.221601
 H    0.855208    2.116356    2.764369
 C    0.856887    0.035056    2.628376
 C    0.635796   -1.130533    3.190538
 H   -0.213228   -1.761876    2.913476
 H    1.309009   -1.497836    3.972687
 P   -2.086669   -0.420265    0.115175
 C   -3.081471   -1.283739    1.381264
 C   -3.186601   -0.692434    2.646639
 C   -3.737521   -2.495151    1.130310
 C   -3.953215   -1.294100    3.642719
 H   -2.657433    0.241583    2.856118
 C   -4.497620   -3.098932    2.130901
 H   -3.649805   -2.973854    0.152010
 C   -4.609035   -2.498285    3.385225
 H   -4.031479   -0.825041    4.625512
 H   -5.003685   -4.045402    1.930060
 H   -5.203382   -2.974559    4.167864
 C   -1.571429   -1.749892   -1.028949
 C   -2.099932   -1.889510   -2.315016
 C   -0.592483   -2.648638   -0.582645
 C   -1.661794   -2.925287   -3.142350
 H   -2.853753   -1.187560   -2.677481
 C   -0.167328   -3.687155   -1.404940
 H   -0.151900   -2.532309    0.411327
 C   -0.701754   -3.826779   -2.687522
 H   -2.078411   -3.026823   -4.146491
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 H    0.592955   -4.385142   -1.048479
 H   -0.361982   -4.636787   -3.336295
 C   -3.262350    0.605138   -0.831107
 C   -4.623284    0.293246   -0.941872
 C   -2.751429    1.736485   -1.481686
 C   -5.463271    1.101444   -1.705673
 H   -5.032403   -0.581153   -0.430491
 C   -3.596677    2.537605   -2.248014
 H   -1.694897    2.009711   -1.395329
 C   -4.950265    2.222264   -2.360781
 H   -6.524148    0.856291   -1.788541
 H   -3.189592    3.417618   -2.749523
 H   -5.610788    2.854665   -2.958078
73
Figure_S8-1_PA-PPh3-ed(1,4) / electronic energy: -3633.73304715 a.u. / lowest freq: 9.83 cm-1
Cu   1.216847   -0.846142    1.178089
 C   -3.520908    0.996171    0.031632
 C   -2.272892    0.470946    0.079803
 H   -3.593024    2.084698    0.110145
 C   -1.970630   -0.986758   -0.062205
 C   -1.087404    1.346865    0.249682
 O   -2.770238   -1.751449    0.671388
 O   -1.103528   -1.430186   -0.777015
 O    0.051328    0.946351    0.378039
 O   -1.376038    2.641451    0.261720
 C   -0.285042    3.533714    0.470471
 H    0.158356    3.373927    1.462993
 H   -0.703085    4.542748    0.397286
 H    0.494514    3.382590   -0.289659
 C   -2.498264   -3.147774    0.666935
 H   -2.557444   -3.556015   -0.351270
 H   -3.259156   -3.605788    1.307067
 H   -1.495668   -3.325776    1.080473
 C   -4.769014    0.285351   -0.133825
 H   -4.732808   -0.801463   -0.221143
 C   -5.946720    0.943879   -0.167667
 H   -5.928566    2.034530   -0.060316
 C   -7.279488    0.353312   -0.332263
 C   -8.401195    1.198512   -0.317526
 C   -7.485330   -1.026980   -0.506066
 C   -9.687352    0.685375   -0.470249
 H   -8.258602    2.273597   -0.182155
 C   -8.768905   -1.538937   -0.659221
 H   -6.635677   -1.712180   -0.523412
 C   -9.874961   -0.685292   -0.642068
 H  -10.546006    1.359878   -0.455514
 H   -8.910407   -2.613154   -0.794566
 H  -10.881332   -1.091702   -0.763354
 C    0.190479   -1.608257    2.652621
 H    0.393294   -2.563670    3.161730
 C   -0.826447   -0.922208    3.094514
 C   -1.854601   -0.177922    3.474604
 H   -1.754827    0.584648    4.254481
 H   -2.838514   -0.310934    3.012655
 P    2.983611   -0.244506   -0.068752
 C    4.610869   -0.839005    0.520204
 C    5.801450   -0.126396    0.327588
 C    4.648008   -2.070043    1.186329
 C    7.011990   -0.648541    0.780671
 H    5.782875    0.844559   -0.173784
 C    5.859928   -2.593727    1.633471
 H    3.714871   -2.611457    1.365523
 C    7.043108   -1.883502    1.430125
 H    7.936435   -0.087611    0.627775
 H    5.878318   -3.554840    2.151424
 H    7.992134   -2.289746    1.786925
 C    3.171951    1.580338   -0.080173
 C    3.236670    2.340804   -1.250897
 C    3.196521    2.231298    1.161126
 C    3.333460    3.732526   -1.180935
 H    3.208498    1.850799   -2.226320
 C    3.304185    3.617083    1.229589
 H    3.126222    1.649342    2.084516
 C    3.370876    4.372100    0.056351
 H    3.381992    4.316535   -2.102596
 H    3.327170    4.112041    2.202733
 H    3.449926    5.460114    0.109514
 C    2.932820   -0.694341   -1.841952
 C    4.079867   -0.903930   -2.617110
 C    1.667850   -0.798021   -2.435898
 C    3.962946   -1.199909   -3.974447
 H    5.070759   -0.838591   -2.162463
 C    1.556770   -1.087562   -3.795483
 H    0.765299   -0.669331   -1.831849
 C    2.702233   -1.287455   -4.566103
 H    4.862431   -1.364605   -4.571540
 H    0.567679   -1.168576   -4.251517
 H    2.612442   -1.518472   -5.629910
73
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Figure_S8-1_PA-PPh3-ts(1,4) / electronic energy: -3633.70950892 a.u. / lowest freq: -429.98 cm-1
Cu     0.553150   -0.020871   -0.228599
 C    -3.272739   -0.937299   -0.059909
 C    -2.084270   -0.725732    0.667208
 H    -3.448463   -1.986999   -0.299887
 C    -1.564989    0.592937    0.997294
 C    -1.177993   -1.861902    0.840900
 O    -2.354236    1.601812    0.602133
 O    -0.497917    0.834534    1.568585
 O     0.027571   -1.798351    1.063222
 O    -1.775148   -3.050686    0.707987
 C    -0.938960   -4.197147    0.743871
 H    -0.166388   -4.143564   -0.036190
 H    -1.594908   -5.056204    0.566631
 H    -0.447712   -4.294010    1.721832
 C    -1.852558    2.914628    0.787539
 H    -1.676840    3.126643    1.851151
 H    -2.616452    3.591394    0.389447
 H    -0.908657    3.048142    0.238697
 C    -4.505864   -0.156829    0.045175
 H    -4.421737    0.871522    0.394822
 C    -5.703943   -0.694631   -0.249414
 H    -5.733610   -1.728917   -0.612847
 C    -7.012993   -0.034003   -0.139737
 C    -8.161476   -0.726524   -0.556909
 C    -7.172916    1.267253    0.369358
 C    -9.424270   -0.142775   -0.474750
 H    -8.058031   -1.739424   -0.955028
 C    -8.433182    1.850000    0.453125
 H    -6.302612    1.831674    0.710013
 C    -9.565499    1.148579    0.031261
 H   -10.302655   -0.700597   -0.806910
 H    -8.535543    2.860444    0.855229
 H   -10.553485    1.608791    0.100220
 C    -0.289689    0.046288   -2.080282
 H     0.465779    0.296943   -2.830825
 C    -1.523554   -0.186112   -2.268724
 C    -2.856598   -0.460194   -2.224379
 H    -3.208638   -1.427481   -2.596028
 H    -3.558396    0.371779   -2.327657
 P     2.794168    0.211327   -0.074117
 C     3.587553    0.894249   -1.576060
 C     4.767881    0.382603   -2.126124
 C     2.957509    1.983061   -2.195040
 C     5.315637    0.959554   -3.272420
 H     5.263296   -0.472459   -1.660870
 C     3.511358    2.564118   -3.333516
 H     2.022910    2.374932   -1.783028
 C     4.691630    2.051383   -3.874656
 H     6.235342    0.551240   -3.696809
 H     3.015332    3.414820   -3.805501
 H     5.122377    2.501147   -4.771799
 C     3.620777   -1.402620    0.176547
 C     4.794667   -1.557949    0.922293
 C     3.033031   -2.525884   -0.420637
 C     5.378673   -2.817339    1.057610
 H     5.256285   -0.692775    1.403745
 C     3.621314   -3.781727   -0.289828
 H     2.101266   -2.416229   -0.981915
 C     4.795448   -3.928931    0.449824
 H     6.294768   -2.929437    1.641369
 H     3.155584   -4.650921   -0.759117
 H     5.253807   -4.914254    0.559081
 C     3.424954    1.262744    1.282410
 C     4.606769    2.008582    1.195282
 C     2.672915    1.291711    2.464589
 C     5.040033    2.761759    2.285959
 H     5.191962    2.003513    0.272358
 C     3.114165    2.039904    3.554692
 H     1.729938    0.741610    2.519597
 C     4.297516    2.773830    3.467289
 H     5.963194    3.340649    2.212196
 H     2.525155    2.057191    4.474228
 H     4.639079    3.364213    4.320461
73
Figure_S8-1_PA-PPh3-prod(1,4) / electronic energy: -3633.77054729 a.u. / lowest freq: 12.47 cm-1
Cu     0.938058    0.045923   -1.169917
 C    -3.204642    0.129519    0.977202
 C    -2.090513    0.104502   -0.059086
 H    -3.283250    1.169922    1.314879
 C    -1.569802   -1.120825   -0.549202
 C    -1.506614    1.327093   -0.482179
 O    -2.295885   -2.202340   -0.200855
 O    -0.546329   -1.314239   -1.242076
 O    -0.473449    1.489539   -1.171331
 O    -2.160457    2.433051   -0.077853
 C    -1.580946    3.685967   -0.383152
 H    -0.602108    3.803398    0.106008
 H    -2.275562    4.442122    0.000612
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 H   -1.449926    3.816306   -1.466407
 C   -1.777532   -3.476038   -0.531825
 H   -1.656920   -3.591623   -1.617929
 H   -2.505608   -4.205777   -0.159283
 H   -0.803978   -3.644818   -0.048236
 C   -4.547370   -0.260085    0.416073
 H   -4.603170   -1.262291   -0.022381
 C   -5.616645    0.546452    0.418310
 H   -5.509546    1.541085    0.868458
 C   -6.953531    0.256294   -0.134887
 C   -7.966512    1.219692   -0.006646
 C   -7.267971   -0.944966   -0.793741
 C   -9.245786    0.996907   -0.514363
 H   -7.743731    2.162469    0.500412
 C   -8.544397   -1.169502   -1.301127
 H   -6.503781   -1.715499   -0.915762
 C   -9.540964   -0.200178   -1.164754
 H  -10.015123    1.764409   -0.402081
 H   -8.763923   -2.110761   -1.810443
 H  -10.540752   -0.377954   -1.566911
 C   -0.365120   -0.357490    3.082301
 H    0.661941   -0.238301    3.381646
 C   -1.512065   -0.514496    2.726392
 C   -2.879945   -0.712184    2.244164
 H   -3.596579   -0.446898    3.038044
 H   -3.023314   -1.781742    2.031145
 P    2.965343    0.022589   -0.371393
 C    2.888281   -0.928025    1.194525
 C    3.498444   -0.515589    2.383660
 C    2.153803   -2.122487    1.175697
 C    3.388064   -1.297432    3.535063
 H    4.058491    0.421291    2.418882
 C    2.057528   -2.907287    2.321592
 H    1.637011   -2.427056    0.261125
 C    2.674759   -2.495404    3.503617
 H    3.863625   -0.966328    4.460574
 H    1.483499   -3.835819    2.296380
 H    2.589523   -3.103955    4.406325
 C    3.596219    1.670552    0.112068
 C    4.954670    1.938943    0.319953
 C    2.653748    2.689412    0.301513
 C    5.361561    3.207678    0.730178
 H    5.700609    1.156354    0.160225
 C    3.063399    3.955326    0.717140
 H    1.595526    2.491252    0.107057
 C    4.416698    4.214503    0.933572
 H    6.422396    3.410659    0.890834
 H    2.321960    4.743808    0.863405
 H    4.738641    5.207651    1.254544
 C    4.342130   -0.735986   -1.303767
 C    5.324046   -1.531856   -0.703051
 C    4.407301   -0.481692   -2.680032
 C    6.364736   -2.056088   -1.469817
 H    5.276727   -1.746348    0.367199
 C    5.451575   -1.000472   -3.442027
 H    3.632460    0.124264   -3.158121
 C    6.431655   -1.788693   -2.836890
 H    7.126634   -2.677826   -0.995041
 H    5.496534   -0.796208   -4.513735
 H    7.247235   -2.200858   -3.434873
24
Figure_S9-1_Me2NHC-Cu-allenyl / electronic energy: -2062.03073671 a.u. / lowest freq: 16.19 cm-1
 C    2.918206    1.315894    0.091326
 H    3.172197    1.838768    1.027814
 C    3.315499   -0.166410    0.114484
 H    3.900547   -0.463518   -0.771327
 C    0.986753    0.001938   -0.023023
Cu   -0.888943   -0.488741   -0.126170
 N    1.467261    1.248504   -0.070934
 N    2.017665   -0.838526    0.111392
 H    3.894306   -0.441143    1.009295
 H    3.378330    1.869933   -0.740626
 C   -2.762590   -0.927759   -0.229714
 H   -3.145854   -1.915697   -0.535398
 C   -3.673890   -0.041198    0.066597
 C   -4.559952    0.891767    0.375842
 H   -4.957585    1.574386   -0.383123
 H   -4.930838    1.010617    1.399723
 C    0.676712    2.451280   -0.144453
 H   -0.378542    2.179900   -0.275011
 H    0.779042    3.047038    0.777227
 H    0.992071    3.072048   -0.997685
 C    1.929271   -2.276075    0.147590
 H    2.401143   -2.673321    1.059948
 H    0.871323   -2.567362    0.139575
 H    2.428683   -2.724632   -0.726592
56
Figure_S9-1_PA-Me2NHC-ed(1,6) / electronic energy: -2903.98097792 a.u. / lowest freq: 19.51 cm-1
 C   -4.384922   -1.833221    0.636783
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 H   -4.634841   -1.919709   -0.434322
 C   -3.396733   -2.910945    1.085904
 H   -3.620704   -3.300003    2.094154
 C   -2.315108   -0.845625    1.021657
Cu   -0.754442    0.400416    0.861053
 N   -3.617773   -0.607663    0.857217
 N   -2.136199   -2.169597    1.104980
 C    0.458577    1.102813   -0.669229
 C   -0.825033    0.799053   -1.182082
 H   -3.345735   -3.764056    0.394266
 H   -5.319672   -1.831842    1.214585
 H    0.629788    2.161898   -0.456390
 C   -1.282062   -0.482972   -1.782620
 C   -1.748429    1.959468   -1.383138
 O   -0.331398   -1.426356   -1.807512
 O   -2.408721   -0.701012   -2.161206
 O   -2.496581    2.122085   -2.312535
 O   -1.631377    2.852968   -0.386812
 C   -2.395555    4.044603   -0.500390
 H   -2.153759    4.575544   -1.431465
 H   -2.131647    4.659261    0.366416
 H   -3.471313    3.817839   -0.489057
 C   -0.737671   -2.717016   -2.235770
 H   -1.549397   -3.095191   -1.597533
 H    0.145090   -3.359466   -2.148304
 H   -1.087121   -2.693518   -3.277124
 C    1.665843    0.292477   -0.691683
 H    1.560309   -0.775100   -0.878865
 C    2.876382    0.842661   -0.466763
 H    2.933432    1.922101   -0.299843
 C    4.161125    0.132326   -0.413819
 C    5.328890    0.864632   -0.142998
 C    4.281125   -1.254307   -0.613340
 C    6.571658    0.239466   -0.071457
 H    5.253546    1.942951    0.019716
 C    5.522243   -1.879393   -0.544270
 H    3.394247   -1.854979   -0.825154
 C    6.673665   -1.136738   -0.272331
 H    7.465299    0.829591    0.143556
 H    5.593945   -2.957719   -0.703045
 H    7.645849   -1.631020   -0.216002
 C    0.277032    0.715208    2.515883
 H   -0.177368    0.372549    3.458611
 C    1.438197    1.294250    2.594390
 C    2.630056    1.867868    2.597096
 H    2.744436    2.952595    2.693779
 H    3.543595    1.270274    2.508963
 C   -0.896335   -2.826193    1.439286
 H   -0.966288   -3.314241    2.425237
 H   -0.645738   -3.592509    0.689815
 H   -0.091466   -2.080819    1.472981
 C   -4.178084    0.676200    0.515223
 H   -3.498587    1.465849    0.859017
 H   -4.313528    0.770007   -0.574744
 H   -5.150326    0.809319    1.011360
56
Figure_S9-1_PA-Me2NHC-ts(1,6) / electronic energy: -2903.96575719 a.u. / lowest freq: -471.62 cm-1
 C   -4.301112    2.032828   -0.371878
 H   -4.571488    1.961864    0.695532
 C   -3.288722    3.148626   -0.639327
 H   -3.490986    3.685300   -1.582436
 C   -2.239770    1.079936   -0.874459
Cu   -0.760725   -0.252397   -0.886773
 N   -3.548263    0.840817   -0.761811
 N   -2.039399    2.397064   -0.751014
 C    0.452714   -1.302516    0.502281
 C   -0.843682   -1.107458    1.090820
 H   -3.236749    3.890062    0.170703
 H   -5.225239    2.134476   -0.957761
 H    0.595381   -2.302888    0.082396
 C   -1.273573    0.054490    1.882644
 C   -1.782786   -2.249062    1.041641
 O   -0.308955    0.991991    2.005414
 O   -2.378969    0.236835    2.347080
 O   -2.654468   -2.517759    1.834224
 O   -1.571676   -3.019660   -0.053244
 C   -2.369748   -4.183342   -0.173806
 H   -2.233009   -4.848748    0.690658
 H   -2.041150   -4.686951   -1.089626
 H   -3.435573   -3.923518   -0.251563
 C   -0.687268    2.202882    2.631758
 H   -1.534403    2.667664    2.105615
 H    0.189645    2.858973    2.586407
 H   -0.974869    2.035658    3.679480
 C    1.602817   -0.494489    0.508312
 H    1.556658    0.499294    0.950224
 C    2.780564   -0.934008   -0.111858
 H    2.860946   -2.013343   -0.266441
 C    4.081394   -0.263187    0.134830
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 C    5.262746   -1.017886    0.122834
 C    4.177701    1.117971    0.368059
 C    6.501064   -0.418052    0.349020
 H    5.207333   -2.093988   -0.062594
 C    5.413377    1.718392    0.592760
 H    3.275313    1.733931    0.358727
 C    6.582009    0.953416    0.585937
 H    7.408041   -1.027069    0.339879
 H    5.467285    2.794965    0.770473
 H    7.550574    1.426776    0.760668
 C    0.185865   -0.329639   -2.673419
 H   -0.508009   -0.140783   -3.492916
 C    1.435581   -0.518562   -2.627011
 C    2.740753   -0.662004   -2.255467
 H    3.253117   -1.600302   -2.488872
 H    3.370473    0.231354   -2.311395
 C   -0.780147    3.070632   -0.945376
 H   -0.791802    3.674418   -1.868013
 H   -0.562730    3.737046   -0.096530
 H    0.017585    2.321229   -1.023908
 C   -4.125134   -0.472054   -0.600064
 H   -3.443960   -1.217090   -1.030870
 H   -4.273472   -0.706182    0.466258
 H   -5.089587   -0.530538   -1.125066
56
Figure_S9-1_PA-Me2NHC-prod(1,6) / electronic energy: -2904.01565681 a.u. / lowest freq: 26.64 cm-1
 C    4.371510   -0.111585    0.084988
 H    4.286227    0.682804    0.845097
 C    4.279979   -1.509608    0.698378
 H    4.983362   -2.225255    0.237684
 C    2.327692   -1.062877   -0.504951
Cu    0.429279   -1.229565   -1.024010
 N    3.183831   -0.076114   -0.769086
 N    2.902625   -1.884630    0.386285
 C   -0.528954    0.936944   -0.157397
 C    0.497628    1.602406    0.580246
 H    4.454641   -1.513205    1.784302
 H    5.289475    0.047534   -0.498020
 H   -0.837213    1.513492   -1.036173
 C    1.185447    1.020309    1.716635
 C    0.972356    2.888037    0.093204
 O    0.628405   -0.160892    2.106127
 O    2.170869    1.438129    2.299742
 O    1.820850    3.608486    0.586299
 O    0.363511    3.273521   -1.068856
 C    0.773567    4.510704   -1.607237
 H    0.585703    5.337438   -0.905934
 H    0.187524    4.660953   -2.522037
 H    1.846789    4.507482   -1.852570
 C    1.253526   -0.819427    3.183828
 H    2.316980   -1.007583    2.974810
 H    0.725629   -1.772181    3.313891
 H    1.186296   -0.229904    4.110676
 C   -1.225788   -0.249657   -0.002683
 H   -1.137404   -0.812557    0.930623
 C   -2.456596   -0.528764   -0.856109
 H   -2.403067    0.119456   -1.745797
 C   -3.755980   -0.212966   -0.135274
 C   -4.654300    0.725267   -0.653044
 C   -4.078312   -0.848095    1.071869
 C   -5.843985    1.023505    0.013960
 H   -4.418363    1.232924   -1.592373
 C   -5.264618   -0.555090    1.740307
 H   -3.387898   -1.578360    1.503117
 C   -6.153552    0.383370    1.212653
 H   -6.531456    1.761435   -0.406075
 H   -5.495425   -1.059042    2.681668
 H   -7.083606    0.615250    1.736302
 C   -0.067275   -2.725793   -2.413815
 H    0.690820   -3.232849   -2.989905
 C   -1.117478   -2.324599   -1.909019
 C   -2.441626   -1.986832   -1.361402
 H   -3.223686   -2.164619   -2.116075
 H   -2.639817   -2.678016   -0.525564
 C    2.369352   -3.150503    0.817441
 H    2.890919   -3.993151    0.331973
 H    2.474759   -3.261221    1.906981
 H    1.302961   -3.203375    0.563303
 C    2.949860    1.048950   -1.638257
 H    1.917888    1.018441   -2.007548
 H    3.096010    1.988731   -1.084909
 H    3.643872    1.031831   -2.493951
56
Figure_S9-1_PA-Me2NHC-ed(1,4AA) / electronic energy: -2903.98119581 a.u. / lowest freq: 16.11 cm-1
 C    4.856147   -1.465620   -0.651853
 H    5.573297   -0.962199    0.015518
 C    4.154017   -2.653199    0.021097
 H    4.253731   -3.589199   -0.551504
 C    2.562154   -1.031587   -0.527288
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Cu    0.793073   -0.132239   -0.717347
 N    3.738769   -0.574239   -0.959522
 N    2.757308   -2.220900    0.046320
 C   -0.486121    1.289706    0.011878
 C    0.684838    1.249451    0.809576
 H    4.519578   -2.841718    1.042121
 H    5.390193   -1.748273   -1.572189
 H   -0.493349    2.054192   -0.769157
 C    0.725058    0.542934    2.125258
 C    1.795033    2.211981    0.568488
 O    0.165171   -0.675329    2.054104
 O    1.176026    0.986827    3.149264
 O    2.843655    2.233745    1.166762
 O    1.523996    3.059368   -0.436024
 C    2.515844    4.026653   -0.743131
 H    2.736302    4.650394    0.134278
 H    2.102673    4.641835   -1.549329
 H    3.445785    3.546199   -1.077593
 C    0.067045   -1.407504    3.267307
 H    1.064115   -1.592408    3.690669
 H   -0.418679   -2.355574    3.013266
 H   -0.536216   -0.858797    4.004113
 C   -1.792237    0.743205    0.353527
 H   -1.851406    0.066205    1.206673
 C   -2.888894    1.018132   -0.376367
 H   -2.777083    1.671028   -1.249085
 C   -4.247457    0.510401   -0.144194
 C   -5.256849    0.825061   -1.068109
 C   -4.587811   -0.289962    0.960381
 C   -6.557356    0.351140   -0.904061
 H   -5.011883    1.447014   -1.933235
 C   -5.885530   -0.761538    1.126303
 H   -3.830000   -0.551010    1.701570
 C   -6.877331   -0.445486    0.194225
 H   -7.323918    0.606475   -1.638977
 H   -6.128202   -1.382536    1.991658
 H   -7.894860   -0.819505    0.326653
 C   -0.177108   -0.829795   -2.285469
 H    0.353735   -0.859807   -3.250321
 C   -1.350375   -1.391122   -2.240446
 C   -2.541972   -1.954975   -2.132611
 H   -2.651630   -3.010520   -1.860507
 H   -3.461530   -1.386442   -2.307466
 C    1.726988   -3.092007    0.551196
 H    1.727910   -4.048741    0.004433
 H    1.881333   -3.303186    1.621223
 H    0.751548   -2.608928    0.420733
 C    3.961237    0.681067   -1.627671
 H    2.994340    1.168329   -1.808139
 H    4.587128    1.347795   -1.013705
 H    4.458719    0.521764   -2.597299
56
Figure_S9-1_PA-Me2NHC-ts(1,4AA) / electronic energy: -2903.95210289 a.u. / lowest freq: -325.50 cm-1
 C    5.425295   -0.608934   -0.552769
 H    6.085128   -0.057864    0.133764
 C    4.971887   -1.963554    0.010437
 H    5.348854   -2.817659   -0.571784
 C    3.091096   -0.665496   -0.473290
Cu    1.228920   -0.113434   -0.549382
 N    4.157248    0.096826   -0.727809
 N    3.516414   -1.871577   -0.086734
 C   -0.680896    0.787748   -0.389389
 C    0.170190    1.111215    0.778437
 H    5.273763   -2.109355    1.060518
 H    5.945224   -0.704444   -1.520014
 H   -0.726614    1.640430   -1.070033
 C    0.197821    0.257733    1.966790
 C    0.899896    2.374724    0.817171
 O   -0.110434   -1.032915    1.634953
 O    0.480555    0.549687    3.105881
 O    1.495745    2.858742    1.755744
 O    0.883936    3.007930   -0.391889
 C    1.554763    4.250702   -0.457020
 H    1.144289    4.964657    0.271821
 H    1.404705    4.629734   -1.474599
 H    2.630637    4.132803   -0.258898
 C   -0.141550   -1.975363    2.688462
 H    0.840883   -2.056718    3.176175
 H   -0.411729   -2.934980    2.232460
 H   -0.887776   -1.698188    3.447188
 C   -2.023986    0.202859   -0.147019
 H   -2.052065   -0.715796    0.439798
 C   -3.147971    0.779282   -0.593057
 H   -3.068996    1.710821   -1.165622
 C   -4.520513    0.286011   -0.379247
 C   -5.603487    1.088858   -0.770330
 C   -4.801293   -0.963664    0.200239
 C   -6.919325    0.668303   -0.582313
 H   -5.408055    2.062372   -1.227893
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 C   -6.114139   -1.384507    0.389085
 H   -3.984450   -1.622329    0.502688
 C   -7.180821   -0.570626    0.000491
 H   -7.743884    1.313754   -0.893407
 H   -6.307530   -2.359541    0.842116
 H   -8.210113   -0.904057    0.149408
 C   -0.208669   -0.504237   -1.911439
 H   -0.241555    0.045321   -2.858301
 C   -0.555043   -1.759353   -1.844040
 C   -0.939213   -3.007527   -1.682577
 H   -0.230331   -3.838038   -1.759355
 H   -1.989309   -3.246539   -1.482679
 C    2.671478   -2.953141    0.351826
 H    2.908456   -3.877726   -0.197323
 H    2.803502   -3.144969    1.429429
 H    1.621788   -2.690357    0.166955
 C    4.119515    1.459508   -1.192559
 H    3.073177    1.782844   -1.268369
 H    4.646271    2.126141   -0.491518
 H    4.592777    1.551717   -2.183482
56
Figure_S9-1_PA-Me2NHC-prod(1,4AA) / electronic energy: -2904.00315785 a.u. / lowest freq: 12.12 cm-1
 C    6.114348    0.218837   -0.632728
 H    6.803252    0.459290    0.192843
 C    5.744038   -1.270658   -0.682289
 H    5.898485   -1.714713   -1.678914
 C    3.826382   -0.016348   -0.234672
Cu    1.961130    0.367679    0.102378
 N    4.817972    0.858524   -0.410411
 N    4.319372   -1.251568   -0.354436
 C   -0.755915   -0.060988   -0.800015
 C   -0.016849    0.553051    0.419420
 H    6.302926   -1.875719    0.047201
 H    6.569047    0.579006   -1.567704
 H   -0.767328    0.737590   -1.551249
 C   -0.031850   -0.213863    1.686379
 C   -0.136115    2.018838    0.580225
 O   -0.288923   -1.527984    1.464325
 O    0.173753    0.185182    2.813854
 O    0.191770    2.690230    1.536440
 O   -0.645022    2.618826   -0.526861
 C   -0.736196    4.028508   -0.494118
 H   -1.398451    4.366677    0.316026
 H   -1.150974    4.332726   -1.462338
 H    0.252002    4.490487   -0.349777
 C   -0.280489   -2.377143    2.592123
 H    0.705052   -2.381302    3.081669
 H   -0.513207   -3.381939    2.219972
 H   -1.033893   -2.069736    3.332093
 C   -2.187955   -0.411244   -0.490800
 H   -2.338458   -1.326081    0.089789
 C   -3.229534    0.349923   -0.849145
 H   -3.027746    1.269655   -1.410320
 C   -4.652659    0.096048   -0.552880
 C   -5.611950    1.033241   -0.967435
 C   -5.102789   -1.049409    0.126456
 C   -6.969376    0.839722   -0.714502
 H   -5.283382    1.931527   -1.497248
 C   -6.457133   -1.244766    0.379675
 H   -4.385434   -1.801785    0.460450
 C   -7.398735   -0.301633   -0.039173
 H   -7.694961    1.585361   -1.047576
 H   -6.782910   -2.143599    0.908431
 H   -8.461139   -0.458472    0.159738
 C    0.010530   -1.200728   -1.451097
 H    0.931637   -0.910526   -1.975896
 C   -0.318094   -2.467771   -1.460930
 C   -0.639765   -3.737044   -1.456314
 H   -0.288167   -4.405498   -0.663004
 H   -1.270792   -4.169742   -2.239649
 C    3.556890   -2.473447   -0.277380
 H    3.543610   -2.992566   -1.249433
 H    3.988222   -3.151839    0.474951
 H    2.523022   -2.238871    0.008951
 C    4.704134    2.291122   -0.299352
 H    3.655967    2.551194   -0.105476
 H    5.322107    2.669692    0.530441
 H    5.029190    2.782287   -1.229740
56
Figure_S9-1_PA-Me2NHC-ed(1,4) / electronic energy: -2903.97461848 a.u. / lowest freq: 13.61 cm-1
 H    4.587567   -1.860525   -0.426336
 C    4.532984   -0.768376   -0.350224
 C    3.312892   -0.193112   -0.390389
 C    2.120266   -1.002355   -0.519290
 H    2.283883   -2.081755   -0.581840
 C    0.830574   -0.593533   -0.597718
 C   -0.266511   -1.593096   -0.724530
Cu   -2.566568    0.334619    0.860360
 C   -4.256890    0.511056   -0.107404
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 N   -5.451255    0.508498    0.503707
 N   -4.471104    0.588801   -1.424569
 C    0.405413    0.838221   -0.589398
 O    1.070595    1.568957    0.301214
 O   -1.447615   -1.329155   -0.753297
 C   -5.884469    0.704425   -1.776755
 H   -6.165629   -0.055406   -2.521394
 C   -6.578119    0.503552   -0.424889
 H   -7.291833    1.305393   -0.182764
 H   -7.116853   -0.457089   -0.363816
 H   -6.085842    1.696054   -2.215742
 O   -0.431180    1.304139   -1.325603
 C    0.673736    2.926713    0.427090
 H    0.781828    3.458944   -0.528123
 H    1.329645    3.366834    1.185327
 H   -0.374749    2.980451    0.754513
 O    0.184246   -2.845968   -0.788746
 C   -0.792280   -3.874045   -0.728938
 H   -0.247976   -4.819793   -0.820582
 H   -1.520283   -3.774335   -1.545647
 H   -1.321875   -3.834095    0.234183
 C    5.826709   -0.090208   -0.212127
 C    5.948655    1.304133   -0.074608
 C    6.998304   -0.865025   -0.213168
 C    7.199650    1.896970    0.056284
 H    5.058159    1.935654   -0.066565
 C    8.251570   -0.271094   -0.082683
 H    6.920487   -1.950196   -0.318357
 C    8.355981    1.112558    0.052685
 H    7.276193    2.980884    0.164825
 H    9.150192   -0.891677   -0.085667
 H    9.336356    1.582120    0.157531
 H    3.196731    0.888178   -0.311015
 C   -1.171232    0.231931    2.215468
 H   -0.903598    1.065654    2.885914
 C   -0.519348   -0.877849    2.423682
 C    0.122054   -2.027563    2.573757
 H   -0.245695   -2.806980    3.250150
 H    1.052744   -2.229888    2.032007
 C   -5.667789    0.346751    1.918361
 H   -6.321327    1.144736    2.305033
 H   -6.139007   -0.625595    2.139855
 H   -4.698442    0.396895    2.430723
 C   -3.456542    0.690562   -2.443129
 H   -3.537445    1.655471   -2.971391
 H   -2.465112    0.614647   -1.982494
 H   -3.573153   -0.117100   -3.183732
56
Figure_S9-1_PA-Me2NHC-ts(1,4) / electronic energy: -2903.94929051 a.u. / lowest freq: -449.97 cm-1
 H   -4.076734   -1.893338    0.321712
 C   -4.151167   -0.811217    0.160746
 C   -3.012954   -0.097248    0.105715
 C   -1.698096   -0.725697    0.275980
 H   -1.758022   -1.785238    0.526266
 C   -0.560160   -0.088302    0.808413
 C    0.485336   -0.910947    1.391716
Cu    2.208224   -0.347626   -0.417187
 C    4.113645    0.187564   -0.234191
 N    5.151912   -0.414606   -0.829653
 N    4.586029    1.210370    0.482964
 C   -0.285834    1.343475    0.652705
 O   -1.013048    1.901214   -0.338882
 O    1.623848   -0.541667    1.698338
 C    6.027339    1.404279    0.335701
 H    6.516840    1.458948    1.319577
 C    6.442917    0.170811   -0.474438
 H    7.020396    0.423129   -1.376625
 H    7.037349   -0.544975    0.117869
 H    6.231405    2.349232   -0.195063
 O    0.496489    2.012440    1.297968
 C   -0.822407    3.286381   -0.558601
 H   -1.060085    3.869378    0.343098
 H   -1.499988    3.564436   -1.373810
 H    0.217491    3.496959   -0.847701
 O    0.124668   -2.192579    1.583098
 C    1.136873   -3.088238    2.005057
 H    0.650379   -4.062098    2.128463
 H    1.582984   -2.766619    2.956121
 H    1.932283   -3.163687    1.247798
 C   -5.521060   -0.293261    0.019925
 C   -5.807786    1.064225   -0.209398
 C   -6.598538   -1.189306    0.110449
 C   -7.121311    1.502921   -0.343081
 H   -4.995717    1.790114   -0.285476
 C   -7.914729   -0.750966   -0.024094
 H   -6.397564   -2.249102    0.288183
 C   -8.181803    0.598059   -0.252002
 H   -7.320494    2.562044   -0.521158
 H   -8.734786   -1.468812    0.048397
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 H    -9.211487    0.945950   -0.359498
 H    -3.033907    0.980028   -0.060126
 C     1.197853   -0.880412   -2.061345
 H     1.867354   -0.962932   -2.923215
 C    -0.054355   -1.094561   -2.059572
 C    -1.393885   -1.203722   -1.847977
 H    -1.848338   -2.197879   -1.802200
 H    -2.028561   -0.409454   -2.250725
 C     5.084497   -1.619009   -1.615400
 H     5.555948   -1.471188   -2.600036
 H     5.597382   -2.453351   -1.108037
 H     4.031542   -1.889402   -1.761839
 C     3.788899    2.153435    1.227646
 H     3.776002    3.138582    0.731335
 H     2.760411    1.781282    1.316508
 H     4.208525    2.283960    2.237547
56
Figure_S9-1_PA-Me2NHC-prod(1,4) / electronic energy: -2903.99035566 a.u. / lowest freq: 12.37 cm-1
 H     3.827397   -1.932621    0.015649
 C     4.030263   -0.860593    0.130496
 C     2.990319   -0.029418    0.276268
 C     1.553773   -0.478585    0.295105
 H     1.553565   -1.555930    0.085368
 C     0.636647    0.163972   -0.731753
 C    -0.297628   -0.713618   -1.342214
Cu    -2.125136   -0.288332    0.437187
 C    -4.086347   -0.039705    0.210886
 N    -5.073659   -0.836194    0.635855
 N    -4.628091    0.995067   -0.432020
 C     0.316370    1.560140   -0.690002
 O     1.119958    2.253168    0.180487
 O    -1.515389   -0.491008   -1.542651
 C    -6.090084    0.987207   -0.403274
 H    -6.503084    1.115662   -1.414602
 C    -6.396046   -0.387998    0.201071
 H    -7.095344   -0.340364    1.048838
 H    -6.808563   -1.093980   -0.539322
 H    -6.460957    1.816556    0.221844
 O    -0.536041    2.171391   -1.324229
 C     0.892513    3.640933    0.278190
 H     1.041158    4.144788   -0.688741
 H     1.617424    4.022953    1.007759
 H    -0.129485    3.857834    0.624883
 O     0.178062   -1.941563   -1.645012
 C    -0.764085   -2.929460   -2.013711
 H    -0.194424   -3.851856   -2.176297
 H    -1.295646   -2.654322   -2.935329
 H    -1.507571   -3.090899   -1.217401
 C     5.460039   -0.494066    0.102997
 C     5.913152    0.833923    0.189430
 C     6.422618   -1.509334   -0.012146
 C     7.272888    1.129213    0.165792
 H     5.192966    1.650409    0.273068
 C     7.785473   -1.215792   -0.036085
 H     6.092774   -2.549381   -0.085116
 C     8.217683    0.106482    0.053669
 H     7.600016    2.169377    0.234821
 H     8.513632   -2.025258   -0.125947
 H     9.284361    0.340606    0.034473
 H     3.148293    1.046464    0.394988
 C    -1.635012   -0.480101    2.373532
 H    -2.436293   -0.536579    3.096363
 C    -0.506881   -0.430237    1.863463
 C     0.959973   -0.294397    1.723397
 H     1.431878   -1.001618    2.424614
 H     1.200113    0.720421    2.076841
 C    -4.905555   -2.126066    1.254205
 H    -5.461505   -2.182312    2.203174
 H    -5.268132   -2.929439    0.591588
 H    -3.840172   -2.293108    1.455097
 C    -3.902441    2.110052   -0.992023
 H    -4.065648    3.025375   -0.398785
 H    -2.827403    1.884299   -1.025574
 H    -4.246658    2.301209   -2.020052
20
Figure_S9-1_PMe3-Cu-allenyl / electronic energy: -2217.18081038 a.u. / lowest freq: 11.56 cm-1
Cu    -0.560515   -0.423375   -0.001720
 C    -2.432841   -0.885632    0.001582
 H    -2.795334   -1.927022    0.005243
 C    -3.361235    0.031770    0.000489
 C    -4.267218    0.995319   -0.000581
 H    -4.662553    1.405817   -0.936021
 H    -4.659265    1.410908    0.933996
 P     1.600036    0.123265   -0.000003
 C     2.748935   -1.283966   -0.218460
 H     2.546754   -1.774384   -1.181161
 H     3.795305   -0.944626   -0.195816
 H     2.586607   -2.016869    0.584369
 C     2.107021    1.292052   -1.312942
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 H     1.880617    0.855999   -2.296084
 H     1.540405    2.228072   -1.209306
 H     3.183775    1.509070   -1.250167
 C     2.192732    0.921893    1.535582
 H     2.020015    0.248277    2.386749
 H     3.265620    1.155807    1.467496
 H     1.628085    1.849223    1.706612
52
Figure_S9-1_PA-PMe3-ed(1,6) / electronic energy: -3059.13763951 a.u. / lowest freq: 6.61 cm-1
Cu    0.946134    0.662142   -0.486494
 C   -0.311842    0.112366    1.075112
 C    0.886842   -0.629223    1.129262
 H   -0.339419    1.012421    1.695992
 C    0.958544   -2.047130    0.656424
 C    2.020812   -0.176838    1.980698
 O    0.463314   -2.180604   -0.581756
 O    1.388376   -2.973729    1.292329
 O    3.098544   -0.723933    2.045992
 O    1.745428    0.952257    2.638323
 C    2.796968    1.527773    3.400638
 H    3.175533    0.813865    4.144536
 H    2.366406    2.402458    3.898738
 H    3.624249    1.839328    2.747163
 C    0.400385   -3.498855   -1.111991
 H    1.406758   -3.934366   -1.185665
 H   -0.045441   -3.403832   -2.107336
 H   -0.222039   -4.143260   -0.475810
 C   -1.599882   -0.345001    0.582509
 H   -1.619905   -1.248391   -0.029396
 C   -2.732343    0.336947    0.846088
 H   -2.657518    1.243442    1.453671
 C   -4.088044   -0.000834    0.392753
 C   -5.140863    0.875135    0.704580
 C   -4.387170   -1.159573   -0.344949
 C   -6.445064    0.609716    0.293589
 H   -4.925937    1.783800    1.272966
 C   -5.690191   -1.426828   -0.753765
 H   -3.595689   -1.866138   -0.602503
 C   -6.725383   -0.543958   -0.437935
 H   -7.245838    1.308168    0.546078
 H   -5.901434   -2.334514   -1.323521
 H   -7.746792   -0.756303   -0.760971
 C    0.013970    2.070678   -1.498341
 H    0.490863    2.460920   -2.411316
 C   -1.122201    2.606468   -1.160161
 C   -2.286590    3.098521   -0.772631
 H   -2.348078    3.953926   -0.091670
 H   -3.227662    2.662799   -1.123952
 P    3.056672    0.301910   -1.341566
 C    4.376103    1.238848   -0.488430
 H    4.453766    0.869484    0.544059
 H    5.344546    1.106225   -0.993331
 H    4.117857    2.307148   -0.467805
 C    3.223935    0.801252   -3.091436
 H    2.514205    0.225340   -3.702413
 H    2.975435    1.867720   -3.188506
 H    4.245528    0.631657   -3.462747
 C    3.674816   -1.418430   -1.306574
 H    4.694821   -1.486488   -1.713095
 H    3.669915   -1.766955   -0.263242
 H    3.005794   -2.057348   -1.899851
52
Figure_S9-1_PA-PMe3-ts(1,6) / electronic energy: -3059.12059614 a.u. / lowest freq: -486.10 cm-1
Cu    0.973463   -0.486190   -0.667064
 C   -0.360566    1.096250   -0.063125
 C    0.859541    1.161787    0.687679
 H   -0.356011    1.708343   -0.970943
 C    0.982082    0.599623    2.051507
 C    1.948043    2.048769    0.248970
 O    0.367932   -0.598802    2.155069
 O    1.555705    1.097799    2.989773
 O    3.047309    2.135405    0.759319
 O    1.636875    2.742161   -0.863627
 C    2.665008    3.533640   -1.431971
 H    3.044770    4.268214   -0.708299
 H    2.215928    4.047865   -2.288813
 H    3.502451    2.907289   -1.773320
 C    0.365506   -1.206541    3.436453
 H    1.392043   -1.394981    3.782086
 H   -0.173046   -2.153877    3.324931
 H   -0.142116   -0.567410    4.172775
 C   -1.592458    0.517937    0.270566
 H   -1.687461   -0.039214    1.203016
 C   -2.654334    0.537070   -0.642765
 H   -2.570468    1.280580   -1.440970
 C   -4.053752    0.265115   -0.224743
 C   -5.107928    0.905840   -0.890250
 C   -4.366846   -0.626846    0.812843
 C   -6.433833    0.675070   -0.525474
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 H   -4.883062    1.600820   -1.703940
 C   -5.690266   -0.859680    1.177120
 H   -3.566510   -1.156522    1.334748
 C   -6.730888   -0.208626    0.511004
 H   -7.239252    1.189587   -1.054631
 H   -5.913009   -1.559595    1.985753
 H   -7.768639   -0.393264    0.796808
 C    0.077420   -1.547483   -2.125677
 H    0.746677   -2.216909   -2.667929
 C   -1.174205   -1.373949   -2.212348
 C   -2.491089   -1.047482   -2.060582
 H   -2.985680   -0.503160   -2.871174
 H   -3.122367   -1.783135   -1.552330
 P    3.102831   -1.286392   -0.413075
 C    4.377154   -0.286528   -1.263249
 H    4.368668    0.721446   -0.824011
 H    5.375768   -0.731149   -1.137565
 H    4.141844   -0.213236   -2.334504
 C    3.404233   -2.986645   -1.015154
 H    2.731996   -3.682485   -0.493082
 H    3.187019   -3.038988   -2.091902
 H    4.447505   -3.291551   -0.844828
 C    3.684695   -1.312529    1.318606
 H    4.718412   -1.682126    1.390433
 H    3.629386   -0.286421    1.710648
 H    3.024594   -1.955984    1.917287
52
Figure_S9-1_PA-PMe3-prod(1,6) / electronic energy: -3059.16803726 a.u. / lowest freq: 11.07 cm-1
Cu    0.641392   -1.430481   -0.158173
 C   -0.261848    0.744701   -0.102685
 C    0.707636    1.532490    0.619003
 H   -0.377822    1.045410   -1.150061
 C    1.196600    1.168387    1.932073
 C    1.323333    2.665368   -0.036311
 O    0.892494   -0.134953    2.245746
 O    1.854816    1.828119    2.712321
 O    2.226730    3.372658    0.375618
 O    0.813691    2.888561   -1.289504
 C    1.396221    3.944163   -2.022758
 H    1.271366    4.908433   -1.507920
 H    0.877714    3.972648   -2.988805
 H    2.472031    3.776769   -2.184719
 C    1.352911   -0.609650    3.493015
 H    2.452534   -0.611438    3.540506
 H    0.975828   -1.634984    3.591595
 H    0.974192    0.007696    4.320347
 C   -1.113747   -0.252283    0.323170
 H   -1.184042   -0.477308    1.391467
 C   -2.202460   -0.849509   -0.549080
 H   -1.931584   -0.691537   -1.605462
 C   -3.566017   -0.218254   -0.328675
 C   -4.259715    0.359694   -1.396422
 C   -4.155117   -0.191915    0.942510
 C   -5.509756    0.949995   -1.204396
 H   -3.812300    0.351165   -2.394050
 C   -5.403705    0.394345    1.138322
 H   -3.630458   -0.628345    1.796817
 C   -6.086387    0.968420    0.064211
 H   -6.032711    1.399155   -2.051793
 H   -5.846431    0.407126    2.136828
 H   -7.063610    1.431287    0.218058
 C    0.204828   -3.496730   -0.522113
 H    1.022059   -4.182658   -0.680478
 C   -0.883287   -2.939236   -0.399370
 C   -2.239144   -2.375710   -0.302667
 H   -2.906532   -2.889545   -1.011512
 H   -2.624264   -2.581627    0.709251
 P    2.786707   -0.984455   -0.769054
 C    2.832932    0.089503   -2.250330
 H    2.264394    1.007673   -2.045712
 H    3.867252    0.346246   -2.523506
 H    2.354651   -0.432632   -3.091592
 C    3.801101   -2.426255   -1.265096
 H    3.911744   -3.109549   -0.410578
 H    3.295153   -2.966639   -2.078400
 H    4.798661   -2.113494   -1.608151
 C    3.857254   -0.111163    0.428282
 H    4.874898   -0.003005    0.024243
 H    3.445924    0.885489    0.640462
 H    3.898707   -0.678796    1.368435
52
Figure_S9-1_PA-PMe3-ed(1,4AA) / electronic energy: -3059.13763951 a.u. / lowest freq: 6.60 cm-1
Cu    0.946133    0.662144   -0.486490
 C   -0.311841    0.112360    1.075114
 C    0.886843   -0.629229    1.129260
 H   -0.339417    1.012412    1.695999
 C    0.958546   -2.047133    0.656413
 C    2.020815   -0.176848    1.980697
 O    0.463314   -2.180601   -0.581766
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 O    1.388382   -2.973734    1.292312
 O    3.098547   -0.723942    2.045986
 O    1.745431    0.952242    2.638330
 C    2.796970    1.527753    3.400647
 H    3.175533    0.813842    4.144544
 H    2.366409    2.402438    3.898751
 H    3.624253    1.839310    2.747175
 C    0.400385   -3.498850   -1.112008
 H    1.406759   -3.934359   -1.185687
 H   -0.045444   -3.403822   -2.107351
 H   -0.222036   -4.143258   -0.475828
 C   -1.599881   -0.345003    0.582510
 H   -1.619906   -1.248390   -0.029400
 C   -2.732342    0.336943    0.846093
 H   -2.657517    1.243435    1.453681
 C   -4.088043   -0.000835    0.392756
 C   -5.140863    0.875128    0.704594
 C   -4.387167   -1.159566   -0.344960
 C   -6.445064    0.609710    0.293603
 H   -4.925939    1.783787    1.272991
 C   -5.690188   -1.426819   -0.753777
 H   -3.595684   -1.866125   -0.602524
 C   -6.725382   -0.543955   -0.437934
 H   -7.245839    1.308157    0.546102
 H   -5.901430   -2.334498   -1.323544
 H   -7.746791   -0.756299   -0.760972
 C    0.013969    2.070686   -1.498329
 H    0.490869    2.460939   -2.411297
 C   -1.122208    2.606465   -1.160155
 C   -2.286604    3.098507   -0.772631
 H   -3.227669    2.662782   -1.123965
 H   -2.348104    3.953905   -0.091663
 P    3.056671    0.301920   -1.341565
 C    3.674817   -1.418420   -1.306582
 H    3.005794   -2.057337   -1.899858
 H    4.694821   -1.486475   -1.713107
 H    3.669920   -1.766949   -0.263251
 C    4.376101    1.238855   -0.488424
 H    4.117853    2.307155   -0.467792
 H    4.453766    0.869484    0.544063
 H    5.344543    1.106236   -0.993327
 C    3.223933    0.801272   -3.091432
 H    4.245525    0.631678   -3.462744
 H    2.514201    0.225365   -3.702412
 H    2.975435    1.867742   -3.188495
52
Figure_S9-1_PA-PMe3-ts(1,4AA) / electronic energy: -3059.10503746 a.u. / lowest freq: -349.31 cm-1
Cu   -1.342484    0.211451    0.739081
 C    0.512319    0.525522   -0.332475
 C   -0.468572   -0.221415   -1.141922
 H    0.566119    1.562542   -0.666237
 C   -0.598195   -1.675925   -1.077874
 C   -1.319841    0.502435   -2.083729
 O   -0.125684   -2.150815    0.113679
 O   -1.089356   -2.429035   -1.888888
 O   -2.117073    0.030533   -2.869751
 O   -1.174343    1.847996   -1.970206
 C   -1.996244    2.644949   -2.799898
 H   -1.807922    2.440339   -3.863794
 H   -1.745217    3.687179   -2.571576
 H   -3.061846    2.465963   -2.593582
 C   -0.162806   -3.553617    0.300735
 H   -1.197614   -3.925713    0.305296
 H    0.305494   -3.745689    1.272744
 H    0.392141   -4.072814   -0.493693
 C    1.855878   -0.053901   -0.093999
 H    1.898009   -1.116125    0.148688
 C    2.971884    0.681981   -0.199158
 H    2.868281    1.750803   -0.420468
 C    4.356718    0.209619   -0.033938
 C    5.402810    1.142856   -0.104299
 C    4.684764   -1.137887    0.195657
 C    6.730654    0.750311    0.055841
 H    5.168672    2.195222   -0.285371
 C    6.009856   -1.530976    0.355257
 H    3.896806   -1.891989    0.246277
 C    7.039337   -0.589079    0.287457
 H    7.526955    1.495658   -0.000735
 H    6.242322   -2.583470    0.532117
 H    8.078459   -0.900740    0.413363
 C    0.224607    1.087083    1.631291
 H    0.766668    0.448856    2.339124
 C    0.138302    2.375743    1.818559
 C    0.053211    3.683964    1.917711
 H    0.840436    4.331207    1.517012
 H   -0.797096    4.163263    2.412779
 P   -3.491797   -0.327766    0.982651
 C   -3.764232   -2.113859    0.695469
 H   -3.257271   -2.691188    1.481775
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 H   -4.837034   -2.357845    0.699451
 H   -3.329342   -2.388985   -0.277032
 C   -4.507308    0.473948   -0.309416
 H   -4.473425    1.564509   -0.173927
 H   -4.078463    0.230463   -1.293111
 H   -5.552106    0.132496   -0.263845
 C   -4.389708    0.017843    2.536468
 H   -5.438825   -0.306605    2.467842
 H   -3.898887   -0.507312    3.368128
 H   -4.355294    1.097377    2.740566
52
Figure_S9-1_PA-PMe3-prod(1,4AA) / electronic energy: -3059.15445792 a.u. / lowest freq: 10.07 cm-1
Cu   -1.853285   -0.031563   -0.851074
 C    0.694401   -0.372027   -0.468226
 C   -0.243212    0.165112    0.633960
 H    0.683344   -1.463567   -0.376536
 C   -0.375077    1.591961    0.871401
 C   -0.730680   -0.746376    1.655533
 O    0.231676    2.324802   -0.114856
 O   -0.953721    2.167287    1.775181
 O   -1.417384   -0.486893    2.629603
 O   -0.376892   -2.040647    1.404831
 C   -0.858519   -3.014194    2.306368
 H   -0.570140   -2.783609    3.341974
 H   -0.410002   -3.966573    1.999238
 H   -1.955617   -3.094676    2.261490
 C    0.125313    3.728973   -0.010355
 H   -0.926429    4.052577   -0.015908
 H    0.644525    4.143950   -0.882504
 H    0.595137    4.100208    0.912237
 C    2.126545    0.083633   -0.385878
 H    2.287837    1.163127   -0.450866
 C    3.156066   -0.758177   -0.229049
 H    2.947155   -1.833796   -0.181662
 C    4.582036   -0.395070   -0.116200
 C    5.548794   -1.412274   -0.138967
 C    5.023962    0.932632    0.015043
 C    6.908400   -1.118511   -0.044933
 H    5.225851   -2.452465   -0.235445
 C    6.380620    1.227755    0.109784
 H    4.297596    1.747019    0.053730
 C    7.330629    0.204335    0.078748
 H    7.641563   -1.927922   -0.066573
 H    6.700551    2.266962    0.215311
 H    8.394643    0.437833    0.157319
 C    0.049114   -0.026872   -1.815012
 H    0.177706    1.001636   -2.175638
 C   -0.682274   -0.872417   -2.546071
 C   -1.185883   -1.746022   -3.386792
 H   -0.537218   -2.231592   -4.124118
 H   -2.244330   -2.016929   -3.384047
 P   -3.975001    0.033752   -0.159708
 C   -4.218207    1.591761    0.763393
 H   -4.155066    2.441725    0.068812
 H   -5.193603    1.607530    1.271804
 H   -3.401863    1.682628    1.495856
 C   -4.331801   -1.259346    1.080361
 H   -4.249713   -2.252318    0.615853
 H   -3.579952   -1.175762    1.879624
 H   -5.340337   -1.133774    1.501813
 C   -5.386784   -0.044000   -1.318351
 H   -6.341981    0.065479   -0.783175
 H   -5.294192    0.758636   -2.063502
 H   -5.375298   -1.008947   -1.844973
52
Figure_S9-1_PA-PMe3-ed(1,4) / electronic energy: -3059.13081436 a.u. / lowest freq: 15.01 cm-1
 H   -4.127353    1.771654   -0.567097
 C   -4.025590    0.690314   -0.420134
 C   -2.780252    0.169848   -0.422283
 C   -1.628733    1.025090   -0.607630
 H   -1.841923    2.088027   -0.751779
 C   -0.321548    0.672813   -0.644634
 C    0.735123    1.705122   -0.823233
Cu    2.820474   -0.060464    1.018203
 C    0.174116   -0.729707   -0.517425
 O   -0.422384   -1.402715    0.461131
 O    1.924138    1.497646   -0.706763
 O    1.022602   -1.214079   -1.230102
 C    0.077786   -2.705202    0.732650
 H    0.003416   -3.351518   -0.152709
 H   -0.533735   -3.102682    1.548865
 H    1.129990   -2.636540    1.047504
 O    0.245233    2.906789   -1.111643
 C    1.170248    3.984568   -1.120423
 H    0.590441    4.882616   -1.357840
 H    1.949273    3.825663   -1.878756
 H    1.640039    4.085668   -0.131579
 C   -5.289371   -0.031532   -0.238761
 C   -5.355019   -1.421565   -0.035259
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 C   -6.490112    0.696530   -0.267463
 C   -6.581206   -2.055517    0.132569
 H   -4.439843   -2.016150   -0.006609
 C   -7.718263    0.061477   -0.099455
 H   -6.455539    1.777793   -0.423368
 C   -7.767184   -1.317359    0.101113
 H   -6.614760   -3.135538    0.290433
 H   -8.640734    0.645318   -0.124689
 H   -8.728143   -1.818781    0.234106
 H   -2.614354   -0.897627   -0.270132
 C    1.694147    0.477808    2.511125
 H    1.614321   -0.093316    3.450444
 C    0.959512    1.552765    2.445023
 C    0.228005    2.648611    2.309848
 H    0.602784    3.629916    2.620618
 H   -0.781829    2.605506    1.887137
 P    4.228350   -1.032461   -0.416956
 C    4.127762   -0.354377   -2.111270
 H    4.391922    0.711951   -2.091327
 H    4.795491   -0.892166   -2.800849
 H    3.083408   -0.443726   -2.439272
 C    6.019669   -0.968187   -0.034537
 H    6.613678   -1.470438   -0.813074
 H    6.338193    0.081225    0.043563
 H    6.204237   -1.456060    0.933285
 C    3.921700   -2.820443   -0.669689
 H    4.609530   -3.243301   -1.417530
 H    4.047714   -3.353505    0.283698
 H    2.883310   -2.941087   -1.008378
52
Figure_S9-1_PA-PMe3-ts(1,4) / electronic energy: -3059.10625840 a.u. / lowest freq: -463.12 cm-1
 H    3.758711   -1.837622    0.079067
 C    3.729212   -0.744279   -0.001348
 C    2.528062   -0.140773   -0.033652
 C    1.280498   -0.914439   -0.007891
 H    1.448460   -1.990419   -0.057200
 C    0.067630   -0.523220   -0.619356
 C   -0.881224   -1.567643   -0.986657
Cu   -2.494694   -0.372571    0.730382
 C   -0.358875    0.869066   -0.765832
 O    0.372002    1.709738   -0.002705
 O   -2.067142   -1.407072   -1.270002
 O   -1.258836    1.291650   -1.470110
 C    0.048114    3.085235   -0.068618
 H    0.029126    3.444246   -1.107213
 H    0.825258    3.611520    0.497451
 H   -0.933165    3.276001    0.390574
 O   -0.360215   -2.804207   -0.959116
 C   -1.259544   -3.881596   -1.154923
 H   -0.660488   -4.796188   -1.085347
 H   -1.740490   -3.821234   -2.140894
 H   -2.039427   -3.884838   -0.379416
 C    5.045227   -0.089763   -0.063749
 C    5.204715    1.301130   -0.195890
 C    6.201698   -0.883291    0.008385
 C    6.472559    1.870822   -0.253092
 H    4.328316    1.949438   -0.257705
 C    7.472258   -0.313424   -0.047900
 H    6.098422   -1.966711    0.111824
 C    7.613104    1.067178   -0.179706
 H    6.574207    2.953194   -0.358908
 H    8.356411   -0.952205    0.010039
 H    8.606488    1.518380   -0.227070
 H    2.444069    0.943678   -0.099392
 C   -1.511859   -0.863387    2.391275
 H   -2.183310   -0.923645    3.253525
 C   -0.247968   -0.980507    2.398704
 C    1.092400   -1.024604    2.159885
 H    1.609523   -1.985085    2.240844
 H    1.681570   -0.146058    2.439875
 P   -4.238567    0.839178   -0.037521
 C   -4.571023    0.526911   -1.805738
 H   -4.868989   -0.521983   -1.940369
 H   -5.357108    1.191151   -2.194830
 H   -3.626532    0.686642   -2.342970
 C   -5.873789    0.623448    0.761582
 H   -6.636890    1.263698    0.293701
 H   -6.183732   -0.428065    0.676378
 H   -5.795507    0.873837    1.829319
 C   -3.978569    2.650197    0.013923
 H   -4.837747    3.189528   -0.412645
 H   -3.820628    2.975703    1.052051
 H   -3.074153    2.870684   -0.569900
52
Figure_S9-1_PA-PMe3-prod(1,4) / electronic energy: -3059.16938303 a.u. / lowest freq: 24.51 cm-1
 H   -2.888672    1.319704    1.323779
 C   -3.134930    0.412332    0.759396
 C   -2.163309   -0.487431    0.559318
 C   -0.743882   -0.298985    1.022574
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 H   -0.701371    0.648124    1.574076
 C    0.254574   -0.142124   -0.146460
 C    0.404427    1.207334   -0.703437
Cu    2.143568   -0.326332    0.815999
 C    0.419745   -1.238632   -1.107804
 O   -0.159005   -2.391404   -0.667030
 O    0.919159    1.535021   -1.757864
 O    1.007193   -1.231882   -2.171676
 C    0.008925   -3.533057   -1.482817
 H   -0.456236   -3.390729   -2.469300
 H   -0.480775   -4.362201   -0.958485
 H    1.074252   -3.762545   -1.632194
 O   -0.089527    2.161464    0.130781
 C    0.024315    3.502294   -0.297623
 H   -0.505695    4.108985    0.446214
 H   -0.429892    3.646821   -1.288282
 H    1.077071    3.819914   -0.346889
 C   -4.534334    0.322493    0.300683
 C   -4.983084   -0.655959   -0.602868
 C   -5.468766    1.253863    0.780229
 C   -6.316669   -0.705184   -0.998606
 H   -4.277911   -1.383635   -1.010457
 C   -6.804928    1.205857    0.385650
 H   -5.138706    2.027424    1.478923
 C   -7.235644    0.224019   -0.505382
 H   -6.642130   -1.472577   -1.704725
 H   -7.512884    1.941221    0.774970
 H   -8.281086    0.183634   -0.819091
 H   -2.362825   -1.412954    0.008538
 C    2.294863   -1.231245    2.702490
 H    3.218511   -1.318188    3.253201
 C    1.119191   -1.274489    2.329274
 C   -0.318089   -1.392661    2.027185
 H   -0.896195   -1.310201    2.961096
 H   -0.495741   -2.392548    1.608151
 P    3.968480    0.492094   -0.227315
 C    3.909198    2.302317   -0.480522
 H    3.835575    2.814953    0.489229
 H    4.803913    2.655848   -1.014367
 H    3.010126    2.524581   -1.073412
 C    5.624606    0.208102    0.499178
 H    6.415696    0.622070   -0.144216
 H    5.678237    0.683742    1.489079
 H    5.788878   -0.871679    0.624804
 C    4.099290   -0.163046   -1.926149
 H    4.902842    0.337050   -2.487157
 H    4.294971   -1.244071   -1.886774
 H    3.123828   -0.010904   -2.410503
32
Figure_S10-1_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C   -0.660544   -0.726572    0.059153
 C   -1.860539   -0.097447    0.115996
 H   -0.691600   -1.818492   -0.004770
 C   -1.976243    1.390665    0.160143
 C   -3.120576   -0.891785    0.187355
 O   -3.041424    1.823605   -0.507466
 O   -1.182749    2.134043    0.689285
 O   -4.147702   -0.497504    0.683440
 O   -2.981802   -2.118850   -0.320932
 C   -4.097604   -2.989729   -0.195724
 H   -4.332384   -3.170881    0.862818
 H   -3.810049   -3.927003   -0.683244
 H   -4.981752   -2.562067   -0.688186
 C   -3.254671    3.228152   -0.535442
 H   -3.354009    3.627502    0.483524
 H   -4.184056    3.384216   -1.092621
 H   -2.420438    3.737793   -1.038016
 C    0.656646   -0.129211    0.062308
 H    0.725624    0.955889    0.150505
 C    1.759981   -0.902956   -0.019704
 H    1.621029   -1.988149   -0.089650
 C    3.156351   -0.453635   -0.025165
 C    4.175093   -1.416830   -0.109525
 C    3.522207    0.902114    0.053056
 C    5.517020   -1.042840   -0.114390
 H    3.907556   -2.474776   -0.172060
 C    4.861836    1.275255    0.048166
 H    2.754752    1.675486    0.118691
 C    5.863995    0.305241   -0.035401
 H    6.294080   -1.807149   -0.179427
 H    5.127957    2.332459    0.111300
 H    6.914980    0.602284   -0.038425
50
Figure_S10-1_dienoate-Naborate / electronic energy: -1486.89608401 a.u. / lowest freq: 15.45 cm-1
 H   -4.420128    2.087873    2.299924
 H   -5.923773   -2.547792    1.430468
 C   -3.899637    1.709040    1.397197
 O   -6.388627   -0.555754    1.056848
 H   -2.832933    1.979558    1.487735
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 O   -4.052556    0.323170    1.268895
 C   -6.462160   -1.902837    0.702697
 H   -7.509160   -2.251286    0.668862
Na   -2.589162   -0.954460    0.028443
 B   -5.242902    0.056168    0.401101
 C   -4.549382    2.260434    0.125108
 H   -4.940007    3.284567    0.257486
 O   -5.580090    1.360046   -0.149654
 C   -5.777159   -1.970930   -0.665207
 O   -4.794555   -0.975836   -0.589590
 H   -3.802053    2.287356   -0.695287
 H   -6.503487   -1.753783   -1.474182
 H   -5.329092   -2.957849   -0.872632
 C    2.217972    0.782767   -0.357663
 C    0.968244    0.253780   -0.477916
 H    2.268783    1.873090   -0.426363
 C    0.656300   -1.199329   -0.386928
 C   -0.192151    1.162783   -0.688524
 O    1.634875   -1.973268   -0.831358
 O   -0.381350   -1.656994    0.046156
 O   -1.335622    0.796830   -0.869352
 O    0.144585    2.445194   -0.682767
 C   -0.892656    3.394615   -0.904656
 H   -1.373335    3.224078   -1.877338
 H   -0.410674    4.376881   -0.885452
 H   -1.650282    3.328425   -0.112354
 C    1.442759   -3.383139   -0.742768
 H    1.291967   -3.686873    0.301829
 H    2.354400   -3.836025   -1.144545
 H    0.572193   -3.688467   -1.338576
 C    3.478653    0.126613   -0.118869
 H    3.499709   -0.957579   -0.015571
 C    4.611174    0.860860   -0.028545
 H    4.527241    1.946558   -0.152174
 C    5.966988    0.366461    0.217775
 C    7.021202    1.293347    0.272402
 C    6.260030   -0.996390    0.405467
 C    8.328905    0.875902    0.507087
 H    6.809143    2.355652    0.127725
 C    7.565616   -1.412370    0.640052
 H    5.462269   -1.740462    0.369434
 C    8.603756   -0.478381    0.691959
 H    9.135264    1.610831    0.545810
 H    7.777281   -2.473596    0.785169
 H    9.627956   -0.809398    0.876235
56
Figure_S10-1_SIMes-Cu-allenyl / electronic energy: -2680.78923765 a.u. / lowest freq: 16.67 cm-1
 C    0.255100   -2.802091    0.505112
 H    0.668208   -3.196427    1.444813
 C   -1.270500   -2.619391    0.554864
 H   -1.800083   -3.253354   -0.170485
 C   -0.267703   -0.553149    0.091367
 C   -2.705673   -0.570588    0.110299
 C   -3.379878   -0.614762   -1.117966
 C   -3.248840    0.082482    1.227243
 C   -4.637370   -0.011781   -1.202344
 C   -4.506955    0.673704    1.096602
 C   -5.220520    0.629249   -0.105733
Cu    0.110016    1.307604   -0.228361
 N    0.723169   -1.433012    0.264097
 N   -1.429749   -1.197347    0.221108
 H   -1.690544   -2.824163    1.551562
 H    0.576639   -3.468534   -0.309931
 C    0.774672    3.096038   -0.486998
 H    0.208773    4.016056   -0.700711
 C    2.071525    3.214162   -0.388898
 C    3.389142    3.271273   -0.276397
 H    4.042154    3.124597   -1.143427
 H    3.872005    3.450329    0.690170
 H   -4.940744    1.189169    1.958286
 H   -5.171125   -0.034945   -2.156636
 C   -2.739174   -1.258856   -2.318184
 H   -1.764393   -0.794441   -2.533026
 H   -2.557008   -2.332599   -2.157552
 H   -3.373859   -1.155030   -3.207828
 C   -2.466468    0.177007    2.509466
 H   -2.161688   -0.814837    2.876499
 H   -1.543922    0.758395    2.352392
 H   -3.052793    0.668434    3.296712
 C    2.100609   -1.074402    0.152530
 C    2.710868   -1.089540   -1.109969
 C    2.796150   -0.676303    1.303159
 C    4.054490   -0.718966   -1.196317
 C    4.137867   -0.315360    1.170431
 C    4.783410   -0.329256   -0.069282
 H    4.541691   -0.721123   -2.175444
 H    4.690272    0.002663    2.059240
 C    1.914463   -1.435151   -2.339256
 H    1.411113   -2.409070   -2.245646
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 H    1.129881   -0.679297   -2.505515
 H    2.554756   -1.464444   -3.230551
 C    2.087510   -0.585650    2.627443
 H    1.295980    0.179314    2.581836
 H    1.603679   -1.535221    2.901538
 H    2.783525   -0.310564    3.430477
 C   -6.591070    1.245868   -0.208877
 H   -6.854724    1.465524   -1.252764
 H   -7.356052    0.560144    0.189860
 H   -6.655115    2.179427    0.368353
 C    6.214528    0.121736   -0.194929
 H    6.791322   -0.109785    0.711774
 H    6.712484   -0.348829   -1.054371
 H    6.258068    1.212948   -0.343793
106
Figure_S10-1_PA-SIMes(Naborate)-ed(1,6) / electronic energy: -4167.72984142 a.u. / lowest freq: 15.67 cm-1
 C   -0.908032    1.743554    3.577161
 H   -1.874873    1.278942    3.826794
 C    0.291319    0.862313    3.956263
 H    1.053361    1.413080    4.527899
 C    0.208121    1.092135    1.625601
 C    1.844946   -0.499626    2.464151
 C    1.459344   -1.832551    2.241745
 C    3.194398   -0.124516    2.527962
 C    3.815745   -2.445807    2.082551
Cu    0.980742    1.136268   -0.190580
 N   -0.767917    1.858850    2.118438
 N    0.821139    0.478664    2.641928
 C    1.603344    0.443008   -1.983620
 C    0.301630   -0.108416   -1.750044
 H    0.006005   -0.026639    4.537031
 H   -0.873389    2.734290    4.050714
 H    1.639312    1.291448   -2.668615
 C    0.020924   -1.511992   -1.378981
 C   -0.851505    0.685195   -2.254380
 O    1.109234   -2.262582   -1.246759
 O   -1.089377   -1.987814   -1.217962
 O   -1.982231    0.285162   -2.453566
 O   -0.519720    1.955690   -2.479628
 C   -1.539970    2.827821   -2.949353
 H   -1.946410    2.470408   -3.905369
 H   -1.061663    3.803624   -3.080840
 H   -2.347081    2.898321   -2.209001
 C    0.922788   -3.646019   -0.980820
 H    0.328102   -3.795681   -0.071117
 H    1.926198   -4.064449   -0.850781
 H    0.415578   -4.133077   -1.825231
 C    2.886056   -0.172176   -1.696501
 H    2.915657   -1.001659   -0.990408
 C    4.027265    0.294287   -2.246849
 H    3.959025    1.108225   -2.975794
 C    5.378857   -0.225318   -2.002819
 C    6.437660    0.207614   -2.816236
 C    5.661124   -1.142977   -0.977005
 C    7.733359   -0.266865   -2.621337
 H    6.238270    0.928984   -3.613106
 C    6.954300   -1.615215   -0.779856
 H    4.863183   -1.473396   -0.310365
 C    7.996919   -1.181847   -1.602560
 H    8.541397    0.081344   -3.268453
 H    7.152916   -2.325303    0.026093
 H    9.011406   -1.554656   -1.445885
 C    2.108688    2.769125   -0.228970
 H    1.527641    3.686118   -0.048742
 C    3.391830    2.866153   -0.384617
 C    4.705479    2.873320   -0.534187
 H    5.169696    2.999827   -1.517212
 H    5.375640    2.765543    0.325441
 C    2.459595   -2.786794    2.053781
 H    2.174262   -3.829494    1.889306
 C    4.161047   -1.114153    2.325577
 H    5.217261   -0.833242    2.362867
 C    0.003991   -2.216389    2.214080
 H   -0.537546   -1.825938    3.088183
 H   -0.503202   -1.814319    1.324366
 H   -0.116672   -3.307982    2.207579
 C    3.589344    1.294990    2.829165
 H    3.038789    2.001668    2.192713
 H    3.378295    1.546642    3.880897
 H    4.663474    1.445757    2.659611
 C   -1.786359    2.456640    1.317426
 C   -1.798616    3.842009    1.116130
 C   -2.788135    1.623876    0.788456
 C   -2.840757    4.385524    0.355619
 C   -3.810651    2.208127    0.042461
 C   -3.853952    3.589133   -0.182933
 H   -4.587746    1.558446   -0.369811
 C   -0.739329    4.723080    1.721383
 H   -0.637881    5.662864    1.162104
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 H   -0.994791    4.984580    2.761369
 H    0.236959    4.219743    1.743731
 C   -2.752209    0.138883    1.009474
 H   -1.972606   -0.321250    0.382397
 H   -2.509928   -0.115833    2.051301
 H   -3.715846   -0.322533    0.760367
 C    4.871901   -3.492073    1.840567
 H    4.612770   -4.443252    2.327210
 H    4.978624   -3.697486    0.762599
 H    5.852455   -3.168198    2.216614
 C   -4.970888    4.188174   -0.996983
 H   -4.829183    5.266970   -1.148224
 H   -5.038285    3.709192   -1.986012
 H   -5.942169    4.038412   -0.500605
 H   -2.858464    5.465312    0.182034
Na   -3.263373   -1.478165   -1.811538
 B   -5.371878   -2.401991   -0.145528
 O   -5.268814   -1.052652   -0.789637
 O   -4.947835   -2.464831    1.248104
 O   -4.386898   -3.269419   -0.861110
 C   -3.768356   -3.204319    1.357365
 C   -3.735061   -4.064984    0.090831
 O   -6.774432   -2.757271   -0.294907
 C   -6.556416   -0.603597   -1.106539
 C   -7.368840   -1.897380   -1.218931
 H   -3.758196   -3.808832    2.281290
 H   -2.878198   -2.542307    1.383977
 H   -4.273525   -5.020608    0.249095
 H   -2.707857   -4.302272   -0.233178
 H   -6.553434   -0.015331   -2.040133
 H   -6.958945    0.043354   -0.301539
 H   -7.302244   -2.299799   -2.252328
 H   -8.438493   -1.746103   -0.993694
106
Figure_S10-1_PA-SIMes(Naborate)-ts(1,6) / electronic energy: -4167.72041851 a.u. / lowest freq: -419.80 cm-1
 C   -0.891009    1.770988    3.591828
 H   -1.850548    1.288868    3.836756
 C    0.322183    0.913475    3.980342
 H    1.070669    1.479295    4.555165
 C    0.243167    1.126691    1.647091
 C    1.902029   -0.431762    2.505604
 C    1.534496   -1.767401    2.271750
 C    3.245961   -0.042542    2.593725
 C    3.899117   -2.358523    2.167181
Cu    0.945276    1.129521   -0.193607
 N   -0.744941    1.883708    2.133451
 N    0.866098    0.535171    2.669826
 C    1.575019    0.416170   -2.032692
 C    0.250515   -0.130118   -1.801979
 H    0.050129    0.020571    4.561463
 H   -0.879402    2.764183    4.061868
 H    1.599926    1.260529   -2.725470
 C   -0.013040   -1.519274   -1.423519
 C   -0.886661    0.664216   -2.293348
 O    1.093645   -2.231283   -1.190787
 O   -1.113339   -2.043424   -1.322753
 O   -2.033854    0.288706   -2.469274
 O   -0.545036    1.937140   -2.540873
 C   -1.565346    2.808930   -3.002616
 H   -1.993719    2.445647   -3.947197
 H   -1.083691    3.780493   -3.155771
 H   -2.361128    2.897909   -2.251568
 C    0.936187   -3.617949   -0.938901
 H    0.305376   -3.793315   -0.057820
 H    1.944486   -4.008415   -0.763864
 H    0.483118   -4.120330   -1.805247
 C    2.832396   -0.091943   -1.657242
 H    2.892545   -0.924132   -0.955825
 C    4.003165    0.501087   -2.132517
 H    3.900655    1.116547   -3.028973
 C    5.338932   -0.110292   -1.958780
 C    6.349284    0.159350   -2.893265
 C    5.640313   -0.950415   -0.875871
 C    7.618716   -0.400784   -2.758493
 H    6.133764    0.816770   -3.740020
 C    6.908808   -1.506310   -0.737912
 H    4.878529   -1.155069   -0.121584
 C    7.904416   -1.236715   -1.679558
 H    8.388875   -0.181422   -3.501356
 H    7.124691   -2.153675    0.115122
 H    8.898505   -1.675282   -1.569401
 C    2.054408    2.853980   -0.144623
 H    1.476504    3.622162    0.368953
 C    3.250346    2.805002   -0.553871
 C    4.457419    2.417100   -1.036265
 H    4.851640    2.875957   -1.946694
 H    5.206898    2.058728   -0.323060
 C    2.547540   -2.711404    2.102648
 H    2.275462   -3.755148    1.923182
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 C    4.226297   -1.024036    2.420907
 H    5.278915   -0.733566    2.482329
 C    0.084642   -2.163917    2.203286
 H   -0.490989   -1.759148    3.048384
 H   -0.391659   -1.783790    1.286835
 H   -0.027409   -3.256185    2.215559
 C    3.621177    1.386505    2.876440
 H    3.065925    2.076370    2.225743
 H    3.399158    1.655510    3.921569
 H    4.694643    1.549075    2.712350
 C   -1.774838    2.455443    1.327274
 C   -1.828116    3.839306    1.125700
 C   -2.751331    1.594149    0.791863
 C   -2.881616    4.352130    0.357762
 C   -3.784622    2.148276    0.039981
 C   -3.866718    3.527773   -0.187062
 H   -4.539166    1.475445   -0.376739
 C   -0.808183    4.769224    1.727798
 H   -0.504087    5.539174    1.004478
 H   -1.225989    5.290600    2.603695
 H    0.089207    4.231259    2.061450
 C   -2.676767    0.110012    1.007569
 H   -1.901185   -0.329083    0.360895
 H   -2.407938   -0.143478    2.043051
 H   -3.634399   -0.371542    0.774448
 C    4.969868   -3.392512    1.939228
 H    4.710875   -4.350007    2.413368
 H    5.097322   -3.586484    0.861532
 H    5.940131   -3.062193    2.335933
 C   -4.996174    4.092812   -1.007949
 H   -4.881492    5.173969   -1.165439
 H   -5.048334    3.605855   -1.993931
 H   -5.964725    3.921518   -0.513104
 H   -2.929699    5.431315    0.185478
Na   -3.278640   -1.495288   -1.852541
 B   -5.310157   -2.451252   -0.105513
 O   -5.234076   -1.090907   -0.731673
 O   -4.822550   -2.537371    1.265501
 O   -4.363765   -3.308195   -0.880815
 C   -3.627867   -3.259961    1.302206
 C   -3.649601   -4.104900    0.024835
 O   -6.719829   -2.799950   -0.195052
 C   -6.533189   -0.633127   -0.979081
 C   -7.355449   -1.922248   -1.073444
 H   -3.560234   -3.874554    2.217015
 H   -2.747148   -2.585129    1.288402
 H   -4.164923   -5.070660    0.199037
 H   -2.638054   -4.320178   -0.357653
 H   -6.572832   -0.029594   -1.902184
 H   -6.894886    0.002040   -0.145570
 H   -7.342284   -2.306620   -2.115802
 H   -8.412119   -1.771278   -0.792977
106
Figure_S10-1_PA-SIMes(Naborate)-prod(1,6) / electronic energy: -4167.77319994 a.u. / lowest freq: 11.49 cm-1
 C   -0.522938    2.673260    3.142399
 H   -1.442902    2.283513    3.603903
 C    0.747336    2.001699    3.685535
 H    1.476727    2.728463    4.071166
 C    0.534363    1.518639    1.400742
 C    2.410379    0.461453    2.543070
 C    2.205091   -0.926937    2.589085
 C    3.698322    1.016456    2.550174
 C    4.625176   -1.240643    2.657829
Cu    0.905229    0.797313   -0.351975
 N   -0.488631    2.314365    1.718627
 N    1.275220    1.321773    2.495371
 C    1.258485   -0.085053   -2.181693
 C   -0.101741   -0.584776   -1.949713
 H    0.539571    1.270941    4.480794
 H   -0.513756    3.765137    3.268825
 H    1.312781    0.664868   -2.976640
 C   -0.396843   -1.847829   -1.307389
 C   -1.196082    0.144370   -2.569311
 O    0.688689   -2.443386   -0.772927
 O   -1.492144   -2.388312   -1.203002
 O   -2.375970   -0.181388   -2.622569
 O   -0.802841    1.312357   -3.119330
 C   -1.800230    2.095230   -3.749181
 H   -2.268008    1.549534   -4.581296
 H   -1.290426    2.987546   -4.129739
 H   -2.576620    2.387796   -3.030063
 C    0.493062   -3.703723   -0.156480
 H   -0.282138   -3.649166    0.620567
 H    1.456626   -3.973529    0.290846
 H    0.197748   -4.461685   -0.896220
 C    2.441643   -0.352692   -1.540524
 H    2.510469   -1.146002   -0.792548
 C    3.737067    0.296129   -1.981279
 H    3.589078    0.710172   -2.990646
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 C    4.869718   -0.710647   -2.056047
 C    5.535250   -0.945598   -3.262917
 C    5.275323   -1.420791   -0.918317
 C    6.580374   -1.867712   -3.336509
 H    5.229693   -0.401475   -4.160727
 C    6.318928   -2.341644   -0.988044
 H    4.768475   -1.254981    0.036051
 C    6.975713   -2.568841   -2.198633
 H    7.085608   -2.038790   -4.289774
 H    6.620467   -2.886854   -0.091068
 H    7.791261   -3.293221   -2.253476
 C    2.332763    3.455050   -1.244122
 H    1.601813    4.237863   -1.335575
 C    3.162002    2.578173   -1.140254
 C    4.133967    1.488864   -1.070538
 H    5.123751    1.867303   -1.371976
 H    4.224346    1.144274   -0.027886
 C    3.326283   -1.757997    2.637301
 H    3.179777   -2.841355    2.667575
 C    4.790240    0.146297    2.609312
 H    5.800046    0.566161    2.603187
 C    0.813382   -1.498787    2.571108
 H    0.167421   -1.018678    3.321067
 H    0.338989   -1.339237    1.590897
 H    0.828128   -2.578155    2.768971
 C    3.899263    2.506150    2.472725
 H    3.225123    2.959251    1.730765
 H    3.698198    2.988650    3.442558
 H    4.933997    2.747403    2.194806
 C   -1.577927    2.605041    0.844178
 C   -1.690030    3.883590    0.278264
 C   -2.532811    1.604182    0.600991
 C   -2.783279    4.141540   -0.552875
 C   -3.611751    1.908741   -0.230700
 C   -3.755144    3.170516   -0.812776
 H   -4.351919    1.126797   -0.417172
 C   -0.671425    4.953431    0.569178
 H   -0.625543    5.688295   -0.246277
 H   -0.928627    5.503158    1.489386
 H    0.329646    4.524459    0.716537
 C   -2.396633    0.227014    1.186041
 H   -1.697683   -0.369513    0.577922
 H   -1.991340    0.246094    2.207726
 H   -3.360731   -0.297497    1.200994
 C    5.817832   -2.155819    2.746123
 H    6.076246   -2.354137    3.798751
 H    5.615735   -3.126075    2.270316
 H    6.701797   -1.709923    2.268482
 C   -4.942550    3.479571   -1.687117
 H   -4.700213    4.240426   -2.442924
 H   -5.302177    2.578074   -2.203519
 H   -5.779370    3.868452   -1.084703
 H   -2.876400    5.130065   -1.012230
Na   -3.627937   -1.683062   -1.499843
 B   -5.256376   -2.355059    0.733585
 O   -5.280071   -1.072405   -0.043071
 O   -4.458195   -2.330831    1.954794
 O   -4.560255   -3.345305   -0.135619
 C   -3.327401   -3.137273    1.801032
 C   -3.693370   -4.099623    0.666919
 O   -6.659735   -2.616461    1.019374
 C   -6.581870   -0.558097   -0.028942
 C   -7.452288   -1.794164    0.218922
 H   -3.080891   -3.662299    2.740634
 H   -2.439928   -2.537881    1.507877
 H   -4.201652   -5.001171    1.064501
 H   -2.811536   -4.424737    0.091140
 H   -6.817836   -0.049419   -0.979530
 H   -6.706996    0.180615    0.788200
 H   -7.702656   -2.282271   -0.747177
 H   -8.404439   -1.547963    0.719769
106
Figure_S10-1_PA-SIMes(Naborate)-ed(1,4AA) / electronic energy: -4167.73112443 a.u. / lowest freq: 14.64 cm-1
 H    2.828236    4.129247    1.574539
 C    2.785534    3.370824    0.787306
 H    0.673226    4.933337    0.988284
 H    0.431128    2.954346    3.888704
 H    2.008889    2.488474    3.149785
 C    1.600278    3.221723    0.061221
 C    0.391794    4.058409    0.387007
 H   -2.422259    4.716065    2.716256
 H    1.381157    1.582551    4.564465
 C    1.102918    2.123389    3.648797
 H   -0.118940    4.412221   -0.520561
 H   -2.416532    3.473901    4.113955
 H   -0.347032    3.479567    0.964874
 C   -2.498418    3.672146    3.039724
 C    1.565811    2.253446   -0.955045
 O    0.363962    1.275354    2.781123
```

H	0.262083	3.776631	-2.998124
C	-2.696986	2.693425	2.169762
N	0.380539	2.092146	-1.729669
C	0.995899	0.257760	2.203457
C	0.235226	2.677423	-3.070152
H	1.049345	2.358060	-3.733362
H	-3.058791	3.572475	-0.795706
C	-0.750512	1.547972	-1.278359
Cu	-1.233193	0.835593	0.505056
C	-2.814621	1.731802	1.305812
H	-3.382251	3.870221	-2.517985
H	-1.464674	-0.131152	2.854554
C	-3.787831	3.409235	-1.604527
H	-4.715143	3.935412	-1.342618
C	0.051257	-0.590088	1.418172
C	-1.134697	2.147144	-3.509063
H	-1.789482	2.931969	-3.911214
C	-1.293129	-0.625824	1.897291
H	-3.811514	1.374907	1.008204
N	-1.665899	1.606967	-2.252395
H	-1.056546	1.348029	-4.263494
C	0.672324	-1.516496	0.448235
C	-4.034783	1.936775	-1.781777
C	-2.982194	1.072597	-2.109313
H	-3.722912	-0.846579	2.923959
C	-2.376763	-1.492361	1.443907
C	-3.579410	-1.495669	2.053183
H	-6.125190	2.043281	-1.289911
H	-1.253897	-1.181508	-1.824080
C	-5.298861	1.381085	-1.563432
H	-2.205638	-2.099831	0.557497
O	-0.170487	-2.405785	-0.076540
C	-3.178688	-0.310766	-2.243754
C	-2.030706	-1.215301	-2.600505
H	-1.557398	-0.918377	-3.548671
H	-6.024435	-1.327120	3.111567
C	-5.525151	0.005856	-1.655400
C	-4.756920	-2.267027	1.637118
C	-4.454794	-0.822098	-2.009764
C	-5.977145	-2.058316	2.300610
H	-2.365078	-2.256667	-2.698819
H	-6.853015	-1.087090	-0.365138
H	-3.787537	-3.403591	0.063695
C	-6.873257	-0.587774	-1.347006
H	-0.477759	-3.959889	-1.327757
C	-4.721460	-3.210903	0.595131
H	-7.657946	0.180758	-1.320696
H	-4.620437	-1.899078	-2.098139
C	-7.123296	-2.763337	1.937462
H	-8.062098	-2.582517	2.465137
H	-7.156083	-1.347958	-2.089860
C	-5.864439	-3.914553	0.232298
C	-7.071088	-3.694667	0.901419
H	-5.815436	-4.644613	-0.578514
H	-7.967359	-4.248421	0.614035
H	5.200914	3.664794	1.896521
C	5.153920	2.700692	1.371173
H	5.176208	1.904519	2.133531
H	6.061854	2.589077	0.761829
C	3.909521	2.583029	0.531558
C	3.844141	1.642177	-0.499977
H	4.711449	1.006224	-0.699823
C	2.682594	1.455083	-1.250359
H	3.456476	-0.313210	-2.205979
C	2.645379	0.416631	-2.338788
H	2.773739	0.877097	-3.332112
H	1.685820	-0.119894	-2.342511
O	1.843529	-1.501764	0.125696
H	0.739242	-2.772587	-1.914248
O	2.187669	0.077190	2.349376
C	0.356169	-3.312628	-1.037172
H	1.167472	-3.910873	-0.602277
Na	3.849689	-0.875718	1.086586
B	5.864598	-2.063255	-0.500210
O	5.904373	-0.685234	0.064498
O	5.239970	-2.180542	-1.814245
O	4.964256	-2.850930	0.392036
C	4.178486	-3.092567	-1.767866
C	4.326078	-3.799959	-0.412988
O	7.259475	-2.483972	-0.515983
C	7.235478	-0.324395	0.311407
C	7.975545	-1.666607	0.358022
H	4.221024	-3.802881	-2.613059
H	3.206051	-2.566215	-1.815843
H	4.942223	-4.716413	-0.511754
H	3.356198	-4.093202	0.022243
H	7.325830	0.243242	1.253110
H	7.626718	0.314015	-0.505351
H	7.968846	-2.069415	1.393277

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 H    9.030639   -1.576405    0.047354
106
Figure_S10-1_PA-SIMes(Naborate)-ts(1,4AA) / electronic energy: -4167.71268692 a.u. / lowest freq: -301.99 cm-1
 H   -6.638772   -1.150855   -1.344087
 H   -8.128633   -2.622996    0.461905
 H   -6.810409   -0.597595    0.345837
 C   -6.440553   -1.424312   -0.293386
 H   -7.118716   -3.442050   -0.760025
 C   -7.090517   -2.751528    0.109850
 O   -5.075453   -1.648501   -0.080185
Na   -3.144267   -2.136720   -1.210925
 O   -6.270268   -3.239930    1.126867
 B   -4.915652   -2.744319    0.930088
 O   -3.938717   -3.704053    0.341800
 O   -4.303644   -2.344309    2.192723
 H   -3.458677   -5.020945    1.873248
 C   -3.068312   -4.119599    1.359344
 C   -3.035829   -2.920195    2.311017
 H   -2.825686   -3.210827    3.355400
 H   -2.239973   -2.214906    1.992262
 H   -2.074055   -4.357520    0.948167
 C   -1.230774    3.298087    2.588593
 H   -2.135400    2.874697    3.050862
 C    0.061414    2.867173    3.304485
 H    0.676782    3.724355    3.615066
 C    0.075522    2.042476    1.112445
 C    1.952959    1.354866    2.466226
 C    1.863736    0.001803    2.830508
 C    3.185805    1.983221    2.249161
 C    4.299314   -0.131606    2.747077
Cu    0.760382    1.132167   -0.448305
 N   -1.050093    2.745433    1.238385
 N    0.745928    2.088959    2.265661
 C    1.609395   -0.040422   -1.926403
 C    0.273117   -0.589300   -1.554415
 H   -0.128436    2.247535    4.193257
 H   -1.349685    4.390079    2.548507
 H    1.637307    0.216104   -2.987065
 C    0.062852   -1.726060   -0.669182
 C   -0.858885   -0.141224   -2.364903
 O    1.138103   -2.059225    0.061093
 O   -0.973415   -2.365465   -0.550208
 O   -1.981432   -0.618651   -2.422829
 O   -0.548500    0.943774   -3.098328
 C   -1.577802    1.496164   -3.903148
 H   -1.913300    0.775006   -4.661665
 H   -1.141583    2.375633   -4.389109
 H   -2.432964    1.794668   -3.282342
 C    1.049023   -3.237344    0.843521
 H    0.212829   -3.181520    1.553567
 H    1.999136   -3.310977    1.383957
 H    0.912906   -4.121411    0.204256
 C    2.864278   -0.683492   -1.467762
 H    3.026396   -0.760868   -0.391129
 C    3.792546   -1.127030   -2.324360
 H    3.591655   -1.060730   -3.400060
 C    5.084020   -1.731417   -1.952792
 C    5.794381   -2.473193   -2.908717
 C    5.644526   -1.587172   -0.671754
 C    7.013760   -3.071164   -2.594786
 H    5.377061   -2.588342   -3.912651
 C    6.862852   -2.182794   -0.358553
 H    5.129502   -0.984935    0.080547
 C    7.552167   -2.930008   -1.316664
 H    7.546605   -3.648553   -3.353637
 H    7.285711   -2.055458    0.640494
 H    8.509038   -3.393971   -1.068098
 C    2.110130    1.963819   -1.687546
 H    1.540410    2.590620   -2.385122
 C    3.370635    2.192172   -1.454844
 C    4.660653    2.318829   -1.238396
 H    5.049708    2.905523   -0.401063
 H    5.385078    1.833431   -1.901371
 C    3.049191   -0.722268    2.961690
 H    2.996839   -1.777805    3.243534
 C    4.347375    1.218940    2.391308
 H    5.317093    1.693106    2.216519
 C    0.522513   -0.645353    3.044939
 H   -0.112998   -0.056323    3.722088
 H   -0.023637   -0.734504    2.093654
 H    0.632937   -1.650510    3.471409
 C    3.240006    3.431580    1.847213
 H    2.738021    3.581489    0.878616
 H    2.733010    4.074620    2.582047
 H    4.277589    3.779227    1.757750
 C   -2.108604    2.713961    0.280851
 C   -2.298435    3.802309   -0.580429
 C   -2.944003    1.585861    0.243788
 C   -3.372154    3.752554   -1.474945
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 C   -4.000728    1.577118   -0.666680
 C   -4.234681    2.653372   -1.527605
 H   -3.532174    4.593570   -2.155784
 H   -4.645225    0.695024   -0.696970
 C    5.561563   -0.932776    2.930383
 H    5.794088   -1.052168    4.000530
 H    5.457775   -1.942323    2.505938
 H    6.422974   -0.442712    2.455099
 C   -2.681989    0.394037    1.120174
 H   -1.834371   -0.181281    0.713469
 H   -2.408798    0.680067    2.146259
 H   -3.550083   -0.275990    1.164062
 C   -1.352455    4.973102   -0.552212
 H   -1.390069    5.501521    0.413012
 H   -0.312934    4.640320   -0.696819
 H   -1.596898    5.697143   -1.340466
 C   -5.370180    2.596997   -2.515814
 H   -5.161038    1.857259   -3.305463
 H   -6.306495    2.289880   -2.026773
 H   -5.536526    3.568910   -3.000497
106
Figure_S10-1_PA-SIMes(Naborate)-prod(1,4AA) / electronic energy: -4167.75978235 a.u. / lowest freq: 13.88 cm-1
 H    6.396640   -1.868249    0.915764
 H    7.547323   -3.495233   -1.004734
 H    6.587205   -1.287813   -0.762850
 C    6.113382   -2.066787   -0.132258
 H    6.472419   -4.184142    0.241099
 C    6.518922   -3.466426   -0.605223
 O    4.721943   -2.057289   -0.287417
Na    2.777355   -2.252702    0.912131
 O    5.586348   -3.777277   -1.595027
 B    4.341497   -3.076209   -1.317931
 O    3.246728   -3.881409   -0.707362
 O    3.746830   -2.538728   -2.538836
 H    2.487919   -5.047511   -2.249066
 C    2.274928   -4.114089   -1.690136
 C    2.397554   -2.892197   -2.605526
 H    2.089955   -3.104054   -3.644531
 H    1.746932   -2.074901   -2.226029
 H    1.276082   -4.202608   -1.233530
 C    1.454766    3.808032   -2.299716
 H    2.264705    3.451357   -2.952812
 C    0.057610    3.608127   -2.919652
 H   -0.498587    4.551161   -3.020310
 C    0.208915    2.373480   -0.941095
 C   -1.897853    2.159905   -2.102715
 C   -2.034718    0.889368   -2.678810
 C   -3.005713    2.878353   -1.625604
 C   -4.446439    1.034291   -2.321795
Cu   -0.183281    1.060946    0.399694
 N    1.383395    2.985707   -1.085191
 N   -0.592051    2.716980   -1.949018
 C   -1.840382   -0.140893    2.345189
 C   -0.472959   -0.479144    1.667700
 H    0.096339    3.130750   -3.910008
 H    1.656456    4.859131   -2.047995
 H   -1.802741   -0.562920    3.364515
 C   -0.383737   -1.571569    0.680395
 C    0.715286   -0.327976    2.517199
 O   -1.407162   -1.584189   -0.190365
 O    0.514089   -2.392128    0.564678
 O    1.851090   -0.724784    2.290456
 O    0.470190    0.379810    3.633454
 C    1.593064    0.747878    4.418148
 H    2.102928   -0.138262    4.820579
 H    1.202203    1.358771    5.239265
 H    2.309665    1.331575    3.821025
 C   -1.475890   -2.664704   -1.102771
 H   -0.596160   -2.682542   -1.761479
 H   -2.383867   -2.500819   -1.693651
 H   -1.545012   -3.625234   -0.572493
 C   -3.041123   -0.725429    1.656926
 H   -3.302357   -0.267897    0.698456
 C   -3.781429   -1.723932    2.147970
 H   -3.519496   -2.147497    3.124731
 C   -4.942661   -2.338005    1.477110
 C   -5.789389   -3.188448    2.204246
 C   -5.232091   -2.119659    0.118770
 C   -6.895519   -3.789440    1.605202
 H   -5.577021   -3.377374    3.259988
 C   -6.336338   -2.719588   -0.480330
 H   -4.578870   -1.480889   -0.481036
 C   -7.174933   -3.556215    0.259408
 H   -7.541530   -4.444343    2.194356
 H   -6.541495   -2.538484   -1.537852
 H   -8.038842   -4.027502   -0.214221
 C   -2.022094    1.368097    2.504979
 H   -1.164879    1.924362    2.899354
 C   -3.138697    2.013296    2.264166
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 C   -4.262325    2.644815    2.038997
 H   -4.491876    3.061834    1.054320
 H   -5.010781    2.764884    2.829064
 C   -3.319788    0.346032   -2.776523
 H   -3.442886   -0.641939   -3.229374
 C   -4.268698    2.299783   -1.750173
 H   -5.143483    2.848964   -1.389837
 C   -0.828714    0.117547   -3.141499
 H   -0.180177    0.718648   -3.795514
 H   -0.215919   -0.191636   -2.280377
 H   -1.123308   -0.787528   -3.688017
 C   -2.815625    4.211914   -0.954642
 H   -2.275058    4.088402   -0.002332
 H   -2.227267    4.903911   -1.574462
 H   -3.781088    4.688972   -0.740094
 C    2.491400    2.703962   -0.228372
 C    2.853935    3.625909    0.762721
 C    3.150389    1.469671   -0.365852
 C    3.901964    3.286361    1.625263
 C    4.187101    1.173437    0.517590
 C    4.575079    2.066650    1.520877
 H    4.188065    3.992778    2.409814
 H    4.680967    0.203831    0.420519
 C   -5.825899    0.442940   -2.442599
 H   -6.484698    1.098350   -3.032367
 H   -5.799972   -0.540396   -2.932004
 H   -6.289992    0.318494   -1.452087
 C    2.712904    0.457255   -1.387832
 H    1.780763   -0.028742   -1.050998
 H    2.490237    0.917027   -2.361813
 H    3.461838   -0.333444   -1.525914
 C    2.119033    4.931484    0.909307
 H    2.421248    5.651936    0.132329
 H    1.032373    4.787506    0.815887
 H    2.325111    5.393098    1.883985
 C    5.686187    1.698818    2.468814
 H    5.465102    0.748363    2.978422
 H    6.636150    1.562167    1.929334
 H    5.839228    2.470741    3.235760
106
Figure_S10-1_PA-SIMes(Naborate)-ed(1,4) / electronic energy: -4167.72594722 a.u. / lowest freq: -12.73 cm-1
 H   -0.748540   -1.415425    3.403760
 H   -0.221270   -1.364166    5.110248
 C    0.127467   -1.283929    4.062046
 H    1.118179   -3.235967    4.334915
 C    1.243489   -2.292200    3.776960
 O    0.741111   -0.042830    3.828331
 H    1.256334   -2.538821    2.694472
 O    2.409713   -1.627654    4.160802
Na    0.942673    0.455368    1.584604
 B    2.207485   -0.190692    4.030600
 O    2.799677    0.531326    5.143173
 O    2.850661    0.439284    2.816637
 C    3.647067    1.534618    4.672005
 H    4.535918    1.644172    5.317171
 C    4.008314    1.091203    3.252262
 H    4.872723    0.396771    3.262284
 H    4.264857    1.938535    2.593254
 H    3.135167    2.519297    4.640537
 H    5.397836    0.342660   -1.107460
 H    4.584030    2.590437   -1.343638
 C    4.540336    0.565787   -0.458237
 C    4.107830    2.037942   -0.517676
 H    4.783539    0.250729    0.566481
 N    3.337885   -0.134490   -0.934284
 N    2.662895    1.928162   -0.760403
 H    4.312859    2.580459    0.415223
 H    4.851095   -2.020454    1.272093
 H    2.184537    4.221900    2.088853
 C    3.765476   -2.170500    1.145867
 C    1.670776    3.388293    1.587124
 H    3.275011   -1.259303    1.509977
 H    2.329231    2.515133    1.654173
 H    3.476159   -2.988535    1.817729
 H   -0.604056   -3.292106   -4.450203
 H   -5.876938   -2.468078    0.518588
 C   -5.935689   -1.376424    0.440713
 C   -7.291979   -0.821351    0.467717
 C   -7.557695    0.551196    0.315002
 H   -8.185385   -2.765838    0.772756
 C   -8.375119   -1.696132    0.653510
 C   -8.863409    1.027661    0.351267
 H   -9.052683    2.095978    0.228457
 C   -9.682909   -1.218186    0.691769
 C   -9.930330    0.145438    0.540540
 H  -10.511130   -1.914355    0.838917
 H  -10.954244    0.524236    0.569022
 H    3.300880   -1.312771   -4.686293
 H    3.674609   -0.003551   -3.534815
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 C    3.015551   -0.861519   -3.726600
 H    1.990740   -0.470962   -3.832939
 H    2.755663   -3.514280   -3.977609
 C    3.087865   -1.883376   -2.622825
 C    2.940237   -3.235699   -2.936306
 H   -1.897402    0.142280   -2.963452
 C    3.295404   -1.524494   -1.276168
 C    2.286461    0.680068   -1.079526
 C    3.026228   -4.234179   -1.964360
 C   -1.012516   -0.466596   -2.721770
Cu    0.558542    0.137753   -1.768426
 C    3.444273   -2.506784   -0.282260
 C    3.304518   -3.847953   -0.653073
 H    0.459575   -3.569495   -0.805710
 H    3.399259   -4.613845    0.122044
 C   -0.262083   -3.913010   -0.051364
 O    0.055664   -1.403784    0.592734
 H   -0.686368   -4.879914   -0.339703
 C   -1.077578   -1.756962    0.326515
 H    0.239474   -3.990415    0.923116
 O   -1.363362   -3.009742    0.020414
 C   -2.262560   -0.857457    0.293553
 H    1.929729    3.378710   -4.360909
 H    3.118085    2.535050   -3.336878
 C    2.050244    2.767627   -3.457078
 H    1.528278    1.811885   -3.621434
 H    0.354902    4.862872   -3.430957
 C    1.491934    3.475844   -2.252258
 C    0.617508    4.549627   -2.416541
 C    1.815500    3.067741   -0.942521
 C    0.075287    5.237202   -1.325312
 C   -1.038691   -1.709676   -3.118441
 C    1.317856    3.758884    0.171641
 C    0.451141    4.835720   -0.044932
 C   -1.015720   -2.981222   -3.484234
 H   -1.415814   -3.762562   -2.829694
 H    0.051294    5.366017    0.824184
 H   -1.462009    2.740684   -1.226420
 H    0.761214    3.179763    2.170640
 H   -3.222407    3.009601   -1.505640
 C   -2.471258    2.642631   -0.799450
 O   -2.776663    1.265870   -0.584110
 C   -1.968437    0.602274    0.223271
 C   -3.512329   -1.384601    0.327755
 H   -3.569091   -2.475164    0.389669
 O   -1.070410    1.153006    0.828677
 H   -2.518912    3.204961    0.142707
 C   -4.777577   -0.689014    0.338299
 H   -4.773406    0.398520    0.259295
 H   -6.738571    1.256535    0.162329
 C   -0.913274    6.353800   -1.532506
 C    2.798070   -5.678096   -2.324478
 H    3.167780   -6.355135   -1.542016
 H    3.294130   -5.938344   -3.270940
 H    1.721785   -5.874245   -2.457529
 H   -0.909704    7.059190   -0.689981
 H   -1.934875    5.949936   -1.622554
 H   -0.701256    6.912314   -2.455251
106
Figure_S10-1_PA-SIMes(Naborate)-ts(1,4) / electronic energy: -4167.70362749 a.u. / lowest freq: -447.01 cm-1
 H   -0.305055   -3.103406    2.122030
 H    0.147868   -3.833233    3.688376
 C    0.494787   -3.158934    2.880176
 H    1.916605   -4.746328    2.308253
 C    1.825078   -3.646233    2.299517
 O    0.800796   -1.886899    3.379936
 H    1.921060   -3.310171    1.245483
 O    2.797038   -3.052091    3.107498
Na    0.937158   -0.091943    1.925858
 B    2.250658   -1.846175    3.726259
 O    2.579462   -1.787726    5.142597
 O    2.760230   -0.541969    3.185023
 C    3.010399   -0.502125    5.471212
 H    3.766823   -0.527540    6.274626
 C    3.567693    0.054745    4.158824
 H    4.629475   -0.236934    4.028571
 H    3.513068    1.154975    4.101276
 H    2.170812    0.132751    5.827042
 H    5.150670    1.357224   -2.304530
 H    4.312009    3.439572   -1.492195
 C    4.625163    1.258460   -1.343146
 C    4.091846    2.599221   -0.816718
 H    5.302845    0.764245   -0.632827
 N    3.394461    0.477121   -1.515495
 N    2.643684    2.362107   -0.759089
 H    4.485101    2.852648    0.178699
 H    5.230038   -1.315834    0.472254
 H    3.203654    3.411170    2.457854
 C    4.146894   -1.518189    0.424543
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 C    2.343623    2.826538    2.093633
 H    3.629851   -0.622754    0.792051
 H    2.743570    1.880009    1.705414
 H    3.930816   -2.318403    1.143976
 H   -3.746273   -1.170258   -3.151059
 H   -5.533958   -2.411471   -0.912876
 C   -5.683061   -1.452011   -0.403480
 C   -7.065156   -1.176783    0.016672
 C   -7.444806    0.011387    0.666052
 H   -7.780938   -3.068624   -0.741409
 C   -8.056463   -2.137902   -0.238600
 C   -8.766483    0.226157    1.042417
 H   -9.040016    1.156144    1.545640
 C   -9.380955   -1.923365    0.138006
 C   -9.741238   -0.739768    0.780539
 H  -10.134883   -2.685259   -0.071495
 H  -10.778395   -0.567831    1.076151
 H    2.621904   -0.563090   -5.246414
 H    3.542275    0.617354   -4.276765
 C    2.746716   -0.141968   -4.240263
 H    1.817852    0.380960   -3.969314
 H    2.767641   -2.836632   -4.624738
 C    3.064387   -1.220324   -3.239145
 C    3.033417   -2.569558   -3.597896
 H   -0.448164    1.008468   -3.843279
 C    3.400030   -0.893221   -1.915438
 C    2.282950    1.145723   -1.186336
 C    3.336960   -3.581924   -2.681438
 C   -0.905809    0.545993   -2.960059
Cu    0.464094    0.451167   -1.489131
 C    3.737326   -1.879281   -0.975404
 C    3.694703   -3.216131   -1.381858
 H    0.675213   -2.758315   -1.970667
 H    3.941140   -3.992780   -0.652200
 C    0.011533   -3.367410   -1.338990
 O    0.264982   -1.204064    0.075898
 H   -0.378245   -4.217571   -1.908542
 C   -0.892348   -1.483258   -0.268150
 H    0.581911   -3.722368   -0.470184
 O   -1.124254   -2.616064   -0.932450
 C   -2.068658   -0.666740   -0.042107
 H    0.720938    4.626549   -3.349103
 H    2.282010    3.831135   -3.016643
 C    1.216096    3.855356   -2.744795
 H    0.792074    2.877964   -3.018861
 H   -0.415047    5.682569   -1.562735
 C    1.026444    4.116136   -1.274938
 C    0.142999    5.096727   -0.826734
 C    1.731625    3.364597   -0.316438
 C   -0.045194    5.352948    0.537268
 C   -2.123064    0.175454   -2.940293
 C    1.573553    3.599461    1.055814
 C    0.679301    4.597922    1.458251
 C   -3.391914   -0.241756   -2.694000
 H   -4.152436    0.523023   -2.512549
 H    0.540985    4.779508    2.527794
 H   -1.770804    3.305192    0.377988
 H    1.712526    2.609255    2.967847
 H   -3.567308    3.392668    0.428388
 C   -2.685862    2.838426    0.768834
 O   -2.829292    1.522247    0.256947
 C   -1.875749    0.641383    0.576413
 C   -3.276592   -1.063473   -0.655535
 H   -3.241290   -2.075859   -1.058436
 O   -0.948258    0.974186    1.303371
 H   -2.641486    2.834240    1.866876
 C   -4.614644   -0.655326   -0.220725
 H   -4.711457    0.310709    0.274057
 H   -6.699976    0.779943    0.881556
 C   -1.029929    6.399227    0.988276
 C    3.242216   -5.032290   -3.076433
 H    3.923146   -5.657010   -2.481615
 H    3.476296   -5.177350   -4.140599
 H    2.220557   -5.411904   -2.911611
 H   -0.941610    6.597811    2.064994
 H   -2.063546    6.073750    0.789394
 H   -0.880121    7.346575    0.449472
106
Figure_S10-1_PA-SIMes(Naborate)-prod(1,4) / electronic energy: -4167.77405497 a.u. / lowest freq: 15.51 cm-1
 H    0.194828   -3.917143    1.927800
 H    1.325519   -4.388355    3.229844
 C    1.073225   -3.587088    2.507921
 H    2.919356   -4.124265    1.427722
 C    2.269677   -3.252575    1.612336
 O    0.804590   -2.382978    3.180505
 H    1.920596   -2.875110    0.632386
 O    2.958198   -2.260200    2.321580
Na   -0.773499   -0.915696    2.453272
 B    2.010478   -1.522080    3.114848
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O	2.560109	-1.086387	4.381209
O	1.537352	-0.201231	2.483400
C	2.246611	0.252390	4.618354
H	3.036619	0.748257	5.206929
C	2.096441	0.857268	3.225076
H	3.085185	1.135658	2.813155
H	1.446026	1.746086	3.191466
H	1.295899	0.356789	5.182987
H	3.936077	1.038280	-3.488244
H	2.942411	3.147936	-2.985937
C	4.032234	1.311881	-2.426929
C	3.421531	2.683406	-2.110146
H	5.098101	1.247310	-2.158761
N	3.235875	0.413926	-1.584922
N	2.417971	2.353633	-1.091669
H	4.158672	3.396379	-1.712051
H	5.446112	0.340768	0.000330
H	4.125445	4.283099	0.595243
C	4.990220	-0.554820	0.448359
C	3.307827	3.849422	1.193603
H	4.184397	-0.228505	1.123378
H	3.505783	2.771993	1.281312
H	5.746946	-1.069094	1.054297
H	-4.139904	0.641821	-3.374033
H	-5.080127	-2.279895	-1.283099
C	-5.365516	-1.325793	-0.823114
C	-6.653588	-1.343730	-0.102055
C	-7.220771	-0.199564	0.485584
H	-6.932535	-3.457028	-0.442609
C	-7.354158	-2.555067	0.009284
C	-8.436099	-0.269478	1.160175
H	-8.858041	0.633640	1.607255
C	-8.571227	-2.627567	0.685579
C	-9.118148	-1.484008	1.265300
H	-9.094002	-3.583902	0.759454
H	-10.072313	-1.536050	1.794126
H	1.384386	-2.080470	-4.011706
H	2.207293	-0.502762	-4.029131
C	1.799097	-1.288040	-3.374306
H	0.967545	-0.832152	-2.813183
H	2.643129	-3.872535	-3.096616
C	2.840199	-1.834495	-2.435299
C	3.147062	-3.197674	-2.398517
H	-0.451288	-0.037313	-5.307424
C	3.493760	-0.986217	-1.531971
C	2.329933	1.042409	-0.823386
C	4.070971	-3.717219	-1.487757
C	-1.230573	0.171874	-4.597558
Cu	1.223505	0.148802	0.457884
C	4.406549	-1.475773	-0.585656
C	4.687192	-2.841843	-0.589183
H	0.615175	-3.173911	-1.474180
H	5.388935	-3.237473	0.150184
C	-0.440293	-3.461434	-1.375787
O	-0.155139	-1.429529	0.191103
H	-0.720569	-4.141259	-2.188677
C	-1.104190	-1.328619	-0.621636
H	-0.573454	-3.967600	-0.407895
O	-1.297699	-2.341570	-1.488446
C	-2.028550	-0.258738	-0.721461
H	-1.060615	3.074623	-2.760657
H	0.629978	2.643373	-3.108157
C	-0.129172	2.703640	-2.314027
H	-0.304307	1.672355	-1.968732
H	-1.463488	4.776764	-1.154011
C	0.314644	3.573666	-1.173231
C	-0.496277	4.592742	-0.677579
C	1.554594	3.349506	-0.553368
C	-0.115070	5.366428	0.424769
C	-2.105923	0.412266	-3.796583
C	1.971302	4.103814	0.550505
C	1.115826	5.102783	1.028740
C	-3.177499	0.671992	-2.836693
H	-3.071336	1.687226	-2.424992
H	1.425285	5.692309	1.896661
H	-1.842276	3.288165	1.171192
H	3.357495	4.297362	2.195029
H	-3.512115	3.609962	0.592799
C	-2.826157	2.844261	0.974395
O	-2.751503	1.846442	-0.026546
C	-1.866460	0.841227	0.171204
C	-3.210031	-0.356254	-1.677541
H	-3.152456	-1.348971	-2.140371
O	-1.034801	0.954103	1.088753
H	-3.227967	2.426710	1.911022
C	-4.530144	-0.286622	-0.949916
H	-4.774400	0.678760	-0.496868
H	-6.709129	0.762375	0.411517
C	-1.038007	6.429676	0.959728

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 C    4.358258   -5.194616   -1.431167
 H    5.430287   -5.388712   -1.281471
 H    4.038534   -5.705405   -2.350089
 H    3.823631   -5.659741   -0.586774
 H   -1.936621    5.975081    1.406811
 H   -1.379966    7.101335    0.158194
 H   -0.549845    7.038400    1.733104
32
Figure_S10-1_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C   -0.660544   -0.726572    0.059153
 C   -1.860539   -0.097447    0.115996
 H   -0.691600   -1.818492   -0.004770
 C   -1.976243    1.390665    0.160143
 C   -3.120576   -0.891785    0.187355
 O   -3.041424    1.823605   -0.507466
 O   -1.182749    2.134043    0.689285
 O   -4.147702   -0.497504    0.683440
 O   -2.981802   -2.118850   -0.320932
 C   -4.097604   -2.989729   -0.195724
 H   -4.332384   -3.170881    0.862818
 H   -3.810049   -3.927003   -0.683244
 H   -4.981752   -2.562067   -0.688186
 C   -3.254671    3.228152   -0.535442
 H   -3.354009    3.627502    0.483524
 H   -4.184056    3.384216   -1.092621
 H   -2.420438    3.737793   -1.038016
 C    0.656646   -0.129211    0.062308
 H    0.725624    0.955889    0.150505
 C    1.759981   -0.902956   -0.019704
 H    1.621029   -1.988149   -0.089650
 C    3.156351   -0.453635   -0.025165
 C    4.175093   -1.416830   -0.109525
 C    3.522207    0.902114    0.053056
 C    5.517020   -1.042840   -0.114390
 H    3.907556   -2.474776   -0.172060
 C    4.861836    1.275255    0.048166
 H    2.754752    1.675486    0.118691
 C    5.863995    0.305241   -0.035401
 H    6.294080   -1.807149   -0.179427
 H    5.127957    2.332459    0.111300
 H    6.914980    0.602284   -0.038425
50
Figure_S10-1_dienoate-Naborate / electronic energy: -1486.89608401 a.u. / lowest freq: 15.45 cm-1
 H   -4.420128    2.087873    2.299924
 H   -5.923773   -2.547792    1.430468
 C   -3.899637    1.709040    1.397197
 O   -6.388627   -0.555754    1.056848
 H   -2.832933    1.979558    1.487735
 O   -4.052556    0.323170    1.268895
 C   -6.462160   -1.902837    0.702697
 H   -7.509160   -2.251286    0.668862
Na   -2.589162   -0.954460    0.028443
 B   -5.242902    0.056168    0.401101
 C   -4.549382    2.260434    0.125108
 H   -4.940007    3.284567    0.257486
 O   -5.580090    1.360046   -0.149654
 C   -5.777159   -1.970930   -0.665207
 O   -4.794555   -0.975836   -0.589590
 H   -3.802053    2.287356   -0.695287
 H   -6.503487   -1.753783   -1.474182
 H   -5.329092   -2.957849   -0.872632
 C    2.217972    0.782767   -0.357663
 C    0.968244    0.253780   -0.477916
 H    2.268783    1.873090   -0.426363
 C    0.656300   -1.199329   -0.386928
 C   -0.192151    1.162783   -0.688524
 O    1.634875   -1.973268   -0.831358
 O   -0.381350   -1.656994    0.046156
 O   -1.335622    0.796830   -0.869352
 O    0.144585    2.445194   -0.682767
 C   -0.892656    3.394615   -0.904656
 H   -1.373335    3.224078   -1.877338
 H   -0.410674    4.376881   -0.885452
 H   -1.650282    3.328425   -0.112354
 C    1.442759   -3.383139   -0.742768
 H    1.291967   -3.686873    0.301829
 H    2.354400   -3.836025   -1.144545
 H    0.572193   -3.688467   -1.338576
 C    3.478653    0.126613   -0.118869
 H    3.499709   -0.957579   -0.015571
 C    4.611174    0.860860   -0.028545
 H    4.527241    1.946558   -0.152174
 C    5.966988    0.366461    0.217775
 C    7.021202    1.293347    0.272402
 C    6.260030   -0.996390    0.405467
 C    8.328905    0.875902    0.507087
 H    6.809143    2.355652    0.127725
 C    7.565616   -1.412370    0.640052
 H    5.462269   -1.740462    0.369434
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 C    8.603756   -0.478381    0.691959
 H    9.135264    1.610831    0.545810
 H    7.777281   -2.473596    0.785169
 H    9.627956   -0.809398    0.876235
41
Figure_S10-1_PPh3-Cu-allenyl / electronic energy: -2791.78064609 a.u. / lowest freq: -8.52 cm-1
Cu    1.925957    0.441034   -0.969324
 C    3.695423    0.782212   -1.650311
 H    3.901621    1.250294   -2.626132
 C    4.739409    0.464057   -0.934464
 C    5.764894    0.124180   -0.171645
 H    6.228054   -0.865398   -0.246897
 H    6.190086    0.825011    0.554818
 P   -0.093017    0.040978   -0.106258
 C   -0.713342    1.391986    0.957863
 C   -1.380331    1.168166    2.166791
 C   -0.511650    2.705927    0.513218
 C   -1.849259    2.247854    2.915852
 H   -1.535294    0.149778    2.529631
 C   -0.989950    3.780817    1.258089
 H    0.022539    2.889678   -0.423318
 C   -1.658731    3.552160    2.461671
 H   -2.365753    2.066564    3.860640
 H   -0.832329    4.800736    0.901689
 H   -2.027713    4.394962    3.049984
 C   -0.164393   -1.456811    0.937848
 C   -1.315396   -2.246691    1.042854
 C    0.979917   -1.802657    1.668371
 C   -1.322993   -3.362695    1.878346
 H   -2.210179   -1.992779    0.469631
 C    0.967011   -2.915256    2.507351
 H    1.889455   -1.202122    1.577400
 C   -0.184532   -3.695898    2.612619
 H   -2.223689   -3.975283    1.954422
 H    1.863220   -3.177711    3.073131
 H   -0.192646   -4.571265    3.265682
 C   -1.410845   -0.201190   -1.350523
 C   -2.710237    0.290159   -1.183020
 C   -1.089521   -0.925749   -2.506174
 C   -3.679067    0.050420   -2.157376
 H   -2.969562    0.864064   -0.290291
 C   -2.061407   -1.169847   -3.473746
 H   -0.072030   -1.299724   -2.651497
 C   -3.357069   -0.680980   -3.300219
 H   -4.690190    0.439664   -2.021497
 H   -1.803574   -1.735870   -4.371205
 H   -4.117079   -0.866243   -4.062285
91
Figure_S10-1_PA-PPh3(Naborate)-ed(1,6) / electronic energy: -4278.71914908 a.u. / lowest freq: 17.78 cm-1
Na   -2.695931   -2.493458   -0.662928
 B   -5.288381   -1.991207    0.509827
 O   -4.990905   -2.090748   -0.960071
 O   -5.841208   -0.728046    0.969819
 O   -3.965261   -2.081441    1.183658
 C   -4.897909   -0.034640    1.728669
 C   -3.889810   -1.102699    2.180923
 O   -6.213687   -3.091901    0.749593
 C   -5.910665   -2.977469   -1.536731
 C   -6.273790   -3.909516   -0.378164
 H   -5.371252    0.474581    2.586939
 H   -4.393781    0.750003    1.128417
 H   -4.174660   -1.518644    3.168078
 H   -2.861523   -0.711751    2.269671
 H   -5.465363   -3.506759   -2.396177
 H   -6.809122   -2.439405   -1.899327
 H   -5.541690   -4.744334   -0.319028
 H   -7.274571   -4.360718   -0.494187
Cu    1.677452    0.602805   -0.644752
 C    2.363867   -1.288113   -1.110241
 C    0.971964   -1.375942   -0.825600
 H    2.605470   -1.177053   -2.170383
 C    0.373438   -1.879181    0.435358
 C    0.052760   -1.309436   -2.000609
 O    1.253003   -2.074599    1.412979
 O   -0.810842   -2.087096    0.602657
 O   -1.002577   -1.894021   -2.123576
 O    0.531948   -0.517478   -2.955827
 C   -0.233605   -0.395604   -4.151123
 H   -0.334371   -1.372445   -4.642980
 H    0.321520    0.296950   -4.791230
 H   -1.229250    0.008401   -3.926082
 C    0.757765   -2.630909    2.628492
 H   -0.080002   -2.037468    3.015672
 H    1.597882   -2.614806    3.330227
 H    0.421217   -3.663395    2.463197
 C    3.489022   -1.656950   -0.274869
 H    3.308913   -1.847493    0.780569
 C    4.732392   -1.746553   -0.793864
 H    4.863209   -1.553170   -1.863608
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 C    5.954559   -2.119115   -0.071000
 C    7.146204   -2.281945   -0.795555
 C    5.988449   -2.320667    1.319663
 C    8.332812   -2.635008   -0.157271
 H    7.138294   -2.124892   -1.877366
 C    7.173029   -2.672908    1.957825
 H    5.081571   -2.192852    1.913748
 C    8.350472   -2.831999    1.223097
 H    9.248820   -2.755249   -0.739569
 H    7.180378   -2.822599    3.039677
 H    9.279400   -3.106078    1.727634
 C    3.195735    1.715604   -1.227739
 H    2.906315    2.653273   -1.728929
 C    4.465315    1.515793   -1.037468
 C    5.741228    1.258160   -0.810570
 H    6.353615    0.722422   -1.542556
 H    6.233260    1.578206    0.113731
 P   -0.091633    1.911733    0.067007
 C   -1.481160    1.761602   -1.108679
 C   -1.494788    2.519576   -2.287359
 C   -2.484882    0.809193   -0.896316
 C   -2.522768    2.354023   -3.213554
 H   -0.708710    3.253340   -2.481139
 C   -3.513393    0.641963   -1.823586
 H   -2.472189    0.198007    0.009950
 C   -3.533979    1.420718   -2.980667
 H   -2.530720    2.957172   -4.123896
 H   -4.286717   -0.108830   -1.631709
 H   -4.339561    1.296341   -3.707426
 C    0.269907    3.703369    0.184314
 C   -0.717895    4.685891    0.031076
 C    1.569329    4.084667    0.539443
 C   -0.405712    6.029334    0.224752
 H   -1.737553    4.407702   -0.245073
 C    1.876985    5.430478    0.737795
 H    2.348051    3.326490    0.652253
 C    0.891779    6.403367    0.578836
 H   -1.180936    6.788250    0.100546
 H    2.894426    5.717183    1.011598
 H    1.133070    7.457611    0.730515
 C   -0.804991    1.565200    1.715540
 C   -0.060787    0.801927    2.619630
 C   -2.020284    2.129019    2.127890
 C   -0.526124    0.600296    3.920147
 H    0.891974    0.364005    2.310488
 C   -2.484418    1.923807    3.423390
 H   -2.613624    2.729158    1.434023
 C   -1.737430    1.158621    4.321484
 H    0.063548    0.005410    4.620593
 H   -3.435436    2.360963    3.733485
 H   -2.103859    0.998145    5.337423
91
Figure_S10-1_PA-PPh3(Naborate)-ts(1,6) / electronic energy: -4278.70801041 a.u. / lowest freq: -446.52 cm-1
Na   -2.723342   -2.381323   -0.647764
 B   -5.309110   -1.909486    0.577168
 O   -5.040664   -2.013536   -0.896953
 O   -5.846173   -0.641325    1.045469
 O   -3.974917   -2.005534    1.225747
 C   -4.889481    0.042513    1.796297
 C   -3.879527   -1.033044    2.226743
 O   -6.236786   -3.004029    0.837239
 C   -5.964228   -2.908342   -1.453824
 C   -6.310475   -3.831272   -0.282656
 H   -5.348361    0.547504    2.664906
 H   -4.390364    0.830301    1.195321
 H   -4.150006   -1.452596    3.216470
 H   -2.848031   -0.648124    2.300969
 H   -5.527729   -3.444185   -2.313777
 H   -6.868899   -2.376588   -1.810595
 H   -5.576301   -4.664324   -0.226244
 H   -7.312092   -4.284721   -0.381820
Cu    1.662642    0.592230   -0.698960
 C    2.382593   -1.360760   -1.125643
 C    0.965609   -1.456857   -0.860145
 H    2.625384   -1.288679   -2.189927
 C    0.378237   -1.954396    0.388651
 C    0.065926   -1.380143   -2.027574
 O    1.275333   -2.176408    1.356182
 O   -0.807387   -2.153092    0.588878
 O   -1.049446   -1.856228   -2.132208
 O    0.611349   -0.686123   -3.036446
 C   -0.152056   -0.561854   -4.228529
 H   -0.327693   -1.547347   -4.681892
 H    0.444902    0.061301   -4.902588
 H   -1.116134   -0.078759   -4.020840
 C    0.789209   -2.740196    2.567493
 H   -0.031010   -2.138820    2.980650
 H    1.639772   -2.753867    3.257412
 H    0.426653   -3.763500    2.396818
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 C    3.485431   -1.509500   -0.272433
 H    3.330114   -1.607750    0.800092
 C    4.784820   -1.475424   -0.789285
 H    4.879311   -1.654871   -1.862906
 C    5.960069   -1.901644    0.006032
 C    7.057233   -2.481198   -0.646526
 C    6.020515   -1.739763    1.399171
 C    8.176761   -2.901364    0.070029
 H    7.028430   -2.609090   -1.732004
 C    7.139199   -2.156327    2.114978
 H    5.190202   -1.267600    1.929148
 C    8.221768   -2.741244    1.454306
 H    9.018696   -3.356158   -0.456542
 H    7.169899   -2.019220    3.198196
 H    9.098883   -3.066881    2.017583
 C    3.155698    1.791784   -1.348804
 H    2.786141    2.789229   -1.596124
 C    4.334271    1.328400   -1.318268
 C    5.465358    0.594055   -1.155405
 H    6.042482    0.304443   -2.038001
 H    6.047724    0.749752   -0.242208
 P   -0.056084    1.906482    0.055904
 C   -1.445031    1.738071   -1.115713
 C   -1.408545    2.418496   -2.340574
 C   -2.487434    0.840384   -0.861951
 C   -2.426134    2.233333   -3.273924
 H   -0.589951    3.106544   -2.566754
 C   -3.505667    0.652925   -1.796819
 H   -2.509356    0.284868    0.078784
 C   -3.476126    1.355017   -3.001320
 H   -2.394910    2.775707   -4.221165
 H   -4.308261   -0.058114   -1.576870
 H   -4.272717    1.212924   -3.734762
 C    0.291239    3.700629    0.170514
 C   -0.666695    4.687392   -0.094965
 C    1.556872    4.079722    0.636504
 C   -0.358384    6.032627    0.098074
 H   -1.659645    4.410929   -0.456512
 C    1.860171    5.425801    0.834643
 H    2.311430    3.317079    0.847130
 C    0.903817    6.403566    0.563136
 H   -1.110844    6.794984   -0.113565
 H    2.849208    5.710154    1.199599
 H    1.141185    7.458660    0.714613
 C   -0.749409    1.554824    1.710112
 C   -0.034193    0.726252    2.579025
 C   -1.923019    2.176615    2.159204
 C   -0.485742    0.520007    3.883772
 H    0.884067    0.241129    2.237931
 C   -2.374912    1.964338    3.457748
 H   -2.490924    2.829661    1.491994
 C   -1.654879    1.136807    4.322401
 H    0.081907   -0.123717    4.558685
 H   -3.293745    2.445845    3.797750
 H   -2.010101    0.972789    5.341757
91
Figure_S10-1_PA-PPh3(Naborate)-prod(1,6) / electronic energy: -4278.76045462 a.u. / lowest freq: 14.94 cm-1
Na   -2.622955   -2.540640   -0.144605
 B   -5.331395   -1.733535    0.530656
 O   -4.853926   -2.129985   -0.838059
 O   -5.908962   -0.402668    0.646337
 O   -4.108728   -1.679818    1.376123
 C   -4.998574    0.455426    1.260834
 C   -4.073703   -0.466642    2.070618
 O   -6.306124   -2.761881    0.869154
 C   -5.725599   -3.104312   -1.341030
 C   -6.259704   -3.784732   -0.078111
 H   -5.513480    1.192417    1.902054
 H   -4.418409    1.035785    0.512703
 H   -4.450785   -0.588237    3.105997
 H   -3.041634   -0.081449    2.139763
 H   -5.196843   -3.798479   -2.016216
 H   -6.555096   -2.641441   -1.912724
 H   -5.571679   -4.600277    0.234174
 H   -7.255440   -4.237335   -0.228323
Cu    2.293872    1.222640    0.006960
 C    2.253912   -1.150912   -0.537993
 C    0.948356   -1.715572   -0.352024
 H    2.545644   -1.133781   -1.593693
 C    0.337808   -1.935653    0.937175
 C    0.242854   -2.196654   -1.526463
 O    1.131949   -1.587774    1.976199
 O   -0.775658   -2.394386    1.168848
 O   -0.866747   -2.717403   -1.564340
 O    0.948113   -2.067846   -2.671363
 C    0.381071   -2.626751   -3.840066
 H    0.269411   -3.716607   -3.741088
 H    1.076811   -2.397602   -4.655546
 H   -0.603136   -2.189257   -4.053233
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 C    0.649447   -1.892621    3.272773
 H   -0.337826   -1.443323    3.446524
 H    1.382822   -1.480531    3.976150
 H    0.567702   -2.979904    3.415201
 C    3.232237   -0.690394    0.324995
 H    3.100976   -0.813980    1.403392
 C    4.661581   -0.503228   -0.166694
 H    4.635435   -0.413959   -1.264736
 C    5.544093   -1.691306    0.175575
 C    6.139255   -2.449645   -0.837362
 C    5.771525   -2.060541    1.507922
 C    6.943169   -3.548707   -0.530883
 H    5.968965   -2.179150   -1.882977
 C    6.574756   -3.155781    1.818302
 H    5.310004   -1.491594    2.319782
 C    7.165036   -3.904170    0.798385
 H    7.398186   -4.128478   -1.337170
 H    6.740133   -3.427282    2.863315
 H    7.794119   -4.763437    1.041022
 C    3.659752    2.902849   -0.200230
 H    3.222018    3.857858   -0.448637
 C    4.355790    1.931531    0.074492
 C    5.255911    0.812708    0.378362
 H    6.251415    1.010259   -0.048053
 H    5.377113    0.753448    1.472013
 P    0.170027    2.035672   -0.166315
 C   -0.833044    1.187643   -1.429164
 C   -0.319945    1.120251   -2.731189
 C   -2.070527    0.602976   -1.149083
 C   -1.064550    0.527464   -3.746720
 H    0.662245    1.544629   -2.957649
 C   -2.808812   -0.008782   -2.162225
 H   -2.465452    0.614916   -0.132108
 C   -2.310070   -0.034463   -3.463417
 H   -0.661306    0.489850   -4.760793
 H   -3.760577   -0.489648   -1.917181
 H   -2.887530   -0.510570   -4.258914
 C    0.097638    3.813907   -0.621378
 C   -0.574584    4.309051   -1.741919
 C    0.755629    4.710468    0.234419
 C   -0.580259    5.680375   -2.006567
 H   -1.104726    3.630502   -2.412646
 C    0.744377    6.076993   -0.029010
 H    1.271291    4.338360    1.124914
 C    0.078143    6.564659   -1.155310
 H   -1.109021    6.056551   -2.884715
 H    1.256703    6.764054    0.647511
 H    0.069918    7.636330   -1.364628
 C   -0.804374    2.020863    1.378901
 C   -0.312609    1.330069    2.489766
 C   -1.997351    2.750066    1.490346
 C   -1.001902    1.370862    3.703008
 H    0.614457    0.758509    2.402636
 C   -2.686167    2.782708    2.698808
 H   -2.385245    3.302518    0.630891
 C   -2.185730    2.097300    3.808037
 H   -0.607872    0.836704    4.569707
 H   -3.617224    3.347261    2.777412
 H   -2.723648    2.129735    4.757645
91
Figure_S10-1_PA-PPh3(Naborate)-ed(1,4AA) / electronic energy: -4278.72067874 a.u. / lowest freq: 13.62 cm-1
Na   3.203491    1.752391   -1.207225
 B   5.510153    2.111525    0.413926
 O   5.387495    1.235304   -0.784571
 O   5.253851    1.449395    1.697562
 O   4.413270    3.112850    0.306956
 C   4.127668    2.006937    2.307548
 C   3.922175    3.348795    1.597519
 O   6.869753    2.627072    0.343358
 C   6.649757    1.093813   -1.372167
 C   7.400651    2.349374   -0.917010
 H   4.272998    2.120000    3.396045
 H   3.233068    1.365548    2.156615
 H   4.495745    4.152260    2.102022
 H   2.862696    3.649227    1.564158
 H   6.569342    1.013094   -2.469470
 H   7.157724    0.179953   -1.003250
 H   7.219365    3.181093   -1.630801
 H   8.491926    2.193157   -0.863682
Cu  -1.840818   -0.390251   -0.446973
 C  -1.903008    1.426687   -1.375833
 C  -0.548897    1.109210   -1.101034
 H  -2.243669    1.173929   -2.384884
 C   0.167882    1.641346    0.089787
 C   0.284519    0.528639   -2.187505
 O  -0.577318    1.562978    1.189742
 O   1.297570    2.075039    0.105018
 O   1.476854    0.689194   -2.333698
 O  -0.434781   -0.231156   -3.010346
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 C    0.247785   -0.835571   -4.105171
 H    0.652940   -0.067423   -4.777681
 H   -0.499793   -1.439945   -4.628343
 H    1.066272   -1.470202   -3.740403
 C   -0.014384    2.054840    2.403980
 H    0.916586    1.521625    2.638735
 H   -0.764416    1.868472    3.178445
 H    0.194735    3.129815    2.320725
 C   -2.747793    2.372009   -0.660158
 H   -2.404876    2.730220    0.311389
 C   -3.932426    2.769268   -1.164593
 H   -4.237760    2.365812   -2.136682
 C   -4.888146    3.695977   -0.545504
 C   -6.090993    3.972355   -1.215720
 C   -4.657471    4.321369    0.692714
 C   -7.033628    4.841934   -0.671426
 H   -6.287212    3.494254   -2.178905
 C   -5.597762    5.190584    1.235630
 H   -3.732285    4.130698    1.240169
 C   -6.790128    5.454636    0.556964
 H   -7.963425    5.040654   -1.208615
 H   -5.400795    5.667427    2.198199
 H   -7.526102    6.137948    0.986011
 C   -3.750167   -0.827175   -0.334735
 H   -4.522475   -0.111631   -0.656472
 C   -4.123909   -1.980034    0.144568
 C   -4.410216   -3.169070    0.641773
 H   -4.486460   -4.048351   -0.006794
 H   -4.561935   -3.315452    1.716169
 P   -0.517266   -2.124543    0.296260
 C   -1.067131   -3.689725   -0.466776
 C   -0.910054   -4.934118    0.151608
 C   -1.667399   -3.616790   -1.729529
 C   -1.349484   -6.092081   -0.487678
 H   -0.454674   -5.005802    1.141480
 C   -2.097304   -4.776362   -2.371113
 H   -1.814680   -2.644547   -2.206976
 C   -1.941899   -6.014887   -1.748701
 H   -1.230526   -7.059922    0.003633
 H   -2.567306   -4.709741   -3.354361
 H   -2.288378   -6.923605   -2.245576
 C   -0.580059   -2.361946    2.103884
 C    0.412933   -3.054815    2.810156
 C   -1.674941   -1.828840    2.796154
 C    0.303461   -3.220291    4.189191
 H    1.281618   -3.460051    2.285716
 C   -1.781668   -1.998632    4.175894
 H   -2.448958   -1.282545    2.250655
 C   -0.793987   -2.694075    4.872411
 H    1.081149   -3.760456    4.732964
 H   -2.639125   -1.580894    4.707225
 H   -0.877203   -2.824540    5.953483
 C    1.263991   -2.020831   -0.106136
 C    1.800569   -2.692159   -1.209301
 C    2.084574   -1.158380    0.636455
 C    3.135630   -2.498169   -1.567359
 H    1.177261   -3.370713   -1.796178
 C    3.419626   -0.976174    0.287447
 H    1.681015   -0.633107    1.506253
 C    3.942595   -1.640994   -0.824070
 H    3.543256   -3.024118   -2.433403
 H    4.064647   -0.302138    0.858645
 H    4.983946   -1.473825   -1.103261
91
Figure_S10-1_PA-PPh3(Naborate)-ts(1,4AA) / electronic energy: -4278.69171118 a.u. / lowest freq: -303.45 cm-1
Na   -2.999672   -2.236202   -0.189698
 B   -5.872398   -2.380440   -0.054254
 O   -5.039030   -1.172674   -0.369702
 O   -6.669795   -2.297751    1.157462
 O   -4.892704   -3.478917    0.223619
 C   -6.049949   -3.036352    2.166196
 C   -5.268250   -4.116445    1.413675
 O   -6.704600   -2.549856   -1.234077
 C   -5.538898   -0.576054   -1.535551
 C   -6.223091   -1.737290   -2.261321
 H   -6.792330   -3.458260    2.865628
 H   -5.353959   -2.408369    2.763509
 H   -5.914141   -4.994017    1.209118
 H   -4.383868   -4.473273    1.968979
 H   -4.726191   -0.115610   -2.123058
 H   -6.272224    0.218700   -1.291274
 H   -5.486235   -2.275134   -2.896061
 H   -7.041015   -1.401431   -2.921884
Cu    1.408156    0.524595    0.042920
 C    2.096821   -1.326330   -0.699579
 C    0.634273   -1.347093   -0.461464
 H    2.306812   -1.204999   -1.763540
 C    0.055828   -1.702905    0.828243
 C   -0.266004   -1.112463   -1.586284
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 O    0.940407   -1.545467    1.834598
 O   -1.091684   -2.046248    1.063809
 O   -1.465170   -1.337851   -1.625439
 O    0.359190   -0.565296   -2.645038
 C   -0.436872   -0.262367   -3.780961
 H   -0.914753   -1.167904   -4.179481
 H    0.248506    0.157823   -4.525085
 H   -1.214144    0.471825   -3.526598
 C    0.482389   -1.807696    3.153702
 H   -0.310929   -1.101543    3.435668
 H    1.351014   -1.673403    3.806787
 H    0.098463   -2.833175    3.239661
 C    2.962013   -2.347022   -0.068140
 H    2.752973   -2.599432    0.971511
 C    3.951944   -2.947966   -0.745051
 H    4.138275   -2.633517   -1.778660
 C    4.851807   -3.997604   -0.240106
 C    5.911124   -4.429220   -1.053690
 C    4.702212   -4.590389    1.025653
 C    6.798313   -5.412113   -0.618652
 H    6.041405   -3.981499   -2.042463
 C    5.586460   -5.572488    1.460212
 H    3.882606   -4.286505    1.680057
 C    6.639360   -5.987352    0.641050
 H    7.616290   -5.730492   -1.268564
 H    5.452036   -6.022594    2.446281
 H    7.331928   -6.758501    0.985016
 C    3.378334    0.279748   -0.201901
 H    3.935217    0.077726    0.720325
 C    3.926339    0.882078   -1.219789
 C    4.420628    1.451833   -2.296328
 H    4.947070    0.863782   -3.055346
 H    4.323834    2.530039   -2.458770
 P    0.480294    2.534319    0.351053
 C    1.061576    3.641468   -0.982266
 C    1.330286    5.000445   -0.783781
 C    1.225113    3.082103   -2.256277
 C    1.745559    5.792395   -1.853631
 H    1.221322    5.443605    0.209148
 C    1.635248    3.877396   -3.324018
 H    1.043665    2.014901   -2.414197
 C    1.895654    5.233093   -3.123056
 H    1.953423    6.852254   -1.693452
 H    1.763114    3.432553   -4.312929
 H    2.222980    5.856241   -3.958059
 C    1.013689    3.341019    1.899777
 C    0.121484    3.865050    2.839445
 C    2.393117    3.386423    2.153557
 C    0.605297    4.439821    4.016417
 H   -0.954876    3.825847    2.660157
 C    2.870993    3.969506    3.323194
 H    3.096515    2.965053    1.428845
 C    1.976271    4.496941    4.257366
 H   -0.098057    4.844852    4.746899
 H    3.946095    4.008666    3.509720
 H    2.351899    4.950013    5.177215
 C   -1.337521    2.655751    0.299414
 C   -1.988437    3.881591    0.102152
 C   -2.094484    1.488029    0.448129
 C   -3.379267    3.934924    0.068405
 H   -1.409812    4.798935   -0.030829
 C   -3.488572    1.541297    0.412245
 H   -1.596214    0.524826    0.579725
 C   -4.127556    2.765796    0.223175
 H   -3.881033    4.892374   -0.086011
 H   -4.072073    0.620564    0.500005
 H   -5.218432    2.808590    0.186677
91
Figure_S10-1_PA-PPh3(Naborate)-prod(1,4AA) / electronic energy: -4278.74542342 a.u. / lowest freq: 12.03 cm-1
Na   1.237607   -2.982167   -0.555057
 B   1.269972   -5.803548    0.052664
 O   0.154136   -5.031671   -0.594186
 O   0.979807   -6.345109    1.369791
 O   2.358106   -4.807747    0.294553
 C   1.585666   -5.542743    2.337835
 C   2.794136   -4.935187    1.619946
 O   1.567311   -6.855401   -0.906977
 C  -0.300088   -5.753097   -1.706121
 C   0.921674   -6.581143   -2.112981
 H   1.871910   -6.134319    3.224840
 H   0.904178   -4.735926    2.683966
 H   3.668870   -5.613271    1.687455
 H   3.091516   -3.957445    2.035338
 H  -0.648725   -5.073751   -2.503046
 H  -1.145832   -6.415570   -1.431553
 H   1.568388   -5.991156   -2.797782
 H   0.647648   -7.511617   -2.639544
Cu  -0.594211    1.452941    0.491386
 C   1.842076    2.183052   -0.004966
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 C    1.335238    0.724352   -0.072742
 H    1.658069    2.620997   -0.992596
 C    1.566201   -0.183078    1.037776
 C    1.050615    0.145041   -1.376957
 O    1.985678    0.457422    2.151187
 O    1.387904   -1.395467    1.070274
 O    0.926935   -1.040081   -1.658874
 O    0.884712    1.076809   -2.342331
 C    0.576527    0.604750   -3.642910
 H    1.362731   -0.065769   -4.017160
 H    0.509136    1.493969   -4.279815
 H   -0.381840    0.065292   -3.649116
 C    2.188409   -0.329813    3.312708
 H    1.259279   -0.832643    3.615976
 H    2.510839    0.365065    4.095895
 H    2.963787   -1.090396    3.144383
 C    3.308878    2.330648    0.300170
 H    3.639901    1.928504    1.261384
 C    4.180324    2.907110   -0.537099
 H    3.804333    3.314506   -1.483450
 C    5.629624    3.073805   -0.313679
 C    6.370632    3.874076   -1.196726
 C    6.309034    2.464163    0.754850
 C    7.738538    4.072989   -1.013946
 H    5.862878    4.351096   -2.039429
 C    7.674102    2.661283    0.938529
 H    5.766517    1.819113    1.448970
 C    8.395958    3.468597    0.056460
 H    8.293707    4.703111   -1.712386
 H    8.181335    2.177000    1.776086
 H    9.467372    3.621455    0.202546
 C    0.959954    2.944008    0.991430
 H    1.155171    2.783871    2.059081
 C   -0.033250    3.747246    0.627883
 C   -0.902056    4.659263    0.264067
 H   -0.591607    5.706041    0.178675
 H   -1.942353    4.417381    0.028529
 P   -2.752428    1.023900    0.170311
 C   -3.444455    2.117554   -1.120229
 C   -4.737435    2.647586   -1.054972
 C   -2.618228    2.438356   -2.206677
 C   -5.201808    3.481055   -2.072591
 H   -5.384720    2.415948   -0.205776
 C   -3.088070    3.264877   -3.224095
 H   -1.596162    2.049763   -2.250777
 C   -4.380469    3.788081   -3.156882
 H   -6.210225    3.895631   -2.014145
 H   -2.438053    3.511312   -4.066095
 H   -4.745411    4.444657   -3.949481
 C   -3.803461    1.305047    1.636885
 C   -4.904050    0.505773    1.963249
 C   -3.475878    2.396570    2.453536
 C   -5.675090    0.805845    3.086774
 H   -5.161911   -0.356213    1.343963
 C   -4.252970    2.698657    3.568527
 H   -2.603727    3.013349    2.216783
 C   -5.354368    1.902461    3.886052
 H   -6.530959    0.176117    3.338161
 H   -3.991996    3.552557    4.196941
 H   -5.960193    2.133880    4.764708
 C   -3.089436   -0.673513   -0.398154
 C   -4.230260   -1.007666   -1.139360
 C   -2.159261   -1.668051   -0.070391
 C   -4.444550   -2.328225   -1.529104
 H   -4.951390   -0.236068   -1.420359
 C   -2.377118   -2.990208   -0.457100
 H   -1.247186   -1.406845    0.475279
 C   -3.521101   -3.317255   -1.185758
 H   -5.334921   -2.584844   -2.107003
 H   -1.638193   -3.759413   -0.213457
 H   -3.688989   -4.351195   -1.495473
91
Figure_S10-1_PA-PPh3(Naborate)-ed(1,4) / electronic energy: -4278.71589517 a.u. / lowest freq: 9.25 cm-1
 H   -0.852673    3.719231    3.095791
 C   -0.470025    3.324873    2.138573
 H   -0.066313    2.310006    2.331625
 H   -2.265593    4.100426    1.164305
 O    0.510253    4.160996    1.601542
 H   -2.129968    2.324688    1.079819
 C   -1.548839    3.262198    1.055012
 B    0.426244    4.140304    0.144103
 O   -0.822815    3.372101   -0.137542
 O    0.494750    5.485982   -0.404412
 H    3.167210    4.665602   -0.522157
 O    1.522470    3.403907   -0.564775
Na    0.230950    1.656733   -1.257477
 C    2.344851    4.348593   -1.194285
 C    1.392646    5.513134   -1.472229
 H    1.916011    6.483254   -1.529848
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 H    0.877259    5.358708   -2.444462
 H    2.796312    3.930703   -2.107603
Cu    1.068720   -2.409236   -0.069549
 C   -3.550995   -0.409555    0.653862
 C   -2.336775   -0.398246    0.044327
 H   -3.532659   -0.310068    1.743149
 C   -2.131659   -0.510576   -1.426550
 C   -1.106423   -0.278477    0.865618
 O   -2.978753   -1.346989   -2.001275
 O   -1.281936    0.087500   -2.056730
 O   -0.010596    0.025517    0.426834
 O   -1.300871   -0.558636    2.140538
 C   -0.150291   -0.627124    2.979081
 H    0.538185   -1.397511    2.604645
 H   -0.518789   -0.897921    3.972987
 H    0.376870    0.335707    3.009836
 C   -2.850578   -1.537256   -3.407146
 H   -2.969458   -0.584302   -3.939964
 H   -3.643975   -2.235769   -3.690027
 H   -1.866932   -1.966257   -3.641509
 C   -4.862634   -0.490509    0.059758
 H   -4.941770   -0.595746   -1.022167
 C   -5.965040   -0.442897    0.840557
 H   -5.821314   -0.337543    1.921975
 C   -7.361258   -0.513511    0.402590
 C   -8.376165   -0.396981    1.366634
 C   -7.730895   -0.693780   -0.942480
 C   -9.719306   -0.454732    1.002423
 H   -8.104892   -0.257263    2.416036
 C   -9.071686   -0.752317   -1.305420
 H   -6.965857   -0.792813   -1.714664
 C  -10.070078   -0.632722   -0.335200
 H  -10.494239   -0.361871    1.765922
 H   -9.341947   -0.894616   -2.353696
 H  -11.122206   -0.680835   -0.623956
 C   -0.499670   -3.489452   -0.412586
 H   -0.632093   -3.998968   -1.381963
 C   -1.477994   -3.659309    0.435753
 C   -2.451548   -3.800963    1.317366
 H   -2.453438   -4.620118    2.043854
 H   -3.293066   -3.100002    1.342591
 P    2.951451   -1.198211    0.072383
 C    4.523596   -2.133061    0.016189
 C    5.732188   -1.619257    0.503522
 C    4.507178   -3.394993   -0.590171
 C    6.907672   -2.356686    0.377808
 H    5.757379   -0.643734    0.995115
 C    5.685921   -4.128207   -0.721141
 H    3.564123   -3.806553   -0.961373
 C    6.886494   -3.609378   -0.237569
 H    7.844977   -1.950590    0.763786
 H    5.663470   -5.110539   -1.197170
 H    7.809822   -4.184348   -0.335407
 C    3.089288   -0.123236    1.541897
 C    2.740742    1.230345    1.507461
 C    3.413430   -0.719768    2.769523
 C    2.720638    1.979353    2.685163
 H    2.459269    1.735422    0.579838
 C    3.400633    0.032466    3.941391
 H    3.674457   -1.780880    2.814786
 C    3.050896    1.384263    3.901168
 H    2.406671    3.024503    2.627807
 H    3.656483   -0.441956    4.891176
 H    3.030368    1.969943    4.823036
 C    3.063122   -0.096674   -1.387701
 C    4.091261    0.840474   -1.550479
 C    2.107894   -0.248705   -2.400377
 C    4.157492    1.613322   -2.706173
 H    4.845587    0.971094   -0.771131
 C    2.171221    0.532375   -3.555849
 H    1.299562   -0.976273   -2.283490
 C    3.196510    1.463853   -3.708421
 H    4.960348    2.343832   -2.823114
 H    1.416177    0.408796   -4.334960
 H    3.249406    2.075710   -4.611361
91
Figure_S10-1_PA-PPh3(Naborate)-ts(1,4) / electronic energy: -4278.69317096 a.u. / lowest freq: -422.93 cm-1
Na   -0.780394    1.830266   -0.336477
 H   -3.271108    4.438886    3.232364
 C   -2.618527    3.988561    2.463857
 H   -1.703968    3.623147    2.978750
 H   -3.189141    1.863269    2.237424
 H   -4.378170    3.029751    1.590852
 C   -3.294487    2.832567    1.722702
 O   -2.308319    4.909553    1.459600
 O   -2.635145    2.822401    0.490106
 B   -2.240006    4.227544    0.174685
 O   -3.056972    4.901299   -0.828796
 C   -2.386485    4.874575   -2.050509
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 H   -2.639096    3.962907   -2.634700
 H   -2.650778    5.748293   -2.671578
 O   -0.889314    4.130978   -0.461875
 H   -0.524904    5.883608   -1.512714
 C   -0.905213    4.853381   -1.662751
 H   -0.268215    4.370131   -2.424202
 H    6.260060   -0.427357   -1.783093
 C    6.186100   -0.209735   -0.710914
 C    4.964374   -0.207460   -0.145880
 C    3.767032   -0.466326   -0.944263
 H    3.974164   -0.587492   -2.007523
 C    2.472758    0.032578   -0.683614
 C    1.526218    0.066163   -1.779696
Cu   -0.079029   -1.585163   -0.572440
 C    1.963017    0.309119    0.656341
 O    2.731091   -0.183108    1.629519
 O    0.309038    0.312502   -1.682457
 O    0.929920    0.912551    0.925605
 C    2.310863    0.038186    2.968469
 H    2.154175    1.108141    3.160754
 H    3.113210   -0.348812    3.605370
 H    1.377899   -0.505581    3.173995
 O    2.041965   -0.216651   -2.971121
 C    1.142882   -0.322832   -4.066375
 H    1.757577   -0.573433   -4.936922
 H    0.616530    0.626147   -4.234861
 H    0.406523   -1.119280   -3.884991
 C    7.467577    0.053036   -0.041273
 C    7.575439    0.292328    1.340275
 C    8.643115    0.059338   -0.809675
 C    8.814606    0.528486    1.926100
 H    6.682714    0.290951    1.968887
 C    9.884686    0.296277   -0.223342
 H    8.578229   -0.125193   -1.885127
 C    9.974895    0.531538    1.147754
 H    8.878556    0.710348    3.001090
 H   10.785764    0.296221   -0.840579
 H   10.946110    0.715473    1.611974
 H    4.832701    0.000460    0.915222
 C    1.192493   -3.127896   -0.594889
 H    0.651241   -4.077906   -0.522170
 C    2.458919   -3.022533   -0.661763
 C    3.773636   -2.689405   -0.705118
 H    4.336550   -2.860206   -1.627053
 H    4.345373   -2.738808    0.225778
 P   -2.258700   -1.512818    0.055210
 C   -2.546909   -1.223087    1.838308
 C   -3.658960   -1.746640    2.509969
 C   -1.632287   -0.424164    2.536354
 C   -3.862532   -1.457701    3.858059
 H   -4.368713   -2.386598    1.980051
 C   -1.841043   -0.135980    3.884703
 H   -0.750705   -0.021085    2.030784
 C   -2.956148   -0.649689    4.545868
 H   -4.733086   -1.868124    4.373710
 H   -1.126068    0.492929    4.419458
 H   -3.117652   -0.426306    5.602545
 C   -3.098542   -3.106693   -0.266567
 C   -4.287757   -3.210449   -0.993939
 C   -2.497594   -4.267496    0.241836
 C   -4.873379   -4.460641   -1.202103
 H   -4.763226   -2.314911   -1.399480
 C   -3.088604   -5.511338    0.040033
 H   -1.562995   -4.195977    0.805654
 C   -4.278660   -5.609467   -0.684431
 H   -5.803503   -4.533104   -1.769612
 H   -2.617178   -6.408616    0.446127
 H   -4.741257   -6.585365   -0.846204
 C   -3.279665   -0.260549   -0.798618
 C   -4.446486    0.276930   -0.243556
 C   -2.861873    0.164562   -2.067124
 C   -5.184893    1.222537   -0.948734
 H   -4.773653   -0.028251    0.752413
 C   -3.603870    1.112515   -2.769874
 H   -1.938369   -0.230036   -2.497445
 C   -4.765534    1.642366   -2.210381
 H   -6.086114    1.647445   -0.502689
 H   -3.266860    1.443346   -3.754630
 H   -5.339004    2.396365   -2.753299
91
Figure_S10-1_PA-PPh3(Naborate)-prod(1,4) / electronic energy: -4278.76423088 a.u. / lowest freq: 15.32 cm-1
 H   -0.416938    4.699840    2.746527
 C   -0.105547    4.163797    1.832788
 H   -0.143162    3.076733    2.039995
 H   -1.356178    5.532740    0.671955
 O    1.175794    4.559734    1.431312
 H   -1.873407    3.822963    0.567168
 C   -0.993817    4.485592    0.629075
 B    1.261012    4.513046   -0.024222
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 O   -0.144193    4.291452   -0.468732
 O    1.925346    5.697598   -0.549254
 H    4.056079    3.876507   -0.447629
 O    2.050882    3.371817   -0.597308
Na    0.230762    2.131429   -1.257984
 C    3.218595    3.886615   -1.174303
 C    2.834390    5.322485   -1.537929
 H    3.704964    6.001284   -1.558215
 H    2.372609    5.348544   -2.548468
 H    3.524974    3.287822   -2.046233
Cu    0.072205   -2.181656   -0.238765
 C   -2.813379   -2.003677   -0.043807
 C   -1.695449   -0.999707   -0.409354
 H   -2.741233   -2.142404    1.041556
 C   -1.568308   -0.552771   -1.793814
 C   -1.388529    0.013011    0.607975
 O   -2.236256   -1.338231   -2.661470
 O   -0.920858    0.396674   -2.223028
 O   -0.800654    1.072576    0.446733
 O   -1.814773   -0.329810    1.835510
 C   -1.553418    0.590985    2.881734
 H   -0.475743    0.773563    2.986433
 H   -1.947975    0.131572    3.794875
 H   -2.059535    1.549112    2.695954
 C   -2.117034   -1.030039   -4.039921
 H   -2.490031   -0.018617   -4.252320
 H   -2.724829   -1.771506   -4.570116
 H   -1.070790   -1.099827   -4.370744
 C   -4.188566   -1.468438   -0.340512
 H   -4.428026   -1.327828   -1.399710
 C   -5.068681   -1.128955    0.609930
 H   -4.775222   -1.270473    1.656803
 C   -6.413118   -0.554056    0.413124
 C   -7.161840   -0.180100    1.539839
 C   -6.986773   -0.359278   -0.854990
 C   -8.434524    0.373809    1.409823
 H   -6.733242   -0.324275    2.535296
 C   -8.257504    0.192570   -0.986860
 H   -6.435046   -0.643966   -1.753503
 C   -8.988210    0.563123    0.144712
 H   -8.995425    0.658967    2.302821
 H   -8.684383    0.334921   -1.982300
 H   -9.984347    0.997966    0.037683
 C   -0.094857   -4.301785   -0.170824
 H    0.763530   -4.918664    0.046525
 C   -1.209663   -3.840982   -0.412833
 C   -2.590453   -3.401117   -0.660559
 H   -3.287872   -4.131780   -0.221859
 H   -2.762233   -3.381169   -1.745226
 P    2.149912   -1.397271    0.224225
 C    3.424387   -2.682227    0.532092
 C    4.397544   -2.584491    1.532456
 C    3.447025   -3.778978   -0.340210
 C    5.371988   -3.574354    1.661753
 H    4.400629   -1.734539    2.217955
 C    4.425508   -4.762470   -0.214486
 H    2.698610   -3.857822   -1.133936
 C    5.387960   -4.663113    0.791155
 H    6.126060   -3.489879    2.446982
 H    4.435183   -5.609260   -0.903832
 H    6.152891   -5.435596    0.894342
 C    2.151923   -0.350178    1.720283
 C    2.269139    1.040596    1.644704
 C    1.938919   -0.959344    2.966911
 C    2.214728    1.810761    2.807832
 H    2.384177    1.561783    0.689673
 C    1.901945   -0.188977    4.125940
 H    1.815566   -2.043616    3.039271
 C    2.046236    1.198563    4.047674
 H    2.276670    2.897275    2.709652
 H    1.750768   -0.673253    5.092984
 H    2.009344    1.802457    4.957207
 C    2.943811   -0.409906   -1.094468
 C    4.259569    0.054599   -0.955219
 C    2.259511   -0.186982   -2.292415
 C    4.878871    0.726464   -2.003428
 H    4.806164   -0.117027   -0.024670
 C    2.880862    0.493981   -3.341597
 H    1.230403   -0.531483   -2.411586
 C    4.191326    0.943399   -3.200350
 H    5.903093    1.086074   -1.887002
 H    2.337358    0.664979   -4.273115
 H    4.680801    1.468980   -4.023070
32
Figure S11-1_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C   -0.660544   -0.726572    0.059153
 C   -1.860539   -0.097447    0.115996
 H   -0.691600   -1.818492   -0.004770
 C   -1.976243    1.390665    0.160143
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 C   -3.120576   -0.891785    0.187355
 O   -3.041424    1.823605   -0.507466
 O   -1.182749    2.134043    0.689285
 O   -4.147702   -0.497504    0.683440
 O   -2.981802   -2.118850   -0.320932
 C   -4.097604   -2.989729   -0.195724
 H   -4.332384   -3.170881    0.862818
 H   -3.810049   -3.927003   -0.683244
 H   -4.981752   -2.562067   -0.688186
 C   -3.254671    3.228152   -0.535442
 H   -3.354009    3.627502    0.483524
 H   -4.184056    3.384216   -1.092621
 H   -2.420438    3.737793   -1.038016
 C    0.656646   -0.129211    0.062308
 H    0.725624    0.955889    0.150505
 C    1.759981   -0.902956   -0.019704
 H    1.621029   -1.988149   -0.089650
 C    3.156351   -0.453635   -0.025165
 C    4.175093   -1.416830   -0.109525
 C    3.522207    0.902114    0.053056
 C    5.517020   -1.042840   -0.114390
 H    3.907556   -2.474776   -0.172060
 C    4.861836    1.275255    0.048166
 H    2.754752    1.675486    0.118691
 C    5.863995    0.305241   -0.035401
 H    6.294080   -1.807149   -0.179427
 H    5.127957    2.332459    0.111300
 H    6.914980    0.602284   -0.038425
83
Figure S11-1_PA-9d(Na)-prod(1,6major) / electronic energy: -3681.07040691 a.u. / lowest freq: 16.84 cm-1
 C    3.359716    2.192561    0.186378
 H    4.084937    2.045474   -0.623987
 C    2.301682    3.253634   -0.084287
 H    2.487627    4.197878    0.443917
 C    1.252797    1.255216    0.519749
 C   -0.154011    3.268993    0.464251
 C   -0.319177    4.494082   -0.187628
 C   -1.234976    2.721506    1.168563
 C   -1.560009    5.142558   -0.190544
 C   -2.481791    3.342500    1.164703
 C   -2.635440    4.552248    0.475124
 H   -3.608401    5.051384    0.474548
Cu   -0.121667   -0.113799    0.916922
 N    2.533441    0.987727    0.317927
 N    1.081772    2.599858    0.407618
 C   -0.564338   -1.667253   -0.868412
 C    0.339764   -1.258115   -1.914799
Na    3.394344   -0.054629   -3.260847
 H    2.204253    3.468661   -1.162679
 H    3.895673    2.382327    1.131622
 H   -0.320887   -2.664768   -0.488597
 C    0.330184    0.057031   -2.510178
 C    1.379788   -2.181028   -2.311050
 O   -0.739871    0.790831   -2.142238
 O    1.175437    0.555265   -3.250797
 O    2.232930   -2.017594   -3.178391
 O    1.379155   -3.338978   -1.604480
 C    2.407538   -4.265605   -1.896842
 H    2.351645   -4.607837   -2.940246
 H    2.254729   -5.113124   -1.218654
 H    3.399527   -3.823111   -1.723251
 C   -0.815652    2.115161   -2.630712
 H    0.107083    2.670519   -2.414192
 H   -1.657088    2.587839   -2.110041
 H   -0.986911    2.126332   -3.717459
 C    3.068782   -0.375270    0.295079
 H    2.466909   -0.929703   -0.436890
 C    2.913517   -1.055084    1.632471
 C    3.331851   -0.440029    2.819155
 C    2.353206   -2.335772    1.700930
 C    3.189746   -1.088835    4.045036
 H    3.762730    0.563840    2.785479
 C    2.209549   -2.987696    2.926046
 H    2.009673   -2.814301    0.779042
 C    2.626782   -2.366278    4.102388
 H    3.519665   -0.595379    4.962203
 H    1.758775   -3.981983    2.962468
 H    2.509601   -2.871378    5.063609
 C    4.523399   -0.386753   -0.259662
 H    4.841665   -1.457743   -0.141037
 H    5.143480    0.155563    0.512282
 O    4.619823    0.106165   -1.502499
 C   -1.673705   -1.103385   -0.279100
 H   -2.108769   -0.183596   -0.678769
 C   -2.533340   -1.923593    0.669128
 H   -1.995303   -2.860483    0.883000
 C   -3.870211   -2.293151    0.052170
 C   -4.201326   -3.633394   -0.170953
 C   -4.792318   -1.306787   -0.322316
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 C   -5.420834   -3.983663   -0.751757
 H   -3.491248   -4.415155    0.111738
 C   -6.012090   -1.651995   -0.900811
 H   -4.555115   -0.250350   -0.169659
 C   -6.330977   -2.993550   -1.117888
 H   -5.658039   -5.036680   -0.919528
 H   -6.717437   -0.868909   -1.187771
 H   -7.285637   -3.264252   -1.574113
 C   -3.642936    2.709122    1.886248
 H   -3.302719    2.104875    2.739717
 H   -4.349242    3.464481    2.258237
 H   -4.204892    2.044533    1.209744
 C   -1.716402    6.449919   -0.923143
 H   -2.717092    6.878335   -0.776058
 H   -0.974363    7.186701   -0.580138
 H   -1.561701    6.313378   -2.004789
 H    0.512466    4.951260   -0.725950
 H   -1.094165    1.812936    1.754301
 C   -0.345908   -0.525533    3.086856
 H    0.549898   -0.328070    3.656043
 C   -1.418580   -0.828411    2.582812
 C   -2.721248   -1.202714    2.022067
 H   -3.270254   -1.835958    2.736222
 H   -3.314996   -0.284862    1.882176
83
Figure S11-1_PA-9d(Na)-ts(1,6major) / electronic energy: -3681.01674239 a.u. / lowest freq: -425.84 cm-1
 C    2.866803    2.675946    1.037241
 H    3.618483    3.073400    0.344267
 C    1.496643    3.345149    0.935558
 H    1.285729    4.038149    1.760640
 C    1.246966    1.039170    0.692392
 C   -0.796962    2.290790    1.180897
 C   -1.490484    3.438376    0.798338
 C   -1.479557    1.247321    1.820637
 C   -2.874586    3.531001    0.998245
 C   -2.851518    1.327151    2.045160
 C   -3.540848    2.470137    1.614215
 H   -4.618525    2.543255    1.788127
Cu    0.443095   -0.673683    0.087133
 N    2.545629    1.293601    0.660974
 N    0.593216    2.188102    0.972750
 C   -0.520351   -1.415746   -1.646627
 C    0.525645   -0.530428   -2.098307
Na    3.541048    1.559954   -2.683597
 H    1.377226    3.887276   -0.017588
 H    3.266719    2.708454    2.064537
 H   -0.293059   -2.477742   -1.765329
 C    0.359803    0.903986   -2.362672
 C    1.798868   -1.136899   -2.511518
 O   -0.906702    1.322018   -2.270671
 O    1.249489    1.695745   -2.636288
 O    2.729106   -0.577606   -3.070754
 O    1.883062   -2.439152   -2.201216
 C    3.067140   -3.118499   -2.585350
 H    3.157940   -3.161586   -3.680079
 H    2.981622   -4.130150   -2.174801
 H    3.957585   -2.618517   -2.178973
 C   -1.154302    2.696016   -2.515703
 H   -0.506982    3.328730   -1.895213
 H   -2.204989    2.866151   -2.256610
 H   -0.981270    2.936927   -3.574367
 C    3.541140    0.255101    0.406446
 H    3.238270   -0.254293   -0.521579
 C    3.569791   -0.776710    1.510104
 C    3.338648   -0.440898    2.848798
 C    3.833792   -2.114224    1.194831
 C    3.358980   -1.418274    3.843111
 H    3.114557    0.593821    3.117691
 C    3.857616   -3.094769    2.184782
 H    4.001163   -2.392857    0.151635
 C    3.616254   -2.750116    3.514915
 H    3.167032   -1.139253    4.881685
 H    4.052018   -4.135263    1.915236
 H    3.623372   -3.516908    4.292376
 C    4.920609    0.898773    0.075156
 H    5.615125    0.019787   -0.011122
 H    5.252989    1.400160    1.029742
 O    4.871332    1.700685   -0.997615
 C   -1.825621   -1.113976   -1.224459
 H   -2.112915   -0.072661   -1.093273
 C   -2.736375   -2.126181   -0.917369
 H   -2.504266   -3.121690   -1.302082
 C   -4.180716   -1.862138   -0.728250
 C   -5.091188   -2.927133   -0.811338
 C   -4.686171   -0.577836   -0.471120
 C   -6.457825   -2.720791   -0.638977
 H   -4.716894   -3.934837   -1.011349
 C   -6.052175   -0.370517   -0.297835
 H   -4.007551    0.273745   -0.389597
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 C   -6.945620   -1.439678   -0.379347
 H   -7.147072   -3.565407   -0.707643
 H   -6.421400    0.637572   -0.095148
 H   -8.016271   -1.274778   -0.241455
 C   -3.571403    0.223601    2.775210
 H   -2.873392   -0.563606    3.091738
 H   -4.079472    0.612349    3.670806
 H   -4.340469   -0.236372    2.136249
 C   -3.621699    4.751481    0.526618
 H   -4.614503    4.821204    0.991853
 H   -3.067914    5.673798    0.755415
 H   -3.766496    4.721037   -0.565435
 H   -0.962707    4.269764    0.326130
 H   -0.924754    0.375016    2.167759
 C    0.058354   -2.071084    1.498789
 H    0.887162   -2.110107    2.209329
 C   -1.081011   -2.617436    1.438593
 C   -2.349736   -2.995465    1.131882
 H   -2.536143   -4.018874    0.794614
 H   -3.176879   -2.515024    1.662542
83
Figure S11-1_PA-9d(Na)-pc(1,6major) / electronic energy: -3681.03006649 a.u. / lowest freq: 18.39 cm-1
 C   -3.023393    1.926663   -1.975684
 H   -3.734352    2.631185   -1.527316
 C   -1.644732    2.532563   -2.247739
 H   -1.460479    2.735628   -3.310896
 C   -1.402412    0.617317   -0.940675
 C    0.652603    1.501882   -1.882637
 C    1.359014    2.709201   -1.868560
 C    1.339277    0.294672   -2.012511
 C    2.754866    2.706409   -1.925556
 C    2.736594    0.269001   -2.064975
 C    3.429058    1.480180   -2.007548
 H    4.522556    1.472153   -2.038805
Cu   -0.443186   -0.653845    0.252837
 N   -2.699485    0.874906   -1.002373
 N   -0.752993    1.482267   -1.747403
 C    0.760117   -0.627317    1.919256
 C   -0.135673    0.472048    1.979585
Na   -2.935225    2.839754    1.562535
 H   -1.490409    3.465715   -1.680749
 H   -3.469084    1.485925   -2.882489
 H    0.498041   -1.513492    2.501012
 C    0.207989    1.890904    1.671427
 C   -1.433009    0.294213    2.680471
 O    1.493583    2.169302    1.832244
 O   -0.595730    2.739101    1.334695
 O   -2.173521    1.191039    3.035081
 O   -1.735423   -0.985506    2.885773
 C   -2.968272   -1.264192    3.539023
 H   -2.954150   -0.882689    4.569069
 H   -3.070482   -2.353768    3.537429
 H   -3.805816   -0.801485    2.998386
 C    1.914143    3.504478    1.577594
 H    1.653824    3.801238    0.554086
 H    3.001317    3.507010    1.706997
 H    1.445484    4.196091    2.290993
 C   -3.700064    0.104960   -0.274107
 H   -3.278032   -0.077292    0.727101
 C   -3.981229   -1.240056   -0.906391
 C   -3.683604   -1.525988   -2.242664
 C   -4.571875   -2.243679   -0.127525
 C   -3.970192   -2.778103   -2.787385
 H   -3.199125   -0.773480   -2.867716
 C   -4.859570   -3.495455   -0.667201
 H   -4.794098   -2.045174    0.924454
 C   -4.560659   -3.767787   -2.002909
 H   -3.725232   -2.981151   -3.832436
 H   -5.311379   -4.266157   -0.038477
 H   -4.778748   -4.749920   -2.427927
 C   -4.966335    0.987140   -0.041987
 H   -5.669686    0.316865    0.520821
 H   -5.450089    1.080375   -1.056977
 O   -4.682120    2.151527    0.554778
 C    2.115488   -0.564051    1.404286
 H    2.390812    0.312596    0.816910
 C    3.021022   -1.546790    1.581871
 H    2.733256   -2.447012    2.132268
 C    4.396575   -1.501236    1.064643
 C    5.099492   -2.697931    0.854882
 C    5.033063   -0.289850    0.747261
 C    6.380136   -2.688708    0.307980
 H    4.618139   -3.647511    1.100718
 C    6.315497   -0.279590    0.206101
 H    4.521311    0.657534    0.929358
 C    6.991629   -1.478918   -0.024015
 H    6.903693   -3.632149    0.138402
 H    6.793165    0.672861   -0.034727
 H    7.995958   -1.470087   -0.452964
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 C    3.446063   -1.050686   -2.204236
 H    3.261668   -1.486079   -3.199144
 H    4.530878   -0.945210   -2.068617
 H    3.074793   -1.767014   -1.456599
 C    3.532102    3.996742   -1.888974
 H    4.034947    4.178828   -2.851532
 H    2.881034    4.857467   -1.681796
 H    4.313956    3.964250   -1.115311
 H    0.822078    3.656540   -1.786138
 H    0.780604   -0.641757   -2.065925
 C   -0.303029   -2.519919   -0.382309
 H   -1.202178   -2.890478   -0.900205
 C    0.724707   -3.306767   -0.288710
 C    1.813396   -4.049150   -0.162957
 H    1.955701   -4.710844    0.698034
 H    2.600336   -4.042421   -0.924324
51
Figure S11-1_9d(Na)-Cu-allenyl / electronic energy: -2839.06020575 a.u. / lowest freq: 14.37 cm-1
 C    1.401449   -2.075087    0.781893
 H    1.679476   -1.881296    1.831858
 C   -0.006213   -2.648365    0.652932
 H   -0.062301   -3.424044   -0.128912
 C    0.006182   -0.440008   -0.139162
 C   -2.189160   -1.531257    0.133738
 C   -2.845361   -2.761728    0.235329
 C   -2.951250   -0.369985   -0.075492
 C   -4.240763   -2.845245    0.119017
 C   -4.334525   -0.435941   -0.206321
 C   -4.972785   -1.681355   -0.104919
 H   -6.061043   -1.738645   -0.201130
Cu   -0.329372    1.490047   -0.372686
 N    1.273764   -0.812875    0.054580
 N   -0.787308   -1.470553    0.258845
Na    0.498306    3.958728    1.355621
 H   -0.381218   -3.078008    1.591814
 H    2.168593   -2.723176    0.339289
 C    2.372398    0.146754   -0.035438
 H    2.178954    0.736216   -0.947149
 C    3.689483   -0.579021   -0.225630
 C    4.620192   -0.739015    0.805951
 C    3.975802   -1.139609   -1.477409
 C    5.810682   -1.435686    0.589342
 H    4.421442   -0.318405    1.793568
 C    5.159152   -1.840488   -1.696033
 H    3.252345   -1.025120   -2.289480
 C    6.083241   -1.989386   -0.660216
 H    6.529017   -1.546552    1.404836
 H    5.363247   -2.270600   -2.679186
 H    7.015148   -2.533630   -0.828612
 C    2.308388    1.165951    1.128058
 H    3.266929    1.737018    1.072498
 H    2.373701    0.583431    2.082237
 O    1.207712    1.962082    1.066314
 C   -5.135842    0.816899   -0.451875
 H   -5.658483    0.763844   -1.419613
 H   -5.904556    0.954837    0.324125
 H   -4.492476    1.707881   -0.461773
 C   -4.919272   -4.186120    0.236349
 H   -6.004229   -4.101088    0.086278
 H   -4.527345   -4.895642   -0.508698
 H   -4.747592   -4.631017    1.228910
 H   -2.283360   -3.682514    0.397907
 H   -2.449009    0.596199   -0.147487
 C   -1.307163    3.029167   -1.145241
 H   -1.961130    2.829821   -2.012024
 C   -1.311845    4.265224   -0.742674
 C   -1.248636    5.503922   -0.256051
 H   -0.536999    6.236564   -0.653695
 H   -1.960491    5.856163    0.499142
83
Figure S11-1_PA-9d(Na)-pc(1,4AA) / electronic energy: -3681.02869646 a.u. / lowest freq: 15.32 cm-1
 C   -3.253675   -2.256189   -0.102901
 H   -3.622490   -2.800857    0.775342
 C   -3.924662   -0.896147   -0.279506
 H   -4.629595   -0.870074   -1.121358
 C   -1.602447   -0.620466   -0.214017
 C   -2.941598    1.319361   -0.932102
 C   -4.180292    1.952469   -0.772779
 C   -1.889254    2.019258   -1.534109
 C   -4.366578    3.274307   -1.192997
 C   -2.047934    3.346158   -1.931960
 C   -3.293322    3.961795   -1.765025
 H   -3.431417    4.996098   -2.092936
Cu    0.207426    0.221923   -0.208507
 N   -1.849404   -1.887602    0.067032
 N   -2.778499   -0.016761   -0.525315
 C    1.492357    1.536151    0.668178
 C    0.519056    1.125969    1.614522
Na   -1.957112   -0.490652    3.597226
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 H    -4.460065   -0.581208    0.631309
 H    -3.368025   -2.900511   -0.988751
 H     1.254172    2.467102    0.143064
 C    -0.693885    1.948848    1.862885
 C     0.789422    0.079983    2.643411
 O    -0.630067    3.153591    1.311632
 O    -1.669469    1.574208    2.487450
 O     0.379406    0.127681    3.783425
 O     1.539574   -0.915403    2.190403
 C     1.745042   -2.014806    3.081898
 H     2.313477   -1.690709    3.964565
 H     2.318535   -2.752722    2.511186
 H     0.756053   -2.404319    3.369559
 C    -1.784267    3.977586    1.427102
 H    -2.662187    3.473487    1.001760
 H    -1.563854    4.888360    0.861291
 H    -1.974606    4.220562    2.481615
 C    -0.849214   -2.848597    0.519073
 H     0.075780   -2.263686    0.617570
 C    -0.617591   -3.932827   -0.515130
 C    -1.501218   -5.009119   -0.672308
 C     0.504424   -3.866382   -1.350600
 C    -1.273342   -5.986223   -1.641659
 H    -2.381261   -5.091992   -0.030768
 C     0.736730   -4.842004   -2.319116
 H     1.192650   -3.022658   -1.251958
 C    -0.153740   -5.905829   -2.468922
 H    -1.976492   -6.815379   -1.749692
 H     1.616219   -4.767934   -2.963023
 H     0.024739   -6.670225   -3.228698
 C    -1.199661   -3.360406    1.943797
 H    -0.348980   -4.054446    2.190507
 H    -2.078042   -4.053606    1.843785
 O    -1.387513   -2.364115    2.820548
 C     2.895953    1.146976    0.610706
 H     3.208429    0.290992    1.209613
 C     3.775879    1.797381   -0.173885
 H     3.412508    2.647522   -0.762556
 C     5.204643    1.491508   -0.331964
 C     5.994449    2.333476   -1.131668
 C     5.823841    0.387330    0.280511
 C     7.354179    2.088289   -1.312113
 H     5.530656    3.195500   -1.618351
 C     7.181225    0.142145    0.100829
 H     5.238617   -0.294001    0.901229
 C     7.953768    0.990977   -0.695557
 H     7.948230    2.757085   -1.938787
 H     7.641873   -0.722525    0.583698
 H     9.018811    0.794814   -0.836230
 C    -0.878554    4.098647   -2.509404
 H    -1.200977    4.849606   -3.244284
 H    -0.335889    4.629258   -1.709633
 H    -0.164325    3.417646   -2.993484
 C    -5.696968    3.951942   -0.989234
 H    -6.526540    3.232613   -1.040543
 H    -5.740494    4.434342    0.000677
 H    -5.868421    4.732855   -1.743333
 H    -0.941747    1.514850   -1.732363
 H    -5.018791    1.422052   -0.318795
 C     1.146118   -0.088268   -1.916732
 H     2.200628    0.192315   -2.062009
 C     0.509184   -0.674153   -2.890053
 C    -0.207543   -1.276342   -3.822618
 H    -0.782271   -0.703189   -4.557630
 H    -0.245324   -2.369575   -3.883371
83
Figure S11-1_PA-9d(Na)-ts(1,4AA) / electronic energy: -3681.00195136 a.u. / lowest freq: -312.43 cm-1
 C     4.176048    1.135057   -0.090047
 H     4.668575    1.567707    0.789996
 C     4.335759   -0.384746   -0.166833
 H     5.014900   -0.708775   -0.967121
 C     2.064657    0.167229   -0.232720
 C     2.643444   -2.173764   -0.699438
 C     3.544523   -3.186939   -0.344149
 C     1.446529   -2.515264   -1.337083
 C     3.250300   -4.527365   -0.604390
 C     1.122649   -3.852780   -1.579408
 C     2.033878   -4.847078   -1.216798
 H     1.793140   -5.895798   -1.413924
Cu     0.127370    0.018715   -0.177629
 N     2.725908    1.287904   -0.001289
 N     2.963388   -0.828840   -0.431824
 C    -1.866795   -0.581305    0.180416
 C    -1.089312   -0.541418    1.435416
Na     1.478134    0.211717    3.617748
 H     4.698384   -0.803351    0.785745
 H     4.554428    1.650803   -0.987156
 H    -1.888642   -1.587476   -0.247600
 C    -0.397907   -1.723976    1.932641
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 C   -1.064010    0.656235    2.274045
 O   -0.685861   -2.842420    1.246485
 O    0.401521   -1.755272    2.861065
 O   -0.828941    0.703778    3.468843
 O   -1.299770    1.781016    1.569809
 C   -1.104679    3.009807    2.262795
 H   -1.844006    3.127387    3.067723
 H   -1.236737    3.798951    1.513998
 H   -0.085887    3.026249    2.677885
 C    0.059139   -4.000970    1.583714
 H    1.133725   -3.835718    1.417594
 H   -0.296323   -4.796055    0.919495
 H   -0.107500   -4.281912    2.632877
 C    2.103661    2.556889    0.352052
 H    1.023242    2.345492    0.357132
 C    2.375168    3.586907   -0.729865
 C    3.311495    4.614811   -0.581722
 C    1.676418    3.486906   -1.941176
 C    3.541375    5.522835   -1.617767
 H    3.869590    4.714526    0.351081
 C    1.904597    4.388731   -2.977487
 H    0.942192    2.684943   -2.067725
 C    2.841276    5.412216   -2.817512
 H    4.275881    6.320585   -1.484755
 H    1.349741    4.294706   -3.913792
 H    3.022317    6.123326   -3.626722
 C    2.455835    2.944766    1.810831
 H    1.953962    3.942442    1.953146
 H    3.551948    3.196415    1.835726
 O    2.094166    1.997594    2.686340
 C   -3.203807    0.059755    0.164916
 H   -3.278547    1.040241    0.637294
 C   -4.281056   -0.541545   -0.359020
 H   -4.148244   -1.515496   -0.844679
 C   -5.657818   -0.018647   -0.366931
 C   -6.652409   -0.732963   -1.053163
 C   -6.027185    1.171610    0.283616
 C   -7.967860   -0.273746   -1.099173
 H   -6.386374   -1.663441   -1.561684
 C   -7.339715    1.630630    0.238760
 H   -5.282839    1.747047    0.837675
 C   -8.316841    0.911361   -0.453618
 H   -8.723390   -0.846080   -1.641999
 H   -7.604446    2.558116    0.751398
 H   -9.346252    1.274762   -0.486863
 C   -0.209941   -4.201181   -2.185788
 H   -0.197991   -5.196898   -2.650118
 H   -0.990109   -4.201373   -1.406591
 H   -0.513240   -3.460450   -2.938859
 C    4.219149   -5.616960   -0.224173
 H    5.125778   -5.208692    0.242800
 H    3.759590   -6.322683    0.484733
 H    4.523249   -6.197974   -1.108367
 H    0.762446   -1.734344   -1.674625
 H    4.487844   -2.938890    0.144431
 C   -1.289662    0.402614   -1.553822
 H   -1.610777    1.450677   -1.515066
 C   -1.368143   -0.275693   -2.663607
 C   -1.464388   -1.021506   -3.742501
 H   -2.392965   -1.552914   -3.977516
 H   -0.630084   -1.121775   -4.444135
83
Figure S11-1_PA-9d(Na)-prod(1,4AA) / electronic energy: -3681.06975124 a.u. / lowest freq: 13.19 cm-1
 C    4.490641    1.254330    0.027949
 H    5.055997    1.040248   -0.891707
 C    3.685722    2.555452   -0.076348
 H    3.939082    3.282006    0.710202
 C    2.207631    0.746738    0.202315
 C    1.216752    2.989147    0.146705
 C    1.326232    4.263172   -0.424746
 C    0.038377    2.631093    0.808972
 C    0.265305    5.170439   -0.351512
 C   -1.032758    3.521834    0.886965
 C   -0.907869    4.787257    0.305207
 H   -1.740930    5.493988    0.368282
Cu    0.805760   -0.494609   -0.391620
 N    3.444105    0.250631    0.229341
 N    2.302099    2.092295    0.080430
 C   -1.941841   -0.711521    0.689351
 C   -1.236603   -0.961158   -0.657302
Na    0.715485   -1.499175   -3.409062
 H    3.829888    3.045487   -1.050422
 H    5.202150    1.253495    0.866092
 H   -1.977997    0.375248    0.815879
 C   -1.352862    0.079903   -1.674284
 C   -1.110437   -2.327161   -1.149150
 O   -2.026564    1.168928   -1.258614
 O   -0.889178    0.055076   -2.815011
 O   -0.855511   -2.704822   -2.288156
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 O   -1.312433   -3.248898   -0.180538
 C   -1.137419   -4.606803   -0.536226
 H   -1.843765   -4.908399   -1.322669
 H   -1.326632   -5.185711    0.375087
 H   -0.113166   -4.792985   -0.890167
 C   -1.987847    2.307552   -2.096483
 H   -0.959307    2.690067   -2.188648
 H   -2.611151    3.066409   -1.610009
 H   -2.381889    2.081755   -3.096996
 C    3.695375   -1.183479    0.091846
 H    2.952462   -1.680598    0.737317
 C    5.072861   -1.530989    0.619443
 C    6.179727   -1.692078   -0.221038
 C    5.257932   -1.663071    2.001585
 C    7.439354   -1.978546    0.307471
 H    6.065121   -1.589406   -1.301884
 C    6.514142   -1.945647    2.533531
 H    4.400296   -1.539103    2.668694
 C    7.611007   -2.104217    1.684958
 H    8.291872   -2.101974   -0.364271
 H    6.638258   -2.046819    3.614002
 H    8.597244   -2.326045    2.098615
 C    3.376338   -1.657525   -1.348056
 H    3.742450   -2.710853   -1.399373
 H    4.044334   -1.082424   -2.037669
 O    2.058367   -1.536812   -1.669817
 C   -3.365934   -1.211468    0.685256
 H   -3.487633   -2.293967    0.573657
 C   -4.434629   -0.409741    0.775847
 H   -4.262397    0.666404    0.890795
 C   -5.853214   -0.812789    0.733738
 C   -6.844452    0.167281    0.899258
 C   -6.268667   -2.140067    0.528768
 C   -8.199261   -0.160294    0.865054
 H   -6.544017    1.206624    1.057745
 C   -7.620378   -2.469395    0.494766
 H   -5.525881   -2.928332    0.389443
 C   -8.593977   -1.481880    0.662529
 H   -8.950289    0.622281    0.995830
 H   -7.917821   -3.508047    0.332587
 H   -9.654278   -1.742397    0.632512
 C   -2.313420    3.103647    1.558850
 H   -2.826798    3.958087    2.022310
 H   -2.999170    2.661740    0.817737
 H   -2.131127    2.341128    2.329539
 C    0.379927    6.541029   -0.968645
 H    1.354144    6.686668   -1.455306
 H   -0.404405    6.699730   -1.724737
 H    0.259648    7.327280   -0.207389
 H   -0.035895    1.646817    1.268917
 H    2.241669    4.561274   -0.938354
 C   -1.175701   -1.263085    1.882862
 H   -1.018908   -2.345021    1.927080
 C   -0.702838   -0.507137    2.842038
 C   -0.207304    0.270045    3.773146
 H   -0.778149    0.525503    4.671887
 H    0.799267    0.690970    3.673043
15
Figure S12-1_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
 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
32
Figure S12-1_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C   -0.660544   -0.726572    0.059153
 C   -1.860539   -0.097447    0.115996
 H   -0.691600   -1.818492   -0.004770
 C   -1.976243    1.390665    0.160143
 C   -3.120576   -0.891785    0.187355
 O   -3.041424    1.823605   -0.507466
 O   -1.182749    2.134043    0.689285
 O   -4.147702   -0.497504    0.683440
 O   -2.981802   -2.118850   -0.320932
 C   -4.097604   -2.989729   -0.195724
 H   -4.332384   -3.170881    0.862818
 H   -3.810049   -3.927003   -0.683244
 H   -4.981752   -2.562067   -0.688186
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 C   -3.254671    3.228152   -0.535442
 H   -3.354009    3.627502    0.483524
 H   -4.184056    3.384216   -1.092621
 H   -2.420438    3.737793   -1.038016
 C    0.656646   -0.129211    0.062308
 H    0.725624    0.955889    0.150505
 C    1.759981   -0.902956   -0.019704
 H    1.621029   -1.988149   -0.089650
 C    3.156351   -0.453635   -0.025165
 C    4.175093   -1.416830   -0.109525
 C    3.522207    0.902114    0.053056
 C    5.517020   -1.042840   -0.114390
 H    3.907556   -2.474776   -0.172060
 C    4.861836    1.275255    0.048166
 H    2.754752    1.675486    0.118691
 C    5.863995    0.305241   -0.035401
 H    6.294080   -1.807149   -0.179427
 H    5.127957    2.332459    0.111300
 H    6.914980    0.602284   -0.038425
103
Figure S12-1_PA-SIMes(NaOtBu)-prod(1,4) / electronic energy: -3917.95611486 a.u. / lowest freq: 10.44 cm-1
Cu   -2.225107   -0.135198    0.570753
 C    3.652191   -0.029908   -0.596619
 C    3.055741    0.177758    0.789288
 H    3.728154    0.963511   -1.053669
 C    2.839153   -0.912542    1.676247
 C    2.580450    1.474033    1.153906
 O    3.318599   -2.098807    1.193129
 O    2.292124   -0.913949    2.787632
 O    1.869296    1.787836    2.118429
 O    2.973878    2.460368    0.301812
 C    2.465524    3.750978    0.549425
 H    1.366359    3.751948    0.563652
 H    2.822544    4.387183   -0.270274
 H    2.826021    4.152773    1.508857
 C    3.213204   -3.229140    2.030255
 H    3.695764   -3.057381    3.003689
 H    3.721572   -4.048014    1.506026
 H    2.163207   -3.504457    2.206132
 C    5.039346   -0.619153   -0.609459
 H    5.139293   -1.616333   -0.171670
 C    6.108421    0.013242   -1.111242
 H    5.969640    1.019710   -1.525316
 C    7.494098   -0.493108   -1.164028
 C    8.516255    0.362770   -1.604228
 C    7.847417   -1.804235   -0.799813
 C    9.840940   -0.066685   -1.673790
 H    8.265059    1.386836   -1.893968
 C    9.169064   -2.235474   -0.869280
 H    7.077901   -2.501662   -0.462317
 C   10.174122   -1.369483   -1.306445
 H   10.616077    0.621850   -2.018218
 H    9.417124   -3.260493   -0.583602
 H   11.209972   -1.711455   -1.362657
 C    0.314058    0.336010   -1.655711
 H   -0.633116    0.841361   -1.678126
 C    1.384131   -0.229794   -1.611176
 C    2.701245   -0.856238   -1.509156
 H    3.139779   -0.955978   -2.515999
 H    2.590163   -1.872338   -1.099775
Na    0.327265    0.259574    2.757118
 O   -1.301942   -1.005582    1.911558
 C   -1.190680   -2.404905    1.879330
 C   -0.333153   -2.827293    0.676119
 H   -0.174955   -3.917462    0.638594
 H   -0.823810   -2.518627   -0.261745
 H    0.648213   -2.331116    0.716829
 C   -2.579882   -3.049728    1.764677
 H   -2.525709   -4.150438    1.780933
 H   -3.219701   -2.720449    2.599038
 H   -3.066096   -2.749259    0.823167
 C   -0.522284   -2.864508    3.182679
 H   -0.413888   -3.960272    3.223437
 H    0.479315   -2.417653    3.275194
 H   -1.129777   -2.548072    4.045802
 C   -5.037276    0.924323   -2.312495
 H   -6.120342    0.801615   -2.177000
 C   -4.539638    2.322738   -1.927516
 H   -4.229046    2.919030   -2.795536
 C   -3.338813    0.723720   -0.711356
 C   -2.602047    3.041466   -0.461467
 C   -1.656318    3.713404   -1.249236
 C   -2.798881    3.374397    0.892751
 C   -0.892392    4.721058   -0.651218
 C   -2.001082    4.374673    1.447031
 C   -1.042626    5.061065    0.692914
 N   -4.290347    0.068719   -1.383391
 N   -3.397705    2.017702   -1.053953
 H   -5.290652    2.900783   -1.365442
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 H   -4.792844    0.659449   -3.353474
 H   -2.138149    4.634640    2.500620
 H   -0.145852    5.242823   -1.256470
 C   -1.462252    3.387082   -2.706746
 H   -1.769192    2.358790   -2.942610
 H   -2.059403    4.060896   -3.342419
 H   -0.409792    3.508710   -2.996810
 C   -3.832537    2.671420    1.733099
 H   -4.767280    2.506035    1.177758
 H   -3.474201    1.679167    2.052515
 H   -4.063623    3.252329    2.635664
 C   -4.512030   -1.336220   -1.262971
 C   -3.726787   -2.225740   -2.008037
 C   -5.499699   -1.789209   -0.373376
 C   -3.961607   -3.596065   -1.856255
 C   -5.704987   -3.163657   -0.261582
 C   -4.945847   -4.082995   -0.994310
 H   -3.349902   -4.300965   -2.426000
 H   -6.464753   -3.530458    0.434404
 C   -2.623559   -1.722837   -2.898544
 H   -2.961630   -0.908525   -3.556176
 H   -1.792434   -1.325308   -2.294291
 H   -2.225256   -2.529272   -3.527802
 C   -6.264780   -0.812590    0.478236
 H   -5.575388   -0.237305    1.116207
 H   -6.825562   -0.086230   -0.129513
 H   -6.979807   -1.332897    1.128535
 C   -0.196841    6.131750    1.330069
 H    0.532101    6.545887    0.619930
 H   -0.821245    6.959762    1.699431
 H    0.355997    5.731102    2.193396
 C   -5.175083   -5.561347   -0.823100
 H   -6.227195   -5.822672   -1.012621
 H   -4.546584   -6.150922   -1.504150
 H   -4.943820   -5.872844    0.207438
103
Figure S12-1_PA-SIMes(NaOtBu)-ts(1,4) / electronic energy: -3917.87960041 a.u. / lowest freq: -420.30 cm-1
Cu    1.179850   -0.046333    0.058207
 C   -3.650430   -1.022435   -0.017570
 C   -2.734301   -1.129692    1.040310
 H   -3.786057   -1.957956   -0.555798
 C   -2.573476   -0.131989    2.093310
 C   -1.869257   -2.309339    1.062855
 O   -3.071020    1.070646    1.766133
 O   -2.067932   -0.312115    3.191998
 O   -1.028702   -2.596011    1.906475
 O   -2.064552   -3.121484    0.014078
 C   -1.056289   -4.081521   -0.234810
 H   -0.095973   -3.575833   -0.416355
 H   -1.364619   -4.625784   -1.135010
 H   -0.943303   -4.780057    0.606354
 C   -3.101747    2.065963    2.774706
 H   -3.540938    1.675242    3.702943
 H   -3.718017    2.881326    2.378944
 H   -2.090600    2.439766    2.986141
 C   -4.795340   -0.122544   -0.126259
 H   -4.746641    0.835235    0.388923
 C   -5.884390   -0.477438   -0.834989
 H   -5.874533   -1.448985   -1.343439
 C   -7.116756    0.302651   -1.012874
 C   -8.146581   -0.230921   -1.805013
 C   -7.319128    1.564334   -0.425152
 C   -9.335974    0.465950   -2.007191
 H   -8.007921   -1.210431   -2.270297
 C   -8.506706    2.260517   -0.626111
 H   -6.540417    2.007711    0.198751
 C   -9.521010    1.715702   -1.417590
 H  -10.121822    0.030360   -2.628214
 H   -8.644386    3.238509   -0.159482
 H  -10.452808    2.264070   -1.571696
 C   -0.071193   -0.734508   -1.460498
 H    0.690955   -0.942110   -2.219475
 C   -1.284224   -0.518757   -1.775186
 C   -2.613969   -0.322145   -1.978611
 H   -3.191247   -1.131588   -2.431344
 H   -2.989787    0.689927   -2.161824
Na    0.068539   -1.188547    3.241836
 O    0.991091    0.333259    1.998382
 C    1.314325    1.591252    2.490055
 C    0.721945    2.685353    1.583783
 H    0.891981    3.702255    1.975571
 H    1.181270    2.626305    0.583907
 H   -0.361829    2.526013    1.468804
 C    2.840559    1.764297    2.553375
 H    3.142233    2.779055    2.862312
 H    3.276614    1.039711    3.260270
 H    3.259439    1.563116    1.559201
 C    0.738955    1.742991    3.911482
 H    0.921596    2.743037    4.337145
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 H   -0.345850    1.557386    3.901259
 H    1.203311    1.006202    4.590000
 C    4.830944    0.590248   -2.204910
 H    5.761101    1.117795   -1.956561
 C    4.883175   -0.899706   -1.872874
 H    4.999075   -1.532174   -2.762985
 C    2.962542    0.040923   -0.882696
 C    3.152897   -2.396582   -0.807933
 C    2.696546   -3.309946   -1.771841
 C    3.207921   -2.742047    0.555296
 C    2.295490   -4.580361   -1.349914
 C    2.777992   -4.017408    0.929448
 C    2.324263   -4.952414   -0.004738
 N    3.710206    1.046387   -1.371950
 N    3.580999   -1.104925   -1.228532
 H    5.693509   -1.149019   -1.167012
 H    4.606153    0.777566   -3.268289
 H    2.805585   -4.290783    1.988537
 H    1.926430   -5.291348   -2.095026
 C    2.630724   -2.943032   -3.230713
 H    2.453706   -1.867444   -3.370786
 H    3.573117   -3.189951   -3.746763
 H    1.826627   -3.495004   -3.736179
 C    3.691203   -1.766889    1.595169
 H    4.576985   -1.212906    1.250372
 H    2.910906   -1.017968    1.817340
 H    3.952186   -2.290377    2.525620
 C    3.420786    2.431904   -1.211105
 C    2.337334    3.007191   -1.892756
 C    4.240872    3.203002   -0.367257
 C    2.061125    4.360964   -1.677536
 C    3.927806    4.550397   -0.186256
 C    2.836179    5.147152   -0.824081
 H    1.208507    4.811463   -2.193703
 H    4.550810    5.151543    0.482894
 C    1.467622    2.190331   -2.807258
 H    2.062312    1.501609   -3.425423
 H    0.766636    1.570168   -2.228136
 H    0.880989    2.838179   -3.472393
 C    5.436373    2.607223    0.328706
 H    5.297116    1.536496    0.530621
 H    6.345240    2.715886   -0.285712
 H    5.623935    3.114927    1.284551
 C    1.886734   -6.326957    0.429469
 H    1.171535   -6.763204   -0.282433
 H    2.747674   -7.012050    0.493454
 H    1.413578   -6.300813    1.421522
 C    2.515043    6.599731   -0.586872
 H    3.353544    7.246322   -0.888683
 H    1.624579    6.913055   -1.149003
 H    2.326907    6.789911    0.481027
103
Figure S12-1_PA-SIMes(NaOtBu)-ed(1,4) / electronic energy: -3917.90470258 a.u. / lowest freq: 9.65 cm-1
Cu   -1.626308    0.035665    0.021274
 C    4.547675    1.130909   -0.032858
 C    3.404339    1.275941    0.693959
 H    4.710466    1.899734   -0.792821
 C    2.944727    0.340961    1.758111
 C    2.526072    2.446839    0.402352
 O    3.538457   -0.845482    1.704750
 O    2.101744    0.589855    2.594259
 O    1.619313    2.846090    1.104609
 O    2.836169    3.047006   -0.741228
 C    2.047682    4.169694   -1.113239
 H    0.985235    3.893445   -1.165853
 H    2.409811    4.480983   -2.098281
 H    2.170529    4.986736   -0.388673
 C    3.082885   -1.837518    2.618295
 H    3.233794   -1.511522    3.656106
 H    3.676182   -2.733287    2.408962
 H    2.016316   -2.041754    2.452491
 C    5.594698    0.142984    0.054363
 H    5.523727   -0.632768    0.813632
 C    6.637900    0.186616   -0.804795
 H    6.652571    0.982054   -1.558584
 C    7.774481   -0.737187   -0.850256
 C    8.755370   -0.556205   -1.839438
 C    7.926149   -1.801125    0.057392
 C    9.853282   -1.409493   -1.922840
 H    8.650903    0.264512   -2.553645
 C    9.022687   -2.651428   -0.025294
 H    7.181118   -1.968798    0.837335
 C    9.989866   -2.459180   -1.015330
 H   10.605062   -1.254157   -2.699384
 H    9.125898   -3.471492    0.688244
 H   10.849214   -3.130244   -1.077546
 C    0.158056    0.484788   -0.812894
 H    0.317767    1.460668   -1.306961
 C    1.088941   -0.397476   -1.045859
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 C    1.978996   -1.358408   -1.268647
 H    2.851462   -1.491527   -0.620244
 H    1.871665   -2.044997   -2.116396
Na    0.008556    1.420705    2.002058
 O   -1.477578   -0.150558    2.062748
 C   -1.762134   -1.380728    2.623722
 C   -1.245513   -2.521064    1.721588
 H   -1.419593   -3.520102    2.156223
 H   -1.752291   -2.482786    0.742048
 H   -0.163703   -2.398541    1.546982
 C   -3.282906   -1.547554    2.795599
 H   -3.565217   -2.542548    3.179296
 H   -3.674142   -0.784281    3.487768
 H   -3.761964   -1.400559    1.816876
 C   -1.076687   -1.487705    3.998267
 H   -1.270206   -2.452002    4.497697
 H    0.012528   -1.369662    3.878618
 H   -1.433363   -0.680023    4.658383
 C   -5.371241   -0.168965   -2.026224
 H   -6.337625   -0.592267   -1.721106
 C   -5.233340    1.316291   -1.669482
 H   -5.318425    1.974550   -2.545532
 C   -3.380165    0.140367   -0.817189
 C   -3.212132    2.540165   -0.679935
 C   -2.459726    3.251673   -1.625953
 C   -3.232356    2.915649    0.673618
 C   -1.727776    4.361398   -1.196827
 C   -2.468994    4.020961    1.061141
 C   -1.706007    4.751472    0.145364
 N   -4.257851   -0.767424   -1.280418
 N   -3.889233    1.355934   -1.090948
 H   -5.981764    1.641586   -0.926879
 H   -5.243147   -0.353323   -3.106020
 H   -2.464700    4.314525    2.115587
 H   -1.140033    4.923056   -1.928962
 C   -2.380044    2.769654   -3.048556
 H   -1.956362    1.753172   -3.074970
 H   -3.369894    2.721702   -3.526800
 H   -1.742096    3.426329   -3.655079
 C   -3.972082    2.096698    1.695234
 H   -4.930323    1.722529    1.307430
 H   -3.354897    1.219827    1.964847
 H   -4.167473    2.682839    2.604133
 C   -4.049152   -2.170413   -1.167469
 C   -3.011122   -2.778708   -1.895821
 C   -4.860654   -2.916215   -0.297538
 C   -2.778491   -4.141775   -1.702896
 C   -4.594769   -4.279628   -0.143765
 C   -3.551638   -4.908490   -0.826215
 H   -1.964191   -4.619552   -2.255690
 H   -5.215322   -4.863810    0.542237
 C   -2.152632   -1.981065   -2.839890
 H   -2.762772   -1.323806   -3.477985
 H   -1.462746   -1.328830   -2.280042
 H   -1.560937   -2.643487   -3.485987
 C   -5.993699   -2.274880    0.459165
 H   -5.773508   -1.226131    0.702536
 H   -6.924408   -2.290669   -0.131931
 H   -6.191093   -2.811041    1.397359
 C   -0.839050    5.892557    0.609120
 H   -0.562367    6.556445   -0.222031
 H   -1.341449    6.494120    1.380487
 H    0.092462    5.502029    1.050047
 C   -3.243602   -6.365632   -0.599464
 H   -4.134146   -6.920369   -0.271581
 H   -2.855080   -6.841187   -1.511478
 H   -2.475271   -6.480854    0.182325
56
Figure S12-1_SIMes-Cu-allenyl / electronic energy: -2680.78923765 a.u. / lowest freq: 16.67 cm-1
 C    0.255100   -2.802091    0.505112
 H    0.668208   -3.196427    1.444813
 C   -1.270500   -2.619391    0.554864
 H   -1.800083   -3.253354   -0.170485
 C   -0.267703   -0.553149    0.091367
 C   -2.705673   -0.570588    0.110299
 C   -3.379878   -0.614762   -1.117966
 C   -3.248840    0.082482    1.227243
 C   -4.637370   -0.011781   -1.202344
 C   -4.506955    0.673704    1.096602
 C   -5.220520    0.629249   -0.105733
Cu    0.110016    1.307604   -0.228361
 N    0.723169   -1.433012    0.264097
 N   -1.429749   -1.197347    0.221108
 H   -1.690544   -2.824163    1.551562
 H    0.576639   -3.468534   -0.309931
 C    0.774672    3.096038   -0.486998
 H    0.208773    4.016056   -0.700711
 C    2.071525    3.214162   -0.388898
 C    3.389142    3.271273   -0.276397
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 H    4.042154    3.124597   -1.143427
 H    3.872005    3.450329    0.690170
 H   -4.940744    1.189169    1.958286
 H   -5.171125   -0.034945   -2.156636
 C   -2.739174   -1.258856   -2.318184
 H   -1.764393   -0.794441   -2.533026
 H   -2.557008   -2.332599   -2.157552
 H   -3.373859   -1.155030   -3.207828
 C   -2.466468    0.177007    2.509466
 H   -2.161688   -0.814837    2.876499
 H   -1.543922    0.758395    2.352392
 H   -3.052793    0.668434    3.296712
 C    2.100609   -1.074402    0.152530
 C    2.710868   -1.089540   -1.109969
 C    2.796150   -0.676303    1.303159
 C    4.054490   -0.718966   -1.196317
 C    4.137867   -0.315360    1.170431
 C    4.783410   -0.329256   -0.069282
 H    4.541691   -0.721123   -2.175444
 H    4.690272    0.002663    2.059240
 C    1.914463   -1.435151   -2.339256
 H    1.411113   -2.409070   -2.245646
 H    1.129881   -0.679297   -2.505515
 H    2.554756   -1.464444   -3.230551
 C    2.087510   -0.585650    2.627443
 H    1.295980    0.179314    2.581836
 H    1.603679   -1.535221    2.901538
 H    2.783525   -0.310564    3.430477
 C   -6.591070    1.245868   -0.208877
 H   -6.854724    1.465524   -1.252764
 H   -7.356052    0.560144    0.189860
 H   -6.655115    2.179427    0.368353
 C    6.214528    0.121736   -0.194929
 H    6.791322   -0.109785    0.711774
 H    6.712484   -0.348829   -1.054371
 H    6.258068    1.212948   -0.343793
71
Figure S12-1_SIMes-Cu(NaOtBu)-allenyl / electronic energy: -3075.94872495 a.u. / lowest freq: 27.33 cm-1
 C   -1.416490   -3.051166    1.140808
 H   -1.938914   -3.883350    0.647034
 C    0.105264   -3.256272    1.189618
 H    0.489715   -3.368543    2.214600
 C   -0.367529   -1.221115    0.094618
 C    1.974999   -1.659754    0.536902
 C    2.505484   -0.907061    1.595408
 C    2.754988   -2.014511   -0.575804
 C    3.855470   -0.537550    1.531896
 C    4.092020   -1.614239   -0.604374
 C    4.663223   -0.881829    0.442809
Cu    0.053612    0.461472   -0.784402
 N   -1.541523   -1.811212    0.365637
 N    0.599348   -2.021713    0.574536
 H    0.429247   -4.136362    0.611310
 H   -1.859299   -2.922390    2.141774
 C    0.755622    1.005974   -2.588005
 H    0.218429    0.826130   -3.532293
 C    1.953933    1.491432   -2.679501
 C    3.189398    2.000319   -2.625307
 H    4.075143    1.356894   -2.689774
 H    3.357584    3.084119   -2.621768
 H    4.704175   -1.873694   -1.472896
 H    4.283319    0.043656    2.354482
 C    1.617360   -0.420541    2.707522
 H    0.978381    0.393096    2.317317
 H    0.955459   -1.212613    3.085486
 H    2.210910   -0.033680    3.547183
 C    2.127896   -2.738861   -1.734054
 H    1.621845   -3.660932   -1.412143
 H    1.367444   -2.092973   -2.200743
 H    2.877234   -3.001217   -2.492195
 C   -2.794261   -1.162873    0.170946
 C   -3.195153   -0.171583    1.079603
 C   -3.592941   -1.525176   -0.923657
 C   -4.433269    0.445296    0.876635
 C   -4.823279   -0.885304   -1.085667
 C   -5.261292    0.100708   -0.195229
 H   -4.757840    1.219932    1.577567
 H   -5.455052   -1.158544   -1.936089
 C   -2.285625    0.246411    2.203719
 H   -1.940340   -0.617407    2.792372
 H   -1.387471    0.744744    1.796547
 H   -2.795900    0.942716    2.883254
 C   -3.105647   -2.549996   -1.912506
 H   -2.132899   -2.249759   -2.331343
 H   -2.964276   -3.535448   -1.442255
 H   -3.818050   -2.670411   -2.739483
 C    6.113342   -0.477713    0.387804
 H    6.368706    0.224936    1.192898
 H    6.768696   -1.356952    0.487869
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 H     6.354502   -0.001942   -0.574561
 C    -6.579967    0.796614   -0.412766
 H    -7.347464    0.095753   -0.772100
 H    -6.946163    1.265949    0.510984
 H    -6.480947    1.589574   -1.171569
 O     0.444757    1.917070    0.659573
 C    -0.144448    3.170287    0.563690
 C    -0.341069    3.749935    1.976032
 H    -0.987186    3.082226    2.567061
 H     0.630883    3.822894    2.491044
 H    -0.799504    4.753042    1.961947
 C    -1.515147    3.082233   -0.136176
 H    -2.004584    4.066198   -0.228684
 H    -1.384991    2.663904   -1.147752
 H    -2.188626    2.415496    0.422473
 C     0.749528    4.130584   -0.252219
 H     0.940046    3.694674   -1.245968
 H     0.291861    5.123935   -0.390364
 H     1.716489    4.288346    0.258633
Na     2.583401    1.756705    0.072139
103
Figure S12-1_PA-SIMes(NaOtBu)-ed(1,6) / electronic energy: -3917.90118513 a.u. / lowest freq: 13.39 cm-1
 C    -1.352497    1.651473    3.417535
 H    -2.228596    1.084571    3.769157
 C    -0.020885    1.045133    3.886581
 H     0.632679    1.788481    4.366856
 C    -0.149230    0.918148    1.549169
 C     1.753969   -0.210934    2.552786
 C     1.610750   -1.606883    2.472329
 C     3.015954    0.399133    2.570494
 C     4.039515   -1.810226    2.361991
Cu     0.604485    0.839273   -0.273997
 N    -1.246491    1.558823    1.955536
 N     0.571533    0.584326    2.624950
 C     1.308134    0.054654   -1.997302
 C     0.097372   -0.642329   -1.681227
 H    -0.152511    0.206455    4.585718
 H    -1.476234    2.697727    3.730597
 H     1.217868    0.825586   -2.764218
 C     0.011316   -2.019492   -1.148993
 C    -1.149762   -0.086995   -2.273562
 O     1.196192   -2.590261   -0.953779
 O    -1.022112   -2.619115   -0.908550
 O    -2.190214   -0.682772   -2.467633
 O    -1.017020    1.198365   -2.599233
 C    -2.140432    1.839508   -3.190710
 H    -2.395807    1.364474   -4.147830
 H    -1.841959    2.880517   -3.350664
 H    -3.002795    1.791987   -2.514059
 C     1.217042   -3.939162   -0.508849
 H     0.661665   -4.053344    0.430440
 H     2.272806   -4.185942   -0.355847
 H     0.779645   -4.602181   -1.268069
 C     2.669308   -0.341229   -1.684783
 H     2.826824   -1.091159   -0.910007
 C     3.722033    0.234835   -2.303187
 H     3.523064    0.961060   -3.098012
 C     5.139763   -0.051080   -2.049384
 C     6.104848    0.424522   -2.950992
 C     5.576215   -0.780442   -0.930639
 C     7.460655    0.172571   -2.750906
 H     5.783195    1.000737   -3.822651
 C     6.929608   -1.030599   -0.729170
 H     4.850129   -1.132251   -0.195955
 C     7.878541   -0.557496   -1.638786
 H     8.194476    0.549696   -3.466666
 H     7.249639   -1.594062    0.150019
 H     8.940590   -0.753054   -1.476072
 C     1.505689    2.596081   -0.481979
 H     0.810078    3.441461   -0.370691
 C     2.765652    2.841447   -0.660558
 C     4.068224    3.002355   -0.820966
 H     4.516795    3.102626   -1.814186
 H     4.743798    3.051699    0.039833
 C     2.764038   -2.384998    2.372526
 H     2.665955   -3.472859    2.315074
 C     4.144068   -0.421563    2.465265
 H     5.133844    0.043074    2.465298
 C     0.247035   -2.242630    2.508992
 H    -0.375448   -1.823037    3.312335
 H    -0.303086   -2.080950    1.570124
 H     0.324764   -3.325446    2.674267
 C     3.154576    1.888262    2.725721
 H     2.482217    2.421557    2.039742
 H     2.912511    2.199759    3.754602
 H     4.183719    2.208615    2.516786
 C    -2.344246    1.876760    1.101121
 C    -2.576509    3.203210    0.718628
 C    -3.192545    0.832313    0.693771
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 C   -3.687526    3.466740   -0.092381
 C   -4.281737    1.135198   -0.122793
 C   -4.547643    2.452206   -0.517918
 H   -4.912350    0.299738   -0.451579
 C   -1.677765    4.319041    1.181160
 H   -1.651611    5.133810    0.444632
 H   -2.038523    4.746851    2.130950
 H   -0.650641    3.966383    1.347415
 C   -2.936191   -0.589292    1.111592
 H   -2.029042   -0.976493    0.622778
 H   -2.771083   -0.676289    2.196499
 H   -3.792307   -1.217959    0.817920
 C    5.263240   -2.681228    2.247174
 H    5.235580   -3.500672    2.980594
 H    5.327412   -3.143448    1.248860
 H    6.184652   -2.106336    2.413273
 C   -5.728712    2.747549   -1.405418
 H   -5.860889    3.826682   -1.564297
 H   -5.606433    2.270523   -2.390928
 H   -6.657155    2.347194   -0.970873
 H   -3.879080    4.498609   -0.401375
Na   -3.314477   -2.358532   -1.416399
 O   -5.235512   -2.053576   -0.636948
 H   -7.415357   -1.598929   -2.084290
 H   -6.959107   -3.985778   -1.293126
 C   -7.475303   -1.293373   -1.026976
 H   -7.171773   -0.235327   -0.966111
 C   -7.004337   -3.629439   -0.250588
 H   -8.528426   -1.367761   -0.704516
 C   -6.517014   -2.163321   -0.179865
 H   -6.338077   -4.267747    0.353191
 H   -8.036868   -3.764212    0.116155
 C   -6.615962   -1.694007    1.291873
 H   -5.949860   -2.307581    1.920765
 H   -6.282723   -0.646516    1.373810
 H   -7.638432   -1.765296    1.701738
103
Figure S12-1_PA-SIMes(NaOtBu)-ts(1,6) / electronic energy: -3917.89152237 a.u. / lowest freq: -424.76 cm-1
 C   -1.327443    1.038541    3.668426
 H   -2.210756    0.423824    3.901635
 C   -0.004491    0.343137    4.025938
 H    0.646936    0.972705    4.650394
 C   -0.109668    0.656281    1.704763
 C    1.785491   -0.640465    2.505548
 C    1.646740   -2.006762    2.210612
 C    3.044922   -0.034654    2.614230
 C    4.076546   -2.185139    2.082363
Cu    0.562033    0.859296   -0.137174
 N   -1.207744    1.219254    2.215522
 N    0.602422    0.131061    2.705800
 C    1.288497    0.358141   -2.007278
 C    0.064663   -0.396301   -1.815297
 H   -0.149498   -0.615062    4.545738
 H   -1.447836    2.009306    4.170142
 H    1.179352    1.230165   -2.656157
 C    0.016228   -1.823902   -1.494320
 C   -1.174939    0.224228   -2.312203
 O    1.223379   -2.364546   -1.295592
 O   -0.990614   -2.513170   -1.410134
 O   -2.239740   -0.326183   -2.530877
 O   -1.036100    1.542058   -2.519700
 C   -2.172400    2.244463   -2.999208
 H   -2.499345    1.845614   -3.969660
 H   -1.858481    3.288250   -3.106619
 H   -2.997984    2.170930   -2.279831
 C    1.292032   -3.766796   -1.098980
 H    0.665602   -4.082251   -0.254860
 H    2.344614   -3.989191   -0.892645
 H    0.965279   -4.300655   -2.002822
 C    2.610945    0.041537   -1.644760
 H    2.804895   -0.806047   -0.987080
 C    3.668728    0.841276   -2.082717
 H    3.462190    1.474796   -2.948218
 C    5.088404    0.451810   -1.936716
 C    6.035469    0.947575   -2.844730
 C    5.531604   -0.391199   -0.906080
 C    7.382719    0.607902   -2.733284
 H    5.708691    1.610125   -3.650845
 C    6.877365   -0.728342   -0.792031
 H    4.817812   -0.769179   -0.172036
 C    7.809996   -0.231876   -1.705364
 H    8.102759    1.002056   -3.454025
 H    7.202850   -1.382489    0.020020
 H    8.865638   -0.495543   -1.611894
 C    1.374840    2.740157    0.010598
 H    0.680589    3.370941    0.565052
 C    2.559660    2.909488   -0.397633
 C    3.811116    2.746757   -0.896456
 H    4.120660    3.310417   -1.780437
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 H    4.612239    2.480349   -0.199258
 C    2.803548   -2.757838    2.000292
 H    2.708405   -3.823460    1.773595
 C    4.176075   -0.827581    2.397108
 H    5.164457   -0.365517    2.472139
 C    0.284089   -2.637517    2.118228
 H   -0.344651   -2.381483    2.983431
 H   -0.255794   -2.292483    1.223817
 H    0.360511   -3.731627    2.068885
 C    3.175330    1.423452    2.959373
 H    2.534769    2.040415    2.313626
 H    2.881871    1.612770    4.004131
 H    4.212432    1.763146    2.837934
 C   -2.301988    1.670986    1.417438
 C   -2.551087    3.040094    1.266893
 C   -3.125288    0.702387    0.813939
 C   -3.645135    3.425822    0.481019
 C   -4.197845    1.128422    0.033117
 C   -4.475623    2.490402   -0.137887
 H   -4.808595    0.355708   -0.448890
 C   -1.692515    4.082537    1.933665
 H   -1.457775    4.900909    1.237692
 H   -2.214054    4.527625    2.795897
 H   -0.748387    3.659250    2.302138
 C   -2.858190   -0.767572    0.983204
 H   -1.957727   -1.059726    0.420951
 H   -2.675590   -1.034076    2.035223
 H   -3.717295   -1.341795    0.600374
 C    5.303957   -3.012965    1.806511
 H    5.221722   -4.012343    2.257696
 H    5.439490   -3.156074    0.721935
 H    6.211695   -2.532067    2.196845
 C   -5.652941    2.917707   -0.975152
 H   -5.651766    4.001432   -1.157568
 H   -5.653618    2.402225   -1.947486
 H   -6.600644    2.660360   -0.476191
 H   -3.845033    4.493309    0.347998
Na   -3.277778   -2.191105   -1.756681
 O   -5.189879   -1.963861   -0.917809
 H   -7.362523   -1.239999   -2.263073
 H   -7.009248   -3.717115   -1.783415
 C   -7.398163   -1.063948   -1.175393
 H   -7.046962   -0.035472   -0.990896
 C   -7.025161   -3.495804   -0.703405
 H   -8.449987   -1.132632   -0.847356
 C   -6.469941   -2.073318   -0.457948
 H   -6.381242   -4.234076   -0.197731
 H   -8.058170   -3.630281   -0.337797
 C   -6.534963   -1.786653    1.062180
 H   -5.889798   -2.499381    1.602099
 H   -6.156378   -0.771940    1.266575
 H   -7.555942   -1.865511    1.474371
103
Figure S12-1_PA-SIMes(NaOtBu)-prod(1,6) / electronic energy: -3917.94472680 a.u. / lowest freq: 14.26 cm-1
 C    1.022383    3.805280   -0.691424
 H    1.892754    3.859216   -1.360750
 C   -0.314724    3.815127   -1.444651
 H   -0.921725    4.703601   -1.223058
 C   -0.164274    1.855939   -0.167419
 C   -2.249711    2.185050   -1.400410
 C   -2.340683    1.230980   -2.425332
 C   -3.394679    2.759908   -0.826669
 C   -4.772963    1.433661   -2.344844
Cu   -0.600353    0.146935    0.621116
 N    0.987154    2.508225   -0.004363
 N   -0.963484    2.595598   -0.944462
 C   -1.006708   -1.749203    1.329365
 C    0.284452   -2.033128    0.695202
 H   -0.188836    3.751606   -2.536777
 H    1.101779    4.622383    0.041312
 H   -0.960713   -1.768551    2.422643
 C    0.432557   -2.481835   -0.672305
 C    1.459207   -2.040552    1.552719
 O   -0.731896   -2.501695   -1.354751
 O    1.467980   -2.814200   -1.239240
 O    2.588266   -2.418638    1.268551
 O    1.208888   -1.555299    2.787518
 C    2.291693   -1.526741    3.699396
 H    2.697423   -2.534565    3.867779
 H    1.887581   -1.125429    4.635833
 H    3.094045   -0.874279    3.329800
 C   -0.687041   -2.954444   -2.695713
 H    0.009982   -2.352803   -3.296032
 H   -1.705451   -2.845267   -3.086120
 H   -0.378294   -4.008439   -2.746599
 C   -2.224023   -1.407062    0.795447
 H   -2.398739   -1.452190   -0.281589
 C   -3.426517   -1.153888    1.682750
 H   -3.236717   -1.618398    2.662750
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 C   -4.686245   -1.777232    1.111875
 C   -5.399029   -2.739408    1.833663
 C   -5.163967   -1.395791   -0.148650
 C   -6.561554   -3.309484    1.312017
 H   -5.037482   -3.050334    2.817656
 C   -6.323823   -1.962979   -0.672664
 H   -4.621525   -0.647383   -0.732101
 C   -7.027905   -2.922548    0.056729
 H   -7.103581   -4.060940    1.890698
 H   -6.680271   -1.654932   -1.657967
 H   -7.936089   -3.368412   -0.354697
 C   -1.583681    1.406494    3.277923
 H   -0.745438    1.805223    3.819961
 C   -2.533885    0.962689    2.671310
 C   -3.651724    0.359807    1.947573
 H   -4.577897    0.496883    2.528125
 H   -3.791983    0.886297    0.989483
 C   -3.612072    0.867854   -2.878055
 H   -3.695442    0.121016   -3.672550
 C   -4.643735    2.370617   -1.314697
 H   -5.543508    2.804423   -0.869360
 C   -1.103668    0.597282   -3.001303
 H   -0.333646    1.344494   -3.241712
 H   -0.657694   -0.101985   -2.277300
 H   -1.337234    0.034879   -3.914587
 C   -3.274609    3.747669    0.302528
 H   -2.562740    3.391989    1.062373
 H   -2.914171    4.725676   -0.054364
 H   -4.246797    3.910128    0.786348
 C    2.123369    1.984851    0.682730
 C    2.420466    2.432426    1.977165
 C    2.939332    1.052862    0.019468
 C    3.561632    1.919463    2.603293
 C    4.072854    0.572657    0.676252
 C    4.398393    0.998634    1.968270
 H    4.705009   -0.146211    0.134914
 C    1.552448    3.448455    2.671530
 H    1.620310    3.342178    3.763231
 H    1.868576    4.475401    2.425304
 H    0.498624    3.350938    2.374603
 C    2.604647    0.551985   -1.359871
 H    1.733074   -0.120739   -1.320483
 H    2.344693    1.372720   -2.045893
 H    3.462558   -0.007971   -1.763123
 C   -6.132966    1.053828   -2.867478
 H   -6.513002    1.823865   -3.557703
 H   -6.101210    0.103169   -3.417942
 H   -6.862594    0.958541   -2.050120
 C    5.636599    0.471436    2.645541
 H    5.617191    0.653608    3.729535
 H    5.750283   -0.609222    2.474650
 H    6.539126    0.957134    2.240939
 H    3.797661    2.250174    3.619300
Na    3.666998   -2.517475   -0.724942
 O    5.288494   -1.450974   -1.499086
 H    7.713806   -1.722934   -0.450022
 H    7.232026   -2.839743   -2.691769
 C    7.508581   -0.749737   -0.925357
 H    7.135756   -0.066671   -0.144857
 C    7.008701   -1.849595   -3.121803
 H    8.460127   -0.344329   -1.311448
 C    6.433021   -0.925248   -2.023921
 H    6.256906   -1.989688   -3.916088
 H    7.931341   -1.456009   -3.582870
 C    6.163352    0.462961   -2.652885
 H    5.403935    0.369511   -3.446728
 H    5.764097    1.146999   -1.886017
 H    7.066814    0.921932   -3.090578
88
Figure S12-1_PA-PPh3(NaOtBu)-prod(1,4) / electronic energy: -4028.96421775 a.u. / lowest freq: 14.38 cm-1
Cu   -1.003543   -1.050129   -0.600510
 C    1.928108   -0.531587   -0.812347
 C    1.196734   -1.485863    0.135687
 H    1.647197    0.477098   -0.497176
 C    1.171095   -2.903831   -0.135928
 C    1.028839   -1.076481    1.511529
 O    1.788182   -3.220557   -1.299834
 O    0.662769   -3.803764    0.532320
 O    0.594820   -1.744303    2.450872
 O    1.418063    0.199997    1.748542
 C    1.318593    0.664358    3.082220
 H    0.285585    0.606068    3.451912
 H    1.645411    1.711330    3.064484
 H    1.971488    0.083188    3.749374
 C    1.635284   -4.544957   -1.767611
 H    2.051708   -5.273781   -1.057847
 H    2.178440   -4.599438   -2.718356
 H    0.573460   -4.781773   -1.934153
 C    3.425594   -0.628715   -0.692316
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 H     3.854243   -1.616585   -0.897122
 C     4.206659    0.402280   -0.345467
 H     3.724062    1.370543   -0.166940
 C     5.671585    0.396622   -0.176511
 C     6.335128    1.615068    0.036539
 C     6.444639   -0.776526   -0.215067
 C     7.718968    1.666735    0.196856
 H     5.751683    2.539279    0.074286
 C     7.826468   -0.727270   -0.054585
 H     5.959270   -1.743411   -0.364328
 C     8.471891    0.494294    0.151032
 H     8.210708    2.628596    0.359337
 H     8.405942   -1.652967   -0.085823
 H     9.555965    0.529816    0.279290
 C    -1.003659   -1.479786   -2.778278
 H    -1.902973   -1.875679   -3.218946
 C     0.104344   -1.043978   -2.486132
 C     1.501616   -0.631682   -2.301473
 H     1.655598    0.347636   -2.781708
 H     2.125917   -1.358388   -2.840474
Na    -1.020258   -3.230321    1.936310
 O    -2.288878   -2.069183    0.517257
 C    -3.458869   -2.668082    0.063170
 C    -3.124557   -3.917246   -0.772566
 H    -4.024141   -4.415361   -1.169558
 H    -2.477502   -3.639177   -1.618398
 H    -2.569778   -4.647836   -0.161748
 C    -4.285030   -1.691956   -0.788159
 H    -5.228741   -2.139535   -1.140039
 H    -4.521707   -0.786237   -0.208275
 H    -3.706295   -1.370460   -1.666638
 C    -4.302846   -3.087554    1.281351
 H    -5.253781   -3.561799    0.989727
 H    -3.751782   -3.808710    1.908360
 H    -4.530804   -2.204491    1.899159
 P    -1.430514    1.276217   -0.150201
 C    -3.044439    1.654909   -0.938906
 C    -3.193983    1.344527   -2.298231
 C    -4.135538    2.180882   -0.239703
 C    -4.406351    1.564843   -2.946622
 H    -2.352761    0.920787   -2.853327
 C    -5.354873    2.386848   -0.886062
 H    -4.040327    2.423578    0.820565
 C    -5.493353    2.080264   -2.238839
 H    -4.507855    1.322360   -4.006671
 H    -6.201585    2.791030   -0.326964
 H    -6.449125    2.241142   -2.742277
 C    -0.384600    2.704886   -0.661407
 C     0.885528    2.847460   -0.078952
 C    -0.779015    3.625548   -1.639562
 C     1.735722    3.879432   -0.468100
 H     1.210446    2.139764    0.685792
 C     0.078295    4.653927   -2.035082
 H    -1.764254    3.548523   -2.102291
 C     1.337044    4.784737   -1.452889
 H     2.717606    3.975787    0.001253
 H    -0.247574    5.360808   -2.801276
 H     2.006292    5.590208   -1.762786
 C    -1.751786    1.571579    1.628456
 C    -1.526624    2.791979    2.274431
 C    -2.265546    0.486064    2.353586
 C    -1.802064    2.925370    3.635340
 H    -1.129607    3.644285    1.718695
 C    -2.552403    0.631100    3.710458
 H    -2.427686   -0.473320    1.840294
 C    -2.316249    1.846310    4.355057
 H    -1.617531    3.879277    4.134371
 H    -2.953148   -0.216905    4.271069
 H    -2.530538    1.954193    5.420779
88
Figure S12-1_PA-PPh3(NaOtBu)-ts(1,4) / electronic energy: -4028.89777635 a.u. / lowest freq: -353.66 cm-1
Cu    -0.737850   -0.679811   -0.643617
 C     3.141478    0.604844    0.239369
 C     2.149668   -0.188984    0.837225
 H     3.008057    1.673580    0.406296
 C     2.191495   -1.652802    0.830504
 C     1.072626    0.466370    1.572480
 O     2.897057   -2.147835   -0.194534
 O     1.676239   -2.403184    1.645618
 O     0.202030   -0.080109    2.238300
 O     1.112015    1.807201    1.497316
 C     0.181819    2.521965    2.293430
 H    -0.849959    2.219192    2.073004
 H     0.320795    3.580418    2.047796
 H     0.376649    2.354361    3.362861
 C     3.029207   -3.557420   -0.264899
 H     3.495831   -3.958716    0.645817
 H     3.663611   -3.760137   -1.134626
 H     2.047735   -4.033345   -0.401168
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 C     4.535239    0.209294    0.039789
 H     4.743812   -0.851675   -0.099304
 C     5.530606    1.114757    0.049595
 H     5.268909    2.170765    0.185490
 C     6.967006    0.844973   -0.109228
 C     7.869094    1.920094   -0.054067
 C     7.487369   -0.444670   -0.319672
 C     9.239842    1.719902   -0.204388
 H     7.484044    2.930383    0.107860
 C     8.855708   -0.645449   -0.469377
 H     6.815210   -1.303791   -0.369154
 C     9.739457    0.435172   -0.412871
 H     9.921412    2.572264   -0.159494
 H     9.238865   -1.655232   -0.632740
 H    10.812806    0.273874   -0.533167
 C     0.366726   -0.037470   -2.176475
 H    -0.257178   -0.131843   -3.075253
 C     1.533091    0.471062   -2.194276
 C     2.786965    0.948375   -2.012460
 H     2.959729    2.028462   -1.966142
 H     3.634945    0.340211   -2.337927
Na    -0.506241   -2.226650    2.257122
 O    -1.321823   -2.364115    0.221047
 C    -1.641060   -3.513520   -0.490125
 C    -0.890181   -3.562467   -1.831011
 H    -1.062453   -4.506582   -2.373253
 H    -1.212979   -2.730412   -2.477757
 H     0.190933   -3.446506   -1.657194
 C    -3.155870   -3.552538   -0.762893
 H    -3.460096   -4.448990   -1.328449
 H    -3.710815   -3.541205    0.189390
 H    -3.454447   -2.660087   -1.335398
 C    -1.242279   -4.743705    0.346873
 H    -1.478981   -5.696293   -0.154064
 H    -0.159245   -4.719404    0.550320
 H    -1.773529   -4.730173    1.313504
 P    -2.508250    0.767917   -0.172711
 C    -3.894769    0.197894   -1.235089
 C    -3.612197    0.006884   -2.595636
 C    -5.172526   -0.110989   -0.758459
 C    -4.587855   -0.478186   -3.462066
 H    -2.614687    0.235038   -2.980127
 C    -6.148017   -0.604871   -1.626204
 H    -5.410733    0.025037    0.298432
 C    -5.859058   -0.791047   -2.976722
 H    -4.353111   -0.622840   -4.518741
 H    -7.141097   -0.845032   -1.239945
 H    -6.623023   -1.180340   -3.653213
 C    -2.405281    2.551456   -0.572540
 C    -1.130618    3.108894   -0.727576
 C    -3.535974    3.361632   -0.750009
 C    -0.986789    4.464315   -1.027027
 H    -0.248030    2.472891   -0.618440
 C    -3.390992    4.713712   -1.050676
 H    -4.535836    2.929999   -0.653095
 C    -2.115344    5.267181   -1.185217
 H     0.011400    4.891759   -1.144572
 H    -4.276409    5.338971   -1.184409
 H    -2.002750    6.327739   -1.421166
 C    -3.213516    0.681021    1.513961
 C    -3.595263    1.787327    2.277795
 C    -3.320274   -0.606295    2.065416
 C    -4.081710    1.611021    3.575389
 H    -3.511166    2.795599    1.866375
 C    -3.820557   -0.778492    3.353113
 H    -2.984807   -1.463098    1.467091
 C    -4.200018    0.331319    4.113448
 H    -4.373120    2.482765    4.165610
 H    -3.910593   -1.783924    3.771856
 H    -4.587280    0.196195    5.125778
88
Figure S12-1_PA-PPh3(NaOtBu)-ed(1,4) / electronic energy: -4028.91570865 a.u. / lowest freq: 15.81 cm-1
Cu    -0.570023    0.562313   -1.431087
 C     0.998863   -2.748327    0.151397
 C    -0.241966   -2.996970   -0.350070
 H     1.165458   -3.079027    1.181621
 C    -0.674776   -2.741002   -1.750259
 C    -1.269008   -3.584256    0.557395
 O     0.332155   -2.632609   -2.601725
 O    -1.833443   -2.695826   -2.112666
 O    -2.458205   -3.345045    0.507083
 O    -0.749250   -4.416324    1.449148
 C    -1.651960   -5.047455    2.351772
 H    -2.235479   -4.299783    2.903121
 H    -1.032411   -5.634382    3.037079
 H    -2.336930   -5.707261    1.801765
 C    -0.007443   -2.325274   -3.950889
 H    -0.598175   -3.138601   -4.393464
 H     0.944148   -2.214288   -4.480382
```

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 H   -0.579339   -1.387902   -3.988264
 C    2.101917   -2.049379   -0.456954
 H    1.940937   -1.554934   -1.414556
 C    3.291108   -1.978431    0.180761
 H    3.397561   -2.500649    1.138596
 C    4.473805   -1.242333   -0.266774
 C    5.668381   -1.363985    0.461004
 C    4.438184   -0.363131   -1.363486
 C    6.797250   -0.629117    0.107317
 H    5.705307   -2.037027    1.321432
 C    5.562723    0.377782   -1.709088
 H    3.511912   -0.215229   -1.922943
 C    6.745837    0.247262   -0.976913
 H    7.718620   -0.734248    0.683815
 H    5.509310    1.074144   -2.548422
 H    7.626250    0.833229   -1.249759
 C    0.985259    0.801422   -2.624594
 H    1.218026    0.133595   -3.471102
 C    1.801684    1.808876   -2.488788
 C    2.606271    2.838971   -2.257573
 H    2.433053    3.820525   -2.712222
 H    3.476073    2.738018   -1.597364
Na   -3.270908   -1.512185   -0.713052
 O   -2.558940    0.436928   -1.410323
 C   -3.309369    1.196634   -2.299214
 C   -2.977236    0.817846   -3.753750
 H   -3.560941    1.400327   -4.485587
 H   -1.905524    0.992038   -3.941268
 H   -3.179472   -0.252745   -3.921080
 C   -3.028654    2.694716   -2.092539
 H   -3.640616    3.333217   -2.751142
 H   -3.225193    2.975354   -1.045503
 H   -1.965930    2.903732   -2.294532
 C   -4.804212    0.930041   -2.040241
 H   -5.460896    1.540180   -2.681127
 H   -5.046957   -0.128619   -2.235630
 H   -5.047229    1.152366   -0.988323
 P   -0.391215    0.950690    0.893545
 C   -1.009983    2.680454    1.030729
 C   -0.455257    3.593212    0.121512
 C   -1.949023    3.135174    1.961509
 C   -0.837520    4.931987    0.141691
 H    0.285402    3.254368   -0.611078
 C   -2.341288    4.474732    1.970672
 H   -2.383871    2.446546    2.688922
 C   -1.789742    5.375438    1.060374
 H   -0.397619    5.630146   -0.574011
 H   -3.080159    4.815572    2.699601
 H   -2.098939    6.423123    1.069148
 C    1.194593    1.145633    1.801526
 C    2.364779    1.134799    1.037020
 C    1.276134    1.422518    3.174627
 C    3.602497    1.387811    1.632834
 H    2.297238    0.937991   -0.035587
 C    2.511457    1.656652    3.771849
 H    0.367119    1.461142    3.780791
 C    3.677422    1.640126    3.000218
 H    4.508465    1.377842    1.021918
 H    2.567221    1.864327    4.842858
 H    4.645149    1.830738    3.469839
 C   -1.468285   -0.032805    1.998532
 C   -0.963959   -0.941472    2.937578
 C   -2.858834    0.032912    1.805234
 C   -1.828988   -1.731790    3.695259
 H    0.113221   -1.029360    3.094367
 C   -3.719842   -0.756458    2.564201
 H   -3.254144    0.700514    1.035226
 C   -3.207839   -1.638765    3.516923
 H   -1.417171   -2.423097    4.434160
 H   -4.798739   -0.681660    2.408554
 H   -3.882264   -2.254919    4.115500
41
Figure S12-1_PPh3-Cu-allenyl / electronic energy: -2791.78064609 a.u. / lowest freq: -8.52 cm-1
Cu    1.925957    0.441034   -0.969324
 C    3.695423    0.782212   -1.650311
 H    3.901621    1.250294   -2.626132
 C    4.739409    0.464057   -0.934464
 C    5.764894    0.124180   -0.171645
 H    6.228054   -0.865398   -0.246897
 H    6.190086    0.825011    0.554818
 P   -0.093017    0.040978   -0.106258
 C   -0.713342    1.391986    0.957863
 C   -1.380331    1.168166    2.166791
 C   -0.511650    2.705927    0.513218
 C   -1.849259    2.247854    2.915852
 H   -1.535294    0.149778    2.529631
 C   -0.989950    3.780817    1.258089
 H    0.022539    2.889678   -0.423318
 C   -1.658731    3.552160    2.461671
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 H   -2.365753    2.066564    3.860640
 H   -0.832329    4.800736    0.901689
 H   -2.027713    4.394962    3.049984
 C   -0.164393   -1.456811    0.937848
 C   -1.315396   -2.246691    1.042854
 C    0.979917   -1.802657    1.668371
 C   -1.322993   -3.362695    1.878346
 H   -2.210179   -1.992779    0.469631
 C    0.967011   -2.915256    2.507351
 H    1.889455   -1.202122    1.577400
 C   -0.184532   -3.695898    2.612619
 H   -2.223689   -3.975283    1.954422
 H    1.863220   -3.177711    3.073131
 H   -0.192646   -4.571265    3.265682
 C   -1.410845   -0.201190   -1.350523
 C   -2.710237    0.290159   -1.183020
 C   -1.089521   -0.925749   -2.506174
 C   -3.679067    0.050420   -2.157376
 H   -2.969562    0.864064   -0.290291
 C   -2.061407   -1.169847   -3.473746
 H   -0.072030   -1.299724   -2.651497
 C   -3.357069   -0.680980   -3.300219
 H   -4.690190    0.439664   -2.021497
 H   -1.803574   -1.735870   -4.371205
 H   -4.117079   -0.866243   -4.062285
56
Figure S12-1_PPh3-Cu(NaOtBu)-allenyl / electronic energy: -3186.94946047 a.u. / lowest freq: 17.55 cm-1
 O    2.679707    0.458749    0.336658
 C    2.876149    1.711501   -0.232810
 C    2.633294    1.652168   -1.752236
 H    2.809636    2.620386   -2.249231
 H    3.294363    0.899036   -2.210771
 H    1.589467    1.355851   -1.946640
 C    4.326321    2.161911    0.022150
 H    4.533981    3.164074   -0.386653
 H    4.527002    2.185912    1.105618
 H    5.034277    1.457346   -0.446128
 C    1.921287    2.752429    0.378207
 H    2.082453    2.826681    1.465553
 H    2.064136    3.752928   -0.061754
 H    0.876391    2.454588    0.207938
Na    4.192004   -1.067646    0.727870
Cu    1.288500   -0.822764   -0.375650
 C    1.862085   -2.640772   -0.993184
 H    1.147514   -3.293574   -1.520932
 C    3.055867   -3.124853   -0.836663
 C    4.312629   -3.520639   -0.623418
 H    4.581162   -4.116181    0.256848
 H    5.095647   -3.351353   -1.371235
 P   -0.849096   -0.136694   -0.070969
 C   -1.422126    1.401939   -0.887995
 C   -1.965520    2.490874   -0.198747
 C   -1.242163    1.495869   -2.276049
 C   -2.324058    3.651887   -0.885475
 H   -2.105372    2.438775    0.882938
 C   -1.609174    2.650658   -2.961685
 H   -0.805874    0.656470   -2.825549
 C   -2.148620    3.734255   -2.265657
 H   -2.743417    4.497278   -0.335680
 H   -1.463921    2.710205   -4.042426
 H   -2.427750    4.644810   -2.800279
 C   -1.109293    0.184208    1.717995
 C   -2.355102    0.071958    2.347964
 C    0.013135    0.561068    2.468941
 C   -2.480470    0.346901    3.708744
 H   -3.233946   -0.233334    1.774683
 C   -0.118773    0.842233    3.829048
 H    0.989112    0.631426    1.974082
 C   -1.363114    0.735464    4.449972
 H   -3.454915    0.255060    4.193448
 H    0.758739    1.139359    4.408150
 H   -1.464204    0.948820    5.516554
 C   -2.179813   -1.336092   -0.471572
 C   -3.448087   -0.965991   -0.934674
 C   -1.891947   -2.693953   -0.277907
 C   -4.415282   -1.938638   -1.189436
 H   -3.683903    0.088070   -1.099146
 C   -2.862629   -3.663398   -0.521896
 H   -0.894077   -2.988180    0.059831
 C   -4.126367   -3.286819   -0.979558
 H   -5.400936   -1.639769   -1.553207
 H   -2.629320   -4.718478   -0.363103
 H   -4.885415   -4.046554   -1.178719
88
Figure S12-1_PA-PPh3(NaOtBu)-ed(1,6) / electronic energy: -4028.88980074 a.u. / lowest freq: 13.33 cm-1
Na    2.450641   -3.074338    1.308034
 O    4.423596   -2.746492    0.623327
Cu   -1.192041    0.723724    0.500555
 C   -2.296177   -0.875188    1.205317
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 C   -0.944971   -1.296006    1.048034
 H   -2.548774   -0.532170    2.211862
 C   -0.426622   -2.119540   -0.072870
 C   -0.091323   -1.239508    2.272298
 O   -1.263293   -2.207318   -1.104345
 O    0.657300   -2.664089   -0.095355
 O    0.814374   -1.994039    2.554660
 O   -0.448134   -0.240526    3.076182
 C    0.250182   -0.115965    4.311120
 H    0.067850   -0.996119    4.942833
 H   -0.148054    0.783942    4.789974
 H    1.327226   -0.007056    4.131627
 C   -0.870613   -3.045202   -2.187870
 H    0.117651   -2.754627   -2.566426
 H   -1.633639   -2.911144   -2.961625
 H   -0.838837   -4.094978   -1.865325
 C   -3.444083   -1.153356    0.365828
 H   -3.273364   -1.577065   -0.621043
 C   -4.693782   -0.880824    0.798743
 H   -4.813151   -0.456411    1.801027
 C   -5.944527   -1.128629    0.071100
 C   -7.164861   -0.881118    0.719939
 C   -5.978861   -1.605565   -1.250649
 C   -8.379664   -1.101588    0.075302
 H   -7.156562   -0.505740    1.746589
 C   -7.191638   -1.826142   -1.895243
 H   -5.047912   -1.800615   -1.786489
 C   -8.397447   -1.575601   -1.236010
 H   -9.317121   -0.901471    0.598533
 H   -7.197946   -2.195614   -2.923076
 H   -9.348008   -1.747934   -1.745237
 C   -2.458129    2.214523    0.737033
 H   -1.992452    3.157329    1.066256
 C   -3.733808    2.240140    0.492451
 C   -5.027576    2.202883    0.226669
 H   -5.761737    1.965517    1.002853
 H   -5.412665    2.415785   -0.775933
 P    0.869641    1.499836   -0.208565
 C    2.115088    1.243418    1.101485
 C    2.172419    2.113067    2.200850
 C    2.955128    0.126638    1.073202
 C    3.089098    1.884969    3.225169
 H    1.511378    2.982070    2.252725
 C    3.868569   -0.106085    2.100936
 H    2.938155   -0.585810    0.244922
 C    3.941502    0.778559    3.175498
 H    3.134948    2.577041    4.068909
 H    4.498761   -0.996274    1.990857
 H    4.661996    0.609438    3.979098
 C    0.929245    3.290949   -0.591894
 C    2.086757    4.060967   -0.415644
 C   -0.204803    3.877707   -1.166172
 C    2.103668    5.399713   -0.800650
 H    2.980891    3.619695    0.030197
 C   -0.182757    5.216755   -1.555565
 H   -1.114983    3.288396   -1.301389
 C    0.969477    5.979492   -1.370701
 H    3.009668    5.991677   -0.655558
 H   -1.073534    5.665475   -1.999818
 H    0.984752    7.029845   -1.669741
 C    1.594175    0.767283   -1.720091
 C    0.770295    0.035107   -2.579299
 C    2.929750    0.997607   -2.077776
 C    1.275460   -0.465420   -3.780967
 H   -0.274673   -0.143820   -2.313177
 C    3.433801    0.489995   -3.270263
 H    3.584660    1.571267   -1.417903
 C    2.606464   -0.241797   -4.124130
 H    0.624949   -1.034140   -4.448627
 H    4.479838    0.660931   -3.531117
 H    3.004631   -0.641835   -5.058924
 H    6.298504   -1.307492   -1.775557
 H    5.075966   -0.528071   -0.735786
 H    6.534500   -1.239940   -0.003799
 C    5.783565   -1.368924   -0.800824
 H    3.238652   -2.043289   -1.658827
 C    5.031521   -2.707048   -0.597598
 H    6.585961   -3.855881   -1.707421
 H    6.807690   -3.776031    0.066194
 H    3.463633   -3.811364   -1.640746
 C    3.990422   -2.846445   -1.736170
 C    6.057815   -3.856119   -0.737796
 H    4.434826   -2.797210   -2.745864
 H    5.546554   -4.826628   -0.623546
88
Figure S12-1_PA-PPh3(NaOtBu)-ts(1,6) / electronic energy: -4028.87865129 a.u. / lowest freq: -449.09 cm-1
Na   -2.536603   -2.902598   -1.322606
 O   -4.488787   -2.632480   -0.546129
Cu    1.170459    0.711231   -0.577139
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 C    2.314675   -0.930227   -1.276563
 C    0.942024   -1.366477   -1.149405
 H    2.582064   -0.611776   -2.288274
 C    0.431605   -2.205511   -0.058587
 C    0.094528   -1.257183   -2.353017
 O    1.307990   -2.382277    0.938174
 O   -0.673902   -2.714191   -0.001108
 O   -0.909897   -1.894847   -2.608539
 O    0.545820   -0.322835   -3.203551
 C   -0.167664   -0.156093   -4.420616
 H   -0.107934   -1.067232   -5.032488
 H    0.314750    0.678517   -4.940199
 H   -1.221569    0.078971   -4.221998
 C    0.914414   -3.250026    1.992825
 H   -0.035763   -2.923895    2.435936
 H    1.718262   -3.206838    2.735487
 H    0.798940   -4.278230    1.622419
 C    3.386522   -1.010982   -0.375766
 H    3.208366   -1.341189    0.645295
 C    4.669031   -0.611301   -0.765284
 H    4.846181   -0.549475   -1.841789
 C    5.872480   -0.939473    0.034895
 C    7.106482   -1.099075   -0.611260
 C    5.825206   -1.092619    1.429530
 C    8.256742   -1.418034    0.108800
 H    7.163735   -0.974462   -1.695998
 C    6.973373   -1.410075    2.149423
 H    4.882410   -0.949631    1.961884
 C    8.194362   -1.576750    1.492644
 H    9.207038   -1.543700   -0.414718
 H    6.915539   -1.526478    3.233952
 H    9.094414   -1.825774    2.058890
 C    2.397006    2.295018   -0.867599
 H    1.829769    3.223632   -0.960687
 C    3.645453    2.087775   -0.813072
 C    4.899520    1.582513   -0.680523
 H    5.572747    1.597170   -1.542180
 H    5.385429    1.671924    0.295953
 P   -0.826110    1.499240    0.229268
 C   -2.096070    1.266745   -1.059685
 C   -2.092460    2.091730   -2.194536
 C   -3.002169    0.205888   -0.992029
 C   -3.014291    1.877456   -3.216894
 H   -1.375648    2.913130   -2.278248
 C   -3.919009   -0.015458   -2.019383
 H   -3.025612   -0.478639   -0.141077
 C   -3.931022    0.826062   -3.129906
 H   -3.012315    2.534332   -4.089625
 H   -4.592729   -0.869911   -1.887287
 H   -4.652159    0.664402   -3.934467
 C   -0.865108    3.282708    0.645853
 C   -1.974489    4.103239    0.406591
 C    0.253664    3.814704    1.300288
 C   -1.958573    5.437560    0.809735
 H   -2.857151    3.704256   -0.098002
 C    0.264643    5.147746    1.707208
 H    1.124743    3.182304    1.492148
 C   -0.840336    5.961673    1.458526
 H   -2.827188    6.070372    0.616180
 H    1.142716    5.552697    2.214273
 H   -0.830144    7.008179    1.770770
 C   -1.508394    0.738890    1.744404
 C   -0.695703   -0.097530    2.513979
 C   -2.801418    1.045527    2.190931
 C   -1.168164   -0.621159    3.718991
 H    0.314751   -0.338642    2.173772
 C   -3.273832    0.514737    3.386087
 H   -3.446360    1.698242    1.597500
 C   -2.455616   -0.316902    4.153540
 H   -0.525785   -1.268770    4.319269
 H   -4.287186    0.746602    3.719245
 H   -2.828448   -0.733301    5.091602
 H   -6.325259   -1.229222    1.903418
 H   -5.108642   -0.434171    0.868768
 H   -6.577976   -1.123711    0.135923
 C   -5.819970   -1.273250    0.922649
 H   -3.267062   -1.968533    1.726309
 C   -5.077042   -2.611324    0.684139
 H   -6.619816   -3.772484    1.798684
 H   -6.867879   -3.661553    0.029980
 H   -3.494075   -3.735140    1.683600
 C   -4.018485   -2.771969    1.803184
 C   -6.106384   -3.758210    0.821257
 H   -4.446309   -2.738271    2.820764
 H   -5.600839   -4.728434    0.682782
88
Figure S12-1_PA-PPh3(NaOtBu)-prod(1,6) / electronic energy: -4028.93073582 a.u. / lowest freq: 14.54 cm-1
Na    2.130369   -3.399350    0.637885
 O    4.218213   -3.003469    0.406807
```

```
Cu   -1.523334    1.465568   -0.026093
 C   -2.180909   -0.733345    0.698604
 C   -1.084557   -1.657801    0.635074
 H   -2.471263   -0.515266    1.732093
 C   -0.601207   -2.258553   -0.585413
 C   -0.502467   -2.105040    1.888290
 O   -1.298598   -1.883774   -1.682702
 O    0.328282   -3.048401   -0.713686
 O    0.401157   -2.919418    2.038071
 O   -1.079300   -1.552136    2.978069
 C   -0.646407   -2.021766    4.239604
 H   -0.875997   -3.090395    4.364449
 H   -1.194563   -1.436042    4.986839
 H    0.433785   -1.874726    4.369303
 C   -0.949173   -2.513513   -2.901982
 H    0.121939   -2.397351   -3.116129
 H   -1.547184   -2.025088   -3.680516
 H   -1.184827   -3.587289   -2.870433
 C   -2.973863   -0.116522   -0.252808
 H   -2.857065   -0.380826   -1.307182
 C   -4.302486    0.513726    0.143229
 H   -4.297331    0.660905    1.235240
 C   -5.481672   -0.383017   -0.193747
 C   -6.317663   -0.870138    0.815644
 C   -5.751983   -0.749137   -1.519019
 C   -7.398371   -1.699741    0.512353
 H   -6.119585   -0.599125    1.856219
 C   -6.830291   -1.575942   -1.826315
 H   -5.108485   -0.390410   -2.327014
 C   -7.659057   -2.054343   -0.810118
 H   -8.039767   -2.069836    1.315399
 H   -7.023880   -1.849417   -2.865988
 H   -8.503826   -2.703702   -1.050110
 C   -2.360796    3.483963    0.083138
 H   -1.671208    4.280515    0.316851
 C   -3.296610    2.741309   -0.189852
 C   -4.464701    1.908472   -0.498071
 H   -5.380392    2.407325   -0.145108
 H   -4.545948    1.817811   -1.593253
 P    0.747788    1.653523    0.049686
 C    1.544926    0.756522    1.420662
 C    1.162938    1.067719    2.733876
 C    2.513605   -0.225717    1.207002
 C    1.791936    0.445697    3.808620
 H    0.384256    1.812928    2.920977
 C    3.133127   -0.862152    2.282442
 H    2.805262   -0.526099    0.199014
 C    2.782578   -0.514235    3.584516
 H    1.499626    0.704288    4.828811
 H    3.867586   -1.636773    2.027728
 H    3.267907   -1.002116    4.433127
 C    1.346749    3.383110    0.211445
 C    2.260391    3.805924    1.181214
 C    0.865853    4.309452   -0.726090
 C    2.678327    5.137771    1.217419
 H    2.654503    3.097078    1.911928
 C    1.287496    5.635630   -0.690857
 H    0.161334    3.988913   -1.499417
 C    2.193483    6.053453    0.286047
 H    3.393032    5.456976    1.978720
 H    0.908681    6.345973   -1.428633
 H    2.523169    7.094026    0.318027
 C    1.601582    1.116105   -1.473825
 C    0.882351    0.439719   -2.462683
 C    2.954591    1.417140   -1.687776
 C    1.506558    0.073535   -3.656609
 H   -0.169496    0.194054   -2.297718
 C    3.576469    1.040267   -2.873073
 H    3.525189    1.951213   -0.923810
 C    2.850854    0.372494   -3.861607
 H    0.937126   -0.445900   -4.429851
 H    4.633151    1.266629   -3.027082
 H    3.339127    0.081951   -4.794013
 H    6.279139   -1.088847   -1.446087
 H    4.977839   -0.546027   -0.351896
 H    6.372527   -1.435674    0.306290
 C    5.687926   -1.363329   -0.554692
 H    3.227503   -1.770819   -1.746980
 C    4.922333   -2.698868   -0.721374
 H    6.566481   -3.587457   -1.936530
 H    6.636434   -3.928340   -0.181243
 H    3.437856   -3.503779   -2.107238
 C    3.977813   -2.555799   -1.941359
 C    5.957694   -3.803929   -1.040920
 H    4.500710   -2.293399   -2.877813
 H    5.440226   -4.764518   -1.200696
6
Figure S13-1_NaOMe / electronic energy: -277.276605389 a.u. / lowest freq: 96.46 cm-1
 O   -0.316755   -0.000577    0.003879
```

```
 C   -1.665390    0.000187   -0.001547
Na    1.722853    0.000166   -0.001070
 H   -2.140426   -0.936765   -0.408364
 H   -2.138619    0.820140   -0.612161
 H   -2.145961    0.118290    1.010551
32
Figure S13-1_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C   -0.660544   -0.726572    0.059153
 C   -1.860539   -0.097447    0.115996
 H   -0.691600   -1.818492   -0.004770
 C   -1.976243    1.390665    0.160143
 C   -3.120576   -0.891785    0.187355
 O   -3.041424    1.823605   -0.507466
 O   -1.182749    2.134043    0.689285
 O   -4.147702   -0.497504    0.683440
 O   -2.981802   -2.118850   -0.320932
 C   -4.097604   -2.989729   -0.195724
 H   -4.332384   -3.170881    0.862818
 H   -3.810049   -3.927003   -0.683244
 H   -4.981752   -2.562067   -0.688186
 C   -3.254671    3.228152   -0.535442
 H   -3.354009    3.627502    0.483524
 H   -4.184056    3.384216   -1.092621
 H   -2.420438    3.737793   -1.038016
 C    0.656646   -0.129211    0.062308
 H    0.725624    0.955889    0.150505
 C    1.759981   -0.902956   -0.019704
 H    1.621029   -1.988149   -0.089650
 C    3.156351   -0.453635   -0.025165
 C    4.175093   -1.416830   -0.109525
 C    3.522207    0.902114    0.053056
 C    5.517020   -1.042840   -0.114390
 H    3.907556   -2.474776   -0.172060
 C    4.861836    1.275255    0.048166
 H    2.754752    1.675486    0.118691
 C    5.863995    0.305241   -0.035401
 H    6.294080   -1.807149   -0.179427
 H    5.127957    2.332459    0.111300
 H    6.914980    0.602284   -0.038425
94
Figure S13-1_PA-SIMes(NaOMe)-prod(1,4) / electronic energy: -3800.11624361 a.u. / lowest freq: 12.17 cm-1
Cu    1.108693    0.499494    0.119494
 C   -2.828671    0.260716   -0.350504
 C   -2.268989   -1.026042    0.240738
 H   -2.729190    0.169040   -1.438290
 C   -2.320476   -1.288497    1.639702
 C   -1.582941   -1.942977   -0.610331
 O   -3.034084   -0.353677    2.336049
 O   -1.818122   -2.226490    2.272044
 O   -0.883024   -2.911223   -0.284408
 O   -1.733814   -1.679264   -1.939326
 C   -1.046503   -2.523300   -2.833482
 H    0.028125   -2.557057   -2.608469
 H   -1.204541   -2.105932   -3.835753
 H   -1.434989   -3.552838   -2.798091
 C   -3.160550   -0.550378    3.726399
 H   -3.640050   -1.513459    3.955704
 H   -3.787613    0.270249    4.096634
 H   -2.181664   -0.520501    4.227582
 C   -4.289569    0.511131   -0.075430
 H   -4.556852    0.696729    0.967875
 C   -5.232484    0.506515   -1.026793
 H   -4.926043    0.317904   -2.063151
 C   -6.679495    0.728636   -0.838665
 C   -7.515440    0.769989   -1.966004
 C   -7.272247    0.902706    0.424197
 C   -8.888052    0.981816   -1.843061
 H   -7.076267    0.633035   -2.958041
 C   -8.642050    1.114817    0.549300
 H   -6.655406    0.866933    1.324736
 C   -9.458770    1.156402   -0.583391
 H   -9.514507    1.009229   -2.737842
 H   -9.079533    1.246512    1.541799
 H  -10.533537    1.321509   -0.481107
 C    0.287196    1.534123   -1.358472
 H    0.801246    1.836214   -2.259023
 C   -0.614511    1.407899   -0.507513
 C   -1.975809    1.492121    0.061451
 H   -2.440670    2.414348   -0.325497
 H   -1.942876    1.571319    1.156569
Na    0.338315   -2.413054    1.558475
 O    0.983141   -0.274579    1.903562
 C    0.332618    0.414343    2.908417
 C    5.244325    0.943407   -0.828908
 H    5.895573    1.269251   -0.003013
 C    5.153547   -0.585183   -0.947226
 H    5.389587   -0.946302   -1.959507
 C    3.030367    0.267866   -0.413736
 C    3.226542   -2.160122   -0.473049
```

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 C    2.721276   -2.835780   -1.593025
 C    3.245409   -2.749634    0.800042
 C    2.211129   -4.122397   -1.414077
 C    2.729256   -4.043955    0.930789
 C    2.199037   -4.740435   -0.160615
 N    3.851589    1.315549   -0.555622
 N    3.743048   -0.841677   -0.625761
 H    5.812301   -1.110496   -0.240197
 H    5.603537    1.419913   -1.752231
 H    2.735749   -4.518287    1.916904
 H    1.795601   -4.651983   -2.275604
 C    2.706722   -2.164922   -2.940295
 H    2.141608   -1.220708   -2.900894
 H    3.724747   -1.918301   -3.278904
 H    2.248756   -2.811685   -3.700107
 C    3.727582   -1.974135    1.995664
 H    4.700754   -1.495224    1.813466
 H    2.991997   -1.179542    2.216328
 H    3.823269   -2.626025    2.874698
 C    3.446094    2.654778   -0.285569
 C    3.193689    3.529732   -1.349118
 C    3.277924    3.050959    1.053458
 C    2.748954    4.821996   -1.050636
 C    2.826864    4.346695    1.302442
 C    2.554182    5.246340    0.264634
 H    2.536215    5.510972   -1.873012
 H    2.681813    4.665631    2.338773
 C    3.388516    3.094256   -2.777074
 H    4.435795    3.230215   -3.092875
 H    3.147073    2.029784   -2.910985
 H    2.762141    3.685909   -3.458432
 C    3.553822    2.087430    2.177325
 H    2.817178    1.267021    2.177453
 H    4.547897    1.625761    2.074712
 H    3.509506    2.596270    3.149244
 C    1.585385   -6.103511    0.016755
 H    0.491791   -6.016318    0.118827
 H    1.783084   -6.749250   -0.850570
 H    1.966726   -6.603981    0.917571
 C    2.054838    6.633872    0.572321
 H    2.758730    7.172830    1.224699
 H    1.917292    7.224767   -0.343459
 H    1.089174    6.594426    1.099440
 H    0.292465   -0.175442    3.850912
 H   -0.718557    0.672376    2.664889
 H    0.831471    1.374543    3.174043
94
Figure S13-1_PA-SIMes(NaOMe)-ts(1,4) / electronic energy: -3800.03623090 a.u. / lowest freq: -400.14 cm-1
Cu    0.939238    0.005732    0.018743
 C   -3.150573   -1.382755   -0.066425
 C   -2.186619   -1.426850    0.948253
 H   -3.235960   -2.314076   -0.623615
 C   -2.108337   -0.440553    2.030223
 C   -1.229167   -2.527335    0.955997
 O   -2.491833    0.785904    1.658495
 O   -1.774537   -0.673044    3.181766
 O   -0.362445   -2.747568    1.796124
 O   -1.369335   -3.352458   -0.092490
 C   -0.299108   -4.239963   -0.346029
 H    0.618518   -3.671999   -0.565685
 H   -0.589052   -4.829722   -1.223471
 H   -0.112388   -4.905116    0.509070
 C   -2.419827    1.800435    2.645221
 H   -3.040217    1.550453    3.517956
 H   -2.791463    2.714865    2.169361
 H   -1.378795    1.937998    2.965750
 C   -4.371400   -0.578426   -0.056767
 H   -4.350469    0.360788    0.496320
 C   -5.488144   -0.980012   -0.692154
 H   -5.460229   -1.932552   -1.234784
 C   -6.775686   -0.271862   -0.740789
 C   -7.858734   -0.875185   -1.401133
 C   -6.979722    0.991042   -0.155941
 C   -9.100304   -0.246839   -1.475138
 H   -7.720633   -1.855815   -1.864386
 C   -8.218831    1.619294   -0.229569
 H   -6.158615    1.492655    0.360367
 C   -9.286134    1.004294   -0.888717
 H   -9.927193   -0.737630   -1.993482
 H   -8.354367    2.600321    0.231488
 H  -10.257216    1.500763   -0.945466
 C    0.235585   -0.806984   -1.679366
 H    1.043523   -0.931120   -2.404381
 C   -0.997870   -0.641646   -1.939469
 C   -2.347544   -0.517048   -2.051591
 H   -2.909031   -1.327188   -2.523112
 H   -2.789329    0.480793   -2.144044
Na    0.463290   -1.246000    3.253293
 O    0.723990    0.476614    1.932420
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 C    1.245614    1.689497    2.310466
 C    4.651656    1.725900   -1.557495
 H    5.375512    2.421589   -1.112970
 C    5.024865    0.258226   -1.347283
 H    5.405226   -0.220764   -2.259622
 C    2.815404    0.604495   -0.605988
 C    3.597951   -1.702860   -0.634247
 C    3.481512   -2.623328   -1.688678
 C    3.578978   -2.123764    0.706732
 C    3.331017   -3.975920   -1.376724
 C    3.416289   -3.486757    0.969204
 C    3.290418   -4.427660   -0.054839
 N    3.344797    1.804719   -0.890027
 N    3.740955   -0.316838   -0.928917
 H    5.776234    0.121906   -0.551056
 H    4.541069    1.983368   -2.623963
 H    3.387336   -3.823342    2.009750
 H    3.223703   -4.697599   -2.192118
 C    3.514373   -2.175005   -3.125727
 H    3.136865   -1.149030   -3.238101
 H    4.542316   -2.191900   -3.523738
 H    2.908435   -2.839154   -3.757122
 C    3.701839   -1.133153    1.834062
 H    4.525011   -0.423724    1.660876
 H    2.775361   -0.538992    1.921377
 H    3.887581   -1.647777    2.787256
 C    2.689960    3.049691   -0.665343
 C    1.604563    3.424471   -1.471022
 C    3.151052    3.883760    0.368904
 C    0.959633    4.634752   -1.194510
 C    2.482835    5.086081    0.601087
 C    1.377302    5.475420   -0.161810
 H    0.107464    4.929529   -1.813877
 H    2.828451    5.734514    1.411888
 C    1.129453    2.551172   -2.599648
 H    1.971375    2.090118   -3.136556
 H    0.507206    1.725820   -2.222117
 H    0.532229    3.130607   -3.316665
 C    4.338281    3.503590    1.213904
 H    4.409378    2.414816    1.344442
 H    5.279502    3.846579    0.753233
 H    4.273753    3.967274    2.207628
 C    3.111351   -5.892855    0.245477
 H    2.251535   -6.306847   -0.302692
 H    3.998428   -6.470010   -0.059903
 H    2.947905   -6.067559    1.317724
 C    0.658839    6.765395    0.138299
 H    1.363816    7.608094    0.200014
 H   -0.089596    6.999486   -0.631157
 H    0.138402    6.705677    1.107184
 H    1.067185    1.907364    3.391475
 H    0.825238    2.559047    1.755088
 H    2.350297    1.761968    2.169567
94
Figure S13-1_PA-SIMes(NaOMe)-ed(1,4) / electronic energy: -3800.05869359 a.u. / lowest freq: 13.79 cm-1
Cu   1.478307    0.095461    0.271493
 C   -4.192674   -1.466072   -0.014437
 C   -3.009673   -1.653931    0.619934
 H   -4.482480   -2.233748   -0.737071
 C   -2.446173   -0.725754    1.643836
 C   -2.165294   -2.838661    0.302519
 O   -2.607304    0.549525    1.348753
 O   -1.867520   -1.101790    2.642762
 O   -1.194285   -3.199132    0.937860
 O   -2.567265   -3.479770   -0.786948
 C   -1.780427   -4.586663   -1.207743
 H   -0.739742   -4.274833   -1.376713
 H   -2.228219   -4.939396   -2.142172
 H   -1.798638   -5.385597   -0.453674
 C   -1.888918    1.485829    2.156668
 H   -2.300526    1.508565    3.175535
 H   -2.025047    2.457623    1.671738
 H   -0.823762    1.201846    2.187100
 C   -5.133486   -0.383714    0.168995
 H   -4.874279    0.410081    0.870439
 C   -6.294587   -0.350174   -0.518499
 H   -6.511941   -1.176667   -1.204751
 C   -7.324582    0.691703   -0.445155
 C   -8.549074    0.482829   -1.100598
 C   -7.136202    1.899091    0.250834
 C   -9.559004    1.441094   -1.054298
 H   -8.709328   -0.448478   -1.649827
 C   -8.142831    2.857413    0.293126
 H   -6.188764    2.099010    0.754936
 C   -9.358682    2.631815   -0.357071
 H  -10.505733    1.258581   -1.566916
 H   -7.977406    3.792289    0.832642
 H  -10.146192    3.387513   -0.323018
 C   -0.011239   -0.695240   -0.804154
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 H     0.088773   -1.759536   -1.087389
 C    -0.983880   -0.073416   -1.408478
 C    -1.961723    0.613579   -1.984973
 H    -2.951590    0.681130   -1.518044
 H    -1.815377    1.135259   -2.937813
Na     0.311055   -1.827290    2.135908
 O     1.265773    0.128409    2.298737
 C     2.009926    1.057982    2.977929
 C     5.284195    1.168881   -1.370423
 H     6.130421    1.682305   -0.892984
 C     5.364153   -0.358972   -1.228535
 H     5.574225   -0.864602   -2.182167
 C     3.289886    0.389944   -0.397793
 C     3.515222   -2.004656   -0.568124
 C     2.867626   -2.621457   -1.648070
 C     3.583432   -2.618641    0.692212
 C     2.297486   -3.881888   -1.449496
 C     2.995689   -3.876765    0.848400
 C     2.343536   -4.521782   -0.208143
 N     4.018199    1.477846   -0.694493
 N     4.024756   -0.684140   -0.734598
 H     6.132014   -0.673962   -0.502854
 H     5.240461    1.492716   -2.423603
 H     3.038037   -4.362729    1.828081
 H     1.785589   -4.367560   -2.285757
 C     2.709612   -1.891216   -2.952487
 H     2.102349   -0.986251   -2.789040
 H     3.676063   -1.569878   -3.369030
 H     2.205408   -2.518040   -3.699962
 C     4.178348   -1.889319    1.865130
 H     5.140111   -1.418099    1.616682
 H     3.485364   -1.088104    2.171549
 H     4.331902   -2.565807    2.717002
 C     3.514911    2.802428   -0.558936
 C     2.514509    3.250246   -1.436861
 C     4.013283    3.627541    0.463332
 C     2.017508    4.546203   -1.267320
 C     3.490262    4.915664    0.591260
 C     2.490972    5.393287   -0.263001
 H     1.234858    4.902002   -1.943575
 H     3.865426    5.562169    1.390403
 C     1.966900    2.350043   -2.512097
 H     2.774208    1.857784   -3.075581
 H     1.355480    1.546894   -2.067883
 H     1.344299    2.915863   -3.217932
 C     5.075716    3.129394    1.406407
 H     4.914782    2.071146    1.656893
 H     6.079377    3.214438    0.958506
 H     5.080776    3.712100    2.337511
 C     1.662740   -5.848052    0.008504
 H     1.475973   -6.365996   -0.942696
 H     2.262886   -6.509146    0.650486
 H     0.690399   -5.699197    0.505195
 C     1.937043    6.783494   -0.086498
 H     2.735762    7.539133   -0.139664
 H     1.191197    7.021464   -0.857234
 H     1.453932    6.892287    0.896993
 H     1.879987    0.992334    4.084169
 H     1.763287    2.113454    2.710856
 H     3.110256    0.965041    2.801302
56
Figure S13-1_SIMes-Cu-allenyl / electronic energy: -2680.78923765 a.u. / lowest freq: 16.67 cm-1
 C     0.255100   -2.802091    0.505112
 H     0.668208   -3.196427    1.444813
 C    -1.270500   -2.619391    0.554864
 H    -1.800083   -3.253354   -0.170485
 C    -0.267703   -0.553149    0.091367
 C    -2.705673   -0.570588    0.110299
 C    -3.379878   -0.614762   -1.117966
 C    -3.248840    0.082482    1.227243
 C    -4.637370   -0.011781   -1.202344
 C    -4.506955    0.673704    1.096602
 C    -5.220520    0.629249   -0.105733
Cu     0.110016    1.307604   -0.228361
 N     0.723169   -1.433012    0.264097
 N    -1.429749   -1.197347    0.221108
 H    -1.690544   -2.824163    1.551562
 H     0.576639   -3.468534   -0.309931
 C     0.774672    3.096038   -0.486998
 H     0.208773    4.016056   -0.700711
 C     2.071525    3.214162   -0.388898
 C     3.389142    3.271273   -0.276397
 H     4.042154    3.124597   -1.143427
 H     3.872005    3.450329    0.690170
 H    -4.940744    1.189169    1.958286
 H    -5.171125   -0.034945   -2.156636
 C    -2.739174   -1.258856   -2.318184
 H    -1.764393   -0.794441   -2.533026
 H    -2.557008   -2.332599   -2.157552
```

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 H   -3.373859   -1.155030   -3.207828
 C   -2.466468    0.177007    2.509466
 H   -2.161688   -0.814837    2.876499
 H   -1.543922    0.758395    2.352392
 H   -3.052793    0.668434    3.296712
 C    2.100609   -1.074402    0.152530
 C    2.710868   -1.089540   -1.109969
 C    2.796150   -0.676303    1.303159
 C    4.054490   -0.718966   -1.196317
 C    4.137867   -0.315360    1.170431
 C    4.783410   -0.329256   -0.069282
 H    4.541691   -0.721123   -2.175444
 H    4.690272    0.002663    2.059240
 C    1.914463   -1.435151   -2.339256
 H    1.411113   -2.409070   -2.245646
 H    1.129881   -0.679297   -2.505515
 H    2.554756   -1.464444   -3.230551
 C    2.087510   -0.585650    2.627443
 H    1.295980    0.179314    2.581836
 H    1.603679   -1.535221    2.901538
 H    2.783525   -0.310564    3.430477
 C   -6.591070    1.245868   -0.208877
 H   -6.854724    1.465524   -1.252764
 H   -7.356052    0.560144    0.189860
 H   -6.655115    2.179427    0.368353
 C    6.214528    0.121736   -0.194929
 H    6.791322   -0.109785    0.711774
 H    6.712484   -0.348829   -1.054371
 H    6.258068    1.212948   -0.343793
62
Figure S13-1_SIMes-Cu(NaOMe)-allenyl / electronic energy: -2958.10335257 a.u. / lowest freq: 26.87 cm-1
 C    1.491287   -2.854838   -0.612571
 H    2.057388   -3.568609    0.002574
 C   -0.023431   -3.104601   -0.566334
 H   -0.429277   -3.451467   -1.528274
 C    0.415890   -0.880695    0.077778
 C   -1.919959   -1.431945   -0.249070
 C   -2.472924   -0.954826   -1.447881
 C   -2.681317   -1.518549    0.927535
 C   -3.826265   -0.593993   -1.453640
 C   -4.021889   -1.130531    0.880942
 C   -4.615656   -0.674885   -0.301233
Cu   -0.042716    0.947660    0.537790
 N    1.600626   -1.490844   -0.080800
 N   -0.539013   -1.777234   -0.221584
 H   -0.304569   -3.841693    0.202777
 H    1.895857   -2.897564   -1.637142
 C   -0.732595    2.021360    2.081781
 H   -0.170218    2.178112    3.015913
 C   -1.955323    2.456236    2.070462
 C   -3.225569    2.851533    1.938962
 H   -4.057349    2.205516    2.244183
 H   -3.475501    3.870546    1.619747
 H   -4.618672   -1.178907    1.796191
 H   -4.270866   -0.225950   -2.383480
 C   -1.603476   -0.732191   -2.655001
 H   -0.948780    0.136992   -2.460124
 H   -0.959191   -1.597021   -2.868565
 H   -2.210704   -0.524945   -3.546837
 C   -2.036311   -1.949774    2.215139
 H   -1.525119   -2.918028    2.109014
 H   -1.277419   -1.209487    2.513676
 H   -2.777162   -2.035106    3.020783
 C    2.838621   -0.786557   -0.048737
 C    3.174588    0.050575   -1.127422
 C    3.687687   -0.939460    1.055272
 C    4.393720    0.728969   -1.075556
 C    4.901683   -0.245613    1.060195
 C    5.271183    0.592817    0.005789
 H    4.668200    1.386011   -1.906320
 H    5.571510   -0.356554    1.917870
 C    2.228390    0.233585   -2.283605
 H    1.895638   -0.733797   -2.690944
 H    1.320353    0.775393   -1.961182
 H    2.708030    0.797740   -3.095104
 C    3.275430   -1.800431    2.219340
 H    2.302945   -1.472002    2.617145
 H    3.163971   -2.856467    1.928078
 H    4.016324   -1.751822    3.028280
 C   -6.071727   -0.289871   -0.326705
 H   -6.317753    0.303128   -1.218640
 H   -6.711142   -1.186932   -0.336587
 H   -6.344672    0.294120    0.564521
 C    6.568354    1.358964    0.036023
 H    7.242637    0.982957    0.817988
 H    7.091289    1.294451   -0.929686
 H    6.386027    2.426852    0.236044
 O   -0.436925    2.012250   -1.223160
 C    0.285590    3.176770   -1.324220
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Na   -2.568931    2.027829   -0.660984
 H   -0.042972    3.825511   -2.171476
 H    1.377184    3.007058   -1.494610
 H    0.229234    3.819942   -0.412386
94
Figure S13-1_PA-SIMes(NaOMe)-ed(1,6) / electronic energy: -3800.05935298 a.u. / lowest freq: 16.09 cm-1
 C    1.934056   -0.183601    3.659131
 H    2.729263    0.565910    3.796633
 C    0.532447    0.374851    3.951149
 H   -0.039452   -0.264934    4.639882
 C    0.678834   -0.196976    1.684343
 C   -1.349723    0.973380    2.336149
 C   -1.362200    2.304551    1.885082
 C   -2.534935    0.245119    2.511015
 C   -3.794010    2.186480    1.725406
Cu   -0.035108   -0.770598   -0.063183
 N    1.835482   -0.559348    2.242547
 N   -0.088252    0.369543    2.620774
 C   -0.848110   -0.607184   -1.902430
 C    0.252774    0.307180   -1.852041
 H    0.552996    1.391374    4.370192
 H    2.180011   -1.058834    4.276700
 H   -0.659591   -1.544486   -2.428092
 C    0.147433    1.777332   -1.728513
 C    1.563894   -0.219544   -2.321458
 O   -1.104193    2.222237   -1.671046
 O    1.090032    2.549424   -1.693999
 O    2.508276    0.431993   -2.719829
 O    1.613548   -1.549927   -2.268064
 C    2.814735   -2.177113   -2.699022
 H    2.992584   -1.980424   -3.765260
 H    2.669290   -3.248819   -2.529958
 H    3.665729   -1.811515   -2.110927
 C   -1.303252    3.627892   -1.623786
 H   -0.781574    4.071680   -0.766586
 H   -2.383825    3.774128   -1.524631
 H   -0.940250    4.098455   -2.547952
 C   -2.245190   -0.322001   -1.631468
 H   -2.490331    0.592025   -1.091119
 C   -3.219578   -1.183225   -1.995474
 H   -2.936264   -2.082945   -2.550490
 C   -4.659272   -1.012547   -1.762745
 C   -5.552231   -1.967366   -2.274956
 C   -5.189746    0.075757   -1.049720
 C   -6.926453   -1.843410   -2.082770
 H   -5.157501   -2.822788   -2.829420
 C   -6.561640    0.201271   -0.858032
 H   -4.520019    0.828739   -0.631453
 C   -7.437547   -0.757200   -1.372967
 H   -7.602218   -2.599376   -2.488761
 H   -6.952985    1.055785   -0.301869
 H   -8.514045   -0.655225   -1.220359
 C   -0.623895   -2.644879    0.235413
 H    0.209647   -3.297647    0.535778
 C   -1.816828   -3.146162    0.167413
 C   -3.068170   -3.567981    0.095391
 H   -3.476415   -4.000237   -0.823476
 H   -3.735577   -3.514483    0.962314
 C   -2.592627    2.889568    1.586610
 H   -2.617219    3.927980    1.243878
 C   -3.744032    0.869777    2.187634
 H   -4.675058    0.308714    2.305628
 C   -0.078804    3.075992    1.734049
 H    0.566702    2.971189    2.617978
 H    0.507298    2.720103    0.873488
 H   -0.277963    4.146052    1.587647
 C   -2.508906   -1.158113    3.050603
 H   -1.780390   -1.776749    2.508245
 H   -2.234630   -1.164597    4.117702
 H   -3.495686   -1.630258    2.957235
 C    2.970913   -0.975893    1.484384
 C    3.373412   -2.317479    1.496040
 C    3.674665   -0.001716    0.756519
 C    4.504201   -2.667582    0.749235
 C    4.788588   -0.394007    0.012794
 C    5.220661   -1.725411    0.005951
 H    5.298680    0.379403   -0.575767
 C    2.633713   -3.348698    2.305991
 H    2.725429   -4.344927    1.851834
 H    3.044415   -3.414862    3.326887
 H    1.566607   -3.103150    2.395847
 C    3.245262    1.439858    0.763304
 H    2.293332    1.560278    0.223613
 H    3.078392    1.815085    1.784433
 H    4.014734    2.050981    0.263713
 C   -5.104016    2.846582    1.383237
 H   -5.194560    3.826690    1.874528
 H   -5.187834    3.021553    0.298344
 H   -5.958394    2.229059    1.692812
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 C    6.414468   -2.131731   -0.818409
 H    6.858533   -3.069157   -0.454956
 H    6.128787   -2.286716   -1.871976
 H    7.188215   -1.351039   -0.806655
 H    4.830708   -3.711987    0.748685
Na    3.395075    2.467038   -2.175137
 O    5.346217    2.527464   -1.421682
 C    6.624300    2.715199   -1.022869
 H    7.012996    1.908781   -0.337946
 H    6.807666    3.665946   -0.451399
 H    7.381261    2.748461   -1.853508
94
Figure S13-1_PA-SIMes(NaOMe)-ts(1,6) / electronic energy: -3800.04969158 a.u. / lowest freq: -424.88 cm-1
 C    1.985245    3.661962    0.081206
 H    2.756814    3.759451   -0.698557
 C    0.573584    3.981123   -0.433088
 H    0.043804    4.700051    0.209898
 C    0.680909    1.719863    0.176828
 C   -1.371814    2.414493   -0.925266
 C   -1.444384    1.874523   -2.221117
 C   -2.524900    2.707909   -0.185502
 C   -3.876827    1.880091   -2.045914
Cu   -0.035495   -0.027375    0.743979
 N    1.862281    2.256421    0.491723
 N   -0.081515    2.669075   -0.374583
 C   -0.865777   -1.920987    0.645066
 C    0.274137   -1.914019   -0.252351
 H    0.567942    4.374537   -1.459957
 H    2.280965    4.290993    0.932720
 H   -0.675557   -2.404616    1.606254
 C    0.176969   -1.860068   -1.711736
 C    1.565263   -2.328673    0.321210
 O   -1.073368   -1.694300   -2.157027
 O    1.105229   -1.954703   -2.502448
 O    2.553972   -2.709313   -0.280291
 O    1.575552   -2.240190    1.660180
 C    2.773915   -2.610398    2.324836
 H    3.006258   -3.670115    2.148922
 H    2.592736   -2.436466    3.390831
 H    3.611313   -1.991422    1.978085
 C   -1.280953   -1.730177   -3.558754
 H   -0.668005   -0.977566   -4.071118
 H   -2.344894   -1.518358   -3.710781
 H   -1.035388   -2.722424   -3.963311
 C   -2.209817   -1.584635    0.398431
 H   -2.483387   -1.089145   -0.532806
 C   -3.183609   -1.833260    1.366853
 H   -2.917501   -2.562469    2.135323
 C   -4.634713   -1.737480    1.094819
 C   -5.525874   -2.528394    1.834572
 C   -5.160485   -0.869597    0.125162
 C   -6.899914   -2.463773    1.608850
 H   -5.133907   -3.207550    2.596632
 C   -6.532871   -0.803059   -0.098983
 H   -4.489123   -0.225221   -0.445799
 C   -7.409640   -1.599663    0.640608
 H   -7.574841   -3.091815    2.194668
 H   -6.923509   -0.118729   -0.855111
 H   -8.485807   -1.542970    0.463646
 C   -0.683549    0.493448    2.620952
 H    0.075391    1.123116    3.085167
 C   -1.861839    0.178934    2.956443
 C   -3.135897   -0.285908    2.994387
 H   -3.420943   -1.028861    3.743728
 H   -3.937620    0.379713    2.658026
 C   -2.703246    1.610423   -2.758665
 H   -2.773023    1.190743   -3.766386
 C   -3.766514    2.427677   -0.766327
 H   -4.675018    2.643395   -0.196918
 C   -0.190224    1.593263   -3.002393
 H    0.503516    2.446355   -2.980091
 H    0.355771    0.734903   -2.583910
 H   -0.421128    1.373512   -4.052893
 C   -2.435705    3.331626    1.180340
 H   -1.610064    2.900998    1.761924
 H   -2.268237    4.418243    1.103026
 H   -3.367231    3.179698    1.741826
 C    2.996731    1.492233    0.900831
 C    3.448971    1.558139    2.224795
 C    3.660197    0.716081   -0.065403
 C    4.584414    0.814582    2.567578
 C    4.781523   -0.019623    0.318987
 C    5.259604    0.024491    1.634049
 H    5.261998   -0.641257   -0.448224
 C    2.762731    2.420867    3.250733
 H    2.763807    1.936108    4.237001
 H    3.279445    3.388047    3.360776
 H    1.722588    2.636649    2.970741
 C    3.182468    0.662699   -1.490470
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 H    2.236468    0.103974   -1.558367
 H    2.987334    1.666308   -1.898025
 H    3.939651    0.151616   -2.106856
 C   -5.220620    1.579498   -2.655901
 H   -5.322949    2.055321   -3.642709
 H   -5.351758    0.495780   -2.804730
 H   -6.041081    1.937259   -2.018648
 C    6.459555   -0.794975    2.031435
 H    6.912956   -0.426827    2.962525
 H    6.177181   -1.848501    2.191648
 H    7.225007   -0.784417    1.242364
 H    4.948454    0.856817    3.598662
Na    3.398465   -2.326545   -2.356279
 O    5.321253   -1.514848   -2.542411
 C    6.577919   -1.074029   -2.773260
 H    6.966147   -0.365625   -1.986786
 H    6.712788   -0.508236   -3.735630
 H    7.362628   -1.878013   -2.820153
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Figure S13-1_PA-SIMes(NaOMe)-prod(1,6) / electronic energy: -3800.10311238 a.u. / lowest freq: 6.39 cm-1
 C   -1.498233    3.784527    0.685135
 H   -2.227490    3.868246    1.503492
 C   -0.047537    3.967690    1.152390
 H    0.436019    4.845655    0.702489
 C   -0.278206    1.854946    0.163512
 C    1.971136    2.458174    0.905898
 C    2.350076    1.624777    1.969815
 C    2.922175    3.049256    0.058872
 C    4.688544    1.963197    1.349225
Cu    0.134590    0.084473   -0.498513
 N   -1.485993    2.417955    0.150072
 N    0.588454    2.726158    0.692247
 C    0.431530   -1.900104   -0.994857
 C   -0.811490   -2.112708   -0.250860
 H    0.042025    4.053439    2.246302
 H   -1.784381    4.499538   -0.100724
 H    0.311001   -2.042457   -2.073316
 C   -0.866999   -2.371422    1.171180
 C   -2.036693   -2.241835   -1.022926
 O    0.328814   -2.230740    1.784055
 O   -1.847769   -2.680651    1.838065
 O   -3.136836   -2.603886   -0.625585
 O   -1.875143   -1.903946   -2.320768
 C   -3.012432   -1.997243   -3.157948
 H   -3.438226   -3.010464   -3.142407
 H   -2.666074   -1.753550   -4.168865
 H   -3.783354   -1.279225   -2.846189
 C    0.374995   -2.491356    3.175218
 H   -0.294597   -1.817515    3.728786
 H    1.413844   -2.319341    3.479367
 H    0.089243   -3.530447    3.392082
 C    1.689035   -1.523466   -0.587966
 H    1.938287   -1.453693    0.472362
 C    2.835611   -1.413043   -1.573818
 H    2.563306   -1.966902   -2.485730
 C    4.105473   -2.030090   -1.017046
 C    4.719438   -3.112061   -1.654845
 C    4.690322   -1.522843    0.150488
 C    5.889004   -3.675385   -1.140952
 H    4.274864   -3.522970   -2.565318
 C    5.857929   -2.081224    0.665989
 H    4.226522   -0.678595    0.666553
 C    6.462679   -3.161352    0.020881
 H    6.352270   -4.522544   -1.651879
 H    6.297755   -1.670462    1.577869
 H    7.376751   -3.601980    0.424869
 C    0.986496    1.063932   -3.291277
 H    0.132299    1.449812   -3.817540
 C    1.957861    0.635130   -2.707697
 C    3.101682    0.053048   -2.008390
 H    3.983605    0.085195   -2.668220
 H    3.338895    0.670118   -1.126731
 C    3.713110    1.391481    2.170926
 H    4.020958    0.741761    2.995131
 C    4.272800    2.789479    0.300959
 H    5.022456    3.233473   -0.360224
 C    1.315736    0.982628    2.853700
 H    0.552676    1.704541    3.179224
 H    0.789677    0.180196    2.313079
 H    1.778888    0.541254    3.745827
 C    2.498828    3.919548   -1.093495
 H    1.603305    3.513702   -1.584446
 H    2.264881    4.943116   -0.758603
 H    3.298727    3.993273   -1.842088
 C   -2.669012    1.778728   -0.328490
 C   -3.097540    2.013334   -1.641558
 C   -3.388041    0.947929    0.546610
 C   -4.277655    1.393088   -2.066969
 C   -4.565290    0.358233    0.087204
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 C   -5.021554    0.570414   -1.218483
 H   -5.114811   -0.295057    0.783607
 C   -2.324323    2.919011   -2.563183
 H   -2.527638    2.678591   -3.615850
 H   -2.601954    3.974586   -2.409579
 H   -1.242048    2.840076   -2.389461
 C   -2.901820    0.680629    1.946318
 H   -1.925770    0.170861    1.926091
 H   -2.764430    1.614923    2.513362
 H   -3.626658    0.038838    2.469827
 C    6.150178    1.665879    1.553689
 H    6.759153    2.577959    1.472948
 H    6.335586    1.210798    2.536459
 H    6.509778    0.961846    0.785969
 C   -6.274612   -0.117531   -1.692686
 H   -6.623519    0.282416   -2.655225
 H   -6.096033   -1.197924   -1.817877
 H   -7.085104   -0.011811   -0.956618
 H   -4.620478    1.560423   -3.092556
Na   -4.078997   -2.597833    1.448060
 O   -5.522684   -1.460232    2.435143
 C   -6.458271   -0.659517    2.989935
 H   -6.568926    0.337944    2.474552
 H   -6.271957   -0.388628    4.065077
 H   -7.501323   -1.078995    2.991831
79
Figure S13-1_PA-PPh3(NaOMe)-prod(1,4) / electronic energy: -3911.12006641 a.u. / lowest freq: 12.79 cm-1
Cu   -1.049738   -1.389978   -0.560504
 C    1.748016   -0.530199   -0.831180
 C    1.157778   -1.568519    0.127685
 H    1.308885    0.429379   -0.542788
 C    1.347179   -2.978837   -0.125447
 C    0.917035   -1.184365    1.500560
 O    2.048428   -3.211709   -1.259866
 O    0.950516   -3.935766    0.538210
 O    0.531302   -1.900916    2.424695
 O    1.170322    0.123910    1.748536
 C    1.006683    0.568949    3.082356
 H   -0.020151    0.407619    3.437714
 H    1.230112    1.642867    3.074038
 H    1.704152    0.051985    3.757248
 C    2.138980   -4.551665   -1.698164
 H    2.686825   -5.174365   -0.976361
 H    2.680858   -4.526140   -2.650883
 H    1.139956   -4.986455   -1.850947
 C    3.240741   -0.385875   -0.703030
 H    3.822615   -1.294134   -0.897350
 C    3.840539    0.761299   -0.360573
 H    3.202563    1.635520   -0.184993
 C    5.284573    1.001252   -0.184958
 C    5.726102    2.305022    0.091191
 C    6.250902   -0.014976   -0.278844
 C    7.079801    2.589120    0.264068
 H    4.989364    3.109316    0.170104
 C    7.603030    0.266382   -0.106297
 H    5.943175   -1.042677   -0.483354
 C    8.025734    1.569957    0.165392
 H    7.396057    3.612917    0.476880
 H    8.336423   -0.539841   -0.181518
 H    9.087405    1.786481    0.302456
 C   -0.965876   -2.027257   -2.716378
 H   -1.806102   -2.617560   -3.041696
 C    0.051425   -1.382991   -2.500156
 C    1.354746   -0.730529   -2.324018
 H    1.343421    0.251432   -2.822321
 H    2.099346   -1.350521   -2.843541
Na   -0.880493   -3.606688    1.849262
 O   -2.235575   -2.684295    0.381024
 C   -3.560627   -2.711729    0.012567
 P   -1.850184    0.770115   -0.165156
 C   -3.514797    0.941098   -0.921792
 C   -3.722696    0.354566   -2.176811
 C   -4.570821    1.620219   -0.303102
 C   -4.960131    0.458220   -2.810170
 H   -2.905808   -0.185853   -2.661287
 C   -5.811727    1.713470   -0.931791
 H   -4.428236    2.076558    0.678932
 C   -6.008068    1.134914   -2.186224
 H   -5.108464   -0.000407   -3.790158
 H   -6.631036    2.240641   -0.437995
 H   -6.981062    1.209658   -2.676715
 C   -1.000121    2.308758   -0.704658
 C    0.214352    2.654975   -0.091141
 C   -1.475448    3.106034   -1.752678
 C    0.931101    3.771541   -0.512520
 H    0.604414    2.037005    0.719432
 C   -0.750731    4.220963   -2.178951
 H   -2.419754    2.862936   -2.244139
 C    0.452250    4.557720   -1.561842
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 H    1.872126    4.026698   -0.019505
 H   -1.135734    4.831490   -2.998688
 H    1.015488    5.431583   -1.896288
 C   -2.172317    1.028388    1.619201
 C   -2.134066    2.274337    2.255013
 C   -2.492642   -0.117897    2.360440
 C   -2.409678    2.373598    3.618541
 H   -1.883005    3.173566    1.687763
 C   -2.782804   -0.010709    3.719851
 H   -2.484719   -1.095148    1.860518
 C   -2.737379    1.232510    4.351804
 H   -2.370085    3.348159    4.109935
 H   -3.030789   -0.907467    4.292411
 H   -2.951952    1.313638    5.419750
 H   -4.118729   -3.541186    0.502704
 H   -3.721064   -2.846342   -1.083121
 H   -4.112063   -1.776421    0.275399
79
Figure S13-1_PA-PPh3(NaOMe)-ts(1,4) / electronic energy: -3911.05049032 a.u. / lowest freq: -356.71 cm-1
Cu   -0.893475   -0.846713   -0.979551
 C    2.909614    0.404809    0.249052
 C    1.962121   -0.538206    0.679023
 H    2.704750    1.420050    0.590042
 C    2.086347   -1.972148    0.405497
 C    0.867815   -0.094404    1.538619
 O    2.858133   -2.232418   -0.657250
 O    1.587075   -2.884314    1.046194
 O    0.002738   -0.798303    2.044269
 O    0.888779    1.223731    1.793614
 C   -0.054069    1.713844    2.731376
 H   -1.077021    1.426190    2.458152
 H    0.041759    2.805003    2.717633
 H    0.165037    1.327077    3.737693
 C    3.101538   -3.597037   -0.957311
 H    3.590177   -4.104644   -0.113234
 H    3.761427   -3.602097   -1.831863
 H    2.162044   -4.115534   -1.192026
 C    4.328520    0.139485    0.017306
 H    4.609372   -0.866965   -0.293096
 C    5.262802    1.088643    0.211240
 H    4.931846    2.085144    0.527292
 C    6.715669    0.935152    0.045798
 C    7.556877    2.003067    0.399025
 C    7.309241   -0.236150   -0.457824
 C    8.940266    1.906939    0.261076
 H    7.114617    2.923027    0.790429
 C    8.690050   -0.332583   -0.596602
 H    6.685676   -1.082740   -0.752342
 C    9.512970    0.737711   -0.237342
 H    9.573755    2.750674    0.543867
 H    9.130042   -1.250361   -0.993062
 H   10.596354    0.658542   -0.349866
 C    0.234312    0.015770   -2.391043
 H   -0.342802    0.019210   -3.325041
 C    1.369661    0.575618   -2.263428
 C    2.585896    1.079704   -1.946109
 H    2.698224    2.148090   -1.734549
 H    3.477771    0.568243   -2.316547
Na   -0.649900   -2.906113    1.542614
 O   -1.193400   -2.757498   -0.597112
 C   -0.710516   -3.669066   -1.510510
 P   -2.663290    0.370094   -0.186034
 C   -4.078614    0.249224   -1.352879
 C   -3.796741    0.450243   -2.711608
 C   -5.395101   -0.020280   -0.963156
 C   -4.814066    0.395839   -3.661051
 H   -2.769316    0.652174   -3.026593
 C   -6.412213   -0.082519   -1.916791
 H   -5.631951   -0.186368    0.090144
 C   -6.125420    0.127120   -3.264843
 H   -4.582024    0.557043   -4.715963
 H   -7.436346   -0.294443   -1.601655
 H   -6.922905    0.077895   -4.009356
 C   -2.505526    2.183758    0.013868
 C   -1.236092    2.747395   -0.156221
 C   -3.600501    3.020557    0.274042
 C   -1.056658    4.126149   -0.036504
 H   -0.387002    2.098348   -0.384826
 C   -3.419236    4.395424    0.397617
 H   -4.602442    2.594793    0.374847
 C   -2.145300    4.949146    0.246186
 H   -0.061986    4.557365   -0.168845
 H   -4.275407    5.040503    0.606594
 H   -2.005183    6.028174    0.341581
 C   -3.359783   -0.276908    1.378331
 C   -3.698794    0.487874    2.497122
 C   -3.496057   -1.673967    1.434401
 C   -4.169748   -0.132759    3.656714
 H   -3.591104    1.574315    2.476875
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 C   -3.980467   -2.287752    2.586207
 H   -3.187565   -2.274982    0.570310
 C   -4.316008   -1.517363    3.703222
 H   -4.426038    0.474406    4.527745
 H   -4.091195   -3.374383    2.617101
 H   -4.689618   -1.998686    4.609565
 H   -0.458168   -4.650341   -1.043450
 H    0.216605   -3.332003   -2.028024
 H   -1.435694   -3.905776   -2.323511
79
Figure S13-1_PA-PPh3(NaOMe)-ed(1,4) / electronic energy: -3911.06860824 a.u. / lowest freq: 16.23 cm-1
Cu   -0.336172   -0.239591   -1.529854
 C    2.183745   -1.481701    1.297381
 C    1.095802   -2.226865    0.954658
 H    2.131187   -1.024828    2.289669
 C    0.914517   -3.004417   -0.299676
 C   -0.074543   -2.201962    1.873765
 O    1.829036   -2.771368   -1.223352
 O    0.010920   -3.801179   -0.465071
 O   -1.231177   -2.338343    1.524607
 O    0.253243   -1.946347    3.132856
 C   -0.808793   -1.678281    4.040825
 H   -1.330732   -0.755484    3.748988
 H   -0.341522   -1.546862    5.021807
 H   -1.521468   -2.513209    4.065073
 C    1.552362   -3.270857   -2.531121
 H    1.536934   -4.369298   -2.533675
 H    2.362748   -2.901726   -3.168232
 H    0.579023   -2.871405   -2.854500
 C    3.359284   -1.140832    0.540904
 H    3.462287   -1.527752   -0.469795
 C    4.270093   -0.295996    1.074189
 H    4.113843    0.052661    2.101894
 C    5.460912    0.232806    0.407965
 C    6.392088    0.966875    1.160066
 C    5.695944    0.055874   -0.966860
 C    7.533492    1.497177    0.563678
 H    6.214797    1.122416    2.227328
 C    6.834883    0.586289   -1.561836
 H    4.970428   -0.481673   -1.579888
 C    7.758282    1.306242   -0.799221
 H    8.246903    2.065577    1.163916
 H    7.001549    0.445739   -2.631743
 H    8.649559    1.725116   -1.271328
 C    1.488595    0.372357   -2.001547
 H    2.089882   -0.134372   -2.776024
 C    2.081650    1.356842   -1.389693
 C    2.616856    2.362955   -0.709641
 H    2.527188    3.400782   -1.049135
 H    3.180715    2.183381    0.213432
Na   -2.134761   -2.788501   -0.614928
 O   -1.430326   -1.710631   -2.373667
 C   -1.775372   -1.492660   -3.684126
 P   -1.799120    0.783837   -0.085031
 C   -2.269543    2.422929   -0.774381
 C   -1.263752    3.134321   -1.442572
 C   -3.534947    3.002587   -0.620517
 C   -1.520429    4.410139   -1.943368
 H   -0.275198    2.681665   -1.567167
 C   -3.790461    4.274881   -1.130426
 H   -4.330364    2.457833   -0.105611
 C   -2.783740    4.980976   -1.790843
 H   -0.729192    4.956669   -2.461340
 H   -4.781148    4.718758   -1.008897
 H   -2.986156    5.977239   -2.190436
 C   -1.252904    1.259535    1.599966
 C    0.121059    1.187905    1.853175
 C   -2.106934    1.765591    2.590505
 C    0.632848    1.582862    3.090086
 H    0.790521    0.838717    1.062198
 C   -1.595894    2.153139    3.826822
 H   -3.177727    1.865036    2.396426
 C   -0.225118    2.055716    4.080589
 H    1.707614    1.523418    3.275993
 H   -2.269269    2.539355    4.595033
 H    0.173727    2.361222    5.050419
 C   -3.404290   -0.080204    0.104806
 C   -3.841652   -0.693331    1.284968
 C   -4.143478   -0.281144   -1.073584
 C   -5.001943   -1.470603    1.292779
 H   -3.264174   -0.589900    2.203603
 C   -5.304154   -1.049696   -1.063308
 H   -3.797315    0.159125   -2.012116
 C   -5.738386   -1.647204    0.122582
 H   -5.328431   -1.941219    2.222638
 H   -5.866403   -1.191170   -1.988724
 H   -6.646895   -2.253398    0.131135
 H   -2.459794   -2.277521   -4.082990
 H   -0.900036   -1.476896   -4.378316
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 H   -2.304953   -0.524448   -3.859097
41
Figure S13-1_PPh3-Cu-allenyl / electronic energy: -2791.78064609 a.u. / lowest freq: -8.52 cm-1
Cu    1.925957    0.441034   -0.969324
 C    3.695423    0.782212   -1.650311
 H    3.901621    1.250294   -2.626132
 C    4.739409    0.464057   -0.934464
 C    5.764894    0.124180   -0.171645
 H    6.228054   -0.865398   -0.246897
 H    6.190086    0.825011    0.554818
 P   -0.093017    0.040978   -0.106258
 C   -0.713342    1.391986    0.957863
 C   -1.380331    1.168166    2.166791
 C   -0.511650    2.705927    0.513218
 C   -1.849259    2.247854    2.915852
 H   -1.535294    0.149778    2.529631
 C   -0.989950    3.780817    1.258089
 H    0.022539    2.889678   -0.423318
 C   -1.658731    3.552160    2.461671
 H   -2.365753    2.066564    3.860640
 H   -0.832329    4.800736    0.901689
 H   -2.027713    4.394962    3.049984
 C   -0.164393   -1.456811    0.937848
 C   -1.315396   -2.246691    1.042854
 C    0.979917   -1.802657    1.668371
 C   -1.322993   -3.362695    1.878346
 H   -2.210179   -1.992779    0.469631
 C    0.967011   -2.915256    2.507351
 H    1.889455   -1.202122    1.577400
 C   -0.184532   -3.695898    2.612619
 H   -2.223689   -3.975283    1.954422
 H    1.863220   -3.177711    3.073131
 H   -0.192646   -4.571265    3.265682
 C   -1.410845   -0.201190   -1.350523
 C   -2.710237    0.290159   -1.183020
 C   -1.089521   -0.925749   -2.506174
 C   -3.679067    0.050420   -2.157376
 H   -2.969562    0.864064   -0.290291
 C   -2.061407   -1.169847   -3.473746
 H   -0.072030   -1.299724   -2.651497
 C   -3.357069   -0.680980   -3.300219
 H   -4.690190    0.439664   -2.021497
 H   -1.803574   -1.735870   -4.371205
 H   -4.117079   -0.866243   -4.062285
47
Figure S13-1_PPh3-Cu(NaOMe)-allenyl / electronic energy: -3069.10617160 a.u. / lowest freq: 20.67 cm-1
 O   -2.507715   -1.614477   -0.117319
 C   -1.791502   -2.691059   -0.588600
Na   -4.570078   -0.950440    0.015508
Cu   -1.747352    0.240623   -0.324777
 C   -2.934205    1.822009   -0.588788
 H   -2.493566    2.799687   -0.845319
 C   -4.226582    1.809945   -0.460645
 C   -5.546103    1.685346   -0.309565
 H   -6.029401    1.872223    0.656057
 H   -6.199853    1.483996   -1.165999
 P    0.500749    0.132935   -0.046191
 C    1.409747   -1.024413   -1.140897
 C    2.295589   -2.003003   -0.678527
 C    1.156627   -0.928767   -2.516933
 C    2.923888   -2.865528   -1.578263
 H    2.494887   -2.100221    0.390797
 C    1.792140   -1.782752   -3.414800
 H    0.451136   -0.179778   -2.888657
 C    2.677232   -2.755298   -2.945796
 H    3.612265   -3.627355   -1.205736
 H    1.590088   -1.694004   -4.484388
 H    3.170569   -3.431164   -3.647726
 C    0.883904   -0.460490    1.647375
 C    2.067822   -0.154805    2.330084
 C   -0.077500   -1.274059    2.263866
 C    2.295159   -0.671259    3.605220
 H    2.818097    0.490100    1.866043
 C    0.156562   -1.793279    3.536862
 H   -1.014360   -1.488192    1.736299
 C    1.342422   -1.494400    4.207704
 H    3.221750   -0.429738    4.130669
 H   -0.595016   -2.429495    4.009562
 H    1.523126   -1.899145    5.206102
 C    1.468399    1.684685   -0.189255
 C    2.792219    1.738270   -0.642221
 C    0.823478    2.872021    0.181927
 C    3.462486    2.959673   -0.711716
 H    3.303866    0.822103   -0.947034
 C    1.497420    4.090255    0.121320
 H   -0.219502    2.835593    0.509566
 C    2.818164    4.135708   -0.327292
 H    4.493744    2.992215   -1.070297
 H    0.985723    5.009627    0.414113
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 H     3.343697    5.091448   -0.385136
 H    -2.344288   -3.652437   -0.483068
 H    -0.822713   -2.845875   -0.056194
 H    -1.519890   -2.613832   -1.666644
79
Figure S13-1_PA-PPh3(NaOMe)-ed(1,6) / electronic energy: -3911.04850322 a.u. / lowest freq: 12.82 cm-1
Na    -1.972247   -4.264442    0.100655
 O    -3.947246   -4.597387    0.631312
Cu     0.662078    0.561800   -0.709108
 C     1.826965   -1.052797   -1.227912
 C     0.585468   -1.525664   -0.731302
 H     1.882172   -0.950382   -2.316967
 C     0.380154   -1.958448    0.676482
 C    -0.457635   -1.928474   -1.716995
 O     1.085571   -1.227082    1.532831
 O    -0.380323   -2.827811    1.048654
 O    -1.162660   -2.909934   -1.642805
 O    -0.549280   -1.058806   -2.718688
 C    -1.578513   -1.284002   -3.679775
 H    -1.448782   -2.259870   -4.165978
 H    -1.486034   -0.477437   -4.413581
 H    -2.561740   -1.243538   -3.189231
 C     0.893116   -1.477599    2.923259
 H    -0.139879   -1.232429    3.209281
 H     1.592565   -0.817505    3.444826
 H     1.102883   -2.529202    3.158631
 C     3.114718   -1.089588   -0.553373
 H     3.121166   -1.275041    0.520071
 C     4.260082   -0.854442   -1.220565
 H     4.197690   -0.641603   -2.293552
 C     5.612980   -0.821828   -0.652543
 C     6.691560   -0.495496   -1.489864
 C     5.879642   -1.085336    0.702898
 C     7.992393   -0.427888   -0.993706
 H     6.503712   -0.287143   -2.546306
 C     7.176968   -1.019540    1.198081
 H     5.064224   -1.338680    1.382972
 C     8.239737   -0.689093    0.352729
 H     8.815128   -0.167731   -1.663120
 H     7.362960   -1.224269    2.254607
 H     9.256849   -0.634403    0.746692
 C     1.892225    2.079277   -0.902338
 H     1.678689    2.927656   -1.568718
 C     2.912547    2.173958   -0.099207
 C     3.929259    2.196108    0.745101
 H     4.913742    1.811023    0.458198
 H     3.819585    2.602447    1.756494
 P    -1.388781    1.306696    0.043366
 C    -2.889708    0.389522   -0.453090
 C    -3.811644    0.923166   -1.362238
 C    -3.065876   -0.924278    0.002900
 C    -4.885293    0.148531   -1.802907
 H    -3.695658    1.943709   -1.732745
 C    -4.140019   -1.699791   -0.429719
 H    -2.354333   -1.359126    0.709805
 C    -5.048876   -1.157246   -1.340885
 H    -5.598158    0.572905   -2.513516
 H    -4.225019   -2.738381   -0.064047
 H    -5.889783   -1.758732   -1.693635
 C    -1.745182    3.035186   -0.421754
 C    -2.515043    3.873411    0.393515
 C    -1.265856    3.512153   -1.647136
 C    -2.801125    5.174286   -0.014916
 H    -2.892141    3.509742    1.352521
 C    -1.559029    4.812369   -2.056677
 H    -0.658696    2.863360   -2.283412
 C    -2.324303    5.644141   -1.239733
 H    -3.399906    5.824447    0.626204
 H    -1.180462    5.179183   -3.012941
 H    -2.546884    6.665429   -1.556188
 C    -1.346461    1.320944    1.871274
 C    -0.160004    1.786444    2.458934
 C    -2.402658    0.903334    2.687445
 C    -0.038695    1.839772    3.844418
 H     0.674905    2.103588    1.826472
 C    -2.269752    0.943641    4.076289
 H    -3.332437    0.540661    2.244728
 C    -1.091582    1.412698    4.655408
 H     0.886776    2.206684    4.292898
 H    -3.096072    0.609852    4.707132
 H    -0.991605    1.444678    5.742416
 C    -5.224974   -4.856013    0.988699
 H    -5.691471   -5.741370    0.477169
 H    -5.939985   -4.012039    0.771105
 H    -5.379845   -5.060610    2.082906
79
Figure S13-1_PA-PPh3(NaOMe)-ts(1,6) / electronic energy: -3911.03470938 a.u. / lowest freq: -446.88 cm-1
Na    -2.668687   -3.697635    0.307189
 O    -4.717032   -3.856097    0.600942
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Cu    0.674660    0.408546   -0.851083
 C    1.804112   -1.363958   -1.000989
 C    0.494818   -1.741346   -0.521311
 H    1.934680   -1.480517   -2.081360
 C    0.181165   -2.126690    0.858218
 C   -0.502114   -2.105808   -1.547150
 O    1.185191   -1.929264    1.716510
 O   -0.882920   -2.584577    1.244231
 O   -1.399007   -2.920332   -1.448936
 O   -0.330155   -1.403630   -2.677185
 C   -1.246885   -1.645086   -3.736793
 H   -1.175936   -2.685355   -4.083073
 H   -0.962831   -0.958871   -4.541298
 H   -2.274594   -1.439647   -3.406971
 C    0.975864   -2.340640    3.060502
 H    0.079563   -1.866399    3.480980
 H    1.867621   -2.026011    3.613472
 H    0.864787   -3.432644    3.116904
 C    2.970480   -1.038874   -0.291400
 H    2.924186   -0.908349    0.788530
 C    4.177140   -0.828642   -0.967587
 H    4.244975   -1.255825   -1.970876
 C    5.471282   -0.742899   -0.251397
 C    6.635505   -1.212912   -0.874856
 C    5.578298   -0.194741    1.036569
 C    7.868693   -1.152937   -0.227618
 H    6.570277   -1.637854   -1.880026
 C    6.809742   -0.131450    1.682195
 H    4.690640    0.204442    1.532720
 C    7.960872   -0.612393    1.054235
 H    8.762586   -1.531269   -0.728404
 H    6.874515    0.303080    2.682258
 H    8.926384   -0.560412    1.561774
 C    1.720618    1.730060   -1.970666
 H    1.067696    2.513264   -2.360724
 C    2.975009    1.571152   -2.037497
 C    4.266692    1.169830   -1.906866
 H    4.797067    0.797395   -2.787715
 H    4.888253    1.681348   -1.165726
 P   -1.171447    1.406895    0.058337
 C   -2.655597    0.673090   -0.709604
 C   -3.125306    1.154403   -1.939737
 C   -3.235861   -0.475142   -0.158421
 C   -4.182250    0.512358   -2.582595
 H   -2.672087    2.036736   -2.398373
 C   -4.284840   -1.127938   -0.806460
 H   -2.855782   -0.876813    0.784383
 C   -4.760848   -0.625782   -2.018062
 H   -4.550017    0.902235   -3.534369
 H   -4.678967   -2.056064   -0.360086
 H   -5.583350   -1.129912   -2.530630
 C   -1.343089    3.220204   -0.122688
 C   -2.586828    3.863942   -0.161131
 C   -0.171466    3.987205   -0.133416
 C   -2.654025    5.253925   -0.223994
 H   -3.510717    3.281362   -0.146221
 C   -0.242064    5.378991   -0.189179
 H    0.803459    3.494130   -0.096428
 C   -1.482572    6.012840   -0.239273
 H   -3.627383    5.747385   -0.259172
 H    0.677502    5.967781   -0.198002
 H   -1.539032    7.102297   -0.290534
 C   -1.354125    1.181277    1.863545
 C   -0.202427    0.927664    2.615392
 C   -2.582599    1.346247    2.517117
 C   -0.276244    0.839532    4.006101
 H    0.759650    0.790976    2.114530
 C   -2.656380    1.241935    3.903003
 H   -3.489920    1.549241    1.943242
 C   -1.502690    0.990706    4.649185
 H    0.628273    0.643036    4.585240
 H   -3.618714    1.361474    4.404521
 H   -1.563608    0.911434    5.736622
 C   -6.045566   -3.956871    0.825394
 H   -6.546834   -4.831445    0.326986
 H   -6.639163   -3.067499    0.467691
 H   -6.338755   -4.056295    1.906315
79
Figure S13-1_PA-PPh3(NaOMe)-prod(1,6) / electronic energy: -3911.08630820 a.u. / lowest freq: -6.95 cm-1
Na   -1.588288   -4.245478    0.402898
 O   -3.654203   -4.511477    0.541988
Cu    0.872233    1.566394   -0.168494
 C    1.899193   -0.617114   -0.558179
 C    1.036664   -1.709045   -0.217463
 H    2.079739   -0.562443   -1.637255
 C    0.716686   -2.098575    1.135805
 C    0.548124   -2.548876   -1.298357
 O    1.349546   -1.354671    2.072088
 O   -0.031801   -2.999630    1.498721
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 O   -0.110684   -3.576971   -1.198623
 O    0.927727   -2.125703   -2.523942
 C    0.608359   -2.963339   -3.617284
 H    1.087346   -3.948066   -3.512963
 H    0.992092   -2.457824   -4.511108
 H   -0.476856   -3.106242   -3.706739
 C    1.176498   -1.748488    3.421294
 H    0.111866   -1.818154    3.682352
 H    1.667466   -0.979122    4.029226
 H    1.647877   -2.724766    3.606934
 C    2.595780    0.328105    0.176496
 H    2.605796    0.259997    1.267741
 C    3.748207    1.089926   -0.465178
 H    3.616695    1.045873   -1.558459
 C    5.099293    0.474237   -0.143635
 C    5.943739    0.039475   -1.169748
 C    5.526768    0.323293    1.182249
 C    7.183896   -0.533051   -0.883370
 H    5.625376    0.148479   -2.210106
 C    6.764178   -0.247130    1.472636
 H    4.882211    0.647080    2.004011
 C    7.598099   -0.678130    0.439489
 H    7.828309   -0.868162   -1.699258
 H    7.078160   -0.360236    2.512773
 H    8.566861   -1.128617    0.665986
 C    1.310924    3.650978   -0.667832
 H    0.474453    4.267683   -0.958880
 C    2.385411    3.139355   -0.374891
 C    3.706811    2.580444   -0.067170
 H    4.485598    3.158013   -0.588668
 H    3.888736    2.691517    1.014072
 P   -1.392272    1.329987   -0.081445
 C   -2.033696   -0.033181   -1.107275
 C   -1.800262    0.011588   -2.488956
 C   -2.695752   -1.135263   -0.558847
 C   -2.276269   -1.005995   -3.310741
 H   -1.254278    0.850604   -2.930071
 C   -3.145956   -2.172127   -1.377618
 H   -2.855922   -1.207433    0.519244
 C   -2.947773   -2.096544   -2.755115
 H   -2.103921   -0.954944   -4.388064
 H   -3.590082   -3.057137   -0.895186
 H   -3.300031   -2.904173   -3.401149
 C   -2.343088    2.815753   -0.592832
 C   -3.344494    2.804699   -1.567930
 C   -2.042497    4.017949    0.065471
 C   -4.025590    3.980863   -1.887969
 H   -3.603506    1.877082   -2.081444
 C   -2.726596    5.188106   -0.251593
 H   -1.274096    4.038302    0.844103
 C   -3.717979    5.172126   -1.234834
 H   -4.805427    3.959946   -2.651875
 H   -2.485925    6.116280    0.270812
 H   -4.252504    6.090209   -1.487461
 C   -2.036090    1.036461    1.602287
 C   -1.146121    0.698958    2.625495
 C   -3.402725    1.166161    1.887589
 C   -1.616690    0.492996    3.923488
 H   -0.082284    0.583023    2.404350
 C   -3.869943    0.951837    3.180523
 H   -4.105513    1.438236    1.096253
 C   -2.976079    0.617540    4.200399
 H   -0.916402    0.235557    4.720403
 H   -4.935786    1.050802    3.395019
 H   -3.343960    0.455742    5.215781
 C   -4.983055   -4.545439    0.777041
 H   -5.484338   -5.526734    0.547591
 H   -5.575862   -3.797099    0.175805
 H   -5.283903   -4.331944    1.839810
15
Figure S14-1_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
 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
32
Figure S14-1_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C   -0.660544   -0.726572    0.059153
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 C   -1.860539   -0.097447    0.115996
 H   -0.691600   -1.818492   -0.004770
 C   -1.976243    1.390665    0.160143
 C   -3.120576   -0.891785    0.187355
 O   -3.041424    1.823605   -0.507466
 O   -1.182749    2.134043    0.689285
 O   -4.147702   -0.497504    0.683440
 O   -2.981802   -2.118850   -0.320932
 C   -4.097604   -2.989729   -0.195724
 H   -4.332384   -3.170881    0.862818
 H   -3.810049   -3.927003   -0.683244
 H   -4.981752   -2.562067   -0.688186
 C   -3.254671    3.228152   -0.535442
 H   -3.354009    3.627502    0.483524
 H   -4.184056    3.384216   -1.092621
 H   -2.420438    3.737793   -1.038016
 C    0.656646   -0.129211    0.062308
 H    0.725624    0.955889    0.150505
 C    1.759981   -0.902956   -0.019704
 H    1.621029   -1.988149   -0.089650
 C    3.156351   -0.453635   -0.025165
 C    4.175093   -1.416830   -0.109525
 C    3.522207    0.902114    0.053056
 C    5.517020   -1.042840   -0.114390
 H    3.907556   -2.474776   -0.172060
 C    4.861836    1.275255    0.048166
 H    2.754752    1.675486    0.118691
 C    5.863995    0.305241   -0.035401
 H    6.294080   -1.807149   -0.179427
 H    5.127957    2.332459    0.111300
 H    6.914980    0.602284   -0.038425
71
Figure S14-1_PA-Me2NHC(NaOtBu)-prod(1,4) / electronic energy: -3299.19328289 a.u. / lowest freq: 18.20 cm-1
Cu    3.148821    0.380493    0.095403
 C   -2.096180   -0.563248   -0.615986
 C   -1.289612    0.081912    0.505879
 H   -1.981774   -1.646054   -0.493329
 C   -1.342209    1.483088    0.744019
 C   -0.379081   -0.722243    1.253323
 O   -2.096551    2.153849   -0.177162
 O   -0.813788    2.141494    1.649719
 O    0.490073   -0.360722    2.061365
 O   -0.512920   -2.054128    1.004693
 C    0.481732   -2.917957    1.496821
 H    1.430158   -2.772527    0.955460
 H    0.120298   -3.939163    1.322842
 H    0.661611   -2.766660    2.570849
 C   -2.232804    3.547353   -0.009851
 H   -2.613929    3.799907    0.990297
 H   -2.946734    3.880471   -0.773223
 H   -1.272215    4.063626   -0.158001
 C   -3.575987   -0.282169   -0.554112
 H   -3.876305    0.760757   -0.687075
 C   -4.499916   -1.229369   -0.344817
 H   -4.165197   -2.268355   -0.233887
 C   -5.959262   -1.031164   -0.246709
 C   -6.803366   -2.153204   -0.239329
 C   -6.553948    0.239129   -0.152571
 C   -8.188148   -2.016442   -0.153015
 H   -6.361443   -3.151182   -0.305615
 C   -7.936289    0.377899   -0.066297
 H   -5.926028    1.132720   -0.134598
 C   -8.762073   -0.748841   -0.067062
 H   -8.821778   -2.906604   -0.150866
 H   -8.375348    1.375428    0.010365
 H   -9.846070   -0.636687    0.005684
 C    0.947390   -1.204127   -2.283723
 H    1.935617   -1.615737   -2.358460
 C   -0.166669   -0.739519   -2.186891
 C   -1.524676   -0.223429   -2.020495
 H   -2.170397   -0.658033   -2.802135
 H   -1.527706    0.867895   -2.165561
Na    1.277659    1.736154    2.303748
 O    2.564611    2.076788    0.523505
 C    2.342503    3.082536   -0.421684
 C    1.349894    2.596132   -1.487676
 H    1.103556    3.382220   -2.220081
 H    1.768809    1.733854   -2.031329
 H    0.420305    2.257648   -1.007107
 C    3.667882    3.475105   -1.092176
 H    3.539266    4.281514   -1.832168
 H    4.391011    3.810374   -0.332098
 H    4.099092    2.600275   -1.606691
 C    1.752238    4.299934    0.305794
 H    1.558812    5.138699   -0.381837
 H    0.800354    4.020933    0.784109
 H    2.447749    4.647955    1.086322
 C    5.012600   -3.196000   -1.057734
 H    6.060171   -3.266023   -1.385453
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 C    4.840255   -3.416305    0.449832
 H    4.320473   -4.354831    0.690216
 C    3.927598   -1.346026   -0.129174
 C    3.703114   -2.026620    2.229345
 N    4.501613   -1.837137   -1.233034
 N    4.038026   -2.259710    0.844064
 H    5.802394   -3.411712    0.989001
 H    4.419281   -3.902682   -1.660861
 C    4.623089   -1.155779   -2.497370
 H    3.348530   -2.961500    2.686847
 H    2.890727   -1.289325    2.284683
 H    4.576531   -1.668049    2.799736
 H    4.160719   -1.741594   -3.308423
 H    5.681951   -0.990991   -2.752230
 H    4.120134   -0.182769   -2.427519
71
Figure S14-1_PA-Me2NHC(NaOtBu)-ts(1,4) / electronic energy: -3299.12254340 a.u. / lowest freq: -363.32 cm-1
Cu   2.220225   -0.114446   -0.526722
 C  -2.230909   -0.848040    0.372173
 C  -1.213524   -0.176815    1.063075
 H  -2.125321   -1.931492    0.386553
 C  -1.218886    1.258790    1.343622
 C  -0.069163   -0.960404    1.520700
 O  -2.033221    1.954121    0.536407
 O  -0.587430    1.830512    2.219290
 O   0.896113   -0.546326    2.155922
 O  -0.156993   -2.256837    1.196558
 C   0.991366   -3.057319    1.399776
 H   1.815809   -2.698538    0.764590
 H   0.711398   -4.075436    1.107475
 H   1.309714   -3.042211    2.451721
 C  -2.177960    3.339547    0.802681
 H  -2.527528    3.509205    1.830830
 H  -2.919185    3.709494    0.085729
 H  -1.224286    3.865743    0.656487
 C  -3.599373   -0.391330    0.151733
 H  -3.783208    0.682027    0.141701
 C  -4.606280   -1.269130   -0.020140
 H  -4.369181   -2.339609   -0.003117
 C  -6.024124   -0.949019   -0.236283
 C  -6.952521   -1.999518   -0.322486
 C  -6.500330    0.367823   -0.369045
 C  -8.307322   -1.748808   -0.530299
 H  -6.601414   -3.030131   -0.223603
 C  -7.852467    0.618784   -0.577417
 H  -5.805325    1.208142   -0.315526
 C  -8.763249   -0.437482   -0.658486
 H  -9.010726   -2.582035   -0.592948
 H  -8.200882    1.648823   -0.681221
 H  -9.824064   -0.237333   -0.823562
 C   0.860461   -0.755593   -1.924661
 H   1.480740   -0.824315   -2.829424
 C  -0.401318   -0.916747   -1.993527
 C  -1.751360   -1.011973   -1.920577
 H  -2.238352   -1.990380   -1.968230
 H  -2.360344   -0.155103   -2.225309
Na   1.687087    1.604818    2.243013
 O   2.056141    1.773535    0.123205
 C   2.047645    2.871915   -0.712429
 C   0.824666    2.839955   -1.646800
 H   0.750031    3.742418   -2.276544
 H   0.874303    1.955293   -2.299260
 H  -0.095077    2.745302   -1.050473
 C   3.329246    2.907592   -1.567734
 H   3.378364    3.789229   -2.228540
 H   4.215733    2.910045   -0.913027
 H   3.378966    2.003627   -2.196266
 C   1.988431    4.151122    0.145421
 H   1.987713    5.073664   -0.458283
 H   1.073329    4.145771    0.760533
 H   2.855260    4.188159    0.826417
 C   5.975284   -2.076453   -0.949841
 H   6.906384   -1.632369   -1.331624
 C   5.889106   -2.079478    0.575531
 H   6.036523   -3.076022    1.017107
 C   3.959171   -1.067316   -0.293913
 C   4.064002   -1.409683    2.155277
 N   4.815371   -1.267044   -1.312094
 N   4.530456   -1.593308    0.805295
 H   6.619892   -1.392369    1.038162
 H   5.881250   -3.089618   -1.379205
 C   4.542187   -0.976371   -2.695067
 H   4.140556   -2.354851    2.715801
 H   3.013779   -1.095284    2.140373
 H   4.667466   -0.650371    2.684615
 H   4.275891   -1.887685   -3.258342
 H   5.424630   -0.520591   -3.169739
 H   3.708346   -0.267134   -2.753228
71
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Figure S14-1_PA-Me2NHC(NaOtBu)-ed(1,4) / electronic energy: -3299.13603253 a.u. / lowest freq: 18.99 cm-1
Cu     1.721380    -0.926895    -0.012157
 C    -1.829087     0.846149     1.402381
 C    -0.874542     1.805731     1.238413
 H    -1.558257     0.062202     2.110738
 C    -0.947876     2.928537     0.274161
 C     0.403816     1.601877     1.969467
 O    -2.195537     3.235758    -0.068831
 O     0.002383     3.537447    -0.176849
 O     1.489597     2.029201     1.621332
 O     0.255776     0.871569     3.062680
 C     1.433835     0.342768     3.657768
 H     1.935877    -0.322299     2.939850
 H     1.100535    -0.234993     4.525013
 H     2.114091     1.148741     3.965505
 C    -2.362871     4.244255    -1.058249
 H    -1.934064     5.196212    -0.717597
 H    -3.442686     4.346807    -1.205990
 H    -1.877706     3.945204    -1.998066
 C    -3.082485     0.622443     0.728492
 H    -3.466896     1.370792     0.037387
 C    -3.711439    -0.558383     0.926830
 H    -3.241442    -1.272854     1.613765
 C    -4.946802    -1.021761     0.292393
 C    -5.376996    -2.335114     0.543557
 C    -5.718323    -0.213904    -0.561980
 C    -6.538721    -2.831669    -0.042304
 H    -4.784234    -2.973307     1.203736
 C    -6.880343    -0.708815    -1.143489
 H    -5.411061     0.812605    -0.771005
 C    -7.293720    -2.018965    -0.887085
 H    -6.854907    -3.856875     0.160632
 H    -7.471422    -0.069234    -1.802297
 H    -8.205794    -2.404777    -1.347475
 C     0.123091    -1.896366     0.688577
 H    -0.578885    -2.221228    -0.103564
 C    -0.304772    -2.186855     1.883664
 C    -0.728063    -2.427691     3.120727
 H    -0.495643    -3.363101     3.642290
 H    -1.319178    -1.687491     3.675407
Na     1.994317     2.350928    -0.621913
 O     1.269225     0.506324    -1.457660
 C     0.447265     0.263315    -2.537338
 C    -1.037206     0.248774    -2.121013
 H    -1.710774     0.003408    -2.959536
 H    -1.192440    -0.485606    -1.318153
 H    -1.330773     1.235430    -1.729577
 C     0.791716    -1.094904    -3.179565
 H     0.201494    -1.305324    -4.087385
 H     1.860945    -1.112398    -3.444148
 H     0.611625    -1.903228    -2.452732
 C     0.642473     1.373619    -3.590703
 H     0.007366     1.236909    -4.482033
 H     0.396906     2.353052    -3.145956
 H     1.695003     1.401344    -3.917855
 C     5.727836    -1.772925    -1.043092
 H     5.937274    -1.408372    -2.064473
 C     6.019315    -0.717245     0.022663
 H     6.511041    -1.145790     0.914395
 C     3.699235    -1.054153    -0.100616
 C     4.515191     0.744633     1.390027
 N     4.295289    -1.986130    -0.866307
 N     4.677472    -0.252099     0.365075
 H     6.647915     0.107447    -0.344611
 H     6.291033    -2.706319    -0.895265
 C     3.605381    -2.982505    -1.642196
 H     4.950773     0.405531     2.346886
 H     3.448932     0.946690     1.541961
 H     5.018157     1.682792     1.103628
 H     4.076957    -3.968662    -1.506224
 H     3.613072    -2.738759    -2.718410
 H     2.563326    -3.034677    -1.300944
24
Figure S14-1_Me2NHC-Cu-allenyl / electronic energy: -2062.03078001 a.u. / lowest freq: 21.55 cm-1
 C     2.887888     1.358348    -0.035346
 H     3.277552     1.952832     0.804727
 C     3.319391    -0.113704     0.022402
 H     3.958317    -0.407007    -0.824313
 C     0.983177     0.001577     0.005623
 C     1.985205    -2.256890    -0.012542
Cu    -0.884678    -0.527874     0.007239
 N     1.431216     1.260707     0.032296
 N     2.039332    -0.817337    -0.026916
 H     3.855467    -0.362962     0.952614
 H     3.193238     1.854637    -0.970895
 C    -2.756787    -0.987275     0.006275
 H    -3.144691    -2.019394     0.014800
 C    -3.661352    -0.046202    -0.005276
 C    -4.537280     0.945925    -0.016393
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 H   -4.916550    1.362518   -0.955914
 H   -4.921179    1.378936    0.913749
 C    0.611326    2.445877    0.008128
 H   -0.443456    2.155748    0.095145
 H    0.750709    3.002155   -0.933173
 H    0.867325    3.111400    0.847231
 H    0.934995   -2.573150   -0.046960
 H    2.448897   -2.660356    0.902272
 H    2.511789   -2.676553   -0.884111
39
Figure S14-1_Me2NHC-Cu(NaOtBu)-allenyl / electronic energy: -2457.18214053 a.u. / lowest freq: 21.95 cm-1
 C   -4.054956   -0.330905   -0.412546
 H   -4.842737   -1.086415   -0.274017
 C   -3.825790    0.533366    0.831328
 H   -4.204421    1.560139    0.717717
 C   -1.783980   -0.401412    0.163591
 C   -1.679461    1.287251    1.949001
Cu    0.154006   -0.789109    0.161368
 N   -2.747405   -0.956421   -0.591115
 N   -2.371193    0.516421    0.946728
 H   -4.290088    0.099680    1.734523
 H   -4.315960    0.270790   -1.301294
 C    1.349335   -2.400801    0.166366
 H    0.881293   -3.396889    0.086776
 C    2.647612   -2.408852    0.120935
 C    3.977366   -2.302739    0.096620
 H    4.575544   -2.419615    1.008256
 H    4.522522   -2.183133   -0.846117
 C   -2.514262   -1.889256   -1.661388
 O    1.221742    0.999702    0.356666
 C    1.300124    1.921772   -0.670988
 C    1.854605    3.251545   -0.124956
 H    1.189651    3.638566    0.663808
 H    2.849643    3.088098    0.322214
 H    1.954147    4.025418   -0.904340
 C   -0.083610    2.184365   -1.297295
 H   -0.044524    2.956047   -2.083896
 H   -0.480425    1.256822   -1.739759
 H   -0.794731    2.510515   -0.522949
 C    2.243430    1.405378   -1.778431
 H    1.880990    0.430889   -2.144306
 H    2.316256    2.096287   -2.635232
 H    3.260750    1.256363   -1.378436
Na    2.943697    0.062658    1.291580
 H   -0.610791    1.304664    1.682357
 H   -1.818895    0.863086    2.959373
 H   -2.061944    2.320366    1.955920
 H   -1.484231   -2.259859   -1.579418
 H   -2.644792   -1.412161   -2.648406
 H   -3.210342   -2.740603   -1.595876
71
Figure S14-1_PA-Me2NHC(NaOtBu)-ed(1,6) / electronic energy: -3299.13575585 a.u. / lowest freq: 13.68 cm-1
 C    3.334554    0.963341    2.093971
 H    4.164538    0.976693    1.364841
 C    2.512660    2.256769    2.132353
 H    2.572938    2.781671    3.097492
 C    1.114792    0.482696    1.538541
 C    0.045568    2.690609    1.818145
Cu   -0.526525   -0.439230    0.879588
 N    2.342968   -0.014252    1.632278
 N    1.153634    1.776163    1.882082
 C   -1.661598   -0.777557   -0.803931
 C   -0.400631   -0.225026   -1.166222
 H    2.807469    2.968878    1.341720
 H    3.711606    0.670052    3.088208
 H   -1.730813   -1.865085   -0.887699
 C   -0.139006    1.209653   -1.463224
 C    0.695646   -1.160478   -1.536109
 O   -1.241374    1.910053   -1.698142
 O    0.960080    1.728874   -1.490354
 O    1.735436   -0.854285   -2.083845
 O    0.430388   -2.423260   -1.203484
 C    1.404710   -3.402807   -1.546573
 H    1.533783   -3.454518   -2.636105
 H    1.019848   -4.353367   -1.164103
 H    2.371212   -3.167363   -1.080792
 C   -1.089110    3.298560   -1.968497
 H   -0.587617    3.805429   -1.133068
 H   -2.101810    3.693598   -2.097614
 H   -0.503804    3.450463   -2.885163
 C   -2.938569   -0.100401   -0.669913
 H   -2.937421    0.980576   -0.536945
 C   -4.098771   -0.788779   -0.676157
 H   -4.059267   -1.870240   -0.834605
 C   -5.445064   -0.228195   -0.498691
 C   -6.551735   -1.091665   -0.554410
 C   -5.683265    1.137977   -0.267993
 C   -7.849099   -0.612092   -0.388291
 H   -6.385986   -2.158247   -0.727089
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 C   -6.978774    1.618219   -0.103539
 H   -4.848209    1.839249   -0.213992
 C   -8.068363    0.746347   -0.162553
 H   -8.692651   -1.304434   -0.433763
 H   -7.141285    2.683541    0.074396
 H   -9.083592    1.126812   -0.031016
 C   -1.598275   -1.203096    2.344546
 H   -1.180415   -1.087888    3.355640
 C   -2.719089   -1.847388    2.217989
 C   -3.867830   -2.469366    2.014982
 H   -3.909842   -3.546651    1.823613
 H   -4.816739   -1.924025    2.043664
 C    2.743678   -1.370737    1.352815
Na    3.133607    0.901431   -1.465780
 O    4.914055    0.359131   -0.483799
 H    5.934165   -1.435164   -2.178152
 H    7.016025    0.857027   -2.071439
 C    6.180587   -1.578793   -1.113165
 H    5.422335   -2.252489   -0.680578
 C    7.233892    0.692404   -1.003052
 H    7.161604   -2.081159   -1.052211
 C    6.149430   -0.217053   -0.380795
 H    7.221474    1.673799   -0.501326
 H    8.251665    0.273376   -0.919550
 C    6.525852   -0.463886    1.100577
 H    6.541089    0.492439    1.649008
 H    5.773063   -1.112308    1.577489
 H    7.513542   -0.941537    1.217897
 H   -0.873666    2.134674    1.588278
 H    0.207604    3.452113    1.036610
 H   -0.093003    3.208397    2.780029
 H    1.870011   -1.944746    1.017939
 H    3.148559   -1.848885    2.259910
 H    3.525114   -1.351768    0.575667
71
Figure S14-1_PA-Me2NHC(NaOtBu)-ts(1,6) / electronic energy: -3299.12365436 a.u. / lowest freq: -453.31 cm-1
 C   -3.286118   -1.585501    1.644382
 H   -4.109096   -1.389444    0.933108
 C   -2.433101   -2.812434    1.306453
 H   -2.519090   -3.619755    2.048906
 C   -1.063554   -0.921265    1.347666
 C    0.060971   -3.098171    1.029612
Cu    0.532262    0.207231    0.982055
 N   -2.310736   -0.496464    1.524662
 N   -1.078484   -2.259171    1.288128
 C    1.684870    1.059137   -0.600225
 C    0.391930    0.657809   -1.102239
 H   -2.673859   -3.236074    0.315474
 H   -3.683581   -1.616977    2.673418
 H    1.744854    2.119440   -0.340477
 C    0.103506   -0.623287   -1.761945
 C   -0.680960    1.664444   -1.125039
 O    1.196208   -1.351195   -2.012596
 O   -1.000902   -1.047802   -2.064272
 O   -1.766639    1.561224   -1.669218
 O   -0.369575    2.778927   -0.443843
 C   -1.339865    3.815870   -0.433050
 H   -1.513064    4.199542   -1.448137
 H   -0.929395    4.606913    0.203178
 H   -2.292932    3.454720   -0.022258
 C    1.010245   -2.599526   -2.661318
 H    0.344541   -3.251751   -2.079854
 H    2.004881   -3.051005   -2.741035
 H    0.579411   -2.457605   -3.662028
 C    2.903273    0.364662   -0.550962
 H    2.936238   -0.683420   -0.842333
 C    4.052010    0.984577   -0.050492
 H    4.032027    2.077075   -0.020986
 C    5.404415    0.405194   -0.232449
 C    6.517481    1.256852   -0.283312
 C    5.620608   -0.977429   -0.344676
 C    7.804165    0.748105   -0.454342
 H    6.369587    2.336007   -0.188821
 C    6.904928   -1.486652   -0.515454
 H    4.777026   -1.668606   -0.285506
 C    8.003682   -0.626595   -0.572979
 H    8.655102    1.431886   -0.494799
 H    7.051289   -2.565690   -0.602007
 H    9.010200   -1.028913   -0.706386
 C    1.540332    0.599036    2.682194
 H    0.893621    0.509558    3.555481
 C    2.780033    0.826788    2.560980
 C    4.067386    0.980856    2.149455
 H    4.534652    1.966871    2.227324
 H    4.744611    0.132385    2.285319
 C   -2.741960    0.873162    1.659185
Na   -3.137088   -0.283663   -1.694742
 O   -4.922198   -0.203749   -0.578296
 H   -6.040686    1.989637   -1.598508
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 H   -7.026160   -0.262607   -2.239202
 C   -6.282487    1.770720   -0.545207
 H   -5.551060    2.303225    0.084981
 C   -7.233964   -0.460761   -1.174577
 H   -7.284793    2.180642   -0.330854
 C   -6.179780    0.248521   -0.293167
 H   -7.171384   -1.549914   -1.016608
 H   -8.268023   -0.139132   -0.960632
 C   -6.540318   -0.016631    1.188896
 H   -6.504844   -1.098899    1.395985
 H   -5.805948    0.475001    1.847550
 H   -7.545073    0.351432    1.458281
 H    0.966310   -2.478405    0.982097
 H   -0.053867   -3.633312    0.072585
 H    0.188476   -3.847527    1.826840
 H   -1.885493    1.541434    1.500873
 H   -3.147224    1.054785    2.668794
 H   -3.531871    1.064400    0.914715
71
Figure S14-1_PA-Me2NHC(NaOtBu)-prod(1,6) / electronic energy: -3299.17749962 a.u. / lowest freq: 16.45 cm-1
 C   -3.130428   -1.973009    0.292674
 H   -3.831028   -1.222594   -0.124943
 C   -2.550280   -2.972814   -0.704680
 H   -2.985499   -3.978801   -0.615807
 C   -0.800544   -1.941006    0.448086
 C   -0.211056   -3.888701   -0.965149
Cu    1.072982   -1.486223    0.889242
 N   -1.919076   -1.297854    0.772097
 N   -1.132114   -2.975259   -0.343299
 C    1.402115    0.811534    0.191280
 C    0.255514    1.167169   -0.607445
 H   -2.668423   -2.641934   -1.752780
 H   -3.620209   -2.478262    1.145289
 H    1.449307    1.387546    1.121621
 C   -0.126058    0.472550   -1.809539
 C   -0.628113    2.196922   -0.107167
 O    0.743942   -0.501850   -2.158689
 O   -1.130901    0.644709   -2.497047
 O   -1.640841    2.636503   -0.642153
 O   -0.258022    2.691707    1.098860
 C   -1.126346    3.637780    1.691226
 H   -1.228852    4.535884    1.065647
 H   -0.674818    3.904658    2.653661
 H   -2.126458    3.208527    1.854102
 C    0.427848   -1.252392   -3.313525
 H   -0.555507   -1.734966   -3.216619
 H    1.210985   -2.014028   -3.407111
 H    0.416137   -0.617653   -4.211509
 C    2.467782   -0.040287    0.004021
 H    2.604215   -0.545511   -0.955716
 C    3.673861   -0.004304    0.930296
 H    3.386633    0.541831    1.843027
 C    4.854871    0.719241    0.306405
 C    5.386978    1.868609    0.898823
 C    5.430774    0.254635   -0.883762
 C    6.468225    2.536863    0.321501
 H    4.947107    2.248638    1.824924
 C    6.510217    0.917527   -1.462782
 H    5.029026   -0.636909   -1.373095
 C    7.034324    2.062569   -0.860537
 H    6.869428    3.433238    0.799851
 H    6.945078    0.538651   -2.390471
 H    7.881164    2.583017   -1.313130
 C    1.952237   -2.890051    2.210914
 H    1.325432   -3.620029    2.698230
 C    2.865643   -2.177740    1.796521
 C    4.057450   -1.436763    1.356578
 H    4.819294   -1.433421    2.151242
 H    4.488973   -1.980984    0.500712
 C   -2.041288   -0.176708    1.669034
Na   -3.150932    1.372165   -1.772825
 O   -4.643812    0.569529   -0.492293
 H   -5.312560    3.073190    0.160208
 H   -6.899692    1.763429   -1.317259
 C   -5.444704    2.311512    0.947137
 H   -4.513548    2.277523    1.536816
 C   -7.003618    1.006073   -0.522209
 H   -6.263328    2.641019    1.610633
 C   -5.696208    0.928460    0.301045
 H   -7.188574    0.033108   -1.006350
 H   -7.888225    1.265625    0.085431
 C   -5.910643   -0.099552    1.438974
 H   -6.110124   -1.095435    1.010485
 H   -4.998122   -0.175634    2.051870
 H   -6.751032    0.164489    2.103636
 H    0.806944   -3.675677   -0.614127
 H   -0.232742   -3.790516   -2.062568
 H   -0.458705   -4.931587   -0.710193
 H   -1.059539    0.287243    1.821046
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 H   -2.444634   -0.497711    2.645397
 H   -2.740250    0.548989    1.223559
67
Figure S14-1_PA-PMe3(NaOtBu)-prod(1,4) / electronic energy: -3454.34900971 a.u. / lowest freq: -2.20 cm-1
Cu    2.128826   -0.372875   -0.884453
 C   -1.672103   -0.563133   -0.429984
 C   -0.890517   -0.117142    0.800470
 H   -1.662973   -1.659046   -0.418441
 C   -0.850307    1.251715    1.194184
 C   -0.057723   -1.062311    1.467773
 O   -1.582764    2.062894    0.375419
 O   -0.263302    1.768977    2.152050
 O    0.821327   -0.854831    2.318202
 O   -0.268524   -2.350320    1.072729
 C    0.663782   -3.308994    1.507889
 H    1.671226   -3.078294    1.126431
 H    0.334428   -4.271467    1.097416
 H    0.714633   -3.369901    2.604591
 C   -1.678250    3.424325    0.729986
 H   -2.041193    3.549395    1.760390
 H   -2.392061    3.873827    0.028408
 H   -0.707440    3.934416    0.636398
 C   -3.122025   -0.150335   -0.459739
 H   -3.319216    0.909885   -0.634687
 C   -4.137511   -1.005458   -0.282716
 H   -3.905747   -2.064792   -0.117068
 C   -5.576725   -0.677048   -0.283195
 C   -6.515230   -1.718914   -0.213911
 C   -6.062701    0.640589   -0.349519
 C   -7.885405   -1.461152   -0.220093
 H   -6.159704   -2.751349   -0.154583
 C   -7.429971    0.900136   -0.356900
 H   -5.361942    1.477239   -0.387547
 C   -8.350158   -0.148862   -0.293579
 H   -8.594119   -2.290883   -0.166797
 H   -7.782866    1.932902   -0.408853
 H   -9.422739    0.057367   -0.297829
 C    1.203391   -1.676608   -2.075808
 H    1.660954   -2.580834   -2.450483
 C    0.351662   -0.798453   -1.855443
 C   -0.958754   -0.133272   -1.743474
 H   -1.564240   -0.427081   -2.617405
 H   -0.845587    0.958477   -1.763314
Na    1.891712    1.118797    2.198696
 O    2.402274    1.300845    0.055413
 C    2.529228    2.530135   -0.580519
 C    1.395995    2.745463   -1.595462
 H    1.460078    3.727152   -2.091738
 H    1.432770    1.964690   -2.373203
 H    0.424187    2.670287   -1.085898
 C    3.882032    2.612198   -1.308531
 H    4.029938    3.578804   -1.817021
 H    4.703531    2.473163   -0.587290
 H    3.950776    1.811093   -2.063007
 C    2.458720    3.638801    0.484112
 H    2.541889    4.647321    0.048837
 H    1.500076    3.571940    1.023064
 H    3.277146    3.518638    1.213924
 P    4.089669   -1.425938   -0.226004
 C    4.301984   -3.229375   -0.480696
 H    4.284704   -3.445189   -1.559202
 H    5.251711   -3.589809   -0.057637
 H    3.470997   -3.774777   -0.011065
 C    5.645286   -0.747165   -0.912788
 H    5.675209   -0.920974   -1.998069
 H    5.668426    0.336877   -0.737129
 H    6.526251   -1.213778   -0.446836
 C    4.315638   -1.215024    1.580306
 H    3.388962   -1.506226    2.097025
 H    5.162388   -1.804766    1.961491
 H    4.505604   -0.149859    1.775993
67
Figure S14-1_PA-PMe3(NaOtBu)-ts(1,4) / electronic energy: -3454.28410031 a.u. / lowest freq: -357.37 cm-1
Cu    2.195907   -0.251986   -0.746317
 C   -1.970110   -0.842094    0.140522
 C   -0.870449   -0.318606    0.839521
 H   -1.966147   -1.929164    0.076413
 C   -0.730578    1.095789    1.181545
 C    0.166837   -1.245469    1.286096
 O   -1.485877    1.895615    0.414422
 O   -0.035234    1.569278    2.067964
 O    1.175528   -0.972462    1.927716
 O   -0.091335   -2.519241    0.951083
 C    0.890004   -3.485932    1.264619
 H    1.814512   -3.284424    0.706478
 H    0.477150   -4.452977    0.957556
 H    1.113765   -3.495815    2.340677
 C   -1.525634    3.273426    0.748440
 H   -1.801890    3.416751    1.802342
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 H   -2.281904    3.721237    0.094240
 H   -0.551397    3.747624    0.565991
 C   -3.307533   -0.258560    0.061232
 H   -3.399843    0.821638    0.166837
 C   -4.396397   -1.033259   -0.102553
 H   -4.250926   -2.115062   -0.206591
 C   -5.795281   -0.584723   -0.153921
 C   -6.813582   -1.547423   -0.248013
 C   -6.167123    0.771067   -0.113034
 C   -8.155658   -1.174927   -0.294204
 H   -6.545017   -2.606542   -0.284362
 C   -7.506608    1.143721   -0.159863
 H   -5.401568    1.546678   -0.047835
 C   -8.507656    0.173358   -0.249840
 H   -8.929599   -1.942207   -0.365762
 H   -7.773194    2.202517   -0.127442
 H   -9.558282    0.469363   -0.287396
 C    0.960835   -0.643965   -2.267935
 H    1.579513   -0.651846   -3.175873
 C   -0.307404   -0.755189   -2.299327
 C   -1.653127   -0.821916   -2.153394
 H   -2.167373   -1.781473   -2.262053
 H   -2.251593    0.070771   -2.359142
Na    2.196325    1.068629    2.186551
 O    2.732453    1.467530    0.106982
 C    2.722585    2.708412   -0.509276
 C    1.567076    2.822266   -1.518429
 H    1.483264    3.833863   -1.949188
 H    1.710023    2.104906   -2.341236
 H    0.615212    2.563642   -1.030753
 C    4.052486    2.935871   -1.251343
 H    4.090290    3.909681   -1.767637
 H    4.893853    2.889242   -0.541032
 H    4.196293    2.139779   -1.999613
 C    2.554872    3.800148    0.566189
 H    2.561173    4.818968    0.145540
 H    1.601653    3.653401    1.099294
 H    3.372898    3.731586    1.302940
 P    4.025806   -1.563633   -0.224748
 C    4.315220   -3.212301   -0.986413
 H    4.192648   -3.126494   -2.076039
 H    5.322890   -3.597031   -0.765188
 H    3.570435   -3.934501   -0.621158
 C    5.498200   -0.624068   -0.788792
 H    5.454848   -0.503538   -1.881263
 H    5.446567    0.377165   -0.338699
 H    6.442764   -1.118048   -0.514040
 C    4.443371   -1.877765    1.538372
 H    3.628097   -2.434310    2.019949
 H    5.386933   -2.435769    1.639752
 H    4.545631   -0.915341    2.060106
67
Figure S14-1_PA-PMe3(NaOtBu)-ed(1,4) / electronic energy: -3454.29818810 a.u. / lowest freq: 18.18 cm-1
Cu   -1.634374   -0.792249    0.649156
 C    1.338301    0.009218   -1.567567
 C    0.343944    0.901335   -1.843097
 H    1.068376   -1.034258   -1.741861
 C    0.413219    2.361074   -1.601707
 C   -0.960892    0.331141   -2.280602
 O    1.658305    2.815828   -1.493344
 O   -0.541343    3.108643   -1.511950
 O   -2.051084    0.850491   -2.130696
 O   -0.822054   -0.854108   -2.855360
 C   -1.991159   -1.646701   -3.006485
 H   -2.419854   -1.849296   -2.014494
 H   -1.663034   -2.583893   -3.466202
 H   -2.731612   -1.140059   -3.640408
 C    1.819851    4.192472   -1.173873
 H    1.376421    4.827632   -1.952309
 H    2.899614    4.363124   -1.114931
 H    1.347707    4.420306   -0.208030
 C    2.648474    0.194707   -0.997720
 H    3.030686    1.201855   -0.844486
 C    3.353444   -0.895585   -0.620232
 H    2.900026   -1.879362   -0.789293
 C    4.667064   -0.912981    0.026948
 C    5.262195   -2.153434    0.309406
 C    5.358442    0.259269    0.382048
 C    6.511439   -2.224939    0.921184
 H    4.733030   -3.072266    0.044331
 C    6.604697    0.187512    0.994086
 H    4.916237    1.237581    0.184837
 C    7.186266   -1.054036    1.264335
 H    6.959662   -3.198216    1.130877
 H    7.128224    1.106762    1.265012
 H    8.165104   -1.106652    1.745716
 C   -0.275127   -2.235427    0.586050
 H    0.279484   -2.396682    1.530025
 C    0.130688   -3.006687   -0.381902
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 C     0.535775   -3.746353   -1.408677
 H     0.096385   -4.726793   -1.624979
 H     1.320961   -3.398170   -2.092382
Na    -2.407772    2.310614   -0.374655
 O    -1.411100    1.145435    1.144321
 C    -0.579906    1.534978    2.179019
 C     0.889622    1.202534    1.863275
 H     1.568215    1.455536    2.694885
 H     0.989574    0.129737    1.636944
 H     1.219558    1.760318    0.973289
 C    -0.988397    0.819347    3.480494
 H    -0.381601    1.125360    4.349133
 H    -2.047189    1.031764    3.701965
 H    -0.881871   -0.270075    3.348350
 C    -0.709695    3.057194    2.374822
 H    -0.059788    3.443699    3.177084
 H    -0.439296    3.571109    1.436993
 H    -1.752441    3.319150    2.620419
 P    -3.920925   -1.061981    0.663532
 C    -4.761104   -2.386510   -0.296898
 H    -4.214743   -3.331225   -0.161796
 H    -5.806738   -2.523623    0.020107
 H    -4.745495   -2.132712   -1.367154
 C    -4.334102   -1.540388    2.390784
 H    -3.820233   -2.480632    2.638493
 H    -3.965165   -0.761476    3.074132
 H    -5.417715   -1.670313    2.536482
 C    -5.078110    0.348825    0.403575
 H    -5.023752    0.681524   -0.643967
 H    -6.119775    0.074281    0.632028
 H    -4.784137    1.184455    1.056512
20
Figure S14-1_PMe3-Cu-allenyl / electronic energy: -2217.18081039 a.u. / lowest freq: 11.62 cm-1
Cu    -0.560515   -0.423386    0.001726
 C    -2.432842   -0.885638   -0.001587
 H    -2.795343   -1.927024   -0.005273
 C    -3.361227    0.031773   -0.000490
 C    -4.267199    0.995333    0.000581
 H    -4.659226    1.410942   -0.933995
 H    -4.662543    1.405822    0.936022
 P     1.600033    0.123266    0.000003
 C     2.106979    1.292186    1.312838
 C     2.192749    0.921748   -1.535650
 C     2.748943   -1.283932    0.218620
 H     2.020056    0.248047   -2.386753
 H     3.265634    1.155681   -1.467568
 H     1.628095    1.849055   -1.706781
 H     2.586640   -2.016914   -0.584141
 H     2.546747   -1.774259    1.181365
 H     3.795310   -0.944582    0.195966
 H     1.880559    0.856225    2.296017
 H     1.540356    2.228190    1.209099
 H     3.183733    1.509209    1.250065
35
Figure S14-1_PMe3-Cu(NaOtBu)-allenyl / electronic energy: -2612.34261472 a.u. / lowest freq: 8.82 cm-1
 O     1.376816    0.842483    0.055204
 C     1.131329    2.203974   -0.029191
 C     0.442096    2.537528   -1.363889
 H     0.228937    3.613224   -1.477266
 H     1.081544    2.219009   -2.202677
 H    -0.505791    1.982636   -1.433540
 C     2.467922    2.963757    0.048059
 H     2.337641    4.056072   -0.022094
 H     2.974878    2.741450    1.001471
 H     3.129371    2.646726   -0.775067
 C     0.231203    2.658089    1.133982
 H     0.716704    2.429272    2.096023
 H     0.009323    3.737495    1.103295
 H    -0.720021    2.104473    1.098333
Na     3.084495   -0.455719    0.171642
Cu    -0.032157   -0.549381   -0.011145
 C     0.586035   -2.477899    0.035776
 H    -0.183685   -3.266188    0.088586
 C     1.806658   -2.909131   -0.047656
 C     3.099190   -3.236035   -0.132842
 H     3.695751   -3.433002    0.765551
 H     3.579367   -3.415708   -1.101330
 P    -2.271743   -0.275085   -0.018208
 C    -3.158051    1.194342   -0.682451
 C    -2.962645   -0.386102    1.682269
 C    -3.153926   -1.643230   -0.870792
 H    -4.063547   -0.386273    1.677483
 H    -2.604439    0.465260    2.279309
 H    -2.601336   -1.310203    2.156320
 H    -2.943506    1.296239   -1.756527
 H    -2.798531    2.102815   -0.177539
 H    -4.246646    1.109074   -0.540966
 H    -2.912686   -1.619117   -1.943624
 H    -4.245180   -1.571053   -0.744156
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 H   -2.802276   -2.602588   -0.464532
67
Figure S14-1_PA-PMe3(NaOtBu)-ed(1,6) / electronic energy: -3454.28842449 a.u. / lowest freq: 19.30 cm-1
Na   -3.242113   -0.795157   -2.211819
 O   -3.708256   -1.375966   -0.179950
Cu    0.366956    1.286753    0.562587
 C    1.492643    0.659942   -1.042368
 C    0.125953    0.382352   -1.281560
 H    1.876320    1.589046   -1.473869
 C   -0.431500   -0.997473   -1.145336
 C   -0.715351    1.333158   -2.044369
 O   -0.207296   -1.531559    0.043380
 O   -1.027492   -1.573680   -2.029741
 O   -1.850792    1.115028   -2.423062
 O   -0.118560    2.505029   -2.242072
 C   -0.869453    3.518577   -2.898435
 H   -1.137603    3.205026   -3.916558
 H   -0.220231    4.399158   -2.933511
 H   -1.786206    3.746872   -2.337593
 C   -0.839286   -2.790450    0.309205
 H   -1.928171   -2.651358    0.194993
 H   -0.574269   -3.039620    1.341951
 H   -0.461573   -3.559064   -0.378887
 C    2.497438   -0.302881   -0.625838
 H    2.152481   -1.232050   -0.167308
 C    3.814940   -0.058317   -0.772014
 H    4.120175    0.866269   -1.270641
 C    4.910151   -0.936281   -0.338632
 C    6.204132   -0.711975   -0.836373
 C    4.720426   -1.992739    0.569017
 C    7.269602   -1.526906   -0.460317
 H    6.371748    0.112544   -1.534284
 C    5.785213   -2.804958    0.947584
 H    3.733058   -2.171073    1.000024
 C    7.063395   -2.578646    0.432323
 H    8.266360   -1.338709   -0.865284
 H    5.618933   -3.616933    1.659028
 H    7.897094   -3.216961    0.732904
 C    1.679554    2.078808    1.802989
 H    1.308174    2.445437    2.772481
 C    2.947032    2.244610    1.564601
 C    4.229904    2.365362    1.269846
 H    4.619526    3.253191    0.761040
 H    4.945398    1.580289    1.535416
 P   -1.703469    1.417304    1.564318
 C   -3.208038    1.748465    0.583377
 C   -1.716481    2.697786    2.871969
 C   -2.129375   -0.137152    2.421498
 H   -6.571771   -1.252002    1.596030
 H   -5.019560   -0.448788    1.965580
 H   -5.915168   -0.008570    0.493629
 C   -5.644630   -0.849836    1.152894
 H   -3.852383   -2.731184    2.108791
 C   -4.853633   -1.910923    0.353020
 H   -6.704966   -2.912209   -0.375055
 H   -6.070559   -1.632351   -1.441942
 H   -3.990502   -3.875991    0.751778
 C   -4.519352   -3.082421    1.305122
 C   -5.779619   -2.452188   -0.762467
 H   -5.415275   -3.528832    1.769469
 H   -5.242203   -3.211657   -1.354675
 H   -2.520282   -0.815311    1.640040
 H   -2.913366    0.032762    3.175284
 H   -1.240340   -0.565334    2.904724
 H   -1.512578    3.682855    2.427882
 H   -0.928763    2.479745    3.606873
 H   -2.690125    2.723960    3.383666
 H   -3.029849    2.538871   -0.158612
 H   -4.038623    2.042567    1.242954
 H   -3.474170    0.794434    0.091042
67
Figure S14-1_PA-PMe3(NaOtBu)-ts(1,6) / electronic energy: -3454.27252064 a.u. / lowest freq: -463.81 cm-1
Na   -3.264628   -1.042155   -2.112070
 O   -4.277061   -0.871422   -0.246233
Cu    0.360336    1.165573    0.465391
 C    1.566282    0.412256   -1.118029
 C    0.194212    0.022761   -1.337824
 H    1.849596    1.329492   -1.642332
 C   -0.328940   -1.305136   -0.979162
 C   -0.647451    0.872665   -2.190165
 O    0.262428   -1.823439    0.104725
 O   -1.211368   -1.913890   -1.555095
 O   -1.763506    0.613651   -2.609063
 O   -0.084584    2.062536   -2.450786
 C   -0.848857    2.984726   -3.211428
 H   -1.059972    2.585993   -4.213464
 H   -0.240064    3.891800   -3.289000
 H   -1.800258    3.211145   -2.710171
 C   -0.192855   -3.097805    0.539376
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 H   -1.259657   -3.056166    0.800315
 H    0.403020   -3.344947    1.424477
 H   -0.042738   -3.855508   -0.241904
 C    2.625458   -0.295966   -0.534789
 H    2.430427   -1.245144   -0.037328
 C    3.909585    0.257633   -0.498996
 H    4.099678    1.065489   -1.210782
 C    5.105432   -0.558211   -0.174578
 C    6.334654   -0.247706   -0.772452
 C    5.054923   -1.635477    0.724064
 C    7.477017   -0.997418   -0.494701
 H    6.393374    0.590961   -1.471486
 C    6.195282   -2.382985    1.004219
 H    4.115269   -1.882966    1.223261
 C    7.411999   -2.069042    0.394595
 H    8.423216   -0.742168   -0.977071
 H    6.136330   -3.215002    1.709584
 H    8.306289   -2.655359    0.616529
 C    1.609513    2.345805    1.535657
 H    1.063896    3.034709    2.182181
 C    2.853748    2.140575    1.415373
 C    4.103081    1.680774    1.132053
 H    4.792630    2.331785    0.586679
 H    4.571406    1.017864    1.865995
 P   -1.640737    1.231827    1.587405
 C   -3.099180    1.892919    0.705589
 C   -1.522618    2.253205    3.103914
 C   -2.216248   -0.398532    2.180537
 H   -6.891035   -0.521701    1.850407
 H   -5.189110   -0.057126    2.134581
 H   -6.118341    0.736984    0.843342
 C   -5.950319   -0.224191    1.356173
 H   -4.468734   -2.492871    1.871329
 C   -5.443963   -1.276957    0.342246
 H   -7.512355   -1.814475   -0.285705
 H   -6.722044   -0.544905   -1.264279
 H   -4.889009   -3.385113    0.388383
 C   -5.240412   -2.613872    1.093906
 C   -6.550839   -1.487369   -0.718283
 H   -6.161231   -2.983834    1.577408
 H   -6.228367   -2.249503   -1.447989
 H   -2.753169   -0.872241    1.334928
 H   -2.929250   -0.280176    3.010784
 H   -1.365933   -1.008898    2.514192
 H   -1.295286    3.295410    2.834663
 H   -0.714317    1.874240    3.746197
 H   -2.470562    2.229269    3.662097
 H   -2.804516    2.703244    0.024204
 H   -3.839130    2.272890    1.426498
 H   -3.562109    1.046105    0.156668
67
Figure S14-1_PA-PMe3(NaOtBu)-prod(1,6) / electronic energy: -3454.32484583 a.u. / lowest freq: 17.63 cm-1
Na   -3.049317   -2.226155    0.755051
 O   -4.456425   -0.688750    0.303549
Cu    0.812971    1.780150   -0.168877
 C    1.385063   -0.544508   -0.434460
 C    0.296474   -1.379069    0.016703
 H    1.527258   -0.603011   -1.518894
 C   -0.090978   -1.528142    1.396976
 C   -0.464740   -2.103169   -0.980300
 O    0.672518   -0.802531    2.245786
 O   -1.018721   -2.193999    1.851062
 O   -1.464402   -2.791426   -0.802803
 O    0.011958   -1.952345   -2.239804
 C   -0.713770   -2.586500   -3.275946
 H   -0.772833   -3.672083   -3.114939
 H   -0.169536   -2.375657   -4.203642
 H   -1.736020   -2.185432   -3.345023
 C    0.363991   -0.890989    3.624538
 H   -0.658349   -0.539148    3.827107
 H    1.086099   -0.246973    4.139610
 H    0.458468   -1.923828    3.988416
 C    2.309355    0.242136    0.219583
 H    2.339315    0.247626    1.312069
 C    3.546857    0.771927   -0.488884
 H    3.354349    0.764400   -1.573872
 C    4.772320   -0.089485   -0.235708
 C    5.434621   -0.709885   -1.299532
 C    5.259415   -0.291202    1.062546
 C    6.556314   -1.509865   -1.076955
 H    5.065011   -0.566933   -2.318571
 C    6.379912   -1.087592    1.289087
 H    4.755322    0.173619    1.914320
 C    7.033691   -1.700210    0.218496
 H    7.057943   -1.986464   -1.922256
 H    6.744693   -1.233284    2.308393
 H    7.911631   -2.325186    0.395841
 C    1.584494    3.757160   -0.390200
 H    0.894103    4.571572   -0.544069
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 C     2.556381    3.019777   -0.241853
 C     3.791628    2.239118   -0.078003
 H     4.605337    2.694768   -0.662868
 H     4.087169    2.291830    0.982515
 P    -1.459769    1.781014   -0.225382
 C    -2.215347    0.730781   -1.529808
 C    -2.281441    3.401629   -0.466562
 C    -2.185302    1.193754    1.353538
 H    -6.692290    1.762889   -0.272337
 H    -5.284034    1.794515    0.825801
 H    -5.039493    1.616983   -0.930246
 C    -5.692444    1.333787   -0.088701
 H    -6.277603   -0.135288    2.165036
 C    -5.714070   -0.206702    0.063097
 H    -7.302651   -0.441312   -1.476133
 H    -5.625058   -0.558894   -2.084777
 H    -6.725204   -1.653686    1.346382
 C    -6.669533   -0.558953    1.226014
 C    -6.288371   -0.807363   -1.240122
 H    -7.694266   -0.177050    1.076047
 H    -6.329805   -1.905998   -1.156161
 H    -3.139056    0.666001    1.145813
 H    -2.340364    2.054452    2.020405
 H    -1.488075    0.505927    1.845661
 H    -2.001758    3.818328   -1.444868
 H    -1.956656    4.100373    0.317774
 H    -3.374618    3.288956   -0.418909
 H    -1.471685    0.028560   -1.925261
 H    -2.557546    1.370692   -2.356254
 H    -3.073467    0.180691   -1.093110
13
Figure_S15-1_NaOPh / electronic energy: -468.853649444 a.u. / lowest freq: 15.68 cm-1
 C    -1.912599   -1.200838   -0.011375
 C    -0.521476   -1.206572    0.015351
 C     0.241248    0.001459    0.028090
 C    -0.524240    1.207747    0.015228
 C    -1.915348    1.198823   -0.011498
 C    -2.633248   -0.001829   -0.025828
 H    -2.448993   -2.155315   -0.021458
 H     0.025710   -2.154567    0.026010
 H     0.020847    2.156944    0.025804
 H    -2.453903    2.152085   -0.021671
 H    -3.725390   -0.003095   -0.047610
 O     1.527681    0.002959    0.048939
Na     3.632205   -0.001133   -0.037490
32
Figure_S15-1_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C    -0.660544   -0.726572    0.059153
 C    -1.860539   -0.097447    0.115996
 H    -0.691600   -1.818492   -0.004770
 C    -1.976243    1.390665    0.160143
 C    -3.120576   -0.891785    0.187355
 O    -3.041424    1.823605   -0.507466
 O    -1.182749    2.134043    0.689285
 O    -4.147702   -0.497504    0.683440
 O    -2.981802   -2.118850   -0.320932
 C    -4.097604   -2.989729   -0.195724
 H    -4.332384   -3.170881    0.862818
 H    -3.810049   -3.927003   -0.683244
 H    -4.981752   -2.562067   -0.688186
 C    -3.254671    3.228152   -0.535442
 H    -3.354009    3.627502    0.483524
 H    -4.184056    3.384216   -1.092621
 H    -2.420438    3.737793   -1.038016
 C     0.656646   -0.129211    0.062308
 H     0.725624    0.955889    0.150505
 C     1.759981   -0.902956   -0.019704
 H     1.621029   -1.988149   -0.089650
 C     3.156351   -0.453635   -0.025165
 C     4.175093   -1.416830   -0.109525
 C     3.522207    0.902114    0.053056
 C     5.517020   -1.042840   -0.114390
 H     3.907556   -2.474776   -0.172060
 C     4.861836    1.275255    0.048166
 H     2.754752    1.675486    0.118691
 C     5.863995    0.305241   -0.035401
 H     6.294080   -1.807149   -0.179427
 H     5.127957    2.332459    0.111300
 H     6.914980    0.602284   -0.038425
64
Figure_S15-1_9d(NaOPh)-Cu-allenyl / electronic energy: -3146.25617778 a.u. / lowest freq: 11.92 cm-1
Cu    -0.619467   -0.796156    0.827096
 C    -0.346515   -2.401130    1.871679
 C    -0.937222    0.741398   -0.321533
 N    -2.143873    1.194277   -0.727784
 N     0.001999    1.491143   -0.883402
 C     1.428889    1.329861   -0.605320
 C     0.000505   -3.552073    1.370637
 C     0.379012   -4.681143    0.783804
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 C   -0.538280    2.590848   -1.682850
 H   -0.064878    2.614677   -2.671898
 C   -2.024791    2.234507   -1.754997
 H   -2.687930    3.081346   -1.533017
 C   -3.384438    0.644678   -0.341043
 C   -4.475496    0.689404   -1.214462
 C   -3.536012    0.067039    0.924065
 C   -5.702527    0.127497   -0.846977
 C   -4.745649   -0.518589    1.301216
 C   -5.819800   -0.481859    0.406051
 H   -6.774855   -0.927927    0.697213
 H    1.928082   -0.165857   -2.634416
 H   -2.295340    1.829362   -2.742745
 H   -0.361921    3.553497   -1.177043
 H    1.548128    0.269518   -0.343982
 C    1.868628    2.158545    0.586139
 C    2.053601    3.544278    0.504275
 C    2.081183    1.523956    1.815389
 C    2.431048    4.278172    1.628804
 H    1.910466    4.065296   -0.445429
 C    2.459838    2.254661    2.940604
 H    1.953127    0.439958    1.885623
 C    2.633553    3.635791    2.850098
 H    2.572759    5.358128    1.547429
 H    2.623645    1.742288    3.891151
 H    2.931610    4.210602    3.729810
 C    2.268177    1.568157   -1.865892
 H    3.322384    1.385089   -1.581130
 H    2.205771    2.626217   -2.173769
 O    1.853004    0.780671   -2.934328
 H   -0.497865   -2.385581    2.963745
 H    1.440706   -4.937140    0.691804
 H   -0.352724   -5.417789    0.434912
 O    2.095699   -1.595484   -1.830360
 C    3.222727   -1.564585   -1.170414
 C    4.447353   -1.226071   -1.804986
 C    3.281741   -1.828571    0.224015
 C    5.640423   -1.157639   -1.091733
 H    4.422841   -1.005951   -2.875978
 C    4.482514   -1.757915    0.926085
 H    2.350068   -2.074064    0.744595
 C    5.675802   -1.422792    0.280923
 H    6.562662   -0.890149   -1.616402
 H    4.483811   -1.961209    2.001267
 H    6.614856   -1.365732    0.835649
Na    0.382018   -2.891610   -1.448261
 C   -4.878061   -1.148536    2.663108
 H   -4.770153   -0.392767    3.456561
 H   -5.854279   -1.635792    2.789687
 H   -4.092521   -1.902634    2.823354
 C   -6.862411    0.151859   -1.808539
 H   -7.814286   -0.041059   -1.295092
 H   -6.937309    1.122263   -2.320462
 H   -6.741086   -0.619441   -2.586003
 H   -2.706191    0.090239    1.634257
 H   -4.376491    1.152925   -2.197690
96
Figure_S15-1_PA-9d(NaOPh)-ts(1,6major)_O1 / electronic energy: -3988.22213482 a.u. / lowest freq: -455.12 cm-1
 C   -3.327935   -0.170787   -1.529052
 H   -4.192691   -0.031508   -0.867769
 C   -2.662458    1.167411   -1.862437
 H   -2.655559    1.391704   -2.938936
 C   -1.099710   -0.222582   -0.802762
 C   -0.307353    1.984154   -1.521281
 C   -0.693752    3.326459   -1.474443
 C    1.035198    1.654344   -1.714125
 C    0.261227    4.341403   -1.568307
 C    2.003898    2.654658   -1.817377
 C    1.606037    3.992765   -1.733262
 H    2.359633    4.782000   -1.811087
Cu    0.589861   -0.977070   -0.055773
 N   -2.252470   -0.892686   -0.840558
 N   -1.286505    0.971906   -1.385249
 C    1.965462   -1.086241    1.563534
 C    0.662027   -0.741864    2.082639
 H   -4.346931   -0.894357    1.133336
 H   -3.149871    1.996130   -1.333085
 H   -3.658809   -0.718542   -2.424534
 H    2.207410   -2.145612    1.676566
 C    0.156130    0.624372    2.257305
 C   -0.154870   -1.838740    2.621282
 O    0.994914    1.557152    1.797065
 O   -0.924652    0.939399    2.729923
 O   -1.159894   -1.740230    3.305429
 O    0.294497   -3.051590    2.257921
 C   -0.426588   -4.176792    2.732978
 H   -0.354837   -4.256153    3.826921
 H    0.033866   -5.051897    2.262414
 H   -1.487690   -4.108639    2.454327
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 C    0.542522    2.902684    1.797709
 H   -0.423369    2.988225    1.282248
 H    1.301639    3.473870    1.251265
 H    0.442156    3.281767    2.824648
 C   -2.373061   -2.267514   -0.386333
 H   -1.685211   -2.369161    0.467484
 C   -1.937462   -3.280305   -1.436109
 C   -1.683413   -4.598887   -1.038105
 C   -1.742102   -2.940560   -2.777612
 C   -1.251371   -5.553514   -1.955278
 H   -1.807979   -4.881373    0.010719
 C   -1.310564   -3.895215   -3.700081
 H   -1.897914   -1.914732   -3.115175
 C   -1.064815   -5.205010   -3.293562
 H   -1.051187   -6.573748   -1.621048
 H   -1.159109   -3.607622   -4.742649
 H   -0.721669   -5.950079   -4.014199
 C   -3.778561   -2.558934    0.165904
 H   -3.812528   -3.629966    0.416967
 H   -4.528915   -2.408374   -0.633139
 O   -4.078303   -1.835000    1.314456
 C    3.032978   -0.282111    1.136206
 H    2.890660    0.791420    1.033708
 C    4.242865   -0.875850    0.766478
 H    4.381132   -1.910989    1.088387
 C    5.509869   -0.119045    0.623319
 C    6.721975   -0.824116    0.557491
 C    5.556988    1.282101    0.564712
 C    7.937097   -0.157824    0.422689
 H    6.708202   -1.916124    0.613352
 C    6.771171    1.950494    0.426032
 H    4.636864    1.864097    0.632769
 C    7.966812    1.235301    0.350907
 H    8.866906   -0.728969    0.374719
 H    6.782858    3.041911    0.380514
 H    8.917917    1.760896    0.242826
 C    3.438840    2.280829   -2.079289
 H    3.687790    1.316241   -1.615480
 H    3.621636    2.181143   -3.161356
 H    4.135300    3.039489   -1.695484
 C   -0.150970    5.784508   -1.437302
 H    0.455210    6.436575   -2.082376
 H   -1.209991    5.926549   -1.694249
 H   -0.013809    6.131473   -0.400079
 H   -1.741173    3.589623   -1.321334
 H    1.331896    0.608822   -1.811012
 C    1.564418   -1.991444   -1.528407
 H    0.834209   -2.419130   -2.217874
 C    2.826855   -1.914298   -1.540685
 C    4.141091   -1.648662   -1.309680
 H    4.813686   -2.478652   -1.076657
 H    4.601615   -0.814920   -1.849771
 O   -4.369248    0.677629    1.574864
Na   -2.871114   -0.291780    2.919350
 C   -4.435046    1.836235    0.998837
 C   -3.478783    2.858527    1.261779
 C   -5.450364    2.153186    0.052960
 C   -3.526907    4.085453    0.607708
 H   -2.682447    2.640935    1.979065
 C   -5.478837    3.380657   -0.603153
 H   -6.208769    1.393480   -0.157842
 C   -4.517069    4.362197   -0.341689
 H   -2.765505    4.839045    0.832557
 H   -6.268084    3.577275   -1.335127
 H   -4.544731    5.324404   -0.857420
96
Figure_S15-1_PA-9d(NaOPh)-ts(1,6major)_O2 / electronic energy: -3988.22242215 a.u. / lowest freq: -444.57 cm-1
 C    3.357333    0.184090   -1.554637
 H    4.252495    0.098351   -0.924952
 C    2.732862   -1.185072   -1.827107
 H    2.769970   -1.473732   -2.887023
 C    1.130680    0.206924   -0.835199
 C    0.394025   -2.040882   -1.504401
 C    0.828452   -3.369464   -1.454373
 C   -0.964995   -1.764430   -1.656379
 C   -0.092836   -4.418260   -1.502234
 C   -1.901141   -2.798705   -1.710393
 C   -1.454522   -4.120582   -1.623423
 H   -2.181919   -4.936798   -1.662472
Cu   -0.600918    0.952335   -0.163764
 N    2.278707    0.885819   -0.852151
 N    1.339810   -0.993094   -1.404738
 C   -1.998169    1.159341    1.436183
 C   -0.689013    0.889510    1.985938
 H    4.422183    0.991342    1.101979
 H    3.217291   -1.969232   -1.231667
 H    3.624675    0.712384   -2.482105
 H   -2.266463    2.217925    1.464781
 C   -0.140459   -0.453506    2.221629
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 C     0.076887    2.032137    2.504002
 O    -0.932719   -1.427444    1.762715
 O     0.929546   -0.720338    2.744692
 O     1.159149    1.993469    3.066303
 O    -0.517882    3.216440    2.283202
 C     0.159786    4.373946    2.749190
 H     0.298891    4.333928    3.838251
 H    -0.476860    5.223773    2.480883
 H     1.143871    4.474704    2.268816
 C    -0.437877   -2.757096    1.820525
 H     0.530924   -2.832332    1.308913
 H    -1.176818   -3.374872    1.297672
 H    -0.327068   -3.088531    2.862561
 C     2.383183    2.264047   -0.372795
 H     1.751181    2.318879    0.524306
 C     1.847792    3.267059   -1.377015
 C     0.730895    4.040476   -1.046326
 C     2.439876    3.443747   -2.633920
 C     0.207506    4.964571   -1.949723
 H     0.248123    3.900388   -0.075788
 C     1.917106    4.364357   -3.540744
 H     3.320701    2.862755   -2.916602
 C     0.798584    5.127290   -3.201257
 H    -0.672384    5.550635   -1.675977
 H     2.388526    4.488919   -4.517999
 H     0.389926    5.847367   -3.913475
 C     3.799495    2.619424    0.099747
 H     3.787341    3.697838    0.321913
 H     4.522965    2.484744   -0.727453
 O     4.192388    1.948157    1.252082
 C    -3.046062    0.298746    1.076043
 H    -2.878441   -0.775793    1.068369
 C    -4.269719    0.825250    0.654095
 H    -4.435951    1.882806    0.874342
 C    -5.514172    0.020680    0.585003
 C    -6.745332    0.676142    0.424651
 C    -5.520508   -1.378723    0.689262
 C    -7.938805   -0.037908    0.357068
 H    -6.764194    1.766778    0.348505
 C    -6.713036   -2.095084    0.619469
 H    -4.585706   -1.921920    0.833657
 C    -7.927652   -1.430100    0.450368
 H    -8.883866    0.495145    0.231991
 H    -6.692286   -3.183910    0.704953
 H    -8.862014   -1.992928    0.397448
 C    -3.357332   -2.473994   -1.913945
 H    -3.619235   -1.520767   -1.434063
 H    -3.586314   -2.373640   -2.987143
 H    -4.012025   -3.257522   -1.507292
 C     0.373947   -5.845081   -1.373126
 H    -0.205521   -6.517027   -2.022566
 H     1.438089   -5.946846   -1.627802
 H     0.246044   -6.201454   -0.338038
 H     1.887738   -3.597876   -1.333402
 H    -1.304629   -0.732947   -1.753267
 C    -1.613457    1.730724   -1.754838
 H    -0.895123    2.073004   -2.500579
 C    -2.876068    1.649111   -1.751799
 C    -4.186066    1.396624   -1.488902
 H    -4.868815    2.238189   -1.342810
 H    -4.636529    0.503465   -1.933552
 O     4.385965   -0.554589    1.602115
Na     2.879680    0.502921    2.871915
 C     4.459372   -1.733700    1.072494
 C     3.498829   -2.744205    1.364584
 C     5.485878   -2.088335    0.152351
 C     3.551328   -3.995121    0.758803
 H     2.696389   -2.495515    2.064615
 C     5.519487   -3.340785   -0.454643
 H     6.247298   -1.338030   -0.079951
 C     4.552489   -4.309888   -0.167054
 H     2.784717   -4.737647    1.001709
 H     6.316574   -3.567343   -1.169235
 H     4.583807   -5.290794   -0.646039
96
Figure_S15-1_PA-9d(NaOPh)-ts(1,6major)_03 / electronic energy: -3988.21826606 a.u. / lowest freq: -458.70 cm-1
 C     3.050145    1.078887   -1.500604
 H     3.987240    1.185367   -0.937596
 C     2.787325   -0.377335   -1.888232
 H     2.756921   -0.533053   -2.975953
 C     0.986716    0.424532   -0.619927
 C     0.832725   -1.889699   -1.400388
 C     1.619466   -3.044593   -1.478475
 C    -0.559274   -2.000116   -1.410851
 C     1.023706   -4.305987   -1.534102
 C    -1.174166   -3.254565   -1.444439
 C    -0.372744   -4.397455   -1.510302
 H    -0.846359   -5.382627   -1.548000
Cu    -0.871618    0.664914    0.054094
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 N     1.890393    1.400976   -0.666476
 N     1.459744   -0.626776   -1.311540
 C    -2.481238    0.497995    1.446044
 C    -1.265695   -0.042468    2.004019
 H     3.682423    1.166410    1.509683
 H     3.540382   -1.050633   -1.459496
 H     3.085208    1.743547   -2.376326
 H    -2.655393    1.553597    1.674544
 C    -1.016146   -1.498090    1.979637
 C    -0.435755    0.828507    2.838313
 O     0.282060   -1.847634    2.125651
 O    -1.860646   -2.345046    1.789679
 O     0.452481    0.470874    3.597320
 O    -0.720621    2.132602    2.692246
 C     0.066686    3.048654    3.443580
 H    -0.109182    2.920036    4.520599
 H    -0.251715    4.047751    3.126987
 H     1.135116    2.899440    3.233561
 C     0.560484   -3.242715    2.051241
 H     0.050408   -3.783640    2.859907
 H     1.646205   -3.345875    2.160170
 H     0.240719   -3.648348    1.082384
 C     1.749173    2.658921    0.058725
 H     0.901032    2.497035    0.738550
 C     1.402166    3.834545   -0.834188
 C     0.130920    4.412246   -0.740820
 C     2.322793    4.379484   -1.738699
 C    -0.222619    5.496353   -1.542457
 H    -0.595417    3.997698   -0.036702
 C     1.970099    5.460917   -2.545615
 H     3.330627    3.965711   -1.818243
 C     0.696138    6.020942   -2.450999
 H    -1.220693    5.931371   -1.457064
 H     2.697795    5.870110   -3.249833
 H     0.421018    6.868048   -3.083148
 C     2.971034    2.936427    0.948450
 H     2.774816    3.889369    1.466688
 H     3.868542    3.106907    0.323563
 O     3.186835    1.942403    1.896333
 C    -3.546257   -0.177951    0.833588
 H    -3.462552   -1.251138    0.670820
 C    -4.657250    0.525389    0.363540
 H    -4.777970    1.539232    0.755808
 C    -5.935333   -0.141047    0.013314
 C    -7.131326    0.587525    0.087364
 C    -5.998806   -1.481129   -0.399188
 C    -8.353605   -0.002580   -0.230125
 H    -7.101077    1.634097    0.403095
 C    -7.218540   -2.071450   -0.718264
 H    -5.083923   -2.070246   -0.477634
 C    -8.402636   -1.336131   -0.634519
 H    -9.273239    0.582712   -0.159752
 H    -7.245193   -3.116351   -1.035825
 H    -9.358451   -1.802137   -0.883261
 C    -2.673048   -3.358695   -1.375022
 H    -3.156003   -2.489245   -1.844377
 H    -3.042482   -4.270655   -1.864001
 H    -2.986356   -3.386975   -0.318718
 C     1.870994   -5.551194   -1.569942
 H     1.516828   -6.253179   -2.339170
 H     2.925160   -5.317948   -1.773742
 H     1.824485   -6.078140   -0.603661
 H     2.707759   -2.969174   -1.469382
 H    -1.179923   -1.100376   -1.422149
 C    -1.668131    1.662065   -1.535396
 H    -0.883877    2.084541   -2.164436
 C    -2.924844    1.606389   -1.683427
 C    -4.261079    1.362170   -1.613270
 H    -4.945753    2.201669   -1.461533
 H    -4.657841    0.542902   -2.221137
 O     4.009052   -0.392423    1.270414
Na     2.212723   -0.467347    2.511718
 C     4.903856   -1.041242    0.591912
 C     4.803268   -2.444849    0.382742
 C     6.013494   -0.392170   -0.014344
 C     5.724042   -3.133944   -0.400372
 H     3.961467   -2.972628    0.840502
 C     6.928212   -1.093558   -0.796022
 H     6.134047    0.683177    0.148765
 C     6.794896   -2.469014   -1.005943
 H     5.600770   -4.211553   -0.544703
 H     7.764789   -0.554930   -1.251081
 H     7.513267   -3.013008   -1.622582
96
Figure_S15-1_PA-9d(NaOPh)-ts(1,6minor)_01 / electronic energy: -3988.21792967 a.u. / lowest freq: -450.44 cm-1
 C     2.947852   -1.853253    1.292620
 H     3.636009   -2.242294    0.530857
 C     3.291331   -0.408970    1.667599
 H     3.492434   -0.274941    2.740739
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C	1.121921	-0.476297	0.781732
C	1.983263	1.727379	1.434222
C	3.147647	2.496801	1.459914
C	0.740052	2.361285	1.548608
C	3.078034	3.892791	1.552925
C	0.648625	3.748597	1.620576
C	1.827043	4.506250	1.621827
H	1.764113	5.596357	1.686889
Cu	-0.755762	0.011850	0.301166
N	1.591961	-1.721432	0.749736
N	2.072511	0.323670	1.296305
C	-2.059354	1.038188	-1.066307
C	-0.953404	0.439594	-1.774156
H	2.968430	-2.887236	-1.454515
H	4.157379	-0.048443	1.098707
H	2.962229	-2.535511	2.155470
H	-1.835292	2.036698	-0.674990
C	0.240514	1.251315	-2.060058
C	-1.025600	-0.884182	-2.404348
O	0.109489	2.526422	-1.682795
O	1.278087	0.851598	-2.563347
O	-0.268341	-1.330817	-3.249899
O	-2.023718	-1.641971	-1.926776
C	-2.160949	-2.945326	-2.472590
H	-2.346251	-2.899492	-3.554395
H	-3.015918	-3.398966	-1.960268
H	-1.252544	-3.539319	-2.295974
C	1.264349	3.348333	-1.771322
H	2.062027	2.967890	-1.116630
H	0.953987	4.342508	-1.432833
H	1.632659	3.395868	-2.805279
C	0.782273	-2.850435	0.323874
H	0.094406	-2.459963	-0.442337
C	-0.073497	-3.427600	1.442287
C	-1.147768	-4.259261	1.103237
C	0.148552	-3.141701	2.791753
C	-1.976139	-4.796735	2.084966
H	-1.350812	-4.476581	0.051234
C	-0.677987	-3.680511	3.778918
H	0.956848	-2.470961	3.087892
C	-1.741573	-4.510077	3.430303
H	-2.813655	-5.435884	1.797175
H	-0.490606	-3.442499	4.828196
H	-2.392400	-4.925014	4.202740
C	1.633016	-3.921768	-0.378528
H	0.968934	-4.771779	-0.597040
H	2.397865	-4.302802	0.324972
O	2.185070	-3.486558	-1.577706
C	-3.411297	0.676238	-1.013817
H	-3.740212	-0.238365	-1.504379
C	-4.309035	1.410480	-0.240619
H	-3.959336	2.388635	0.103806
C	-5.779080	1.312363	-0.402577
C	-6.581030	2.409017	-0.054926
C	-6.408837	0.155625	-0.888536
C	-7.966706	2.360356	-0.199429
H	-6.108584	3.315786	0.332444
C	-7.792624	0.105451	-1.032280
H	-5.813989	-0.722460	-1.149303
C	-8.578608	1.207940	-0.690469
H	-8.570623	3.228776	0.073451
H	-8.262977	-0.803707	-1.413509
H	-9.663826	1.165699	-0.805359
C	-0.700495	4.415791	1.671096
H	-0.952933	4.846097	0.688441
H	-1.491391	3.699156	1.933822
H	-0.717897	5.236896	2.402316
C	4.349549	4.700826	1.543868
H	4.153328	5.766504	1.723904
H	5.051977	4.344864	2.312389
H	4.861295	4.609640	0.572872
H	4.125428	2.022775	1.374119
H	-0.175029	1.770787	1.607872
C	-1.787100	-0.179647	2.036798
H	-1.174648	-0.659549	2.801312
C	-2.993111	0.208894	2.062094
C	-4.257774	0.645955	1.828583
H	-5.037649	-0.107471	1.686176
H	-4.587903	1.585159	2.282960
O	3.878431	-1.599328	-1.883493
Na	2.006085	-1.285180	-3.033121
C	4.731029	-0.761716	-1.381871
C	4.568302	0.645878	-1.526398
C	5.865781	-1.190932	-0.638046
C	5.465525	1.543087	-0.957652
H	3.691963	1.009661	-2.070241
C	6.747784	-0.279936	-0.062416
H	6.023561	-2.266959	-0.519254
C	6.561258	1.098359	-0.209630

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 H    5.296666    2.616652   -1.086971
 H    7.601364   -0.653082    0.511686
 H    7.257897    1.809077    0.240241
96
Figure_S15-1_PA-9d(NaOPh)-ts(1,6minor)_O2 / electronic energy: -3988.21925399 a.u. / lowest freq: -446.90 cm-1
 C   -2.295989   -1.963389   -1.648467
 H   -2.833526   -2.697259   -1.035686
 C   -3.088636   -0.661703   -1.784927
 H   -3.408400   -0.457852   -2.816617
 C   -0.985258   -0.190958   -0.874332
 C   -2.433338    1.729201   -1.334833
 C   -3.760087    2.137412   -1.178384
 C   -1.428978    2.690132   -1.493179
 C   -4.087277    3.498328   -1.154791
 C   -1.733961    4.050410   -1.470640
 C   -3.067138    4.441874   -1.296017
 H   -3.313884    5.507141   -1.273605
Cu    0.708394    0.690252   -0.311865
 N   -1.066690   -1.511736   -0.990936
 N   -2.120371    0.352504   -1.347267
 C    2.062982    1.429229    1.151577
 C    0.793124    1.107244    1.763631
 H   -2.057757   -2.841079    1.131538
 H   -3.974511   -0.666276   -1.135187
 H   -2.071591   -2.421493   -2.623612
 H    2.152576    2.478165    0.854589
 C   -0.204488    2.186885    1.911343
 C    0.507502   -0.141443    2.485932
 O    0.279190    3.397720    1.614961
 O   -1.368791    2.053712    2.252617
 O   -0.493579   -0.381390    3.140640
 O    1.470064   -1.064881    2.372254
 C    1.249707   -2.312048    3.028503
 H    1.141471   -2.164287    4.111463
 H    2.140329   -2.915557    2.820025
 H    0.348037   -2.801413    2.630885
 C   -0.612741    4.494349    1.752930
 H   -1.528981    4.329967    1.170474
 H   -0.075897    5.371210    1.376189
 H   -0.878174    4.642660    2.809259
 C   -0.021891   -2.392032   -0.476584
 H    0.387219   -1.883397    0.405801
 C    1.136385   -2.583583   -1.437215
 C    2.437805   -2.555321   -0.923448
 C    0.960415   -2.775702   -2.809901
 C    3.541183   -2.710897   -1.758730
 H    2.584429   -2.379814    0.145637
 C    2.063154   -2.928143   -3.650740
 H   -0.042833   -2.792683   -3.239705
 C    3.356031   -2.894868   -3.128781
 H    4.549917   -2.671532   -1.340735
 H    1.909623   -3.070751   -4.722628
 H    4.217889   -3.006554   -3.790142
 C   -0.603164   -3.711094    0.046373
 H    0.251891   -4.363385    0.286223
 H   -1.154783   -4.218471   -0.772328
 O   -1.365974   -3.562671    1.198621
 C    3.247063    0.680637    1.060556
 H    3.254385   -0.345417    1.419488
 C    4.382181    1.201418    0.438440
 H    4.410469    2.286749    0.309040
 C    5.714490    0.565934    0.577678
 C    6.869211    1.353552    0.467809
 C    5.869862   -0.811361    0.802845
 C    8.138376    0.789206    0.588485
 H    6.768046    2.427244    0.287694
 C    7.136257   -1.376860    0.920844
 H    4.989969   -1.453917    0.878266
 C    8.277982   -0.579210    0.815370
 H    9.023451    1.423912    0.504668
 H    7.234501   -2.450759    1.094874
 H    9.270499   -1.024967    0.909185
 C   -0.641724    5.068419   -1.668053
 H    0.309273    4.715125   -1.244027
 H   -0.475255    5.256054   -2.740818
 H   -0.896902    6.029285   -1.199699
 C   -5.523948    3.919147   -0.985251
 H   -5.612580    5.004014   -0.837917
 H   -6.116432    3.649091   -1.873524
 H   -5.985903    3.416670   -0.122271
 H   -4.553305    1.397393   -1.056197
 H   -0.396823    2.376613   -1.657016
 C    1.670094    0.883596   -2.092649
 H    0.980169    0.783998   -2.931563
 C    2.933222    0.971377   -2.063616
 C    4.253847    0.988031   -1.746858
 H    4.796573    0.041912   -1.832693
 H    4.841189    1.890093   -1.940842
 O   -3.220105   -1.694601    1.258129
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Na   -2.572561    0.112068    2.349233
 C   -4.435020   -2.057428    0.973282
 C   -5.499291   -1.115289    0.898068
 C   -4.770151   -3.410044    0.684857
 C   -6.793513   -1.499782    0.557500
 H   -5.277896   -0.063901    1.110982
 C   -6.068049   -3.779696    0.344724
 H   -3.973916   -4.157016    0.749503
 C   -7.096015   -2.834368    0.273642
 H   -7.580861   -0.741547    0.510987
 H   -6.282860   -4.831535    0.133046
 H   -8.112389   -3.131962    0.007207
96
Figure_S15-1_PA-9d(NaOPh)-ts(1,6minor)_03 / electronic energy: -3988.21926870 a.u. / lowest freq: -449.72 cm-1
 C    2.298140   -1.963367    1.647079
 H    2.835681   -2.697003    1.034036
 C    3.090092   -0.661164    1.782858
 H    3.409303   -0.456559    2.814578
 C    0.985889   -0.191927    0.873198
 C    2.432082    1.729481    1.334852
 C    3.760261    2.139148    1.180232
 C    1.427541    2.688848    1.489719
 C    4.086030    3.498953    1.156582
 C    1.731565    4.050627    1.465240
 C    3.063260    4.442648    1.292886
 H    3.309222    5.508147    1.267216
Cu   -0.708295    0.688615    0.311530
 N    1.068113   -1.512587    0.990343
 N    2.121431    0.352346    1.344214
 C   -2.063981    1.428392   -1.151909
 C   -0.794205    1.106224   -1.764336
 H    2.058776   -2.842464   -1.132259
 H    3.976246   -0.665671    1.133512
 H    2.074695   -2.421495    2.622432
 H   -2.153132    2.477327   -0.854726
 C    0.203094    2.185824   -1.913252
 C   -0.508662   -0.142822   -2.485765
 O   -0.280889    3.397101   -1.618748
 O    1.367481    2.052556   -2.254240
 O    0.492303   -0.383249   -3.140542
 O   -1.471203   -1.066301   -2.371284
 C   -1.250989   -2.313729   -3.027020
 H   -1.143346   -2.166498   -4.110116
 H   -2.141388   -2.917315   -2.817788
 H   -0.349024   -2.802822   -2.629740
 C    0.610910    4.493587   -1.758764
 H    1.525645    4.332025   -1.173123
 H    0.072620    5.371715   -1.387040
 H    0.879212    4.637860   -2.814917
 C    0.023543   -2.393570    0.476646
 H   -0.386054   -1.885461   -0.405812
 C   -1.134291   -2.585091    1.437795
 C   -2.435986   -2.556228    0.924769
 C   -0.957590   -2.777743    2.810320
 C   -3.538931   -2.711782    1.760638
 H   -2.583166   -2.380265   -0.144162
 C   -2.059892   -2.930120    3.651738
 H    0.045917   -2.795243    3.239512
 C   -3.353060   -2.896272    3.130517
 H   -4.547896   -2.672031    1.343226
 H   -1.905809   -3.073146    4.723491
 H   -4.214569   -3.007939    3.792335
 C    0.605144   -3.712624   -0.045955
 H   -0.249756   -4.365378   -0.285092
 H    1.157354   -4.219403    0.772722
 O    1.367333   -3.564430   -1.198640
 C   -3.247577    0.679948   -1.059320
 H   -3.255475   -0.346185   -1.418043
 C   -4.382212    1.201036   -0.435457
 H   -4.410236    2.286572   -0.307436
 C   -5.714992    0.566353   -0.575113
 C   -6.869260    1.354664   -0.465633
 C   -5.871110   -0.810873   -0.800092
 C   -8.138734    0.791041   -0.586509
 H   -6.767511    2.428331   -0.285689
 C   -7.137814   -1.375657   -0.918301
 H   -4.991580   -1.453963   -0.875235
 C   -8.279091   -0.577324   -0.813222
 H   -9.023447    1.426295   -0.503013
 H   -7.236644   -2.449521   -1.092211
 H   -9.271848   -1.022513   -0.907221
 C   -1.668504    0.881852    2.093989
 H   -0.976982    0.781950    2.931434
 C   -2.931284    0.969954    2.064341
 C   -4.252244    0.986891    1.747009
 H   -4.794811    0.040776    1.834135
 H   -4.839375    1.888638    1.943204
 O    3.220475   -1.695321   -1.259818
Na    2.571591    0.111179   -2.350598
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 C    4.435849   -2.056756   -0.975202
 C    5.499110   -1.113418   -0.900386
 C    4.772543   -3.408956   -0.686617
 C    6.793859   -1.496464   -0.560200
 H    5.276522   -0.062287   -1.113279
 C    6.070955   -3.777135   -0.346836
 H    3.977094   -4.156797   -0.750861
 C    7.097912   -2.830684   -0.276245
 H    7.580412   -0.737375   -0.514057
 H    6.286965   -4.828708   -0.135045
 H    8.114705   -3.127122   -0.010120
 C    0.636377    5.066676    1.656462
 H   -0.309936    4.714225    1.221352
 H    0.459006    5.248908    2.728395
 H    0.895076    6.029863    1.194927
 C    5.521242    3.933053    1.010110
 H    6.001001    4.022145    1.998112
 H    6.104854    3.207764    0.425729
 H    5.595863    4.913427    0.519108
 H    0.394916    2.375269    1.650410
 H    4.553224    1.399020    1.058543
96
Figure_S15-1_PA-9d(NaOPh)-ts(1,6minor)_O4 / electronic energy: -3988.21743768 a.u. / lowest freq: -446.62 cm-1
 C   -2.140802   -2.213680   -1.811121
 H   -2.622075   -2.970061   -1.176968
 C   -3.033356   -0.985629   -2.000461
 H   -3.199607   -0.734898   -3.059247
 C   -1.083525   -0.352943   -0.869841
 C   -2.748936    1.407855   -1.308514
 C   -4.094293    1.654506   -1.593376
 C   -1.907705    2.491316   -1.016607
 C   -4.608401    2.956831   -1.567909
 C   -2.395617    3.795699   -1.006099
 C   -3.753057    4.017898   -1.272726
 H   -4.144936    5.039002   -1.257673
Cu    0.505797    0.601513   -0.138009
 N   -0.973116   -1.648496   -1.136799
 N   -2.263216    0.085138   -1.350918
 C    1.852159    1.266393    1.339746
 C    0.727701    0.622569    1.989432
 H   -1.562517   -3.257919    0.945994
 H   -4.007010   -1.120889   -1.511993
 H   -1.866200   -2.686809   -2.764665
 H    1.735479    2.347659    1.221969
 C   -0.426152    1.449002    2.386080
 C    0.794405   -0.722464    2.583004
 O   -0.277986    2.746860    2.084874
 O   -1.452886    1.055104    2.915192
 O    0.073078   -1.156919    3.464195
 O    1.760559   -1.497070    2.072128
 C    1.830980   -2.837800    2.551588
 H    1.954545   -2.856859    3.642318
 H    2.708521   -3.281344    2.067522
 H    0.919114   -3.384945    2.267069
 C   -1.361012    3.603830    2.414807
 H   -2.251753    3.350284    1.821976
 H   -1.027642    4.618649    2.175062
 H   -1.604221    3.529136    3.483308
 C    0.196492   -2.420362   -0.736281
 H    0.553995   -1.964253    0.195451
 C    1.333213   -2.317861   -1.739509
 C    2.644908   -2.212979   -1.263488
 C    1.118793   -2.296866   -3.120246
 C    3.717764   -2.085749   -2.142715
 H    2.819895   -2.199376   -0.185384
 C    2.190064   -2.169636   -4.004191
 H    0.105810   -2.359422   -3.521591
 C    3.492752   -2.060756   -3.518740
 H    4.732898   -1.987453   -1.750796
 H    2.003547   -2.147018   -5.080163
 H    4.329592   -1.951181   -4.211855
 C   -0.166433   -3.865740   -0.378670
 H    0.785543   -4.407710   -0.252240
 H   -0.670479   -4.337928   -1.247902
 O   -0.899470   -3.992837    0.795519
 C    3.135309    0.765031    1.068359
 H    3.334308   -0.289295    1.243020
 C    4.121856    1.564085    0.492033
 H    3.961784    2.644673    0.540471
 C    5.547299    1.155866    0.459906
 C    6.544558    2.138453    0.383564
 C    5.944416   -0.190742    0.485864
 C    7.894399    1.792205    0.341750
 H    6.255429    3.192699    0.357095
 C    7.291669   -0.538513    0.442104
 H    5.191458   -0.979991    0.533969
 C    8.274354    0.450999    0.369763
 H    8.653327    2.575769    0.286351
 H    7.577288   -1.592781    0.463041
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 H    9.330865    0.176731    0.333978
 C   -1.462165    4.951488   -0.755938
 H   -0.500139    4.608920   -0.349848
 H   -1.256721    5.491343   -1.693894
 H   -1.899168    5.676154   -0.052951
 C   -6.067213    3.186205   -1.867546
 H   -6.356835    4.229787   -1.683544
 H   -6.292201    2.953370   -2.920206
 H   -6.705233    2.537514   -1.248329
 H   -4.772040    0.829716   -1.812909
 H   -0.848766    2.328518   -0.817885
 C    1.298910    1.271742   -1.894641
 H    0.547438    1.242268   -2.683908
 C    2.540393    1.516210   -1.928999
 C    3.869256    1.661955   -1.690659
 H    4.522002    0.826858   -1.963050
 H    4.320757    2.655826   -1.758073
 O   -2.566788   -2.100452    1.494938
Na   -2.176578   -1.055364    3.418386
 C   -3.785721   -1.929218    1.080852
 C   -4.415122   -0.653312    1.127964
 C   -4.562034   -2.995942    0.546147
 C   -5.711956   -0.463191    0.660243
 H   -3.834207    0.196820    1.499576
 C   -5.852079   -2.788298    0.068366
 H   -4.106742   -3.990165    0.512011
 C   -6.445750   -1.521695    0.116173
 H   -6.151713    0.537703    0.703744
 H   -6.409431   -3.633120   -0.347444
 H   -7.459345   -1.365437   -0.258936
96
Figure_S15-1_PA-9d(NaOPh)-ts(1,6minor)_O5 / electronic energy: -3988.21946363 a.u. / lowest freq: -425.99 cm-1
 C   -1.096829   -2.912236   -0.846531
 H   -1.534559   -3.584789   -0.097249
 C   -2.171342   -2.164273   -1.636288
 H   -2.040406   -2.288037   -2.721613
 C   -0.859637   -0.615755   -0.460516
 C   -2.819104    0.258138   -1.644006
 C   -3.675425    0.053039   -2.727106
 C   -2.891276    1.461563   -0.927752
 C   -4.600727    1.033630   -3.105476
 C   -3.806722    2.447597   -1.288199
 C   -4.654353    2.224066   -2.382034
 H   -5.382294    2.991088   -2.661221
Cu    0.243309    1.019773   -0.205517
 N   -0.364005   -1.821899   -0.201652
 N   -1.940114   -0.766313   -1.250453
 C    1.712283    2.201493    0.701641
 C    0.636907    1.999655    1.645853
 H   -1.240628   -1.972701    2.296911
 H   -3.191483   -2.470711   -1.362767
 H   -0.419862   -3.494115   -1.489833
 H    1.709891    3.177636    0.210899
 C   -0.396837    3.053631    1.728587
 C    0.673379    1.059709    2.773596
 O    0.009086    4.217994    1.219441
 O   -1.519216    2.923576    2.194518
 O   -0.190558    0.943085    3.628778
 O    1.793218    0.335791    2.830789
 C    1.918758   -0.577570    3.917436
 H    1.949356   -0.036067    4.873219
 H    2.869181   -1.098263    3.755038
 H    1.076383   -1.282365    3.909269
 C   -0.904822    5.304347    1.217580
 H   -1.708906    5.133390    0.490749
 H   -0.325382    6.186928    0.926543
 H   -1.342677    5.449584    2.214027
 C    0.812870   -2.078275    0.609097
 H    1.095888   -1.104602    1.037300
 C    1.976085   -2.564090   -0.254059
 C    2.916104   -3.497868    0.196103
 C    2.144868   -2.020495   -1.535777
 C    3.990684   -3.878208   -0.611208
 H    2.825476   -3.948599    1.184866
 C    3.214233   -2.400315   -2.342389
 H    1.435994   -1.277552   -1.906643
 C    4.143829   -3.333368   -1.883290
 H    4.710465   -4.610022   -0.237775
 H    3.323757   -1.959001   -3.335570
 H    4.985586   -3.629383   -2.512750
 C    0.453413   -2.976746    1.799957
 H    1.379775   -3.195822    2.352026
 H    0.082723   -3.951983    1.420721
 O   -0.421881   -2.386388    2.699841
 C    2.825817    1.386067    0.430407
 H    2.909665    0.411588    0.909133
 C    3.814702    1.790963   -0.468200
 H    3.861259    2.860395   -0.685727
 C    5.107728    1.080781   -0.588441
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 C    6.246719    1.793606   -0.991564
 C    5.240041   -0.290549   -0.318399
 C    7.483756    1.163136   -1.110115
 H    6.158618    2.861240   -1.210610
 C    6.475323   -0.920742   -0.438713
 H    4.367101   -0.881838   -0.032909
 C    7.603413   -0.198469   -0.832653
 H    8.358621    1.738771   -1.420907
 H    6.553259   -1.990322   -0.231278
 H    8.570669   -0.696640   -0.927658
 C   -3.902547    3.728092   -0.501764
 H   -3.443688    4.562977   -1.056059
 H   -4.951878    4.001280   -0.317770
 H   -3.390496    3.639268    0.466176
 C   -5.536993    0.774450   -4.257006
 H   -6.076811    1.685139   -4.550324
 H   -4.993657    0.397915   -5.136369
 H   -6.283824    0.011746   -3.985450
 H   -3.643671   -0.883084   -3.285850
 H   -2.262041    1.607040   -0.048830
 C    0.612428    1.396670   -2.184933
 H   -0.326873    1.334800   -2.737558
 C    1.821096    1.497923   -2.546337
 C    3.176994    1.524784   -2.605313
 H    3.699429    0.588490   -2.825555
 H    3.688633    2.439231   -2.916920
 O   -2.625449   -1.160220    2.015709
Na   -2.361972    0.830469    2.905204
 C   -3.575124   -1.831311    1.437574
 C   -4.635207   -1.190926    0.738681
 C   -3.603143   -3.254195    1.454394
 C   -5.613524   -1.919779    0.070573
 H   -4.645911   -0.098033    0.701680
 C   -4.586422   -3.972391    0.780289
 H   -2.814579   -3.772121    2.008696
 C   -5.599866   -3.318716    0.071925
 H   -6.398542   -1.384052   -0.471876
 H   -4.562320   -5.066099    0.809290
 H   -6.367457   -3.886485   -0.458326
96
Figure_S15-1_PA-9d(NaOPh)-ts(1,6minor)_06 / electronic energy: -3988.21636174 a.u. / lowest freq: -441.94 cm-1
 C   -1.200470   -2.842007   -0.565079
 H   -1.703377   -3.344902    0.273895
 C   -2.196096   -2.124749   -1.476300
 H   -1.983459   -2.304867   -2.541941
 C   -0.858092   -0.537621   -0.398222
 C   -2.793529    0.313561   -1.634209
 C   -2.793878    1.583951   -1.042819
 C   -3.671209    0.047661   -2.687499
 C   -3.657825    2.578898   -1.498025
 C   -4.550822    1.031097   -3.152471
 C   -4.532899    2.290860   -2.552537
 H   -5.224096    3.062838   -2.902107
Cu    0.346694    1.036362   -0.232428
 N   -0.379823   -1.734436   -0.077179
 N   -1.960217   -0.711151   -1.151185
 C    1.912179    2.157692    0.600373
 C    0.899316    1.967173    1.612557
 H   -1.468459   -1.894648    2.368724
 H   -3.238389   -2.402073   -1.267910
 H   -0.581007   -3.576466   -1.098817
 H    1.892791    3.123845    0.088700
 C   -0.144174    3.009102    1.741973
 C    1.121239    1.030358    2.724588
 O    0.258061    4.205310    1.319292
 O   -1.281782    2.829922    2.153200
 O    2.060661    0.266873    2.823369
 O    0.187902    1.110063    3.695859
 C    0.407083    0.311908    4.857538
 H    0.294205   -0.749669    4.603862
 H   -0.363035    0.616518    5.575138
 H    1.405310    0.500754    5.273883
 C   -0.693083    5.260890    1.315995
 H   -1.494613    5.056111    0.594991
 H   -0.145341    6.161184    1.018921
 H   -1.130792    5.395109    2.314113
 C    0.791263   -1.942768    0.751478
 H    1.143930   -0.937912    1.021830
 C    1.914510   -2.611823   -0.028181
 C    2.808737   -3.509940    0.563413
 C    2.109151   -2.266119   -1.373434
 C    3.867285   -4.050297   -0.170340
 H    2.694155   -3.799134    1.608892
 C    3.161407   -2.807530   -2.106719
 H    1.434908   -1.550133   -1.849364
 C    4.046382   -3.704651   -1.507452
 H    4.554270   -4.748986    0.312160
 H    3.295141   -2.522064   -3.152492
 H    4.875510   -4.126512   -2.079197
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 C    0.397390   -2.604323    2.078503
 H    1.296685   -2.651843    2.710175
 H    0.069716   -3.647984    1.900987
 O   -0.555253   -1.862564    2.769369
 C    2.998244    1.313154    0.310226
 H    3.083753    0.367280    0.844161
 C    3.947742    1.642881   -0.659080
 H    4.006421    2.696765   -0.942226
 C    5.219447    0.894763   -0.790439
 C    6.358192    1.552904   -1.276739
 C    5.325654   -0.464735   -0.455516
 C    7.571603    0.881086   -1.413856
 H    6.289635    2.610152   -1.547293
 C    6.536553   -1.136409   -0.595365
 H    4.449696   -1.014029   -0.103057
 C    7.665820   -0.467904   -1.072626
 H    8.447594    1.413966   -1.790500
 H    6.593823   -2.196198   -0.336610
 H    8.614546   -0.997759   -1.182187
 C    0.662726    1.286349   -2.236730
 H   -0.291813    1.239943   -2.763959
 C    1.865436    1.292490   -2.630697
 C    3.219242    1.239586   -2.724933
 H    3.766312    2.095428   -3.129141
 H    3.681864    0.261109   -2.890091
Na   -1.937746    0.600438    2.528212
 O   -2.934374   -1.284922    2.015422
 C   -3.917617   -1.829630    1.365769
 C   -4.117553   -3.237638    1.345617
 C   -4.839291   -1.053336    0.611975
 C   -5.128022   -3.820145    0.585227
 H   -3.442811   -3.860619    1.940949
 C   -5.844827   -1.646414   -0.143997
 H   -4.715211    0.033046    0.603696
 C   -5.999283   -3.036215   -0.177401
 H   -5.238658   -4.908797    0.587503
 H   -6.514861   -1.009950   -0.729928
 H   -6.787675   -3.497574   -0.775943
 H   -3.695418   -0.939705   -3.149883
 H   -2.138597    1.795958   -0.196782
 C   -5.515391    0.707501   -4.263376
 H   -6.274975   -0.012349   -3.919700
 H   -6.037527    1.606111   -4.618973
 H   -4.998255    0.249065   -5.119509
 C   -3.645025    3.941670   -0.857344
 H   -2.897470    4.591594   -1.340903
 H   -4.620616    4.438634   -0.950225
 H   -3.389252    3.873416    0.209615
96
Figure_S15-1_PA-9d(NaOPh)-ts(1,6minor)_07 / electronic energy: -3988.21954606 a.u. / lowest freq: -424.42 cm-1
 C   -1.019663   -2.889396   -0.963671
 H   -1.437576   -3.606749   -0.245238
 C   -2.117156   -2.140358   -1.724803
 H   -1.995357   -2.236454   -2.813632
 C   -0.839916   -0.602955   -0.498503
 C   -2.811326    0.275380   -1.640159
 C   -3.011044    1.358568   -0.772141
 C   -3.559952    0.181675   -2.812588
 C   -3.962788    2.332152   -1.065363
 C   -4.506814    1.163252   -3.135296
 C   -4.698195    2.226961   -2.255217
 H   -5.450557    2.986552   -2.486617
Cu    0.233067    1.039129   -0.197854
 N   -0.319707   -1.805413   -0.271771
 N   -1.907324   -0.749289   -1.302200
 C    1.671770    2.221811    0.741026
 C    0.585915    1.995019    1.670707
 H   -1.216623   -1.917645    2.225082
 H   -3.128654   -2.471570   -1.447657
 H   -0.324807   -3.421503   -1.630687
 H    1.661451    3.200706    0.256771
 C   -0.491831    3.002939    1.708169
 C    0.630846    1.053880    2.798222
 O   -0.152810    4.145606    1.106044
 O   -1.600213    2.854930    2.203434
 O   -0.239095    0.911470    3.643064
 O    1.769211    0.360553    2.867521
 C    1.908274   -0.548396    3.955321
 H    1.920293   -0.005601    4.910922
 H    2.870984   -1.048325    3.800095
 H    1.082039   -1.271154    3.941696
 C   -1.133871    5.164283    0.991305
 H   -1.887219    4.888743    0.241787
 H   -0.601172    6.063677    0.664627
 H   -1.628646    5.344676    1.954624
 C    0.849414   -2.051625    0.552896
 H    1.123132   -1.072246    0.974744
 C    2.024277   -2.534839   -0.292877
 C    2.953985   -3.475569    0.162843
```

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 C    2.215501   -1.975123   -1.564556
 C    4.043183   -3.846177   -0.629560
 H    2.843987   -3.938061    1.144340
 C    3.298506   -2.346083   -2.356511
 H    1.512258   -1.226676   -1.936210
 C    4.219432   -3.285174   -1.891565
 H    4.756021   -4.582990   -0.252648
 H    3.426477   -1.893256   -3.342282
 H    5.072582   -3.573826   -2.509048
 C    0.477801   -2.929401    1.754131
 H    1.398356   -3.152179    2.314538
 H    0.092152   -3.904617    1.390171
 O   -0.392240   -2.307725    2.638647
 C    2.800813    1.424611    0.479451
 H    2.891034    0.447007    0.950633
 C    3.796375    1.848821   -0.402796
 H    3.835211    2.920832   -0.608626
 C    5.096672    1.151186   -0.518562
 C    6.232828    1.877941   -0.904810
 C    5.239037   -0.221944   -0.262560
 C    7.476081    1.259293   -1.020619
 H    6.137323    2.947062   -1.113234
 C    6.480653   -0.840217   -0.379699
 H    4.369265   -0.824543    0.008790
 C    7.605480   -0.104147   -0.756987
 H    8.348262    1.845744   -1.318572
 H    6.566195   -1.911237   -0.183065
 H    8.577604   -0.593145   -0.850009
 C    0.615229    1.451333   -2.165916
 H   -0.319602    1.389204   -2.726014
 C    1.827383    1.565566   -2.510896
 C    3.183744    1.603372   -2.551890
 H    3.692296    2.525682   -2.844708
 H    3.716345    0.674132   -2.777795
Na   -2.413908    0.767180    2.946974
 O   -2.635849   -1.157144    1.921567
 C   -3.534677   -1.906330    1.358500
 C   -3.446473   -3.326685    1.384727
 C   -4.652163   -1.360099    0.668986
 C   -4.372138   -4.128592    0.723841
 H   -2.614801   -3.774701    1.936554
 C   -5.573222   -2.172626    0.015627
 H   -4.756030   -0.272769    0.631388
 C   -5.442605   -3.565485    0.022005
 H   -4.256771   -5.216238    0.759491
 H   -6.408183   -1.707783   -0.517502
 H   -6.165190   -4.197928   -0.498140
 H   -3.416799   -0.660983   -3.491263
 H   -2.458293    1.400748    0.166879
 C   -5.291163    1.054427   -4.416943
 H   -6.068065    1.828255   -4.480789
 H   -4.630251    1.165301   -5.290862
 H   -5.777723    0.070979   -4.501511
 C   -4.256307    3.443312   -0.091685
 H   -4.178746    4.428864   -0.576410
 H   -5.284578    3.355795    0.293168
 H   -3.567759    3.418526    0.763347
96
Figure_S15-1_PA-9d(NaOPh)-ts(1,6minor)_O8 / electronic energy: -3988.21575574 a.u. / lowest freq: -451.85 cm-1
 C   -2.165913   -2.012204   -1.688241
 H   -2.697437   -2.750637   -1.075101
 C   -2.990201   -0.735201   -1.862504
 H   -3.279315   -0.548118   -2.906477
 C   -0.931545   -0.195036   -0.891983
 C   -2.441698    1.672906   -1.378610
 C   -3.798312    2.018365   -1.339919
 C   -1.477009    2.683117   -1.403591
 C   -4.190533    3.359428   -1.307511
 C   -1.847338    4.028915   -1.351432
 C   -3.206528    4.353832   -1.307216
 H   -3.505474    5.405169   -1.268853
Cu    0.731462    0.726643   -0.310520
 N   -0.965519   -1.517601   -1.010283
 N   -2.070264    0.311535   -1.398396
 C    2.069556    1.518022    1.135574
 C    0.812230    1.174446    1.759843
 H   -1.960772   -2.847132    1.104221
 H   -3.897407   -0.761891   -1.243891
 H   -1.908473   -2.479657   -2.650431
 H    2.118370    2.569305    0.831166
 C   -0.155372    2.294384    1.830019
 C    0.585730   -0.042993    2.540843
 O   -1.422913    1.943784    2.133170
 O    0.121646    3.448327    1.579640
 O   -0.343553   -0.245898    3.308698
 O    1.518608   -0.984895    2.357922
 C    1.346455   -2.217859    3.052868
 H    1.271634   -2.047864    4.135051
 H    2.240063   -2.810594    2.826907
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 H    0.443677   -2.733844    2.692192
 C   -2.376508    3.002060    2.152009
 H   -2.080842    3.779916    2.868270
 H   -3.327978    2.553131    2.459977
 H   -2.482288    3.445469    1.153438
 C    0.096780   -2.361006   -0.470491
 H    0.481414   -1.825156    0.407048
 C    1.270167   -2.535149   -1.416498
 C    2.565353   -2.457759   -0.891965
 C    1.113701   -2.751858   -2.787988
 C    3.680739   -2.587991   -1.715714
 H    2.696926   -2.262856    0.175692
 C    2.228269   -2.878295   -3.617329
 H    0.116002   -2.808233   -3.226918
 C    3.514440   -2.795106   -3.084803
 H    4.683863   -2.509014   -1.289941
 H    2.088822   -3.038825   -4.688600
 H    4.385744   -2.885604   -3.736964
 C   -0.454840   -3.685655    0.070022
 H    0.414085   -4.308512    0.336618
 H   -0.980013   -4.224765   -0.745623
 O   -1.240416   -3.534569    1.207479
 C    3.271643    0.800463    1.045902
 H    3.305432   -0.222518    1.412981
 C    4.390708    1.341478    0.410717
 H    4.393570    2.426370    0.274952
 C    5.737576    0.736369    0.548616
 C    6.875218    1.545936    0.421976
 C    5.923144   -0.634615    0.788138
 C    8.156467    1.008563    0.539262
 H    6.750997    2.615378    0.231481
 C    7.201454   -1.173436    0.902508
 H    5.057310   -1.294192    0.877769
 C    8.325868   -0.354149    0.779531
 H    9.027508    1.660579    0.442175
 H    7.322504   -2.243233    1.087190
 H    9.327948   -0.778668    0.870401
 C   -0.781336    5.089192   -1.299481
 H   -0.015510    4.922515   -2.071643
 H   -1.201741    6.094728   -1.437217
 H   -0.276478    5.049069   -0.321889
 C   -5.653097    3.720896   -1.291305
 H   -5.822343    4.683923   -0.789555
 H   -6.042395    3.811908   -2.318206
 H   -6.251817    2.953345   -0.780473
 H   -4.563931    1.241443   -1.322067
 H   -0.418037    2.428494   -1.472758
 C    1.670647    0.957432   -2.101070
 H    0.969858    0.856474   -2.930447
 C    2.931706    1.065994   -2.078300
 C    4.253887    1.109106   -1.766579
 H    4.815108    0.174120   -1.857258
 H    4.820950    2.022523   -1.967539
 O   -3.136027   -1.716962    1.204518
Na   -2.481458   -0.200666    2.643950
 C   -4.354798   -2.049394    0.897361
 C   -5.394466   -1.081748    0.809089
 C   -4.714594   -3.392355    0.598078
 C   -6.691658   -1.436102    0.447130
 H   -5.149389   -0.035694    1.022825
 C   -6.014803   -3.731623    0.235665
 H   -3.935884   -4.156986    0.671612
 C   -7.019502   -2.762605    0.153335
 H   -7.461191   -0.660479    0.390024
 H   -6.249854   -4.777325    0.015532
 H   -8.037993   -3.035799   -0.130451
32
Figure_S15-2_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C   -0.660544   -0.726572    0.059153
 C   -1.860539   -0.097447    0.115996
 H   -0.691600   -1.818492   -0.004770
 C   -1.976243    1.390665    0.160143
 C   -3.120576   -0.891785    0.187355
 O   -3.041424    1.823605   -0.507466
 O   -1.182749    2.134043    0.689285
 O   -4.147702   -0.497504    0.683440
 O   -2.981802   -2.118850   -0.320932
 C   -4.097604   -2.989729   -0.195724
 H   -4.332384   -3.170881    0.862818
 H   -3.810049   -3.927003   -0.683244
 H   -4.981752   -2.562067   -0.688186
 C   -3.254671    3.228152   -0.535442
 H   -3.354009    3.627502    0.483524
 H   -4.184056    3.384216   -1.092621
 H   -2.420438    3.737793   -1.038016
 C    0.656646   -0.129211    0.062308
 H    0.725624    0.955889    0.150505
 C    1.759981   -0.902956   -0.019704
 H    1.621029   -1.988149   -0.089650
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 C    3.156351   -0.453635   -0.025165
 C    4.175093   -1.416830   -0.109525
 C    3.522207    0.902114    0.053056
 C    5.517020   -1.042840   -0.114390
 H    3.907556   -2.474776   -0.172060
 C    4.861836    1.275255    0.048166
 H    2.754752    1.675486    0.118691
 C    5.863995    0.305241   -0.035401
 H    6.294080   -1.807149   -0.179427
 H    5.127957    2.332459    0.111300
 H    6.914980    0.602284   -0.038425
64
Figure_S15-2_9b(NaOPh)-Cu-allenyl / electronic energy: -3146.25183127 a.u. / lowest freq: 14.48 cm-1
Cu   -1.159994   -0.590393    1.249005
 C   -1.116318   -1.661983    2.858319
 C   -1.308620    0.472985   -0.363800
 N   -2.371853    0.399588   -1.177453
 N   -0.493582    1.418385   -0.819509
 C    0.814281    1.723428   -0.265472
 C   -0.596166   -2.849269    2.995372
 C   -0.025278   -4.043820    3.070053
 C   -0.945998    2.002813   -2.084278
 H   -0.272077    1.686950   -2.894296
 C   -2.351352    1.408165   -2.240987
 H   -3.149298    2.149610   -2.075173
 C   -3.440408   -0.525568   -0.997211
 C   -3.475273   -1.678430   -1.799498
 C   -4.415212   -0.266257   -0.018691
 C   -4.525858   -2.580829   -1.607528
 C   -5.446875   -1.195447    0.143691
 C   -5.503845   -2.341479   -0.645832
 H   -6.315317   -3.058967   -0.505594
 H    2.120613   -0.435489   -1.301376
 H   -2.511030    0.949494   -3.226320
 H   -0.945517    3.100865   -2.029370
 H    0.971060    0.976016    0.528978
 C    0.814478    3.104087    0.377621
 C    1.750663    4.094003    0.065960
 C   -0.169357    3.389740    1.334883
 C    1.702016    5.341374    0.693971
 H    2.532536    3.907255   -0.671765
 C   -0.220119    4.630799    1.961712
 H   -0.905210    2.621803    1.589754
 C    0.718062    5.614499    1.640496
 H    2.440976    6.102966    0.435574
 H   -0.993041    4.832638    2.706634
 H    0.680478    6.590470    2.129154
 C    1.902113    1.482826   -1.323653
 H    2.887379    1.589112   -0.831044
 H    1.848654    2.269951   -2.096199
 O    1.751113    0.246580   -1.937746
 H   -1.654416   -1.288009    3.746046
 H    0.986244   -4.167031    3.474573
 H   -0.566270   -4.953493    2.789462
 O    2.821164   -1.346953   -0.192222
 C    4.108122   -1.475818   -0.364930
 C    4.777182   -0.916478   -1.488893
 C    4.920292   -2.188977    0.557579
 C    6.149052   -1.066440   -1.667172
 H    4.175796   -0.369004   -2.219089
 C    6.291874   -2.333409    0.366447
 H    4.444043   -2.630613    1.438885
 C    6.926653   -1.775348   -0.746475
 H    6.622021   -0.621629   -2.548077
 H    6.877295   -2.893512    1.101940
 H    8.002320   -1.892512   -0.894117
Na    1.484647   -2.445468    1.154493
 H   -6.214114   -1.015553    0.900660
 H   -4.568838   -3.488419   -2.214687
 C   -4.327742    0.958995    0.851507
 H   -5.265653    1.121622    1.398270
 H   -3.517629    0.850456    1.591941
 H   -4.103510    1.862442    0.265913
 C   -2.409874   -1.938363   -2.830953
 H   -2.615164   -1.387375   -3.763086
 H   -1.418478   -1.620506   -2.477586
 H   -2.364271   -3.005637   -3.085514
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6major)_01 / electronic energy: -3988.21834759 a.u. / lowest freq: -441.84 cm-1
 C    2.922414    0.429802   -1.695778
 H    3.860551    0.219443   -1.172217
 C    2.236525   -0.867157   -2.138580
 H    2.104802   -0.937626   -3.228128
 C    0.803687    0.313433   -0.707976
 C   -0.086863   -1.763320   -1.622590
 C    0.049225   -2.992460   -0.954587
 C   -1.184815   -1.485804   -2.456696
 C   -0.982581   -3.928515   -1.084987
 C   -2.190373   -2.451526   -2.562200
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 C   -2.098720   -3.657111   -1.870965
 H   -2.895943   -4.398509   -1.959475
Cu   -0.823872    0.859921    0.284910
 N    1.936156    1.015424   -0.780295
 N    0.930242   -0.774923   -1.474145
 C   -2.204880    0.628600    1.847805
 C   -0.921242    0.176567    2.329538
 H    4.077180    0.564705    0.992854
 H    2.790138   -1.753458   -1.795804
 H    3.132125    1.111568   -2.533749
 H   -2.507817    1.623409    2.184343
 C   -0.546841   -1.239987    2.458831
 C   -0.031665    1.156508    2.958134
 O   -1.590857   -2.066677    2.386390
 O    0.580755   -1.669343    2.644655
 O    1.032929    0.932331    3.514633
 O   -0.483842    2.417118    2.845236
 C    0.324283    3.441986    3.400822
 H    0.421573    3.320535    4.488542
 H   -0.180740    4.385652    3.169340
 H    1.329525    3.432000    2.955675
 C   -1.345345   -3.453132    2.553836
 H   -0.637956   -3.820614    1.800685
 H   -2.314315   -3.948155    2.429703
 H   -0.941082   -3.657638    3.555114
 C    2.126148    2.287406   -0.107837
 H    1.467591    2.261116    0.775679
 C    1.708036    3.483835   -0.951465
 C    1.606399    4.742155   -0.343838
 C    1.369123    3.369512   -2.302922
 C    1.188186    5.855869   -1.068067
 H    1.835467    4.854126    0.719168
 C    0.953179    4.484373   -3.032581
 H    1.395613    2.396899   -2.795903
 C    0.863325    5.731873   -2.419552
 H    1.106210    6.824933   -0.571308
 H    0.690386    4.369611   -4.086295
 H    0.532116    6.603217   -2.988264
 C    3.561746    2.419386    0.431664
 H    3.650166    3.413057    0.896434
 H    4.272621    2.414195   -0.417198
 O    3.875870    1.462009    1.388460
 C   -3.155308   -0.100368    1.114443
 H   -2.888659   -1.086867    0.731842
 C   -4.415233    0.429156    0.820228
 H   -4.778472    1.214346    1.486097
 C   -5.472465   -0.394296    0.191487
 C   -6.822089   -0.124418    0.457978
 C   -5.162555   -1.443195   -0.688304
 C   -7.832602   -0.887518   -0.125885
 H   -7.082654    0.692768    1.136063
 C   -6.170352   -2.204162   -1.272758
 H   -4.120020   -1.657003   -0.931701
 C   -7.511333   -1.931460   -0.993155
 H   -8.878393   -0.665085    0.097958
 H   -5.905855   -3.013860   -1.957192
 H   -8.302268   -2.527931   -1.452967
 C   -1.737108    2.375541   -0.741870
 H   -0.974778    3.010437   -1.195899
 C   -2.998603    2.344286   -0.821026
 C   -4.314415    2.014075   -0.751116
 H   -5.004423    2.673653   -0.218062
 H   -4.747561    1.453889   -1.585663
 O    4.000986   -1.037809    0.898803
Na    2.528816   -0.462660    2.461997
 C    4.800380   -1.840980    0.264080
 C    5.836089   -1.361067   -0.584407
 C    4.679956   -3.253978    0.369114
 C    6.660905   -2.230265   -1.294378
 H    5.986997   -0.279601   -0.659401
 C    5.511410   -4.111757   -0.343643
 H    3.909763   -3.654591    1.033348
 C    6.507407   -3.615023   -1.191084
 H    7.442598   -1.816898   -1.938860
 H    5.380576   -5.192608   -0.234208
 H    7.155322   -4.292610   -1.751099
 C    1.292224   -3.319854   -0.175094
 H    1.100874   -4.089163    0.584691
 H    2.068210   -3.721131   -0.846549
 H    1.721990   -2.439705    0.321344
 C   -1.272830   -0.195750   -3.225584
 H   -1.548916    0.639870   -2.565194
 H   -0.308796    0.061131   -3.688869
 H   -2.030718   -0.266451   -4.017047
 H   -3.052668   -2.254308   -3.203920
 H   -0.901157   -4.887259   -0.566807
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6major)_O2 / electronic energy: -3988.21729738 a.u. / lowest freq: -451.32 cm-1
 C    2.986343    0.318627   -1.694713
```

H	3.967462	0.112327	-1.251196
C	2.269258	-0.970144	-2.107823
H	2.201159	-1.093289	-3.197403
C	0.879621	0.278834	-0.699110
C	-0.139113	-1.700868	-1.665153
C	-0.138001	-2.881040	-0.901783
C	-1.173512	-1.400139	-2.568826
C	-1.251177	-3.723647	-0.995237
C	-2.268961	-2.267152	-2.627963
C	-2.316078	-3.411335	-1.835239
H	-3.180448	-4.077221	-1.889283
Cu	-0.792261	0.850813	0.202659
N	2.062901	0.895522	-0.711346
N	0.938278	-0.774967	-1.522329
C	-2.271925	0.736024	1.687884
C	-1.033963	0.234154	2.238183
H	4.019944	0.173928	1.162225
H	2.753641	-1.862285	-1.682024
H	3.114662	1.008979	-2.542972
H	-2.521148	1.765368	1.957917
C	-0.752349	-1.195887	2.445957
C	-0.115506	1.179196	2.879359
O	-1.843551	-1.960153	2.381430
O	0.338455	-1.684555	2.691367
O	0.926585	0.909437	3.456473
O	-0.509010	2.460406	2.760410
C	0.319250	3.443460	3.362920
H	0.418117	3.266821	4.442699
H	-0.172072	4.405375	3.181665
H	1.322316	3.443339	2.912047
C	-1.688746	-3.347853	2.627360
H	-0.975555	-3.794781	1.924013
H	-2.679790	-3.792707	2.487897
H	-1.336349	-3.523790	3.653337
C	2.340195	2.111678	0.046992
H	1.629781	2.091705	0.885540
C	2.086558	3.385060	-0.738407
C	1.038547	4.228747	-0.354225
C	2.888145	3.763790	-1.823410
C	0.781713	5.413405	-1.042738
H	0.402344	3.942889	0.487208
C	2.631844	4.946531	-2.516423
H	3.729793	3.140300	-2.133507
C	1.577208	5.773788	-2.129581
H	-0.045159	6.054275	-0.729316
H	3.265160	5.226191	-3.361179
H	1.379433	6.701010	-2.671573
C	3.741847	2.096895	0.673908
H	3.866009	3.064131	1.186804
H	4.510188	2.073956	-0.124075
O	3.925002	1.077466	1.597391
C	-3.254391	0.024616	0.980592
H	-3.052354	-1.003008	0.676351
C	-4.459506	0.625937	0.607799
H	-4.754110	1.507205	1.182096
C	-5.590994	-0.160816	0.063880
C	-6.903831	0.294599	0.250257
C	-5.393711	-1.351738	-0.652747
C	-7.989256	-0.421351	-0.252511
H	-7.075418	1.225055	0.798307
C	-6.476995	-2.067104	-1.155126
H	-4.380854	-1.716965	-0.834231
C	-7.780548	-1.606849	-0.956421
H	-9.003864	-0.049400	-0.092989
H	-6.301975	-2.992321	-1.709338
H	-8.629291	-2.168261	-1.352817
C	-1.624544	2.252756	-1.031211
H	-0.828849	2.802010	-1.535135
C	-2.882459	2.256068	-1.164392
C	-4.210162	1.970549	-1.127901
H	-4.910778	2.713122	-0.736310
H	-4.608055	1.315814	-1.909739
O	3.811127	-1.368592	0.973880
Na	2.380849	-0.651584	2.557033
C	4.668019	-2.088176	0.313374
C	5.788522	-1.507441	-0.343455
C	4.532753	-3.498191	0.194937
C	6.676056	-2.275878	-1.092146
H	5.952183	-0.430616	-0.233573
C	5.426072	-4.254914	-0.557275
H	3.703702	-3.980456	0.718331
C	6.503650	-3.656667	-1.218277
H	7.522796	-1.786486	-1.582861
H	5.279736	-5.336949	-0.628568
H	7.198921	-4.255996	-1.809824
C	1.053386	-3.271676	-0.073690
H	0.773259	-3.949268	0.743021
H	1.779373	-3.809838	-0.704007
H	1.582692	-2.411477	0.357498

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 C   -1.095699   -0.193546   -3.463271
 H   -1.270310    0.731139   -2.896036
 H   -0.105194   -0.108209   -3.933914
 H   -1.852610   -0.250354   -4.256829
 H   -3.089777   -2.042730   -3.313478
 H   -1.274967   -4.644465   -0.407224
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6major)_O3 / electronic energy: -3988.21368855 a.u. / lowest freq: -436.08 cm-1
 C    3.075670    0.237310   -1.712348
 H    4.026605   -0.139063   -1.316446
 C    2.211194   -0.896817   -2.272765
 H    2.160467   -0.900573   -3.370075
 C    0.972236    0.334434   -0.721365
 C   -0.324006   -1.214358   -2.052979
 C   -0.744993   -2.358628   -1.356623
 C   -1.101000   -0.631328   -3.069230
 C   -2.001706   -2.890227   -1.661917
 C   -2.349419   -1.196403   -3.346234
 C   -2.800449   -2.310051   -2.643457
 H   -3.784188   -2.730777   -2.863615
Cu   -0.686317    0.857529    0.230930
 N    2.227071    0.783882   -0.647224
 N    0.905087   -0.588352   -1.685659
 C   -2.116164    0.711739    1.749323
 C   -0.860797    0.212181    2.278893
 H    4.128288   -0.087967    1.147173
 H    2.560656   -1.884881   -1.929137
 H    3.284468    1.013955   -2.466663
 H   -2.344480    1.751575    1.995873
 C   -0.685029   -1.237066    2.475791
 C    0.057031    1.178485    2.887938
 O    0.522102   -1.617155    2.956989
 O   -1.532756   -2.074647    2.251894
 O    1.110678    0.947677    3.463406
 O   -0.346142    2.453408    2.727498
 C    0.471500    3.464594    3.297158
 H    0.567275    3.325964    4.382692
 H   -0.028459    4.414560    3.080292
 H    1.476069    3.459941    2.849726
 C    0.659719   -2.996206    3.282242
 H   -0.133464   -3.315000    3.970889
 H    1.637478   -3.100380    3.765833
 H    0.624511   -3.618606    2.378914
 C    2.599570    1.956578    0.140396
 H    1.935902    1.941629    1.016847
 C    2.334152    3.247374   -0.615826
 C    1.174784    3.977763   -0.331073
 C    3.198716    3.722416   -1.610593
 C    0.875092    5.146833   -1.028260
 H    0.486594    3.613875    0.436233
 C    2.901508    4.892378   -2.309905
 H    4.120297    3.185488   -1.846304
 C    1.738518    5.606505   -2.022472
 H   -0.038777    5.697217   -0.794314
 H    3.586566    5.248693   -3.082246
 H    1.507375    6.522668   -2.570149
 C    4.031336    1.860983    0.678200
 H    4.240407    2.808615    1.198972
 H    4.751398    1.804521   -0.160903
 O    4.217184    0.816614    1.576957
 C   -3.148813   -0.027356    1.148240
 H   -2.977501   -1.078507    0.921072
 C   -4.356574    0.573293    0.793262
 H   -4.579117    1.530705    1.271274
 C   -5.549380   -0.215280    0.406431
 C   -6.828739    0.322630    0.606047
 C   -5.445331   -1.489417   -0.173579
 C   -7.971185   -0.390888    0.246068
 H   -6.929051    1.315276    1.053649
 C   -6.585148   -2.201553   -0.535431
 H   -4.460385   -1.922032   -0.358379
 C   -7.854197   -1.656614   -0.327109
 H   -8.958002    0.046543    0.413749
 H   -6.481698   -3.190323   -0.988550
 H   -8.747621   -2.216415   -0.612356
 C   -1.614745    2.128636   -1.065154
 H   -0.863226    2.689745   -1.620370
 C   -2.868771    2.027191   -1.200000
 C   -4.176090    1.670356   -1.133655
 H   -4.923643    2.404870   -0.822598
 H   -4.528775    0.896046   -1.822840
 O    3.632282   -1.601365    1.089559
Na    2.657990   -0.582953    2.822644
 C    4.145403   -2.489011    0.293979
 C    5.310845   -2.222969   -0.477422
 C    3.568762   -3.778317    0.134133
 C    5.824835   -3.158507   -1.371382
 H    5.807380   -1.256188   -0.346008
 C    4.092098   -4.705359   -0.762030
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 H     2.689520   -4.023671    0.735008
 C     5.219923   -4.407667   -1.534005
 H     6.719667   -2.908265   -1.949433
 H     3.609481   -5.682424   -0.861028
 H     5.623432   -5.137731   -2.238844
 C     0.146507   -3.027036   -0.349983
 H    -0.447495   -3.614941    0.360490
 H     0.849815   -3.705516   -0.858451
 H     0.756872   -2.307495    0.213358
 C    -0.603807    0.545931   -3.863335
 H     0.062659    1.187823   -3.273800
 H    -0.037687    0.202046   -4.744568
 H    -1.442001    1.157572   -4.222659
 H    -2.978166   -0.748093   -4.119362
 H    -2.354357   -3.770588   -1.119048
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6major)_04 / electronic energy: -3988.21708629 a.u. / lowest freq: -456.14 cm-1
 C     2.911653    0.439055   -1.696940
 H     3.885451    0.158815   -1.271244
 C     2.153742   -0.773867   -2.248380
 H     2.035833   -0.741151   -3.340875
 C     0.828070    0.317727   -0.657719
 C    -0.286621   -1.438892   -1.916442
 C    -0.354408   -2.775365   -1.486949
 C    -1.311195   -0.855246   -2.686333
 C    -1.511743   -3.503418   -1.784752
 C    -2.455763   -1.614435   -2.947400
 C    -2.563246   -2.924496   -2.488242
 H    -3.464070   -3.504668   -2.700646
Cu    -0.774598    0.746500    0.417106
 N     2.003745    0.946274   -0.660549
 N     0.851638   -0.645615   -1.586420
 C    -2.248228    0.360097    1.834807
 C    -1.109356   -0.465247    2.176370
 H     3.420152   -0.250343    1.342198
 H     2.638149   -1.722575   -1.972364
 H     3.069862    1.206751   -2.469058
 H    -2.352814    1.283299    2.412406
 C    -1.081468   -1.926749    2.014812
 C    -0.060806    0.112092    3.025590
 O    -2.261593   -2.451246    1.680176
 O    -0.111158   -2.647297    2.191124
 O     0.807859   -0.493520    3.630991
 O    -0.113202    1.455706    3.070705
 C     0.916719    2.108536    3.803512
 H     0.814005    1.909276    4.879661
 H     0.790194    3.179339    3.609283
 H     1.900707    1.760635    3.460045
 C    -2.350177   -3.862813    1.590770
 H    -1.583682   -4.265646    0.917729
 H    -3.348170   -4.078435    1.194162
 H    -2.231395   -4.321845    2.582868
 C     2.340542    2.033779    0.252242
 H     1.490893    2.086719    0.947571
 C     2.477193    3.385608   -0.424786
 C     3.504018    3.660040   -1.338651
 C     1.595608    4.419120   -0.085689
 C     3.617513    4.919504   -1.926279
 H     4.237125    2.892327   -1.594219
 C     1.708193    5.680789   -0.668948
 H     0.810062    4.233946    0.651778
 C     2.716119    5.932094   -1.598805
 H     4.419959    5.111491   -2.641875
 H     1.005134    6.469418   -0.392444
 H     2.806060    6.917576   -2.060744
 C     3.580033    1.707614    1.099165
 H     3.764404    2.581689    1.745617
 H     4.466950    1.622495    0.438109
 O     3.415334    0.587191    1.896937
 C    -3.318465    0.032623    0.986463
 H    -3.247009   -0.865017    0.371166
 C    -4.441599    0.855207    0.866263
 H    -4.640634    1.528532    1.702928
 C    -5.649516    0.405282    0.134863
 C    -6.912182    0.874478    0.523212
 C    -5.572880   -0.476510   -0.955452
 C    -8.066021    0.464418   -0.143529
 H    -6.989646    1.569411    1.363818
 C    -6.724457   -0.886297   -1.621474
 H    -4.599946   -0.837132   -1.297360
 C    -7.977694   -0.420121   -1.217755
 H    -9.039931    0.839043    0.179889
 H    -6.643235   -1.574612   -2.466153
 H    -8.880213   -0.742692   -1.741363
 C    -1.418753    2.525700   -0.359989
 H    -0.564222    3.061826   -0.772346
 C    -2.663823    2.746159   -0.394733
 C    -4.018144    2.646333   -0.344313
 H    -4.532507    2.328679   -1.256498
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 H   -4.584231    3.325705    0.299112
Na    2.080077   -2.048281    2.497610
 O    3.374344   -1.710946    0.728569
 C    4.458389   -2.073226    0.103991
 C    5.642126   -1.284474    0.136821
 C    4.518745   -3.266827   -0.664462
 C    6.784347   -1.654162   -0.567875
 H    5.637390   -0.376757    0.746692
 C    5.668446   -3.625476   -1.363142
 H    3.633426   -3.906239   -0.694345
 C    6.813788   -2.824778   -1.330775
 H    7.671839   -1.016130   -0.516563
 H    5.670708   -4.552392   -1.944710
 H    7.712231   -3.110498   -1.881951
 H   -3.264864   -1.173356   -3.534991
 H   -1.584467   -4.544144   -1.459689
 C    0.798724   -3.431127   -0.780327
 H    1.430315   -2.712250   -0.240155
 H    0.449158   -4.189645   -0.067553
 H    1.440707   -3.942941   -1.516334
 C   -1.184832    0.540082   -3.234897
 H   -1.838161    0.671642   -4.107905
 H   -1.473448    1.287115   -2.481023
 H   -0.151485    0.764726   -3.534712
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6major)_05 / electronic energy: -3988.21870349 a.u. / lowest freq: -445.32 cm-1
 C    2.857606    0.592709   -1.657269
 H    3.810642    0.227948   -1.249852
 C    2.064957   -0.524779   -2.346424
 H    1.892918   -0.335298   -3.416182
 C    0.784756    0.368607   -0.598812
 C   -0.345287   -1.262930   -2.014535
 C   -0.361046   -2.652570   -1.809214
 C   -1.413768   -0.595041   -2.645824
 C   -1.498583   -3.364267   -2.208437
 C   -2.533867   -1.343847   -3.016737
 C   -2.582419   -2.717703   -2.791748
 H   -3.464648   -3.288522   -3.089900
Cu   -0.747078    0.692040    0.612170
 N    1.952753    1.007847   -0.581720
 N    0.792390   -0.503400   -1.614060
 C   -2.204273    0.099012    1.965043
 C   -1.076638   -0.785336    2.165243
 H    3.255348   -0.321148    1.301105
 H    2.560233   -1.500330   -2.234882
 H    3.067495    1.442674   -2.325207
 H   -2.306164    0.907980    2.693884
 C   -1.072316   -2.201629    1.774568
 C   -0.019614   -0.358663    3.091418
 O   -2.259583   -2.646820    1.356992
 O   -0.116735   -2.959966    1.840400
 O    0.851992   -1.058060    3.581573
 O   -0.075233    0.955512    3.363114
 C    0.962058    1.482974    4.181405
 H    0.924289    1.044478    5.188580
 H    0.780124    2.561863    4.236965
 H    1.938451    1.272627    3.723783
 C   -2.375699   -4.030685    1.074989
 H   -1.604075   -4.357752    0.367946
 H   -3.369456   -4.168720    0.635276
 H   -2.287813   -4.619853    1.999401
 C    2.296746    2.061691    0.353150
 H    1.431902    2.137522    1.032506
 C    2.463739    3.397518   -0.364716
 C    3.386496    4.361527    0.057091
 C    1.649261    3.698679   -1.465926
 C    3.484594    5.591583   -0.594641
 H    4.045004    4.167040    0.904317
 C    1.743904    4.926394   -2.117203
 H    0.930281    2.956712   -1.821908
 C    2.663819    5.880621   -1.682432
 H    4.213068    6.327466   -0.247298
 H    1.095271    5.136965   -2.970327
 H    2.742631    6.843355   -2.191747
 C    3.486279    1.646551    1.230795
 H    3.656964    2.438304    1.976299
 H    4.404319    1.590596    0.610661
 O    3.240386    0.467052    1.918904
 C   -3.261428   -0.064078    1.053689
 H   -3.183884   -0.840518    0.291453
 C   -4.379843    0.773108    1.064718
 H   -4.583088    1.292472    2.003702
 C   -5.580660    0.471567    0.251432
 C   -6.844980    0.877588    0.700514
 C   -5.494885   -0.206330   -0.975020
 C   -7.991820    0.602596   -0.043331
 H   -6.930404    1.411309    1.650922
 C   -6.638880   -0.479579   -1.719117
 H   -4.519913   -0.514577   -1.358570
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 C   -7.894132   -0.078058   -1.256411
 H   -8.967732    0.922730    0.328835
 H   -6.549318   -1.007035   -2.671800
 H   -8.791564   -0.293262   -1.840485
 C   -1.342665    2.632887    0.290566
 H   -0.472588    3.261794    0.098343
 C   -2.584966    2.862434    0.228316
 C   -3.939296    2.760171    0.189715
 H   -4.539174    3.286907    0.936805
 H   -4.413991    2.634785   -0.788734
 O    3.297676   -1.739048    0.531693
Na    2.079434   -2.463842    2.228412
 C    4.438206   -1.969298   -0.054934
 C    5.609854   -1.228330    0.266472
 C    4.577851   -2.959185   -1.064867
 C    6.816513   -1.450875   -0.390549
 H    5.540220   -0.476889    1.057518
 C    5.791626   -3.171777   -1.713504
 H    3.701835   -3.558659   -1.324154
 C    6.925425   -2.420860   -1.391002
 H    7.692164   -0.856438   -0.112365
 H    5.853347   -3.942282   -2.487934
 H    7.874427   -2.591255   -1.903722
 C    0.817412   -3.375766   -1.218378
 H    0.489231   -4.224859   -0.603666
 H    1.450493   -3.780776   -2.025489
 H    1.448531   -2.721835   -0.600456
 C   -1.355479    0.881085   -2.934760
 H   -1.527498    1.473385   -2.023261
 H   -0.371528    1.173257   -3.331044
 H   -2.120810    1.162503   -3.670071
 H   -3.371101   -0.842140   -3.508500
 H   -1.528322   -4.446216   -2.057162
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6major)_O6 / electronic energy: -3988.21476261 a.u. / lowest freq: -437.71 cm-1
 C    2.950144    0.143167   -1.752991
 H    3.936623   -0.098917   -1.338843
 C    2.169783   -1.118553   -2.139877
 H    2.058139   -1.235906   -3.226388
 C    0.880813    0.179502   -0.683163
 C   -0.245213   -1.760592   -1.603420
 C   -0.387304   -2.793846   -0.664793
 C   -1.181304   -1.554527   -2.633772
 C   -1.529040   -3.601260   -0.741437
 C   -2.305640   -2.381955   -2.675075
 C   -2.483206   -3.392711   -1.730872
 H   -3.370494   -4.028489   -1.775280
Cu   -0.763125    0.858742    0.177576
 N    2.080115    0.760418   -0.745021
 N    0.871673   -0.877266   -1.501331
 C   -2.280410    1.030357    1.604552
 C   -1.073987    0.598098    2.277020
 H    3.988308   -0.004353    1.136119
 H    2.632665   -2.033665   -1.736404
 H    3.079255    0.824236   -2.608252
 H   -2.490964    2.099719    1.700017
 C   -0.869630   -0.762868    2.782287
 C   -0.199172    1.704012    2.706103
 O   -1.970466   -1.514748    2.723605
 O    0.167153   -1.223289    3.242627
 O   -0.468026    2.881780    2.558555
 O    0.982531    1.335842    3.243204
 C    1.816014    2.389995    3.713040
 H    2.059225    3.091393    2.903252
 H    2.730024    1.912500    4.079965
 H    1.319757    2.940851    4.523495
 C   -1.905660   -2.832100    3.247003
 H   -1.173112   -3.443047    2.702383
 H   -2.907826   -3.254950    3.118998
 H   -1.636154   -2.816102    4.311999
 C    2.408854    1.982781   -0.017440
 H    1.701091    2.006446    0.821276
 C    2.183838    3.249139   -0.820547
 C    1.170796    4.129389   -0.421670
 C    2.966918    3.580958   -1.933606
 C    0.929137    5.305250   -1.130468
 H    0.559596    3.884028    0.452270
 C    2.723356    4.755164   -2.645725
 H    3.782093    2.926513   -2.250736
 C    1.702091    5.618550   -2.248008
 H    0.131606    5.977834   -0.807746
 H    3.339394    4.999426   -3.513993
 H    1.513603    6.538593   -2.805493
 C    3.806970    1.919028    0.610968
 H    3.979226    2.889325    1.103911
 H    4.577155    1.836809   -0.181107
 O    3.929741    0.909597    1.559388
 C   -3.264358    0.245073    0.981619
 H   -3.088459   -0.823099    0.847981
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 C   -4.434143    0.813502    0.473644
 H   -4.718675    1.781841    0.890949
 C   -5.566406   -0.015836    0.002372
 C   -6.877243    0.464723    0.128042
 C   -5.370097   -1.274372   -0.588127
 C   -7.963070   -0.293343   -0.308342
 H   -7.046829    1.445959    0.579474
 C   -6.453509   -2.030625   -1.025683
 H   -4.357040   -1.658472   -0.726758
 C   -7.755963   -1.545162   -0.886405
 H   -8.976526    0.098507   -0.195703
 H   -6.280107   -3.006078   -1.486463
 H   -8.604748   -2.139374   -1.231814
 C   -1.487592    2.112708   -1.264643
 H   -0.651219    2.586574   -1.779220
 C   -2.736441    2.117131   -1.465458
 C   -4.072571    1.879121   -1.452352
 H   -4.761335    2.686248   -1.188925
 H   -4.465898    1.130121   -2.146879
 O    3.690861   -1.521901    0.918662
Na    2.227096   -0.680470    2.441171
 C    4.527280   -2.249837    0.237690
 C    5.714703   -1.700421   -0.320248
 C    4.294304   -3.629282   -0.012049
 C    6.585617   -2.470381   -1.086385
 H    5.939500   -0.647360   -0.122864
 C    5.173546   -4.387853   -0.779553
 H    3.401796   -4.089584    0.418126
 C    6.326293   -3.821267   -1.331601
 H    7.486424   -2.006034   -1.498577
 H    4.955425   -5.446400   -0.949800
 H    7.010125   -4.421950   -1.934918
 C    0.642899   -3.038084    0.402330
 H    0.312051   -2.632297    1.368269
 H    0.801718   -4.116670    0.544664
 H    1.610592   -2.568890    0.185897
 C   -0.967745   -0.478469   -3.662704
 H   -0.840750    0.502986   -3.186072
 H   -0.065188   -0.676631   -4.261746
 H   -1.821940   -0.418430   -4.349903
 H   -3.053262   -2.229680   -3.457264
 H   -1.661083   -4.407999   -0.015899
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6major)_07 / electronic energy: -3988.20625665 a.u. / lowest freq: -462.49 cm-1
 C    2.960599    1.158813   -1.339132
 H    3.910886    1.304323   -0.810933
 C    2.830141   -0.260563   -1.894371
 H    2.905030   -0.301173   -2.989799
 C    0.956061    0.232439   -0.582079
 C    0.948267   -1.931828   -1.723154
 C    1.225245   -2.979377   -0.829924
 C    0.205986   -2.129166   -2.898186
 C    0.755023   -4.256470   -1.147910
 C   -0.261134   -3.418484   -3.170793
 C    0.016842   -4.474717   -2.307244
 H   -0.346783   -5.477989   -2.539729
Cu   -0.944258    0.240447    0.001250
 N    1.813467    1.247344   -0.429429
 N    1.483396   -0.638537   -1.447369
 C   -2.562497    0.056757    1.366116
 C   -1.425734   -0.689899    1.853441
 H    3.833002    1.113078    1.548563
 H    3.581853   -0.946356   -1.472078
 H    2.873128    1.918204   -2.131797
 H   -2.608883    1.091080    1.720889
 C   -1.397556   -2.153914    1.658162
 C   -0.471436   -0.038056    2.748104
 O   -0.721458   -2.822227    2.599185
 O   -1.964447   -2.735312    0.753791
 O    0.556375   -0.526599    3.198084
 O   -0.785339    1.239669    3.024394
 C    0.112438    1.962765    3.855268
 H    0.151859    1.520487    4.860625
 H   -0.284197    2.982206    3.910455
 H    1.126386    1.972552    3.430127
 C   -0.669988   -4.232161    2.460299
 H   -1.669276   -4.675902    2.576972
 H   -0.005819   -4.592814    3.253485
 H   -0.274043   -4.514930    1.475675
 C    1.549877    2.393744    0.432326
 H    0.799347    2.035665    1.149985
 C    0.947707    3.584799   -0.289914
 C    1.668705    4.330999   -1.231354
 C   -0.363840    3.969243    0.008398
 C    1.080466    5.420063   -1.874195
 H    2.704442    4.074908   -1.465927
 C   -0.952967    5.059333   -0.628951
 H   -0.936723    3.392569    0.739051
 C   -0.232750    5.785128   -1.576791
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 H    1.654808    5.990070   -2.607709
 H   -1.982027    5.336170   -0.389994
 H   -0.692308    6.638160   -2.080722
 C    2.789875    2.788947    1.247440
 H    2.494414    3.639434    1.883006
 H    3.580331    3.168975    0.572789
 O    3.262544    1.762612    2.059791
 C   -3.715214   -0.415403    0.722546
 H   -3.757029   -1.460535    0.417409
 C   -4.744414    0.460660    0.373884
 H   -4.733721    1.433428    0.874203
 C   -6.101154   -0.015756    0.008785
 C   -7.211521    0.794083    0.285972
 C   -6.319871   -1.254403   -0.614738
 C   -8.502977    0.377001   -0.033968
 H   -7.059374    1.764849    0.765660
 C   -7.608761   -1.671204   -0.936166
 H   -5.471689   -1.896270   -0.862988
 C   -8.707292   -0.859163   -0.645317
 H   -9.353587    1.022157    0.197625
 H   -7.757697   -2.638627   -1.421175
 H   -9.717592   -1.188830   -0.897297
 C   -1.689465    1.407506   -1.499463
 H   -0.877891    1.817196   -2.100974
 C   -2.946077    1.509635   -1.618842
 C   -4.300177    1.430200   -1.522692
 H   -4.818224    0.734665   -2.190043
 H   -4.861136    2.333986   -1.266144
Na    2.707294   -0.571273    2.597720
 O    4.369564   -0.330366    1.147279
 C    5.410955   -0.586552    0.410849
 C    6.289191    0.439613   -0.030394
 C    5.712700   -1.905845   -0.022372
 C    7.377097    0.162870   -0.854475
 H    6.097431    1.464020    0.304228
 C    6.802932   -2.169010   -0.846662
 H    5.062308   -2.720152    0.308092
 C    7.647131   -1.141266   -1.277319
 H    8.028944    0.982431   -1.171402
 H    6.997727   -3.199097   -1.159595
 H    8.500480   -1.353735   -1.924744
 H   -0.844133   -3.594118   -4.078051
 H    0.973223   -5.090235   -0.475873
 C    1.960175   -2.721265    0.456879
 H    2.792283   -2.012912    0.333959
 H    1.267645   -2.291205    1.199385
 H    2.358089   -3.654521    0.878521
 C   -0.107416   -0.978884   -3.815774
 H   -0.546481   -1.336994   -4.756273
 H   -0.828085   -0.294777   -3.341758
 H    0.789337   -0.389563   -4.057214
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6minor)_01 / electronic energy: -3988.21330777 a.u. / lowest freq: -465.41 cm-1
 C   -2.703452    1.527561    1.353933
 H   -3.342978    1.905825    0.548817
 C   -3.155336    0.143503    1.821047
 H   -3.272644    0.071523    2.913922
 C   -1.014417   -0.030756    0.881243
 C   -2.102740   -2.123289    1.644653
 C   -2.975158   -2.920971    0.883049
 C   -1.370947   -2.661514    2.721948
 C   -3.092329   -4.276835    1.209117
 C   -1.500112   -4.026170    2.996819
 C   -2.357832   -4.829913    2.251286
 H   -2.457981   -5.891270    2.488351
Cu    0.859807   -0.558380    0.410665
 N   -1.350496    1.261217    0.853276
 N   -2.047049   -0.720818    1.386494
 C    2.331979   -1.418163   -0.920109
 C    1.048918   -1.306588   -1.572761
 H   -2.438726    1.975637   -1.581425
 H   -4.101670   -0.162762    1.352981
 H   -2.688138    2.269838    2.164430
 H    2.461082   -2.357793   -0.374127
 C    0.147202   -2.468699   -1.550408
 C    0.692124   -0.195381   -2.465502
 O    0.702653   -3.542964   -0.980137
 O   -1.000453   -2.506542   -1.968308
 O   -0.228000   -0.181820   -3.267190
 O    1.481597    0.873607   -2.320431
 C    1.192088    2.009920   -3.130770
 H    1.301819    1.762723   -4.195843
 H    1.929614    2.768787   -2.846745
 H    0.170278    2.362424   -2.931149
 C   -0.107745   -4.698383   -0.833584
 H   -1.000735   -4.474812   -0.236347
 H    0.513163   -5.438721   -0.317822
 H   -0.416811   -5.085609   -1.814710
 C   -0.482404    2.304778    0.336006
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 H    0.254405    1.798385   -0.307085
 C    0.293606    3.040450    1.418193
 C    1.348131    3.878162    1.033349
 C    0.033677    2.884306    2.781895
 C    2.112520    4.551342    1.982683
 H    1.588681    3.991999   -0.027258
 C    0.796379    3.558260    3.737016
 H   -0.752112    2.204916    3.116019
 C    1.836308    4.396519    3.341790
 H    2.934312    5.194253    1.659717
 H    0.579539    3.416732    4.798059
 H    2.436228    4.920867    4.088588
 C   -1.263157    3.260334   -0.584936
 H   -0.578174    4.072129   -0.874175
 H   -2.076458    3.740584   -0.003726
 O   -1.722358    2.655935   -1.746480
 C    3.502782   -0.663839   -1.072041
 H    3.490791    0.224788   -1.700418
 C    4.646293   -0.980088   -0.337409
 H    4.657466   -1.966834    0.134946
 C    5.990060   -0.461868   -0.692620
 C    7.125634   -1.216212   -0.365546
 C    6.173511    0.771167   -1.338108
 C    8.405143   -0.761858   -0.682127
 H    7.001564   -2.176422    0.142453
 C    7.450542    1.226768   -1.653352
 H    5.308632    1.390169   -1.586721
 C    8.573059    0.462274   -1.327830
 H    9.275623   -1.367996   -0.420911
 H    7.572271    2.189941   -2.154033
 H    9.574174    0.822709   -1.574003
 C    1.952881    0.073812    2.000379
 H    1.299089    0.480418    2.772223
 C    3.218731    0.050390    1.946370
 C    4.535742   -0.023082    1.621950
 H    5.032841    0.906130    1.328877
 H    5.171147   -0.754209    2.131239
 O   -3.569546    0.815804   -1.575626
Na   -2.323226   -0.706554   -2.549778
 C   -4.803419    1.207097   -1.425874
 C   -5.131349    2.570645   -1.189136
 C   -5.893282    0.296363   -1.470665
 C   -6.446899    2.980098   -0.989008
 H   -4.318714    3.302700   -1.187844
 C   -7.204161    0.719154   -1.269195
 H   -5.682421   -0.757126   -1.671689
 C   -7.500188    2.062491   -1.019664
 H   -6.652998    4.039557   -0.809779
 H   -8.012740   -0.016900   -1.308984
 H   -8.530570    2.387595   -0.860949
 C   -3.783597   -2.374056   -0.261061
 H   -3.538461   -2.920323   -1.184349
 H   -4.859107   -2.512488   -0.073296
 H   -3.611323   -1.304644   -0.435043
 C   -0.473954   -1.808441    3.575976
 H    0.522893   -1.709706    3.121311
 H   -0.871488   -0.791004    3.700403
 H   -0.345925   -2.256461    4.570381
 H   -0.935187   -4.456049    3.827526
 H   -3.766485   -4.905046    0.621477
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6minor)_O2 / electronic energy: -3988.21880720 a.u. / lowest freq: -417.00 cm-1
 C    1.761905   -1.791282    1.776076
 H    2.352441   -2.592969    1.312869
 C    2.635032   -0.586340    2.140199
 H    2.735898   -0.438022    3.224153
 C    0.892449    0.114582    0.745694
 C    2.206003    1.889925    1.783489
 C    3.017393    2.607055    0.892413
 C    1.671614    2.481089    2.945623
 C    3.258748    3.960129    1.166275
 C    1.937896    3.831168    3.181852
 C    2.721138    4.568538    2.294576
 H    2.916206    5.625246    2.489832
Cu   -0.468886    1.217321   -0.177184
 N    0.810460   -1.213644    0.824160
 N    1.899198    0.523326    1.524319
 C   -1.822999    1.533024   -1.731317
 C   -0.569736    1.148249   -2.351838
 H    1.955579   -2.306060   -1.229788
 H    3.642677   -0.659118    1.701259
 H    1.219202   -2.206824    2.641436
 H   -2.047615    2.602227   -1.744604
 C    0.450227    2.186598   -2.553060
 C   -0.347493   -0.136575   -3.028769
 O    0.036031    3.401846   -2.163131
 O    1.589596    2.022774   -2.967595
 O    0.647469   -0.443922   -3.666474
 O   -1.375927   -0.982807   -2.933039
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 C   -1.237337   -2.240028   -3.586645
 H   -1.189894   -2.103724   -4.676284
 H   -2.133752   -2.811938   -3.321808
 H   -0.327991   -2.744800   -3.235409
 C    0.990699    4.450743   -2.157730
 H    1.757031    4.271473   -1.388872
 H    0.436611    5.363558   -1.914323
 H    1.475628    4.551777   -3.137759
 C   -0.253813   -1.998110    0.222809
 H   -0.678555   -1.355490   -0.563075
 C   -1.368369   -2.292388    1.226963
 C   -1.994074   -3.539574    1.326520
 C   -1.829256   -1.253921    2.049408
 C   -3.050618   -3.739929    2.218893
 H   -1.668763   -4.377769    0.708991
 C   -2.879151   -1.451499    2.940965
 H   -1.376691   -0.263371    1.975903
 C   -3.497165   -2.699374    3.029305
 H   -3.523755   -4.722489    2.279242
 H   -3.220575   -0.621999    3.564278
 H   -4.323739   -2.857825    3.725056
 C    0.320669   -3.217779   -0.502052
 H   -0.517609   -3.771359   -0.952477
 H    0.788139   -3.903700    0.235054
 O    1.186240   -2.871986   -1.530066
 C   -2.839397    0.684273   -1.254705
 H   -2.659053   -0.389137   -1.216437
 C   -4.062226    1.168496   -0.789024
 H   -4.357403    2.162663   -1.131121
 C   -5.183262    0.260755   -0.456578
 C   -6.503158    0.708524   -0.612013
 C   -4.972860   -1.040699    0.028207
 C   -7.582123   -0.119692   -0.307154
 H   -6.684531    1.721243   -0.982132
 C   -6.050263   -1.865916    0.337097
 H   -3.958015   -1.409061    0.194187
 C   -7.360034   -1.411481    0.168986
 H   -8.601853    0.248295   -0.441340
 H   -5.861528   -2.870151    0.723444
 H   -8.203291   -2.060945    0.414047
 C   -1.309473    2.457953    1.208127
 H   -0.509410    2.962847    1.750992
 C   -2.563981    2.397696    1.356395
 C   -3.884772    2.104229    1.262011
 H   -4.594768    2.886824    0.983181
 H   -4.286067    1.298529    1.885111
Na    2.694022   -0.062505   -2.748602
 O    3.299535   -1.392028   -1.082354
 C    4.310180   -2.019851   -0.554632
 C    4.267463   -3.417591   -0.287140
 C    5.509863   -1.347612   -0.192493
 C    5.335241   -4.078242    0.313386
 H    3.367910   -3.966187   -0.580603
 C    6.570754   -2.022055    0.406260
 H    5.584215   -0.275502   -0.391853
 C    6.499364   -3.392555    0.671859
 H    5.257280   -5.153375    0.501360
 H    7.474505   -1.464877    0.671449
 H    7.334853   -3.914726    1.142964
 H    1.519159    4.311401    4.069422
 H    3.886166    4.537323    0.482075
 C    3.616791    1.963700   -0.327367
 H    3.517050    0.869756   -0.310204
 H    3.121823    2.330658   -1.239821
 H    4.683989    2.217853   -0.409733
 C    0.824285    1.681967    3.899951
 H    0.260260    2.342870    4.571150
 H    0.108422    1.043659    3.363047
 H    1.445185    1.022478    4.527103
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6minor)_03 / electronic energy: -3988.21880751 a.u. / lowest freq: -416.95 cm-1
 C   -1.762011   -1.790553   -1.777467
 H   -2.352725   -2.591915   -1.313889
 C   -2.634895   -0.585471   -2.141797
 H   -2.734931   -0.436781   -3.225783
 C   -0.892797    0.115193   -0.746512
 C   -2.206558    1.890622   -1.783994
 C   -3.018371    2.607449   -0.893056
 C   -1.672004    2.481984   -2.945959
 C   -3.260117    3.960443   -1.167000
 C   -1.938691    3.831966   -3.182253
 C   -2.722459    4.569031   -2.295187
 H   -2.917881    5.625661   -2.490513
Cu    0.468417    1.217117    0.177560
 N   -0.810351   -1.212926   -0.825789
 N   -1.899612    0.524043   -1.524995
 C    1.822505    1.532443    1.731716
 C    0.569205    1.148205    2.352494
 H   -1.955278   -2.303266    1.230862
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 H   -3.642912   -0.658406   -1.703768
 H   -1.219558   -2.206544   -2.642752
 H    2.047155    2.601642    1.744773
 C   -0.450417    2.187084    2.553105
 C    0.346581   -0.136157    3.030326
 O   -0.035552    3.402179    2.163484
 O   -1.590290    2.023602    2.966396
 O   -0.645838   -0.439867    3.673781
 O    1.371310   -0.986075    2.928274
 C    1.231063   -2.244553    3.579544
 H    1.175925   -2.109948    4.668972
 H    2.130601   -2.813872    3.319766
 H    0.325145   -2.750794    3.220846
 C   -0.990209    4.451090    2.156201
 H   -1.755844    4.271094    1.386817
 H   -0.435878    5.363664    1.912440
 H   -1.476020    4.553063    3.135695
 C    0.253735   -1.997402   -0.224199
 H    0.678782   -1.354488    0.561266
 C    1.368152   -2.292616   -1.228128
 C    1.830798   -1.254091   -2.049527
 C    1.992259   -3.540536   -1.328275
 C    2.880996   -1.452336   -2.940572
 H    1.379400   -0.263025   -1.975502
 C    3.049154   -3.741539   -2.220098
 H    1.665464   -4.378792   -0.711604
 C    3.497550   -2.700914   -3.029395
 H    3.223872   -0.622819   -3.563062
 H    3.521131   -4.724630   -2.280876
 H    4.324414   -2.859863   -3.724687
 C   -0.321227   -3.215971    0.501955
 H    0.516885   -3.770459    0.951573
 H   -0.790954   -3.901780   -0.233754
 O   -1.184743   -2.867900    1.531043
 C    2.839134    0.683754    1.255473
 H    2.659049   -0.389686    1.217372
 C    4.061868    1.168420    0.789983
 H    4.356552    2.162758    1.132005
 C    5.183352    0.261162    0.457808
 C    6.503007    0.709595    0.613353
 C    4.973610   -1.040452   -0.026833
 C    7.582405   -0.118139    0.308734
 H    6.683840    1.722451    0.983362
 C    6.051450   -1.865193   -0.335479
 H    3.958940   -1.409283   -0.192873
 C    7.360981   -1.410095   -0.167263
 H    8.601940    0.250362    0.442994
 H    5.863272   -2.869585   -0.721690
 H    8.204588   -2.059180   -0.412123
 C    1.309305    2.457836   -1.207554
 H    0.509301    2.962711   -1.750526
 C    2.563825    2.397519   -1.355680
 C    3.884593    2.103982   -1.261180
 H    4.594613    2.886546   -0.982328
 H    4.285894    1.298237   -1.884217
Na   -2.692875   -0.062239    2.750168
 O   -3.298822   -1.391054    1.083207
 C   -4.308552   -2.020369    0.555389
 C   -4.264388   -3.418364    0.289525
 C   -5.508505   -1.349562    0.191615
 C   -5.331145   -4.080627   -0.311038
 H   -3.364582   -3.965874    0.584228
 C   -6.568371   -2.025615   -0.407147
 H   -5.583923   -0.277299    0.389735
 C   -6.495590   -3.396354   -0.671123
 H   -5.252095   -5.155895   -0.497765
 H   -7.472412   -1.469531   -0.673624
 H   -7.330279   -3.919786   -1.142245
 H   -1.519898    4.312349   -4.069717
 H   -3.887876    4.537440   -0.482949
 C   -3.617753    1.963901    0.326652
 H   -3.517250    0.870022    0.309820
 H   -3.123250    2.331323    1.239173
 H   -4.685143    2.217382    0.408642
 C   -0.824170    1.683132   -3.900085
 H   -0.260047    2.344223   -4.571017
 H   -0.108353    1.044899   -3.363018
 H   -1.444713    1.023599   -4.527546
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6minor)_O4 / electronic energy: -3988.21355466 a.u. / lowest freq: -462.55 cm-1
 C    2.669864   -1.580950    1.448171
 H    3.302887   -1.969887    0.642104
 C    3.141221   -0.202102    1.912590
 H    3.261398   -0.129538    3.005043
 C    1.006551    0.000027    0.966176
 C    2.131050    2.081920    1.701338
 C    3.035291    2.834309    0.930101
 C    1.395567    2.669725    2.748713
 C    3.182021    4.195697    1.215871
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 C    1.555831    4.038934    2.984352
 C    2.445093    4.798063    2.229405
 H    2.567399    5.863513    2.435820
Cu   -0.837961    0.562515    0.432757
 N    1.321235   -1.296723    0.947529
 N    2.045131    0.676084    1.477206
 C   -2.236240    1.396724   -0.978693
 C   -0.939204    1.231083   -1.592682
 H    2.338256   -2.135464   -1.453576
 H    4.090595    0.088438    1.441709
 H    2.646068   -2.320721    2.260989
 H   -2.359955    2.362582   -0.479212
 C   -0.011211    2.372156   -1.590732
 C   -0.598912    0.088885   -2.453378
 O   -0.532807    3.461584   -1.015025
 O    1.128330    2.385343   -2.031274
 O    0.310784    0.040556   -3.264978
 O   -1.401622   -0.964566   -2.271143
 C   -1.142466   -2.125796   -3.056161
 H   -1.222874   -1.894557   -4.127295
 H   -1.913959   -2.850495   -2.772538
 H   -0.140130   -2.515967   -2.827980
 C    0.292070    4.611949   -0.923205
 H    1.213958    4.389067   -0.371916
 H   -0.295389    5.362122   -0.382878
 H    0.549245    4.987213   -1.923994
 C    0.421961   -2.326901    0.456753
 H   -0.265995   -1.826608   -0.242249
 C   -0.429368   -2.952571    1.551031
 C   -1.568916   -3.675562    1.177789
 C   -0.153973   -2.800221    2.911984
 C   -2.409989   -4.233856    2.136510
 H   -1.815007   -3.783306    0.117699
 C   -0.992775   -3.360815    3.876666
 H    0.704767   -2.210022    3.236287
 C   -2.123048   -4.079501    3.493612
 H   -3.300727   -4.782856    1.823147
 H   -0.764528   -3.222949    4.935856
 H   -2.784661   -4.509632    4.248507
 C    1.180103   -3.375716   -0.374527
 H    0.467687   -4.180558   -0.613471
 H    1.963421   -3.840108    0.259080
 O    1.680911   -2.882454   -1.570661
 C   -3.420211    0.662723   -1.132282
 H   -3.409628   -0.257086   -1.714019
 C   -4.578955    1.041656   -0.453338
 H   -4.581090    2.051069   -0.031282
 C   -5.923399    0.538764   -0.828214
 C   -7.050492    1.328716   -0.560789
 C   -6.117223   -0.712838   -1.433736
 C   -8.330931    0.891325   -0.896594
 H   -6.918825    2.303228   -0.082762
 C   -7.395362   -1.151244   -1.768821
 H   -5.260853   -1.359761   -1.636035
 C   -8.508846   -0.351363   -1.503023
 H   -9.193993    1.525387   -0.681289
 H   -7.524970   -2.128562   -2.239303
 H   -9.510703   -0.698415   -1.765006
 C   -1.993930    0.035968    2.016974
 H   -1.371005   -0.355655    2.821318
 C   -3.256232    0.091952    1.924257
 C   -4.559788    0.184316    1.552761
 H   -5.072435   -0.745564    1.289949
 H   -5.191194    0.956109    2.003728
 O    3.421689   -0.927835   -1.560886
Na    2.445465    0.645103   -2.779092
 C    4.674051   -1.271214   -1.456858
 C    5.727365   -0.335368   -1.647117
 C    5.065648   -2.601149   -1.136491
 C    7.062691   -0.698751   -1.498877
 H    5.465848    0.691784   -1.916246
 C    6.405186   -2.951427   -0.991395
 H    4.281594   -3.356155   -1.029880
 C    7.421377   -2.007523   -1.162560
 H    7.840617    0.055854   -1.650153
 H    6.660142   -3.986742   -0.745470
 H    8.470615   -2.286385   -1.044660
 H    0.988412    4.508238    3.791811
 H    3.879310    4.789785    0.619759
 C    0.463227    1.865442    3.611916
 H   -0.536568    1.804129    3.157155
 H    0.817589    0.833755    3.748381
 H    0.352767    2.330572    4.600688
 C    3.851727    2.216282   -0.169960
 H    4.906280    2.121887    0.134333
 H    3.499333    1.213128   -0.442469
 H    3.825692    2.853024   -1.066256
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6minor)_O5 / electronic energy: -3988.21868997 a.u. / lowest freq: -417.87 cm-1
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C	-1.771710	-1.783857	-1.728103
H	-2.363349	-2.579641	-1.256203
C	-2.642269	-0.581067	-2.104337
H	-2.737458	-0.439997	-3.189737
C	-0.899977	0.130613	-0.713643
C	-2.214831	1.897009	-1.768665
C	-3.023418	2.624791	-0.883482
C	-1.687587	2.473532	-2.941145
C	-3.265996	3.974321	-1.171738
C	-1.954869	3.821023	-3.191814
C	-2.733038	4.569269	-2.309621
H	-2.928870	5.623633	-2.516371
Cu	0.482618	1.228677	0.185860
N	-0.818470	-1.198415	-0.782967
N	-1.908530	0.533261	-1.493454
C	1.871928	1.557257	1.708793
C	0.626534	1.195288	2.358059
H	-2.014212	-2.292609	1.245778
H	-3.651805	-0.649902	-1.669836
H	-1.230097	-2.209544	-2.589079
H	2.104961	2.624686	1.696685
C	-0.385511	2.244084	2.551097
C	0.400197	-0.075291	3.059724
O	0.041909	3.456527	2.169469
O	-1.532200	2.084874	2.946598
O	-0.593194	-0.361069	3.710422
O	1.416707	-0.936100	2.964151
C	1.264361	-2.185874	3.628767
H	1.232052	-2.041455	4.717833
H	2.147226	-2.775518	3.357395
H	0.342283	-2.679103	3.293976
C	-0.913276	4.505023	2.133904
H	-1.675057	4.307215	1.364903
H	-0.357590	5.412239	1.873896
H	-1.404261	4.627749	3.108433
C	0.240124	-1.980891	-0.170329
H	0.675008	-1.326209	0.600316
C	1.346332	-2.310184	-1.172015
C	1.981561	-3.555879	-1.217726
C	1.790179	-1.309528	-2.048554
C	3.029118	-3.792084	-2.111508
H	1.670340	-4.364487	-0.555288
C	2.831793	-1.542976	-2.941461
H	1.329079	-0.320769	-2.020460
C	3.458070	-2.789213	-2.976996
H	3.509375	-4.772856	-2.128652
H	3.159275	-0.743047	-3.609227
H	4.277673	-2.975459	-3.674046
C	-0.345389	-3.179476	0.581861
H	0.486031	-3.722343	1.056957
H	-0.807222	-3.884462	-0.140157
O	-1.221918	-2.799846	1.588841
C	2.871327	0.690008	1.229588
H	2.681297	-0.382419	1.220170
C	4.087894	1.153122	0.727029
H	4.398419	2.152416	1.039221
C	5.193843	0.228509	0.390599
C	6.520510	0.669747	0.501177
C	4.962028	-1.083381	-0.054454
C	7.585483	-0.174995	0.192623
H	6.718448	1.691085	0.837602
C	6.025426	-1.925610	-0.365815
H	3.940824	-1.447552	-0.187700
C	7.342256	-1.477695	-0.241622
H	8.610878	0.188347	0.291775
H	5.819924	-2.938717	-0.718922
H	8.174239	-2.140760	-0.488691
C	1.309935	2.438849	-1.234264
H	0.505853	2.945640	-1.769392
C	2.559613	2.356372	-1.410142
C	3.877863	2.045422	-1.340980
H	4.605267	2.822778	-1.094273
H	4.253090	1.221570	-1.956627
Na	-2.565241	-0.040385	2.582500
O	-3.350840	-1.395953	1.033513
C	-4.370264	-2.033577	0.535795
C	-4.333572	-3.436855	0.302566
C	-5.571416	-1.365531	0.172835
C	-5.412245	-4.109544	-0.264431
H	-3.431273	-3.981076	0.596622
C	-6.643100	-2.051663	-0.392128
H	-5.638557	-0.288428	0.347444
C	-6.579484	-3.429080	-0.622262
H	-5.340320	-5.189201	-0.426769
H	-7.549198	-1.498874	-0.658264
H	-7.423608	-3.960452	-1.066804
H	-1.541151	4.290287	-4.087570
H	-3.890755	4.559425	-0.491934
C	-3.615539	1.995165	0.347112

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 H   -3.582898    0.897679    0.304699
 H   -3.065865    2.318011    1.245458
 H   -4.661322    2.310299    0.475086
 C   -0.849722    1.663026   -3.894266
 H   -0.272855    2.316350   -4.561982
 H   -0.146046    1.011565   -3.357430
 H   -1.479758    1.016049   -4.525434
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6minor)_06 / electronic energy: -3988.21301922 a.u. / lowest freq: -426.05 cm-1
 C    1.674736   -2.144028    1.237588
 H    2.237573   -2.855498    0.619276
 C    2.585521   -1.064924    1.827213
 H    2.722632   -1.169581    2.911590
 C    0.823904   -0.045419    0.668600
 C    2.285142    1.454467    1.907752
 C    2.908682    2.289815    0.964868
 C    2.075454    1.856947    3.238041
 C    3.300929    3.566942    1.377213
 C    2.483201    3.142196    3.608250
 C    3.086762    3.992395    2.685575
 H    3.395339    4.994993    2.989518
Cu   -0.554956    1.301238    0.208956
 N    0.732598   -1.357023    0.436486
 N    1.849383    0.161963    1.501834
 C   -2.028461    2.104467   -1.026509
 C   -0.791545    2.119245   -1.771430
 H    2.079752   -2.192937   -1.681048
 H    3.575970   -1.047872    1.347833
 H    1.124668   -2.707367    2.009619
 H   -2.312966    3.081235   -0.625113
 C   -0.048242    3.392285   -1.652980
 C   -0.398752    1.099564   -2.743447
 O    0.987202    3.525834   -2.487815
 O   -0.338584    4.269318   -0.859894
 O    0.692701    0.991118   -3.286154
 O   -1.377344    0.229589   -3.020815
 C   -1.094696   -0.803519   -3.955496
 H   -0.874470   -0.378825   -4.945086
 H   -2.003976   -1.412673   -4.007984
 H   -0.244916   -1.413012   -3.618006
 C    1.762757    4.702872   -2.343599
 H    1.163937    5.601506   -2.549111
 H    2.577048    4.622154   -3.072330
 H    2.172811    4.779033   -1.325897
 C   -0.325715   -1.978846   -0.336499
 H   -0.770242   -1.162178   -0.927729
 C   -1.420990   -2.554093    0.560532
 C   -2.122399   -3.721819    0.236557
 C   -1.783838   -1.866260    1.726599
 C   -3.156412   -4.184595    1.053093
 H   -1.875888   -4.289969   -0.661343
 C   -2.815562   -2.325785    2.540866
 H   -1.270347   -0.942699    1.997744
 C   -3.508559   -3.488957    2.207116
 H   -3.688328   -5.098701    0.779983
 H   -3.080386   -1.766343    3.440973
 H   -4.320484   -3.849183    2.842139
 C    0.264097   -2.975508   -1.345027
 H   -0.552223   -3.335903   -1.988770
 H    0.657235   -3.862121   -0.809821
 O    1.225881   -2.398966   -2.168457
 C   -2.960284    1.063271   -0.855826
 H   -2.733930    0.070043   -1.242121
 C   -4.166467    1.261145   -0.181037
 H   -4.519148    2.292037   -0.107468
 C   -5.232551    0.234393   -0.176595
 C   -6.576991    0.631625   -0.135157
 C   -4.943431   -1.139335   -0.205938
 C   -7.603648   -0.311347   -0.142765
 H   -6.819033    1.697381   -0.101309
 C   -5.968291   -2.080684   -0.211923
 H   -3.906007   -1.481668   -0.195989
 C   -7.303483   -1.672655   -0.183898
 H   -8.644135    0.020452   -0.115439
 H   -5.718524   -3.144007   -0.227290
 H   -8.105399   -2.414011   -0.187127
 C   -1.344224    1.846295    2.018249
 H   -0.523971    2.146553    2.670862
 C   -2.583850    1.671061    2.195759
 C   -3.898448    1.363309    2.055927
 H   -4.650390    2.152568    2.135493
 H   -4.229887    0.359331    2.340590
Na    2.523993   -0.240048   -2.926787
 O    3.463239   -1.473416   -1.354314
 C    4.450565   -2.142274   -0.832596
 C    4.414995   -3.557842   -0.713338
 C    5.604669   -1.491688   -0.320194
 C    5.453281   -4.263362   -0.110913
 H    3.546131   -4.086769   -1.117278
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 C    6.636864   -2.209179    0.277729
 H    5.662338   -0.402541   -0.402596
 C    6.575068   -3.601139    0.394787
 H    5.384389   -5.352599   -0.034652
 H    7.507461   -1.670993    0.664176
 H    7.386814   -4.157699    0.867874
 H    2.316125    3.480350    4.633786
 H    3.787927    4.233074    0.660478
 C    3.134768    1.825574   -0.448384
 H    3.431809    0.766091   -0.488800
 H    2.210535    1.923278   -1.038980
 H    3.907566    2.433688   -0.938787
 C    1.428204    0.936534    4.239043
 H    0.973905    1.507134    5.060239
 H    0.648677    0.317057    3.772571
 H    2.168599    0.252599    4.684779
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6minor)_07 / electronic energy: -3988.21538734 a.u. / lowest freq: -421.57 cm-1
 C   -1.762942   -1.724382   -1.759653
 H   -2.381504   -2.506352   -1.298391
 C   -2.599641   -0.504720   -2.162073
 H   -2.664162   -0.367483   -3.250058
 C   -0.880452    0.177577   -0.730000
 C   -2.143166    1.967071   -1.809682
 C   -2.911177    2.714720   -0.904192
 C   -1.630278    2.530495   -2.994223
 C   -3.140009    4.065597   -1.194459
 C   -1.883884    3.880788   -3.246495
 C   -2.630213    4.645007   -2.351393
 H   -2.816669    5.700673   -2.560127
Cu    0.534011    1.207727    0.204238
 N   -0.821094   -1.152516   -0.795924
 N   -1.859119    0.598222   -1.536686
 C    1.970428    1.449727    1.694163
 C    0.758138    1.029520    2.372108
 H   -2.190753   -2.195321    1.168406
 H   -3.620744   -0.550234   -1.753176
 H   -1.210826   -2.166235   -2.605439
 H    2.187521    2.520216    1.720967
 C   -0.249238    2.050428    2.686049
 C    0.696373   -0.309743    2.981491
 O    0.171566    3.295741    2.426861
 O   -1.393083    1.851354    3.076559
 O    1.525467   -1.184016    2.824273
 O   -0.357096   -0.509646    3.800549
 C   -0.379760   -1.752410    4.500428
 H   -0.550836   -2.573484    3.792714
 H   -1.214268   -1.679120    5.207374
 H    0.561838   -1.907825    5.042905
 C   -0.780134    4.343532    2.527206
 H   -1.554766    4.239549    1.753045
 H   -0.225048    5.273730    2.366750
 H   -1.256886    4.352022    3.516234
 C    0.196665   -1.942457   -0.129886
 H    0.657152   -1.263536    0.601244
 C    1.302590   -2.372532   -1.088078
 C    1.914462   -3.627940   -1.013939
 C    1.781750   -1.454438   -2.034414
 C    2.974821   -3.957230   -1.861593
 H    1.575686   -4.369074   -0.288910
 C    2.835812   -1.782107   -2.882521
 H    1.337009   -0.458760   -2.098034
 C    3.438148   -3.038216   -2.799547
 H    3.439141   -4.942716   -1.783499
 H    3.193518   -1.047631   -3.607460
 H    4.268108   -3.296164   -3.460667
 C   -0.442119   -3.060638    0.699379
 H    0.355592   -3.554307    1.273957
 H   -0.880530   -3.828312    0.029974
 O   -1.372689   -2.569722    1.609821
 C    2.968504    0.606380    1.172656
 H    2.787728   -0.467606    1.161175
 C    4.164455    1.096784    0.648027
 H    4.459131    2.102369    0.956666
 C    5.284265    0.198587    0.286245
 C    6.599794    0.682477    0.332941
 C    5.075697   -1.129084   -0.121283
 C    7.677495   -0.134965   -0.003412
 H    6.779066    1.716526    0.639842
 C    6.151673   -1.944409   -0.459998
 H    4.062229   -1.528885   -0.198789
 C    7.457671   -1.453465   -0.400975
 H    8.693999    0.262088    0.045429
 H    5.963926   -2.971900   -0.780050
 H    8.299502   -2.095896   -0.668593
 C    1.340794    2.422148   -1.221292
 H    0.530227    2.937797   -1.738035
 C    2.582149    2.312943   -1.438001
 C    3.895184    1.973981   -1.411724
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 H    4.647073    2.737758   -1.197845
 H    4.230992    1.139584   -2.036077
Na   -2.407353   -0.177331    2.490297
 O   -3.497742   -1.299587    0.923459
 C   -4.516184   -1.886207    0.364539
 C   -4.526554   -3.286207    0.114920
 C   -5.664500   -1.161228   -0.053448
 C   -5.601442   -3.905875   -0.516314
 H   -3.665014   -3.874246    0.446256
 C   -6.733041   -1.793965   -0.682883
 H   -5.691860   -0.083866    0.130781
 C   -6.717161   -3.170593   -0.925846
 H   -5.567913   -4.985756   -0.688901
 H   -7.598159   -1.199005   -0.990975
 H   -7.558962   -3.660161   -1.420055
 H   -1.481809    4.339548   -4.152947
 H   -3.735635    4.665056   -0.501298
 C   -3.464784    2.102969    0.353118
 H   -3.582296    1.013564    0.266617
 H   -2.793733    2.296649    1.205748
 H   -4.439301    2.546658    0.601400
 C   -0.811496    1.707659   -3.953287
 H   -0.231459    2.353278   -4.625725
 H   -0.111351    1.049959   -3.418666
 H   -1.452446    1.066972   -4.579782
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6minor)_O8 / electronic energy: -3988.21376729 a.u. / lowest freq: -435.90 cm-1
 C    1.785568   -1.972006    1.393388
 H    2.364716   -2.721021    0.837527
 C    2.665814   -0.811765    1.865234
 H    2.822424   -0.809464    2.952227
 C    0.854095    0.033912    0.647299
 C    2.279849    1.694046    1.705229
 C    2.863961    2.441916    0.667542
 C    2.077788    2.229315    2.988612
 C    3.226538    3.764823    0.936858
 C    2.450929    3.558324    3.213763
 C    3.017590    4.321318    2.196412
 H    3.301532    5.358469    2.387479
Cu   -0.570599    1.284349    0.078269
 N    0.808132   -1.295305    0.536104
 N    1.880365    0.353592    1.443040
 C   -2.053004    1.930872   -1.227027
 C   -0.818368    1.884430   -1.975586
 H    2.160977   -2.252636   -1.531382
 H    3.647598   -0.805868    1.367552
 H    1.264033   -2.476806    2.223655
 H   -2.368781    2.932300   -0.924289
 C   -0.021660    3.125814   -2.064734
 C   -0.418033    0.785137   -2.852282
 O   -0.355001    3.999807   -1.089321
 O    0.843086    3.386495   -2.871030
 O    0.678119    0.657092   -3.379539
 O   -1.377382   -0.124693   -3.051935
 C   -1.064969   -1.235686   -3.882874
 H   -0.871931   -0.904717   -4.913250
 H   -1.949796   -1.881666   -3.861616
 H   -0.187191   -1.772015   -3.497362
 C    0.346500    5.229887   -1.069988
 H    1.423037    5.061130   -0.926776
 H   -0.056270    5.797311   -0.223931
 H    0.193673    5.785906   -2.005976
 C   -0.231082   -2.018150   -0.172636
 H   -0.702963   -1.271095   -0.830619
 C   -1.305899   -2.548058    0.775162
 C   -1.962466   -3.765584    0.558623
 C   -1.699317   -1.769828    1.872594
 C   -2.982985   -4.189860    1.412011
 H   -1.689862   -4.405030   -0.281861
 C   -2.717608   -2.191225    2.723861
 H   -1.221456   -0.806473    2.057117
 C   -3.365679   -3.405175    2.497078
 H   -3.479725   -5.144086    1.223018
 H   -3.008463   -1.561047    3.567380
 H   -4.166586   -3.735646    3.161617
 C    0.386343   -3.079866   -1.094561
 H   -0.424522   -3.529035   -1.687707
 H    0.818627   -3.897968   -0.484643
 O    1.313391   -2.548402   -1.983513
 C   -2.962429    0.890268   -0.955175
 H   -2.711426   -0.131502   -1.238978
 C   -4.174485    1.124489   -0.301294
 H   -4.556834    2.146870   -0.339482
 C   -5.214439    0.075671   -0.196591
 C   -6.568469    0.440563   -0.202250
 C   -4.890768   -1.285997   -0.082659
 C   -7.571342   -0.523894   -0.115978
 H   -6.837163    1.497349   -0.282530
 C   -5.892032   -2.248710    0.005109
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 H   -3.844920   -1.598144   -0.033295
 C   -7.237203   -1.874014   -0.014306
 H   -8.620059   -0.218100   -0.128833
 H   -5.616294   -3.301250    0.101401
 H   -8.020594   -2.631779    0.055510
 C   -1.367256    1.956617    1.841174
 H   -0.551242    2.317278    2.467525
 C   -2.606383    1.787857    2.024987
 C   -3.917692    1.455289    1.901987
 H   -4.675986    2.242541    1.907713
 H   -4.242312    0.482937    2.286659
Na    2.600444   -0.410795   -2.984311
 O    3.525847   -1.484258   -1.283674
 C    4.521605   -2.113929   -0.729940
 C    4.496757   -3.520244   -0.526083
 C    5.675540   -1.426491   -0.268033
 C    5.546779   -4.182527    0.104300
 H    3.627203   -4.077217   -0.888654
 C    6.719382   -2.101169    0.358895
 H    5.724525   -0.343731   -0.414934
 C    6.669657   -3.484432    0.556758
 H    5.486872   -5.265988    0.243890
 H    7.590361   -1.535300    0.702786
 H    7.491454   -4.007161    1.050713
 H    2.288947    3.998812    4.200585
 H    3.687719    4.362098    0.146257
 C    3.086675    1.833959   -0.689891
 H    3.457605    0.800001   -0.617491
 H    2.144797    1.796074   -1.259079
 H    3.798534    2.433808   -1.273012
 C    1.477288    1.401054    4.093992
 H    0.993848    2.040825    4.844689
 H    0.731393    0.691026    3.708728
 H    2.252490    0.814610    4.613486
96
Figure_S15-2_PA-9b(NaOPh)-ts(1,6minor)_09 / electronic energy: -3988.20604707 a.u. / lowest freq: -449.99 cm-1
 C    2.416792   -1.605250    1.749273
 H    3.069782   -2.149551    1.057244
 C    3.012806   -0.246490    2.133857
 H    3.080152   -0.098727    3.222606
 C    0.993915    0.095475    0.997007
 C    2.267013    2.112635    1.611456
 C    3.236381    2.676800    0.759801
 C    1.558977    2.903893    2.534080
 C    3.440795    4.058722    0.803976
 C    1.783127    4.285307    2.533454
 C    2.707656    4.862647    1.670941
 H    2.870662    5.942396    1.686470
Cu   -0.773887    0.779438    0.371271
 N    1.166393   -1.224078    1.084935
 N    2.047851    0.702397    1.560789
 C   -2.174961    1.427305   -1.106700
 C   -0.881118    1.208085   -1.715018
 H    2.312709   -2.460484   -1.125887
 H    4.014075   -0.099823    1.704970
 H    2.225933   -2.241751    2.625001
 H   -2.302431    2.459658   -0.762091
 C   -0.042831    2.423594   -1.780245
 C   -0.544421    0.013366   -2.495511
 O    1.197314    2.255122   -2.292350
 O   -0.396985    3.515943   -1.388544
 O    0.416026   -0.127946   -3.238267
 O   -1.407909   -0.994361   -2.326319
 C   -1.128627   -2.211696   -3.013916
 H   -1.084164   -2.044071   -4.098365
 H   -1.959748   -2.884196   -2.773000
 H   -0.176334   -2.635979   -2.662126
 C    1.942709    3.450873   -2.497409
 H    1.395350    4.137284   -3.157099
 H    2.879701    3.144523   -2.977095
 H    2.145952    3.953074   -1.542690
 C    0.210432   -2.170096    0.520392
 H   -0.243221   -1.661017   -0.340918
 C   -0.929303   -2.523374    1.459068
 C   -2.202018   -2.715298    0.909383
 C   -0.769257   -2.648399    2.840576
 C   -3.292851   -3.020031    1.718306
 H   -2.344346   -2.585944   -0.166949
 C   -1.860390   -2.952779    3.655552
 H    0.208208   -2.487085    3.298877
 C   -3.124767   -3.137345    3.098279
 H   -4.281444   -3.149495    1.271686
 H   -1.720260   -3.041245    4.735159
 H   -3.978929   -3.367390    3.738859
 C    0.900850   -3.411299   -0.063758
 H    0.105183   -4.135933   -0.298215
 H    1.526507   -3.887641    0.719205
 O    1.603869   -3.159418   -1.234506
 C   -3.342741    0.651043   -1.115291
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 H   -3.313999   -0.354426   -1.529082
 C   -4.513537    1.118266   -0.517110
 H   -4.559536    2.191722   -0.312893
 C   -5.831266    0.486765   -0.771587
 C   -6.991050    1.273334   -0.738515
 C   -5.966391   -0.886344   -1.032775
 C   -8.246241    0.712096   -0.971086
 H   -6.905211    2.343335   -0.531189
 C   -7.218840   -1.448285   -1.262707
 H   -5.082343   -1.528266   -1.040370
 C   -8.365876   -0.651508   -1.234569
 H   -9.135843    1.345647   -0.945231
 H   -7.303091   -2.519267   -1.460668
 H   -9.347762   -1.095008   -1.413037
 C   -1.900632    0.605730    2.054174
 H   -1.266060    0.337496    2.897510
 C   -3.163111    0.682185    1.990349
 C   -4.472654    0.710513    1.635482
 H   -4.987638   -0.252380    1.572522
 H   -5.095642    1.562605    1.924165
 O    3.459862   -1.326233   -1.236083
Na    2.502152    0.198209   -2.502579
 C    4.688512   -1.709204   -1.027811
 C    5.795665   -0.873889   -1.337181
 C    4.995664   -2.981017   -0.471229
 C    7.104316   -1.271043   -1.078965
 H    5.597660    0.100319   -1.793269
 C    6.309270   -3.366123   -0.216689
 H    4.170466   -3.669416   -0.267732
 C    7.380104   -2.517216   -0.508507
 H    7.926371   -0.594383   -1.330975
 H    6.499881   -4.353210    0.215024
 H    8.408581   -2.823468   -0.306153
 H    1.226883    4.911652    3.235179
 H    4.186046    4.506564    0.141518
 C    0.589524    2.321109    3.524807
 H   -0.447500    2.458176    3.185206
 H    0.749555    1.245655    3.676188
 H    0.689663    2.825827    4.495905
 C    4.080580    1.830604   -0.151290
 H    5.070821    1.652179    0.297882
 H    3.643416    0.841772   -0.341808
 H    4.260649    2.341219   -1.108405
32
Figure_S15-3_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C   -0.660544   -0.726572    0.059153
 C   -1.860539   -0.097447    0.115996
 H   -0.691600   -1.818492   -0.004770
 C   -1.976243    1.390665    0.160143
 C   -3.120576   -0.891785    0.187355
 O   -3.041424    1.823605   -0.507466
 O   -1.182749    2.134043    0.689285
 O   -4.147702   -0.497504    0.683440
 O   -2.981802   -2.118850   -0.320932
 C   -4.097604   -2.989729   -0.195724
 H   -4.332384   -3.170881    0.862818
 H   -3.810049   -3.927003   -0.683244
 H   -4.981752   -2.562067   -0.688186
 C   -3.254671    3.228152   -0.535442
 H   -3.354009    3.627502    0.483524
 H   -4.184056    3.384216   -1.092621
 H   -2.420438    3.737793   -1.038016
 C    0.656646   -0.129211    0.062308
 H    0.725624    0.955889    0.150505
 C    1.759981   -0.902956   -0.019704
 H    1.621029   -1.988149   -0.089650
 C    3.156351   -0.453635   -0.025165
 C    4.175093   -1.416830   -0.109525
 C    3.522207    0.902114    0.053056
 C    5.517020   -1.042840   -0.114390
 H    3.907556   -2.474776   -0.172060
 C    4.861836    1.275255    0.048166
 H    2.754752    1.675486    0.118691
 C    5.863995    0.305241   -0.035401
 H    6.294080   -1.807149   -0.179427
 H    5.127957    2.332459    0.111300
 H    6.914980    0.602284   -0.038425
51
Figure_S15-3_9d(Na)-Cu-allenyl / electronic energy: -2839.06020575 a.u. / lowest freq: 14.37 cm-1
 C    1.401449   -2.075087    0.781893
 H    1.679476   -1.881296    1.831858
 C   -0.006213   -2.648365    0.652932
 H   -0.062301   -3.424044   -0.128912
 C    0.006182   -0.440008   -0.139162
 C   -2.189160   -1.531257    0.133738
 C   -2.845361   -2.761728    0.235329
 C   -2.951250   -0.369985   -0.075492
 C   -4.240763   -2.845245    0.119017
 C   -4.334525   -0.435941   -0.206321
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 C   -4.972785   -1.681355   -0.104919
 H   -6.061043   -1.738645   -0.201130
Cu   -0.329372    1.490047   -0.372686
 N    1.273764   -0.812875    0.054580
 N   -0.787308   -1.470553    0.258845
Na    0.498306    3.958728    1.355621
 H   -0.381218   -3.078008    1.591814
 H    2.168593   -2.723176    0.339289
 C    2.372398    0.146754   -0.035438
 H    2.178954    0.736216   -0.947149
 C    3.689483   -0.579021   -0.225630
 C    4.620192   -0.739015    0.805951
 C    3.975802   -1.139609   -1.477409
 C    5.810682   -1.435686    0.589342
 H    4.421442   -0.318405    1.793568
 C    5.159152   -1.840488   -1.696033
 H    3.252345   -1.025120   -2.289480
 C    6.083241   -1.989386   -0.660216
 H    6.529017   -1.546552    1.404836
 H    5.363247   -2.270600   -2.679186
 H    7.015148   -2.533630   -0.828612
 C    2.308388    1.165951    1.128058
 H    3.266929    1.737018    1.072498
 H    2.373701    0.583431    2.082237
 O    1.207712    1.962082    1.066314
 C   -5.135842    0.816899   -0.451875
 H   -5.658483    0.763844   -1.419613
 H   -5.904556    0.954837    0.324125
 H   -4.492476    1.707881   -0.461773
 C   -4.919272   -4.186120    0.236349
 H   -6.004229   -4.101088    0.086278
 H   -4.527345   -4.895642   -0.508698
 H   -4.747592   -4.631017    1.228910
 H   -2.283360   -3.682514    0.397907
 H   -2.449009    0.596199   -0.147487
 C   -1.307163    3.029167   -1.145241
 H   -1.961130    2.829821   -2.012024
 C   -1.311845    4.265224   -0.742674
 C   -1.248636    5.503922   -0.256051
 H   -0.536999    6.236564   -0.653695
 H   -1.960491    5.856163    0.499142
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_01 / electronic energy: -3681.01695194 a.u. / lowest freq: -446.94 cm-1
 C   -3.226581    2.332635   -1.099792
 H   -3.981826    2.696365   -0.392182
 C   -1.952093    3.174225   -1.130718
 H   -1.864290    3.800961   -2.028060
 C   -1.393366    0.950832   -0.697085
 C    0.460213    2.435636   -1.287072
 C    0.945886    3.722322   -1.043710
 C    1.334004    1.439963   -1.738679
 C    2.307971    4.007354   -1.191490
 C    2.692364    1.707668   -1.903845
 C    3.170185    2.991641   -1.611807
 H    4.235084    3.207680   -1.735868
Cu   -0.361303   -0.618995   -0.050701
 N   -2.713169    1.039318   -0.632534
 N   -0.905783    2.145518   -1.100657
 C    0.758401   -1.298588    1.616162
 C   -0.230641   -0.363073    2.094236
 H   -1.871191    3.822340   -0.241903
 H   -3.680267    2.225737   -2.098989
 H    0.493335   -2.346059    1.780902
 C   -0.020004    1.079559    2.270752
 C   -1.484968   -0.915010    2.625198
 O    1.249904    1.456008    2.100822
 O   -0.883817    1.904959    2.528767
 O   -2.318296   -0.324773    3.292244
 O   -1.673477   -2.201496    2.290638
 C   -2.859367   -2.820510    2.762928
 H   -2.855723   -2.891668    3.859795
 H   -2.874378   -3.822245    2.320724
 H   -3.747949   -2.253603    2.449506
 C    1.547858    2.835952    2.240397
 H    0.879199    3.446561    1.620801
 H    2.582406    2.958716    1.900916
 H    1.454117    3.145937    3.291059
 C   -3.566652   -0.077618   -0.245289
 H   -3.087142   -0.548829    0.626715
 C   -3.677318   -1.125759   -1.329634
 C   -4.017204   -2.437128   -0.974302
 C   -3.449762   -0.842212   -2.680603
 C   -4.121438   -3.438724   -1.937160
 H   -4.185433   -2.678822    0.078175
 C   -3.552282   -1.842158   -3.648364
 H   -3.162875    0.166087   -2.985815
 C   -3.887032   -3.145110   -3.281016
 H   -4.375793   -4.457366   -1.635430
 H   -3.362611   -1.601552   -4.696926
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 H   -3.959099   -3.929365   -4.037584
 C   -4.933617    0.463474    0.278907
 H   -5.513112   -0.464153    0.535180
 H   -5.464197    0.858009   -0.635511
 O   -4.791623    1.347635    1.273688
 C    2.055796   -1.075617    1.129882
 H    2.393609   -0.054898    0.960302
 C    2.882028   -2.152242    0.795953
 H    2.592116   -3.122015    1.207031
 C    4.339205   -2.001103    0.570172
 C    5.155568   -3.143319    0.570779
 C    4.948676   -0.753766    0.365609
 C    6.529716   -3.046902    0.366110
 H    4.700613   -4.124286    0.733326
 C    6.322585   -0.655618    0.159318
 H    4.348155    0.157691    0.365763
 C    7.120357   -1.800509    0.156326
 H    7.143096   -3.950819    0.372049
 H    6.774847    0.326349    0.002250
 H    8.197466   -1.720166   -0.004761
 C    3.601725    0.638271   -2.448500
 H    3.372100   -0.339092   -2.001760
 H    3.471570    0.539741   -3.538049
 H    4.659430    0.863134   -2.255186
 C    2.821235    5.385935   -0.866739
 H    3.884285    5.493178   -1.121541
 H    2.257610    6.158775   -1.410789
 H    2.708425    5.598582    0.208281
 H    0.270188    4.511381   -0.707593
 H    0.945888    0.449890   -1.984325
 C   -0.044963   -2.021817   -1.478777
 H   -0.905887   -2.059369   -2.149181
 C    1.088129   -2.582247   -1.459085
 C    2.362775   -2.985956   -1.204035
 H    2.534802   -4.016903   -0.882160
 H    3.171656   -2.544415   -1.794630
Na   -3.199420    1.713999    2.660794
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_O2 / electronic energy: -3681.01674239 a.u. / lowest freq: -425.84 cm-1
 C    2.866803    2.675946    1.037241
 H    3.618483    3.073400    0.344267
 C    1.496643    3.345149    0.935558
 H    1.285729    4.038149    1.760640
 C    1.246966    1.039170    0.692392
 C   -0.796962    2.290790    1.180897
 C   -1.490484    3.438376    0.798338
 C   -1.479557    1.247321    1.820637
 C   -2.874586    3.531001    0.998245
 C   -2.851518    1.327151    2.045160
 C   -3.540848    2.470137    1.614215
 H   -4.618525    2.543255    1.788127
Cu    0.443095   -0.673683    0.087133
 N    2.545629    1.293601    0.660974
 N    0.593216    2.188102    0.972750
 C   -0.520351   -1.415746   -1.646627
 C    0.525645   -0.530428   -2.098307
Na    3.541048    1.559954   -2.683597
 H    1.377226    3.887276   -0.017588
 H    3.266719    2.708454    2.064537
 H   -0.293059   -2.477742   -1.765329
 C    0.359803    0.903986   -2.362672
 C    1.798868   -1.136899   -2.511518
 O   -0.906702    1.322018   -2.270671
 O    1.249489    1.695745   -2.636288
 O    2.729106   -0.577606   -3.070754
 O    1.883062   -2.439152   -2.201216
 C    3.067140   -3.118499   -2.585350
 H    3.157940   -3.161586   -3.680079
 H    2.981622   -4.130150   -2.174801
 H    3.957585   -2.618517   -2.178973
 C   -1.154302    2.696016   -2.515703
 H   -0.506982    3.328730   -1.895213
 H   -2.204989    2.866151   -2.256610
 H   -0.981270    2.936927   -3.574367
 C    3.541140    0.255101    0.406446
 H    3.238270   -0.254293   -0.521579
 C    3.569791   -0.776710    1.510104
 C    3.338648   -0.440898    2.848798
 C    3.833792   -2.114224    1.194831
 C    3.358980   -1.418274    3.843111
 H    3.114557    0.593821    3.117691
 C    3.857616   -3.094769    2.184782
 H    4.001163   -2.392857    0.151635
 C    3.616254   -2.750116    3.514915
 H    3.167032   -1.139253    4.881685
 H    4.052018   -4.135263    1.915236
 H    3.623372   -3.516908    4.292376
 C    4.920609    0.898773    0.075156
 H    5.615125    0.019787   -0.011122
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 H    5.252989    1.400160    1.029742
 O    4.871332    1.700685   -0.997615
 C   -1.825621   -1.113976   -1.224459
 H   -2.112915   -0.072661   -1.093273
 C   -2.736375   -2.126181   -0.917369
 H   -2.504266   -3.121690   -1.302082
 C   -4.180716   -1.862138   -0.728250
 C   -5.091188   -2.927133   -0.811338
 C   -4.686171   -0.577836   -0.471120
 C   -6.457825   -2.720791   -0.638977
 H   -4.716894   -3.934837   -1.011349
 C   -6.052175   -0.370517   -0.297835
 H   -4.007551    0.273745   -0.389597
 C   -6.945620   -1.439678   -0.379347
 H   -7.147072   -3.565407   -0.707643
 H   -6.421400    0.637572   -0.095148
 H   -8.016271   -1.274778   -0.241455
 C   -3.571403    0.223601    2.775210
 H   -2.873392   -0.563606    3.091738
 H   -4.079472    0.612349    3.670806
 H   -4.340469   -0.236372    2.136249
 C   -3.621699    4.751481    0.526618
 H   -4.614503    4.821204    0.991853
 H   -3.067914    5.673798    0.755415
 H   -3.766496    4.721037   -0.565435
 H   -0.962707    4.269764    0.326130
 H   -0.924754    0.375016    2.167759
 C    0.058354   -2.071084    1.498789
 H    0.887162   -2.110107    2.209329
 C   -1.081011   -2.617436    1.438593
 C   -2.349736   -2.995465    1.131882
 H   -2.536143   -4.018874    0.794614
 H   -3.176879   -2.515024    1.662542
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_03 / electronic energy: -3681.01674622 a.u. / lowest freq: -439.73 cm-1
 C    2.808814   -2.155459    0.867278
 H    2.553608   -3.125374    1.299515
 C    0.645853   -1.348172    1.640382
 H    0.393753   -2.400391    1.793550
 C    1.945842   -1.099536    1.173681
 H    2.262952   -0.072111    1.004400
 C   -0.363994   -0.426156    2.099330
 C   -0.162220    1.013225    2.308185
 O   -1.033668    1.832224    2.560143
 C   -1.631585   -0.991440    2.581687
 O   -2.499734   -0.409023    3.211347
 O   -1.789292   -2.281866    2.248390
 C    4.258701   -1.953309    0.639065
 C    4.813223   -0.692756    0.368262
 C    6.182994   -0.544500    0.165599
 C    7.031058   -1.650951    0.229364
 C    6.494394   -2.909912    0.500960
 C    5.124360   -3.056782    0.703459
 C    2.317169   -3.075692   -1.112372
 H    2.452588   -4.097230   -0.745805
 H    3.155391   -2.676195   -1.691208
 C    1.061610   -2.647178   -1.414693
 C   -0.056218   -2.059963   -1.477192
 H   -0.900188   -2.091476   -2.169400
Cu   -0.393334   -0.642863   -0.068642
 C   -1.326599    0.991489   -0.706060
 N   -2.640136    1.152228   -0.658671
 N   -0.765752    2.169386   -1.059994
 C   -3.557079    0.067641   -0.323259
 C   -3.070794    2.486793   -1.094005
 H   -3.827865    2.866419   -0.396578
 C   -1.751946    3.256868   -1.064717
 H   -1.610896    3.915419   -1.931889
 C    0.614888    2.378644   -1.247517
 C    1.412893    1.354546   -1.764070
 C    1.189075    3.617264   -0.941495
 C    2.786349    1.540429   -1.936004
 C    2.562839    3.818881   -1.095447
 C    3.351328    2.768930   -1.580853
 H    4.427231    2.921401   -1.706843
Na   -3.340514    1.671157    2.667336
 H   -1.653168    3.859455   -0.146211
 H   -3.500011    2.436997   -2.108564
 O    1.111307    1.396635    2.182488
 C   -2.978581   -2.918544    2.686524
 H   -3.007629   -2.986180    3.783334
 H   -2.963425   -3.921940    2.248014
 H   -3.866926   -2.368158    2.344847
 C    1.400361    2.771817    2.375827
 H    0.749976    3.401241    1.755884
 H    2.445213    2.907679    2.075769
 H    1.270055    3.046968    3.432298
 H   -3.155275   -0.415260    0.581129
 C   -3.626891   -0.978321   -1.412178
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 C   -3.404414   -0.673511   -2.759506
 C   -3.922618   -2.303115   -1.070013
 C   -3.465417   -1.667464   -3.736230
 H   -3.154690    0.348372   -3.052553
 C   -3.986347   -3.299402   -2.042085
 H   -4.085991   -2.559109   -0.020348
 C   -3.754297   -2.985340   -3.381585
 H   -3.279599   -1.411384   -4.781809
 H   -4.205530   -4.329222   -1.751157
 H   -3.793185   -3.765008   -4.145210
 C   -4.936438    0.651496    0.110936
 H   -5.566004   -0.258700    0.304393
 H   -5.384928    1.084253   -0.829631
 O   -4.834592    1.509566    1.134264
 H    4.711641   -4.047158    0.914239
 H    4.171845    0.188692    0.307457
 H    7.147585   -3.783689    0.556683
 H    6.592147    0.446757   -0.043318
 H    8.104791   -1.531377    0.070245
 C    3.185094    5.150087   -0.762421
 H    2.536661    5.748687   -0.107567
 H    4.156168    5.021194   -0.262820
 H    3.364994    5.735118   -1.678574
 C    3.612863    0.443390   -2.553017
 H    3.443854    0.399540   -3.640750
 H    4.686900    0.597523   -2.383320
 H    3.337647   -0.536131   -2.138397
 H    0.956625    0.405791   -2.051294
 H    0.569449    4.429308   -0.555900
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_O4 / electronic energy: -3681.01671223 a.u. / lowest freq: -455.50 cm-1
 C   -3.591662    1.934032   -1.025909
 H   -4.376220    2.203010   -0.309573
 C   -2.471326    2.965707   -1.102990
 H   -2.497852    3.568894   -2.020242
 C   -1.557520    0.869179   -0.629234
 C    0.021205    2.662842   -1.203677
 C    0.219318    4.042421   -1.096995
 C    1.117960    1.831766   -1.469917
 C    1.502698    4.592197   -1.216003
 C    2.400648    2.360276   -1.589527
 C    2.583606    3.742749   -1.451729
 H    3.588454    4.164297   -1.545338
Cu   -0.271453   -0.562506   -0.101471
 N   -2.873432    0.751771   -0.542232
 N   -1.270897    2.123061   -1.059204
 C    1.020512   -1.310189    1.428926
 C    0.047247   -0.414400    2.005520
 H   -2.485320    3.648118   -0.236225
 H   -4.034998    1.732332   -2.014128
 H    0.748748   -2.365412    1.517933
 C    0.239788    1.030608    2.203814
 C   -1.146136   -1.009299    2.624387
 O    1.499126    1.426055    2.015251
 O   -0.633256    1.838459    2.484011
 O   -1.932762   -0.449495    3.367913
 O   -1.331915   -2.296913    2.286940
 C   -2.470000   -2.945038    2.837357
 H   -2.414768   -2.969106    3.934430
 H   -2.459567   -3.964394    2.436862
 H   -3.394525   -2.430530    2.537343
 C    1.761896    2.820228    2.062553
 H    1.170001    3.351754    1.304949
 H    2.829548    2.933611    1.845832
 H    1.533380    3.227528    3.057124
 C   -3.552678   -0.443528   -0.040163
 H   -2.882572   -0.856621    0.726289
 C   -3.733709   -1.496472   -1.108699
 C   -3.099113   -2.736993   -0.976228
 C   -4.529471   -1.270830   -2.240037
 C   -3.248807   -3.727778   -1.945998
 H   -2.458201   -2.917385   -0.108844
 C   -4.678336   -2.257344   -3.214059
 H   -5.040656   -0.313721   -2.366277
 C   -4.038923   -3.489618   -3.070083
 H   -2.739046   -4.686291   -1.825590
 H   -5.298667   -2.062606   -4.091983
 H   -4.154778   -4.261261   -3.834497
 C   -4.859395   -0.032339    0.701798
 H   -5.267946   -1.008640    1.082855
 H   -5.591323    0.253100   -0.107871
 O   -4.660518    0.913328    1.627665
 C    2.317445   -1.068657    0.951442
 H    2.681853   -0.045012    0.891633
 C    3.096381   -2.123411    0.468973
 H    2.751193   -3.127009    0.731857
 C    4.564465   -2.024083    0.277565
 C    5.310412   -3.196739    0.079852
 C    5.251319   -0.800945    0.295254
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 C    6.689494   -3.150786   -0.109368
 H    4.796722   -4.161965    0.072949
 C    6.630111   -0.752175    0.102635
 H    4.709322    0.129623    0.467606
 C    7.356329   -1.925484   -0.104175
 H    7.245738   -4.078505   -0.260867
 H    7.142277    0.212524    0.119965
 H    8.437266   -1.884674   -0.254365
 C    3.558706    1.457342   -1.922602
 H    3.355121    0.418399   -1.627433
 H    3.752526    1.460944   -3.007274
 H    4.482842    1.785800   -1.425836
 C    1.697039    6.077182   -1.052718
 H    2.724810    6.377713   -1.297767
 H    1.009602    6.643240   -1.698906
 H    1.494692    6.384677   -0.014523
 H   -0.620462    4.710262   -0.899291
 H    0.968599    0.761655   -1.620692
 C    0.124239   -1.713730   -1.727074
 H   -0.724219   -1.701444   -2.411874
 C    1.288287   -2.204155   -1.800736
 C    2.587385   -2.572051   -1.627358
 H    2.820632   -3.633874   -1.508898
 H    3.358138   -1.980658   -2.132381
Na   -2.932710    1.536012    2.718431
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_O5 / electronic energy: -3681.01685875 a.u. / lowest freq: -455.87 cm-1
 C   -3.544314    1.987791   -0.997868
 H   -4.302445    2.257405   -0.253080
 C   -2.404127    2.999453   -1.091434
 H   -2.423494    3.591482   -2.016339
 C   -1.520200    0.887070   -0.627346
 C    0.085462    2.648442   -1.206686
 C    0.316633    4.024064   -1.123616
 C    1.158122    1.785962   -1.472418
 C    1.611814    4.540394   -1.264511
 C    2.451661    2.281206   -1.614207
 C    2.668769    3.661021   -1.498599
 H    3.682428    4.056685   -1.608784
Cu   -0.285931   -0.566678   -0.053637
 N   -2.837904    0.782072   -0.552886
 N   -1.216041    2.139317   -1.041840
 C    0.983556   -1.281003    1.499720
 C    0.031332   -0.347394    2.049079
Na   -2.953243    1.608695    2.661366
 H   -2.402741    3.694084   -0.234833
 H   -4.030499    1.812310   -1.970928
 H    0.694261   -2.327538    1.628440
 C    0.246729    1.099521    2.204251
 C   -1.174748   -0.897139    2.684780
 O    1.518158    1.465251    2.039021
 O   -0.621238    1.929544    2.431290
 O   -1.922815   -0.307451    3.445577
 O   -1.419651   -2.171541    2.340944
 C   -2.585516   -2.769008    2.888588
 H   -2.512598   -2.842513    3.982574
 H   -2.647764   -3.769358    2.447205
 H   -3.480025   -2.182880    2.630114
 C    1.807930    2.854730    2.055244
 H    1.247255    3.376575    1.267928
 H    2.883047    2.941398    1.864526
 H    1.561559    3.293571    3.031972
 C   -3.524998   -0.424180   -0.113142
 H   -2.880102   -0.875351    0.656304
 C   -3.699776   -1.443248   -1.217182
 C   -4.032771   -2.760254   -0.872696
 C   -3.534477   -1.134269   -2.571613
 C   -4.199144   -3.738196   -1.850648
 H   -4.148905   -3.024840    0.181499
 C   -3.698780   -2.111765   -3.554339
 H   -3.249752   -0.123545   -2.870293
 C   -4.032661   -3.417555   -3.198734
 H   -4.449801   -4.760514   -1.558297
 H   -3.557221   -1.850199   -4.605471
 H   -4.155087   -4.184117   -3.966986
 C   -4.848048   -0.025362    0.617579
 H   -5.285470   -1.004007    0.953244
 H   -5.549112    0.303543   -0.203409
 O   -4.650738    0.876275    1.585002
 C    2.279943   -1.078139    1.000549
 H    2.663391   -0.063700    0.904671
 C    3.033274   -2.163179    0.545910
 H    2.667240   -3.149841    0.842429
 C    4.500839   -2.105430    0.336975
 C    5.215130   -3.301929    0.166529
 C    5.218614   -0.900299    0.312790
 C    6.592639   -3.296747   -0.038230
 H    4.677927   -4.253952    0.193970
 C    6.596068   -0.892324    0.104367
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 H     4.701995    0.047984    0.464976
 C     7.290145   -2.089120   -0.076107
 H     7.123780   -4.242237   -0.168461
 H     7.132287    0.059280    0.088192
 H     8.370047   -2.080656   -0.238686
 C     3.583721    1.346157   -1.947518
 H     3.762243    1.326860   -3.034640
 H     4.522042    1.661262   -1.469101
 H     3.360498    0.317348   -1.631696
 C     1.844472    6.022272   -1.125417
 H     2.878141    6.292551   -1.380609
 H     1.167801    6.595565   -1.776607
 H     1.655850    6.350956   -0.091147
 H    -0.504599    4.714732   -0.926303
 H     0.978698    0.717605   -1.605561
 C     0.031340   -1.818947   -1.618019
 H    -0.843703   -1.833823   -2.270119
 C     1.193864   -2.310751   -1.698485
 C     2.495826   -2.674244   -1.536184
 H     2.729106   -3.730884   -1.379126
 H     3.259351   -2.105175   -2.076885
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_O6 / electronic energy: -3681.01677377 a.u. / lowest freq: -425.81 cm-1
 C     2.738942   -2.118966    0.923536
 H     2.507597   -3.112529    1.313677
 C     0.523057   -1.406407    1.650699
 H     0.296559   -2.467977    1.774669
 C     1.827683   -1.105771    1.225910
 H     2.113890   -0.064860    1.089111
 C    -0.523012   -0.519574    2.099049
 C    -0.357444    0.915968    2.357490
 O    -1.247517    1.708590    2.627333
 C    -1.795584   -1.124733    2.516028
 O    -2.725428   -0.563523    3.073998
 O    -1.879614   -2.428300    2.211112
 C     4.183163   -1.855284    0.732650
 C     4.688680   -0.571287    0.474151
 C     6.054592   -0.364374    0.299533
 C     6.947899   -1.433619    0.381030
 C     6.460080   -2.714431    0.642167
 C     5.093579   -2.920347    0.815959
 C     2.350722   -2.999543   -1.120349
 H     2.537368   -4.021140   -0.777770
 H     3.177452   -2.521943   -1.654142
 C     1.081712   -2.623509   -1.428507
 C    -0.057909   -2.077991   -1.491133
 H    -0.886966   -2.120992   -2.201156
Cu    -0.442908   -0.673965   -0.086100
 C    -1.249373    1.035194   -0.698157
 N    -2.548012    1.289651   -0.665578
 N    -0.596241    2.183032   -0.984310
 C    -3.542934    0.251906   -0.405669
 C    -2.869705    2.670482   -1.047014
 H    -3.620953    3.070566   -0.355106
 C    -1.499517    3.340174   -0.948886
 H    -1.289667    4.031154   -1.775926
 C     0.794148    2.284667   -1.191702
 C     1.475668    1.239506   -1.831028
 C     1.489496    3.429188   -0.805775
 C     2.848222    1.314643   -2.049798
 C     2.875132    3.517720   -1.001222
 C     3.540104    2.455027   -1.613937
 H     4.619298    2.522786   -1.780258
Na    -3.539101    1.571729    2.677577
 H    -1.378983    3.884528    0.002859
 H    -3.270246    2.698872   -2.074203
 O     0.909072    1.333802    2.264789
 C    -3.062762   -3.106675    2.599793
 H    -3.152375   -3.144469    3.694810
 H    -2.976896   -4.120248    2.194084
 H    -3.954048   -2.609389    2.191945
 C     1.156772    2.708311    2.507092
 H     0.506977    3.339905    1.888086
 H     2.206449    2.878884    2.244188
 H     0.987032    2.950315    3.566059
 H    -3.239100   -0.253360    0.524292
 C    -3.571981   -0.784709   -1.504800
 C    -3.834252   -2.121130   -1.183498
 C    -3.342715   -0.454375   -2.845189
 C    -3.858277   -3.105909   -2.169254
 H    -4.000143   -2.395380   -0.138907
 C    -3.363197   -1.435991   -3.835292
 H    -3.119951    0.579405   -3.118756
 C    -3.618779   -2.766685   -3.501119
 H    -4.051382   -4.145426   -1.895044
 H    -3.172698   -1.161258   -4.875274
 H    -3.626049   -3.536739   -4.275348
 C    -4.922352    0.896482   -0.075986
 H    -5.616493    0.017636    0.014660
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 H   -5.255709    1.393696   -1.032421
 O   -4.872456    1.703009    0.993306
 H    4.719336   -3.927815    1.017260
 H    4.010325    0.280512    0.393027
 H    7.149231   -3.559113    0.710973
 H    6.423864    0.643536    0.096075
 H    8.018467   -1.269010    0.242147
 C    3.616284    4.749167   -0.548970
 H    3.476491    4.918583    0.529924
 H    4.694050    4.664411   -0.742973
 H    3.244935    5.646291   -1.067815
 C    3.568347    0.208613   -2.775655
 H    4.079885    0.594904   -3.670358
 H    4.334710   -0.251337   -2.133410
 H    2.869918   -0.577898   -3.092962
 H    0.919321    0.368335   -2.178545
 H    0.963334    4.260699   -0.331868
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_07 / electronic energy: -3681.01671535 a.u. / lowest freq: -426.21 cm-1
 C    2.740000   -2.119828    0.920462
 H    2.508209   -3.114044    1.308662
 C    0.524323   -1.408985    1.648876
 H    0.298245   -2.470926    1.770411
 C    1.828912   -1.107033    1.224970
 H    2.114930   -0.065749    1.090290
 C   -0.522364   -0.523750    2.098955
 C   -0.357669    0.911138    2.361532
 O   -1.248367    1.702231    2.633862
 C   -1.794928   -1.130772    2.513300
 O   -2.725113   -0.572007    3.073135
 O   -1.878596   -2.433152    2.203121
 C    4.184426   -1.856712    0.730277
 C    4.691342   -0.572242    0.476964
 C    6.057444   -0.366270    0.302495
 C    6.949502   -1.436904    0.379018
 C    6.460294   -2.718205    0.635146
 C    5.093662   -2.923173    0.808815
 C    2.351319   -2.996488   -1.124643
 H    2.537734   -4.018813   -0.784113
 H    3.178104   -2.518267   -1.657779
 C    1.082349   -2.619843   -1.432416
 C   -0.057264   -2.074291   -1.494357
 H   -0.886304   -2.115847   -2.204473
Cu   -0.442374   -0.673421   -0.086184
 C   -1.250265    1.036261   -0.694639
 N   -2.549014    1.290057   -0.661645
 N   -0.597563    2.184957   -0.978243
 C   -3.543513    0.251131   -0.404941
 C   -2.871335    2.671576   -1.040012
 H   -3.622564    3.069873   -0.347041
 C   -1.501378    3.341666   -0.940822
 H   -1.291946    4.034147   -1.766711
 C    0.792517    2.287254   -1.187206
 C    1.473908    1.244447   -1.828490
 C    1.488287    3.431159   -0.796699
 C    2.847785    1.319361   -2.044425
 C    2.872982    3.520493   -0.991506
 C    3.539067    2.457316   -1.604443
 H    4.619101    2.523838   -1.766393
Na   -3.539702    1.563884    2.682000
 H   -1.381004    3.884488    0.011806
 H   -3.272247    2.702088   -2.066994
 O    0.908471    1.330274    2.269819
 C   -3.061836   -3.113291    2.588369
 H   -3.151279   -3.156991    3.683189
 H   -2.976296   -4.124698    2.177209
 H   -3.953040   -2.613558    2.183350
 C    1.154848    2.704295    2.516785
 H    0.504577    3.337164    1.899553
 H    2.204348    2.877050    2.254679
 H    0.984265    2.942585    3.576464
 H   -3.239425   -0.256948    0.523413
 C   -3.572186   -0.781987   -1.507400
 C   -3.341756   -0.447564   -2.846574
 C   -3.835208   -2.119312   -1.190521
 C   -3.361773   -1.426071   -3.839768
 H   -3.118449    0.586985   -3.116756
 C   -3.858727   -3.100999   -2.179361
 H   -4.002088   -2.396842   -0.146957
 C   -3.618042   -2.757711   -3.509971
 H   -3.170389   -1.148097   -4.878727
 H   -4.052389   -4.141309   -1.908572
 H   -3.624933   -3.525375   -4.286574
 C   -4.923144    0.894191   -0.073188
 H   -5.616899    0.014787    0.015048
 H   -5.256868    1.393969   -1.028157
 O   -4.873416    1.697682    0.998368
 H    4.718301   -3.931015    1.006130
 H    4.014025    0.280760    0.399870
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 H    7.148453   -3.564003    0.700065
 H    6.427899    0.642004    0.103042
 H    8.020186   -1.272990    0.240203
 C    3.615976    4.760851   -0.567365
 H    3.210795    5.170630    0.369379
 H    4.686017    4.558635   -0.421106
 H    3.528351    5.548187   -1.333320
 C    3.568392    0.213159   -2.769667
 H    4.083893    0.599945   -3.661849
 H    4.331458   -0.249495   -2.125469
 H    2.869552   -0.571402   -3.090871
 H    0.918293    0.373235   -2.177077
 H    0.961482    4.259939   -0.319022
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_O8 / electronic energy: -3681.01672564 a.u. / lowest freq: -455.71 cm-1
 C   -3.634131    1.861274   -0.997707
 H   -4.406766    2.110048   -0.260734
 C   -2.536784    2.917467   -1.095691
 H   -2.587252    3.511367   -2.018038
 C   -1.570862    0.842341   -0.628888
 C   -0.038144    2.669605   -1.216141
 C    0.129117    4.055431   -1.131411
 C    1.076058    1.860536   -1.476275
 C    1.398008    4.632600   -1.268380
 C    2.345844    2.416739   -1.611825
 C    2.497323    3.804737   -1.499500
 H    3.491302    4.248086   -1.608148
Cu   -0.252796   -0.554912   -0.091780
 N   -2.882440    0.691167   -0.537192
 N   -1.316733    2.103180   -1.058195
 C    1.054192   -1.271833    1.436846
 C    0.091214   -0.361743    2.006813
 H   -2.556424    3.607869   -0.235546
 H   -4.097961    1.656935   -1.975675
 H    0.776063   -2.324075    1.543871
 C    0.284645    1.087287    2.174554
 C   -1.089624   -0.939720    2.664721
 O    1.543596    1.480169    1.980413
 O   -0.591808    1.898672    2.433143
 O   -1.828284   -0.370689    3.449149
 O   -1.321732   -2.216400    2.315889
 C   -2.469289   -2.833524    2.883476
 H   -2.378375   -2.899594    3.976430
 H   -2.519092   -3.837292    2.448156
 H   -3.378171   -2.266527    2.632756
 C    1.802779    2.875880    1.999540
 H    1.202269    3.391704    1.237998
 H    2.868340    2.988343    1.772449
 H    1.581090    3.300129    2.988613
 C   -3.525447   -0.520732   -0.028800
 H   -2.821254   -0.931160    0.707442
 C   -3.728148   -1.565639   -1.101234
 C   -4.558191   -1.338437   -2.207357
 C   -3.084975   -2.804222   -0.993034
 C   -4.731066   -2.320984   -3.181542
 H   -5.078279   -0.383713   -2.313534
 C   -3.258496   -3.790971   -1.963019
 H   -2.420336   -2.986605   -0.143993
 C   -4.082180   -3.550852   -3.062442
 H   -5.378936   -2.125181   -4.039123
 H   -2.742230   -4.748224   -1.861822
 H   -4.217254   -4.319475   -3.826776
 C   -4.812034   -0.141095    0.761717
 H   -5.192246   -1.128522    1.144030
 H   -5.575811    0.141989   -0.018996
 O   -4.594959    0.795541    1.691608
 C    2.351029   -1.046302    0.949836
 H    2.725907   -0.026763    0.881101
 C    3.115248   -2.113262    0.470909
 H    2.758684   -3.110236    0.744116
 C    4.583202   -2.035923    0.270620
 C    5.315946   -3.223727    0.121280
 C    5.281568   -0.819964    0.227579
 C    6.694584   -3.200348   -0.076223
 H    4.792457   -4.183009    0.159842
 C    6.659705   -0.793993    0.026359
 H    4.748545    0.122676    0.356723
 C    7.373425   -1.982930   -0.129459
 H    7.240837   -4.139444   -0.189149
 H    7.181154    0.165373   -0.004997
 H    8.453915   -1.960052   -0.286593
 C    0.134632   -1.715161   -1.712579
 H   -0.715330   -1.707356   -2.395469
 C    1.299922   -2.202497   -1.788865
 C    2.600872   -2.565281   -1.619107
 H    3.367204   -1.970900   -2.127453
 H    2.839536   -3.625869   -1.500092
Na   -2.891492    1.550947    2.724233
 H   -0.725325    4.706163   -0.939920
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 H    0.950866    0.785140   -1.611273
 C    3.524095    1.535227   -1.931976
 H    3.744171    1.559323   -3.011289
 H    4.431118    1.870336   -1.408283
 H    3.329112    0.488832   -1.657516
 C    1.565951    6.122031   -1.115944
 H    1.607897    6.399051   -0.050040
 H    2.494790    6.473147   -1.586179
 H    0.723077    6.668636   -1.562838
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_09 / electronic energy: -3681.01602735 a.u. / lowest freq: -466.70 cm-1
 C   -3.673078    1.708482   -0.921980
 H   -4.426369    1.951325   -0.162937
 C   -2.609933    2.796285   -1.071679
 H   -2.691155    3.350303   -2.016716
 C   -1.574700    0.758105   -0.579868
 C   -0.109986    2.613887   -1.252000
 C    0.021837    4.005815   -1.241995
 C    1.015005    1.822478   -1.524919
 C    1.264764    4.609173   -1.474786
 C    2.259847    2.404568   -1.748777
 C    2.374751    3.800781   -1.720129
 H    3.349035    4.264176   -1.899899
Cu   -0.203872   -0.569599   -0.011417
 N   -2.879067    0.557517   -0.491480
 N   -1.365196    2.023632   -1.020193
 C    1.183956   -1.194919    1.475103
 C    0.284013   -0.218466    2.032175
 H   -2.643147    3.521007   -0.241490
 H   -4.176992    1.490174   -1.876095
 H    0.882204   -2.229737    1.666382
 C    0.520608    1.230855    2.104855
 C   -0.847101   -0.712228    2.838075
 O    1.773059    1.589223    1.823659
 O   -0.330648    2.070195    2.361468
 O   -1.377112   -0.111266    3.754463
 O   -1.272550   -1.928267    2.471553
 C   -2.445984   -2.404176    3.126368
 H   -2.243041   -2.612404    4.186398
 H   -2.723712   -3.328688    2.608473
 H   -3.240898   -1.647800    3.041441
 C    2.052670    2.979950    1.763928
 H    1.399558    3.476027    1.033610
 H    3.098001    3.065674    1.448158
 H    1.916665    3.445504    2.750190
 C   -3.480835   -0.673059    0.018712
 H   -2.666970   -1.176879    0.558190
 C   -3.950435   -1.596207   -1.083868
 C   -5.026455   -1.268701   -1.920761
 C   -3.322142   -2.834848   -1.264946
 C   -5.447416   -2.146002   -2.919855
 H   -5.552954   -0.320981   -1.789547
 C   -3.741950   -3.716253   -2.260794
 H   -2.485121   -3.107810   -0.616043
 C   -4.805522   -3.372015   -3.094967
 H   -6.285851   -1.870728   -3.563932
 H   -3.235114   -4.675867   -2.385601
 H   -5.135992   -4.059593   -3.876673
 C   -4.566833   -0.335843    1.078819
 H   -4.917811   -1.346191    1.428536
 H   -5.454823    0.060610    0.509440
 O   -4.112203    0.477045    2.037850
 C    2.458966   -1.039838    0.907862
 H    2.857686   -0.037253    0.762521
 C    3.165244   -2.154723    0.447673
 H    2.800441   -3.122117    0.804639
 C    4.624344   -2.130829    0.174862
 C    5.325760   -3.343513    0.095248
 C    5.342734   -0.939786   -0.008679
 C    6.694330   -3.369016   -0.164652
 H    4.786794   -4.283915    0.240115
 C    6.710454   -0.962850   -0.271461
 H    4.832286    0.021616    0.057521
 C    7.393678   -2.176931   -0.352874
 H    7.217089   -4.326499   -0.220037
 H    7.247298   -0.021696   -0.410644
 H    8.466422   -2.193324   -0.557036
 C    3.454177    1.542428   -2.061934
 H    3.263556    0.487398   -1.819512
 H    3.707014    1.599833   -3.132503
 H    4.341629    1.873779   -1.502355
 C    1.394273    6.108877   -1.410838
 H    2.306669    6.456076   -1.914797
 H    0.530892    6.606078   -1.876289
 H    1.442360    6.449603   -0.363906
 H   -0.840860    4.642080   -1.038935
 H    0.915325    0.738458   -1.600810
 C    0.086142   -1.809924   -1.598059
 H   -0.786279   -1.810646   -2.252102
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 C    1.238759   -2.322219   -1.699088
 C    2.541845   -2.697304   -1.565054
 H    2.768881   -3.757256   -1.418348
 H    3.289366   -2.140050   -2.139242
Na   -2.597185    1.679307    2.891124
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_10 / electronic energy: -3681.01100626 a.u. / lowest freq: -418.22 cm-1
 C   -2.619613   -2.166296    1.436365
 H   -2.438546   -3.129773    1.915738
 C   -0.527366   -2.328297    0.156714
 H   -0.147396   -2.976247    0.950888
 C   -1.836303   -1.842700    0.325528
 H   -2.236142   -1.136598   -0.403023
 C    0.342975   -2.178209   -0.986058
 C   -0.101484   -1.818821   -2.339334
 O    0.619641   -1.485473   -3.265733
 C    1.718348   -2.683064   -0.871491
 O    2.519430   -2.837659   -1.778603
 O    2.061061   -2.965852    0.395089
 C   -3.995856   -1.635457    1.550741
 C   -4.282993   -0.307246    1.198061
 C   -5.577542    0.192561    1.298148
 C   -6.612626   -0.623782    1.759904
 C   -6.336985   -1.940963    2.126880
 C   -5.038516   -2.440883    2.028403
 C   -1.779086   -1.281555    3.346902
 H   -1.687056   -2.231522    3.881455
 H   -2.665455   -0.687031    3.583761
 C   -0.650441   -0.638644    2.954499
 C    0.306411   -0.119323    2.311359
 H    1.161869    0.496618    2.592678
Cu    0.335815   -0.438789    0.297746
 C    1.089159    1.230249   -0.449275
 N    2.390581    1.479690   -0.471777
 N    0.437016    2.332726   -0.880006
 C    3.424335    0.539320   -0.076125
 C    2.714891    2.776575   -1.072965
 H    3.135299    2.592203   -2.072878
 C    1.350406    3.463166   -1.090750
 H    1.254149    4.197239   -0.274283
 C   -0.967735    2.482498   -0.926917
 C   -1.555429    3.661796   -0.455993
 C   -1.771094    1.473888   -1.461980
 C   -2.940428    3.830738   -0.494083
 C   -3.162511    1.621756   -1.508904
 C   -3.729287    2.800375   -1.018443
 H   -4.815126    2.927389   -1.058801
Na    2.886905   -1.130247   -3.323368
 H    1.130641    3.970161   -2.039781
 H    3.455774    3.321521   -0.472835
 O   -1.426500   -1.897129   -2.511391
 C    3.375125   -3.453678    0.610747
 H    3.510753   -4.438496    0.141716
 H    3.496296   -3.532333    1.696213
 H    4.120243   -2.760158    0.195921
 C   -1.916706   -1.612850   -3.814168
 H   -1.719687   -0.565933   -4.087516
 H   -2.995606   -1.794235   -3.777503
 H   -1.447765   -2.270155   -4.558653
 H    2.961555   -0.459284   -0.116778
 C    3.913052    0.779434    1.339125
 C    3.496135    1.870468    2.110629
 C    4.818867   -0.124241    1.912902
 C    3.974858    2.059268    3.408363
 H    2.769113    2.577499    1.706127
 C    5.298890    0.060376    3.207478
 H    5.148516   -0.994164    1.340895
 C    4.881272    1.157368    3.961971
 H    3.630656    2.917603    3.989968
 H    6.001625   -0.660973    3.630970
 H    5.255743    1.303605    4.977438
 C    4.562693    0.540178   -1.151533
 H    5.294601   -0.228618   -0.785330
 H    5.110584    1.514012   -0.996817
 O    4.103355    0.344599   -2.391137
 H   -4.830621   -3.474574    2.317180
 H   -3.475960    0.349084    0.862443
 H   -7.138467   -2.586254    2.493788
 H   -5.775918    1.231194    1.022470
 H   -7.628235   -0.230529    1.842527
 C   -4.029454    0.553431   -2.120800
 H   -3.978685    0.596623   -3.220222
 H   -3.709388   -0.452890   -1.815627
 H   -5.080621    0.677005   -1.827759
 C   -3.581047    5.083199    0.044513
 H   -2.842540    5.882738    0.193832
 H   -4.359664    5.454891   -0.637612
 H   -4.063979    4.886862    1.014841
 H   -0.931752    4.454919   -0.039908
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 H   -1.301956    0.577595   -1.868887
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_11 / electronic energy: -3681.01145389 a.u. / lowest freq: -445.76 cm-1
 C   -2.966054   -0.929287    1.962501
 H   -2.745388   -1.412993    2.916926
 C   -0.837786   -1.765681    1.100060
 H   -0.555700   -1.941300    2.141825
 C   -2.132255   -1.261045    0.891723
 H   -2.471830   -1.065915   -0.126146
 C    0.114303   -2.242169    0.123464
 C   -0.201811   -2.523949   -1.285698
 O    0.610734   -2.662867   -2.185421
 C    1.411313   -2.742236    0.596059
 O    2.235913   -3.359851   -0.057091
 O    1.651272   -2.443387    1.884972
 C   -4.395959   -0.610578    1.741209
 C   -4.811697    0.155865    0.641183
 C   -6.159627    0.429535    0.431667
 C   -7.121892   -0.049697    1.324005
 C   -6.719716   -0.796226    2.430840
 C   -5.367775   -1.070045    2.639659
 C   -2.380537    0.998832    2.884361
 H   -2.513206    0.649999    3.912627
 H   -3.203230    1.596451    2.481408
 C   -1.127124    1.268922    2.433514
 C   -0.022341    1.307142    1.818300
 H    0.812908    2.007590    1.829110
Cu    0.316734   -0.147034    0.438193
 C    1.428562    0.798344   -0.898030
 N    2.745834    0.853549   -1.013865
 N    0.880450    1.634677   -1.797014
 C    3.681650    0.106733   -0.176365
 C    3.194089    1.747552   -2.084260
 H    3.692600    1.146205   -2.858139
 C    1.880383    2.384792   -2.563409
 H    1.823510    3.460040   -2.332587
 C   -0.516995    1.871068   -1.880860
 C   -1.364302    0.852963   -2.313852
 C   -1.036651    3.109195   -1.498728
 C   -2.748349    1.059128   -2.363724
 C   -2.412892    3.338226   -1.535508
 C   -3.249765    2.303808   -1.973840
 H   -4.329438    2.476195   -2.013265
Na    2.899878   -2.718869   -2.198746
 H    1.713710    2.257171   -3.642428
 H    3.905269    2.492664   -1.699650
 O   -1.509384   -2.647466   -1.533772
 C    2.883132   -2.894212    2.429278
 H    2.970722   -3.986507    2.351537
 H    2.878580   -2.588526    3.481042
 H    3.733705   -2.430370    1.908389
 C   -1.874748   -3.016738   -2.855338
 H   -1.545793   -2.263210   -3.584695
 H   -2.967016   -3.092230   -2.859281
 H   -1.429111   -3.984552   -3.123056
 H    3.112697   -0.761413    0.184688
 C    4.095445    0.926722    1.030390
 C    5.086848    1.914411    0.958880
 C    3.450219    0.721512    2.257047
 C    5.418606    2.674986    2.080652
 H    5.612662    2.092996    0.018600
 C    3.777367    1.480326    3.379683
 H    2.666815   -0.038171    2.325825
 C    4.765002    2.461992    3.294247
 H    6.195043    3.439875    2.005424
 H    3.257391    1.304564    4.324205
 H    5.025413    3.058471    4.171611
 C    4.837953   -0.468380   -1.037611
 H    5.494155   -0.994945   -0.289160
 H    5.467214    0.410492   -1.356071
 O    4.399775   -1.220446   -2.055106
 H   -5.060651   -1.657723    3.508953
 H   -4.063933    0.564624   -0.041823
 H   -7.463058   -1.169035    3.139275
 H   -6.461599    1.029949   -0.430032
 H   -8.180150    0.164727    1.160110
 C   -2.988169    4.647455   -1.063272
 H   -2.284648    5.476592   -1.222242
 H   -3.928716    4.883716   -1.580381
 H   -3.206647    4.601688    0.015811
 C   -3.672041   -0.038589   -2.820078
 H   -4.696833    0.331679   -2.958994
 H   -3.332469   -0.476627   -3.769837
 H   -3.710130   -0.852615   -2.078670
 H   -0.926912   -0.097401   -2.628055
 H   -0.358682    3.889901   -1.145639
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_12 / electronic energy: -3681.01103126 a.u. / lowest freq: -418.42 cm-1
 C    2.626113   -2.179060   -1.414908
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 H    2.441478   -3.146221   -1.885466
 C    0.535938   -2.326386   -0.130734
 H    0.155469   -2.982784   -0.917714
 C    1.845080   -1.843660   -0.305973
 H    2.247257   -1.131510    0.415203
 C   -0.333719   -2.166220    1.011401
 C    0.110343   -1.790789    2.360454
 O   -0.611603   -1.452169    3.284320
 C   -1.707831   -2.676125    0.903030
 O   -2.506871   -2.826191    1.812616
 O   -2.051971   -2.969441   -0.360857
 C    4.004354   -1.654454   -1.535100
 C    4.296808   -0.323601   -1.196961
 C    5.593369    0.169887   -1.302895
 C    6.625034   -0.655756   -1.755717
 C    6.344108   -1.975796   -2.108049
 C    5.043634   -2.469313   -2.004043
 C    1.787873   -1.307400   -3.331205
 H    1.698070   -2.261129   -3.859378
 H    2.673322   -0.712862   -3.571497
 C    0.657622   -0.663521   -2.945002
 C   -0.300768   -0.140644   -2.307046
 H   -1.157051    0.471070   -2.594970
Cu   -0.331999   -0.440817   -0.290575
 C   -1.092885    1.234895    0.434420
 N   -2.395238    1.479859    0.449853
 N   -0.446053    2.346143    0.851021
 C   -3.425317    0.529353    0.069187
 C   -2.725839    2.783636    1.032325
 H   -3.146154    2.611589    2.034470
 C   -1.364418    3.476010    1.041832
 H   -1.269648    4.197248    0.213833
 C    0.957876    2.503270    0.896046
 C    1.766416    1.498740    1.437712
 C    1.540317    3.679924    0.420101
 C    3.154734    1.651559    1.483884
 C    2.927481    3.853986    0.456480
 C    3.718709    2.831004    0.984217
 H    4.804176    2.959688    1.021391
Na   -2.879169   -1.104982    3.340492
 H   -1.148280    3.998938    1.983033
 H   -3.468567    3.316753    0.423913
 O    1.436026   -1.859074    2.531646
 C   -3.365486   -3.461319   -0.570695
 H   -3.498257   -4.443292   -0.094950
 H   -3.488585   -3.547382   -1.655376
 H   -4.111150   -2.766472   -0.159030
 C    1.926224   -1.555741    3.830132
 H    1.727198   -0.505422    4.088666
 H    3.005502   -1.735316    3.795542
 H    1.458920   -2.203437    4.583955
 H   -2.956833   -0.466063    0.119560
 C   -3.920905    0.750744   -1.346876
 C   -4.832823   -0.157624   -1.903465
 C   -3.503684    1.829076   -2.135977
 C   -5.318735    0.010945   -3.198021
 H   -5.162988   -1.018278   -1.317923
 C   -3.988152    2.001631   -3.433774
 H   -2.772155    2.538910   -1.744666
 C   -4.900900    1.095642   -3.969969
 H   -6.026452   -0.713465   -3.607788
 H   -3.643618    2.850276   -4.029237
 H   -5.280367    1.229330   -4.985321
 C   -4.559215    0.536833    1.149403
 H   -5.288362   -0.240416    0.795988
 H   -5.113218    1.505648    0.985242
 O   -4.093577    0.358865    2.389323
 H    4.831549   -3.505308   -2.281296
 H    3.492225    0.339492   -0.868668
 H    7.142898   -2.628340   -2.467925
 H    5.796290    1.210782   -1.039337
 H    7.642189   -0.267499   -1.842849
 C    3.542158    5.118752   -0.083627
 H    3.096595    6.007421    0.388217
 H    4.626362    5.146144    0.090506
 H    3.370757    5.206441   -1.167677
 C    4.027842    0.592617    2.103386
 H    5.076902    0.714881    1.802333
 H    3.984475    0.650025    3.202512
 H    3.708542   -0.418280    1.813232
 H    1.300024    0.603118    1.849164
 H    0.915189    4.469704   -0.000769
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_13 / electronic energy: -3681.01155941 a.u. / lowest freq: -461.85 cm-1
 C   -3.826362    1.199025   -1.066376
 H   -4.550017    1.404218   -0.267897
 C   -2.935386    2.405451   -1.373423
 H   -3.054432    2.783617   -2.398605
 C   -1.601114    0.617447   -0.658988
```

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 C   -0.436408    2.665633   -1.346510
 C   -0.566612    4.049747   -1.506574
 C    0.841469    2.093389   -1.368374
 C    0.564075    4.864175   -1.637040
 C    1.979493    2.890609   -1.471595
 C    1.829620    4.275971   -1.605127
 H    2.718740    4.905825   -1.697706
Cu   -0.106914   -0.522737   -0.000384
 N   -2.857337    0.205130   -0.600058
 N   -1.584383    1.871328   -1.168191
 C    1.321436   -1.032968    1.487520
 C    0.434687   -0.017484    1.992680
Na   -2.778968    1.609218    2.525424
 H   -3.125391    3.239098   -0.679019
 H   -4.368542    0.833755   -1.951152
 H    1.025804   -2.056969    1.735174
 C    0.809621    1.409297    1.954578
 C   -0.685358   -0.431146    2.845734
 O   -0.243458    2.251731    2.050972
 O    1.932028    1.837810    1.795737
 O   -1.278723    0.284990    3.637490
 O   -1.032467   -1.714091    2.687247
 C   -2.182875   -2.152676    3.406406
 H   -2.003594   -2.108270    4.489819
 H   -2.348999   -3.190548    3.097477
 H   -3.043442   -1.517468    3.142963
 C    0.061555    3.638999    2.011027
 H    0.683158    3.927329    2.870641
 H   -0.900722    4.162548    2.053785
 H    0.588224    3.895692    1.081875
 C   -3.263862   -1.063386   -0.014696
 H   -2.415683   -1.385185    0.610104
 C   -3.520664   -2.140518   -1.047314
 C   -3.784825   -3.447355   -0.611908
 C   -3.480117   -1.900464   -2.425304
 C   -4.018277   -4.474677   -1.523110
 H   -3.791914   -3.666344    0.458695
 C   -3.712265   -2.927963   -3.341296
 H   -3.241756   -0.903057   -2.799443
 C   -3.987246   -4.218766   -2.894684
 H   -4.216569   -5.485313   -1.158755
 H   -3.670095   -2.715918   -4.412108
 H   -4.166177   -5.023590   -3.610961
 C   -4.447293   -0.810223    0.973227
 H   -4.661377   -1.814563    1.423207
 H   -5.348976   -0.614046    0.327205
 O   -4.167423    0.152545    1.861141
 C    2.591746   -0.887600    0.906711
 H    2.979788    0.115482    0.731769
 C    3.308416   -2.012427    0.491581
 H    2.964957   -2.966107    0.902425
 C    4.760086   -1.978421    0.189701
 C    5.509098   -3.159471    0.296974
 C    5.422870   -0.807724   -0.209488
 C    6.875200   -3.173144    0.021150
 H    5.010061   -4.082527    0.604686
 C    6.787456   -0.819775   -0.486850
 H    4.867071    0.125407   -0.309689
 C    7.521376   -2.002014   -0.372942
 H    7.436851   -4.105233    0.116035
 H    7.282704    0.103754   -0.795272
 H    8.591831   -2.009049   -0.589527
 C    3.344061    2.262174   -1.400308
 H    3.337430    1.243244   -1.813924
 H    4.095323    2.854392   -1.941024
 H    3.659841    2.193850   -0.346455
 C    0.406023    6.357111   -1.765589
 H    1.297540    6.818260   -2.212377
 H   -0.465003    6.617737   -2.384192
 H    0.255134    6.818473   -0.776208
 H   -1.551544    4.517891   -1.520444
 H    0.959948    1.009073   -1.317088
 C    0.180437   -1.866649   -1.497118
 H   -0.714502   -1.953188   -2.114967
 C    1.347119   -2.345601   -1.602957
 C    2.662654   -2.676330   -1.485659
 H    2.926552   -3.717497   -1.279141
 H    3.380314   -2.129377   -2.105752
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_14 / electronic energy: -3681.00352015 a.u. / lowest freq: -478.56 cm-1
 C   -3.470925    2.180499   -0.462540
 H   -4.214185    2.320067    0.332403
 C   -2.346257    3.215263   -0.407316
 H   -2.402781    3.957308   -1.215212
 C   -1.423165    1.068089   -0.362841
 C    0.136625    2.934978   -0.690687
 C    0.342924    4.293661   -0.443566
 C    1.215916    2.144744   -1.116064
 C    1.611860    4.867957   -0.604424
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 C    2.485098    2.694429   -1.265210
 C    2.672323    4.060523   -1.010581
 H    3.667011    4.498383   -1.133409
Cu   -0.154881   -0.441656   -0.098247
 N   -2.737948    0.926667   -0.281149
 N   -1.147673    2.380279   -0.542211
 C    1.196274   -1.393809    1.252445
 C    0.375214   -0.455826    1.969608
Na   -3.201494   -3.268248    1.913620
 H   -2.327472    3.747485    0.556878
 H   -3.997010    2.170875   -1.430810
 H    0.798410   -2.413290    1.288462
 C    0.742719    0.944175    2.274908
 C   -0.811572   -1.058090    2.600027
 O    2.048512    1.184992    2.060928
 O   -0.004638    1.819598    2.651001
 O   -1.221382   -2.183205    2.319769
 O   -1.399962   -0.322874    3.528969
 C   -2.544369   -0.868721    4.177262
 H   -3.338933   -1.102211    3.448120
 H   -2.882773   -0.098248    4.878462
 H   -2.271840   -1.777393    4.735478
 C    2.480356    2.523204    2.237588
 H    1.877269    3.212216    1.630836
 H    3.525996    2.553389    1.910398
 H    2.408529    2.819087    3.294435
 C   -3.416003   -0.346199   -0.092732
 H   -2.610783   -1.076518    0.096443
 C   -4.153055   -0.767450   -1.356878
 C   -5.330007   -1.523817   -1.279257
 C   -3.660492   -0.425612   -2.622977
 C   -5.993232   -1.924692   -2.438815
 H   -5.696067   -1.803836   -0.288444
 C   -4.322168   -0.828255   -3.783092
 H   -2.749890    0.174021   -2.706878
 C   -5.492989   -1.580760   -3.695202
 H   -6.912222   -2.510760   -2.359429
 H   -3.920260   -0.549164   -4.759907
 H   -6.014329   -1.895426   -4.602118
 C   -4.285118   -0.355224    1.198207
 H   -5.214088    0.234129    0.961959
 H   -3.714625    0.301106    1.912044
 O   -4.527908   -1.596502    1.661111
 C    2.466725   -1.267650    0.668948
 H    2.957757   -0.295815    0.657835
 C    3.048817   -2.367227    0.028143
 H    2.598988   -3.335657    0.264770
 C    4.497961   -2.448636   -0.282840
 C    5.089047   -3.708117   -0.462666
 C    5.312092   -1.312889   -0.406958
 C    6.446033   -3.832142   -0.754433
 H    4.472344   -4.606393   -0.369264
 C    6.667904   -1.434078   -0.700864
 H    4.882710   -0.319473   -0.274603
 C    7.242799   -2.693871   -0.876190
 H    6.884174   -4.824117   -0.886040
 H    7.281552   -0.534869   -0.791939
 H    8.306772   -2.787992   -1.103666
 C    3.644221    1.837544   -1.699337
 H    4.078598    2.203575   -2.642211
 H    4.446529    1.862303   -0.945464
 H    3.341764    0.791217   -1.845611
 C    1.809179    6.333372   -0.315964
 H    2.842335    6.647388   -0.517445
 H    1.137494    6.952375   -0.930100
 H    1.585529    6.558205    0.738415
 H   -0.480451    4.926724   -0.109688
 H    1.060734    1.091998   -1.360026
 C   -0.033697   -1.488507   -1.832697
 H   -0.922406   -1.345645   -2.448425
 C    1.069359   -2.072172   -2.043434
 C    2.340786   -2.563159   -2.007496
 H    2.484049   -3.647612   -2.018367
 H    3.114789   -1.992578   -2.531699
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_15 / electronic energy: -3680.99812292 a.u. / lowest freq: -456.22 cm-1
 C   -3.745612    0.706435   -1.616098
 H   -3.891489    1.110388   -2.626480
 C   -3.993235   -0.801856   -1.537699
 H   -4.888799   -1.061052   -0.956045
 C   -1.830619   -0.328835   -0.773310
 C   -2.613168   -2.648010   -0.535452
 C   -3.493909   -3.606239   -1.043389
 C   -1.575714   -3.059558    0.314371
 C   -3.330088   -4.964766   -0.737719
 C   -1.383947   -4.404672    0.612797
 C   -2.270271   -5.351892    0.080529
 H   -2.129594   -6.410693    0.315948
Cu    0.089623   -0.514937   -0.257230
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 N    -2.343294    0.809530   -1.212390
 N    -2.779248   -1.290908   -0.872053
 C     1.660321   -0.361891    1.162722
 C     0.566797    0.472391    1.598629
Na     1.437437    3.501638   -1.542717
 H    -4.088486   -1.254813   -2.537144
 H    -4.379744    1.280134   -0.922814
 H     1.612390   -1.389892    1.536030
 C     0.656714    1.926079    1.404570
 C    -0.457540   -0.078205    2.509832
 O     0.043303    2.657250    2.322009
 O     1.284666    2.456388    0.492053
 O    -1.479446    0.465218    2.867152
 O    -0.174176   -1.342991    2.894789
 C    -1.163238   -2.003527    3.666224
 H    -1.345956   -1.472249    4.610642
 H    -0.771014   -3.005847    3.870060
 H    -2.109243   -2.078533    3.109927
 C     0.070397    4.067577    2.159660
 H     1.099140    4.449032    2.230654
 H    -0.539104    4.474781    2.972844
 H    -0.366129    4.357183    1.192958
 C    -1.587407    2.048117   -1.314441
 H    -0.613966    1.818860   -0.856390
 C    -2.243480    3.146187   -0.492800
 C    -2.325652    4.461305   -0.966737
 C    -2.757263    2.853618    0.777133
 C    -2.922968    5.456778   -0.192326
 H    -1.874147    4.692051   -1.933742
 C    -3.356965    3.847841    1.548218
 H    -2.656485    1.845709    1.188349
 C    -3.445440    5.153843    1.065009
 H    -2.979665    6.478372   -0.576443
 H    -3.746902    3.601611    2.538597
 H    -3.913948    5.934133    1.669482
 C    -1.245076    2.432471   -2.780357
 H    -2.207418    2.773365   -3.258316
 H    -1.024961    1.447912   -3.279141
 O    -0.248441    3.334622   -2.845099
 C     2.874607    0.000494    0.559308
 H     3.025136    1.034990    0.252811
 C     3.837069   -0.965091    0.262359
 H     3.717302   -1.928964    0.765665
 C     5.245606   -0.615884   -0.044988
 C     6.263901   -1.523046    0.280262
 C     5.605748    0.591781   -0.663805
 C     7.600391   -1.231256    0.011400
 H     6.002448   -2.471792    0.756701
 C     6.939839    0.884093   -0.934354
 H     4.833051    1.309189   -0.949359
 C     7.944775   -0.024969   -0.596749
 H     8.376119   -1.951999    0.279435
 H     7.198029    1.829231   -1.417494
 H     8.990846    0.205528   -0.809597
 C    -0.244622   -4.834289    1.499696
 H    -0.616402   -5.329773    2.410002
 H     0.404390   -5.555130    0.979638
 H     0.372908   -3.977270    1.802445
 C    -4.281649   -5.979863   -1.316562
 H    -4.143035   -6.968009   -0.857024
 H    -5.328148   -5.675076   -1.167050
 H    -4.125946   -6.088826   -2.401510
 H    -4.316979   -3.313012   -1.696465
 H    -0.909809   -2.324524    0.764702
 C     0.803012   -1.658349   -1.779502
 H    -0.006744   -1.954079   -2.446840
 C     2.050161   -1.872607   -1.821609
 C     3.399400   -1.914470   -1.651538
 H     3.866448   -2.865201   -1.377317
 H     4.010318   -1.263232   -2.283972
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_16 / electronic energy: -3681.00337669 a.u. / lowest freq: -462.64 cm-1
 C     0.432632    0.833593    1.624317
 O    -0.331710   -0.952619    2.995834
 C    -0.558071    0.126350    2.451766
 C     0.364498    2.272817    1.302100
 O     1.137388    2.839589    0.551115
 O    -0.601634    2.940222    1.936357
 O    -1.753570    0.696275    2.526200
 C     1.629201    0.096407    1.324418
 C     2.303868   -1.368885   -1.651259
 C     1.043201   -1.263649   -1.709369
 H     0.315219   -1.625701   -2.436860
 C     3.637391   -1.316845   -1.384762
 H     4.150510   -2.240472   -1.099428
 H     4.242288   -0.606797   -1.956472
 H     3.777233   -1.357967    1.062740
 C     3.886672   -0.383622    0.576488
 H     1.617680   -0.926695    1.718948
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 H    2.957945    1.567982    0.490716
 C    5.295117    0.031723    0.369273
 C    5.641114    1.271359   -0.191596
 C    6.328857   -0.844231    0.730191
 C    7.665884   -0.494205    0.547722
 C    7.995750    0.741623   -0.007006
 C    6.976047    1.621513   -0.376186
Cu    0.147415   -0.246845   -0.218866
 N   -2.503102   -1.464465   -0.026259
 N   -2.744104    0.606488   -0.632069
 C   -1.844115   -0.369746   -0.383784
 C   -3.959656   -1.300973   -0.046987
 H   -4.379876   -1.654994    0.903446
 C   -4.106732    0.205138   -0.265124
 H   -4.819755    0.457824   -1.061835
 C   -2.433417    1.909788   -1.061666
 C   -3.364560    2.943103   -0.890736
 C   -1.215284    2.183082   -1.689707
 C   -3.082886    4.236496   -1.336753
 C   -0.902113    3.476269   -2.112376
 C   -1.847032    4.491576   -1.941017
 H   -1.614077    5.505581   -2.278601
Na   -1.406285   -2.838315    3.731496
 H   -4.418349    0.726261    0.654170
 H   -4.403332   -1.886839   -0.867710
 C   -2.783823   -0.011922    3.201508
 H   -2.954365   -1.000747    2.736602
 H   -3.679490    0.614180    3.116812
 H   -2.539655   -0.135235    4.268381
 C   -0.730631    4.316975    1.626736
 H   -0.942404    4.458034    0.557903
 H    0.185224    4.867945    1.885550
 H   -1.571175    4.684771    2.225982
 C   -1.854680   -2.748712    0.219079
 H   -0.947334   -2.528692    0.806144
 C   -1.433928   -3.441351   -1.059691
 C   -0.417194   -4.402334   -1.003335
 C   -2.024394   -3.171845   -2.297969
 C    0.002472   -5.072963   -2.149323
 H    0.070172   -4.608853   -0.046363
 C   -1.605607   -3.839144   -3.450270
 H   -2.804325   -2.412180   -2.378213
 C   -0.590728   -4.792227   -3.381030
 H    0.805428   -5.810752   -2.083998
 H   -2.075209   -3.608217   -4.409178
 H   -0.258256   -5.309586   -4.283582
 C   -2.749451   -3.653358    1.120224
 H   -2.193591   -4.628300    1.155291
 H   -3.653093   -3.897427    0.493721
 O   -3.023932   -3.113591    2.319668
 C    2.856474    0.529984    0.804303
 H    6.078735   -1.816161    1.164304
 H    4.858305    1.967841   -0.499552
 H    8.453180   -1.192536    0.840548
 H    7.222840    2.589992   -0.817179
 H    9.042057    1.017488   -0.154961
 C    0.455012    3.753864   -2.698269
 H    0.742951    2.981673   -3.426663
 H    0.493449    4.733425   -3.194341
 H    1.204408    3.740684   -1.891518
 C   -4.098916    5.338098   -1.179213
 H   -3.619067    6.283858   -0.888427
 H   -4.626393    5.519117   -2.129519
 H   -4.853945    5.086873   -0.421559
 H   -4.320661    2.750492   -0.402240
 H   -0.496916    1.378462   -1.861678
83
Figure_S15-3_PA-9d(Na)-ts(1,6major)_17 / electronic energy: -3680.99860603 a.u. / lowest freq: -447.57 cm-1
 C    4.349904   -2.269685   -0.494220
 C    4.577515   -2.086770    0.878069
 C    5.825601   -2.350420    1.437642
 C    6.875809   -2.804331    0.638984
 C    6.663211   -2.996396   -0.726506
 C    5.414719   -2.731662   -1.284080
 C    3.041338   -1.994218   -1.131752
 C    1.846374   -1.921692   -0.409829
 H    1.864557   -1.848694    0.678978
 C    0.606880   -1.899294   -1.075132
 C   -0.717294   -2.023885   -0.526728
 H    0.635268   -1.977927   -2.166239
 C   -0.963956   -2.469531    0.853994
 O   -1.750740   -3.343357    1.177047
 C   -1.794019   -2.069343   -1.522612
 O   -1.636889   -1.879116   -2.713074
Cu    0.067201    0.039610   -0.584842
 N   -2.013804    1.628292    0.873843
 C   -0.748518    1.531212    0.477120
 N   -0.151162    2.720774    0.697517
 C    1.218866    1.028153   -1.977237
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 H    0.679288    1.922746   -2.287494
 C    2.400840    0.618969   -2.146348
 H    3.985376   -0.532775   -2.967561
 C    3.584846   -0.047144   -2.073624
 H    4.334566    0.323185   -1.367200
 C   -2.948181    0.519121    0.942921
 C   -2.339169    2.926741    1.469203
 H   -2.502574    2.814293    2.551780
 C   -1.091960    3.753473    1.147725
 H   -1.276678    4.485454    0.345655
 C    1.231643    2.978107    0.551589
 C    2.161950    2.092756    1.098081
 C    1.660482    4.126715   -0.114770
 C    3.530381    2.329553    0.953777
 C    3.025176    4.386980   -0.265967
 C    3.943327    3.475956    0.266147
 H    5.013717    3.670722    0.150893
Na   -3.948829   -2.780883    1.300741
 H   -0.691812    4.289506    2.018922
 H   -3.255790    3.337409    1.022979
 O   -0.241289   -1.820125    1.767657
 O   -3.034677   -2.270347   -1.017927
 C   -4.099885   -2.206241   -1.959379
 H   -4.147693   -1.212276   -2.424027
 H   -5.024402   -2.387106   -1.399461
 H   -3.977397   -2.969398   -2.739955
 C   -0.552012   -2.092183    3.133108
 H   -1.613779   -1.856041    3.312312
 H    0.100949   -1.441077    3.724121
 H   -0.354888   -3.145567    3.376270
 H   -2.385086   -0.348372    0.576890
 C   -4.118971    0.723706   -0.004231
 C   -5.401223    0.259488    0.313525
 C   -3.921139    1.341946   -1.245319
 C   -6.454139    0.405792   -0.590086
 H   -5.547980   -0.238304    1.274839
 C   -4.973093    1.491812   -2.148252
 H   -2.925783    1.707933   -1.510319
 C   -6.245790    1.020241   -1.824924
 H   -7.447818    0.035096   -0.326183
 H   -4.796186    1.975481   -3.111747
 H   -7.070366    1.132391   -2.532552
 C   -3.323255    0.170760    2.413598
 H   -4.033922    0.971441    2.764389
 H   -2.374795    0.371541    2.987685
 O   -3.793770   -1.080077    2.552706
 H    2.955757   -2.368193   -2.153947
 H    5.257539   -2.883791   -2.355396
 H    3.774918   -1.724931    1.522877
 H    7.475190   -3.355124   -1.363070
 H    5.979568   -2.196383    2.508050
 H    7.854101   -3.007907    1.079548
 C    3.494675    5.636525   -0.964783
 H    4.462571    5.478712   -1.461029
 H    2.769648    5.972389   -1.719451
 H    3.624630    6.458862   -0.242611
 C    4.540426    1.367792    1.520413
 H    5.473158    1.879575    1.796141
 H    4.150421    0.854551    2.410832
 H    4.797411    0.588311    0.786344
 H    1.805814    1.211629    1.637247
 H    0.926299    4.816348   -0.537766
83
Figure_S15-3_PA-9d(Na)-ts(1,6minor)_01 / electronic energy: -3681.01261478 a.u. / lowest freq: -459.96 cm-1
 C    3.659544    2.047246   -0.366906
 H    4.051864    2.555127    0.522168
 C    4.175987    0.617260   -0.516602
 H    4.864432    0.492678   -1.363392
 C    1.838989    0.587570   -0.437054
 C    2.960065   -1.534459   -0.968542
 C    4.149817   -2.254209   -0.824326
 C    1.799290   -2.212280   -1.368197
 C    4.182549   -3.637772   -1.048592
 C    1.805568   -3.589583   -1.566834
 C    3.006223   -4.294472   -1.407170
 H    3.021482   -5.375544   -1.571763
Cu   -0.052747   -0.026957   -0.282358
 N    2.219273    1.832147   -0.200960
 N    2.940741   -0.148649   -0.723460
 C   -1.406247   -1.192830    0.925565
 C   -0.363215   -0.625273    1.741140
Na    2.414098    1.220797    3.079838
 H    4.685482    0.268478    0.396785
 H    3.857266    2.662778   -1.258609
 H   -1.143551   -2.164928    0.493393
 C    0.833419   -1.426176    2.052715
 C   -0.517378    0.625019    2.497523
 O    0.702309   -2.713141    1.723429
 O    1.872805   -1.002170    2.535225
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 O    0.139354    0.959898    3.467674
 O   -1.461712    1.436263    2.000773
 C   -1.624071    2.695875    2.639351
 H   -1.915876    2.567285    3.690473
 H   -2.414555    3.214145    2.086305
 H   -0.687394    3.271175    2.597527
 C    1.842622   -3.542856    1.887734
 H    2.707214   -3.128827    1.351460
 H    1.573747   -4.516342    1.464302
 H    2.090698   -3.650111    2.953172
 C    1.303488    2.899082    0.174318
 H    0.479763    2.409590    0.715767
 C    0.707716    3.616456   -1.017868
 C    1.158006    3.418929   -2.327548
 C   -0.347302    4.515648   -0.808469
 C    0.580953    4.107297   -3.395645
 H    1.956395    2.701785   -2.527988
 C   -0.925803    5.204561   -1.872244
 H   -0.731667    4.667426    0.203412
 C   -0.460821    5.005697   -3.172922
 H    0.947875    3.934180   -4.409995
 H   -1.749346    5.897443   -1.684748
 H   -0.915430    5.540997   -4.009344
 C    2.011379    3.838889    1.205697
 H    1.223260    4.586326    1.490204
 H    2.737771    4.449566    0.595178
 O    2.556483    3.168668    2.226204
 C   -2.750928   -0.825870    0.784339
 H   -3.117401    0.064702    1.293180
 C   -3.585026   -1.513435   -0.096893
 H   -3.216921   -2.481294   -0.451129
 C   -5.062979   -1.407082   -0.042764
 C   -5.846104   -2.486908   -0.474925
 C   -5.717896   -0.255163    0.421237
 C   -7.238474   -2.427136   -0.433246
 H   -5.353980   -3.389598   -0.846991
 C   -7.108018   -0.193642    0.462069
 H   -5.135871    0.610796    0.744256
 C   -7.875891   -1.280064    0.037321
 H   -7.827715   -3.282881   -0.770557
 H   -7.597389    0.712199    0.827015
 H   -8.966327   -1.228993    0.070852
 C    0.528144   -4.306465   -1.915511
 H   -0.224144   -3.611830   -2.315294
 H    0.698584   -5.101549   -2.655583
 H    0.098276   -4.779192   -1.017398
 C    5.480189   -4.387041   -0.891376
 H    5.911320   -4.227961    0.108759
 H    5.340563   -5.466963   -1.035210
 H    6.224967   -4.040376   -1.624467
 H    5.071431   -1.751542   -0.528467
 H    0.876097   -1.659899   -1.549673
 C   -0.904423    0.218537   -2.097521
 H   -0.241045    0.749398   -2.781396
 C   -2.093103   -0.199342   -2.230770
 C   -3.362822   -0.671765   -2.113501
 H   -3.634098   -1.595490   -2.633831
 H   -4.165872    0.064162   -2.015214
83
Figure_S15-3_PA-9d(Na)-ts(1,6minor)_O2 / electronic energy: -3681.01062138 a.u. / lowest freq: -444.26 cm-1
 C   -3.584500   -2.115325   -0.695902
 H   -4.062522   -2.559701    0.188613
 C   -4.132110   -0.738477   -1.070779
 H   -4.339909   -0.655612   -2.148903
 C   -1.914146   -0.524214   -0.341504
 C   -3.151362    1.555728   -0.830673
 C   -2.199622    2.428895   -0.281987
 C   -4.241501    2.098087   -1.517929
 C   -2.301709    3.805966   -0.450235
 C   -4.374140    3.484274   -1.680781
 C   -3.397302    4.326321   -1.153100
 H   -3.488265    5.408116   -1.285285
Cu   -0.081573    0.216282   -0.041679
 N   -2.193449   -1.814798   -0.359605
 N   -3.032930    0.160045   -0.695152
 C    1.464881    0.945675    1.237968
 C    0.550112    0.132539    2.007738
 H   -5.049337   -0.478943   -0.523183
 H   -3.638538   -2.828714   -1.529852
 H    1.185423    2.003564    1.204212
 C   -0.573112    0.781808    2.705536
 C    0.824102   -1.261784    2.384573
 O   -0.537233    2.120705    2.634162
 O   -1.491978    0.219142    3.277603
 O    0.275529   -1.889944    3.272823
 O    1.761913   -1.843533    1.624217
 C    2.040374   -3.214027    1.876618
 H    2.424700   -3.354322    2.895923
 H    2.797130   -3.507357    1.141377
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 H    1.133711   -3.822536    1.746834
 C   -1.645319    2.822640    3.178255
 H   -2.572425    2.551643    2.652631
 H   -1.431688    3.886496    3.030867
 H   -1.759413    2.605123    4.248732
 C   -1.237268   -2.872153   -0.032157
 H   -0.512549   -2.399469    0.641461
 C   -0.487327   -3.323587   -1.269129
 C   -1.040995   -4.213564   -2.198697
 C    0.790510   -2.806856   -1.520806
 C   -0.336930   -4.569842   -3.349559
 H   -2.032115   -4.638747   -2.025327
 C    1.494499   -3.156573   -2.671438
 H    1.237553   -2.112820   -0.803771
 C    0.931145   -4.040857   -3.591347
 H   -0.783201   -5.266293   -4.063316
 H    2.485535   -2.732881   -2.849744
 H    1.478297   -4.317664   -4.495380
 C   -1.936234   -3.979675    0.801957
 H   -1.116125   -4.725668    0.999570
 H   -2.617528   -4.532487    0.095755
 O   -2.552204   -3.491887    1.886603
 C    2.752066    0.666685    0.752864
 H    3.152264   -0.340931    0.845679
 C    3.480478    1.638378    0.068945
 H    3.130869    2.669386    0.173982
 C    4.934995    1.507723   -0.184328
 C    5.723129    2.663397   -0.280877
 C    5.560871    0.260878   -0.342683
 C    7.095494    2.579601   -0.512495
 H    5.251551    3.643312   -0.167432
 C    6.930637    0.175988   -0.575581
 H    4.968770   -0.656042   -0.297067
 C    7.705729    1.334863   -0.659519
 H    7.689931    3.493684   -0.578542
 H    7.398333   -0.803669   -0.697395
 H    8.780116    1.265130   -0.842463
 C    0.408509    0.835728   -1.909296
 H   -0.422035    0.668625   -2.595768
 C    1.578137    1.281077   -2.104072
 C    2.877809    1.671727   -2.058486
 H    3.119252    2.731485   -2.183081
 H    3.634723    0.970555   -2.422030
Na   -2.044418   -2.030263    3.351863
 H   -5.005373    1.449585   -1.948334
 H   -1.363604    2.041099    0.297086
 C   -5.566563    4.037246   -2.417758
 H   -6.495305    3.855983   -1.854297
 H   -5.473521    5.120109   -2.576712
 H   -5.684707    3.555597   -3.400119
 C   -1.244508    4.721813    0.109009
 H   -0.489223    4.161653    0.677446
 H   -0.728253    5.259288   -0.701482
 H   -1.684840    5.480917    0.773480
83
Figure_S15-3_PA-9d(Na)-ts(1,6minor)_03 / electronic energy: -3681.01372521 a.u. / lowest freq: -473.84 cm-1
 C    3.459868    2.242979   -0.205475
 H    3.814140    2.770864    0.688122
 C    4.089084    0.860370   -0.366599
 H    4.815086    0.811480   -1.189270
 C    1.759060    0.660216   -0.360327
 C    3.049753   -1.341876   -0.982350
 C    4.282995   -1.987520   -0.830339
 C    1.966741   -2.059292   -1.504903
 C    4.432945   -3.335082   -1.177205
 C    2.090275   -3.408446   -1.832605
 C    3.330632   -4.035488   -1.672292
 H    3.440537   -5.090191   -1.940252
Cu   -0.077314   -0.113518   -0.280055
 N    2.040612    1.919636   -0.073875
 N    2.921281    0.016406   -0.640068
 C   -1.427661   -1.383063    0.794631
 C   -0.389160   -0.908463    1.669406
Na    2.227666    0.851759    3.267826
 H    4.590013    0.526959    0.557315
 H    3.623579    2.880802   -1.088373
 H   -1.183684   -2.321040    0.282976
 C    0.810403   -1.725592    1.908525
 C   -0.577241    0.219873    2.600680
 O    0.714679   -2.967026    1.425809
 O    1.830997   -1.340405    2.460269
 O   -0.044092    0.326163    3.689609
 O   -1.395555    1.168885    2.135205
 C   -1.506739    2.350554    2.927056
 H   -1.996575    2.130587    3.885960
 H   -2.121246    3.042557    2.340797
 H   -0.500705    2.761715    3.102094
 C    1.863292   -3.792831    1.544487
 H    2.739345   -3.314041    1.086988
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 H    1.626926   -4.721935    1.015011
 H    2.075859   -4.004924    2.601996
 C    1.043163    2.915067    0.313408
 H    0.161032    2.326438    0.601202
 C    0.652432    3.806012   -0.846796
 C    1.499744    4.811077   -1.333604
 C   -0.595108    3.632896   -1.459626
 C    1.113877    5.610807   -2.409648
 H    2.472058    4.980565   -0.865593
 C   -0.984535    4.430843   -2.534582
 H   -1.266025    2.850855   -1.093841
 C   -0.128737    5.422409   -3.014656
 H    1.789004    6.387952   -2.775410
 H   -1.960539    4.275591   -3.000168
 H   -0.430396    6.049119   -3.857033
 C    1.506964    3.659251    1.594977
 H    0.650286    4.351461    1.825163
 H    2.328625    4.363140    1.284284
 O    1.842174    2.816855    2.579697
 C   -2.757730   -0.956807    0.675706
 H   -3.088100   -0.090259    1.248099
 C   -3.618211   -1.541191   -0.256526
 H   -3.300175   -2.508712   -0.656838
 C   -5.091226   -1.371191   -0.183977
 C   -5.927614   -2.387761   -0.666072
 C   -5.687815   -0.214846    0.343116
 C   -7.315407   -2.263264   -0.611640
 H   -5.481212   -3.292517   -1.087645
 C   -7.073066   -0.088645    0.397205
 H   -5.062461    0.603888    0.706028
 C   -7.894737   -1.113068   -0.077918
 H   -7.947195   -3.070773   -0.988596
 H   -7.516550    0.819374    0.812106
 H   -8.981234   -1.011409   -0.033991
 C    0.888428   -4.175264   -2.317015
 H    0.152529   -3.510260   -2.790835
 H    1.168871   -4.957247   -3.036607
 H    0.386479   -4.669530   -1.469028
 C    5.757180   -4.025592   -0.976959
 H    5.800228   -4.502793    0.015406
 H    5.914600   -4.813669   -1.726871
 H    6.594788   -3.316632   -1.038132
 H    5.145954   -1.449135   -0.436411
 H    1.015512   -1.557098   -1.687042
 C   -0.873424    0.185519   -2.124329
 H   -0.175896    0.707605   -2.779560
 C   -2.071149   -0.189076   -2.293842
 C   -3.358047   -0.625107   -2.197508
 H   -3.654814   -1.512747   -2.764838
 H   -4.135100    0.138116   -2.093224
83
Figure_S15-3_PA-9d(Na)-ts(1,6minor)_O4 / electronic energy: -3681.01376311 a.u. / lowest freq: -473.62 cm-1
 C    3.467132    2.234161   -0.207755
 H    3.823505    2.761080    0.685550
 C    4.092210    0.849749   -0.369127
 H    4.818350    0.798725   -1.191560
 C    1.761705    0.656322   -0.361988
 C    3.047097   -1.349486   -0.983835
 C    4.276770   -1.998573   -0.831228
 C    1.960281   -2.064595   -1.505208
 C    4.421731   -3.348819   -1.175609
 C    2.078480   -3.413671   -1.829593
 C    3.317726   -4.045812   -1.667538
 H    3.422626   -5.101869   -1.931671
Cu   -0.077005   -0.112207   -0.280768
 N    2.047075    1.914782   -0.075085
 N    2.921982    0.009482   -0.643154
 C   -1.430360   -1.378168    0.794992
 C   -0.391194   -0.904621    1.669532
Na    2.228298    0.849371    3.270446
 H    4.591710    0.514467    0.554910
 H    3.631944    2.871358   -1.090914
 H   -1.187767   -2.316859    0.284000
 C    0.806361   -1.724242    1.910176
 C   -0.577030    0.225753    2.598602
 O    0.708070   -2.965728    1.428213
 O    1.827465   -1.341084    2.462379
 O   -0.043370    0.333518    3.687155
 O   -1.393582    1.175533    2.131418
 C   -1.501962    2.359004    2.920893
 H   -1.992341    2.142143    3.880220
 H   -2.114651    3.051420    2.333237
 H   -0.495116    2.768234    3.095550
 C    1.855040   -3.793791    1.547172
 H    2.731620   -3.317596    1.087971
 H    1.616254   -4.723160    1.019258
 H    2.068130   -4.004783    2.604786
 C    1.052847    2.913072    0.313194
 H    0.169914    2.326941    0.603523
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 C    0.661600    3.803564   -0.847180
 C   -0.587804    3.632770   -1.456853
 C    1.510229    4.805932   -1.337230
 C   -0.977790    4.430321   -2.531898
 H   -1.259783    2.852824   -1.088546
 C    1.123764    5.605324   -2.413306
 H    2.484029    4.973633   -0.871665
 C   -0.120710    5.419208   -3.015191
 H   -1.955211    4.276796   -2.995087
 H    1.799894    6.380425   -2.781550
 H   -0.422820    6.045614   -3.857632
 C    1.521478    3.657667    1.592811
 H    0.667218    4.352567    1.823920
 H    2.344294    4.358964    1.279167
 O    1.856829    2.815771    2.577857
 C   -2.759904   -0.950397    0.676063
 H   -3.089344   -0.083281    1.248136
 C   -3.621030   -1.534397   -0.255738
 H   -3.303645   -2.502115   -0.656089
 C   -5.093899   -1.363523   -0.182947
 C   -5.930903   -2.379796   -0.664608
 C   -5.689768   -0.206924    0.344393
 C   -7.318616   -2.254809   -0.609417
 H   -5.485041   -3.284751   -1.086327
 C   -7.074943   -0.080233    0.399231
 H   -5.063913    0.611548    0.707030
 C   -7.897233   -1.104394   -0.075391
 H   -7.950903   -3.062116   -0.985964
 H   -7.517892    0.827932    0.814382
 H   -8.983668   -1.002384   -0.030789
 C    0.874567   -4.178626   -2.311660
 H    0.132022   -3.510303   -2.770151
 H    1.150720   -4.950875   -3.043386
 H    0.382590   -4.685262   -1.465133
 C    5.750416   -4.031449   -0.978350
 H    5.939586   -4.212929    0.091657
 H    5.785254   -5.001167   -1.493207
 H    6.577540   -3.411393   -1.354299
 H    5.142107   -1.463507   -0.437551
 H    1.010699   -1.559127   -1.686902
 C   -0.873992    0.187641   -2.124527
 H   -0.175910    0.708303   -2.780324
 C   -2.072513   -0.184683   -2.293638
 C   -3.360159   -0.618330   -2.197111
 H   -3.658661   -1.505534   -2.764206
 H   -4.135918    0.146132   -2.092283
83
Figure_S15-3_PA-9d(Na)-ts(1,6minor)_05 / electronic energy: -3681.01376311 a.u. / lowest freq: -473.62 cm-1
 C    3.467157    2.234121   -0.207720
 H    3.823530    2.761035    0.685588
 C    4.092216    0.849702   -0.369090
 H    4.818372    0.798674   -1.191509
 C    1.761709    0.656308   -0.361984
 C    3.047080   -1.349513   -0.983829
 C    4.276745   -1.998615   -0.831222
 C    1.960255   -2.064609   -1.505204
 C    4.421690   -3.348863   -1.175601
 C    2.078438   -3.413686   -1.829588
 C    3.317677   -4.045843   -1.667530
 H    3.422564   -5.101902   -1.931661
Cu   -0.077008   -0.112204   -0.280774
 N    2.047094    1.914761   -0.075060
 N    2.921980    0.009456   -0.643146
 C   -1.430371   -1.378147    0.794999
 C   -0.391201   -0.904602    1.669535
Na    2.228310    0.849393    3.270431
 H    4.591691    0.514404    0.554954
 H    3.631982    2.871317   -1.090877
 H   -1.187785   -2.316842    0.284012
 C    0.806352   -1.724227    1.910179
 C   -0.577028    0.225778    2.598600
 O    0.708049   -2.965717    1.428231
 O    1.827462   -1.341067    2.462369
 O   -0.043360    0.333546    3.687149
 O   -1.393579    1.175559    2.131418
 C   -1.501949    2.359035    2.920886
 H   -1.992327    2.142183    3.880216
 H   -2.114634    3.051453    2.333228
 H   -0.495099    2.768259    3.095539
 C    1.855015   -3.793786    1.547190
 H    2.731593   -3.317605    1.087972
 H    1.616217   -4.723161    1.019293
 H    2.068115   -4.004764    2.604805
 C    1.052873    2.913067    0.313195
 H    0.169933    2.326951    0.603531
 C    0.661643    3.803541   -0.847199
 C   -0.587758    3.632746   -1.456879
 C    1.510285    4.805891   -1.337262
 C   -0.977727    4.430277   -2.531945
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 H   -1.259749    2.852816   -1.088561
 C    1.123838    5.605264   -2.413359
 H    2.484083    4.973593   -0.871692
 C   -0.120633    5.419146   -3.015252
 H   -1.955145    4.276752   -2.995139
 H    1.799978    6.380351   -2.781612
 H   -0.422729    6.045536   -3.857709
 C    1.521504    3.657683    1.592800
 H    0.667246    4.352592    1.823893
 H    2.344324    4.358970    1.279148
 O    1.856845    2.815804    2.577864
 C   -2.759913   -0.950370    0.676069
 H   -3.089348   -0.083249    1.248136
 C   -3.621043   -1.534374   -0.255725
 H   -3.303666   -2.502097   -0.656067
 C   -5.093911   -1.363488   -0.182935
 C   -5.930923   -2.379761   -0.664581
 C   -5.689771   -0.206877    0.344390
 C   -7.318636   -2.254762   -0.609390
 H   -5.485068   -3.284726   -1.086288
 C   -7.074945   -0.080174    0.399226
 H   -5.063910    0.611595    0.707014
 C   -7.897243   -1.104336   -0.075380
 H   -7.950930   -3.062070   -0.985926
 H   -7.517887    0.828000    0.814364
 H   -8.983677   -1.002316   -0.030779
 C    0.874518   -4.178628   -2.311656
 H    0.131970   -3.510294   -2.770127
 H    1.150660   -4.950864   -3.043399
 H    0.382548   -4.685278   -1.465134
 C    5.750366   -4.031509   -0.978339
 H    5.939527   -4.212998    0.091667
 H    5.785196   -5.001224   -1.493203
 H    6.577499   -3.411459   -1.354279
 H    5.142088   -1.463559   -0.437543
 H    1.010681   -1.559129   -1.686900
 C   -0.874005    0.187652   -2.124527
 H   -0.175927    0.708324   -2.780322
 C   -2.072524   -0.184679   -2.293638
 C   -3.360169   -0.618328   -2.197109
 H   -3.658669   -1.505536   -2.764199
 H   -4.135929    0.146134   -2.092287
83
Figure_S15-3_PA-9d(Na)-ts(1,6minor)_O6 / electronic energy: -3681.01280902 a.u. / lowest freq: -467.72 cm-1
 C    3.454210    2.248473   -0.020989
 H    3.717559    2.681652    0.952092
 C    4.091862    0.876637   -0.253873
 H    4.810804    0.870579   -1.085060
 C    1.760653    0.672922   -0.340425
 C    3.072108   -1.324012   -0.915390
 C    4.312458   -1.961150   -0.768866
 C    1.994837   -2.047369   -1.437355
 C    4.470555   -3.305910   -1.115654
 C    2.126786   -3.397621   -1.764040
 C    3.369497   -4.015975   -1.604741
 H    3.485540   -5.071251   -1.867954
Cu   -0.083289   -0.078642   -0.285964
 N    2.024762    1.932170   -0.036981
 N    2.932813    0.029615   -0.558511
 C   -1.402059   -1.372076    0.808222
 C   -0.377539   -0.854787    1.674960
Na    2.209413    1.018906    3.229120
 H    4.606209    0.505364    0.646648
 H    3.701753    2.973962   -0.810991
 H   -1.126735   -2.304649    0.302301
 C    0.839858   -1.639020    1.936482
 C   -0.589718    0.293201    2.575573
 O    0.764285   -2.898206    1.499287
 O    1.854621   -1.214188    2.469385
 O   -0.044029    0.450666    3.652222
 O   -1.442421    1.203589    2.094051
 C   -1.574132    2.406277    2.849943
 H   -2.042340    2.204187    3.823376
 H   -2.216960    3.062132    2.252645
 H   -0.578207    2.851848    2.998132
 C    1.924108   -3.703537    1.646202
 H    2.797112   -3.223171    1.184992
 H    1.705682   -4.648506    1.137543
 H    2.130783   -3.887242    2.710238
 C    1.006194    2.926076    0.262499
 H    0.123134    2.356285    0.590352
 C    0.611778    3.743672   -0.951756
 C    1.208559    3.574377   -2.206362
 C   -0.413398    4.693622   -0.831904
 C    0.809596    4.340783   -3.302519
 H    1.985600    2.819960   -2.343786
 C   -0.813833    5.460603   -1.923863
 H   -0.916082    4.825861    0.129063
 C   -0.199993    5.291200   -3.165623
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 H    1.290758    4.187774   -4.271330
 H   -1.615880    6.192916   -1.805381
 H   -0.514381    5.890435   -4.022980
 C    1.466084    3.763870    1.497457
 H    0.614957    4.464885    1.702248
 H    2.278596    4.446244    1.116803
 O    1.814479    2.989335    2.531888
 C   -2.746569   -0.994926    0.689120
 H   -3.108922   -0.141512    1.262223
 C   -3.580568   -1.606369   -0.248315
 H   -3.218913   -2.552287   -0.663237
 C   -5.059150   -1.499428   -0.183879
 C   -5.847500   -2.539475   -0.696337
 C   -5.708967   -0.383226    0.366425
 C   -7.239681   -2.476389   -0.650226
 H   -5.359721   -3.414065   -1.135303
 C   -7.098864   -0.318346    0.412197
 H   -5.123026    0.452631    0.754881
 C   -7.871992   -1.365459   -0.093860
 H   -7.832736   -3.301361   -1.051439
 H   -7.583701    0.559650    0.845008
 H   -8.962194   -1.311910   -0.056488
 C    0.924458   -4.167655   -2.242203
 H    0.260624   -3.536542   -2.850508
 H    1.213364   -5.046086   -2.835872
 H    0.336246   -4.525233   -1.381169
 C    5.801478   -3.991223   -0.943179
 H    5.745308   -4.762057   -0.158792
 H    6.109253   -4.495519   -1.871357
 H    6.590301   -3.280582   -0.661429
 H    5.172486   -1.417322   -0.376858
 H    1.038018   -1.553502   -1.614880
 C   -0.899273    0.266304   -2.104641
 H   -0.232896    0.842369   -2.747370
 C   -2.083203   -0.151776   -2.271037
 C   -3.351213   -0.640247   -2.183393
 H   -3.615703   -1.525508   -2.770242
 H   -4.156948    0.087890   -2.051626
83
Figure_S15-3_PA-9d(Na)-ts(1,6minor)_07 / electronic energy: -3681.01290228 a.u. / lowest freq: -467.74 cm-1
 C    3.458394    2.241642   -0.019233
 H    3.722184    2.674788    0.953728
 C    4.093124    0.868384   -0.251398
 H    4.814613    0.860942   -1.080365
 C    1.761716    0.670062   -0.341717
 C    3.070674   -1.328938   -0.916270
 C    4.305939   -1.968659   -0.771445
 C    1.988234   -2.049781   -1.439612
 C    4.459493   -3.317107   -1.119987
 C    2.114992   -3.396913   -1.767370
 C    3.358890   -4.021226   -1.608795
 H    3.470177   -5.076122   -1.874856
Cu   -0.083740   -0.078358   -0.287088
 N    2.028284    1.928223   -0.035903
 N    2.932882    0.024890   -0.560239
 C   -1.403249   -1.370186    0.809094
 C   -0.377592   -0.853311    1.674698
Na    2.212273    1.018140    3.228094
 H    4.603596    0.494473    0.650331
 H    3.707780    2.966212   -0.809521
 H   -1.129310   -2.303472    0.303718
 C    0.839305   -1.638463    1.935841
 C   -0.588100    0.295199    2.575062
 O    0.762110   -2.897930    1.499989
 O    1.855054   -1.213911    2.467176
 O   -0.041891    0.452205    3.651511
 O   -1.439855    1.206478    2.093575
 C   -1.570147    2.409474    2.849243
 H   -2.038030    2.208012    3.822961
 H   -2.212737    3.065706    2.252106
 H   -0.573770    2.854255    2.996817
 C    1.921485   -3.704102    1.645595
 H    2.794235   -3.224484    1.183108
 H    1.701804   -4.649097    1.137518
 H    2.129422   -3.887715    2.709398
 C    1.011382    2.924269    0.262315
 H    0.127352    2.356465    0.590936
 C    0.618236    3.741012   -0.952912
 C    1.215944    3.570760   -2.206938
 C   -0.406736    4.691340   -0.834411
 C    0.818004    4.336596   -3.303876
 H    1.992879    2.816048   -2.343341
 C   -0.806145    5.457750   -1.927141
 H   -0.910025    4.824293    0.126148
 C   -0.191432    5.287371   -3.168337
 H    1.299835    4.182847   -4.272237
 H   -1.608078    6.190357   -1.809734
 H   -0.505026    5.886115   -4.026329
 C    1.472619    3.762925    1.496141
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 H    0.622823    4.465951    1.699591
 H    2.286589    4.443117    1.114692
 O    1.819191    2.989256    2.531840
 C   -2.747272   -0.991250    0.690317
 H   -3.108076   -0.136742    1.262764
 C   -3.582742   -1.602448   -0.245999
 H   -3.222795   -2.549409   -0.660031
 C   -5.061121   -1.493040   -0.180891
 C   -5.851460   -2.532407   -0.691648
 C   -5.708793   -0.375006    0.368213
 C   -7.243515   -2.466864   -0.645085
 H   -5.365348   -3.408387   -1.129687
 C   -7.098557   -0.307670    0.414421
 H   -5.121245    0.460372    0.755276
 C   -7.873692   -1.354102   -0.089965
 H   -7.838166   -3.291325   -1.044984
 H   -7.581727    0.571732    0.846239
 H   -8.963783   -1.298582   -0.052277
 C    0.914949   -4.168774   -2.248156
 H    0.167447   -3.504302   -2.704240
 H    1.194377   -4.938243   -2.981555
 H    0.428090   -4.679583   -1.401222
 C    5.794236   -3.989873   -0.929985
 H    5.990194   -4.170571    0.138921
 H    5.833815   -4.958920   -1.445734
 H    6.614601   -3.363173   -1.309721
 H    5.169196   -1.429150   -0.379682
 H    1.033918   -1.551255   -1.616767
 C   -0.900377    0.265306   -2.105689
 H   -0.233622    0.839686   -2.749540
 C   -2.084765   -0.151920   -2.271115
 C   -3.353222   -0.639030   -2.182361
 H   -3.618761   -1.524796   -2.767963
 H   -4.158181    0.090091   -2.051333
83
Figure_S15-3_PA-9d(Na)-ts(1,6minor)_O8 / electronic energy: -3681.00936876 a.u. / lowest freq: -472.77 cm-1
 C    2.502018    3.100931   -0.504259
 H    2.746811    3.774759    0.325993
 C    3.576236    2.039625   -0.739346
 H    4.156567    2.209220   -1.656197
 C    1.503041    0.999474   -0.430097
 C    3.371964   -0.433903   -1.141443
 C    4.762872   -0.585326   -1.045419
 C    2.595133   -1.522980   -1.543645
 C    5.366519   -1.816057   -1.311793
 C    3.177267   -2.767996   -1.793355
 C    4.562677   -2.902580   -1.675452
 H    5.028938   -3.871215   -1.876568
Cu    0.008741   -0.311470   -0.325819
 N    1.330505    2.287374   -0.185672
 N    2.782423    0.809180   -0.840363
 C   -1.104178   -1.849611    0.653150
 C   -0.064191   -1.351486    1.514772
Na    2.252280    0.934169    2.838631
 H    4.279270    1.974871    0.107522
 H    2.305094    3.706394   -1.403023
 H   -0.793245   -2.725122    0.070272
 C    1.195575   -2.128633    1.498864
 C   -0.293122   -0.412072    2.620210
 O    2.266720   -1.449630    1.963935
 O    1.312732   -3.250640    1.056610
 O    0.420828   -0.302790    3.604902
 O   -1.376751    0.351274    2.467414
 C   -1.593702    1.353239    3.460953
 H   -1.769600    0.890746    4.442256
 H   -2.486946    1.899617    3.138370
 H   -0.711303    2.012098    3.498201
 C    3.502785   -2.152782    1.974713
 H    3.449138   -3.022185    2.644882
 H    4.252080   -1.442193    2.343065
 H    3.768491   -2.487818    0.963503
 C    0.125107    2.845726    0.418854
 H   -0.477032    1.967685    0.695017
 C   -0.673813    3.677721   -0.560080
 C   -0.280742    4.969790   -0.934449
 C   -1.847853    3.151271   -1.114048
 C   -1.037977    5.710894   -1.842115
 H    0.623838    5.410621   -0.509320
 C   -2.606876    3.888985   -2.020936
 H   -2.161245    2.140511   -0.839059
 C   -2.203100    5.172900   -2.388576
 H   -0.716618    6.717216   -2.120787
 H   -3.516987    3.457479   -2.443955
 H   -2.796478    5.754529   -3.097650
 C    0.487198    3.545262    1.759111
 H   -0.508137    3.878182    2.162840
 H    0.999269    4.512842    1.502517
 O    1.191684    2.747482    2.573597
 C   -2.468755   -1.531266    0.590991
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 H   -2.852794   -0.724908    1.213925
 C   -3.307632   -2.156902   -0.336258
 H   -2.933342   -3.092325   -0.762219
 C   -4.786477   -2.090919   -0.223594
 C   -5.563186   -3.158751   -0.694516
 C   -5.447162   -0.981056    0.326818
 C   -6.954683   -3.128623   -0.607431
 H   -5.067133   -4.028518   -1.133754
 C   -6.836214   -0.949215    0.413627
 H   -4.870097   -0.123479    0.680197
 C   -7.597672   -2.023839   -0.051138
 H   -7.538713   -3.974560   -0.977032
 H   -7.329779   -0.075413    0.845131
 H   -8.687305   -1.996342    0.017980
 C    2.299920   -3.937447   -2.148176
 H    1.522718   -3.647561   -2.870441
 H    2.879527   -4.768117   -2.573505
 H    1.790237   -4.297291   -1.241016
 C    6.858248   -1.984840   -1.182479
 H    7.104735   -2.642149   -0.333818
 H    7.283770   -2.448946   -2.084634
 H    7.363106   -1.022423   -1.021721
 H    5.392835    0.255326   -0.751601
 H    1.518775   -1.407199   -1.682952
 C   -0.793980   -0.119188   -2.188711
 H   -0.158710    0.485543   -2.836067
 C   -1.935413   -0.634680   -2.372314
 C   -3.164423   -1.213333   -2.274285
 H   -3.362391   -2.128983   -2.839737
 H   -4.020565   -0.539557   -2.171108
83
Figure_S15-3_PA-9d(Na)-ts(1,6minor)_09 / electronic energy: -3681.00528804 a.u. / lowest freq: -436.29 cm-1
 C    1.471229   -2.756206    2.248800
 H    1.805684   -3.677320    1.748967
 C    2.618716   -1.814845    2.602633
 H    2.444430   -1.303257    3.563410
 C    1.402216   -0.920114    0.819671
 C    3.542002    0.161591    1.345788
 C    3.748732    0.771624    0.103633
 C    4.306136    0.560552    2.447764
 C    4.666915    1.816172   -0.027558
 C    5.246715    1.587730    2.329757
 C    5.407959    2.212716    1.090586
 H    6.136334    3.022105    0.989705
Cu    0.516807    0.433567   -0.338649
 N    0.723011   -1.960386    1.275066
 N    2.573315   -0.849576    1.497356
 C   -0.734526    1.097056   -1.871586
 C   -0.093036   -0.111222   -2.347045
 H    3.595379   -2.314898    2.648003
 H    0.845561   -3.014331    3.114036
 H   -0.305346    2.035821   -2.234207
 C    1.222218   -0.010812   -3.006503
 C   -0.803225   -1.378362   -2.578177
 O    1.539646    1.237455   -3.373991
 O    1.995022   -0.935450   -3.202652
 O   -0.339200   -2.369346   -3.118324
 O   -2.076878   -1.365890   -2.171322
 C   -2.841286   -2.538538   -2.402000
 H   -2.968038   -2.716832   -3.478938
 H   -3.815065   -2.359284   -1.933420
 H   -2.356526   -3.414953   -1.950069
 C    2.760801    1.407252   -4.076742
 H    3.598354    0.951583   -3.533420
 H    2.912827    2.487511   -4.173339
 H    2.695250    0.947579   -5.073362
 C   -0.519120   -2.443071    0.701745
 H   -0.637305   -1.884716   -0.235961
 C   -1.721753   -2.106866    1.566076
 C   -2.970963   -2.687923    1.304517
 C   -1.642951   -1.149831    2.586405
 C   -4.098725   -2.330533    2.042575
 H   -3.070048   -3.426852    0.507908
 C   -2.769203   -0.791281    3.327295
 H   -0.688360   -0.664034    2.797228
 C   -4.003140   -1.382539    3.061250
 H   -5.060118   -2.798379    1.818592
 H   -2.680445   -0.037927    4.113317
 H   -4.886326   -1.102992    3.640127
 C   -0.318931   -3.938659    0.290013
 H   -1.269368   -4.232538   -0.227963
 H   -0.356521   -4.525314    1.253077
 O    0.792782   -4.111970   -0.435167
 C   -1.932899    1.188429   -1.141429
 H   -2.377025    0.273671   -0.751339
 C   -2.552026    2.404386   -0.850203
 H   -2.304471    3.251222   -1.494318
 C   -3.911755    2.435323   -0.262319
 C   -4.790596    3.476007   -0.592206
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 C   -4.351701    1.447813    0.635161
 C   -6.077353    3.524054   -0.056665
 H   -4.461347    4.255775   -1.284272
 C   -5.634649    1.497543    1.171513
 H   -3.678436    0.641602    0.938216
 C   -6.505623    2.534016    0.826673
 H   -6.749167    4.340167   -0.332361
 H   -5.953293    0.721372    1.871205
 H   -7.511199    2.571974    1.251202
 C    0.671747    2.091141    0.850927
 H    1.626962    2.063122    1.376623
 C   -0.316608    2.878046    0.917095
 C   -1.522820    3.489040    0.801613
 H   -1.586706    4.464159    0.310612
 H   -2.268087    3.303496    1.580549
Na    1.643263   -3.072449   -2.115759
 H    4.164141    0.083752    3.418792
 H    3.192129    0.420188   -0.768296
 C    6.036717    2.030918    3.533712
 H    6.930092    2.599874    3.241627
 H    5.425420    2.679301    4.181674
 H    6.356917    1.171596    4.140635
 C    4.860613    2.490914   -1.359380
 H    3.906824    2.885955   -1.740142
 H    5.571651    3.324894   -1.287588
 H    5.247693    1.782629   -2.107982
51
Figure_S15-4_9b(Na)-Cu-allenyl / electronic energy: -2839.05552233 a.u. / lowest freq: 18.49 cm-1
 C   -1.403505   -1.447218   -1.463778
 H   -1.518968   -0.926587   -2.428424
 C   -0.102320   -2.249278   -1.398621
 H   -0.227521   -3.213821   -0.877881
 C    0.053653   -0.375990   -0.006245
 C    2.115590   -1.646329   -0.323692
 C    2.447529   -2.278240    0.886897
 C    3.093354   -1.289872   -1.267445
 C    3.794134   -2.560894    1.135970
 C    4.427961   -1.594447   -0.983886
 C    4.776145   -2.227614    0.206801
 H    5.823692   -2.456465    0.414766
Cu    0.843286    1.028000    1.058904
 N   -1.218234   -0.464888   -0.392885
 N    0.750379   -1.356185   -0.608944
Na    0.955612    3.102468   -1.264571
 H    0.329842   -2.451327   -2.388040
 H   -2.298582   -2.059781   -1.291665
 C   -2.190235    0.595041   -0.173375
 H   -1.850072    1.110871    0.740288
 C   -3.556987   -0.008997    0.105143
 C   -4.706885    0.356784   -0.601576
 C   -3.677253   -0.973578    1.116074
 C   -5.942423   -0.224050   -0.305173
 H   -4.649878    1.103012   -1.395225
 C   -4.905862   -1.557315    1.412344
 H   -2.783955   -1.272241    1.671962
 C   -6.047178   -1.182627    0.699889
 H   -6.828698    0.076027   -0.869206
 H   -4.975116   -2.307462    2.203595
 H   -7.013189   -1.638603    0.927875
 C   -2.105561    1.652949   -1.307432
 H   -2.876323    2.421016   -1.032266
 H   -2.526837    1.167141   -2.231630
 O   -0.866029    2.140611   -1.461517
 C    1.722811    2.492968    1.972660
 H    1.936525    2.461721    3.053521
 C    2.118112    3.566313    1.350898
 C    2.487290    4.627547    0.641169
 H    1.831345    5.500129    0.544963
 H    3.482307    4.692597    0.187595
 H    5.202845   -1.322373   -1.704686
 H    4.072439   -3.050469    2.072400
 C    1.385066   -2.604535    1.901717
 H    0.998593   -1.681347    2.362588
 H    0.524948   -3.114869    1.443881
 H    1.783860   -3.245588    2.698815
 C    2.712511   -0.567453   -2.531971
 H    2.063535   -1.181523   -3.174815
 H    2.155428    0.354222   -2.305548
 H    3.604292   -0.299794   -3.114044
83
Figure_S15-4_PA-9b(Na)-ts(1,6major)_01 / electronic energy: -3681.01420703 a.u. / lowest freq: -427.03 cm-1
 C    2.979277   -1.816363    1.363890
 H    2.832953   -2.499901    2.202407
 C    0.983754   -0.583498    2.061507
 H    0.687994   -1.482945    2.607573
 C    2.204575   -0.653459    1.365698
 H    2.532869    0.207846    0.781962
 C    0.132807    0.567981    2.261009
 C    0.555516    1.959815    2.064348
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 O   -0.178914    2.937010    2.048099
 C   -1.162905    0.359582    2.919903
 O   -1.901175    1.216398    3.376497
 O   -1.517300   -0.936671    2.962522
 C    4.329569   -1.851716    0.760541
 C    4.682883   -1.022138   -0.315747
 C    5.957777   -1.080815   -0.871037
 C    6.907086   -1.972887   -0.367128
 C    6.566688   -2.806274    0.698073
 C    5.289634   -2.746887    1.253825
 C    2.069231   -3.442207    0.102650
 H    2.261290   -4.216338    0.850501
 H    2.774336   -3.409537   -0.733773
 C    0.793982   -3.030186   -0.121012
 C   -0.269149   -2.357956   -0.241579
 H   -1.246278   -2.540213   -0.691663
Cu   -0.175462   -0.401482    0.359787
 C   -1.144033    0.599950   -1.032719
 N   -2.457990    0.509661   -1.204986
 N   -0.638672    1.394818   -1.990384
 C   -3.354623   -0.132049   -0.259882
 C   -2.947832    1.409435   -2.255697
 H   -3.435672    2.267963   -1.769538
 C   -1.652843    1.791478   -2.974419
 H   -1.504971    1.230046   -3.912538
 C    0.743914    1.707881   -2.131227
 C    1.624394    0.753087   -2.667616
 C    1.181826    2.986763   -1.742460
 C    2.976709    1.094986   -2.779816
 C    2.540838    3.287647   -1.871490
 C    3.433983    2.346862   -2.378552
 H    4.493435    2.594870   -2.472863
Na   -2.500038    2.928818    1.919630
 H   -1.592203    2.862329   -3.208512
 H   -3.670790    0.907902   -2.913030
 O    1.874268    2.097145    1.908907
 C   -2.790716   -1.234933    3.511430
 H   -2.834690   -0.969064    4.576959
 H   -2.929437   -2.313857    3.385119
 H   -3.580634   -0.687293    2.976474
 C    2.385404    3.411637    1.760938
 H    1.910161    3.929061    0.918794
 H    3.458436    3.298031    1.573259
 H    2.222644    3.994940    2.678345
 H   -2.747429   -0.342183    0.636144
 C   -3.895854   -1.450235   -0.775982
 C   -4.702645   -2.239439    0.057043
 C   -3.597217   -1.935173   -2.054595
 C   -5.205944   -3.462897   -0.379836
 H   -4.928757   -1.898010    1.069876
 C   -4.099393   -3.160548   -2.495451
 H   -2.943062   -1.358256   -2.711137
 C   -4.909721   -3.928399   -1.661848
 H   -5.829184   -4.061357    0.288699
 H   -3.849280   -3.517918   -3.497085
 H   -5.302642   -4.888063   -2.004790
 C   -4.448169    0.891868    0.192062
 H   -5.064236    0.335170    0.947141
 H   -5.144368    0.989581   -0.689936
 O   -3.925874    2.043648    0.626926
 H    5.029497   -3.405910    2.086631
 H    3.948303   -0.331158   -0.735039
 H    7.300106   -3.509664    1.099012
 H    6.211953   -0.425913   -1.708111
 H    7.905710   -2.020504   -0.806658
 C    1.138435   -0.602947   -3.100184
 H    0.985301   -1.258390   -2.229315
 H    0.174446   -0.541526   -3.625366
 H    1.866664   -1.084682   -3.766166
 C    0.208212    3.998497   -1.199623
 H    0.728806    4.910812   -0.878466
 H   -0.532200    4.294608   -1.957945
 H   -0.343607    3.594945   -0.338235
 H    3.677310    0.366478   -3.195724
 H    2.901920    4.273721   -1.568872
83
Figure_S15-4_PA-9b(Na)-ts(1,6major)_O2 / electronic energy: -3681.01281667 a.u. / lowest freq: -438.77 cm-1
 C   -3.136864    1.752039    1.146068
 H   -2.969054    2.525961    1.898477
 C   -1.092165    0.652122    1.905771
 H   -0.831937    1.601341    2.381194
 C   -2.326981    0.617768    1.234324
 H   -2.634912   -0.299287    0.732068
 C   -0.195573   -0.445109    2.201877
 C   -0.568174   -1.863059    2.117563
 O    0.189118   -2.815361    2.234520
 C    1.071396   -0.138875    2.879068
 O    1.850366   -0.935762    3.374180
 O    1.348034    1.178388    2.895742
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 C   -4.523051    1.682059    0.630107
 C   -4.909502    0.742204   -0.338685
 C   -6.219317    0.700864   -0.807513
 C   -7.172143    1.599444   -0.321811
 C   -6.799071    2.542392    0.635272
 C   -5.486271    2.584382    1.103108
 C   -2.363670    3.203924   -0.356845
 H   -2.598282    4.071375    0.266362
 H   -3.076335    2.997032   -1.161325
 C   -1.066645    2.850668   -0.551731
 C    0.044457    2.249612   -0.605257
 H    0.985318    2.457955   -1.115413
Cu    0.159590    0.403739    0.262646
 C    1.287883   -0.608692   -1.003521
 N    2.608071   -0.544349   -1.115927
 N    0.805189   -1.361857   -2.006138
 C    3.476379    0.049707   -0.103478
 C    3.120833   -1.409463   -2.183190
 H    3.595303   -2.286333   -1.716339
 C    1.845495   -1.763539   -2.956124
 H    1.743853   -1.188565   -3.891844
 C   -0.584019   -1.622087   -2.182538
 C   -1.403567   -0.680255   -2.825182
 C   -1.094667   -2.834071   -1.681104
 C   -2.774619   -0.953813   -2.909313
 C   -2.466220   -3.071491   -1.791718
 C   -3.303152   -2.131605   -2.391706
 H   -4.375937   -2.324593   -2.463846
Na    2.493226   -2.803967    2.141518
 H    1.775384   -2.831842   -3.203347
 H    3.856258   -0.885129   -2.807152
 O   -1.872240   -2.057764    1.908017
 C    2.565352    1.567554    3.513579
 H    2.580426    1.275588    4.572888
 H    2.616081    2.657983    3.423028
 H    3.425952    1.108430    3.005108
 C   -2.341147   -3.395295    1.871325
 H   -1.804194   -3.983469    1.117184
 H   -3.404580   -3.334724    1.616075
 H   -2.216652   -3.876493    2.851860
 H    2.816657    0.242014    0.755198
 C    4.044436    1.378862   -0.553782
 C    5.049997    1.469671   -1.525983
 C    3.560061    2.565771    0.010940
 C    5.546997    2.710049   -1.926227
 H    5.460107    0.562311   -1.974865
 C    4.054475    3.807808   -0.385546
 H    2.771592    2.512413    0.766465
 C    5.050704    3.883834   -1.358711
 H    6.330181    2.759084   -2.686223
 H    3.656889    4.719229    0.066803
 H    5.441109    4.854331   -1.673184
 C    4.527763   -0.988215    0.381749
 H    5.109539   -0.431626    1.168336
 H    5.271751   -1.098372   -0.457739
 O    3.973787   -2.140286    0.778977
 H   -5.201011    3.328070    1.852040
 H   -4.173011    0.045443   -0.744225
 H   -7.534494    3.252434    1.020518
 H   -6.498503   -0.037236   -1.563194
 H   -8.199062    1.566035   -0.692214
 C   -0.844341    0.565409   -3.458122
 H    0.124223    0.849841   -3.031748
 H   -0.707525    0.409183   -4.540402
 H   -1.530972    1.412713   -3.326548
 C   -0.170702   -3.842075   -1.051947
 H   -0.713944   -4.757906   -0.782270
 H    0.638942   -4.127639   -1.739638
 H    0.302271   -3.441617   -0.143120
 H   -3.433088   -0.226474   -3.390955
 H   -2.883501   -4.003515   -1.402791
83
Figure_S15-4_PA-9b(Na)-ts(1,6major)_03 / electronic energy: -3681.01313518 a.u. / lowest freq: -434.70 cm-1
 C    2.999801   -1.568701   -2.158205
 H    3.481819   -2.397870   -1.617948
 C    1.707790   -1.990629   -2.863349
 H    1.587851   -1.510973   -3.849154
 C    1.193966   -0.654899   -1.016927
 C   -0.696970   -1.813894   -2.048422
 C   -1.150207   -3.019646   -1.483712
 C   -1.563279   -0.938771   -2.724177
 C   -2.513119   -3.318671   -1.568848
 C   -2.919839   -1.276342   -2.789175
 C   -3.393680   -2.449352   -2.208735
 H   -4.456653   -2.693889   -2.266433
Cu    0.161058    0.450662    0.253023
 N    2.513094   -0.602407   -1.167146
 N    0.686970   -1.493593   -1.935964
 C   -1.018405    0.792991    1.926617
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 C   -0.146264   -0.315380    2.247464
 H    1.629569   -3.077055   -3.004998
 H    3.720360   -1.113029   -2.849386
 H   -0.737297    1.751060    2.371407
 C   -0.559583   -1.724430    2.222257
 C    1.137551   -0.020291    2.896525
 O   -1.874479   -1.888852    2.060994
 O    0.175729   -2.692342    2.348618
 O    1.895266   -0.819682    3.420098
 O    1.454715    1.286651    2.852517
 C    2.693089    1.663107    3.434917
 H    2.721829    1.405533    4.502770
 H    2.770798    2.748286    3.307698
 H    3.530947    1.164948    2.924988
 C   -2.378663   -3.213822    2.073015
 H   -1.893501   -3.829045    1.305410
 H   -3.450539   -3.129573    1.864266
 H   -2.221940   -3.680307    3.055986
 C    3.402526    0.040935   -0.203041
 H    2.758336    0.294123    0.652011
 C    3.995975    1.330279   -0.727216
 C    3.627540    2.549633   -0.144870
 C    4.928285    1.350865   -1.773938
 C    4.160611    3.756333   -0.597212
 H    2.896546    2.550767    0.667982
 C    5.463125    2.555296   -2.230644
 H    5.251331    0.416464   -2.237843
 C    5.080335    3.762635   -1.645420
 H    3.852923    4.694549   -0.129904
 H    6.188274    2.549933   -3.047680
 H    5.499862    4.704817   -2.005209
 C    4.449893   -0.980719    0.328433
 H    5.043022   -0.388187    1.079139
 H    5.184369   -1.136235   -0.512704
 O    3.893529   -2.106996    0.789548
 C   -2.248744    0.760848    1.246634
 H   -2.561844   -0.164831    0.762552
 C   -3.056405    1.895600    1.132577
 H   -2.924596    2.667337    1.893631
 C   -4.417181    1.814148    0.555408
 C   -5.415647    2.696894    0.990758
 C   -4.742527    0.877865   -0.439038
 C   -6.704455    2.637139    0.462046
 H   -5.177870    3.438461    1.758146
 C   -6.028473    0.817961   -0.967541
 H   -3.977819    0.196005   -0.817096
 C   -7.017434    1.696106   -0.518406
 H   -7.468423    3.331785    0.818606
 H   -6.259621    0.081344   -1.740833
 H   -8.025651    1.648833   -0.935616
 C    0.133212    2.308082   -0.609289
 H    1.079177    2.463863   -1.128519
 C   -0.940496    2.970889   -0.528779
 C   -2.215986    3.383076   -0.309584
 H   -2.399082    4.239462    0.345270
 H   -2.944858    3.240541   -1.113348
Na    2.481379   -2.736786    2.238966
 C   -0.184850   -3.959390   -0.812243
 H   -0.705627   -4.843001   -0.419388
 H    0.583567   -4.316103   -1.514379
 H    0.336556   -3.468867    0.022726
 C   -1.056585    0.331909   -3.348574
 H   -0.878128    1.097621   -2.578593
 H   -0.103926    0.176723   -3.874665
 H   -1.786469    0.732132   -4.064951
 H   -3.610334   -0.607428   -3.308856
 H   -2.886777   -4.246898   -1.129633
83
Figure_S15-4_PA-9b(Na)-ts(1,6major)_04 / electronic energy: -3681.00780852 a.u. / lowest freq: -440.92 cm-1
 C   -3.049815    0.984897   -2.252606
 H   -3.584829    1.821609   -1.775870
 C   -1.808749    1.448672   -3.008644
 H   -1.582676    0.811573   -3.881131
 C   -1.170789    0.443630   -1.008105
 C    0.535813    1.833916   -2.096631
 C    0.677418    3.219669   -1.890399
 C    1.638079    1.020937   -2.416824
 C    3.061107    2.986433   -2.270013
 H    4.053855    3.436523   -2.333875
Cu   -0.096034   -0.405568    0.405049
 N   -2.457207    0.158155   -1.195947
 N   -0.767975    1.270799   -1.988566
 C    1.192684   -0.467317    2.016976
 C    0.395746    0.732078    2.153285
Na   -2.444378    2.876474    1.776078
 H   -1.877322    2.487582   -3.352667
 H   -3.749351    0.414472   -2.877130
 H    0.898781   -1.308964    2.649934
 C    0.961535    2.041106    1.793698
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 C   -0.852784    0.639721    2.916025
 O    0.062405    3.056150    1.760212
 O    2.124502    2.248957    1.525181
 O   -1.494734    1.560235    3.396760
 O   -1.291755   -0.626188    3.029490
 C   -2.565711   -0.810743    3.628935
 H   -2.564664   -0.471583    4.674175
 H   -2.766587   -1.886412    3.581134
 H   -3.332284   -0.254977    3.068665
 C    0.612336    4.357377    1.605391
 H    1.236307    4.617911    2.472274
 H   -0.236842    5.047431    1.540946
 H    1.224578    4.419424    0.696860
 C   -3.275976   -0.507285   -0.196958
 H   -2.601723   -0.709745    0.651375
 C   -3.832195   -1.830025   -0.683416
 C   -4.616046   -2.609872    0.180369
 C   -3.564697   -2.332550   -1.962345
 C   -5.131728   -3.837456   -0.229398
 H   -4.814133   -2.257282    1.195219
 C   -4.079778   -3.562028   -2.375932
 H   -2.924775   -1.765177   -2.640846
 C   -4.870672   -4.318020   -1.513525
 H   -5.737859   -4.427419    0.462025
 H   -3.854908   -3.931929   -3.378977
 H   -5.274584   -5.280477   -1.835092
 C   -4.345361    0.497582    0.342059
 H   -4.899757   -0.067610    1.135953
 H   -5.105002    0.602453   -0.483508
 O   -3.798292    1.647730    0.752651
 C    2.383916   -0.616297    1.285100
 H    2.709561    0.203553    0.642641
 C    3.126410   -1.800353    1.325451
 H    2.994590   -2.423497    2.212434
 C    4.457438   -1.906561    0.685799
 C    5.408745   -2.799644    1.199178
 C    4.797164   -1.152534   -0.448748
 C    6.663091   -2.930902    0.605286
 H    5.159641   -3.399119    2.079113
 C    6.048990   -1.282713   -1.042735
 H    4.067902   -0.463053   -0.878835
 C    6.989146   -2.172882   -0.518991
 H    7.390058   -3.631316    1.022902
 H    6.292281   -0.687259   -1.926048
 H    7.969879   -2.276893   -0.988132
 C   -0.200664   -2.392537   -0.104310
 H   -1.190481   -2.606408   -0.509892
 C    0.868502   -3.056170    0.006182
 C    2.155679   -3.453052    0.193061
 H    2.381289   -4.199578    0.959491
 H    2.816610   -3.464510   -0.679557
 C    1.954210    3.779424   -1.981194
 H    2.080821    4.852197   -1.815396
 C    2.899793    1.622769   -2.491135
 H    3.766953    1.009083   -2.748634
 C   -0.516051    4.085360   -1.587529
 H   -1.079200    4.324813   -2.503412
 H   -1.209835    3.580630   -0.901163
 H   -0.207723    5.039710   -1.142297
 C    1.490967   -0.454061   -2.673507
 H    1.523432   -1.025697   -1.733335
 H    0.530610   -0.692888   -3.151208
 H    2.303270   -0.818068   -3.317278
83
Figure_S15-4_PA-9b(Na)-ts(1,6major)_O5 / electronic energy: -3681.00473590 a.u. / lowest freq: -469.73 cm-1
 C   -4.002505    0.075621    1.124597
 H   -4.659529   -0.231101    0.296878
 C   -3.491607   -1.101073    1.957204
 H   -3.479967   -0.885270    3.038679
 C   -1.723367   -0.207185    0.714784
 C   -1.308677   -2.356177    1.837374
 C   -1.450606   -3.551765    1.113971
 C   -0.435910   -2.243799    2.930382
 C   -0.732251   -4.670367    1.543524
 C    0.286792   -3.379163    3.311522
 C    0.129490   -4.585124    2.634693
 H    0.689437   -5.466280    2.955503
Cu    0.098211    0.219341    0.044869
 N   -2.760238    0.613347    0.555328
 N   -2.117895   -1.247021    1.462299
 C    1.622972    0.146416   -1.420907
 C    0.653474   -0.889069   -1.690407
 H   -4.068895   -2.023712    1.805481
 H   -4.528788    0.825665    1.729938
 H    1.426912    1.092906   -1.933116
 C    0.973859   -2.278419   -1.307767
 C   -0.476556   -0.592718   -2.575414
 O    0.420385   -3.208396   -2.094674
 O    1.721394   -2.583583   -0.398456
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 O   -1.398083   -1.349037   -2.852514
 O   -0.453790    0.660684   -3.050897
 C   -1.560895    1.092095   -3.834687
 H   -1.618707    0.515785   -4.770116
 H   -1.366572    2.145326   -4.066559
 H   -2.503187    0.989582   -3.268602
 C    0.755114   -4.555707   -1.812465
 H    1.816100   -4.748227   -2.030576
 H    0.123862   -5.171804   -2.462832
 H    0.566743   -4.795569   -0.757930
 C   -2.748406    1.762746   -0.334986
 H   -1.886203    1.618005   -1.004725
 C   -2.558044    3.078576    0.387557
 C   -2.773516    3.232472    1.761022
 C   -2.150321    4.198475   -0.349057
 C   -2.594221    4.470422    2.380228
 H   -3.058764    2.370872    2.367980
 C   -1.971519    5.436224    0.264372
 H   -1.953512    4.091001   -1.419381
 C   -2.195622    5.578473    1.634578
 H   -2.762147    4.566558    3.455418
 H   -1.645415    6.293626   -0.329024
 H   -2.050746    6.546352    2.119393
 C   -4.018470    1.741362   -1.245693
 H   -3.905984    2.645123   -1.900787
 H   -4.878032    2.010051   -0.571224
 O   -4.167464    0.584444   -1.907104
 C    2.876792    0.044194   -0.799058
 H    3.152510   -0.896033   -0.322659
 C    3.708911    1.161241   -0.695526
 H    3.478782    1.990283   -1.371072
 C    5.147872    1.043537   -0.353453
 C    6.056572    1.981845   -0.862988
 C    5.640995    0.024168    0.476476
 C    7.417094    1.898606   -0.569147
 H    5.689821    2.786382   -1.506333
 C    6.998871   -0.059194    0.771911
 H    4.952518   -0.707886    0.904561
 C    7.894926    0.876131    0.249327
 H    8.107439    2.637697   -0.982333
 H    7.361690   -0.860163    1.420221
 H    8.960011    0.807093    0.480938
 C    0.599754    1.813741    1.214489
 H   -0.264220    2.140602    1.793907
 C    1.802970    2.206591    1.195363
 C    3.137221    2.390992    0.997667
 H    3.820848    1.977203    1.745667
 H    3.474504    3.319085    0.526583
Na   -3.656876   -1.309937   -2.660622
 H    0.976458   -3.314742    4.156650
 H   -0.844000   -5.617753    1.010321
 C   -2.312350   -3.594887   -0.119865
 H   -3.357732   -3.322836    0.093595
 H   -1.928057   -2.888873   -0.873186
 H   -2.310215   -4.599482   -0.563709
 C   -0.258432   -0.930418    3.643094
 H    0.267955   -1.067322    4.596850
 H    0.329740   -0.233225    3.024944
 H   -1.222177   -0.440859    3.845806
83
Figure_S15-4_PA-9b(Na)-ts(1,6minor)_01 / electronic energy: -3681.00662586 a.u. / lowest freq: -473.73 cm-1
 C    3.186998    2.460131   -0.440560
 H    3.647008    2.672480    0.537318
 C    3.879383    1.307115   -1.162490
 H    3.958625    1.473301   -2.250094
 C    1.766979    0.614601   -0.437847
 C    3.340236   -1.134927   -1.249282
 C    4.272016   -1.803179   -0.433424
 C    2.869931   -1.709438   -2.445763
 C    4.732775   -3.060109   -0.840604
 C    3.334204   -2.979947   -2.799618
 C    4.266660   -3.648033   -2.011241
 H    4.632013   -4.632387   -2.312038
Cu    0.005988   -0.317213   -0.311251
 N    1.837946    1.930352   -0.237902
 N    2.960739    0.192986   -0.898364
 C   -1.406904   -1.719397    0.496445
 C   -0.338186   -1.474598    1.431045
Na    2.341076   -0.067471    3.032442
 H    4.886791    1.097454   -0.777504
 H    3.170785    3.383701   -1.034047
 H   -1.200541   -2.531888   -0.208867
 C    0.813034   -2.386857    1.470565
 C   -0.466059   -0.542969    2.564299
 O    0.639655   -3.476778    0.715868
 O    1.851190   -2.204395    2.089225
 O    0.131983   -0.633268    3.621496
 O   -1.312435    0.465320    2.332683
 C   -1.369839    1.478520    3.332246
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 H   -1.776586    1.076378    4.270802
 H   -2.035574    2.252660    2.934780
 H   -0.356385    1.872741    3.495396
 C    1.717096   -4.396078    0.640149
 H    2.625415   -3.905373    0.270039
 H    1.401022   -5.176326   -0.060710
 H    1.919875   -4.837944    1.626102
 C    0.844982    2.670435    0.535769
 H    0.035196    1.949400    0.719185
 C    0.262938    3.838181   -0.231649
 C    0.955183    5.044749   -0.404170
 C   -1.021970    3.726903   -0.779375
 C    0.384259    6.100928   -1.115569
 H    1.949721    5.171299    0.029685
 C   -1.595640    4.779306   -1.490778
 H   -1.573371    2.791475   -0.653319
 C   -0.891689    5.971171   -1.663722
 H    0.939063    7.034003   -1.238620
 H   -2.596754    4.666556   -1.913580
 H   -1.337755    6.798924   -2.219723
 C    1.417019    3.020451    1.939439
 H    0.572881    3.569196    2.440717
 H    2.192472    3.820797    1.789144
 O    1.860067    1.939278    2.594087
 C   -2.731472   -1.262023    0.507844
 H   -3.036623   -0.538517    1.262916
 C   -3.620363   -1.624213   -0.506240
 H   -3.318081   -2.475297   -1.124353
 C   -5.090644   -1.472624   -0.366693
 C   -5.940889   -2.321331   -1.089755
 C   -5.671629   -0.494421    0.455571
 C   -7.326841   -2.207031   -0.988907
 H   -5.506790   -3.084553   -1.741503
 C   -7.055394   -0.378967    0.557214
 H   -5.036689    0.192861    1.018626
 C   -7.890623   -1.234940   -0.163654
 H   -7.968862   -2.881076   -1.560515
 H   -7.486341    0.388587    1.204128
 H   -8.975644   -1.141062   -0.082307
 C   -0.895449    0.434790   -1.979520
 H   -0.217607    1.113147   -2.497991
 C   -2.104730    0.136683   -2.208382
 C   -3.399554   -0.282023   -2.185872
 H   -3.737853   -0.995740   -2.943565
 H   -4.151942    0.443970   -1.863978
 C    4.778701   -1.220415    0.859287
 H    4.533305   -1.895982    1.691826
 H    5.872084   -1.099274    0.835471
 H    4.332969   -0.241959    1.073633
 C    1.898989   -0.988383   -3.339136
 H    0.863420   -1.133116   -2.995777
 H    2.080238    0.095521   -3.350399
 H    1.967479   -1.364020   -4.368824
 H    2.973754   -3.438463   -3.723688
 H    5.458275   -3.587110   -0.215691
83
Figure_S15-4_PA-9b(Na)-ts(1,6minor)_O2 / electronic energy: -3681.00610479 a.u. / lowest freq: -471.38 cm-1
 C    3.287832    2.331087   -0.099700
 H    3.641751    2.388425    0.941917
 C    3.974095    1.220340   -0.882220
 H    4.099600    1.466283   -1.951015
 C    1.791155    0.570498   -0.370232
 C    3.350035   -1.183303   -1.197299
 C    4.291841   -1.918942   -0.451484
 C    2.835169   -1.674059   -2.412442
 C    4.710432   -3.159327   -0.942081
 C    3.259019   -2.933742   -2.850287
 C    4.194430   -3.668928   -2.129261
 H    4.524827   -4.642895   -2.496805
Cu   -0.015401   -0.274448   -0.306751
 N    1.897007    1.869016   -0.093632
 N    3.006662    0.122372   -0.744892
 C   -1.435289   -1.679095    0.481627
 C   -0.384787   -1.429446    1.434932
 H    4.956921    0.950468   -0.476179
 H    3.389713    3.319335   -0.566762
 H   -1.202967   -2.472488   -0.237774
 C    0.778735   -2.325340    1.489787
 C   -0.541233   -0.502980    2.568959
 O    0.625689   -3.419961    0.737245
 O    1.807552   -2.126168    2.118514
 O    0.034690   -0.596638    3.638626
 O   -1.384124    0.504985    2.325700
 C   -1.469752    1.508359    3.333440
 H   -1.883786    1.092241    4.262557
 H   -2.141729    2.275912    2.933739
 H   -0.464792    1.916394    3.517068
 C    1.711294   -4.330670    0.678278
 H    2.619703   -3.834764    0.315908
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 H    1.409538   -5.116861   -0.022278
 H    1.906374   -4.766259    1.668604
 C    0.854749    2.643774    0.556569
 H    0.022126    1.944359    0.736138
 C    0.347381    3.775545   -0.314609
 C   -0.644801    4.638580    0.173963
 C    0.811604    3.981929   -1.619226
 C   -1.137906    5.682441   -0.606576
 H   -1.049966    4.484211    1.176555
 C    0.321178    5.026433   -2.403471
 H    1.557174    3.304007   -2.039842
 C   -0.652506    5.885989   -1.898931
 H   -1.911875    6.339752   -0.203406
 H    0.702160    5.164257   -3.418126
 H   -1.038622    6.703793   -2.511325
 C    1.358075    3.071468    1.973833
 H    0.496522    3.621792    2.433224
 H    2.121944    3.879831    1.797844
 O    1.794645    2.026723    2.688976
 C   -2.769500   -1.250692    0.487073
 H   -3.101179   -0.560681    1.262445
 C   -3.632839   -1.588402   -0.555572
 H   -3.296830   -2.396868   -1.212346
 C   -5.108215   -1.479062   -0.437907
 C   -5.923427   -2.315050   -1.214292
 C   -5.728794   -0.556235    0.418861
 C   -7.313370   -2.243004   -1.131738
 H   -5.458253   -3.035426   -1.892787
 C   -7.116555   -0.482782    0.502014
 H   -5.121757    0.120672    1.023643
 C   -7.916457   -1.326282   -0.271657
 H   -7.927901   -2.906798   -1.744151
 H   -7.578740    0.242004    1.176136
 H   -9.004836   -1.265733   -0.204225
 C   -0.918591    0.582884   -1.915210
 H   -0.245463    1.295833   -2.392581
 C   -2.126924    0.290142   -2.155624
 C   -3.417079   -0.142030   -2.164179
 H   -4.179825    0.551827   -1.798989
 H   -3.743938   -0.816028   -2.962313
Na    2.238976    0.010640    3.143407
 H    2.863078   -3.329046   -3.789086
 H    5.438764   -3.738986   -0.369520
 C    1.871489   -0.878349   -3.249505
 H    0.829984   -1.060523   -2.943784
 H    2.042577    0.202992   -3.155497
 H    1.963048   -1.153380   -4.308948
 C    4.856584   -1.402656    0.844152
 H    5.847632   -0.945431    0.691875
 H    4.202608   -0.644743    1.289478
 H    4.978588   -2.221347    1.566163
83
Figure_S15-4_PA-9b(Na)-ts(1,6minor)_03 / electronic energy: -3681.00799031 a.u. / lowest freq: -409.85 cm-1
 C   -1.611495    1.866970    2.833384
 H   -2.038393    2.835963    2.536035
 C   -2.674323    0.777538    3.003521
 H   -2.501268    0.152042    3.893808
 C   -1.398839    0.336824    1.088293
 C   -3.370824   -1.077217    1.425354
 C   -4.389558   -0.825180    0.491848
 C   -3.199447   -2.339032    2.019480
 C   -5.230388   -1.883385    0.131707
 C   -4.064404   -3.369459    1.637133
 C   -5.067722   -3.145665    0.697328
 H   -5.732289   -3.961816    0.405722
Cu   -0.573751   -0.557675   -0.481418
 N   -0.822627    1.360922    1.705460
 N   -2.496049   -0.012870    1.780533
 C    0.583761   -0.582524   -2.207607
 C   -0.226425    0.615669   -2.328144
 H   -3.695606    1.179837    3.064074
 H   -0.986951    2.000409    3.727725
 H    0.268771   -1.443053   -2.803293
 C   -1.619113    0.482080   -2.768500
 C    0.336963    1.969566   -2.338216
 O   -1.928545   -0.773427   -3.131097
 O   -2.471312    1.360056   -2.769062
 O   -0.267262    2.997037   -2.603261
 O    1.647646    2.012576   -2.067449
 C    2.270854    3.284954   -2.116587
 H    2.188538    3.725703   -3.119830
 H    3.323745    3.114315   -1.866745
 H    1.813011    3.972508   -1.390689
 C   -3.287668   -1.060819   -3.415503
 H   -3.890001   -1.028656   -2.495620
 H   -3.303984   -2.075858   -3.826721
 H   -3.699464   -0.349476   -4.143682
 C    0.303198    2.103192    1.171889
 H    0.400952    1.775257    0.128020
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 C    1.604953    1.771356    1.874646
 C    2.789337    2.415986    1.487884
 C    1.683885    0.797183    2.877039
 C    4.004875    2.114095    2.098381
 H    2.763009    3.163127    0.693228
 C    2.899524    0.492780    3.491345
 H    0.782418    0.257537    3.174266
 C    4.064639    1.155817    3.110829
 H    4.913230    2.629031    1.777465
 H    2.933517   -0.271283    4.271209
 H    5.015674    0.923241    3.595156
 C   -0.075892    3.620935    1.113911
 H    0.802202    4.119886    0.624988
 H   -0.019637    3.985234    2.179977
 O   -1.252304    3.827666    0.509561
 C    1.815989   -0.689306   -1.535593
 H    2.135611    0.132061   -0.892652
 C    2.628631   -1.819088   -1.622941
 H    2.504149   -2.447370   -2.506604
 C    3.971954   -1.857280   -1.005625
 C    4.975693   -2.648543   -1.583053
 C    4.277642   -1.133578    0.159445
 C    6.251558   -2.708988   -1.025235
 H    4.750822   -3.222026   -2.486469
 C    5.551927   -1.195509    0.716008
 H    3.512066   -0.527134    0.651591
 C    6.545286   -1.981346    0.127559
 H    7.019642   -3.328508   -1.493780
 H    5.766428   -0.627533    1.623784
 H    7.542310   -2.029824    0.570724
 C   -0.616944   -2.579003   -0.189223
 H   -1.619661   -2.850836    0.142017
 C    0.470581   -3.215240   -0.292490
 C    1.758043   -3.590041   -0.489742
 H    2.002781   -4.274852   -1.305837
 H    2.438145   -3.610290    0.367395
Na   -2.178936    3.299094   -1.347766
 H   -3.940012   -4.361610    2.077679
 H   -6.026328   -1.710471   -0.597009
 C   -4.558769    0.544808   -0.107595
 H   -4.502664    1.330650    0.659867
 H   -3.770869    0.756164   -0.846489
 H   -5.526262    0.630253   -0.620457
 C   -2.096091   -2.579290    3.014641
 H   -1.940833   -3.654105    3.175744
 H   -1.148562   -2.142298    2.665934
 H   -2.330588   -2.126869    3.991109
83
Figure_S15-4_PA-9b(Na)-ts(1,6minor)_O4 / electronic energy: -3681.00623136 a.u. / lowest freq: -470.11 cm-1
 C    3.215583    2.418883   -0.066799
 H    3.567762    2.492518    0.974364
 C    3.943861    1.332114   -0.844065
 H    4.050050    1.573802   -1.916228
 C    1.790820    0.597963   -0.326527
 C    3.410595   -1.083112   -1.188254
 C    4.311558   -1.854768   -0.430485
 C    2.985154   -1.493936   -2.465514
 C    4.779159   -3.054802   -0.975987
 C    3.452324   -2.717239   -2.958415
 C    4.348025   -3.489280   -2.225633
 H    4.718922   -4.431559   -2.634831
Cu    0.010886   -0.305688   -0.290788
 N    1.844045    1.902576   -0.060814
 N    3.025257    0.194942   -0.687999
 C   -1.419541   -1.717868    0.471941
 C   -0.380001   -1.478409    1.440284
Na    2.245900   -0.007809    3.102819
 H    4.942134    1.105103   -0.447646
 H    3.278453    3.408794   -0.537126
 H   -1.179780   -2.507782   -0.248412
 C    0.781919   -2.373918    1.490651
 C   -0.545216   -0.566023    2.585272
 O    0.658974   -3.434382    0.685111
 O    1.789792   -2.201271    2.160963
 O    0.038985   -0.658922    3.650009
 O   -1.406691    0.429710    2.356163
 C   -1.502418    1.421036    3.374977
 H   -1.913833    0.990780    4.298845
 H   -2.181168    2.186621    2.982937
 H   -0.501110    1.835736    3.563676
 C    1.757491   -4.327687    0.603614
 H    2.645706   -3.820507    0.206014
 H    1.448460   -5.124975   -0.080962
 H    1.991729   -4.749773    1.590767
 C    0.775142    2.638384    0.590900
 H   -0.040515    1.913866    0.749478
 C    0.247956    3.769798   -0.269872
 C    0.680258    3.967765   -1.586996
 C   -0.730958    4.637432    0.236889
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 C    0.170869    5.006475   -2.366533
 H    1.416601    3.287092   -2.019884
 C   -1.242836    5.675917   -0.538961
 H   -1.111211    4.492383    1.250349
 C   -0.790178    5.869883   -1.844441
 H    0.526502    5.136872   -3.391316
 H   -2.005822    6.336890   -0.121080
 H   -1.191196    6.683448   -2.452889
 C    1.255483    3.051874    2.020167
 H    0.373919    3.560853    2.488372
 H    1.992081    3.889766    1.867727
 O    1.724006    2.005806    2.713135
 C   -2.753757   -1.290029    0.464249
 H   -3.094342   -0.599949    1.235498
 C   -3.606681   -1.635032   -0.584621
 H   -3.263735   -2.446703   -1.233683
 C   -5.083135   -1.526512   -0.481399
 C   -5.889814   -2.371788   -1.256590
 C   -5.712899   -0.596385    0.360662
 C   -7.280538   -2.302022   -1.186691
 H   -5.417195   -3.097799   -1.923794
 C   -7.101479   -0.525167    0.431074
 H   -5.112472    0.087954    0.963696
 C   -7.892903   -1.378096   -0.341009
 H   -7.888473   -2.973105   -1.797708
 H   -7.571099    0.205266    1.093845
 H   -8.981950   -1.319276   -0.283562
 C   -0.881388    0.530669   -1.918482
 H   -0.210538    1.250846   -2.387865
 C   -2.085116    0.233407   -2.177274
 C   -3.374337   -0.199411   -2.201559
 H   -3.691292   -0.878116   -2.999632
 H   -4.141653    0.495249   -1.847755
 C    4.724997   -1.466226    0.963501
 H    4.011813   -1.906690    1.677508
 H    5.726710   -1.851363    1.197078
 H    4.723915   -0.381175    1.125800
 C    2.059174   -0.652479   -3.300877
 H    1.006832   -0.846286   -3.042939
 H    2.229808    0.422594   -3.147944
 H    2.190807   -0.874720   -4.368249
 H    3.125300   -3.051903   -3.946028
 H    5.480609   -3.662551   -0.399115
83
Figure_S15-4_PA-9b(Na)-ts(1,6minor)_05 / electronic energy: -3681.00676070 a.u. / lowest freq: -408.77 cm-1
 C   -1.508697    1.473585    3.076580
 H   -1.970792    2.450284    2.868091
 C   -2.536913    0.342883    3.163541
 H   -2.319062   -0.364673    3.979424
 C   -1.295230    0.126674    1.190145
 C   -3.215740   -1.374864    1.427608
 C   -4.267538   -1.083655    0.544577
 C   -2.972522   -2.679157    1.891354
 C   -5.078378   -2.137630    0.111138
 C   -3.809933   -3.704469    1.440887
 C   -4.852428   -3.437403    0.556367
 H   -5.494779   -4.250310    0.210950
Cu   -0.527962   -0.534460   -0.519601
 N   -0.716136    1.084314    1.906001
 N   -2.373999   -0.311755    1.860401
 C    0.555754   -0.311162   -2.280440
 C   -0.292108    0.864120   -2.232703
 H   -3.566152    0.705945    3.293714
 H   -0.885105    1.558005    3.976996
 H    0.244136   -1.104782   -2.963606
 C   -1.676677    0.738072   -2.695985
 C    0.320205    2.183726   -2.015188
 O   -1.930706   -0.450606   -3.261806
 O   -2.576840    1.556814   -2.548665
 O    1.465050    2.368836   -1.651161
 O   -0.482332    3.227343   -2.305143
 C    0.062404    4.524041   -2.080129
 H    0.162094    4.693998   -0.999189
 H   -0.663035    5.228749   -2.503060
 H    1.033847    4.635947   -2.578357
 C   -3.279871   -0.750654   -3.579186
 H   -3.893191   -0.801728   -2.667541
 H   -3.264317   -1.731168   -4.066741
 H   -3.704308    0.001928   -4.257407
 C    0.382149    1.894379    1.413854
 H    0.474130    1.650650    0.349585
 C    1.711001    1.567237    2.056566
 C    2.872215    2.155166    1.531504
 C    1.843929    0.675831    3.126371
 C    4.122110    1.888548    2.085318
 H    2.789056    2.805373    0.657503
 C    3.096602    0.402564    3.679173
 H    0.961322    0.171317    3.524969
 C    4.239176    1.015808    3.168725
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 H     5.013656    2.352220    1.656930
 H     3.177362   -0.299067    4.512764
 H     5.218557    0.806137    3.605052
 C    -0.021827    3.401074    1.458579
 H     0.859705    3.941507    1.025105
 H    -0.004347    3.693727    2.546673
 O    -1.184971    3.633399    0.832424
 C     1.816167   -0.449834   -1.669974
 H     2.137287    0.311422   -0.957657
 C     2.655072   -1.537521   -1.920684
 H     2.526878   -2.050371   -2.875459
 C     4.011788   -1.616572   -1.337465
 C     5.028822   -2.293705   -2.026089
 C     4.314658   -1.045301   -0.090296
 C     6.314266   -2.388026   -1.494889
 H     4.807377   -2.751274   -2.994129
 C     5.598153   -1.140037    0.439338
 H     3.539530   -0.531128    0.483897
 C     6.604648   -1.810077   -0.259292
 H     7.092990   -2.916261   -2.049889
 H     5.808541   -0.687107    1.410522
 H     7.609567   -1.885801    0.161818
 C    -0.520339   -2.579263   -0.493903
 H    -1.498209   -2.924125   -0.156085
 C     0.576674   -3.163292   -0.725386
 C     1.863356   -3.470384   -1.022409
 H     2.086745   -4.030562   -1.934167
 H     2.578578   -3.591543   -0.203192
Na    -2.422171    3.109996   -0.805016
 H    -3.631840   -4.727433    1.780891
 H    -5.899074   -1.931754   -0.580507
 C    -4.495325    0.322766    0.062396
 H    -4.450834    1.047962    0.888290
 H    -3.727186    0.613943   -0.670551
 H    -5.473109    0.416856   -0.428679
 C    -1.813659   -2.967750    2.807215
 H    -1.659355   -4.049189    2.915432
 H    -0.885851   -2.524565    2.414431
 H    -1.978481   -2.552252    3.813477
83
Figure_S15-4_PA-9b(Na)-ts(1,6minor)_06 / electronic energy: -3681.00111925 a.u. / lowest freq: -471.06 cm-1
 C     3.278941    2.347933   -0.391932
 H     3.753346    2.344134    0.602556
 C     3.846779    1.267251   -1.302080
 H     3.809916    1.550164   -2.368621
 C     1.750894    0.606951   -0.526797
 C     3.184958   -1.171626   -1.461023
 C     4.161621   -1.891633   -0.745637
 C     2.523445   -1.735672   -2.566658
 C     3.758667   -3.794698   -2.194371
 H     3.973741   -4.827915   -2.474882
Cu    -0.025849   -0.269927   -0.349492
 N     1.889594    1.902326   -0.245776
 N     2.907664    0.165200   -1.057072
 C    -1.394898   -1.725428    0.395272
 C    -0.303188   -1.546291    1.321012
Na     2.392445   -0.072174    3.126552
 H     4.879591    0.992439   -1.056521
 H     3.347330    3.356407   -0.819404
 H    -1.189150   -2.494364   -0.360126
 C     0.766367   -2.554262    1.234141
 C    -0.394069   -0.655665    2.486870
 O     1.832340   -2.310118    2.029879
 O     0.746895   -3.522944    0.504259
 O     0.222243   -0.764853    3.533828
 O    -1.234276    0.369277    2.294634
 C    -1.266791    1.363750    3.312220
 H    -1.623489    0.940923    4.261653
 H    -1.964575    2.130045    2.956913
 H    -0.257899    1.782405    3.443723
 C     2.773123   -3.367366    2.152785
 H     2.293641   -4.261995    2.574766
 H     3.548723   -3.007693    2.838686
 H     3.210260   -3.622262    1.179321
 C     0.936589    2.646346    0.559522
 H     0.128720    1.936144    0.797523
 C     0.326609    3.818057   -0.181781
 C    -0.644124    4.604029    0.456650
 C     0.663203    4.135292   -1.502842
 C    -1.241964    5.680182   -0.195421
 H    -0.948984    4.362526    1.477451
 C     0.066529    5.212612   -2.159734
 H     1.387965    3.518490   -2.038353
 C    -0.885691    5.993459   -1.507794
 H    -1.997639    6.274370    0.323702
 H     0.344115    5.435595   -3.192633
 H    -1.354899    6.835935   -2.020660
 C     1.598382    3.005632    1.929370
 H     0.804654    3.555395    2.498544
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 H    2.358377    3.804556    1.702827
 O    2.084614    1.925512    2.555028
 C   -2.727102   -1.299088    0.473630
 H   -3.026423   -0.641482    1.289693
 C   -3.634461   -1.599486   -0.542609
 H   -3.322894   -2.378302   -1.245482
 C   -5.103618   -1.501568   -0.359829
 C   -5.947424   -2.312352   -1.132393
 C   -5.691066   -0.611019    0.552655
 C   -7.333220   -2.245824   -0.993696
 H   -5.508384   -3.008084   -1.852766
 C   -7.074667   -0.542801    0.691487
 H   -5.060997    0.045902    1.156084
 C   -7.903226   -1.360197   -0.080143
 H   -7.970176   -2.889486   -1.604735
 H   -7.510888    0.158107    1.406955
 H   -8.988278   -1.303380    0.030300
 C   -1.013535    0.692525   -1.853500
 H   -0.363533    1.445824   -2.299378
 C   -2.218400    0.385172   -2.091194
 C   -3.495752   -0.081614   -2.097675
 H   -3.820064   -0.727347   -2.919986
 H   -4.270191    0.570695   -1.684226
 C    4.437042   -3.205963   -1.131400
 H    5.186571   -3.778083   -0.578558
 C    2.816019   -3.061307   -2.906085
 H    2.301463   -3.516274   -3.756004
 C    4.913208   -1.272125    0.402009
 H    5.827487   -0.767807    0.049683
 H    4.307033   -0.519653    0.922406
 H    5.227401   -2.036627    1.124698
 C    1.528453   -0.958780   -3.384225
 H    0.506921   -1.083465   -2.993686
 H    1.740970    0.119075   -3.376058
 H    1.531822   -1.307342   -4.426124
83
Figure_S15-4_PA-9b(Na)-ts(1,6minor)_07 / electronic energy: -3681.00898900 a.u. / lowest freq: -435.85 cm-1
 C    1.081920    3.450821    0.699439
 H    1.189782    3.823516    1.725784
 C    2.430808    3.217937    0.006758
 H    2.608419    3.908501   -0.829086
 C    1.193067    1.227782    0.005479
 C    3.255927    1.180020   -1.283031
 C    4.170321    0.294995   -0.687362
 C    3.246333    1.422123   -2.666984
 C    5.073712   -0.375301   -1.516748
 C    4.167647    0.732783   -3.461887
 C    5.070041   -0.162202   -2.893336
 H    5.777802   -0.698906   -3.528616
Cu    0.581471   -0.580979   -0.514720
 N    0.497516    2.108290    0.715459
 N    2.295730    1.835724   -0.462907
 C   -0.345968   -2.386750   -0.032012
 C    0.749435   -2.220112    0.889124
 H    3.282205    3.301364    0.702019
 H    0.428859    4.136567    0.135206
 H   -0.146704   -3.105294   -0.832193
 C    1.994905   -2.886574    0.457689
 C    0.628980   -1.640402    2.229527
 O    2.938786   -2.986414    1.399896
 O    2.168625   -3.334877   -0.661316
 O    1.553066   -1.256715    2.934702
 O   -0.634969   -1.545816    2.651272
 C   -0.866171   -0.924025    3.912269
 H   -0.399831   -1.507225    4.719533
 H   -1.953922   -0.918667    4.043639
 H   -0.470503    0.106393    3.914512
 C    4.162497   -3.576576    1.000818
 H    4.020588   -4.629550    0.718041
 H    4.831743   -3.509380    1.866007
 H    4.597165   -3.040559    0.144550
 C   -0.767037    1.842502    1.379562
 H   -0.810158    0.746652    1.485143
 C   -1.955232    2.271138    0.523302
 C   -3.140213    2.753823    1.094825
 C   -1.908133    2.130248   -0.870520
 C   -4.240243    3.079720    0.299601
 H   -3.218130    2.877112    2.175551
 C   -3.006177    2.451120   -1.666293
 H   -1.008117    1.738157   -1.346260
 C   -4.180218    2.927472   -1.084306
 H   -5.152094    3.455010    0.770072
 H   -2.941409    2.319900   -2.749042
 H   -5.044163    3.175340   -1.704841
 C   -0.725580    2.419908    2.824427
 H   -1.668578    2.051939    3.307120
 H   -0.889866    3.528822    2.725421
 O    0.390998    2.078515    3.486294
 C   -1.648517   -1.853888    0.016121
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 H   -1.912346   -1.140601    0.796977
 C   -2.613264   -2.201715   -0.932823
 H   -2.442981   -3.135892   -1.472345
 C   -4.036991   -1.831393   -0.767477
 C   -5.034551   -2.696973   -1.238580
 C   -4.428903   -0.630785   -0.153957
 C   -6.384683   -2.386405   -1.083252
 H   -4.745928   -3.631196   -1.727866
 C   -5.776902   -0.319928   -0.000696
 H   -3.674769    0.083217    0.185020
 C   -6.761681   -1.196990   -0.460267
 H   -7.145523   -3.079150   -1.450174
 H   -6.056816    0.622819    0.474692
 H   -7.818847   -0.951611   -0.337204
 C    0.175408   -0.515441   -2.519135
 H    1.045458   -0.117501   -3.041816
 C   -1.001042   -0.812667   -2.873968
 C   -2.310078   -1.174414   -2.905703
 H   -2.608650   -2.072495   -3.452836
 H   -3.065854   -0.384867   -2.839774
Na    2.081552    0.843221    3.620428
 H    4.168400    0.895761   -4.542393
 H    5.792473   -1.070342   -1.075438
 C    4.169845    0.082905    0.802647
 H    4.220650    1.045625    1.335224
 H    3.257015   -0.431549    1.140350
 H    5.031171   -0.523450    1.112994
 C    2.267413    2.391185   -3.275723
 H    2.153180    2.211140   -4.353008
 H    1.277531    2.312575   -2.803238
 H    2.608182    3.431501   -3.149367
83
Figure_S15-4_PA-9b(Na)-ts(1,6minor)_08 / electronic energy: -3681.00969248 a.u. / lowest freq: -442.20 cm-1
 C    1.122922    3.485773   -0.547243
 H    1.242695    4.184417    0.290907
 C    2.466112    3.009010   -1.118685
 H    2.619510    3.317047   -2.162504
 C    1.228481    1.161569   -0.374633
 C    3.348758    0.646207   -1.453954
 C    4.206057    0.066943   -0.501948
 C    3.449261    0.351222   -2.823880
 C    5.169013   -0.841519   -0.950041
 C    4.424714   -0.565372   -3.230467
 C    5.275455   -1.159027   -2.302283
 H    6.030880   -1.873870   -2.635543
Cu    0.610738   -0.706995   -0.185447
 N    0.517686    2.240370   -0.071145
 N    2.345211    1.551889   -1.011004
 C   -0.355443   -2.208102    0.878268
 C    0.687518   -1.693126    1.732554
 H    3.327466    3.364536   -0.530921
 H    0.477828    3.951086   -1.309707
 H   -0.131253   -3.168013    0.406155
 C    1.988156   -2.392983    1.721136
 C    0.495861   -0.682689    2.776018
 O    2.162231   -3.098800    0.580483
 O    2.838895   -2.374413    2.581878
 O    1.391396   -0.093405    3.366279
 O   -0.787022   -0.427328    3.046379
 C   -1.069499    0.604562    3.987086
 H   -0.668136    0.343470    4.976988
 H   -2.162146    0.668368    4.037662
 H   -0.639707    1.562000    3.645057
 C    3.369709   -3.827834    0.461822
 H    4.237312   -3.154544    0.505179
 H    3.332827   -4.322858   -0.514829
 H    3.459800   -4.577275    1.261439
 C   -0.764138    2.233510    0.612163
 H   -0.823075    1.247523    1.099729
 C   -1.925653    2.329033   -0.373312
 C   -3.127336    2.967609   -0.038377
 C   -1.837077    1.713388   -1.629727
 C   -4.202998    2.985906   -0.927822
 H   -3.237817    3.456046    0.930336
 C   -2.911029    1.726045   -2.517557
 H   -0.921536    1.193248   -1.915119
 C   -4.101857    2.362696   -2.170122
 H   -5.128936    3.490865   -0.642565
 H   -2.814403    1.228838   -3.485642
 H   -4.946438    2.370009   -2.862510
 C   -0.751660    3.284951    1.758769
 H   -1.719184    3.125828    2.302921
 H   -0.883458    4.289407    1.268498
 O    0.333386    3.183834    2.542363
 C   -1.657680   -1.711487    0.671309
 H   -1.949414   -0.765455    1.126949
 C   -2.582575   -2.386474   -0.130425
 H   -2.402148   -3.452825   -0.283743
 C   -4.008032   -1.986203   -0.173481
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 C   -4.997564   -2.964812   -0.344346
 C   -4.407580   -0.644717   -0.060614
 C   -6.348109   -2.620270   -0.381338
 H   -4.702843   -4.012873   -0.445798
 C   -5.755687   -0.300864   -0.098611
 H   -3.657585    0.144813    0.028690
 C   -6.733146   -1.285805   -0.255794
 H   -7.103228   -3.399345   -0.509284
 H   -6.040840    0.750257   -0.014902
 H   -7.790364   -1.013081   -0.287638
 C    0.280932   -1.349785   -2.101231
 H    1.172919   -1.146076   -2.693470
 C   -0.879160   -1.772431   -2.370008
 C   -2.187322   -2.138045   -2.314492
 H   -2.464888   -3.175275   -2.520233
 H   -2.941178   -1.386184   -2.569934
Na    1.941559    2.117216    3.371833
 H    4.512773   -0.816610   -4.290256
 H    5.850006   -1.297752   -0.227167
 C    4.088590    0.425074    0.954736
 H    4.092760    1.517324    1.092683
 H    3.152712    0.046946    1.392919
 H    4.919817   -0.000507    1.531489
 C    2.533365    0.999817   -3.828157
 H    2.464758    0.397875   -4.744295
 H    1.520483    1.134697   -3.422110
 H    2.905935    1.995901   -4.117528
89
Figure_S15-5_9d(NaOPh)-Cu-allyl_01 / electronic energy: -3597.06845638 a.u. / lowest freq: 14.75 cm-1
Na    1.466278   -1.713895    0.568774
 H    4.895602   -3.588713    0.817161
 H    4.692117   -0.895972   -2.541156
 O    3.335573   -2.007938   -0.584046
 C    5.271052   -1.564621   -1.896670
 C    4.600612   -2.207337   -0.820863
 H    7.102470   -1.262094   -2.980981
 C    6.625148   -1.776136   -2.141098
 C    5.384324   -3.077572   -0.017672
 C    7.377630   -2.634567   -1.334758
 C    6.737508   -3.280572   -0.272517
 H    8.439672   -2.798024   -1.529682
 H    7.306712   -3.957090    0.372185
 H    1.822369   -0.807067    3.943134
 H   -2.251641   -0.329887    3.139589
 C    0.449649   -2.296353    3.162582
 C   -1.148749   -0.342683    3.068826
 H    0.743177   -3.269591    2.747587
 C   -0.656265   -1.681110    2.668089
 H   -0.722254    0.025625    4.016197
 B   -1.373536   -2.298457    1.423828
 O   -2.713492   -2.319048    1.179742
 H   -1.727987   -0.728011   -0.976153
 O   -0.646091   -2.774963    0.347830
 H   -0.369549   -1.436810   -1.877879
 C   -1.416767   -1.592283   -1.578998
 H   -3.924597   -1.288533   -0.925882
 C   -1.545189   -2.887384   -0.779148
 C   -2.937112   -3.023746   -0.060716
 C   -4.089317   -2.364956   -0.799421
 H   -2.035120   -1.618693   -2.487150
 H   -5.022038   -2.500680   -0.233511
 H   -2.452907   -4.961768    0.822840
 H   -4.156010   -4.465844    0.969667
 C   -3.284310   -4.466581    0.300122
 H   -0.161528   -3.891634   -2.091822
 C   -1.138452   -4.082032   -1.624394
 H   -1.058778   -4.996627   -1.023531
 H   -4.221693   -2.822726   -1.791255
 H   -3.534901   -5.053460   -0.594647
 H   -1.873021   -4.249881   -2.425820
 H    2.084171   -2.447422    4.577693
 C    1.310104   -1.734587    4.260318
 H    0.715848   -1.463962    5.150374
 C    0.319514    2.875268   -1.993392
 H    1.033917    2.506723   -2.740473
 C   -1.127654    2.540540   -2.354801
 H   -1.705390    3.414017   -2.684987
 C   -0.661312    1.729692   -0.210974
 C   -3.004911    1.645974   -0.933491
 C   -3.559642    1.488554    0.340873
 C   -3.804764    1.434619   -2.061581
 C   -4.882144    1.072030    0.498446
 C   -5.140732    1.044490   -1.923628
 C   -5.665477    0.864801   -0.641218
 H   -6.706703    0.550845   -0.526471
Cu   -0.836713    0.775737    1.479326
 N    0.481016    2.176611   -0.718861
 N   -1.650734    2.012129   -1.089715
 H    2.605203   -0.823585   -1.253202
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 H   -1.180566    1.768453   -3.138589
 H    0.488311    3.954711   -1.852253
 C    1.783728    1.989569   -0.103034
 H    1.577644    1.419376    0.818373
 C    2.387717    3.326050    0.305028
 C    3.684660    3.715190   -0.041325
 C    1.611056    4.193427    1.085504
 C    4.194290    4.943729    0.386120
 H    4.319736    3.066305   -0.646305
 C    2.116435    5.418098    1.511249
 H    0.594881    3.899472    1.363203
 C    3.414073    5.797630    1.161301
 H    5.210992    5.230395    0.108577
 H    1.496950    6.078282    2.122170
 H    3.815380    6.756940    1.495184
 C    2.667582    1.110708   -0.990647
 H    3.584280    0.863576   -0.424765
 H    2.991597    1.684656   -1.881421
 O    1.975771   -0.040827   -1.362266
 C   -5.977773    0.764471   -3.144325
 H   -5.678591    1.395447   -3.993282
 H   -5.860945   -0.286000   -3.456591
 H   -7.045661    0.932149   -2.946707
 C   -5.429241    0.820029    1.877761
 H   -6.526964    0.864113    1.893808
 H   -5.127045   -0.182053    2.222954
 H   -5.039940    1.546746    2.605212
 H   -2.959357    1.704718    1.226933
 H   -3.392248    1.559302   -3.063750
121
Figure_S15-5_AA-9d(NaOPh)-ts(1,6major)_01 / electronic energy: -4439.05034678 a.u. / lowest freq: -323.92 cm-1
 H    1.531852    2.790146   -2.844247
 H    0.412404    0.668919   -2.120806
 C    2.797337    1.816802   -1.391465
 C    1.106764    0.026893   -1.562237
 H    3.863212    2.053348   -1.431478
 C    2.443015    0.473043   -1.394451
 H    0.980905   -1.042579   -1.772976
 B    3.549881   -0.575461   -1.074372
 O    3.441876   -1.912723   -1.338260
 H    5.931808   -1.231726   -2.662388
 O    4.741925   -0.257658   -0.472719
 H    7.060334   -0.324564   -1.628083
 C    6.504967   -1.268332   -1.724530
 H    5.229237   -3.418982   -2.572010
 C    5.584466   -1.424315   -0.514875
 C    4.533680   -2.583052   -0.684149
 C    5.003175   -3.742626   -1.548148
 H    7.229857   -2.091893   -1.788292
 H    4.215154   -4.506333   -1.598906
 H    3.651512   -2.278459    1.288468
 H    3.127599   -3.747121    0.434681
 C    3.993170   -3.103209    0.645751
 H    7.113959   -0.653716    0.796776
 C    6.403413   -1.492079    0.764517
 H    5.765500   -1.434395    1.655594
 H    5.903640   -4.204201   -1.116173
 H    4.745148   -3.690144    1.191751
 H    6.978935   -2.428896    0.803870
 H    2.263621    3.895688   -1.653947
 C    1.835048    2.893134   -1.787389
 H    0.911582    2.826075   -1.190317
 C   -3.316186   -2.155874   -1.398300
 H   -4.156754   -2.422195   -0.742036
 C   -3.526707   -0.799318   -2.066112
 H   -3.326121   -0.836908   -3.148082
 C   -1.704143   -0.654114   -0.602983
 C   -2.484833    1.435382   -1.641874
 C   -1.809491    2.309622   -0.779549
 C   -3.152709    1.955574   -2.751481
 C   -1.767565    3.677195   -1.042649
 C   -3.141830    3.329489   -3.019984
 C   -2.438441    4.176874   -2.166502
 H   -2.413719    5.251094   -2.370520
Cu    0.006515   -0.027793    0.205264
 N   -2.104610   -1.925704   -0.604990
 N   -2.531322    0.048634   -1.397788
 C    1.290145    0.606135    1.703137
 C    0.072517    0.119888    2.333086
 H   -3.772351   -2.876610    1.379068
 H   -4.536850   -0.400204   -1.902121
 H   -3.165656   -2.967768   -2.123805
 H    2.089341   -0.139005    1.673567
 C   -1.064345    0.956159    2.742909
 C    0.072792   -1.253207    2.856704
 O   -0.865063    2.269668    2.563347
 O   -2.126197    0.558475    3.193476
 O   -0.778040   -1.764397    3.566541
 O    1.144058   -1.974137    2.479366
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 C    1.222875   -3.294105    2.994442
 H    1.319956   -3.281337    4.088911
 H    2.111922   -3.745191    2.543777
 H    0.326134   -3.872662    2.730344
 C   -1.948725    3.133843    2.880121
 H   -2.757723    3.021644    2.142576
 H   -1.545574    4.150890    2.838491
 H   -2.341646    2.921775    3.882390
 C   -1.362628   -3.015194    0.003200
 H   -0.779124   -2.571576    0.823411
 C   -0.383693   -3.671350   -0.965527
 C    0.492411   -4.657421   -0.493098
 C   -0.310138   -3.311832   -2.314249
 C    1.403379   -5.275553   -1.345862
 H    0.475264   -4.942237    0.561573
 C    0.603113   -3.927137   -3.170944
 H   -0.954685   -2.525176   -2.709034
 C    1.461414   -4.913066   -2.691690
 H    2.078891   -6.038961   -0.953216
 H    0.646441   -3.624325   -4.219179
 H    2.179335   -5.391531   -3.361013
 C   -2.317716   -4.042085    0.638678
 H   -1.705482   -4.860969    1.043526
 H   -2.944550   -4.492864   -0.154612
 O   -3.079136   -3.526747    1.679268
 C    1.706295    1.923543    1.411283
 H    1.000152    2.739469    1.544959
 C    2.975350    2.175312    0.914239
 H    3.702124    1.361087    0.943297
 C    3.574831    3.519582    0.821940
 C    4.958519    3.630495    0.603164
 C    2.828916    4.704466    0.931775
 C    5.574376    4.874565    0.496418
 H    5.551401    2.716561    0.507877
 C    3.443320    5.949760    0.823856
 H    1.751275    4.657613    1.094795
 C    4.818571    6.042924    0.605105
 H    6.651842    4.933812    0.326072
 H    2.841462    6.857418    0.910511
 H    5.298290    7.020266    0.519104
 C   -3.895631    3.862314   -4.210348
 H   -3.611585    3.331642   -5.131537
 H   -4.979789    3.722745   -4.076124
 H   -3.708280    4.934164   -4.360492
 C   -1.017767    4.615813   -0.135240
 H   -0.476459    4.064653    0.643801
 H   -0.285848    5.209369   -0.703696
 H   -1.702311    5.323228    0.357787
 H   -1.322372    1.929538    0.118541
 H   -3.705789    1.299131   -3.423292
 O   -4.649250   -1.533846    1.626024
Na   -3.032395   -1.546919    3.183395
 C   -5.240819   -0.644347    0.889136
 C   -4.783849    0.701559    0.828275
 C   -6.367852   -0.961991    0.080743
 C   -5.390210    1.642867    0.004416
 H   -3.911075    0.968243    1.431189
 C   -6.970611   -0.008573   -0.737110
 H   -6.749076   -1.987051    0.114924
 C   -6.489206    1.303127   -0.792408
 H   -4.982268    2.657726   -0.034847
 H   -7.831630   -0.296643   -1.348353
 H   -6.957778    2.044331   -1.443532
121
Figure_S15-5_AA-9d(NaOPh)-ts(1,6major)_02 / electronic energy: -4439.05088590 a.u. / lowest freq: -338.66 cm-1
 H    1.755897    2.589666   -2.870519
 H    0.496732    0.572282   -2.130016
 C    2.941573    1.546113   -1.400691
 C    1.135981   -0.124094   -1.571108
 H    4.021053    1.709516   -1.435760
 C    2.500831    0.226266   -1.398872
 H    0.929871   -1.177266   -1.796614
 B    3.568194   -0.859344   -1.058929
 O    3.444573   -2.204039   -1.292790
 H    5.961338   -1.580020   -2.617799
 O    4.763550   -0.551410   -0.459043
 H    7.089315   -0.665243   -1.590270
 C    6.525029   -1.604894   -1.673905
 H    5.206763   -3.754731   -2.500092
 C    5.591915   -1.726202   -0.469673
 C    4.529886   -2.876064   -0.623024
 C    4.999448   -4.053245   -1.464898
 H    7.242231   -2.436424   -1.714661
 H    4.230600   -4.838717   -1.482143
 H    3.615090   -2.539550    1.331164
 H    3.131688   -4.043304    0.510227
 C    3.979444   -3.372669    0.711888
 H    7.118694   -0.946040    0.838495
 C    6.398245   -1.776184    0.818589
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H	5.752966	-1.689902	1.702037
H	5.912730	-4.489741	-1.033952
H	4.734055	-3.933425	1.280733
H	6.961829	-2.718609	0.884568
H	2.557024	3.654096	-1.687535
C	2.059422	2.682855	-1.812816
H	1.130228	2.688147	-1.222122
C	-3.609547	-1.849831	-1.375124
H	-4.509146	-1.972048	-0.754668
C	-3.598139	-0.507666	-2.101865
H	-3.409307	-0.629104	-3.178597
C	-1.794791	-0.588269	-0.603491
C	-2.217616	1.547110	-1.751383
C	-1.570562	2.378965	-0.828259
C	-2.657718	2.081795	-2.962721
C	-1.336086	3.720015	-1.125270
C	-2.444953	3.430096	-3.272989
C	-1.778166	4.234611	-2.350950
H	-1.602951	5.289227	-2.581777
Cu	-0.021835	-0.087811	0.180314
N	-2.414257	-1.767139	-0.533520
N	-2.478337	0.192650	-1.461667
C	1.324266	0.461148	1.663787
C	0.084593	0.072118	2.318739
H	-4.166247	-2.262079	1.551284
H	-4.528404	0.060236	-1.961995
H	-3.536596	-2.700817	-2.067489
H	2.063119	-0.343046	1.619227
C	-0.926126	1.008720	2.826949
C	-0.044016	-1.321053	2.765025
O	-0.662638	2.295581	2.552316
O	-1.938372	0.721060	3.443933
O	-0.942700	-1.797637	3.437862
O	0.956546	-2.116301	2.334409
C	0.897767	-3.477227	2.734903
H	0.857623	-3.564012	3.828863
H	1.808888	-3.945775	2.351738
H	0.015523	-3.975341	2.307478
C	-1.598218	3.255414	3.025702
H	-2.556569	3.161624	2.494670
H	-1.153633	4.235622	2.825073
H	-1.772487	3.133159	4.102423
C	-1.892555	-2.948241	0.149890
H	-1.219882	-2.565902	0.926647
C	-1.079939	-3.809979	-0.803789
C	-1.678498	-4.761795	-1.639840
C	0.303467	-3.617855	-0.893033
C	-0.914721	-5.494004	-2.548748
H	-2.753458	-4.945797	-1.589727
C	1.065533	-4.336072	-1.812229
H	0.794647	-2.885450	-0.245694
C	0.459112	-5.278614	-2.641802
H	-1.400157	-6.232187	-3.190891
H	2.133024	-4.130612	-1.885856
H	1.057255	-5.842879	-3.360584
C	-2.999966	-3.738420	0.860575
H	-2.522809	-4.630540	1.296326
H	-3.732195	-4.112333	0.120088
O	-3.633882	-3.042026	1.879807
C	1.837943	1.743809	1.376730
H	1.193274	2.608993	1.504064
C	3.126104	1.905656	0.891444
H	3.797083	1.046287	0.933759
C	3.817928	3.205866	0.806083
C	5.205289	3.218862	0.582856
C	3.159122	4.439630	0.930050
C	5.909050	4.416298	0.486674
H	5.729489	2.265283	0.474684
C	3.861703	5.638491	0.833119
H	2.081677	4.469451	1.098053
C	5.239591	5.634566	0.610832
H	6.987481	4.398709	0.312967
H	3.327609	6.586272	0.932893
H	5.787380	6.576321	0.534702
C	-2.931250	3.979456	-4.588688
H	-2.431426	3.479993	-5.433163
H	-4.012785	3.813877	-4.708393
H	-2.739536	5.057825	-4.671737
C	-0.636046	4.619939	-0.142598
H	-0.211133	4.042726	0.687715
H	0.180949	5.173670	-0.629117
H	-1.332012	5.362101	0.278872
H	-1.272383	1.989004	0.146170
H	-3.178618	1.454173	-3.686457
O	-4.696192	-0.764358	1.746223
Na	-3.167251	-1.180651	3.346452
C	-5.191358	0.108352	0.925300
C	-4.573751	1.370932	0.712314
C	-6.370961	-0.147694	0.171198

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 C   -5.084490    2.293069   -0.194206
 H   -3.653081    1.582277    1.262986
 C   -6.876546    0.784725   -0.731380
 H   -6.872880   -1.108756    0.318592
 C   -6.241316    2.014887   -0.930215
 H   -4.557360    3.240169   -0.344965
 H   -7.784383    0.545701   -1.293991
 H   -6.636061    2.739947   -1.645251
121
Figure_S15-5_AA-9d(NaOPh)-ts(1,6minor)_01 / electronic energy: -4439.04244814 a.u. / lowest freq: -345.54 cm-1
 H    3.639728    4.266447   -2.509121
 H    5.388690    3.936274   -2.539873
 C    4.570082    4.339701   -1.927262
 H    4.776222    5.400836   -1.728982
 H    2.364214    5.468895   -1.006152
 B    2.946946    1.894371   -0.984115
 O    4.293598    2.156885   -1.001008
 C    2.635293    5.247525    0.033642
 C    4.477675    3.534750   -0.631232
 O    2.228194    2.907443   -0.407684
 H    3.388991    5.976410    0.366474
 H    1.738813    5.376955    0.653905
 C    3.165161    3.830546    0.181425
 H    6.626681    3.451917   -0.482954
 C    5.765733    3.668006    0.165820
 H    5.877723    4.691673    0.552952
 H    5.792510    2.967929    1.010573
 C    3.287985    3.458197    1.657553
 H    2.289341    3.473404    2.113079
 H    3.696833    2.444975    1.785362
 H    3.930670    4.164046    2.201901
 C    2.344424    0.558122   -1.513129
 C    3.244296   -0.471752   -1.760560
 H    4.297714   -0.202782   -1.866445
 H    2.376696   -1.689252   -3.316210
 H    2.021748   -2.231701   -1.672481
 C    2.809661   -1.795115   -2.305954
 H    3.640762   -2.510413   -2.366520
 H    0.349399    1.306102   -1.583391
 C    0.940349    0.383521   -1.566859
 H    0.547632   -0.401635   -2.226292
 C   -3.614220   -1.436651   -1.707166
 H   -4.558500   -1.603409   -1.169716
 C   -3.475933    0.016005   -2.162540
 H   -3.158367    0.086578   -3.214195
 C   -1.815917   -0.459907   -0.576082
 C   -2.076995    1.881767   -1.217845
 C   -2.179560    2.678147   -2.359662
 C   -1.637515    2.439404   -0.015250
 C   -1.811119    4.026238   -2.319131
 C   -1.257322    3.780004    0.042553
 C   -1.345121    4.560160   -1.114540
 H   -1.054752    5.613692   -1.071678
Cu    0.021547   -0.275248    0.211713
 N   -2.471127   -1.596063   -0.805778
 N   -2.420161    0.516994   -1.277159
 C    1.619020   -0.416432    1.536495
 C    0.388120   -0.614149    2.281369
 H   -4.254887   -1.851371    1.232830
 H   -4.400194    0.594738   -2.026733
 H   -3.551685   -2.148288   -2.542100
 H    1.990119    0.612563    1.576943
 C   -0.154234    0.525396    3.047909
 C   -0.166797   -1.917443    2.653295
 O    0.746251    1.487446    3.282294
 O   -1.293425    0.625514    3.473233
 O   -1.125458   -2.114787    3.383925
 O    0.481878   -2.958188    2.105610
 C    0.028763   -4.260130    2.446375
 H    0.169204   -4.451895    3.518867
 H    0.636610   -4.953092    1.854504
 H   -1.034509   -4.386019    2.200285
 C    0.350759    2.533149    4.158963
 H   -0.601945    2.977477    3.847655
 H    1.149643    3.281838    4.124912
 H    0.245316    2.147352    5.183117
 C   -2.145968   -2.875864   -0.191980
 H   -1.433247   -2.633400    0.604049
 C   -1.450638   -3.815921   -1.160249
 C   -2.151766   -4.579109   -2.102145
 C   -0.055575   -3.918105   -1.118897
 C   -1.469672   -5.416331   -2.985435
 H   -3.241900   -4.530999   -2.153245
 C    0.628323   -4.755514   -1.998085
 H    0.498624   -3.331243   -0.381614
 C   -0.078822   -5.507119   -2.936148
 H   -2.031277   -6.004778   -3.714209
 H    1.717787   -4.819200   -1.949024
 H    0.453548   -6.164963   -3.626338
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 C   -3.373630   -3.498926    0.487793
 H   -3.059163   -4.474046    0.893392
 H   -4.154179   -3.719565   -0.265879
 O   -3.872841   -2.729916    1.530714
 C    2.534770   -1.365870    1.032272
 H    2.267257   -2.418633    1.073708
 C    3.740545   -0.992813    0.458348
 H    4.077791    0.036735    0.598278
 C    4.826988   -1.945844    0.159574
 C    6.120854   -1.451193   -0.074036
 C    4.627918   -3.334162    0.081078
 C    7.177623   -2.307834   -0.371284
 H    6.291329   -0.371991   -0.026902
 C    5.684061   -4.191939   -0.217170
 H    3.633555   -3.754841    0.244418
 C    6.964399   -3.684816   -0.444924
 H    8.174285   -1.896599   -0.547198
 H    5.504742   -5.268034   -0.275536
 H    7.790074   -4.359898   -0.680124
 C   -0.776633    4.361166    1.342263
 H    0.153973    3.863921    1.652413
 H   -0.582673    5.439156    1.259246
 H   -1.519812    4.209758    2.139606
 C   -1.892147    4.867174   -3.566459
 H   -1.725800    5.930771   -3.347882
 H   -1.133156    4.551414   -4.299404
 H   -2.874483    4.764445   -4.051188
 H   -2.532390    2.248215   -3.298760
 H   -1.625997    1.825902    0.889153
 O   -4.504684   -0.277146    1.383540
Na   -3.012642   -0.835028    2.941519
 C   -5.288857    0.439548    0.638436
 C   -5.075086    1.830932    0.443259
 C   -6.396510   -0.128864   -0.050101
 C   -5.871997    2.577126   -0.418438
 H   -4.236909    2.300536    0.963436
 C   -7.188017    0.628250   -0.909648
 H   -6.607399   -1.191597    0.105874
 C   -6.933041    1.987567   -1.114437
 H   -5.655926    3.640806   -0.556725
 H   -8.022943    0.147865   -1.429036
 H   -7.554034    2.577573   -1.791891
121
Figure_S15-5_AA-9d(NaOPh)-ts(1,6minor)_02 / electronic energy: -4439.04486199 a.u. / lowest freq: -347.74 cm-1
 H   -1.879353   -2.590285    0.942378
 H   -0.498727    0.922645    1.738733
 C   -3.275758   -0.962592    1.157853
 C   -1.032375    0.004756    1.465123
 H   -4.349623   -0.770095    1.197223
 C   -2.427173    0.136121    1.250751
 H   -0.689216   -0.880883    2.016152
 B   -3.043849    1.550765    1.030311
 O   -2.410120    2.727991    1.322528
 H   -3.046105    3.069082   -1.425914
 O   -4.302638    1.751737    0.519213
 H   -4.742295    2.727790   -1.844766
 C   -4.087704    3.359765   -1.227380
 H   -2.171105    4.858350   -0.229659
 C   -4.443534    3.157703    0.244906
 C   -3.383637    3.784557    1.221653
 C   -2.708035    5.044197    0.707289
 H   -4.224388    4.405620   -1.536838
 H   -1.976927    5.401855    1.446262
 H   -4.441842    3.122051    3.013684
 H   -3.105092    4.261323    3.302270
 C   -3.937848    4.019696    2.626649
 H   -6.546412    3.095104   -0.226851
 C   -5.881491    3.576121    0.505071
 H   -6.212931    3.283846    1.509443
 H   -3.450617    5.838813    0.540916
 H   -4.650881    4.855865    2.643007
 H   -5.991445    4.665696    0.399976
 H   -3.571403   -3.101422    1.199794
 C   -2.815291   -2.351887    1.475389
 H   -2.602854   -2.464988    2.553298
 C    3.756434   -0.579894    2.000533
 H    4.702939   -0.830560    1.501651
 C    3.470966    0.920950    1.956127
 H    3.180362    1.313416    2.942908
 C    1.853732   -0.202508    0.690740
 C    1.822608    2.249193    0.609569
 C    1.054405    2.363337   -0.555956
 C    2.097347    3.392005    1.362163
 C    0.532796    3.595116   -0.947099
 C    1.598629    4.641233    0.976176
 C    0.813379    4.727044   -0.172493
 H    0.409626    5.696918   -0.476430
Cu    0.102280   -0.540954   -0.194366
 N    2.624182   -1.133459    1.251048
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 N    2.338597    1.005512    1.025541
 C   -1.188084   -0.906154   -1.780477
 C    0.141383   -1.371804   -2.155389
 H    4.651567   -2.344922   -0.160556
 H    4.321199    1.503207    1.575431
 H    3.784363   -0.977497    3.024996
 H   -1.368621    0.150159   -2.009409
 C    0.996543   -0.523516   -2.993123
 C    0.587641   -2.755637   -1.980165
 O    0.367530    0.563664   -3.467268
 O    2.170643   -0.718374   -3.265600
 O    1.587143   -3.270240   -2.458408
 O   -0.213616   -3.476440   -1.176579
 C    0.103384   -4.848868   -1.012432
 H    0.012649   -5.385800   -1.967001
 H   -0.619665   -5.240157   -0.288453
 H    1.128403   -4.976455   -0.636080
 C    1.145149    1.448831   -4.261177
 H    1.902757    1.958492   -3.646889
 H    0.444080    2.181339   -4.673596
 H    1.647953    0.906789   -5.072511
 C    2.296486   -2.547583    1.260176
 H    1.714485   -2.731987    0.345316
 C    1.418673   -2.936852    2.445823
 C    0.855878   -4.219119    2.490192
 C    1.108682   -2.043573    3.475103
 C    0.006101   -4.595536    3.527179
 H    1.071210   -4.935733    1.695014
 C    0.260865   -2.417695    4.518470
 H    1.504169   -1.027120    3.459323
 C   -0.295515   -3.693878    4.548549
 H   -0.429311   -5.597010    3.533020
 H    0.027053   -1.697404    5.305137
 H   -0.966418   -3.984648    5.359488
 C    3.566144   -3.408030    1.145952
 H    3.264083   -4.462832    1.224789
 H    4.221081   -3.211196    2.016453
 O    4.233207   -3.243897   -0.062541
 C   -2.349843   -1.659022   -1.518361
 H   -2.275111   -2.745024   -1.522232
 C   -3.540148   -1.063636   -1.141144
 H   -3.608717    0.024514   -1.205935
 C   -4.849106   -1.746633   -1.129005
 C   -6.009679   -0.975783   -0.940128
 C   -4.996049   -3.133472   -1.291137
 C   -7.269650   -1.566903   -0.916540
 H   -5.901705    0.101356   -0.786373
 C   -6.257548   -3.725459   -1.265374
 H   -4.117616   -3.763137   -1.445449
 C   -7.400636   -2.947210   -1.079388
 H   -8.156727   -0.946941   -0.767012
 H   -6.348931   -4.806216   -1.396381
 H   -8.387621   -3.414402   -1.061084
 C    1.925629    5.863579    1.793576
 H    1.740091    5.688549    2.863687
 H    2.989355    6.128471    1.686213
 H    1.328921    6.730529    1.478249
 C   -0.283589    3.720358   -2.205795
 H   -0.748210    2.764073   -2.482024
 H   -1.076156    4.474420   -2.095812
 H    0.347753    4.043563   -3.048184
 H    0.877587    1.489532   -1.182724
 H    2.705176    3.326788    2.265049
 O    5.065038   -1.055504   -1.066122
Na    3.635294   -2.216771   -2.324872
 C    5.305292    0.202036   -0.852053
 C    4.467751    1.224653   -1.378211
 C    6.404944    0.636472   -0.060344
 C    4.698986    2.568688   -1.108584
 H    3.607562    0.918372   -1.980600
 C    6.630159    1.986776    0.197850
 H    7.072685   -0.127237    0.349446
 C    5.779547    2.970826   -0.315584
 H    4.007757    3.318004   -1.506983
 H    7.484334    2.277340    0.817399
 H    5.953728    4.027892   -0.103336
121
Figure_S15-5_AA-9d(NaOPh)-ts(1,6minor)_O3 / electronic energy: -4439.04473040 a.u. / lowest freq: -309.80 cm-1
 H   -4.078356   -4.099965   -2.680075
 H   -5.773402   -3.702640   -2.312554
 C   -4.883436   -4.231040   -1.942346
 H   -5.120844   -5.301714   -1.870232
 H   -2.615701   -5.562963   -1.672664
 B   -2.930448   -2.045249   -0.958698
 O   -4.274689   -2.243536   -0.770212
 C   -2.673135   -5.522935   -0.577748
 C   -4.492796   -3.652502   -0.582584
 O   -2.194942   -3.162163   -0.657991
 H   -3.388685   -6.283952   -0.232811
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H	-1.681977	-5.778179	-0.176438
C	-3.081792	-4.142755	-0.085319
H	-6.561763	-3.466336	-0.012275
C	-5.623987	-3.849873	0.414708
H	-5.761941	-4.918361	0.636902
H	-5.434257	-3.316285	1.354466
C	-2.927712	-4.063733	1.430948
H	-1.881502	-4.269288	1.690307
H	-3.180983	-3.064952	1.814942
H	-3.557005	-4.807503	1.939258
C	-2.334196	-0.695307	-1.456632
C	-3.215493	0.359320	-1.656777
H	-4.281586	0.123518	-1.697084
H	-2.326213	1.542396	-3.226385
H	-1.990242	2.132892	-1.597106
C	-2.772152	1.670928	-2.224491
H	-3.600439	2.385732	-2.313411
H	-0.340916	-1.469067	-1.615725
C	-0.929203	-0.542636	-1.569029
H	-0.553826	0.248294	-2.230209
C	3.278417	1.941282	-1.693006
H	4.124540	2.259515	-1.069832
C	3.463781	0.514751	-2.202242
H	3.169253	0.411838	-3.259104
C	1.714628	0.557844	-0.648146
C	2.482155	-1.646130	-1.373413
C	2.984925	-2.346710	-2.472889
C	1.916764	-2.351166	-0.306657
C	2.884797	-3.740672	-2.535151
C	1.778785	-3.737033	-0.365678
C	2.265210	-4.421502	-1.484275
H	2.165076	-5.509268	-1.533294
Cu	-0.009603	0.054701	0.216176
N	2.066754	1.819347	-0.877976
N	2.544657	-0.242124	-1.345573
C	-1.540036	0.062453	1.601600
C	-0.286009	0.057079	2.325720
H	3.527093	2.500240	1.249419
H	4.493700	0.152559	-2.077761
H	3.149810	2.672284	-2.502401
H	-2.028893	-0.915270	1.564688
C	0.144603	-1.226530	2.927407
C	0.370145	1.229534	2.912522
O	-0.872149	-2.046100	3.200584
O	1.291876	-1.542767	3.197971
O	1.359950	1.201867	3.629688
O	-0.226971	2.393047	2.630443
C	0.361419	3.562451	3.194958
H	0.331327	3.516932	4.292215
H	-0.249825	4.401567	2.843655
H	1.402966	3.662341	2.857008
C	-0.573214	-3.246521	3.899007
H	0.065915	-3.905617	3.297919
H	-1.535761	-3.731166	4.092029
H	-0.065792	-3.024327	4.847612
C	1.414111	2.961475	-0.267732
H	0.839077	2.567096	0.581252
C	0.428991	3.654782	-1.196340
C	-0.469399	4.581444	-0.650512
C	0.362065	3.392795	-2.566781
C	-1.396297	5.240565	-1.453285
H	-0.451654	4.780759	0.424321
C	-0.560269	4.057745	-3.375715
H	1.014838	2.642020	-3.014345
C	-1.441415	4.984206	-2.824218
H	-2.092504	5.953073	-1.005521
H	-0.598069	3.836066	-4.444461
H	-2.168793	5.497496	-3.456391
C	2.455895	3.932112	0.315185
H	1.916155	4.828626	0.659304
H	3.118440	4.275867	-0.505663
O	3.162459	3.420459	1.394632
C	-2.329996	1.148052	1.159232
H	-1.925935	2.156342	1.235362
C	-3.583746	0.943593	0.604264
H	-4.038203	-0.042530	0.724048
C	-4.538595	2.029755	0.323967
C	-5.888772	1.714152	0.098058
C	-4.155813	3.379270	0.248962
C	-6.822769	2.705921	-0.189951
H	-6.202923	0.667498	0.143935
C	-5.088508	4.371611	-0.039957
H	-3.110873	3.658046	0.394968
C	-6.426926	4.042471	-0.261137
H	-7.867027	2.434822	-0.361694
H	-4.765911	5.413912	-0.099206
H	-7.156579	4.822273	-0.489726
C	1.107996	-4.459126	0.770057
H	0.080166	-4.084595	0.889309

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 H    1.061668   -5.542862    0.597036
 H    1.640267   -4.281347    1.716791
 C    3.427984   -4.478574   -3.731143
 H    3.267811   -5.561554   -3.641904
 H    2.943430   -4.137353   -4.658754
 H    4.508469   -4.301570   -3.845558
 H    3.449864   -1.812340   -3.302733
 H    1.591379   -1.815543    0.587066
 O    4.104665    0.967855    1.346450
Na    3.107818   -0.126331    2.977446
 C    5.147141    0.560016    0.686993
 C    5.352865   -0.814418    0.383359
 C    6.132624    1.464688    0.202486
 C    6.440650   -1.239836   -0.373068
 H    4.608954   -1.539195    0.727156
 C    7.213100    1.027409   -0.557913
 H    6.009032    2.526161    0.437453
 C    7.381437   -0.327506   -0.861186
 H    6.551073   -2.305722   -0.594187
 H    7.941820    1.759172   -0.919752
 H    8.230580   -0.665373   -1.459048
121
Figure_S15-5_AA-9d(NaOPh)-ts(1,6minor)_O4 / electronic energy: -4439.04421454 a.u. / lowest freq: -323.67 cm-1
 H    3.095969    4.985623   -2.047636
 H    4.866326    4.855899   -2.183862
 C    4.041776    5.094434   -1.497129
 H    4.145217    6.142319   -1.182072
 H    1.763877    5.869620   -0.337892
 B    2.749285    2.389918   -0.810450
 O    4.058211    2.801289   -0.826946
 C    2.123190    5.542810    0.646520
 C    4.099460    4.142137   -0.302837
 O    1.941394    3.255615   -0.122668
 H    2.822613    6.297497    1.035897
 H    1.262688    5.493331    1.327893
 C    2.798789    4.183513    0.574140
 H    6.247790    4.298185   -0.229823
 C    5.396786    4.337314    0.465241
 H    5.406846    5.318653    0.962390
 H    5.539293    3.557841    1.224429
 C    3.016225    3.626312    1.980295
 H    2.040286    3.434277    2.445906
 H    3.564592    2.672574    1.951909
 H    3.583220    4.329464    2.606816
 C    2.275113    1.045415   -1.439538
 C    3.257617    0.100404   -1.710727
 H    4.290370    0.452774   -1.768289
 H    2.475563   -1.105439   -3.318661
 H    2.209767   -1.781191   -1.708252
 C    2.938972   -1.226381   -2.324029
 H    3.831889   -1.853806   -2.441994
 H    0.207451    1.607636   -1.505535
 C    0.893782    0.752102   -1.540485
 H    0.588964   -0.024604   -2.253275
 C   -3.139450   -2.118594   -1.693758
 H   -3.959815   -2.488622   -1.063032
 C   -3.408368   -0.699103   -2.189621
 H   -3.115071   -0.567802   -3.243771
 C   -1.646301   -0.649411   -0.657618
 C   -2.597235    1.511990   -1.309496
 C   -3.183384    2.191108   -2.376351
 C   -2.090086    2.235232   -0.222726
 C   -3.246942    3.590366   -2.380666
 C   -2.122422    3.627354   -0.217078
 C   -2.704318    4.292881   -1.305493
 H   -2.739599    5.386160   -1.305733
Cu    0.069509   -0.107862    0.183526
 N   -1.928329   -1.930098   -0.888024
 N   -2.536594    0.104981   -1.324695
 C    1.588385   -0.041402    1.566860
 C    0.361179   -0.333956    2.290860
 H   -3.556408   -3.064408    1.051426
 H   -4.457568   -0.398972   -2.069236
 H   -2.974604   -2.833825   -2.510502
 H    1.873496    1.014713    1.605415
 C   -0.356813    0.860349    2.785942
 C    0.027235   -1.637025    2.866738
 O   -1.646821    0.641760    3.122715
 O    0.109728    1.979309    2.839249
 O   -0.871136   -1.864609    3.666043
 O    0.815889   -2.639206    2.454956
 C    0.558604   -3.920904    3.012356
 H    0.650463   -3.897665    4.106474
 H    1.315799   -4.591337    2.590667
 H   -0.451632   -4.263262    2.746329
 C   -2.376900    1.750456    3.634446
 H   -1.831163    2.233068    4.455629
 H   -3.327759    1.346861    4.000887
 H   -2.565997    2.489674    2.843829
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 C   -1.144294   -3.023614   -0.347007
 H   -0.593417   -2.605681    0.507699
 C   -0.106052   -3.562456   -1.318869
 C    0.917922   -4.378596   -0.819964
 C   -0.105302   -3.250525   -2.680555
 C    1.905938   -4.882996   -1.661372
 H    0.953292   -4.607942    0.247660
 C    0.879091   -3.761123   -3.527822
 H   -0.860765   -2.579550   -3.092080
 C    1.885969   -4.580020   -3.023259
 H    2.700612   -5.509552   -1.250351
 H    0.863289   -3.503067   -4.588852
 H    2.661562   -4.970118   -3.685393
 C   -2.061266   -4.113538    0.231941
 H   -1.421177   -4.939789    0.576912
 H   -2.696570   -4.531533   -0.571868
 O   -2.810137   -3.664543    1.316653
 C    2.553711   -0.936180    1.056646
 H    2.329013   -2.000673    1.060543
 C    3.750125   -0.499512    0.506983
 H    4.050593    0.534989    0.688173
 C    4.862991   -1.407187    0.172200
 C    6.150445   -0.875379   -0.007931
 C    4.690907   -2.791161    0.002057
 C    7.228163   -1.692865   -0.339752
 H    6.300862    0.201367    0.110464
 C    5.767370   -3.609028   -0.331098
 H    3.699400   -3.235514    0.108221
 C    7.041940   -3.066061   -0.503352
 H    8.219528   -1.253804   -0.473612
 H    5.607506   -4.681634   -0.464356
 H    7.884109   -3.709788   -0.766674
 C   -1.577038    4.405028    0.951011
 H   -1.022450    5.289421    0.606227
 H   -2.396308    4.767110    1.593726
 H   -0.908342    3.788083    1.566812
 C   -3.900101    4.305045   -3.534931
 H   -3.770165    5.393188   -3.459662
 H   -3.478512    3.974557   -4.496171
 H   -4.980553    4.093295   -3.563710
 H   -3.598604    1.640664   -3.221633
 H   -1.680194    1.699693    0.633307
 O   -4.519130   -1.735964    1.290583
Na   -2.891348   -1.425206    2.727466
 C   -5.286897   -0.954950    0.593211
 C   -5.146611    0.459422    0.632268
 C   -6.293401   -1.461321   -0.274923
 C   -5.919678    1.294228   -0.166573
 H   -4.375654    0.885576    1.281434
 C   -7.065777   -0.615770   -1.067335
 H   -6.437739   -2.545048   -0.315647
 C   -6.885999    0.770695   -1.031970
 H   -5.751900    2.374586   -0.125005
 H   -7.820869   -1.047616   -1.731238
 H   -7.488576    1.428627   -1.661741
121
Figure_S15-5_AA-9d(NaOPh)-ts(1,6minor)_05 / electronic energy: -4439.04612350 a.u. / lowest freq: -325.20 cm-1
 C    3.280224   -2.183566    1.587208
 H    4.004142   -2.592082    0.867775
 C    3.680111   -0.789141    2.057873
 H    3.582518   -0.675975    3.149177
 C    1.734564   -0.629761    0.769814
 C    2.804357    1.478988    1.485631
 C    3.714220    2.025101    2.395777
 C    2.021898    2.342433    0.706484
 C    3.833258    3.409437    2.556349
 C    2.092747    3.724178    0.885885
 C    3.008352    4.246962    1.807846
 H    3.074773    5.330306    1.942636
Cu   -0.001261   -0.109941   -0.054383
 N    2.003821   -1.924559    0.921942
 N    2.707022    0.077319    1.378180
 C   -1.465306   -0.092244   -1.485865
 C   -0.232297   -0.407823   -2.197445
 H    3.158125   -3.043968   -1.284763
 H    4.704266   -0.526626    1.759656
 H    3.165515   -2.898480    2.413956
 H   -1.754355    0.960974   -1.536455
 C    0.593931    0.699487   -2.696289
 C    0.061979   -1.722776   -2.784511
 O    0.086090    1.913759   -2.421177
 O    1.660330    0.610304   -3.284866
 O    0.879562   -1.951494   -3.661078
 O   -0.685299   -2.723049   -2.298991
 C   -0.439554   -4.017129   -2.837494
 H   -0.645267   -4.036243   -3.916451
 H   -1.127816   -4.693716   -2.317933
 H    0.605932   -4.302769   -2.656464
 C    0.837459    3.025447   -2.878758
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H	1.817483	3.066860	-2.381864
H	0.251788	3.913987	-2.621295
H	0.989808	2.974836	-3.965451
C	1.129474	-2.983992	0.453930
H	0.545350	-2.560579	-0.373640
C	0.137117	-3.448209	1.509795
C	-0.938406	-4.253556	1.111336
C	0.233508	-3.085334	2.855048
C	-1.879025	-4.702471	2.034040
H	-1.049681	-4.520008	0.057261
C	-0.705819	-3.537134	3.783703
H	1.036240	-2.425550	3.188960
C	-1.761820	-4.349786	3.379111
H	-2.714191	-5.322023	1.699814
H	-0.612317	-3.241557	4.830938
H	-2.499963	-4.696073	4.105319
C	1.933425	-4.149029	-0.147072
H	1.222649	-4.966506	-0.343595
H	2.634480	-4.537217	0.620018
O	2.563054	-3.840589	-1.343424
C	-2.446736	-0.985163	-0.999682
H	-2.211768	-2.046634	-0.970756
C	-3.673705	-0.554136	-0.518118
H	-3.983013	0.469986	-0.737731
C	-4.789679	-1.469461	-0.214412
C	-6.088511	-0.948259	-0.094357
C	-4.611371	-2.848650	-0.016076
C	-7.170690	-1.771344	0.207532
H	-6.243996	0.125258	-0.234219
C	-5.692619	-3.672506	0.285885
H	-3.612428	-3.284163	-0.077799
C	-6.978070	-3.140000	0.399422
H	-8.170509	-1.340153	0.296486
H	-5.528362	-4.741620	0.440093
H	-7.823805	-3.788222	0.639154
C	1.194608	4.642644	0.100549
H	0.268938	4.129340	-0.192385
H	0.920283	5.525439	0.696278
H	1.695196	5.008706	-0.809905
C	4.823480	3.963980	3.547399
H	4.939709	5.050610	3.435371
H	4.500101	3.764092	4.581235
H	5.811871	3.497531	3.419856
H	4.355028	1.379530	2.995261
H	1.329387	1.942461	-0.034811
O	3.988582	-1.691109	-1.646176
Na	3.018298	-1.214134	-3.559530
C	4.892555	-0.952563	-1.077611
C	4.766877	0.463352	-1.024810
C	6.050405	-1.505065	-0.462974
C	5.706448	1.256354	-0.376470
H	3.877050	0.912894	-1.476256
C	6.986824	-0.699676	0.181209
H	6.184008	-2.590312	-0.503591
C	6.826773	0.688264	0.240222
H	5.551627	2.338595	-0.333617
H	7.859520	-1.165147	0.649594
H	7.559035	1.314394	0.754623
H	-3.274924	5.025690	1.827329
C	-4.209194	5.066810	1.248507
H	-4.340612	6.089404	0.867720
H	-5.042339	4.839996	1.928659
H	-1.934633	5.850929	0.107105
O	-2.016491	3.216555	0.014379
C	-2.255312	5.460013	-0.866801
C	-4.204967	4.043924	0.112902
H	-1.372963	5.412058	-1.520943
H	-2.968278	6.168078	-1.314665
C	-2.887555	4.083307	-0.740864
H	-6.355095	4.106236	-0.011491
C	-5.491720	4.143381	-0.691132
H	-5.531508	5.095629	-1.240630
C	-3.061395	3.455211	-2.123156
H	-2.072364	3.292440	-2.570878
H	-5.587078	3.318973	-1.409074
H	-3.563261	2.478314	-2.061445
H	-3.648774	4.104125	-2.787618
B	-2.808393	2.364547	0.741895
O	-4.127335	2.739507	0.715542
C	-2.318072	1.060276	1.440222
C	-3.292671	0.103987	1.701012
H	-4.333656	0.436143	1.705362
H	-2.190143	-1.742220	1.815327
H	-2.585515	-1.038412	3.386278
H	-3.856239	-1.849279	2.439705
C	-2.976019	-1.197451	2.366077
C	-0.937628	0.791644	1.601304
H	-0.265212	1.657246	1.585275
H	-0.650071	0.031383	2.338408

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Figure_S15-5_AA-9d(NaOPh)-ts(1,6minor)_O6 / electronic energy: -4439.04259063 a.u. / lowest freq: -326.29 cm-1
 H    -3.709092    -4.336252    -2.666080
 H    -5.452256    -4.040838    -2.463817
 C    -4.564665    -4.484712    -1.991157
 H    -4.736651    -5.564007    -1.875906
 H    -2.263181    -5.658347    -1.441460
 B    -2.857672    -2.118110    -0.997729
 O    -4.196385    -2.398277    -0.892504
 C    -2.411614    -5.545995    -0.360334
 C    -4.333156    -3.808049    -0.640409
 O    -2.075453    -3.166750    -0.586416
 H    -3.110081    -6.323405    -0.016785
 H    -1.444071    -5.713085     0.133693
 C    -2.938151    -4.163995    -0.005992
 H    -6.452618    -3.763748    -0.251358
 C    -5.526410    -4.038630     0.273333
 H    -5.597193    -5.099647     0.555312
 H    -5.461520    -3.435018     1.187405
 C    -2.906137    -3.961334     1.507073
 H    -1.868394    -4.047466     1.854043
 H    -3.277319    -2.965761     1.790900
 H    -3.505221    -4.720398     2.029078
 C    -2.309573    -0.751814    -1.506011
 C    -3.228470     0.263297    -1.742228
 H    -4.279956    -0.020703    -1.828409
 H    -2.333701     1.484636    -3.280949
 H    -2.077931     2.081963    -1.637976
 C    -2.818035     1.592419    -2.294547
 H    -3.670449     2.274409    -2.409836
 H    -0.282915    -1.440541    -1.601192
 C    -0.909739    -0.539501    -1.573279
 H    -0.548107     0.264473    -2.226619
 C     3.184442     1.982913    -1.710649
 H     4.045151     2.318415    -1.116921
 C     3.370117     0.551443    -2.204638
 H     3.032042     0.424737    -3.245946
 C     1.665741     0.597853    -0.605370
 C     2.491995    -1.610335    -1.269115
 C     3.092309    -2.328212    -2.307004
 C     1.905098    -2.303112    -0.204644
 C     3.087726    -3.726744    -2.303339
 C     1.864953    -3.696740    -0.198479
 C     2.459977    -4.398644    -1.251733
 H     2.438061    -5.491858    -1.248281
Cu    -0.076097     0.107346     0.236362
 N     1.998018     1.859694    -0.858991
 N     2.495375    -0.204819    -1.300991
 C    -1.664175     0.101218     1.572197
 C    -0.436557     0.223484     2.328560
 H     3.663297     2.600483     1.134619
 H     4.409715     0.207844    -2.118654
 H     3.025184     2.700336    -2.526025
 H    -2.083373    -0.909033     1.553872
 C     0.064088    -0.989579     3.015734
 C     0.038649     1.532126     2.790257
 O    -0.908365    -1.832736     3.358031
 O     1.231744    -1.241409     3.272026
 O    -0.474173     2.602680     2.523095
 O     1.135096     1.473329     3.576700
 C     1.600966     2.708885     4.122335
 H     2.073529     3.307332     3.331213
 H     2.341708     2.434442     4.881870
 H     0.773287     3.261388     4.585024
 C    -0.536948    -3.009565     4.063049
 H     0.114547    -3.645306     3.449812
 H    -1.471532    -3.533758     4.287744
 H    -0.013901    -2.753300     4.994317
 C     1.360412     2.995066    -0.216868
 H     0.829085     2.598866     0.657056
 C     0.322886     3.685897    -1.084652
 C    -0.609768     4.521075    -0.454142
 C     0.241938     3.518958    -2.469079
 C    -1.582118     5.190292    -1.192331
 H    -0.581381     4.626639     0.633790
 C    -0.731586     4.190383    -3.210735
 H     0.921909     2.838616    -2.983904
 C    -1.644268     5.029981    -2.577456
 H    -2.302935     5.833012    -0.681820
 H    -0.783575     4.041324    -4.291424
 H    -2.410635     5.548458    -3.157390
 C     2.414048     3.968637     0.337628
 H     1.874777     4.842390     0.733947
 H     3.035682     4.345563    -0.500127
 O     3.175738     3.437681     1.371126
 C    -2.503717     1.124246     1.079836
 H    -2.158889     2.154585     1.158288
 C    -3.721118     0.833313     0.482704
 H    -4.120304    -0.176602     0.603306
```

```
 C   -4.732187    1.855833    0.159614
 C   -6.049200    1.455712   -0.120685
 C   -4.430989    3.225972    0.093916
 C   -7.029418    2.387007   -0.454149
 H   -6.298993    0.391535   -0.082542
 C   -5.409329    4.157751   -0.241602
 H   -3.412972    3.568912    0.284845
 C   -6.714063    3.745113   -0.517669
 H   -8.046665    2.050314   -0.667334
 H   -5.149375    5.217848   -0.293570
 H   -7.479623    4.477524   -0.782610
 C    1.190257   -4.410319    0.941197
 H    0.160181   -4.041396    1.055845
 H    1.151593   -5.495786    0.777355
 H    1.720135   -4.225961    1.888536
 C    3.755000   -4.479476   -3.424903
 H    3.599476   -5.562698   -3.330703
 H    3.364680   -4.160615   -4.403183
 H    4.839902   -4.290889   -3.430232
 H    3.569532   -1.804604   -3.136380
 H    1.475149   -1.757457    0.637529
 O    4.340176    1.103112    1.176977
Na    2.866184    0.157032    2.468613
 C    5.324566    0.638206    0.467494
 C    5.488334   -0.754834    0.233527
 C    6.276327    1.495988   -0.148788
 C    6.500416   -1.242487   -0.587106
 H    4.771331   -1.447885    0.683707
 C    7.282989    0.996269   -0.970313
 H    6.188248    2.571575    0.031787
 C    7.406833   -0.376228   -1.206763
 H    6.577228   -2.321014   -0.754364
 H    7.987382    1.692974   -1.434850
 H    8.196298   -0.762377   -1.854985
121
Figure_S15-5_AA-9d(NaOPh)-ts(1,6minor)_07 / electronic energy: -4439.04642717 a.u. / lowest freq: -374.30 cm-1
 H   -3.454421    3.390575   -0.945764
 H   -2.521045    2.761050   -2.327710
 C   -2.802158    2.570947   -1.277075
 C   -3.455001    1.234622   -1.112302
 H   -4.546182    1.198679   -1.103477
 C   -1.393178    0.024052   -1.681347
 C   -2.782365    0.049015   -1.399722
 B   -3.588789   -1.271192   -1.201062
 O   -4.926458   -1.270234   -0.891074
 H   -4.862338   -2.964233   -3.188883
 O   -3.071873   -2.542027   -1.241830
 H   -6.842788   -2.711118   -1.992203
 C   -5.284777   -2.598252   -0.475430
 C   -4.534240   -3.842069   -2.613385
 C   -6.707289   -2.897587   -0.919428
 H   -3.641010   -4.257394   -3.101373
 C   -4.180170   -3.466593   -1.175423
 H   -5.329418   -4.600032   -2.645393
 H   -6.964502   -3.946164   -0.708234
 C   -3.782996   -4.707395   -0.390820
 H   -3.091509   -5.327265   -0.977140
 H   -4.673576   -5.314791   -0.170800
 H   -1.863338    2.618304   -0.698001
 H   -5.832093   -1.847133    1.468254
 C   -5.186988   -2.633407    1.050738
 H   -5.517806   -3.599445    1.456847
 H   -3.294578   -4.445023    0.556234
 H   -4.157887   -2.448234    1.392916
 H   -7.410167   -2.256071   -0.368901
 H   -0.953053    0.924508   -2.125578
 H   -1.012547   -0.902193   -2.128910
 C    3.401593    1.319011   -1.869720
 H    4.200497    1.843621   -1.331384
 C    3.666093   -0.184832   -1.921110
 H    3.702199   -0.583463   -2.945774
 C    1.642591    0.201653   -0.798620
 C    2.379085   -2.131896   -0.995801
 C    3.513094   -2.876666   -0.659144
 C    1.145812   -2.769510   -1.128791
 C    3.419341   -4.254147   -0.441198
 C    1.031961   -4.146262   -0.927586
 C    2.173755   -4.874706   -0.579901
 H    2.089920   -5.952738   -0.413442
Cu   -0.166922   -0.006003    0.019584
 N    2.132332    1.393364   -1.139087
 N    2.502518   -0.740597   -1.218239
 C   -1.491520   -0.079441    1.629007
 C   -0.140482   -0.279924    2.118858
 H    3.633099    2.158512    0.910520
 H    4.603204   -0.441460   -1.410969
 H    3.301639    1.773734   -2.866561
 H   -2.029566   -1.013321    1.444928
 C    0.335983   -1.664220    2.283741
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 C    0.689410    0.775633    2.717740
 O   -0.622129   -2.579395    2.084390
 O    1.471928   -2.013197    2.566794
 O    1.775323    0.621886    3.254601
 O    0.138984    1.991090    2.640980
 C    0.853504    3.073060    3.231470
 H    1.021524    2.885321    4.300954
 H    0.210836    3.952145    3.105124
 H    1.812657    3.215327    2.715231
 C   -0.262861   -3.938486    2.271680
 H   -1.131288   -4.527280    1.957011
 H   -0.041433   -4.135801    3.330482
 H    0.614256   -4.201225    1.665892
 C    1.538327    2.657786   -0.739433
 H    0.822000    2.414864    0.063665
 C    0.773646    3.342355   -1.864854
 C    0.137652    4.568186   -1.625671
 C    0.633379    2.760520   -3.127998
 C   -0.602057    5.198495   -2.622974
 H    0.199231    5.032659   -0.638683
 C   -0.107419    3.388883   -4.129876
 H    1.088828    1.790623   -3.334010
 C   -0.725137    4.612536   -3.883225
 H   -1.093653    6.150477   -2.411246
 H   -0.205708    2.911170   -5.107030
 H   -1.306880    5.104637   -4.665471
 C    2.611682    3.567715   -0.110847
 H    2.130357    4.519336    0.159223
 H    3.362911    3.818808   -0.887469
 O    3.183812    3.045197    1.037889
 C   -2.289290    1.083800    1.608817
 H   -1.840705    2.033028    1.888422
 C   -3.604777    1.044810    1.169708
 H   -4.070792    0.065879    1.049570
 C   -4.575541    2.138487    1.373462
 C   -5.939726    1.879335    1.158727
 C   -4.203567    3.434915    1.763426
 C   -6.898176    2.874369    1.329791
 H   -6.241081    0.877939    0.838208
 C   -5.161799    4.431817    1.933949
 H   -3.152061    3.672632    1.934835
 C   -6.513236    4.158382    1.718901
 H   -7.952733    2.648017    1.156355
 H   -4.849173    5.433580    2.238074
 H   -7.262445    4.941686    1.853244
 O    4.428448    0.740465    0.984516
Na    3.336543   -0.711447    2.243141
 C    5.673729    0.736446    0.616013
 C    6.446526   -0.458746    0.595052
 C    6.336563    1.919850    0.183933
 C    7.767327   -0.468471    0.154510
 H    5.978772   -1.385189    0.944269
 C    7.656766    1.895108   -0.255491
 H    5.779742    2.860521    0.223933
 C    8.389043    0.704180   -0.282934
 H    8.321897   -1.411689    0.152877
 H    8.126916    2.827983   -0.580939
 H    9.424138    0.691875   -0.630732
 C   -0.298521   -4.820647   -1.119403
 H   -1.117913   -4.092525   -1.056762
 H   -0.351737   -5.300867   -2.109980
 H   -0.463948   -5.606423   -0.367840
 C    4.644146   -5.056533   -0.086221
 H    5.060380   -5.546133   -0.981098
 H    5.432909   -4.420452    0.339248
 H    4.406927   -5.847036    0.639925
 H    0.264279   -2.193691   -1.406417
 H    4.478318   -2.379866   -0.546847
89
Figure_S15-6_9b(NaOPh)-Cu-allyl_O1 / electronic energy: -3597.06856996 a.u. / lowest freq: 15.34 cm-1
Na    0.148120   -2.350929   -0.661887
 H    2.438637   -3.886514    0.418400
 H    4.437536   -1.625816   -2.657585
 O    2.188175   -1.934213   -1.331976
 C    4.457113   -2.409826   -1.896029
 C    3.271723   -2.638718   -1.144621
 H    6.503884   -2.941304   -2.274753
 C    5.611926   -3.155530   -1.678013
 C    3.330703   -3.680261   -0.180384
 C    5.648755   -4.168717   -0.715703
 C    4.491286   -4.420599    0.026190
 H    6.559206   -4.747918   -0.547636
 H    4.492260   -5.208637    0.785191
 H    2.110038   -1.789209    2.251941
 H   -1.683682   -0.084569    3.012140
 C    0.177417   -2.763996    2.184032
 C   -0.716422   -0.448477    2.624984
 H    0.009685   -3.753268    1.738460
 C   -0.814296   -1.836152    2.123482
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 H    0.060429   -0.307140    3.395789
 B   -2.112989   -2.153360    1.318568
 O   -3.369101   -1.737541    1.633548
 H   -2.845676   -0.482203   -0.927861
 O   -2.073350   -2.793843    0.089938
 H   -2.386052   -1.604043   -2.238318
 C   -3.158779   -1.375665   -1.489089
 H   -4.906254   -0.251131    0.103283
 C   -3.345234   -2.575300   -0.562814
 C   -4.288875   -2.263960    0.657935
 C   -5.353692   -1.214414    0.379956
 H   -4.085231   -1.134855   -2.028538
 H   -5.962317   -1.060989    1.282259
 H   -4.158934   -4.286914    1.470992
 H   -5.400718   -3.251670    2.212692
 C   -4.917121   -3.518031    1.262489
 H   -3.003759   -3.952870   -2.186413
 C   -3.717784   -3.812772   -1.361912
 H   -3.704627   -4.717295   -0.741233
 H   -6.020495   -1.543104   -0.431111
 H   -5.677701   -3.946520    0.595013
 H   -4.721339   -3.698819   -1.797645
 H    2.106807   -3.437236    2.912827
 C    1.510733   -2.517409    2.830805
 H    1.401035   -2.091228    3.843076
 C    1.280515    3.069545   -2.003442
 H    1.565108    2.605156   -2.959047
 C   -0.172818    3.561404   -1.995315
 H   -0.276419    4.578520   -1.584882
 C    0.060095    1.792810   -0.476656
 C   -2.217588    2.610963   -0.829080
 C   -2.678385    3.129778    0.395038
 C   -3.100884    2.109301   -1.801083
 C   -4.054535    3.111730    0.641038
 C   -4.470186    2.122037   -1.519756
 C   -4.944329    2.613849   -0.307033
 H   -6.016384    2.608530   -0.098720
Cu   -0.341132    0.639697    1.032050
 N    1.273784    2.050851   -0.951347
 N   -0.819266    2.595349   -1.099937
 H    2.443780   -0.610758   -2.213460
 H   -0.629024    3.549352   -2.994037
 H    1.996706    3.870578   -1.771134
 C    2.484707    1.372525   -0.497575
 H    2.139125    0.425669   -0.056505
 C    3.187276    2.170139    0.586692
 C    4.053990    3.229208    0.291404
 C    2.928357    1.870261    1.929919
 C    4.643739    3.972204    1.314760
 H    4.282158    3.482129   -0.746497
 C    3.515716    2.610503    2.954124
 H    2.250016    1.047192    2.174293
 C    4.375475    3.666125    2.648300
 H    5.320155    4.793092    1.066340
 H    3.303057    2.360630    3.995928
 H    4.838980    4.246461    3.449152
 C    3.374358    0.994741   -1.687423
 H    4.246875    0.448944   -1.277619
 H    3.774104    1.901226   -2.172724
 O    2.681605    0.261974   -2.643836
 H   -4.432045    3.504641    1.588162
 H   -5.170862    1.726395   -2.259259
 C   -2.592705    1.563034   -3.108381
 H   -2.423060    2.369586   -3.840006
 H   -1.639450    1.031325   -2.978681
 H   -3.320420    0.870396   -3.551477
 C   -1.723572    3.682246    1.419703
 H   -1.210134    2.868739    1.959856
 H   -0.940363    4.298843    0.955650
 H   -2.256508    4.292551    2.160509
121
Figure_S15-6_AA-9b(NaOPh)-ts(1,6major)_01 / electronic energy: -4439.04225300 a.u. / lowest freq: -302.37 cm-1
 C    0.994657    0.629022    4.152905
 H    0.816261   -0.280969    3.564092
 H    1.904888    0.462704    4.751414
 H    0.157717    0.752953    4.852850
 H   -2.218728    2.280131    3.090642
 H   -0.785160    0.492325    2.170977
 C   -3.262119    1.334340    1.456737
 C   -1.329610   -0.183510    1.503823
 H   -4.351476    1.420712    1.443181
 C   -2.712988    0.068601    1.315025
 H   -1.039590   -1.237116    1.603453
 B   -3.618360   -1.095557    0.817808
 O   -3.314717   -2.417207    0.995351
 H   -5.983990   -2.257156    2.112316
 O   -4.794050   -0.917791    0.132915
 H   -7.170777   -1.476924    1.039672
 C   -6.461358   -2.312633    1.123140
```

H	-4.926709	-4.301788	1.919199
C	-5.428985	-2.204076	0.002360
C	-4.215837	-3.191005	0.184963
C	-4.548176	-4.487256	0.906230
H	-7.026107	-3.253291	1.059066
H	-3.640887	-5.102642	0.987943
H	-3.234633	-2.560337	-1.657250
H	-2.540355	-3.998836	-0.877860
C	-3.482985	-3.487878	-1.120908
H	-6.941358	-1.564349	-1.395553
C	-6.111421	-2.284360	-1.354170
H	-5.415593	-2.048775	-2.169261
H	-5.303295	-5.058697	0.346199
H	-4.075709	-4.133714	-1.784018
H	-6.523173	-3.290888	-1.520711
H	-3.047810	3.418039	2.000905
C	-2.484748	2.475578	2.036996
H	-1.530048	2.621600	1.501572
C	3.525684	-1.464785	1.445159
H	4.439255	-1.676503	0.879275
C	3.563752	-0.059402	2.049284
H	3.613945	-0.062732	3.146650
C	1.665140	-0.263362	0.689854
C	1.807661	1.771641	2.036639
C	1.146095	1.841934	3.273955
C	2.021140	2.908436	1.241402
C	0.645184	3.082615	3.680133
C	1.492873	4.127062	1.676007
C	0.803203	4.212254	2.883192
H	0.392937	5.170019	3.210406
Cu	-0.099482	0.161163	-0.143852
N	2.358950	-1.398161	0.556361
N	2.294812	0.510423	1.582081
C	-1.421790	0.716156	-1.636072
C	-0.126193	0.505968	-2.260099
H	4.317977	-1.911589	-1.328775
H	4.410994	0.529868	1.663904
H	3.391423	-2.253427	2.202690
H	-2.099185	-0.138345	-1.715683
C	0.782572	1.583898	-2.679487
C	0.163637	-0.813798	-2.832815
O	0.261455	2.807221	-2.553427
O	1.913349	1.442254	-3.120644
O	1.175626	-1.140518	-3.433698
O	-0.814574	-1.716183	-2.640531
C	-0.612902	-2.988096	-3.236977
H	-0.576527	-2.902059	-4.331834
H	-1.463020	-3.607051	-2.935388
H	0.327652	-3.439978	-2.893055
C	1.038131	3.899272	-3.021440
H	2.026087	3.916713	-2.544798
H	0.475833	4.802864	-2.762013
H	1.170927	3.838726	-4.110699
C	1.868628	-2.559587	-0.166404
H	1.278385	-2.168860	-1.008231
C	0.950653	-3.442312	0.674230
C	0.299804	-4.527999	0.072922
C	0.702516	-3.192569	2.027029
C	-0.563666	-5.341404	0.802888
H	0.456067	-4.739028	-0.987382
C	-0.163054	-4.003211	2.761591
H	1.170684	-2.341249	2.522359
C	-0.797802	-5.083012	2.153454
H	-1.061797	-6.179498	0.310090
H	-0.344391	-3.781576	3.815261
H	-1.477473	-5.716615	2.726922
C	3.033926	-3.354156	-0.784286
H	2.607026	-4.236832	-1.282740
H	3.676342	-3.743843	0.029176
O	3.757611	-2.637747	-1.728897
C	-2.033507	1.924162	-1.230037
H	-1.437210	2.833493	-1.208038
C	-3.353814	1.956174	-0.820294
H	-3.963969	1.067412	-0.993847
C	-4.121858	3.197283	-0.612268
C	-5.519929	3.118415	-0.496253
C	-3.523054	4.464126	-0.513055
C	-6.292343	4.258448	-0.289256
H	-6.000857	2.138745	-0.564629
C	-4.294551	5.605130	-0.305701
H	-2.438676	4.564035	-0.590710
C	-5.682500	5.509794	-0.191774
H	-7.377515	4.168661	-0.200933
H	-3.806282	6.579452	-0.229348
H	-6.284090	6.406448	-0.027802
H	1.638670	5.021331	1.065270
H	0.114459	3.157263	4.632228
C	2.834696	2.805511	-0.016249
O	4.891885	-0.411924	-1.258193

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Na     3.260473   -0.381258   -2.788678
 C     5.909448    0.069296   -0.614765
 C     6.224501    1.456656   -0.640249
 C     6.765668   -0.752305    0.170791
 C     7.285932    1.978492    0.092906
 H     5.607582    2.110668   -1.262807
 C     7.823504   -0.217304    0.901258
 H     6.582471   -1.831360    0.179632
 C     8.094641    1.153607    0.881006
 H     7.487648    3.052991    0.046521
 H     8.452672   -0.885961    1.496591
 H     8.925115    1.568487    1.456025
 H     2.967128    3.790755   -0.481698
 H     2.375484    2.130399   -0.750216
 H     3.832566    2.393282    0.194920
121
Figure_S15-6_AA-9b(NaOPh)-ts(1,6major)_02 / electronic energy: -4439.04481123 a.u. / lowest freq: -334.42 cm-1
 H    -5.255192   -3.977951    0.768063
 H    -3.999758   -5.150226   -0.794285
 H    -6.818441   -3.145155    0.588918
 B    -3.638043   -1.652602    0.129695
 C    -6.000203   -3.630112    0.037719
 O    -3.082789   -2.691759   -0.568205
 H    -6.408858   -4.503835   -0.489091
 O    -4.968682   -1.484570   -0.162774
 C    -3.927765   -4.617017   -1.750629
 H    -2.959366   -4.863722   -2.209158
 C    -5.393976   -2.621870   -0.937529
 C    -4.037255   -3.112794   -1.560908
 H    -4.722528   -4.980129   -2.419027
 H    -7.350504   -1.857562   -1.424662
 C    -6.437172   -2.173820   -1.948674
 C    -3.692271   -2.388657   -2.862088
 H    -3.808403   -1.299962   -2.757512
 H    -6.700518   -3.001599   -2.623871
 H    -6.081020   -1.329075   -2.551600
 H    -4.331083   -2.726256   -3.690226
 H    -2.644344   -2.591009   -3.118781
 C    -2.857101   -0.723643    1.107819
 C    -3.514386    0.413439    1.567544
 H    -4.601350    0.445684    1.460180
 C    -2.885910    1.357665    2.543997
 H    -2.610075    0.842020    3.480405
 H    -1.954744    1.777575    2.125494
 H    -3.552818    2.192328    2.796661
 C    -1.486081   -0.957274    1.360627
 H    -1.064339   -0.574524    2.296595
 H    -1.093171   -1.943479    1.084004
 C     3.606184   -0.767606    1.844605
 H     4.465205   -1.125756    1.264334
 C     3.591230    0.764463    1.937533
 H     3.694321    1.135949    2.967500
 C     1.608628    0.028556    0.930731
 C     1.714981    2.406393    1.365457
 C     2.116658    3.305827    0.366585
 C     0.763224    2.749717    2.342676
 C     1.479016    4.551116    0.314876
 C     0.139338    3.995696    2.246091
 C     0.485172    4.885016    1.229697
 H    -0.011696    5.855499    1.163356
Cu    -0.170749    0.075674    0.067888
 N     2.345131   -1.057698    1.153282
 N     2.268175    1.093910    1.398127
 C    -1.478595    0.567812   -1.425299
 C    -0.179655    0.518561   -2.073294
 H     3.749777   -1.804693   -1.003357
 H     4.383681    1.216262    1.321385
 H     3.628469   -1.256801    2.830913
 H    -2.113580   -0.304554   -1.595014
 C     0.528557    1.697233   -2.579361
 C     0.305234   -0.787237   -2.528551
 O    -0.175792    2.829641   -2.484829
 O     1.642721    1.705049   -3.083533
 O     1.231080   -1.015272   -3.292403
 O    -0.386118   -1.800022   -1.978196
 C     0.025406   -3.121779   -2.288783
 H    -0.153026   -3.346728   -3.350638
 H    -0.590212   -3.772115   -1.657326
 H     1.095049   -3.251839   -2.068197
 C     0.390729    4.001107   -3.043438
 H     1.371067    4.219310   -2.601172
 H    -0.309757    4.812562   -2.818047
 H     0.508581    3.896002   -4.131448
 C     1.890950   -2.400175    0.843716
 H     1.120419   -2.276112    0.067916
 C     1.221456   -3.090467    2.024917
 C     0.650400   -4.357340    1.842752
 C     1.066592   -2.467199    3.266426
 C    -0.041994   -4.987189    2.873999
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 H    0.722892   -4.852899    0.871423
 C    0.377280   -3.096907    4.303237
 H    1.461410   -1.462999    3.428422
 C   -0.178110   -4.360077    4.112963
 H   -0.486845   -5.970369    2.705507
 H    0.266599   -2.588667    5.263624
 H   -0.722319   -4.850848    4.922665
 C    3.017222   -3.219645    0.195863
 H    2.659833   -4.252029    0.066429
 H    3.872688   -3.279077    0.900039
 O    3.383175   -2.735360   -1.052170
 C   -2.081299    1.680598   -0.802655
 H   -1.465271    2.558752   -0.605467
 C   -3.412304    1.678253   -0.404193
 H   -4.076236    0.928197   -0.838492
 C   -4.094032    2.876612    0.116397
 C   -5.497477    2.901070    0.170166
 C   -3.396447    3.998919    0.594332
 C   -6.180484    4.003039    0.678952
 H   -6.056921    2.032853   -0.189525
 C   -4.078403    5.101267    1.102557
 H   -2.304729    4.009072    0.587544
 C   -5.473590    5.110830    1.148855
 H   -7.272540    3.996509    0.710416
 H   -3.513520    5.961003    1.471018
 H   -6.005724    5.975813    1.550600
 O    4.388212   -0.320187   -1.209869
Na    3.231165    0.062271   -3.053194
 C    5.638165   -0.196215   -0.869884
 C    6.397413   -1.299655   -0.387018
 C    6.319350    1.049532   -0.945103
 C    7.723015   -1.154471    0.012149
 H    5.910832   -2.278636   -0.352700
 C    7.646450    1.179696   -0.544837
 H    5.773891    1.913918   -1.331723
 C    8.365233    0.085078   -0.055345
 H    8.267219   -2.029862    0.379348
 H    8.131525    2.157797   -0.618588
 H    9.405409    0.194877    0.258677
 C    3.238733    2.965842   -0.573678
 H    3.119625    3.469681   -1.541363
 H    4.195872    3.302579   -0.142409
 H    3.326456    1.884578   -0.752276
 C    0.459871    1.806157    3.475341
 H    0.046666    0.857347    3.107715
 H    1.374652    1.563467    4.037990
 H   -0.265865    2.245529    4.171782
 H   -0.619027    4.273852    2.981834
 H    1.771301    5.269237   -0.454780
121
Figure_S15-6_AA-9b(NaOPh)-ts(1,6minor)_01 / electronic energy: -4439.04644858 a.u. / lowest freq: -305.39 cm-1
 C   -0.816448   -1.703765    3.816329
 H   -0.728413   -0.673569    3.448528
 H   -1.666631   -1.735577    4.517117
 H    0.091652   -1.941629    4.386280
 H    2.074218    2.369535    1.540851
 H    0.950529   -1.411559    1.694922
 C    3.524345    0.779378    1.365728
 C    1.381267   -0.413942    1.547875
 H    4.608238    0.688334    1.255940
 C    2.769530   -0.379659    1.265206
 H    0.968521    0.353206    2.214848
 B    3.424432   -1.675624    0.704774
 O    2.857177   -2.918157    0.817555
 H    3.200795   -2.699393   -1.995908
 O    4.622117   -1.708923    0.036700
 H    4.830442   -2.198008   -2.504259
 C    4.266496   -2.968298   -1.958796
 H    2.506423   -4.721656   -1.074730
 C    4.773777   -3.029879   -0.518678
 C    3.845678   -3.884588    0.418373
 C    3.155100   -5.056594   -0.258178
 H    4.405402   -3.928372   -2.476126
 H    2.529591   -5.589692    0.471891
 H    5.076151   -3.522360    2.185854
 H    3.805632   -4.752332    2.387812
 C    4.554868   -4.353765    1.688973
 H    6.811134   -2.780521   -1.180317
 C    6.242541   -3.420207   -0.490186
 H    6.673107   -3.304490    0.512493
 H    3.895432   -5.764387   -0.659584
 H    5.285605   -5.145917    1.473306
 H    6.369746   -4.465260   -0.809826
 H    3.724035    2.832893    2.022770
 C    2.995015    2.012256    2.032719
 H    2.726907    1.811601    3.084803
 C   -3.479536    0.945164    1.791081
 H   -4.379440    1.279805    1.260737
 C   -3.505537   -0.567237    2.040728
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 H   -3.527530   -0.825400    3.109342
 C   -1.603055   -0.027984    0.788840
 C   -1.765246   -2.345269    1.548648
 C   -1.018260   -2.686169    2.693241
 C   -2.045253   -3.281805    0.542198
 C   -0.481337   -3.972446    2.772567
 C   -1.493040   -4.563534    0.664399
 C   -0.705282   -4.901618    1.758944
 H   -0.271876   -5.901512    1.832403
Cu    0.173531   -0.071472   -0.102109
 N   -2.281709    1.106271    0.959659
 N   -2.249146   -1.009691    1.426484
 C    1.510555    0.262642   -1.637265
 C    0.199135    0.078909   -2.238643
 H   -3.918781    1.755908   -1.047723
 H   -4.361291   -1.052381    1.545017
 H   -3.390830    1.529430    2.720223
 H    2.148130   -0.624004   -1.674116
 C   -0.200935   -1.282629   -2.620828
 C   -0.622124    1.165440   -2.791431
 O    0.750782   -2.201225   -2.393177
 O   -1.281106   -1.617871   -3.084909
 O   -1.647963    1.034203   -3.440127
 O   -0.147827    2.390296   -2.535136
 C   -0.911502    3.485330   -3.031403
 H   -0.918545    3.485577   -4.130249
 H   -0.410460    4.388504   -2.664936
 H   -1.943447    3.424536   -2.657846
 C    0.431483   -3.558414   -2.655994
 H   -0.114583   -3.990292   -1.804582
 H    1.387029   -4.078921   -2.782999
 H   -0.170023   -3.653369   -3.568132
 C   -1.817523    2.381965    0.445817
 H   -1.216891    2.149096   -0.444559
 C   -0.904519    3.135009    1.402194
 C   -0.179411    4.228848    0.909791
 C   -0.730005    2.770350    2.739244
 C    0.673847    4.955221    1.735747
 H   -0.276523    4.509527   -0.142393
 C    0.122470    3.498324    3.571276
 H   -1.249582    1.899692    3.142546
 C    0.821624    4.596156    3.076014
 H    1.233051    5.800485    1.328765
 H    0.245424    3.196231    4.613569
 H    1.491845    5.162006    3.726171
 C   -2.996249    3.230709   -0.053494
 H   -2.604122    4.224328   -0.319732
 H   -3.705897    3.397413    0.782453
 O   -3.610683    2.699079   -1.179774
 C    2.177976    1.457440   -1.284976
 H    1.617997    2.389837   -1.275160
 C    3.509629    1.450840   -0.906315
 H    4.092111    0.547897   -1.101925
 C    4.301308    2.677439   -0.707037
 C    5.702030    2.588135   -0.650833
 C    3.715013    3.943891   -0.543025
 C    6.488907    3.717610   -0.438540
 H    6.176128    1.609801   -0.769603
 C    4.500363    5.073709   -0.330733
 H    2.628625    4.049561   -0.558719
 C    5.891366    4.968166   -0.276233
 H    7.576247    3.619935   -0.396899
 H    4.020547    6.046625   -0.200064
 H    6.504986    5.855581   -0.106527
 H   -1.696383   -5.305960   -0.112022
 H    0.123932   -4.246189    3.640069
 C   -2.927916   -2.949561   -0.629403
 O   -4.497508    0.218862   -1.094721
Na   -3.261915   -0.435559   -2.798175
 C   -5.707532    0.088882   -0.631162
 C   -6.312957   -1.184783   -0.449796
 C   -6.489739    1.216901   -0.253941
 C   -7.594528   -1.314066    0.079291
 H   -5.744827   -2.073802   -0.735687
 C   -7.768831    1.072374    0.275279
 H   -6.057364    2.210276   -0.403628
 C   -8.338969   -0.191462    0.452734
 H   -8.021847   -2.313708    0.203976
 H   -8.334125    1.967478    0.552392
 H   -9.342193   -0.299671    0.870459
 H   -3.729193   -3.698486   -0.721093
 H   -2.356256   -2.963210   -1.568712
 H   -3.391512   -1.958153   -0.532641
121
Figure_S15-6_AA-9b(NaOPh)-ts(1,6minor)_O2 / electronic energy: -4439.04584920 a.u. / lowest freq: -309.05 cm-1
 H    5.185048   -3.617520    2.072278
 H    7.038092   -2.943266    0.850253
 C    4.861673   -4.348375    1.316903
 H    4.037193   -4.937284    1.743399
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B	3.658940	-1.591276	0.671235
O	4.962677	-1.405598	0.281013
H	5.699381	-5.027340	1.104456
C	6.828660	-2.851052	-0.222824
O	3.220451	-2.864636	0.420226
C	4.366450	-3.654653	0.048067
C	5.359813	-2.558766	-0.481913
H	7.129324	-3.784027	-0.722248
C	3.961192	-4.689376	-0.988370
H	5.701014	-1.304128	-2.198493
C	5.136537	-2.215768	-1.955050
H	4.842397	-5.252347	-1.330284
H	4.073349	-2.024235	-2.163986
H	3.486417	-4.225703	-1.861668
H	5.481128	-3.022347	-2.617233
H	3.251745	-5.403685	-0.545637
H	7.446307	-2.034603	-0.623567
C	2.796254	-0.452117	1.292984
C	1.416304	-0.652442	1.543467
H	0.939466	0.000895	2.283245
H	1.066871	-1.693240	1.582260
C	3.397860	0.790195	1.449710
H	4.487233	0.836813	1.379293
H	2.438284	1.715911	3.146224
H	1.739880	2.159565	1.585024
C	2.693771	1.941222	2.095730
H	3.301138	2.855826	2.087168
C	-3.568747	0.986343	1.693768
H	-4.444550	1.276624	1.100761
C	-3.603223	-0.503966	2.049146
H	-3.650228	-0.688590	3.132294
C	-1.655534	-0.050352	0.829810
C	-1.887009	-2.327637	1.694244
C	-2.224391	-3.310367	0.750651
C	-1.139265	-2.630404	2.847263
C	-1.742757	-4.609440	0.951408
C	-0.669420	-3.936526	3.004294
C	-0.960331	-4.917680	2.059277
H	-0.582652	-5.933437	2.195625
Cu	0.134803	-0.171173	-0.024489
N	-2.336613	1.093930	0.904639
N	-2.333001	-0.988539	1.498959
C	1.466500	0.155478	-1.561745
C	0.174489	-0.093228	-2.183124
H	-3.917285	1.613277	-1.199167
H	-4.449079	-1.022209	1.569783
H	-3.522484	1.637037	2.580755
H	2.135644	-0.707887	-1.560753
C	-0.202222	-1.490694	-2.429422
C	-0.640919	0.934548	-2.839169
O	0.703170	-2.359786	-1.955175
O	-1.228155	-1.896398	-2.959786
O	-1.648193	0.739502	-3.501957
O	-0.183346	2.180212	-2.667062
C	-0.940245	3.227684	-3.264861
H	-0.929952	3.135217	-4.359840
H	-0.445706	4.159400	-2.967070
H	-1.977202	3.195391	-2.902232
C	0.408240	-3.741988	-2.059083
H	-0.501026	-3.992224	-1.496925
H	1.261673	-4.260706	-1.613993
H	0.281237	-4.040413	-3.108901
C	-1.856088	2.338206	0.333174
H	-1.212225	2.056433	-0.512627
C	-0.998405	3.156844	1.286399
C	-0.275556	4.241421	0.771412
C	-0.868769	2.856415	2.644461
C	0.537032	5.016876	1.593568
H	-0.340083	4.474119	-0.295186
C	-0.057468	3.634108	3.472381
H	-1.387698	1.995201	3.068290
C	0.644777	4.718326	2.952339
H	1.095823	5.854025	1.169628
H	0.032713	3.381133	4.530965
H	1.284392	5.322501	3.598920
C	-3.016080	3.146082	-0.268610
H	-2.614629	4.120565	-0.586635
H	-3.755873	3.367673	0.527701
O	-3.588776	2.541500	-1.378872
C	2.069463	1.385500	-1.215747
H	1.466257	2.291555	-1.227140
C	3.395392	1.447258	-0.816541
H	4.027054	0.577701	-1.006912
C	4.134789	2.705884	-0.617192
C	5.537579	2.667947	-0.550097
C	3.500535	3.949876	-0.467171
C	6.280951	3.827258	-0.344168
H	6.046036	1.705256	-0.653860
C	4.242823	5.109910	-0.261137

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 H    2.411259    4.013038   -0.490542
 C    5.636409    5.056363   -0.198312
 H    7.370815    3.770207   -0.294284
 H    3.727857    6.066251   -0.142701
 H    6.215238    5.967878   -0.034373
Na   -3.244483   -0.712273   -2.787611
 O   -4.530737    0.091250   -1.180948
 C   -5.756553    0.007811   -0.748576
 C   -6.519165    1.166955   -0.430439
 C   -6.401457   -1.242953   -0.545225
 C   -7.815684    1.072883    0.067067
 H   -6.058626    2.143911   -0.602100
 C   -7.699678   -1.321860   -0.048002
 H   -5.852493   -2.155894   -0.789206
 C   -8.423705   -0.169177    0.269430
 H   -8.364141    1.991077    0.298483
 H   -8.156659   -2.305807    0.094842
 H   -9.440449   -0.238030    0.662056
 H   -0.068556   -4.185663    3.882392
 H   -1.992676   -5.387150    0.224973
 C   -3.080964   -2.998057   -0.445763
 H   -3.545105   -2.004577   -0.382835
 H   -2.482647   -3.026574   -1.369038
 H   -3.877670   -3.749543   -0.549799
 C   -0.874588   -1.594879    3.907603
 H    0.089737   -1.775781    4.401266
 H   -0.862773   -0.578416    3.495142
 H   -1.657272   -1.630355    4.682697
121
Figure_S15-6_AA-9b(NaOPh)-ts(1,6minor)_03 / electronic energy: -4439.04644860 a.u. / lowest freq: -305.38 cm-1
 H    3.724036    2.832901    2.022761
 C    2.995017    2.012263    2.032709
 H    2.726907    1.811607    3.084792
 H    2.074221    2.369541    1.540839
 H    4.608241    0.688345    1.255924
 C    3.524348    0.779386    1.365718
 H    0.968531    0.353208    2.214853
 C    2.769537   -0.379655    1.265203
 C    1.381275   -0.413941    1.547879
 O    4.622124   -1.708913    0.036692
 B    3.424442   -1.675618    0.704773
 H    6.811141   -2.780500   -1.180333
 H    0.950540   -1.411559    1.694928
 H    6.673127   -3.304466    0.512480
 C    6.242555   -3.420188   -0.490197
 C    4.773789   -3.029871   -0.518681
 H    5.076183   -3.522337    2.185851
 O    2.857197   -2.918155    0.817563
 C    3.845701   -3.884581    0.418380
 H    6.369765   -4.465242   -0.809834
 C    4.554902   -4.353747    1.688978
 H    3.805673   -4.752316    2.387823
 H    5.285643   -5.145896    1.473309
 C    3.155128   -5.056594   -0.258162
 H    3.895462   -5.764380   -0.659576
 H    2.529632   -5.589699    0.471914
 C    4.266498   -2.968298   -1.958795
 H    4.830437   -2.198009   -2.504266
 H    4.405406   -3.928375   -2.476122
 H    2.506438   -4.721663   -1.074707
 H    3.200796   -2.699399   -1.995902
 C   -3.479538    0.945170    1.791087
 H   -4.379441    1.279811    1.260742
 C   -3.505538   -0.567231    2.040735
 H   -3.527537   -0.825392    3.109350
 C   -1.603053   -0.027978    0.788851
 C   -1.765242   -2.345261    1.548663
 C   -2.045249   -3.281798    0.542215
 C   -1.018254   -2.686158    2.693256
 C   -1.493033   -4.563526    0.664417
 C   -0.481327   -3.972433    2.772583
 C   -0.705272   -4.901607    1.758960
 H   -0.271864   -5.901500    1.832420
Cu    0.173531   -0.071473   -0.102100
 N   -2.281710    1.106276    0.959664
 N   -2.249144   -1.009684    1.426498
 C    1.510546    0.262633   -1.637265
 C    0.199125    0.078894   -2.238636
 H   -3.918783    1.755910   -1.047718
 H   -4.361289   -1.052376    1.545021
 H   -3.390831    1.529437    2.720228
 H    2.148124   -0.624010   -1.674114
 C   -0.200942   -1.282647   -2.620815
 C   -0.622141    1.165421   -2.791424
 O    0.750776   -2.201240   -2.393154
 O   -1.281110   -1.617894   -3.084898
 O   -1.647989    1.034178   -3.440105
 O   -0.147840    2.390278   -2.535147
 C   -0.911521    3.485308   -3.031415
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 H   -0.918577    3.485546   -4.130260
 H   -0.410474    4.388485   -2.664961
 H   -1.943462    3.424517   -2.657845
 C    0.431482   -3.558430   -2.655970
 H   -0.114592   -3.990307   -1.804563
 H    1.387030   -4.078937   -2.782962
 H   -0.170014   -3.653390   -3.568114
 C   -1.817526    2.381968    0.445816
 H   -1.216899    2.149098   -0.444563
 C   -0.904516    3.135015    1.402185
 C   -0.179403    4.228845    0.909771
 C   -0.730007    2.770371    2.739240
 C    0.673858    4.955224    1.735720
 H   -0.276512    4.509513   -0.142417
 C    0.122471    3.498350    3.571265
 H   -1.249590    1.899720    3.142550
 C    0.821631    4.596173    3.075992
 H    1.233066    5.800481    1.328729
 H    0.245421    3.196270    4.613561
 H    1.491853    5.162028    3.726143
 C   -2.996254    3.230713   -0.053488
 H   -2.604126    4.224332   -0.319729
 H   -3.705896    3.397419    0.782463
 O   -3.610696    2.699086   -1.179766
 C    2.177965    1.457435   -1.284981
 H    1.617982    2.389831   -1.275166
 C    3.509619    1.450841   -0.906326
 H    4.092103    0.547899   -1.101938
 C    4.301295    2.677443   -0.707057
 C    5.702018    2.588145   -0.650869
 C    3.714996    3.943892   -0.543036
 C    6.488893    3.717623   -0.438587
 H    6.176119    1.609813   -0.769645
 C    4.500344    5.073714   -0.330754
 H    2.628607    4.049557   -0.558717
 C    5.891348    4.968177   -0.276272
 H    7.576234    3.619953   -0.396961
 H    4.020525    6.046628   -0.200078
 H    6.504967    5.855594   -0.106574
 O   -4.497502    0.218863   -1.094716
Na   -3.261928   -0.435601   -2.798170
 C   -5.707527    0.088878   -0.631162
 C   -6.312953   -1.184790   -0.449811
 C   -6.489737    1.216892   -0.253933
 C   -7.594526   -1.314079    0.079268
 H   -5.744821   -2.073806   -0.735709
 C   -7.768832    1.072359    0.275278
 H   -6.057363    2.210269   -0.403610
 C   -8.338969   -0.191479    0.452718
 H   -8.021845   -2.313722    0.203941
 H   -8.334128    1.967460    0.552397
 H   -9.342196   -0.299693    0.870437
 H    0.123943   -4.246174    3.640083
 H   -1.696376   -5.305954   -0.112003
 C   -0.816443   -1.703752    3.816342
 H    0.091649   -1.941621    4.386302
 H   -0.728397   -0.673558    3.448538
 H   -1.666634   -1.735553    4.517122
 C   -2.927917   -2.949559   -0.629383
 H   -3.729212   -3.698470   -0.721048
 H   -3.391492   -1.958141   -0.532635
 H   -2.356268   -2.963241   -1.568698
121
Figure_S15-6_AA-9b(NaOPh)-ts(1,6minor)_O4 / electronic energy: -4439.04525456 a.u. / lowest freq: -267.46 cm-1
 H    2.251864    1.398679    3.342243
 H    4.391513    0.942272    1.488803
 C    3.317567    0.758992    1.575581
 C    2.842191   -0.513286    1.290436
 B    3.796407   -1.510152    0.560683
 O    4.913715   -1.097041   -0.122523
 H    7.372780   -2.042732    0.044408
 H    6.011613   -2.929142    1.730185
 H    7.221629   -1.277300   -1.554119
 O    3.633136   -2.870507    0.504859
 C    6.922508   -2.146802   -0.951063
 C    5.406782   -2.221225   -0.874670
 C    5.737618   -3.811255    1.132932
 C    4.844014   -3.428961   -0.047055
 H    5.189141   -4.507183    1.783384
 H    7.328922   -3.050121   -1.429637
 H    6.659693   -4.304878    0.795408
 C    4.516592   -4.662417   -0.872426
 H    4.094511   -5.443531   -0.223626
 H    5.431404   -5.062138   -1.334803
 H    3.008635    2.726290    2.426476
 C    2.497018    1.760043    2.327339
 H    1.532815    1.934817    1.817187
 H    0.965049   -0.359906    2.334025
 C    1.487878   -0.863122    1.515481
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H	1.216963	-1.921864	1.405695
H	3.793077	-4.446001	-1.667292
H	5.024426	-1.139127	-2.697463
C	4.792976	-2.126000	-2.271747
H	3.698844	-2.238110	-2.235539
H	5.198189	-2.895393	-2.944075
C	-3.639641	1.065480	1.448717
H	-4.527466	1.180403	0.814083
C	-3.579602	-0.329194	2.078101
H	-3.673879	-0.312736	3.173250
C	-1.634101	0.034475	0.825068
C	-1.699719	-2.026915	2.133683
C	-1.849812	-3.185581	1.357433
C	-1.017843	-2.037962	3.364563
C	-1.241991	-4.363167	1.811233
C	-0.429953	-3.232741	3.782295
C	-0.530148	-4.385749	3.005361
H	-0.057607	-5.311083	3.341863
Cu	0.164459	-0.204491	0.027424
N	-2.408676	1.107369	0.651040
N	-2.249433	-0.794973	1.674720
C	1.523259	0.068504	-1.481656
C	0.314094	-0.384594	-2.146942
H	-3.898782	0.997848	-1.554817
H	-4.353511	-0.999886	1.671765
H	-3.639808	1.874758	2.196395
H	2.317022	-0.675916	-1.415759
C	0.080415	-1.832313	-2.199512
C	-0.529842	0.461888	-2.991036
O	1.054780	-2.522419	-1.584532
O	-0.888387	-2.411853	-2.672556
O	-1.460849	0.081073	-3.684871
O	-0.185230	1.755001	-2.973763
C	-0.970690	2.636894	-3.767176
H	-0.825732	2.428315	-4.836729
H	-0.610554	3.645877	-3.536231
H	-2.033308	2.527831	-3.511473
C	0.891056	-3.918418	-1.411700
H	-0.066986	-4.145222	-0.926247
H	1.713057	-4.227937	-0.759019
H	0.942252	-4.444115	-2.375939
C	-2.021857	2.269682	-0.127437
H	-1.276216	1.913446	-0.853940
C	-1.355054	3.354290	0.713444
C	-0.986071	4.571617	0.123026
C	-1.037618	3.153429	2.060304
C	-0.343678	5.562492	0.862162
H	-1.186185	4.752331	-0.935030
C	-0.386759	4.140378	2.801362
H	-1.285692	2.206705	2.542272
C	-0.041048	5.351475	2.207309
H	-0.069533	6.502489	0.378165
H	-0.146968	3.954882	3.850501
H	0.468921	6.124666	2.785647
C	-3.214134	2.781968	-0.951182
H	-2.908890	3.708001	-1.459207
H	-4.032275	3.072313	-0.260830
O	-3.628662	1.887680	-1.927121
C	1.898824	1.382500	-1.117951
H	1.158190	2.181981	-1.161485
C	3.183033	1.655784	-0.672465
H	3.961379	0.920038	-0.878819
C	3.663124	3.004137	-0.338697
C	5.046059	3.244411	-0.278900
C	2.792987	4.066225	-0.041960
C	5.544161	4.501426	0.054196
H	5.737063	2.424788	-0.494798
C	3.290464	5.322944	0.290836
H	1.712911	3.907741	-0.044246
C	4.667098	5.548967	0.339875
H	6.623628	4.664571	0.093886
H	2.593113	6.130604	0.524663
H	5.054986	6.535341	0.603641
Na	-2.998379	-1.338445	-2.770880
O	-4.378881	-0.521005	-1.243783
C	-5.603435	-0.615542	-0.809916
C	-6.476075	0.508729	-0.779932
C	-6.136191	-1.838561	-0.318369
C	-7.771277	0.412235	-0.279485
H	-6.100940	1.456336	-1.176904
C	-7.434059	-1.920117	0.179029
H	-5.498176	-2.725573	-0.336232
C	-8.268160	-0.798901	0.210334
H	-8.407992	1.302275	-0.274914
H	-7.802931	-2.880619	0.551740
H	-9.284264	-0.869317	0.604324
H	0.120357	-3.256960	4.725828
H	-1.342113	-5.276319	1.218575
C	-2.649040	-3.188160	0.083401

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 H   -3.204990   -2.253264   -0.066982
 H   -1.998958   -3.323820   -0.793887
 H   -3.365657   -4.023101    0.087534
 C   -0.928608   -0.796942    4.212194
 H   -0.138124   -0.892585    4.968064
 H   -0.718952    0.096012    3.606081
 H   -1.876702   -0.612301    4.742422
32
Figure_S15-7_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C   -0.660544   -0.726572    0.059153
 C   -1.860539   -0.097447    0.115996
 H   -0.691600   -1.818492   -0.004770
 C   -1.976243    1.390665    0.160143
 C   -3.120576   -0.891785    0.187355
 O   -3.041424    1.823605   -0.507466
 O   -1.182749    2.134043    0.689285
 O   -4.147702   -0.497504    0.683440
 O   -2.981802   -2.118850   -0.320932
 C   -4.097604   -2.989729   -0.195724
 H   -4.332384   -3.170881    0.862818
 H   -3.810049   -3.927003   -0.683244
 H   -4.981752   -2.562067   -0.688186
 C   -3.254671    3.228152   -0.535442
 H   -3.354009    3.627502    0.483524
 H   -4.184056    3.384216   -1.092621
 H   -2.420438    3.737793   -1.038016
 C    0.656646   -0.129211    0.062308
 H    0.725624    0.955889    0.150505
 C    1.759981   -0.902956   -0.019704
 H    1.621029   -1.988149   -0.089650
 C    3.156351   -0.453635   -0.025165
 C    4.175093   -1.416830   -0.109525
 C    3.522207    0.902114    0.053056
 C    5.517020   -1.042840   -0.114390
 H    3.907556   -2.474776   -0.172060
 C    4.861836    1.275255    0.048166
 H    2.754752    1.675486    0.118691
 C    5.863995    0.305241   -0.035401
 H    6.294080   -1.807149   -0.179427
 H    5.127957    2.332459    0.111300
 H    6.914980    0.602284   -0.038425
76
Figure_S15-7_9d(Na)-Cu-allyl_01 / electronic energy: -3289.87323919 a.u. / lowest freq: 20.48 cm-1
 C    2.890494    1.919481   -1.277302
 H    3.212834    1.619009   -2.282905
 C    1.580347    2.708660   -1.287786
 H    1.715166    3.773396   -1.053559
 C    1.361334    0.845889    0.116302
 C   -0.476920    2.468998    0.143962
 C   -1.201053    3.344915   -0.672658
 C   -1.049124    2.021662    1.341390
 C   -2.500751    3.731098   -0.327753
 C   -2.353152    2.373080    1.688914
 C   -3.068439    3.232389    0.847613
 H   -4.088296    3.522016    1.116164
Cu    0.549243   -0.521771    1.237838
 N    2.543033    0.749000   -0.472014
 N    0.804179    2.032970   -0.243867
 H    1.066715    2.629079   -2.259433
 H    3.717911    2.468759   -0.801157
 C    3.344698   -0.463934   -0.515154
 H    2.901187   -1.123898    0.249271
 C    4.775968   -0.154327   -0.107352
 C    5.877692   -0.460143   -0.912213
 C    5.005969    0.459152    1.132365
 C    7.175180   -0.164497   -0.487241
 H    5.732823   -0.936167   -1.883022
 C    6.297285    0.758235    1.558327
 H    4.151927    0.706681    1.769782
 C    7.389916    0.445116    0.746743
 H    8.022928   -0.413557   -1.129804
 H    6.453595    1.234919    2.528793
 H    8.405182    0.675575    1.077400
 C    3.137215   -1.190296   -1.873781
 H    3.774689   -2.111853   -1.794461
 H    3.662176   -0.569468   -2.653477
 O    1.845948   -1.423998   -2.140698
 C   -0.451569   -1.910882    2.208955
 H   -1.214664   -1.404047    2.822373
 H    0.177713   -2.546649    2.852851
 C   -1.044927   -2.620703    1.056533
 C   -0.492142   -3.711033    0.455359
 H   -0.988980   -4.153163   -0.417369
 C    0.787250   -4.340968    0.920790
 H    1.118695   -5.149002    0.253404
 H    1.593059   -3.583472    0.969365
 H    0.701537   -4.758930    1.940091
 B   -2.306527   -1.993764    0.382957
 O   -3.373025   -1.412180    1.004517
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 O   -2.415671   -1.921873   -0.995612
 C   -4.386992   -1.159047    0.008097
 C   -3.540932   -1.073394   -1.313835
 C   -5.133677    0.116193    0.360060
 C   -5.338535   -2.354768    0.029500
 C   -4.233816   -1.613380   -2.553791
 C   -2.982138    0.323768   -1.572158
 H   -4.479589   -2.677383   -2.447888
 H   -3.576969   -1.498793   -3.428337
 H   -5.161058   -1.055202   -2.750289
 H   -4.818196   -3.287688   -0.232540
 H   -6.175828   -2.213317   -0.667972
 H   -5.748118   -2.466329    1.043327
 H   -2.476565    0.722952   -0.681484
 H   -3.773968    1.028313   -1.862331
 H   -2.252056    0.281035   -2.394600
 H   -4.449481    0.965059    0.476018
 H   -5.678059   -0.021758    1.305057
 H   -5.865158    0.358733   -0.425131
Na   -0.132379   -1.871828   -1.732083
 C   -3.288355    4.628767   -1.246136
 H   -4.131202    5.101149   -0.723105
 H   -2.656663    5.421816   -1.671818
 H   -3.701543    4.052122   -2.089506
 C   -2.973914    1.790798    2.930585
 H   -2.277050    1.825374    3.780685
 H   -3.894667    2.320460    3.211548
 H   -3.228022    0.732756    2.756237
 H   -0.769050    3.721967   -1.600967
 H   -0.472166    1.385437    2.015110
108
Figure_S15-7_AA-9d(Na)-ts(1,6major)_01 / electronic energy: -4131.84208395 a.u. / lowest freq: -388.75 cm-1
 C   -2.711428   -3.560318   -1.132305
 H   -2.940555   -4.392337   -0.455983
 C   -3.822044   -2.516706   -1.175235
 H   -4.381319   -2.522257   -2.120455
 C   -1.802443   -1.482480   -0.602707
 C   -3.716520   -0.015060   -1.150647
 C   -5.117856    0.045520   -1.100061
 C   -2.992944    1.160810   -1.370541
 C   -5.791194    1.256658   -1.264968
 C   -3.650939    2.385091   -1.527585
 C   -5.045495    2.420104   -1.479188
 H   -5.563011    3.375465   -1.603033
Cu   -0.439091   -0.167115    0.015113
 N   -1.575823   -2.788080   -0.629088
 N   -3.077685   -1.262639   -1.013789
 C    0.291728    1.125930    1.468171
 C   -0.772780    0.338840    2.044785
Na   -2.895378   -2.343495    2.760611
 H   -4.538826   -2.645827   -0.347872
 H   -2.482812   -3.963920   -2.130610
 H    1.292282    0.740652    1.688668
 C   -2.190886    0.724592    2.110135
 C   -0.403830   -0.808671    2.891926
 O   -2.423783    2.007660    1.827688
 O   -3.113091   -0.033989    2.371073
 O   -1.084498   -1.260615    3.795464
 O    0.788673   -1.342336    2.595678
 C    1.119918   -2.532643    3.306770
 H    1.273412   -2.319422    4.374091
 H    2.050045   -2.899797    2.862028
 H    0.306457   -3.262190    3.179765
 C   -3.779397    2.430074    1.825288
 H   -4.391841    1.778338    1.188916
 H   -3.778538    3.450142    1.425814
 H   -4.185106    2.425348    2.847135
 C   -0.396587   -3.433138   -0.055809
 H    0.156777   -2.619573    0.435653
 C    0.509425   -4.065965   -1.088689
 C    0.113697   -5.164826   -1.865135
 C    1.810875   -3.577008   -1.249803
 C    0.986779   -5.735439   -2.792025
 H   -0.883258   -5.593867   -1.743935
 C    2.685025   -4.142105   -2.176962
 H    2.152393   -2.725057   -0.658608
 C    2.274613   -5.223836   -2.955281
 H    0.657605   -6.588742   -3.389761
 H    3.687218   -3.722584   -2.291455
 H    2.954823   -5.668397   -3.685396
 C   -0.830002   -4.414434    1.075110
 H    0.150020   -4.780473    1.489969
 H   -1.246107   -5.326425    0.561704
 O   -1.652875   -3.853165    1.964925
 C    0.822483   -0.011040   -1.639409
 H    0.077293    0.283313   -2.390232
 H    1.052317   -1.082375   -1.669123
 C    1.910067    0.867157   -1.402852
 C    1.836518    2.242102   -1.627255
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 H     2.777802    2.795811   -1.600745
 C     0.705249    2.854033   -2.395762
 H     0.645384    2.446417   -3.420227
 H    -0.257424    2.632002   -1.909175
 H     0.801225    3.945902   -2.469218
 C     0.264652    2.415375    0.896415
 H    -0.697708    2.904028    0.755150
 C     1.439172    3.026760    0.473743
 H     2.379378    2.570306    0.790077
 C     1.545697    4.467074    0.162051
 C     2.820178    5.032955   -0.010463
 C     0.430656    5.309280    0.027744
 C     2.976406    6.382773   -0.313412
 H     3.700017    4.391303    0.091286
 C     0.584028    6.659849   -0.277325
 H    -0.574727    4.909557    0.169458
 C     1.856624    7.204735   -0.451628
 H     3.978803    6.797776   -0.442119
 H    -0.300443    7.293606   -0.375782
 H     1.976010    8.264327   -0.687734
 C    -2.859170    3.645640   -1.749864
 H    -2.328461    3.618546   -2.713672
 H    -3.505951    4.533297   -1.743514
 H    -2.096966    3.771127   -0.967396
 C    -7.296253    1.311504   -1.225679
 H    -7.646217    2.167711   -0.630719
 H    -7.708889    1.430530   -2.240169
 H    -7.724662    0.395764   -0.795613
 H    -5.702509   -0.857679   -0.923482
 H    -1.904206    1.124885   -1.436150
 B     3.212845    0.333471   -0.734838
 O     4.088291    1.142500   -0.055571
 O     3.621695   -0.974140   -0.739793
 C     5.269041    0.376300    0.243014
 C     4.731333   -1.101132    0.169044
 C     5.720025   -2.112219   -0.390335
 H     6.009007   -1.869222   -1.420635
 H     6.626905   -2.150982    0.231366
 H     5.264774   -3.113121   -0.389931
 C     4.163126   -1.602277    1.494787
 H     3.416057   -0.905582    1.902650
 H     3.666328   -2.567336    1.319421
 H     4.952744   -1.754517    2.243763
 C     5.795395    0.793317    1.607106
 H     6.150585    1.833027    1.565445
 H     5.015138    0.729706    2.376080
 H     6.640080    0.155805    1.907801
 C     6.295329    0.694273   -0.843383
 H     7.252426    0.187867   -0.655677
 H     5.929881    0.396781   -1.837088
 H     6.474539    1.778812   -0.857786
108
Figure_S15-7_AA-9d(Na)-ts(1,6major)_02 / electronic energy: -4131.84213530 a.u. / lowest freq: -365.14 cm-1
 C    -1.419996   -4.158800   -1.063704
 H    -1.423259   -4.948513   -0.303228
 C    -2.800665   -3.525033   -1.245112
 H    -3.225434   -3.686782   -2.245904
 C    -1.272076   -1.880809   -0.581363
 C    -3.537127   -1.124424   -1.187134
 C    -4.880185   -1.520318   -1.229227
 C    -3.221916    0.230706   -1.340917
 C    -5.900224   -0.581636   -1.409205
 C    -4.227989    1.183388   -1.512527
 C    -5.561537    0.766298   -1.551044
 H    -6.352456    1.508503   -1.689858
Cu    -0.396853   -0.217777    0.049592
 N    -0.614289   -3.029308   -0.597954
 N    -2.533328   -2.098999   -1.021303
 C    -0.058117    1.190784    1.529318
 C    -0.861374    0.124619    2.081674
Na    -2.083527   -3.077652    2.659084
 H    -3.521328   -3.901532   -0.502496
 H    -1.007198   -4.566243   -1.999414
 H     1.010074    1.093452    1.749790
 C    -2.333880    0.075787    2.108904
 C    -0.203258   -0.867340    2.951533
 O    -2.928952    1.240351    1.843292
 O    -2.996527   -0.927761    2.325445
 O    -0.762366   -1.513045    3.820342
 O     1.108816   -1.010917    2.729586
 C     1.744149   -2.040776    3.483924
 H     1.737924   -1.798081    4.555704
 H     2.774332   -2.091187    3.117412
 H     1.214640   -2.989099    3.309556
 C    -4.349378    1.242616    1.815429
 H    -4.728657    0.451189    1.156183
 H    -4.643842    2.225243    1.430839
 H    -4.753218    1.097825    2.827621
 C     0.713481   -3.227022   -0.036757
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 H     0.960275   -2.283386    0.478898
 C     1.764463   -3.473483   -1.104330
 C     3.034142   -3.952500   -0.749413
 C     1.525689   -3.188838   -2.454209
 C     4.029268   -4.131759   -1.708514
 H     3.257031   -4.180059    0.294494
 C     2.520275   -3.363597   -3.416162
 H     0.550293   -2.805006   -2.760475
 C     3.778702   -3.834676   -3.048008
 H     5.010168   -4.504656   -1.404017
 H     2.308439   -3.125565   -4.461032
 H     4.559732   -3.969084   -3.799526
 C     0.627366   -4.320426    1.078787
 H     1.638104   -4.314664    1.562996
 H     0.600482   -5.309021    0.538448
 O    -0.385593   -4.109503    1.925680
 C     0.673413    0.303294   -1.654776
 H    -0.148581    0.411509   -2.375138
 H     1.186612   -0.662496   -1.731199
 C     1.503232    1.423846   -1.400567
 C     1.091186    2.741699   -1.577826
 H     1.862395    3.514491   -1.531481
 C    -0.168384    3.071428   -2.321317
 H    -0.144510    2.674493   -3.351476
 H    -1.040872    2.614860   -1.826173
 H    -0.343136    4.154099   -2.379454
 C    -0.439328    2.436041    0.983919
 H    -1.499559    2.649644    0.856363
 C     0.522125    3.347458    0.568180
 H     1.555446    3.148133    0.861556
 C     0.237270    4.766281    0.277868
 C     1.310456    5.666481    0.167459
 C    -1.061451    5.269556    0.098455
 C     1.098125    7.013168   -0.114931
 H     2.329215    5.292180    0.302782
 C    -1.276282    6.616022   -0.185938
 H    -1.920946    4.601739    0.178047
 C    -0.198788    7.496171   -0.295455
 H     1.950699    7.691825   -0.193526
 H    -2.296528    6.982251   -0.322583
 H    -0.369230    8.552097   -0.516158
 C    -3.868369    2.638106   -1.657124
 H    -3.358726    2.828483   -2.614199
 H    -4.758418    3.280319   -1.614299
 H    -3.179656    2.949669   -0.858094
 C    -7.341220   -1.021742   -1.411953
 H    -7.981311   -0.296249   -1.932697
 H    -7.461748   -2.000539   -1.898047
 H    -7.720217   -1.118955   -0.381838
 H    -5.148599   -2.571296   -1.115405
 H    -2.179432    0.552088   -1.338431
 B     2.900305    1.143292   -0.775190
 O     3.586702    2.027935    0.016436
 O     3.567834   -0.039161   -0.937640
 C     4.899110    1.482084    0.253376
 C     4.674239   -0.052845   -0.020837
 C     5.848084   -0.767239   -0.671105
 H     6.105642   -0.322021   -1.640237
 H     6.733045   -0.731940   -0.018229
 H     5.583865   -1.820818   -0.841284
 C     4.205842   -0.818302    1.213701
 H     3.344359   -0.322066    1.683250
 H     3.883363   -1.821401    0.898907
 H     5.006136   -0.924896    1.959687
 C     5.323621    1.816090    1.674746
 H     5.456279    2.902594    1.778632
 H     4.572398    1.492446    2.406130
 H     6.281411    1.330820    1.914484
 C     5.845950    2.137676   -0.750465
 H     6.884756    1.814725   -0.593498
 H     5.558429    1.902150   -1.785530
 H     5.799504    3.228732   -0.623480
108
Figure_S15-7_AA-9d(Na)-ts(1,6major)_03 / electronic energy: -4131.84066850 a.u. / lowest freq: -367.11 cm-1
 C    -1.462256   -4.030582   -1.212482
 H    -1.545877   -4.804502   -0.438623
 C    -2.803697   -3.348073   -1.492196
 H    -3.107480   -3.407682   -2.547682
 C    -1.291957   -1.777405   -0.631913
 C    -3.537107   -0.959475   -1.227884
 C    -4.870799   -1.337691   -1.421742
 C    -3.223327    0.404355   -1.155262
 C    -5.884926   -0.377526   -1.510946
 C    -4.222244    1.375551   -1.216613
 C    -5.551108    0.972692   -1.396342
 H    -6.338207    1.729315   -1.452869
Cu    -0.396176   -0.146099    0.050988
 N    -0.642645   -2.928702   -0.708487
 N    -2.545013   -1.953480   -1.112473
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C	0.002205	1.294962	1.486217
C	-0.910784	0.323356	2.041504
Na	-2.263271	-2.875764	2.539197
H	-3.612345	-3.774495	-0.880584
H	-1.010208	-4.475021	-2.111100
H	1.056461	1.126325	1.728831
C	-2.368155	0.569872	2.047648
C	-0.391647	-0.712319	2.940323
O	-3.113836	-0.556089	2.133536
O	-2.901306	1.652040	1.937446
O	-1.058387	-1.330349	3.756936
O	0.920273	-0.939403	2.814000
C	1.437246	-2.016774	3.591558
H	1.333752	-1.806187	4.665033
H	2.496756	-2.097602	3.327739
H	0.891407	-2.936045	3.330861
C	-4.524020	-0.371096	2.143783
H	-4.826595	0.277160	2.977526
H	-4.964314	-1.367148	2.267875
H	-4.864509	0.072496	1.198065
C	0.647795	-3.181676	-0.087034
H	0.929461	-2.235369	0.406447
C	1.716858	-3.530645	-1.106644
C	2.923022	-4.119568	-0.699924
C	1.554606	-3.241775	-2.467198
C	3.930644	-4.402824	-1.620523
H	3.086859	-4.355433	0.352879
C	2.560966	-3.522581	-3.390649
H	0.629756	-2.774663	-2.812006
C	3.755770	-4.104346	-2.971482
H	4.861351	-4.859872	-1.276153
H	2.408211	-3.281683	-4.445066
H	4.545873	-4.323960	-3.692755
C	0.457010	-4.229984	1.059010
H	1.440312	-4.246715	1.596569
H	0.412738	-5.235364	0.553687
O	-0.588465	-3.946399	1.843957
C	0.726852	0.273493	-1.656198
H	-0.086302	0.403103	-2.383044
H	1.192655	-0.717254	-1.701819
C	1.611205	1.356103	-1.421565
C	1.271947	2.687248	-1.646199
H	2.080076	3.422130	-1.608566
C	0.046853	3.056197	-2.429559
H	0.085934	2.645601	-3.453710
H	-0.857368	2.637530	-1.955659
H	-0.083966	4.143880	-2.505515
C	-0.300099	2.543168	0.901893
H	-1.347972	2.807465	0.764611
C	0.705201	3.394922	0.466735
H	1.726125	3.162580	0.778258
C	0.476480	4.813241	0.127302
C	1.581389	5.672596	0.007699
C	-0.801976	5.353046	-0.090148
C	1.419427	7.016997	-0.316975
H	2.584746	5.268991	0.170723
C	-0.965844	6.697306	-0.415815
H	-1.684238	4.715758	-0.008549
C	0.142644	7.537662	-0.531697
H	2.296051	7.663633	-0.401261
H	-1.970736	7.093718	-0.579331
H	0.010989	8.592046	-0.784189
C	-3.871145	2.828464	-1.044043
H	-2.947030	3.086310	-1.581118
H	-4.674361	3.486628	-1.402088
H	-3.701721	3.036651	0.024307
C	-7.310595	-0.814296	-1.727248
H	-8.004955	0.035159	-1.674958
H	-7.429954	-1.288545	-2.713904
H	-7.617948	-1.554076	-0.972787
H	-5.142594	-2.390779	-1.501540
H	-2.186169	0.725682	-1.045498
B	2.967222	1.007262	-0.741757
O	3.659223	1.848521	0.091100
O	3.575053	-0.211530	-0.873843
C	4.917582	1.220504	0.407927
C	4.611733	-0.296410	0.117555
C	5.777824	-1.090785	-0.447712
H	6.137371	-0.667577	-1.394162
H	6.612073	-1.114852	0.269134
H	5.454181	-2.123705	-0.639536
C	4.005039	-1.024092	1.314929
H	3.148535	-0.469439	1.724283
H	3.637167	-2.003568	0.976380
H	4.742534	-1.184155	2.114366
C	5.272876	1.530277	1.853297
H	5.463292	2.607086	1.967620
H	4.459711	1.253927	2.536327
H	6.182902	0.988552	2.151352

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 C    5.963187    1.812435   -0.535508
 H    6.967823    1.423310   -0.317928
 H    5.723552    1.593975   -1.586407
 H    5.980292    2.904446   -0.409102
108
Figure_S15-7_AA-9d(Na)-ts(1,6minor)_01 / electronic energy: -4131.83826859 a.u. / lowest freq: -396.29 cm-1
 C    4.469926   -0.443997    1.672550
 H    5.247146   -1.041689    1.180404
 C    4.499512    1.026998    1.249706
 H    4.746261    1.708953    2.075439
 C    2.421749    0.104477    0.696218
 C    2.694159    2.516174    0.328613
 C    3.622554    3.539170    0.105580
 C    1.335007    2.773658    0.113683
 C    3.206557    4.798635   -0.343625
 C    0.906044    4.009041   -0.365093
 C    1.849125    5.019335   -0.583949
 H    1.518011    5.994382   -0.952441
Cu    0.651461   -0.233012   -0.145874
 N    3.153417   -0.876718    1.197255
 N    3.129732    1.255260    0.775787
 C   -0.449819   -0.377166   -1.908705
 C    0.950711   -0.574103   -2.219945
Na    4.395784   -1.267744   -1.911966
 H    5.218917    1.203147    0.434085
 H    4.556865   -0.574590    2.761710
 H   -0.771980    0.671056   -1.906903
 C    1.796754    0.554814   -2.631366
 C    1.557204   -1.901068   -2.399781
 O    1.102828    1.647176   -2.967186
 O    3.019774    0.554075   -2.655052
 O    2.551044   -2.139089   -3.064543
 O    0.935241   -2.881995   -1.730970
 C    1.568065   -4.158285   -1.755685
 H    1.565912   -4.575960   -2.772163
 H    0.975953   -4.795886   -1.089555
 H    2.604387   -4.059483   -1.397996
 C    1.854176    2.797963   -3.322961
 H    2.591949    3.042654   -2.547584
 H    1.131407    3.614819   -3.423296
 H    2.372569    2.636210   -4.279059
 C    2.729288   -2.269726    1.190057
 H    2.000328   -2.350750    0.369887
 C    2.030512   -2.693264    2.462173
 C    1.303811   -3.891954    2.458310
 C    2.047587   -1.933595    3.636297
 C    0.623887   -4.324069    3.594496
 H    1.253762   -4.484814    1.541294
 C    1.367489   -2.362807    4.776761
 H    2.573226   -0.977399    3.661215
 C    0.654963   -3.560385    4.762348
 H    0.058466   -5.258332    3.564838
 H    1.389462   -1.749953    5.680903
 H    0.118708   -3.893730    5.653464
 C    3.933789   -3.167413    0.769042
 H    3.517506   -4.210119    0.766053
 H    4.635625   -3.170081    1.651187
 O    4.476100   -2.768885   -0.387895
 C   -0.617585   -0.227119    1.499638
 H   -0.259743    0.665067    2.027138
 H   -0.161570   -1.154496    1.875175
 C   -1.998087   -0.258720    1.179527
 C   -2.643875   -1.418897    0.748472
 H   -3.735269   -1.406444    0.754760
 C   -1.975880   -2.758440    0.801979
 H   -0.987700   -2.727335    0.312538
 H   -1.801482   -3.073755    1.845746
 H   -2.581871   -3.532649    0.308588
 C   -1.483318   -1.333013   -1.904628
 H   -1.228083   -2.367889   -2.130937
 C   -2.769548   -1.031796   -1.482698
 H   -3.013770    0.022045   -1.329599
 C   -3.949462   -1.881475   -1.751590
 C   -5.230206   -1.355439   -1.509259
 C   -3.856110   -3.195219   -2.237390
 C   -6.375288   -2.109163   -1.751358
 H   -5.312610   -0.345042   -1.099853
 C   -5.002510   -3.951400   -2.476432
 H   -2.878385   -3.637161   -2.438538
 C   -6.267312   -3.412922   -2.238427
 H   -7.359429   -1.676133   -1.557402
 H   -4.905044   -4.970339   -2.858533
 H   -7.164255   -4.005613   -2.431296
 C   -0.550857    4.210838   -0.677788
 H   -1.177033    3.580697   -0.030806
 H   -0.854242    5.259895   -0.551482
 H   -0.760119    3.927434   -1.722701
 C    4.218891    5.896659   -0.543801
 H    3.849068    6.661840   -1.240298
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 H     4.442114    6.397217    0.412094
 H     5.166978    5.501689   -0.936412
 H     4.686341    3.368745    0.274961
 H     0.589000    2.008960    0.331241
 B    -2.867154    1.034726    1.243105
 O    -4.168686    1.066803    0.807004
 O    -2.470203    2.243035    1.761486
 C    -4.632911    2.425335    0.884714
 C    -3.662798    3.033453    1.958791
 C    -3.349024    4.508225    1.772070
 H    -2.917498    4.718525    0.787415
 H    -4.266143    5.105093    1.885539
 H    -2.630433    4.835287    2.537093
 C    -4.129722    2.778140    3.392489
 H    -4.379700    1.718700    3.550281
 H    -3.317260    3.042675    4.083975
 H    -5.009866    3.386284    3.644266
 C    -6.101976    2.428584    1.276122
 H    -6.702526    1.988364    0.467061
 H    -6.278214    1.844425    2.188036
 H    -6.455168    3.457239    1.442197
 C    -4.450664    3.041417   -0.502266
 H    -4.848405    4.065103   -0.546035
 H    -3.389948    3.064525   -0.792358
 H    -4.992125    2.429854   -1.238270
108
Figure_S15-7_AA-9d(Na)-ts(1,6minor)_O2 / electronic energy: -4131.83828091 a.u. / lowest freq: -396.51 cm-1
 C     4.468564   -0.450417    1.674256
 H     5.244860   -1.051139    1.184404
 C     4.502306    1.019437    1.248039
 H     4.754398    1.702260    2.071402
 C     2.421212    0.102479    0.698743
 C     2.699509    2.513522    0.330767
 C     3.629043    3.533763    0.106848
 C     1.339413    2.774651    0.119898
 C     3.214611    4.795469   -0.340568
 C     0.912112    4.011465   -0.354016
 C     1.857836    5.020559   -0.574020
 H     1.527388    5.998220   -0.935910
Cu     0.650782   -0.231668   -0.144472
 N     3.151258   -0.880547    1.198689
 N     3.131933    1.251599    0.778111
 C    -0.447999   -0.374384   -1.909086
 C     0.952842   -0.571546   -2.218622
Na     4.396551   -1.268747   -1.906743
 H     5.219531    1.191224    0.429483
 H     4.553930   -0.578632    2.763853
 H    -0.769924    0.673905   -1.906947
 C     1.799993    0.557311   -2.627916
 C     1.558879   -1.898614   -2.399849
 O     1.107130    1.650458   -2.963336
 O     3.023058    0.555756   -2.650226
 O     2.552759   -2.136011   -3.064779
 O     0.936464   -2.880139   -1.732501
 C     1.569257   -4.156528   -1.758474
 H     1.566936   -4.573159   -2.775388
 H     0.977032   -4.794704   -1.093000
 H     2.605580   -4.057795   -1.400604
 C     1.859465    2.801019   -3.317675
 H     2.596514    3.044884   -2.541332
 H     1.137307    3.618319   -3.418516
 H     2.378924    2.639416   -4.273218
 C     2.724006   -2.272614    1.191760
 H     1.994640   -2.352124    0.371795
 C     2.024745   -2.694586    2.464147
 C     1.296531   -3.892373    2.461018
 C     2.042584   -1.934169    3.637778
 C     0.615944   -4.322893    3.597416
 H     1.245711   -4.485790    1.544406
 C     1.361819   -2.361782    4.778446
 H     2.569360   -0.978587    3.662147
 C     0.647821   -3.558489    4.764772
 H     0.049354   -5.256468    3.568296
 H     1.384420   -1.748319    5.682158
 H     0.111031   -3.890552    5.656046
 C     3.926419   -3.172822    0.770257
 H     3.507922   -4.214617    0.767056
 H     4.628558   -3.177200    1.652129
 O     4.469195   -2.775195   -0.386826
 C    -0.620484   -0.226187    1.499397
 H    -0.263405    0.665666    2.027989
 H    -0.164891   -1.153752    1.874986
 C    -2.000570   -0.257719    1.177551
 C    -2.645628   -1.417657    0.744647
 H    -3.737031   -1.405413    0.749660
 C    -1.977493   -2.757138    0.798007
 H    -0.988792   -2.725530    0.309659
 H    -1.804163   -3.073175    1.841727
 H    -2.582795   -3.531101    0.303388
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 C   -1.481679   -1.330051   -1.906792
 H   -1.226333   -2.364831   -2.133445
 C   -2.768369   -1.028912   -1.486122
 H   -3.012617    0.024869   -1.332688
 C   -3.948103   -1.878193   -1.757168
 C   -5.229080   -1.352057   -1.516295
 C   -3.854333   -3.191674   -2.243593
 C   -6.373965   -2.105445   -1.760374
 H   -5.311874   -0.341889   -1.106419
 C   -5.000540   -3.947519   -2.484622
 H   -2.876410   -3.633674   -2.443654
 C   -6.265567   -3.408951   -2.248023
 H   -7.358290   -1.672346   -1.567496
 H   -4.902739   -4.966258   -2.867171
 H   -7.162355   -4.001377   -2.442430
 C   -0.545769    4.220994   -0.656877
 H   -1.170912    3.586784   -0.012896
 H   -0.844510    5.269856   -0.518245
 H   -0.761946    3.949588   -1.703545
 C    4.238582    5.877614   -0.566622
 H    3.776375    6.794113   -0.957551
 H    4.756590    6.130645    0.371324
 H    5.006554    5.550288   -1.283926
 H    4.692972    3.362000    0.274867
 H    0.592432    2.011847    0.340611
 B   -2.870227    1.035331    1.241440
 O   -4.170713    1.067624    0.802263
 O   -2.475175    2.242835    1.763182
 C   -4.635672    2.425816    0.881283
 C   -3.668674    3.032278    1.959049
 C   -3.355393    4.507610    1.776030
 H   -2.922690    4.720309    0.792418
 H   -4.273028    5.103682    1.889490
 H   -2.638046    4.833402    2.542759
 C   -4.139109    2.773884    3.391040
 H   -4.388639    1.713952    3.546210
 H   -3.328676    3.037787    4.085144
 H   -5.020412    3.380824    3.641652
 C   -6.105776    2.427757    1.268721
 H   -6.703924    1.988812    0.457191
 H   -6.284211    1.841779    2.179046
 H   -6.459851    3.455945    1.435787
 C   -4.449752    3.044582   -0.504023
 H   -4.848185    4.068029   -0.547085
 H   -3.388126    3.069098   -0.790737
 H   -4.988452    2.433943   -1.242817
108
Figure_S15-7_AA-9d(Na)-ts(1,6minor)_O3 / electronic energy: -4131.83588529 a.u. / lowest freq: -368.17 cm-1
 C   -2.202324    2.335266    1.832175
 H   -0.580844    3.819869    1.475227
 C   -0.821160    2.755301    1.423502
 H   -2.928308    3.153629    1.732796
 H   -1.969920    7.610749   -0.265140
 H   -0.454640    5.656800   -0.437847
 C   -2.387339    6.614389   -0.428638
 C   -1.535430    5.517436   -0.529864
 H   -4.439923    7.299393   -0.459165
 C   -3.767820    6.441930   -0.536826
 C   -2.036563    4.221979   -0.742579
 C   -4.281988    5.161354   -0.746639
 C   -1.084448    3.097981   -0.838751
 H   -0.036857    3.401784   -0.889766
 C   -3.428337    4.065019   -0.847987
 H   -5.360952    5.013403   -0.833814
 H   -3.856287    3.073306   -1.006496
 C   -1.413816    1.852007   -1.350746
 H   -2.457628    1.560238   -1.450345
 C    0.241330    1.854905    1.450314
 H    0.605994    1.296488   -1.679791
 C   -0.417024    0.906421   -1.669420
 H   -0.837655    0.105549    2.159628
 C    0.062539    0.461896    1.640342
 H    0.968121   -0.101205    1.886442
Cu   -0.246935   -0.514590   -0.165770
 C   -0.207205   -2.378418    0.505090
 N    0.847271   -3.168651    0.775518
 H   -2.795088   -1.435367    5.150946
 N   -1.317497   -3.036739    0.807871
 C   -1.831519   -0.969067   -2.728242
 O   -2.914119   -0.459405   -2.131003
 C   -0.555663   -0.408451   -2.261620
 O    0.710556   -2.310638   -2.997771
 C    0.637812   -1.114888   -2.757511
 C   -2.650654   -2.515613    0.564716
 C   -1.069044   -4.414362    1.242001
 H   -1.402953   -5.101113    0.449667
 C    0.450030   -4.418813    1.437690
 H    0.740026   -4.387633    2.501491
 C    2.198554   -2.717665    0.824472
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 C    3.062346   -2.965978   -0.243668
 C    2.657188   -2.070450    1.967806
 C    4.398664   -2.564743   -0.170763
 C    3.983477   -1.635378    2.056706
 C    4.836944   -1.902517    0.984477
 H    5.882768   -1.585686    1.046024
Na   -1.209563   -3.807709   -2.583772
 H    0.942972   -5.284144    0.973896
 H   -1.619948   -4.649881    2.163221
 O    1.700586   -0.315062   -2.910034
 O   -1.943916   -1.827135   -3.588266
 C   -4.160447   -1.052607   -2.486453
 H   -4.392996   -0.862833   -3.543528
 H   -4.911197   -0.575192   -1.846788
 H   -4.110422   -2.136537   -2.303551
 C    2.907600   -0.917044   -3.344956
 H    3.250169   -1.667569   -2.622351
 H    3.643285   -0.108907   -3.418472
 H    2.773211   -1.396217   -4.324642
 H   -2.527235   -1.706539   -0.170166
 C   -3.277019   -1.907248    1.801991
 C   -4.480529   -1.198877    1.673939
 C   -2.684204   -1.977182    3.067109
 C   -5.078085   -0.591386    2.775677
 H   -4.947418   -1.107498    0.690250
 C   -3.279653   -1.369843    4.174017
 H   -1.728308   -2.489869    3.190231
 C   -4.480621   -0.677190    4.034281
 H   -6.013640   -0.041645    2.649623
 H   -4.945268   -0.198782    4.899217
 C   -3.496734   -3.604572   -0.163979
 H   -4.507297   -3.136064   -0.303784
 H   -3.688322   -4.409163    0.601438
 O   -2.906773   -4.021075   -1.292305
 H   -2.552015    1.488243    1.214951
 H   -2.225573    1.984573    2.879173
 C    4.443119   -0.868755    3.266258
 H    4.105176   -1.348652    4.196365
 H    5.537671   -0.777907    3.300231
 H    4.015737    0.145727    3.238398
 C    5.356867   -2.811949   -1.306783
 H    5.625627   -1.866033   -1.803807
 H    6.291725   -3.263769   -0.943573
 H    4.925578   -3.481265   -2.063931
 H    2.674510   -3.473826   -1.129513
 H    1.965882   -1.899015    2.796616
 B    1.674134    2.326823    1.060192
 O    1.938201    3.479112    0.365260
 O    2.808583    1.587851    1.284292
 C    3.365938    3.605432    0.229766
 C    3.849305    2.123912    0.447796
 C    3.848318    1.295020   -0.835693
 H    2.891913    1.382399   -1.370248
 H    4.658652    1.597057   -1.514594
 H    3.986973    0.236711   -0.571364
 C    5.190375    1.994086    1.151068
 H    5.977311    2.500105    0.572194
 H    5.163394    2.425920    2.159445
 H    5.459522    0.932633    1.238299
 C    3.841390    4.557450    1.325919
 H    3.306633    5.512730    1.226267
 H    3.632999    4.151015    2.326255
 H    4.919534    4.755359    1.245728
 C    3.680273    4.179215   -1.142988
 H    4.766489    4.191649   -1.317195
 H    3.202418    3.598051   -1.941944
 H    3.312020    5.213281   -1.207496
108
Figure_S15-7_AA-9d(Na)-ts(1,6minor)_O4 / electronic energy: -4131.83709746 a.u. / lowest freq: -406.05 cm-1
 C    4.409379    0.010152    1.720521
 H    5.328157   -0.460761    1.350171
 C    4.274723    1.466963    1.283767
 H    4.417397    2.176901    2.109627
 C    2.378901    0.269989    0.612624
 C    2.290774    2.721055    0.392753
 C    3.069575    3.871044    0.213618
 C    0.907193    2.804478    0.201146
 C    2.480923    5.084800   -0.160132
 C    0.309032    3.992576   -0.212400
 C    1.102182    5.132298   -0.378815
 H    0.637257    6.071605   -0.690820
Cu    0.636435   -0.172473   -0.244493
 N    3.231666   -0.610472    1.112354
 N    2.898098    1.513268    0.782290
 C   -0.595842   -0.208811   -1.932268
 C    0.788075   -0.218457   -2.353313
Na    4.268120   -0.465351   -2.397868
 H    4.983480    1.724370    0.479716
 H    4.370146   -0.097361    2.815093
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H   -1.025438    0.791294   -1.801567
C    1.456659    1.021629   -2.763280
C    1.517247   -1.458190   -2.665376
O    0.618515    2.043074   -2.967068
O    2.663564    1.166046   -2.903530
O    2.439373   -1.556150   -3.454951
O    1.096742   -2.519660   -1.962642
C    1.865803   -3.711372   -2.099515
H    1.753976   -4.132987   -3.108593
H    1.465923   -4.410566   -1.356156
H    2.923731   -3.483451   -1.900125
C    1.210818    3.285874   -3.312708
H    1.968035    3.578566   -2.573521
H    0.398423    4.020449   -3.325339
H    1.678346    3.224829   -4.305918
C    3.096901   -2.056456    0.956762
H    2.230216   -2.181265    0.292914
C    2.808210   -2.782260    2.251567
C    3.728374   -2.830213    3.308315
C    1.608103   -3.490338    2.389270
C    3.439467   -3.536406    4.476142
H    4.691162   -2.322741    3.221039
C    1.315123   -4.199087    3.553300
H    0.888633   -3.485314    1.567201
C    2.229891   -4.219074    4.605627
H    4.169322   -3.557185    5.288648
H    0.367412   -4.735964    3.637461
H    2.004487   -4.769110    5.521962
C    4.322989   -2.627124    0.183068
H    4.080963   -3.721482    0.082922
H    5.185702   -2.620875    0.907466
O    4.551927   -1.985831   -0.965970
C   -0.533129   -0.456412    1.461914
H   -0.218473    0.407057    2.059849
H    0.018742   -1.370430    1.719070
C   -1.925725   -0.576233    1.221886
C   -2.512838   -1.733164    0.707555
H   -3.599097   -1.807052    0.783541
C   -1.757656   -3.020273    0.578357
H   -0.792480   -2.862208    0.068157
H   -1.539218   -3.450206    1.571651
H   -2.329079   -3.767834    0.008907
C   -1.521372   -1.268946   -1.969677
H   -1.172815   -2.243416   -2.313080
C   -2.804057   -1.149587   -1.455148
H   -3.144829   -0.146097   -1.187618
C   -3.906525   -2.090326   -1.749986
C   -5.213406   -1.744152   -1.365112
C   -3.713002   -3.322893   -2.392925
C   -6.286530   -2.594472   -1.616210
H   -5.371417   -0.798110   -0.839972
C   -4.786721   -4.176505   -2.640944
H   -2.713077   -3.622259   -2.712764
C   -6.078686   -3.817774   -2.255984
H   -7.293150   -2.302503   -1.307490
H   -4.611607   -5.130576   -3.143590
H   -6.918343   -4.487595   -2.454080
C   -1.163185    4.001947   -0.515322
H   -1.695607    3.304278    0.145583
H   -1.601613    5.003581   -0.401897
H   -1.338362    3.673694   -1.553215
C    3.330787    6.320678   -0.304470
H    2.835297    7.077721   -0.927913
H    3.523793    6.776252    0.680089
H    4.306660    6.088212   -0.754597
H    4.149475    3.836610    0.364425
H    0.269646    1.942029    0.398126
B   -2.889705    0.622074    1.481092
O   -4.230491    0.562671    1.190817
O   -2.540142    1.821344    2.050749
C   -4.801431    1.858961    1.438530
C   -3.763530    2.482392    2.439374
C   -3.598047    3.989043    2.330690
H   -3.298117    4.302275    1.324690
H   -4.543623    4.491023    2.584019
H   -2.829410    4.330054    3.038811
C   -4.032216    2.093837    3.893757
H   -4.175569    1.008577    4.000326
H   -3.165506    2.384104    4.504504
H   -4.921205    2.604106    4.289768
C   -6.202586    1.686312    2.003968
H   -6.863731    1.258297    1.236703
H   -6.207425    1.013713    2.870850
H   -6.619083    2.658098    2.308140
C   -4.858421    2.589291    0.097454
H   -5.341696    3.571813    0.193112
H   -3.853177    2.732150   -0.324720
H   -5.442253    1.985642   -0.612228
108
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Figure_S15-7_AA-9d(Na)-ts(1,6minor)_O5 / electronic energy: -4131.83763873 a.u. / lowest freq: -403.75 cm-1

C	-2.283685	-2.324647	1.205320
H	-3.889046	-0.791990	1.120698
C	-2.807317	-0.928909	1.072594
H	-2.996696	-3.066744	0.817918
H	-7.616654	-1.031149	-1.090547
H	-5.486616	0.212287	-0.792428
C	-6.663749	-1.534874	-1.269050
C	-5.471583	-0.832774	-1.113463
H	-7.577300	-3.430307	-1.771957
C	-6.643145	-2.877953	-1.648954
C	-4.229956	-1.451316	-1.338409
C	-5.417547	-3.507098	-1.869685
C	-2.995057	-0.657213	-1.157339
H	-3.183075	0.413517	-1.057217
C	-4.224485	-2.802968	-1.717429
H	-5.388257	-4.558412	-2.165759
H	-3.278068	-3.315849	-1.898937
C	-1.751723	-1.050645	-1.634401
H	-1.579860	-2.102170	-1.852993
C	-2.016819	0.182177	1.379124
H	-0.889794	0.898920	-1.668342
C	-0.656692	-0.170477	-1.723187
H	-0.272060	-0.856350	2.106508
C	-0.631691	0.076970	1.651286
H	-0.150830	0.969062	2.070348
Cu	0.573075	-0.191479	-0.034866
C	2.421102	-0.331264	0.706579
N	3.416821	0.573339	0.859586
H	0.950840	-2.474470	5.407811
N	2.890236	-1.524983	1.040042
C	1.113220	-1.809985	-2.609621
O	0.426420	-2.817157	-2.059830
C	0.691801	-0.471556	-2.161350
O	2.845069	0.472093	-2.626523
C	1.640376	0.608811	-2.461097
C	2.148961	-2.764049	0.859716
C	4.279808	-1.501137	1.503768
H	4.866444	-2.245940	0.954308
C	4.698593	-0.070978	1.170710
H	5.202030	0.440437	2.002388
C	3.334206	1.957569	0.613876
C	4.493810	2.674159	0.293441
C	2.117177	2.638342	0.723409
C	4.445461	4.054538	0.074163
C	2.051406	4.015545	0.510619
C	3.219648	4.713184	0.188869
H	3.171452	5.793767	0.024760
Na	3.960593	-1.626375	-2.156138
H	5.363756	-0.037718	0.291941
H	4.332675	-1.719720	2.581954
O	1.075924	1.823327	-2.495603
O	2.006494	-2.032350	-3.409640
C	0.854433	-4.134356	-2.394754
H	0.713915	-4.327159	-3.467541
H	0.221384	-4.808631	-1.806864
H	1.915089	-4.246862	-2.123996
C	1.939536	2.925737	-2.726307
H	2.789415	2.913986	-2.031552
H	1.336385	3.825637	-2.563894
H	2.316939	2.908085	-3.759176
H	1.385559	-2.548407	0.096042
C	1.436550	-3.227587	2.111372
C	0.588852	-4.342212	2.036221
C	1.550276	-2.566494	3.338893
C	-0.111862	-4.788170	3.153967
H	0.457405	-4.854490	1.080015
C	0.848753	-3.009916	4.461124
H	2.174671	-1.674647	3.420426
C	0.016881	-4.124466	4.375075
H	-0.773143	-5.653551	3.068647
H	-0.535167	-4.470030	5.251804
C	3.098824	-3.818946	0.206928
H	2.451887	-4.718919	0.038497
H	3.797395	-4.150663	1.026399
O	3.699045	-3.344787	-0.892728
H	-1.329253	-2.441836	0.663753
H	-2.070638	-2.574068	2.259717
C	0.738446	4.738105	0.634950
H	-0.070871	4.046273	0.901299
H	0.791215	5.523462	1.404875
H	0.473355	5.234155	-0.312472
C	5.692738	4.822057	-0.281281
H	5.579785	5.325113	-1.253681
H	5.899843	5.603000	0.466279
H	6.571202	4.164851	-0.338582
H	5.452778	2.163316	0.201581
H	1.210861	2.094963	0.987573
B	-2.713592	1.567057	1.208291

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 O   -4.057567    1.675495    0.953140
 O   -2.091612    2.790341    1.206422
 C   -4.408167    3.068388    0.967376
 C   -3.025999    3.751977    0.668778
 C   -2.733295    3.865927   -0.827459
 H   -2.902076    2.909260   -1.343699
 H   -3.360835    4.632735   -1.302616
 H   -1.679687    4.142631   -0.967934
 C   -2.836140    5.097626    1.350665
 H   -3.644016    5.785731    1.060708
 H   -2.834341    4.998367    2.443430
 H   -1.883492    5.550241    1.045050
 C   -4.944975    3.384280    2.363004
 H   -5.783716    2.708084    2.581153
 H   -4.174492    3.230442    3.132575
 H   -5.307813    4.419340    2.432388
 C   -5.480745    3.320479   -0.081096
 H   -5.683893    4.397523   -0.176569
 H   -5.184458    2.931011   -1.063531
 H   -6.414829    2.822135    0.215679
108
Figure_S15-7_AA-9d(Na)-ts(1,6minor)_O6 / electronic energy: -4131.83545844 a.u. / lowest freq: -358.72 cm-1
 C    0.509621   -4.449655    1.410307
 H    0.463506   -5.212815    0.618909
 C    1.935013   -3.952827    1.667958
 H    2.142862   -3.797282    2.739827
 C    0.697772   -2.260007    0.638092
 C    3.090380   -1.826570    0.954328
 C    4.046353   -1.985337   -0.048944
 C    3.268745   -0.875006    1.954648
 C    5.185814   -1.177237   -0.067496
 C    4.386755   -0.034960    1.944707
 C    5.330633   -0.201892    0.927959
 H    6.210106    0.448895    0.908450
Cu    0.030549   -0.541893   -0.091216
 N   -0.155578   -3.233997    0.930370
 N    1.936281   -2.660552    0.970261
 C   -0.650377    0.690657   -1.617106
 C   -0.168443   -0.540775   -2.208373
Na    0.630708   -3.856533   -2.406017
 H    2.706087   -4.622515    1.262958
 H    0.024565   -4.846115    2.312773
 H    0.090965    1.493668   -1.590271
 C    1.259662   -0.667358   -2.547712
 C   -1.041068   -1.563900   -2.802521
 O    1.908036    0.506367   -2.533381
 O    1.847098   -1.710746   -2.787951
 O   -0.692098   -2.373294   -3.646670
 O   -2.298877   -1.549522   -2.352211
 C   -3.150928   -2.581466   -2.842135
 H   -3.306266   -2.474675   -3.924771
 H   -4.103997   -2.456391   -2.315960
 H   -2.695979   -3.558289   -2.619177
 C    3.310629    0.490547   -2.741134
 H    3.822352    0.071178   -1.864818
 H    3.607031    1.536180   -2.882580
 H    3.571277   -0.096898   -3.631646
 C   -1.548985   -3.207703    0.519711
 H   -1.627195   -2.401400   -0.225199
 C   -2.495789   -2.865397    1.649011
 C   -3.843649   -2.617540    1.350577
 C   -2.076716   -2.726287    2.976183
 C   -4.746462   -2.257226    2.347931
 H   -4.186033   -2.690066    0.315263
 C   -2.978392   -2.364471    3.978641
 H   -1.025379   -2.877166    3.229027
 C   -4.317330   -2.131436    3.670372
 H   -5.790368   -2.063397    2.090828
 H   -2.626464   -2.255893    5.007268
 H   -5.022080   -1.842644    4.453090
 C   -1.864747   -4.509929   -0.278283
 H   -2.948282   -4.422101   -0.554683
 H   -1.856353   -5.346917    0.475620
 O   -1.029146   -4.669463   -1.314681
 C   -0.097941    0.529920    1.680131
 H    0.960603    0.388195    1.919020
 H   -0.771401   -0.137313    2.234449
 C   -0.498312    1.867839    1.439742
 C   -1.833779    2.261049    1.418548
 H   -2.041772    3.333928    1.418235
 C   -2.921086    1.343214    1.894104
 H   -2.913152    0.395059    1.326914
 H   -2.782666    1.071921    2.955617
 H   -3.916003    1.796081    1.788308
 C   -1.973179    1.087877   -1.329630
 H   -2.771527    0.355518   -1.430601
 C   -2.248235    2.360262   -0.850858
 H   -1.455799    3.108523   -0.918867
 C   -3.610547    2.920782   -0.762911
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 C   -3.767140    4.306680   -0.593880
 C   -4.770755    2.131245   -0.827212
 C   -5.030302    4.884204   -0.492783
 H   -2.874424    4.936069   -0.536330
 C   -6.034832    2.707211   -0.726258
 H   -4.687555    1.049539   -0.948506
 C   -6.173177    4.085931   -0.557869
 H   -5.124186    5.964652   -0.361026
 H   -6.922188    2.071671   -0.776956
 H   -7.165254    4.535458   -0.476786
 C    4.533962    1.027491    2.999643
 H    4.467995    0.595449    4.009440
 H    5.493788    1.555522    2.913763
 H    3.720519    1.762357    2.899665
 C    6.237036   -1.354289   -1.132258
 H    6.723794   -0.399785   -1.378257
 H    7.023527   -2.046318   -0.790731
 H    5.807727   -1.772846   -2.053599
 H    3.881553   -2.730594   -0.829750
 H    2.519260   -0.785404    2.744091
 B    0.612796    2.867147    0.997111
 O    0.374932    4.033266    0.314384
 O    1.953732    2.640419    1.177097
 C    1.630829    4.494736   -0.218545
 C    2.668187    3.813990    0.748505
 C    3.968791    3.386078    0.085668
 H    3.794291    2.625528   -0.684886
 H    4.472118    4.250059   -0.373164
 H    4.646057    2.954794    0.835981
 C    2.959132    4.652033    1.992611
 H    2.029949    4.969363    2.487691
 H    3.538655    4.049704    2.706212
 H    3.546562    5.547146    1.743907
 C    1.647194    6.014788   -0.209723
 H    0.899503    6.395890   -0.920117
 H    1.410685    6.418091    0.782946
 H    2.633460    6.392380   -0.517968
 C    1.728335    3.973339   -1.651894
 H    2.627593    4.353906   -2.156596
 H    1.752615    2.874558   -1.682727
 H    0.847268    4.310553   -2.216644
108
Figure_S15-7_AA-9d(Na)-ts(1,6minor)_07 / electronic energy: -4131.83586301 a.u. / lowest freq: -394.32 cm-1
 C    3.849090   -1.863501    1.902265
 H    4.454371   -2.620380    1.389282
 C    4.420245   -0.453928    1.730176
 H    4.695513    0.021125    2.682551
 C    2.273406   -0.541608    0.796026
 C    3.413226    1.636784    0.764918
 C    4.664562    2.266255    0.782370
 C    2.282764    2.381789    0.417538
 C    4.791583    3.614352    0.432120
 C    2.391153    3.720591    0.042975
 C    3.650859    4.328024    0.054195
 H    3.744379    5.379723   -0.230856
Cu    0.538022   -0.195418   -0.112190
 N    2.542940   -1.756407    1.248634
 N    3.313211    0.271027    1.094740
 C   -0.686484   -0.028294   -1.787324
 C    0.661257   -0.330412   -2.223808
Na    3.879519   -1.726944   -1.938699
 H    5.307366   -0.449869    1.077965
 H    3.735130   -2.151949    2.957630
 H   -0.897860    1.046849   -1.743501
 C    1.514314    0.839682   -2.518843
 C    1.100775   -1.650390   -2.687892
 O    2.838628    0.569291   -2.519022
 O    1.108438    1.970845   -2.684495
 O    2.073207   -1.863451   -3.397797
 O    0.338469   -2.662842   -2.261890
 C    0.771650   -3.974959   -2.611468
 H    0.758730   -4.110724   -3.701926
 H    0.054729   -4.657767   -2.141453
 H    1.787982   -4.133531   -2.218967
 C    3.711421    1.651854   -2.811309
 H    3.460863    2.106251   -3.779704
 H    4.720055    1.223853   -2.851774
 H    3.659689    2.419269   -2.026827
 C    1.754022   -2.928879    0.901336
 H    1.072901   -2.600027    0.099525
 C    0.909392   -3.447515    2.044765
 C    0.065961   -4.546460    1.826274
 C    0.887762   -2.839815    3.304444
 C   -0.762474   -5.027995    2.836573
 H    0.038924   -5.018969    0.841825
 C    0.058203   -3.319218    4.319446
 H    1.506244   -1.960165    3.492729
 C   -0.768723   -4.416994    4.091326
 H   -1.417040   -5.879980    2.638908
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 H    0.054762   -2.822832    5.292487
 H   -1.422941   -4.789271    4.882668
 C    2.699653   -3.979252    0.233748
 H    2.023095   -4.814153   -0.082470
 H    3.299996   -4.431966    1.071819
 O    3.424334   -3.443344   -0.758126
 C   -0.620723    0.198068    1.586308
 H   -0.054859    1.052872    1.976750
 H   -0.356172   -0.752207    2.067699
 C   -1.989928    0.425094    1.304945
 C   -2.875326   -0.620609    1.036749
 H   -3.941109   -0.386042    1.061968
 C   -2.477074   -2.050999    1.226836
 H   -1.551571   -2.276500    0.668838
 H   -2.254688   -2.273679    2.285658
 H   -3.260827   -2.744617    0.891003
 C   -1.799293   -0.885380   -1.677495
 H   -1.652834   -1.944797   -1.876569
 C   -3.031450   -0.439274   -1.218943
 H   -3.183767    0.639328   -1.147084
 C   -4.288946   -1.201474   -1.370037
 C   -5.510788   -0.539961   -1.159245
 C   -4.326733   -2.564314   -1.705543
 C   -6.724565   -1.210016   -1.285265
 H   -5.493490    0.515851   -0.874957
 C   -5.541145   -3.236559   -1.828912
 H   -3.397023   -3.111052   -1.873971
 C   -6.746307   -2.564595   -1.621561
 H   -7.660996   -0.672891   -1.117419
 H   -5.545366   -4.297431   -2.090429
 H   -7.696969   -3.092906   -1.721443
 C    1.159813    4.458817   -0.399582
 H    0.280869    4.121532    0.165889
 H    1.267396    5.545972   -0.279312
 H    0.964921    4.240459   -1.461412
 C    6.137423    4.289560    0.488830
 H    6.225619    5.071094   -0.279050
 H    6.287284    4.772674    1.467865
 H    6.956454    3.570360    0.347261
 H    5.561110    1.713224    1.064890
 H    1.294803    1.922615    0.431670
 B   -2.557500    1.868070    1.140753
 O   -3.878106    2.102462    0.846163
 O   -1.838931    3.033463    1.242040
 C   -4.018373    3.494675    0.519685
 C   -2.784608    4.125125    1.257921
 C   -2.192096    5.340127    0.563772
 H   -1.832972    5.101779   -0.444966
 H   -2.948723    6.135389    0.487299
 H   -1.345643    5.731325    1.145757
 C   -3.067844    4.445413    2.725420
 H   -3.527278    3.589245    3.240737
 H   -2.118014    4.677030    3.227859
 H   -3.734598    5.313310    2.825964
 C   -5.371859    3.989390    1.003759
 H   -6.172517    3.495495    0.434417
 H   -5.526410    3.770255    2.067686
 H   -5.464325    5.074756    0.849724
 C   -3.923901    3.610421   -1.001989
 H   -4.088899    4.642805   -1.340790
 H   -2.942628    3.275042   -1.369785
 H   -4.694266    2.971922   -1.457870
76
Figure_S15-8_9b(Na)-Cu-allyl_01 / electronic energy: -3289.86902565 a.u. / lowest freq: 17.54 cm-1
 C   -2.892697    1.596089    1.460941
 H   -2.743197    1.250407    2.497136
 C   -1.975473    2.766074    1.108473
 H   -2.463374    3.496160    0.440338
 C   -1.249374    0.839069    0.001489
 C    0.301145    2.736026   -0.016190
 C    1.264409    3.038492    0.964267
 C    0.499150    3.065316   -1.370203
 C    2.449274    3.661177    0.561084
 C    1.705816    3.672713   -1.732198
 C    2.674483    3.968356   -0.777657
 H    3.610370    4.443824   -1.078925
Cu   -0.251244   -0.335231   -1.174432
 N   -2.441060    0.564339    0.526560
 N   -0.895934    2.082234    0.388527
 H   -1.606803    3.302977    1.991271
 H   -3.958000    1.822171    1.319187
 C   -3.044007   -0.760576    0.519412
 H   -2.554189   -1.289301   -0.315468
 C   -4.525217   -0.639770    0.199869
 C   -5.531197   -1.041691    1.083724
 C   -4.902867   -0.081480   -1.029569
 C   -6.878729   -0.890279    0.747507
 H   -5.271410   -1.477151    2.049741
 C   -6.244395    0.073098   -1.368072
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 H   -4.124350    0.241321   -1.727003
 C   -7.240224   -0.331892   -0.476378
 H   -7.649523   -1.209649    1.452726
 H   -6.515806    0.510614   -2.331627
 H   -8.294305   -0.210547   -0.735919
 C   -2.663657   -1.551289    1.799213
 H   -3.213957   -2.525298    1.696342
 H   -3.180113   -1.041428    2.659897
 O   -1.336986   -1.673655    1.957204
 C    0.761487   -1.541323   -2.354457
 H    1.475351   -0.912042   -2.911363
 H    0.108200   -2.075043   -3.064880
 C    1.441426   -2.424103   -1.385089
 C    0.988711   -3.644270   -0.986354
 H    1.556486   -4.204231   -0.232322
 C   -0.265528   -4.273060   -1.519961
 H   -0.471331   -5.246949   -1.053546
 H   -1.139388   -3.618105   -1.339556
 H   -0.221274   -4.425144   -2.613314
 B    2.674857   -1.814147   -0.650999
 O    3.578781   -0.949566   -1.188422
 O    2.893022   -2.014555    0.702220
 C    4.592362   -0.671470   -0.204792
 C    3.868051   -1.044195    1.142553
 C    4.996463    0.790230   -0.319960
 C    5.781401   -1.578686   -0.516488
 C    4.764620   -1.674238    2.195354
 C    3.081412    0.121336    1.736282
 H    5.219611   -2.605750    1.836445
 H    4.178808   -1.903760    3.097250
 H    5.566555   -0.977538    2.480470
 H    5.509876   -2.641027   -0.432057
 H    6.626269   -1.378286    0.157165
 H    6.109124   -1.392230   -1.548824
 H    2.392039    0.553077    0.995092
 H    3.746843    0.918937    2.094387
 H    2.489884   -0.230057    2.595248
 H    4.125398    1.455965   -0.267177
 H    5.494789    0.958336   -1.285293
 H    5.701406    1.061643    0.480029
Na    0.603802   -2.265300    1.509716
 H    1.879983    3.924594   -2.781112
 H    3.211577    3.891914    1.309483
 C   -0.547128    2.775810   -2.413076
 H   -0.507148    1.718738   -2.725077
 H   -1.561952    2.956715   -2.031076
 H   -0.390961    3.397087   -3.304993
 C    1.037472    2.696278    2.412516
 H    0.431839    3.466996    2.916158
 H    0.508160    1.738685    2.519469
 H    1.991775    2.629837    2.951304
108
Figure_S15-8_AA-9b(Na)-ts(1,6major)_01 / electronic energy: -4131.83854441 a.u. / lowest freq: -314.01 cm-1
 C    4.409202   -0.678859   -1.598345
 H    5.207548   -1.054404   -0.941860
 C    3.706139   -1.798193   -2.378042
 H    3.596282   -1.568039   -3.449415
 C    2.223515   -0.871689   -0.812396
 C    1.434987   -2.867925   -1.971666
 C    1.347184   -3.924553   -1.046921
 C    0.621524   -2.813495   -3.113970
 C    0.355907   -4.889661   -1.235793
 C   -0.350795   -3.807478   -3.275246
 C   -0.497135   -4.823552   -2.336606
 H   -1.271345   -5.582115   -2.471515
Cu    0.496181   -0.459771    0.096214
 N    3.333055   -0.149647   -0.757910
 N    2.394188   -1.846363   -1.725962
 C   -0.926695   -0.354216    1.585449
 C    0.319930   -0.747922    2.224491
Na    3.736675   -1.410196    3.015045
 H    4.220373   -2.766437   -2.290448
 H    4.816547    0.103718   -2.254261
 H   -1.153101    0.711394    1.678048
 C    0.654958   -2.121833    2.619202
 C    1.157029    0.309056    2.806858
 O   -0.321657   -3.003783    2.381993
 O    1.707722   -2.496944    3.115524
 O    2.109282    0.160055    3.554073
 O    0.792913    1.550462    2.428543
 C    1.585552    2.615027    2.935263
 H    1.531681    2.656479    4.031831
 H    1.173512    3.531428    2.503325
 H    2.636148    2.498108    2.632803
 C   -0.108171   -4.346218    2.785163
 H    0.789218   -4.765425    2.313326
 H   -0.996803   -4.901057    2.464708
 H    0.002286   -4.412473    3.876704
 C    3.554110    0.965420    0.156830
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 H    2.742115    0.886894    0.890514
 C    3.402118    2.292883   -0.561064
 C    4.453546    2.886630   -1.271342
 C    2.157175    2.936280   -0.558273
 C    4.263440    4.086288   -1.959333
 H    5.436350    2.411024   -1.288785
 C    1.958755    4.123771   -1.259006
 H    1.320349    2.493633   -0.010863
 C    3.014766    4.706662   -1.960045
 H    5.098247    4.535450   -2.502571
 H    0.965982    4.575798   -1.265411
 H    2.863814    5.640228   -2.506772
 C    4.874971    0.758450    0.946498
 H    4.925505    1.656483    1.624995
 H    5.716095    0.938007    0.219524
 O    4.930325   -0.433057    1.556033
 C   -0.446441    0.476821   -1.530405
 H   -0.272218   -0.355557   -2.218822
 H    0.296764    1.278015   -1.622207
 C   -1.792693    0.871003   -1.322151
 C   -2.848236   -0.018189   -1.484198
 H   -3.861083    0.390666   -1.460661
 C   -2.658429   -1.367670   -2.105762
 H   -2.287646   -1.280162   -3.142345
 H   -1.900389   -1.953703   -1.557194
 H   -3.591840   -1.945689   -2.128204
 C   -2.009583   -1.159127    1.163043
 H   -1.875852   -2.237122    1.121905
 C   -3.208743   -0.599180    0.759351
 H   -3.373906    0.460289    0.963227
 C   -4.441509   -1.376310    0.533011
 C   -5.667315   -0.694506    0.451684
 C   -4.454014   -2.773184    0.382699
 C   -6.860582   -1.377878    0.232453
 H   -5.673321    0.393835    0.558437
 C   -5.646781   -3.457753    0.162519
 H   -3.519068   -3.335233    0.426778
 C   -6.856599   -2.765797    0.086217
 H   -7.800575   -0.824145    0.174457
 H   -5.630839   -4.544012    0.046024
 H   -7.790818   -3.304488   -0.086565
 B   -2.128721    2.290733   -0.774518
 O   -3.293047    2.563854   -0.101912
 O   -1.330156    3.398645   -0.892786
 C   -3.397117    3.988156    0.060249
 C   -1.898486    4.448267   -0.084685
 C   -1.720120    5.784224   -0.790331
 H   -2.097458    5.750960   -1.819982
 H   -2.250998    6.579176   -0.245895
 H   -0.655135    6.054910   -0.824320
 C   -1.135774    4.445992    1.237735
 H   -1.227012    3.476967    1.750165
 H   -0.070979    4.621263    1.026726
 H   -1.486740    5.238808    1.912808
 C   -4.025296    4.286900    1.412530
 H   -5.066480    3.933666    1.423106
 H   -3.487559    3.785641    2.227322
 H   -4.030070    5.369807    1.606196
 C   -4.295604    4.500327   -1.065041
 H   -4.477524    5.580422   -0.976214
 H   -3.855182    4.298549   -2.052234
 H   -5.263025    3.981206   -1.010802
 H    0.262632   -5.709887   -0.519615
 H   -1.010160   -3.771735   -4.146018
 C    0.800958   -1.744126   -4.158673
 H   -0.153909   -1.505369   -4.646711
 H    1.213103   -0.819367   -3.733760
 H    1.495772   -2.086658   -4.942798
 C    2.334580   -4.022077    0.084239
 H    3.366807   -3.937008   -0.287161
 H    2.203278   -3.220744    0.824604
 H    2.242445   -4.986516    0.600994
108
Figure_S15-8_AA-9b(Na)-ts(1,6major)_O2 / electronic energy: -4131.83936333 a.u. / lowest freq: -320.04 cm-1
 C   -4.384148    0.925591   -1.426463
 H   -5.108023    1.069669   -0.610092
 C   -3.723185    2.233133   -1.872185
 H   -3.580764    2.284311   -2.964276
 C   -2.178475    0.932736   -0.691215
 C   -1.488250    3.224923   -1.138929
 C   -1.507010    4.063837   -0.012248
 C   -0.580067    3.413197   -2.192179
 C   -0.531790    5.060340    0.085064
 C    0.381971    4.419966   -2.058296
 C    0.415741    5.226155   -0.923327
 H    1.179577    6.001523   -0.830625
Cu   -0.488478    0.280449    0.088387
 N   -3.246410    0.170679   -0.891501
 N   -2.425097    2.154434   -1.194757
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C	0.986602	0.077809	1.482336
C	-0.232197	0.254016	2.250858
Na	-3.645517	0.486967	3.101499
H	-4.282241	3.126098	-1.559682
H	-4.870152	0.388377	-2.252582
H	1.368544	-0.944572	1.459585
C	-0.619621	1.492944	2.925277
C	-0.997431	-0.950546	2.590790
O	0.335489	2.428736	2.915233
O	-1.694550	1.709722	3.469453
O	-1.914254	-1.049593	3.391276
O	-0.599942	-2.014087	1.873643
C	-1.302385	-3.229710	2.045038
H	-1.131286	-3.648768	3.047771
H	-0.909280	-3.905389	1.277707
H	-2.383103	-3.079405	1.906909
C	0.066009	3.651297	3.578966
H	-0.845745	4.121740	3.190054
H	0.931478	4.295430	3.388761
H	-0.052258	3.490477	4.659992
C	-3.401398	-1.170475	-0.359447
H	-2.555276	-1.313897	0.330489
C	-3.308769	-2.231950	-1.439127
C	-3.463364	-3.585466	-1.104590
C	-3.034238	-1.912767	-2.774279
C	-3.359120	-4.582118	-2.072839
H	-3.657369	-3.868008	-0.067919
C	-2.930650	-2.907652	-3.746645
H	-2.877473	-0.869739	-3.055996
C	-3.095797	-4.247774	-3.401616
H	-3.481879	-5.629127	-1.786052
H	-2.713485	-2.631750	-4.781221
H	-3.012994	-5.028038	-4.161364
C	-4.694678	-1.225811	0.519359
H	-4.710757	-2.263346	0.946169
H	-5.551446	-1.231701	-0.214261
O	-4.740740	-0.244423	1.428533
C	0.315133	-0.932404	-1.449531
H	-0.046179	-0.309802	-2.275792
H	-0.343641	-1.780470	-1.219559
C	1.709748	-1.141648	-1.339026
C	2.633925	-0.185590	-1.748966
H	3.688203	-0.472378	-1.764331
C	2.230359	1.021418	-2.532678
H	1.764187	0.735236	-3.491402
H	1.476749	1.604232	-1.975008
H	3.081199	1.680174	-2.750138
C	1.822632	1.076569	0.937628
H	1.468837	2.108618	0.940506
C	3.057790	0.781400	0.372489
H	3.521146	-0.175325	0.620927
C	3.991422	1.819142	-0.095976
C	5.339170	1.489158	-0.314346
C	3.582809	3.135667	-0.369695
C	6.246544	2.436268	-0.782695
H	5.673791	0.466725	-0.117319
C	4.489096	4.083085	-0.837337
H	2.537808	3.423095	-0.238669
C	5.826198	3.740753	-1.046968
H	7.289764	2.154778	-0.943738
H	4.144688	5.099104	-1.045456
H	6.535721	4.484857	-1.415418
B	2.275611	-2.383120	-0.584036
O	3.621868	-2.630103	-0.470256
O	1.522744	-3.323613	0.066469
C	3.780640	-3.941632	0.101637
C	2.416221	-4.129006	0.858536
C	1.898713	-5.557804	0.898657
H	1.708992	-5.947496	-0.109267
H	2.623155	-6.215782	1.401132
H	0.956331	-5.597090	1.463812
C	2.442919	-3.537480	2.267581
H	2.853706	-2.517298	2.266487
H	1.418831	-3.485972	2.658697
H	3.048823	-4.153390	2.946848
C	5.014014	-3.951862	0.990841
H	5.915371	-3.816628	0.376004
H	4.985926	-3.145906	1.734663
H	5.101762	-4.914112	1.516863
C	3.957281	-4.923359	-1.056361
H	4.145791	-5.943091	-0.692144
H	3.069000	-4.941992	-1.704771
H	4.816967	-4.608007	-1.664760
H	-0.520748	5.718046	0.957693
H	1.117136	4.566155	-2.853417
C	-0.664418	2.577157	-3.440213
H	-0.825516	1.515259	-3.206767
H	-1.507537	2.905090	-4.069131
H	0.250747	2.666566	-4.038828

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 C   -2.572361    3.894942    1.036473
 H   -3.575605    3.900857    0.585415
 H   -2.468517    2.941904    1.573819
 H   -2.532339    4.708508    1.773039
108
Figure_S15-8_AA-9b(Na)-ts(1,6major)_03 / electronic energy: -4131.83794438 a.u. / lowest freq: -314.88 cm-1
 C   -4.215782    1.137409   -1.426545
 H   -4.915974    1.603441   -0.718041
 C   -3.478640    2.164664   -2.291629
 H   -3.411792    1.862586   -3.349211
 C   -1.985381    1.208665   -0.755272
 C   -1.131206    3.104594   -2.037974
 C   -0.927958    4.215150   -1.200030
 C   -0.376973    2.907354   -3.205752
 C    0.115757    5.092113   -1.504209
 C    0.658966    3.808780   -3.476429
 C    0.914699    4.880542   -2.626701
 H    1.731626    5.569891   -2.851051
Cu   -0.267319    0.642284    0.091222
 N   -3.125947    0.538347   -0.650770
 N   -2.146828    2.175121   -1.677698
 C    1.124730    0.241412    1.570578
 C   -0.009550    0.901729    2.201732
Na   -3.211863    2.208457    3.032440
 H   -3.935864    3.163657   -2.252185
 H   -4.743817    0.376225   -2.018294
 H    1.075100   -0.849088    1.633638
 C   -0.097683    2.346060    2.433837
 C   -0.978071    0.061546    2.921102
 O    0.938319    3.027670    1.925519
 O   -1.005287    2.942372    2.996442
 O   -1.862527    0.441835    3.669111
 O   -0.820319   -1.254662    2.687799
 C   -1.737407   -2.122706    3.335139
 H   -1.662396   -2.027021    4.426949
 H   -1.468367   -3.137616    3.025413
 H   -2.769036   -1.898054    3.028666
 C    0.992456    4.424151    2.164818
 H    0.086141    4.925998    1.805373
 H    1.867212    4.790042    1.616122
 H    1.110821    4.628375    3.238486
 C   -3.394206   -0.497998    0.326725
 H   -2.501791   -0.528421    0.969431
 C   -3.541656   -1.864705   -0.322361
 C   -4.093289   -2.940744    0.388995
 C   -3.094853   -2.103150   -1.627883
 C   -4.194172   -4.206788   -0.185829
 H   -4.447650   -2.793857    1.410526
 C   -3.192053   -3.368329   -2.205472
 H   -2.653637   -1.285953   -2.201690
 C   -3.743972   -4.427529   -1.487412
 H   -4.627163   -5.027868    0.390181
 H   -2.823993   -3.526610   -3.221631
 H   -3.821825   -5.419443   -1.938140
 C   -4.597090   -0.053288    1.227531
 H   -4.638796   -0.816503    2.050029
 H   -5.521085   -0.274332    0.618503
 O   -4.493017    1.212152    1.648893
 C    0.547448   -0.220345   -1.624098
 H    0.603702    0.722744   -2.177086
 H   -0.345639   -0.815649   -1.849100
 C    1.750116   -0.950159   -1.444453
 C    2.998588   -0.344875   -1.479786
 H    3.877541   -0.994342   -1.492876
 C    3.175405    1.069957   -1.944696
 H    2.869611    1.187134   -2.999443
 H    2.542400    1.758422   -1.357368
 H    4.218489    1.402331   -1.855663
 C    2.404832    0.739943    1.239259
 H    2.579980    1.811962    1.281019
 C    3.409029   -0.111510    0.814814
 H    3.243944   -1.185891    0.918488
 C    4.826289    0.281060    0.698703
 C    5.800182   -0.722953    0.565747
 C    5.257046    1.618233    0.709859
 C    7.151631   -0.407489    0.450241
 H    5.480581   -1.768747    0.547803
 C    6.608303    1.935278    0.593236
 H    4.527782    2.425014    0.804602
 C    7.563432    0.925926    0.462846
 H    7.889091   -1.207253    0.349700
 H    6.918783    2.982832    0.603845
 H    8.622401    1.176683    0.370481
 B    1.611398   -2.446929   -1.037862
 O    2.507429   -3.117139   -0.244850
 O    0.531803   -3.219028   -1.370913
 C    2.079657   -4.490583   -0.155087
 C    0.554787   -4.385944   -0.529953
 C    0.004333   -5.575673   -1.298770
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 H    0.520665   -5.714206   -2.257194
 H    0.106993   -6.497585   -0.706964
 H   -1.063684   -5.415330   -1.502312
 C   -0.336522   -4.069980    0.669084
 H    0.046131   -3.201385    1.224618
 H   -1.344127   -3.819848    0.306969
 H   -0.414067   -4.925500    1.355363
 C    2.351685   -5.000661    1.251230
 H    3.435926   -5.061747    1.423523
 H    1.922413   -4.333682    2.009699
 H    1.927261   -6.006793    1.385527
 C    2.894518   -5.282785   -1.175692
 H    2.672912   -6.357851   -1.119827
 H    2.697448   -4.936613   -2.200722
 H    3.964300   -5.138631   -0.967207
 H    0.296767    5.955866   -0.859565
 H    1.272269    3.661634   -4.368835
 C   -0.685138    1.789849   -4.167066
 H    0.224674    1.449078   -4.680034
 H   -1.137777    0.926328   -3.662755
 H   -1.392016    2.134011   -4.939602
 C   -1.846161    4.454140   -0.032417
 H   -2.900598    4.398902   -0.341351
 H   -1.710861    3.700445    0.756072
 H   -1.673816    5.445531    0.407669
108
Figure_S15-8_AA-9b(Na)-ts(1,6major)_O4 / electronic energy: -4131.83111422 a.u. / lowest freq: -361.44 cm-1
 C   -2.812256   -2.862913   -1.601564
 H   -3.386190   -3.384493   -0.818721
 C   -3.600262   -1.714600   -2.210705
 H   -3.340128   -1.538403   -3.268215
 C   -1.964566   -0.856600   -0.788731
 C   -3.904743    0.615220   -1.326485
 C   -5.159194    0.541330   -0.688140
 C   -3.468809    1.804400   -1.937829
 C   -5.990384    1.664566   -0.714307
 C   -4.319355    2.914485   -1.914504
 C   -5.577793    2.843871   -1.324915
 H   -6.235274    3.715828   -1.332491
Cu   -0.519816    0.289930   -0.028449
 N   -1.691407   -2.152771   -0.982388
 N   -3.133234   -0.579787   -1.401529
 C    0.531581    1.442528    1.339129
 C   -0.756815    1.107935    1.909669
Na   -3.434057   -0.926297    2.404115
 H   -4.686259   -1.849942   -2.145083
 H   -2.469360   -3.595489   -2.343390
 H    1.343765    0.779918    1.653159
 C   -1.903670    2.008736    1.733146
 C   -0.815054    0.028448    2.903912
 O   -3.092035    1.487187    2.121862
 O   -1.859378    3.115374    1.234189
 O   -1.708073   -0.146512    3.718497
 O    0.239971   -0.796850    2.871763
 C    0.166537   -1.918180    3.743975
 H    0.134318   -1.597106    4.794374
 H    1.072126   -2.504602    3.559550
 H   -0.731981   -2.504086    3.504825
 C   -4.204206    2.369089    2.076909
 H   -4.101314    3.154759    2.839565
 H   -5.089044    1.758625    2.291282
 H   -4.299880    2.832337    1.088239
 C   -0.779399   -2.881435   -0.116208
 H   -0.106128   -2.123593    0.321819
 C    0.068240   -3.871424   -0.893459
 C    0.627827   -4.994929   -0.269568
 C    0.350274   -3.667175   -2.250177
 C    1.449337   -5.874454   -0.975113
 H    0.429641   -5.189612    0.785557
 C    1.172180   -4.541570   -2.957914
 H   -0.078842   -2.801574   -2.758962
 C    1.728897   -5.650643   -2.322429
 H    1.875188   -6.741329   -0.464460
 H    1.379359   -4.353034   -4.013801
 H    2.374808   -6.336782   -2.874568
 C   -1.592754   -3.480662    1.081208
 H   -0.812969   -3.858305    1.792004
 H   -2.075469   -4.418737    0.689284
 O   -2.441531   -2.598102    1.622764
 C    0.838004    0.006940   -1.623552
 H    0.243561    0.476258   -2.415896
 H    0.746749   -1.082852   -1.597323
 C    2.139396    0.508596   -1.374670
 C    2.532100    1.806527   -1.680858
 H    3.597824    2.036458   -1.600838
 C    1.701801    2.697048   -2.557621
 H    1.526047    2.236090   -3.545525
 H    0.710207    2.874253   -2.107822
 H    2.178604    3.673196   -2.717433
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 C    0.947389    2.640020    0.717709
 H    0.195643    3.394353    0.491956
 C    2.276640    2.831674    0.371540
 H    3.007603    2.125342    0.771580
 C    2.838955    4.140184   -0.015983
 C    4.233989    4.305954   -0.027413
 C    2.043351    5.237276   -0.385168
 C    4.814499    5.517536   -0.393712
 H    4.869312    3.461159    0.253655
 C    2.622396    6.449590   -0.752687
 H    0.955851    5.143045   -0.393621
 C    4.010267    6.597715   -0.760027
 H    5.902223    5.620351   -0.392983
 H    1.981941    7.287751   -1.037540
 H    4.462242    7.549313   -1.048198
 B    3.106974   -0.427711   -0.593263
 O    4.087363    0.006523    0.261306
 O    3.033715   -1.792266   -0.653491
 C    4.852327   -1.141975    0.678083
 C    3.850697   -2.325368    0.401570
 C    4.496544   -3.616258   -0.074285
 H    5.050626   -3.469900   -1.010207
 H    5.186568   -4.008404    0.687845
 H    3.714917   -4.367665   -0.256975
 C    2.914336   -2.599918    1.575323
 H    2.424792   -1.674612    1.911360
 H    2.130270   -3.294000    1.240772
 H    3.442845   -3.053583    2.425833
 C    5.242722   -0.970185    2.137772
 H    5.948247   -0.132900    2.238563
 H    4.368060   -0.757047    2.765461
 H    5.734818   -1.878788    2.515423
 C    6.099749   -1.191778   -0.202265
 H    6.771982   -2.007723    0.098561
 H    5.837743   -1.326633   -1.261712
 H    6.642519   -0.240868   -0.103223
 H   -3.989737    3.843002   -2.386474
 H   -6.967530    1.614127   -0.227458
 C   -2.124228    1.901221   -2.597862
 H   -1.341038    2.081962   -1.844538
 H   -1.861797    0.972085   -3.122749
 H   -2.094778    2.732493   -3.314422
 C   -5.624194   -0.706924    0.017295
 H   -6.344782   -1.271916   -0.595133
 H   -4.794143   -1.388984    0.249380
 H   -6.141202   -0.448189    0.953524
108
Figure_S15-8_AA-9b(Na)-ts(1,6minor)_01 / electronic energy: -4131.83618193 a.u. / lowest freq: -326.46 cm-1
 C   -1.872866   -2.485834    1.943345
 H   -3.682318   -1.248251    1.557371
 C   -2.590814   -1.244543    1.504419
 H   -2.504522   -3.379663    1.847701
 H   -7.139356   -3.354432   -0.162828
 H   -5.508330   -1.500600   -0.404607
 C   -6.080164   -3.578616   -0.308969
 C   -5.165290   -2.538189   -0.448183
 H   -6.360964   -5.722656   -0.246685
 C   -5.645900   -4.904180   -0.354799
 C   -3.796232   -2.791738   -0.637635
 C   -4.289133   -5.172954   -0.541623
 C   -2.874373   -1.647983   -0.777482
 H   -3.370248   -0.678964   -0.860874
 C   -3.374907   -4.131158   -0.680865
 H   -3.937195   -6.206648   -0.579779
 H   -2.318287   -4.366154   -0.822215
 C   -1.578968   -1.753302   -1.251353
 H   -1.096330   -2.726140   -1.299673
 C   -1.952603   -0.012615    1.452936
 H   -1.419263    0.313860   -1.668529
 C   -0.833975   -0.608723   -1.609773
 H    0.013062   -0.620903    2.154341
 C   -0.550254    0.139212    1.595973
 H   -0.213310    1.162878    1.776427
Cu    0.538394   -0.006112   -0.169540
 C    2.296908    0.501133    0.632387
 N    2.728418    1.674274    1.131238
 H    1.521526   -2.744920    4.838770
 N    3.188913   -0.433178    0.936565
 C    1.274829   -1.685682   -2.623746
 O    0.922131   -2.809443   -1.982830
 C    0.468171   -0.516230   -2.250968
 O    1.974215    1.020360   -3.319210
 C    0.869907    0.754838   -2.864994
 C    3.102081   -1.813526    0.501731
 C    4.396154    0.103404    1.570869
 H    5.221329    0.038573    0.846562
 C    3.984469    1.545151    1.880428
 H    3.805711    1.717167    2.954421
 C    2.076330    2.932948    0.989169
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 C    2.334380    3.683683   -0.173858
 C    1.266117    3.428202    2.022814
 C    1.702140    4.919963   -0.319039
 C    0.647384    4.670689    1.836241
 C    0.853329    5.405479    0.675099
 H    0.360794    6.371927    0.546188
Na    3.926490   -0.280615   -2.810055
 H    4.721795    2.285207    1.537966
 H    4.661603   -0.468610    2.471063
 O   -0.108164    1.672802   -2.870446
 O    2.190636   -1.704440   -3.429634
 C    1.638282   -3.988206   -2.317519
 H    1.514608   -4.232343   -3.381536
 H    1.213755   -4.784699   -1.696647
 H    2.709197   -3.864794   -2.102245
 C    0.203059    2.964261   -3.366504
 H    0.849921    3.505807   -2.662245
 H   -0.752987    3.490203   -3.461819
 H    0.700222    2.901428   -4.343285
 H    2.333833   -1.829739   -0.285084
 C    2.624327   -2.739051    1.604218
 C    2.446167   -4.103657    1.334013
 C    2.284506   -2.272462    2.879543
 C    1.946249   -4.970482    2.303461
 H    2.689463   -4.493748    0.343960
 C    1.784085   -3.137463    3.853619
 H    2.391464   -1.211332    3.112471
 C    1.611209   -4.490732    3.570444
 H    1.810484   -6.028084    2.065739
 H    1.214880   -5.168436    4.329713
 C    4.440836   -2.207565   -0.201187
 H    4.289894   -3.265528   -0.544441
 H    5.198318   -2.312251    0.627751
 O    4.777240   -1.341632   -1.165210
 H   -0.956900   -2.644730    1.347521
 H   -1.551054   -2.410658    2.997038
 B   -2.733112    1.269766    1.037463
 O   -3.901094    1.270715    0.319105
 O   -2.264562    2.537078    1.267299
 C   -4.334316    2.637798    0.176316
 C   -2.996139    3.430662    0.410843
 C   -2.162765    3.591536   -0.859779
 H   -2.042431    2.632254   -1.383703
 H   -2.611021    4.317881   -1.552855
 H   -1.160024    3.945880   -0.579723
 C   -3.167293    4.773039    1.102854
 H   -3.812319    5.433583    0.504410
 H   -3.608868    4.660849    2.101368
 H   -2.187169    5.257525    1.212695
 C   -5.379538    2.892948    1.260575
 H   -6.189041    2.156641    1.155032
 H   -4.946149    2.782302    2.265236
 H   -5.812806    3.899308    1.173446
 C   -4.944626    2.820521   -1.204221
 H   -5.181214    3.879860   -1.383576
 H   -4.263954    2.474545   -1.992489
 H   -5.877992    2.244348   -1.279717
 C    1.094366    2.697262    3.328219
 H    1.341399    1.631704    3.244781
 H    1.750150    3.135731    4.097711
 H    0.059200    2.780918    3.687374
 C    3.296492    3.172175   -1.210887
 H    4.266346    2.913318   -0.759677
 H    2.912881    2.269728   -1.705397
 H    3.473029    3.928770   -1.987535
 H   -0.003765    5.060678    2.622224
 H    1.889426    5.515325   -1.216154
108
Figure_S15-8_AA-9b(Na)-ts(1,6minor)_O2 / electronic energy: -4131.83467184 a.u. / lowest freq: -367.23 cm-1
 C    3.744702   -2.198824    1.501565
 H    4.331218   -2.715679    0.725801
 C    4.231469   -0.774393    1.748637
 H    4.146530   -0.474517    2.807467
 C    2.212658   -0.709560    0.575831
 C    3.530030    1.398801    0.711775
 C    4.360046    1.765199   -0.366707
 C    3.039096    2.356338    1.615910
 C    4.644401    3.119864   -0.557932
 C    3.340496    3.703629    1.381032
 C    4.128535    4.085916    0.302520
 H    4.356215    5.141506    0.138839
Cu    0.423493   -0.257594   -0.184479
 N    2.393602   -1.963477    0.985207
 N    3.292732    0.009439    0.934214
 C   -1.029747    0.073554   -1.641941
 C    0.171884   -0.409647   -2.293452
Na    3.190713   -1.949157   -2.601875
 H    5.269693   -0.606802    1.431182
 H    3.734237   -2.816281    2.409522
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H   -1.059969    1.162210   -1.530525
C    1.184742    0.549850   -2.741702
C    0.323535   -1.785208   -2.791266
O    0.797040    1.827950   -2.623617
O    2.301140    0.269599   -3.158118
O    1.096857   -2.145207   -3.662471
O   -0.476703   -2.671457   -2.184955
C   -0.296011   -4.033147   -2.555688
H   -0.542104   -4.186112   -3.615550
H   -0.982069   -4.609987   -1.925332
H    0.747911   -4.324952   -2.372611
C    1.763035    2.828233   -2.903359
H    2.539740    2.843658   -2.125952
H    1.224234    3.782006   -2.905022
H    2.232048    2.660361   -3.882023
C    1.509131   -3.057510    0.626134
H    0.786893   -2.641637   -0.094484
C    0.717939   -3.589081    1.802350
C   -0.281792   -4.545707    1.573464
C    0.898100   -3.125608    3.109988
C   -1.066147   -5.031170    2.617253
H   -0.460642   -4.902648    0.556434
C    0.114616   -3.609105    4.158794
H    1.640164   -2.350824    3.311715
C   -0.869734   -4.565720    3.918320
H   -1.842729   -5.771427    2.411515
H    0.270388   -3.224879    5.169569
H   -1.487537   -4.940418    4.737343
C    2.318297   -4.117332   -0.185351
H    1.578697   -4.927798   -0.417850
H    3.014946   -4.605770    0.552746
O    2.914561   -3.573122   -1.254187
C   -0.545810   -0.003196    1.640476
H    0.258722    0.621489    2.030102
H   -0.506820   -1.039549    1.999909
C   -1.807081    0.628445    1.513176
C   -2.997468   -0.080121    1.389963
H   -3.928729    0.483252    1.484674
C   -3.054486   -1.561811    1.615612
H   -2.347135   -2.088795    0.951187
H   -2.762763   -1.821822    2.648629
H   -4.059981   -1.965905    1.435861
C   -2.262064   -0.580436   -1.441637
H   -2.331990   -1.642403   -1.669266
C   -3.346622    0.078692   -0.886271
H   -3.289364    1.165822   -0.801670
C   -4.725027   -0.449458   -0.895746
C   -5.789241    0.424133   -0.615996
C   -5.029807   -1.793854   -1.164259
C   -7.107636   -0.024393   -0.606079
H   -5.569379    1.472775   -0.396554
C   -6.348045   -2.244102   -1.153453
H   -4.228762   -2.503631   -1.378937
C   -7.394311   -1.363350   -0.874797
H   -7.916210    0.676509   -0.385954
H   -6.559571   -3.295208   -1.363326
H   -8.426827   -1.719529   -0.866738
B   -1.803044    2.164515    1.259070
O   -2.916762    2.932004    1.036985
O   -0.643557    2.882911    1.117438
C   -2.483014    4.184268    0.471566
C   -0.985738    4.269429    0.954135
C   -0.029313    4.891270   -0.050840
H   -0.017672    4.324720   -0.989418
H   -0.311255    5.932549   -0.266432
H    0.990706    4.884968    0.358288
C   -0.828711    4.936774    2.319279
H   -1.510125    4.496910    3.061999
H    0.202023    4.787983    2.671836
H   -1.021166    6.017379    2.263344
C   -3.381755    5.299873    0.980533
H   -4.399393    5.163300    0.587545
H   -3.437678    5.307338    2.076342
H   -3.012365    6.278127    0.638669
C   -2.612935    4.055383   -1.046541
H   -2.364693    4.997806   -1.554376
H   -1.957007    3.266249   -1.442792
H   -3.651090    3.792092   -1.295001
H    2.962180    4.458613    2.075242
H    5.281821    3.418101   -1.393996
C    2.222766    1.997085    2.827328
H    1.188215    2.347110    2.692683
H    2.195211    0.916541    3.013234
H    2.630332    2.489675    3.722001
C    4.906351    0.742752   -1.325777
H    5.130543   -0.216377   -0.839560
H    4.163427    0.558266   -2.116701
H    5.824044    1.110339   -1.804093
108
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Figure_S15-8_AA-9b(Na)-ts(1,6minor)_O3 / electronic energy: -4131.83689786 a.u. / lowest freq: -278.48 cm-1
 O    -4.345619     1.320086    -0.464245
 H    -0.319067     3.008243    -2.809453
 H    -0.434326     1.382129    -3.529179
 H     0.398212     1.600214    -1.981732
 C    -0.465758     1.944954    -2.579187
 C    -1.747182     1.697752    -1.846203
 H    -0.464119    -0.650336    -2.251076
 H    -2.523385     2.464686    -1.902631
 C    -1.189500    -0.644315    -1.433522
 C    -2.102515     0.436667    -1.387518
 H    -1.567592    -1.642404    -1.174336
 B    -3.456918     0.287291    -0.630669
 O    -3.874982    -0.859750    -0.010877
 H    -6.239483    -2.003129    -0.209873
 H    -6.117221    -0.244288    -1.717454
 H    -6.696258     1.432470    -1.571984
 C    -5.544040     0.781142     0.124980
 C    -6.521080     0.500496    -1.016073
 C    -5.982668    -1.694539     0.811397
 C    -5.008273    -0.527526     0.813676
 H    -5.532709    -2.555875     1.325971
 H    -6.908138    -1.426723     1.342494
 H    -7.486608     0.136796    -0.637103
 C    -4.483785    -0.278825     2.227277
 H    -3.911930    -1.155271     2.559149
 H    -5.305484    -0.103014     2.935603
 H    -6.484102     2.682344     0.513949
 H    -5.396436     2.149813     1.815677
 C    -6.134614     1.806931     1.079909
 H    -6.995707     1.381312     1.616144
 C     4.148988    -1.712769    -1.288264
 H     4.756013    -2.192471    -0.506693
 C     3.332146    -2.721668    -2.103872
 H     3.360087    -2.516036    -3.185921
 C     1.895613    -1.457521    -0.752886
 C     0.873095    -3.330585    -1.945476
 C     0.453207    -4.329405    -1.050283
 C     0.233206    -3.119503    -3.176576
 C    -0.666095    -5.093601    -1.390751
 C    -0.879723    -3.909183    -3.483691
 C    -1.332261    -4.880310    -2.595970
 H    -2.208648    -5.481754    -2.847434
Cu     0.291167    -0.622540     0.055024
 N     3.104036    -0.923552    -0.627940
 N     1.979300    -2.514969    -1.576877
 C    -0.696789     0.506483     1.436639
 C     0.149075    -0.362478     2.244352
 H     3.655034    -3.760963    -1.947505
 H     4.792615    -1.077043    -1.912572
 H    -1.753697     0.235675     1.400636
 C    -0.285536    -1.746355     2.450774
 C     1.242008     0.119730     3.090393
 O    -1.495657    -1.973942     1.916062
 O     0.348116    -2.653408     2.975774
 O     1.879987    -0.546654     3.891758
 O     1.496651     1.428579     2.952681
 C     2.520383     1.972882     3.767402
 H     2.272682     1.872193     4.833357
 H     2.589990     3.032532     3.497475
 H     3.479807     1.469283     3.579658
 C    -1.986789    -3.299899     1.884395
 H    -1.318757    -3.952729     1.305806
 H    -2.959326    -3.237034     1.383665
 H    -2.101362    -3.708045     2.898565
 C     3.424686     0.144054     0.300173
 H     2.539436     0.245512     0.943652
 C     3.632608     1.476159    -0.393739
 C     4.006334     2.603647     0.352735
 C     3.407538     1.642395    -1.765616
 C     4.170444     3.846787    -0.255565
 H     4.166089     2.510517     1.428095
 C     3.567182     2.886145    -2.377324
 H     3.088433     0.787549    -2.365210
 C     3.957094     3.993378    -1.626583
 H     4.461557     4.709232     0.348608
 H     3.381653     2.989149    -3.448879
 H     4.086744     4.966597    -2.105124
 C     4.579380    -0.336380     1.239048
 H     4.725774     0.498839     1.973509
 H     5.515851    -0.296494     0.611168
 O     4.318947    -1.529238     1.788321
 C    -0.331778     1.762558     0.898475
 H     0.721377     2.044719     0.921295
 C    -1.241938     2.630310     0.316990
 H    -2.303994     2.485932     0.522155
 C    -0.875947     3.972965    -0.162348
 C    -1.886568     4.925124    -0.375849
 C     0.451227     4.342388    -0.442830
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 C   -1.586180    6.203507   -0.839920
 H   -2.925869    4.649981   -0.175213
 C    0.751068    5.620783   -0.904953
 H    1.263713    3.622352   -0.319818
 C   -0.262997    6.558913   -1.105532
 H   -2.389623    6.927295   -0.995582
 H    1.790812    5.880083   -1.116411
 H   -0.024082    7.560002   -1.471258
Na    2.770159   -2.451470    2.945891
 H   -1.402439   -3.748800   -4.429724
 H   -1.013399   -5.869911   -0.704384
 C    1.195267   -4.562281    0.238110
 H    2.280348   -4.631053    0.069876
 H    1.029961   -3.741829    0.952112
 H    0.860928   -5.491379    0.719065
 C    0.720069   -2.076071   -4.146708
 H   -0.109196   -1.692962   -4.756603
 H    1.190225   -1.226291   -3.631864
 H    1.469046   -2.498638   -4.836087
 H   -3.808950    0.589046    2.257302
108
Figure_S15-8_AA-9b(Na)-ts(1,6minor)_O4 / electronic energy: -4131.83652085 a.u. / lowest freq: -256.32 cm-1
 H    0.240753    3.102240   -2.948830
 H   -0.250135    1.537782   -3.645488
 H    0.715772    1.576953   -2.159948
 C   -0.101504    2.089142   -2.699962
 C   -1.353857    2.107970   -1.877130
 H   -0.569540   -0.443274   -2.308774
 H   -1.948270    3.025406   -1.882386
 C   -1.276541   -0.302667   -1.486788
 C   -1.941552    0.945340   -1.401470
 H   -1.857420   -1.204747   -1.251514
 B   -3.276770    1.043029   -0.599758
 O   -3.718830    2.207413   -0.022934
 O   -4.124728   -0.006717   -0.358454
 H   -5.952910    1.463678   -1.643946
 H   -6.124425    3.271794   -0.188480
 H   -5.381503    3.907840    1.297322
 C   -4.815393    1.876913    0.850144
 C   -5.823914    3.013835    0.834884
 C   -6.327595    0.736586   -0.908687
 C   -5.327862    0.528462    0.228657
 H   -6.483521   -0.221399   -1.424699
 H   -7.297896    1.088929   -0.531315
 H   -6.722335    2.741223    1.408509
 C   -5.888030   -0.459370    1.239472
 H   -6.200196   -1.380673    0.726638
 H   -6.770009   -0.032303    1.739534
 H   -3.672571    2.601321    2.525943
 H   -3.549595    0.837428    2.296921
 C   -4.234908    1.696767    2.252951
 H   -5.027873    1.544968    2.998847
 C    3.581861   -2.740661   -1.156118
 H    3.988632   -3.375782   -0.355504
 C    2.555491   -3.473123   -2.027412
 H    2.690476   -3.273396   -3.102450
 C    1.468136   -1.865071   -0.715511
 C    0.018744   -3.367350   -1.986466
 C   -0.717623   -4.191249   -1.118507
 C   -0.472750   -2.983677   -3.243708
 C   -1.995251   -4.594396   -1.515224
 C   -1.752209   -3.414872   -3.608176
 C   -2.511441   -4.203606   -2.749369
 H   -3.513957   -4.520797   -3.044810
Cu    0.122663   -0.616158    0.034778
 N    2.770336   -1.692380   -0.530261
 N    1.291123   -2.900128   -1.553925
 C   -0.536117    0.771633    1.380577
 C    0.013531   -0.281765    2.219580
 H    2.568102   -4.562450   -1.879925
 H    4.408987   -2.308239   -1.736604
 H   -1.623964    0.835731    1.342887
 C   -0.793816   -1.485214    2.429149
 C    1.171517   -0.096437    3.096238
 O   -2.002200   -1.385549    1.845843
 O   -0.453363   -2.518054    2.990627
 O    1.575508   -0.888878    3.933712
 O    1.780684    1.086951    2.941159
 C    2.886691    1.356228    3.785122
 H    2.578726    1.392348    4.839699
 H    3.272304    2.333530    3.474171
 H    3.663720    0.586707    3.669790
 C   -2.831388   -2.532708    1.804414
 H   -2.263931   -3.419507    1.494275
 H   -3.609310   -2.305969    1.067774
 H   -3.282851   -2.723745    2.789098
 C    3.337668   -0.752093    0.416474
 H    2.489237   -0.404300    1.021483
 C    3.932076    0.466187   -0.265368
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 C    4.611943    1.433340    0.489572
 C    3.770416    0.699519   -1.636961
 C    5.128962    2.581152   -0.108719
 H    4.737838    1.290357    1.563714
 C    4.285058    1.848160   -2.239128
 H    3.222385   -0.022688   -2.245101
 C    4.973737    2.791400   -1.479113
 H    5.655516    3.317764    0.502386
 H    4.140818    2.006647   -3.310232
 H    5.382490    3.688271   -1.949845
 C    4.272706   -1.530194    1.399652
 H    4.609332   -0.766560    2.149236
 H    5.211714   -1.750319    0.814298
 O    3.671358   -2.605345    1.925176
 C    0.170636    1.861244    0.822076
 H    1.261294    1.831509    0.828060
 C   -0.474762    2.937122    0.238182
 H   -1.532872    3.085428    0.458842
 C    0.236692    4.104001   -0.303732
 C   -0.479565    5.284193   -0.565081
 C    1.611369    4.085562   -0.599736
 C    0.149968    6.407972   -1.094398
 H   -1.551458    5.312547   -0.350060
 C    2.240577    5.209932   -1.126409
 H    2.202359    3.181167   -0.435775
 C    1.516358    6.376701   -1.377211
 H   -0.428533    7.314396   -1.287530
 H    3.309348    5.167851   -1.347480
 H    2.013213    7.255705   -1.793606
Na    1.917420   -3.010587    3.096071
 H   -2.163140   -3.110562   -4.573876
 H   -2.589129   -5.227041   -0.850823
 C   -0.132861   -4.619633    0.200464
 H    0.880352   -5.029729    0.073708
 H   -0.050560   -3.773213    0.898422
 H   -0.758425   -5.386731    0.676542
 C    0.338348   -2.121331   -4.173911
 H   -0.316116   -1.527023   -4.825761
 H    0.992520   -1.431249   -3.622380
 H    0.981405   -2.737423   -4.823276
 H   -5.148749   -0.725213    2.004159
108
Figure_S15-8_AA-9b(Na)-ts(1,6minor)_05 / electronic energy: -4131.83783555 a.u. / lowest freq: -304.38 cm-1
 C   -0.706503   -4.178043    1.732618
 H   -0.874025   -5.039986    1.071225
 C    0.758127   -4.025524    2.171529
 H    0.865581   -3.901055    3.260370
 C    0.153636   -2.211995    0.816525
 C    2.493934   -2.294503    1.474899
 C    3.307845   -2.561649    0.360192
 C    2.949445   -1.539252    2.567080
 C    4.594812   -2.019735    0.340076
 C    4.238864   -1.000439    2.499364
 C    5.053112   -1.234953    1.396010
 H    6.056047   -0.804289    1.358075
Cu    0.200948   -0.433923   -0.043425
 N   -0.941617   -2.945840    0.970678
 N    1.163420   -2.802139    1.472900
 C   -0.083364    0.867462   -1.613544
 C    0.460176   -0.359487   -2.154821
Na   -0.354756   -4.671385   -2.269604
 H    1.387231   -4.874732    1.865367
 H   -1.397178   -4.253693    2.584629
 H    0.659306    1.665675   -1.532677
 C    1.921922   -0.308020   -2.361591
 C   -0.329708   -1.457140   -2.717199
 O    2.399874   -1.185078   -3.248530
 O    2.654027    0.493748   -1.808791
 O    0.092200   -2.566040   -3.019781
 O   -1.625644   -1.159731   -2.858649
 C   -2.496093   -2.191703   -3.312116
 H   -2.223209   -2.506320   -4.329906
 H   -3.498179   -1.748482   -3.321696
 H   -2.462042   -3.057430   -2.628718
 C    3.799712   -1.164010   -3.463580
 H    4.115080   -0.214355   -3.919606
 H    4.017671   -1.994730   -4.144047
 H    4.343225   -1.295293   -2.517816
 C   -2.218873   -2.629423    0.353956
 H   -1.983235   -2.004963   -0.521153
 C   -3.134426   -1.826019    1.253367
 C   -4.278162   -1.236723    0.696177
 C   -2.893511   -1.642012    2.618401
 C   -5.161397   -0.499546    1.481251
 H   -4.470434   -1.348387   -0.374673
 C   -3.776594   -0.904776    3.408227
 H   -1.992530   -2.060228    3.071778
 C   -4.915840   -0.333863    2.844599
 H   -6.040558   -0.040403    1.023604
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 H    -3.565105   -0.767120    4.471072
 H    -5.601377    0.251621    3.460855
 C    -2.870326   -3.932739   -0.205399
 H    -3.839134   -3.592134   -0.656238
 H    -3.192795   -4.523775    0.696365
 O    -2.063350   -4.592339   -1.048821
 C     0.168590    0.733963    1.674200
 H     1.191013    0.420812    1.918111
 H    -0.609531    0.227514    2.258725
 C     0.007570    2.104196    1.353375
 C    -1.234045    2.725439    1.312646
 H    -1.251992    3.810935    1.181086
 C    -2.456454    2.078422    1.891550
 H    -2.668233    1.112381    1.402506
 H    -2.321209    1.858872    2.965226
 H    -3.348899    2.709427    1.786806
 C    -1.417910    1.272470   -1.391256
 H    -2.221424    0.544089   -1.494377
 C    -1.698966    2.575141   -1.004531
 H    -0.905037    3.316119   -1.120465
 C    -3.061887    3.127030   -0.931900
 C    -3.238697    4.519277   -0.865843
 C    -4.209676    2.317108   -0.898875
 C    -4.508562    5.082408   -0.767685
 H    -2.357789    5.167257   -0.884031
 C    -5.480073    2.878576   -0.802859
 H    -4.110350    1.230755   -0.924628
 C    -5.638680    4.263719   -0.735053
 H    -4.617929    6.168192   -0.714467
 H    -6.356454    2.226245   -0.775524
 H    -6.635624    4.702658   -0.655242
 B     1.286912    2.863805    0.887826
 O     1.285192    4.054079    0.208017
 O     2.548197    2.382803    1.099297
 C     2.624391    4.305562   -0.260913
 C     3.496628    3.370840    0.668945
 C     4.643630    2.665738   -0.041715
 H     4.268214    1.995859   -0.824814
 H     5.338022    3.397755   -0.481259
 H     5.202805    2.056803    0.683636
 C     4.003018    4.075673    1.927233
 H     3.184516    4.581595    2.459918
 H     4.434736    3.324731    2.604555
 H     4.779473    4.817055    1.691397
 C     2.921064    5.791780   -0.122995
 H     2.272078    6.363338   -0.802130
 H     2.742965    6.149140    0.899159
 H     3.966886    6.002655   -0.391554
 C     2.668105    3.898502   -1.732646
 H     3.638220    4.147316   -2.186024
 H     2.498051    2.820412   -1.855961
 H     1.883557    4.445763   -2.275691
 C     2.092658   -1.323333    3.786196
 H     2.331803   -0.366040    4.268919
 H     1.022251   -1.324354    3.541091
 H     2.266077   -2.120354    4.527811
 C     2.791716   -3.401267   -0.777233
 H     2.344269   -4.338787   -0.412359
 H     2.011638   -2.872960   -1.346428
 H     3.600500   -3.657638   -1.474718
 H     4.603615   -0.386158    3.326203
 H     5.247890   -2.217918   -0.513400
13
Figure_S15-9_NaOPh / electronic energy: -468.853649444 a.u. / lowest freq: 15.68 cm-1
 C    -1.912599   -1.200838   -0.011375
 C    -0.521476   -1.206572    0.015351
 C     0.241248    0.001459    0.028090
 C    -0.524240    1.207747    0.015228
 C    -1.915348    1.198823   -0.011498
 C    -2.633248   -0.001829   -0.025828
 H    -2.448993   -2.155315   -0.021458
 H     0.025710   -2.154567    0.026010
 H     0.020847    2.156944    0.025804
 H    -2.453903    2.152085   -0.021671
 H    -3.725390   -0.003095   -0.047610
 O     1.527681    0.002959    0.048939
Na     3.632205   -0.001133   -0.037490
46
Figure_S15-9_(PhO)2BpinNa / electronic energy: -1186.36814498 a.u. / lowest freq: 13.97 cm-1
 B    -0.563220    0.044928   -0.178943
 O     0.291267    0.926614    0.688425
 C     1.283536    1.704672    0.236971
 C     1.570313    1.877919   -1.127640
 C     2.065408    2.387362    1.183443
 C     2.618259    2.709596   -1.518355
 H     0.968476    1.357829   -1.872206
 C     3.108859    3.216376    0.779645
 H     1.838595    2.254777    2.244585
 C     3.395857    3.384044   -0.576007
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 H    2.826632    2.832602   -2.584305
 H    3.704622    3.736239    1.534259
 H    4.214297    4.033139   -0.893992
Na   -0.808966    0.523795    2.687870
 O   -1.401273    0.751365   -1.110868
 O   -1.477954   -0.585186    0.786000
 C   -2.750349    0.668453   -0.700149
 C   -2.762683   -0.634075    0.179234
 C   -3.835371   -0.661639    1.260867
 C   -2.856470   -1.909073   -0.666303
 C   -3.649998    0.599972   -1.930115
 C   -3.098822    1.925515    0.107771
 H   -3.332450   -0.201151   -2.609851
 H   -3.597144    1.551134   -2.480503
 H   -4.700038    0.428292   -1.646429
 H   -2.493507    1.994151    1.022809
 H   -4.162427    1.964752    0.386050
 H   -2.867924    2.809936   -0.503853
 H   -3.713572    0.159050    1.981888
 H   -3.788318   -1.612147    1.813558
 H   -4.838966   -0.577840    0.817054
 H   -2.121263   -1.893048   -1.482449
 H   -3.861061   -2.045468   -1.092990
 H   -2.632217   -2.773934   -0.024406
 H    1.663800   -2.361720   -2.479463
 C    1.156468   -1.758231   -0.480048
 C    1.868619   -2.528543   -1.419688
 C    1.421837   -1.970396    0.885132
 C    2.803385   -3.473353   -1.010584
 C    2.361381   -2.920725    1.284246
 H    3.340044   -4.056682   -1.763421
 C    3.059848   -3.680848    0.347231
 H    2.547156   -3.067370    2.351610
 H    3.793490   -4.423052    0.668193
 O    0.272585   -0.884037   -0.951749
 H    0.889028   -1.388098    1.633642
33
Figure_S15-9_PhOBpin / electronic energy: -717.466658936 a.u. / lowest freq: 34.04 cm-1
 B    0.316485   -0.649497    0.152442
 O    0.547339    0.656564   -0.167517
 O    1.450352   -1.390749    0.310010
 C    1.953393    0.765407   -0.475562
 C    2.556556   -0.464329    0.303349
 C    3.750402   -1.118973   -0.372082
 H    4.110941   -1.956020    0.242581
 H    3.490766   -1.511055   -1.363342
 H    4.572751   -0.396645   -0.481985
 C    2.881450   -0.142716    1.761241
 H    3.761317    0.510734    1.842022
 H    2.033939    0.348756    2.261363
 H    3.094875   -1.080566    2.293131
 C    2.090739    0.636050   -1.991454
 H    3.132712    0.771530   -2.312966
 H    1.476060    1.410062   -2.472261
 H    1.740869   -0.345498   -2.343688
 C    2.458430    2.121802   -0.012348
 H    1.979441    2.916387   -0.602078
 H    2.232209    2.298870    1.046507
 H    3.546064    2.197566   -0.158022
 H   -2.930733   -2.174758   -0.976580
 O   -0.912560   -1.220338    0.303715
 C   -3.126356   -1.200585   -0.524893
 C   -2.103803   -0.564658    0.181286
 C   -4.371635   -0.585968   -0.642680
 C   -2.327104    0.678308    0.778803
 C   -4.601602    0.659823   -0.057725
 H   -1.522715    1.166044    1.330768
 C   -3.575625    1.285149    0.651396
 H   -5.577031    1.140857   -0.152884
 H   -3.745791    2.258600    1.116820
 H   -5.168218   -1.087052   -1.197239
32
Figure_S15-9_dienoate / electronic energy: -841.927078481 a.u. / lowest freq: 24.55 cm-1
 C   -0.660544   -0.726572    0.059153
 C   -1.860539   -0.097447    0.115996
 H   -0.691600   -1.818492   -0.004770
 C   -1.976243    1.390665    0.160143
 C   -3.120576   -0.891785    0.187355
 O   -3.041424    1.823605   -0.507466
 O   -1.182749    2.134043    0.689285
 O   -4.147702   -0.497504    0.683440
 O   -2.981802   -2.118850   -0.320932
 C   -4.097604   -2.989729   -0.195724
 H   -4.332384   -3.170881    0.862818
 H   -3.810049   -3.927003   -0.683244
 H   -4.981752   -2.562067   -0.688186
 C   -3.254671    3.228152   -0.535442
 H   -3.354009    3.627502    0.483524
 H   -4.184056    3.384216   -1.092621
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 H   -2.420438    3.737793   -1.038016
 C    0.656646   -0.129211    0.062308
 H    0.725624    0.955889    0.150505
 C    1.759981   -0.902956   -0.019704
 H    1.621029   -1.988149   -0.089650
 C    3.156351   -0.453635   -0.025165
 C    4.175093   -1.416830   -0.109525
 C    3.522207    0.902114    0.053056
 C    5.517020   -1.042840   -0.114390
 H    3.907556   -2.474776   -0.172060
 C    4.861836    1.275255    0.048166
 H    2.754752    1.675486    0.118691
 C    5.863995    0.305241   -0.035401
 H    6.294080   -1.807149   -0.179427
 H    5.127957    2.332459    0.111300
 H    6.914980    0.602284   -0.038425
84
Figure_S15-9_9d(Naborate)-Cu-allenyl_01 / electronic energy: -3556.59972133 a.u. / lowest freq: 6.98 cm-1
Cu   -1.541487    0.512198    1.320622
 C   -1.443241    0.280979    3.240199
 C   -1.708543    0.570437   -0.618345
 N   -2.703782    0.006397   -1.338605
 N   -0.843137    1.117024   -1.462725
 C    0.339276    1.860794   -1.044976
 C   -0.866615   -0.748817    3.789649
 C   -0.244212   -1.818381    4.271722
 C   -1.263213    1.024435   -2.860798
 H   -0.448075    0.654817   -3.495763
 C   -2.431137    0.039099   -2.779181
 H   -3.317691    0.367546   -3.338046
 C   -3.822522   -0.654141   -0.787344
 C   -4.403465   -1.736535   -1.457185
 C   -4.365970   -0.218745    0.424395
 C   -5.499456   -2.405697   -0.905083
 C   -5.446625   -0.887610    1.003749
 C   -6.003346   -1.977169    0.328370
 H   -6.858359   -2.499194    0.767305
 B    2.473873   -0.386637   -0.145228
 H   -2.142357   -0.960910   -3.139177
 H   -1.567888    2.017795   -3.228704
 H    0.425750    1.661748    0.030454
 C    0.140518    3.351059   -1.243250
 C    0.476012    4.004913   -2.433813
 C   -0.434299    4.096566   -0.206338
 C    0.242521    5.372968   -2.583343
 H    0.925428    3.449248   -3.259815
 C   -0.668240    5.461918   -0.351779
 H   -0.701300    3.593157    0.727484
 C   -0.329858    6.104383   -1.543760
 H    0.510325    5.868836   -3.518935
 H   -1.113929    6.027375    0.469545
 H   -0.510495    7.175044   -1.661573
 C    1.610315    1.285819   -1.680398
 H    2.465187    1.898975   -1.342081
 H    1.571928    1.385444   -2.780192
 O    1.764330   -0.050841   -1.356561
 H   -1.933974    0.981211    3.935554
 H    0.802960   -1.764109    4.590003
 H   -0.774863   -2.762088    4.437032
 O    2.387136   -1.895077   -0.046317
 C    2.906397   -2.746670   -0.934513
 C    3.897792   -2.382965   -1.863522
 C    2.453604   -4.077549   -0.921881
 C    4.403362   -3.329794   -2.751874
 H    4.269923   -1.358687   -1.865609
 C    2.970192   -5.015503   -1.812820
 H    1.685663   -4.362359   -0.197613
 C    3.948234   -4.649763   -2.739127
 H    5.172444   -3.027217   -3.467572
 H    2.599853   -6.043636   -1.783062
 H    4.350998   -5.383589   -3.440445
Na    0.677439   -1.839637    1.558925
 C   -6.004871   -0.406331    2.317499
 H   -6.474223    0.583477    2.204724
 H   -6.763194   -1.097279    2.710266
 H   -5.207093   -0.305544    3.068762
 C   -6.098484   -3.596682   -1.607543
 H   -7.177639   -3.675396   -1.414521
 H   -5.943910   -3.542992   -2.694327
 H   -5.632951   -4.530415   -1.252957
 H   -3.951281    0.663371    0.917027
 H   -3.995152   -2.078090   -2.410284
 O    3.803496    0.174961   -0.094134
 O    1.838245    0.061275    1.116929
 C    4.145657    0.442829    1.248766
 C    2.754008    0.810560    1.898020
 C    2.625168    0.410269    3.365027
 C    2.406023    2.296831    1.764430
 C    5.167494    1.574133    1.289393
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 C    4.768010   -0.819633    1.861744
 H    4.817042    2.449860    0.727323
 H    6.111788    1.236674    0.836575
 H    5.376533    1.881148    2.325737
 H    4.046035   -1.647362    1.882875
 H    5.143830   -0.646233    2.880947
 H    5.612458   -1.130820    1.228985
 H    2.776998   -0.668346    3.506644
 H    1.618462    0.664090    3.730275
 H    3.363129    0.942589    3.984708
 H    2.524541    2.648090    0.730035
 H    3.030419    2.926419    2.414920
 H    1.354467    2.440249    2.056858
84
Figure_S15-9_9d(Naborate)-Cu-allenyl_02 / electronic energy: -3556.59879587 a.u. / lowest freq: 11.93 cm-1
 H    0.580931   -0.723113   -5.771843
Cu    2.067226    0.780569   -1.607415
 H    3.632288    0.721699   -3.749757
 C    2.661345    0.338434   -3.392942
 C    2.011812   -0.397797   -4.248386
 C    1.292777   -1.160712   -5.063373
 H    1.439359   -2.245755   -5.102156
 N    0.157987    1.558593    0.464784
 C    1.380105    1.127391    0.175998
 N    2.001011    0.810164    1.330094
 C   -0.822399    1.998254   -0.517386
Na   -0.304550   -1.205401   -2.784307
 C   -0.194521    1.379557    1.873759
 H   -0.892479    0.531236    1.960230
 C    1.162498    1.065723    2.507801
 H    1.577719    1.908172    3.083199
 C    3.338042    0.361378    1.418144
 C    3.710178   -0.544717    2.413845
 C    4.295210    0.820213    0.506943
 C    5.024768   -1.015878    2.490772
 C    5.606531    0.343208    0.549754
 C    5.956911   -0.572285    1.547869
 H    6.984373   -0.943945    1.596614
 H    1.109441    0.191278    3.169515
 H   -0.666022    2.283082    2.284060
 H   -0.284946    1.996615   -1.478510
 C   -1.250005    3.425612   -0.216027
 C   -2.496960    3.746681    0.328391
 C   -0.334717    4.457505   -0.459831
 C   -2.822422    5.074000    0.617810
 H   -3.231245    2.965659    0.535664
 C   -0.656058    5.780695   -0.171635
 H    0.644620    4.214205   -0.882091
 C   -1.905208    6.092479    0.369709
 H   -3.800771    5.308249    1.042882
 H    0.068677    6.572770   -0.372287
 H   -2.161048    7.130022    0.595429
 C   -1.964832    0.994912   -0.638933
 H   -2.713806    1.402694   -1.344059
 H   -2.474947    0.895510    0.335185
 O   -1.463435   -0.224302   -1.071300
 C    6.609576    0.810813   -0.471895
 H    7.639797    0.598039   -0.155311
 H    6.443024    0.304503   -1.436186
 H    6.518580    1.891748   -0.652649
 C    5.419133   -1.975898    3.582782
 H    6.374853   -2.469372    3.359456
 H    5.531985   -1.448430    4.543409
 H    4.654491   -2.753434    3.726049
 H    2.972159   -0.908155    3.131169
 H    4.015455    1.567131   -0.239355
 B   -2.023918   -1.469183   -0.501618
 O   -1.596695   -1.746330    0.860817
 O   -1.449708   -2.543077   -1.316357
 C   -0.666389   -2.812267    0.852190
 C   -1.054814   -3.595762   -0.453026
 C    0.093035   -4.365813   -1.095427
 H   -0.266361   -4.894957   -1.991022
 H    0.908603   -3.695052   -1.399436
 H    0.503060   -5.114995   -0.400969
 C   -2.248143   -4.531525   -0.233803
 H   -1.973103   -5.416305    0.359240
 H   -3.070016   -4.005544    0.271988
 H   -2.616392   -4.872321   -1.212772
 C    0.751840   -2.240137    0.777317
 H    1.524582   -3.019891    0.843478
 H    0.894245   -1.549819    1.618810
 H    0.906232   -1.665398   -0.147125
 C   -0.816573   -3.618857    2.137507
 H   -0.496994   -3.011129    2.997847
 H   -1.861479   -3.912091    2.301762
 H   -0.193464   -4.526429    2.112926
 H   -5.877697   -1.031593   -1.457222
 O   -3.498415   -1.446713   -0.664050
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 C   -5.731586   -0.801612   -0.399415
 C   -4.447650   -0.993229    0.148935
 C   -6.781899   -0.327595    0.380416
 C   -4.258183   -0.697603    1.514324
 C   -6.586757   -0.028328    1.730903
 H   -3.275736   -0.865721    1.953875
 C   -5.319680   -0.219773    2.282812
 H   -7.410304    0.345153    2.343139
 H   -5.148499    0.001290    3.340055
 H   -7.765815   -0.187087   -0.075149
84
Figure_S15-9_9d(Naborate)-Cu-allenyl_03 / electronic energy: -3556.60003110 a.u. / lowest freq: 12.55 cm-1
 H    1.788044    1.466405    5.579331
Cu   -1.195968    1.043557    1.948192
 H   -1.965195    1.482422    4.427752
 C   -1.061626    1.171742    3.874789
 C   -0.025007    0.937774    4.626899
 C    1.070738    0.676946    5.330023
 H    1.254829   -0.320890    5.743249
 N   -0.438975    1.568413   -0.794299
 C   -1.324742    0.986218    0.006683
 N   -2.239340    0.357256   -0.761214
 C    0.702979    2.352060   -0.340362
Na    1.851392   -0.015497    2.739367
 C   -0.709860    1.368358   -2.217470
 H    0.152285    0.901805   -2.714835
 C   -1.928395    0.444068   -2.193917
 H   -2.788620    0.853263   -2.743179
 C   -3.364549   -0.353571   -0.295278
 C   -3.981560   -1.288976   -1.132530
 C   -3.888933   -0.132036    0.983318
 C   -5.081070   -2.030059   -0.690545
 C   -4.976971   -0.871746    1.448935
 C   -5.561407   -1.822193    0.605127
 H   -6.413339   -2.406797    0.963549
 H   -1.691927   -0.548891   -2.600930
 H   -0.911491    2.334381   -2.704197
 H    0.528462    2.523559    0.733213
 C    0.702664    3.702298   -1.036588
 C    1.543626    3.998553   -2.113356
 C   -0.217712    4.669326   -0.614397
 C    1.469781    5.238912   -2.750252
 H    2.264176    3.259741   -2.470276
 C   -0.295210    5.906401   -1.248385
 H   -0.885361    4.442645    0.221913
 C    0.551437    6.194742   -2.320494
 H    2.134756    5.456322   -3.588981
 H   -1.017347    6.650119   -0.904576
 H    0.493640    7.164304   -2.819830
 C    2.017109    1.571128   -0.439564
 H    2.842780    2.290641   -0.286036
 H    2.146642    1.157743   -1.455541
 O    2.072368    0.569579    0.520001
 C   -5.516209   -0.616275    2.832749
 H   -6.242430   -1.384670    3.130771
 H   -4.705941   -0.600340    3.576777
 H   -6.021680    0.361162    2.881707
 C   -5.733087   -3.027639   -1.612614
 H   -6.366304   -3.733519   -1.057760
 H   -6.370575   -2.516559   -2.351723
 H   -4.982656   -3.603887   -2.173558
 H   -3.588822   -1.473777   -2.132424
 H   -3.454182    0.635082    1.627767
 B    2.250906   -0.844472    0.117946
 O    2.770734   -1.557861    1.299453
 O    3.242285   -1.016082   -0.912863
 C    4.125323   -1.896643    1.052206
 C    4.145719   -2.030592   -0.513003
 C    5.504307   -1.769775   -1.152215
 H    5.434610   -1.910996   -2.241233
 H    5.841711   -0.741906   -0.964894
 H    6.263658   -2.467833   -0.767060
 C    3.611886   -3.391156   -0.979004
 H    4.323589   -4.203905   -0.770744
 H    2.654042   -3.626956   -0.493283
 H    3.437859   -3.351559   -2.064003
 C    5.024864   -0.755222    1.542182
 H    6.092780   -0.987192    1.418023
 H    4.845066   -0.587589    2.615841
 H    4.799722    0.176378    1.004006
 C    4.470075   -3.178699    1.800327
 H    4.461733   -2.995537    2.885799
 H    3.741971   -3.971375    1.585034
 H    5.474220   -3.537458    1.526064
 H   -1.152996   -2.894884   -0.099301
 O    0.898946   -1.389653   -0.167011
 C   -0.756799   -2.746624   -1.106121
 C    0.388682   -1.941095   -1.257513
 C   -1.381122   -3.319521   -2.209433
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 C     0.892062   -1.740260   -2.559044
 C    -0.886413   -3.107080   -3.498401
 H     1.796678   -1.147125   -2.686275
 C     0.254377   -2.317092   -3.656006
 H    -1.377196   -3.555047   -4.364821
 H     0.662366   -2.144835   -4.655748
 H    -2.272517   -3.933924   -2.058422
84
Figure_S15-9_9d(Naborate)-Cu-allenyl_04 / electronic energy: -3556.60702129 a.u. / lowest freq: 23.73 cm-1
Cu   -1.211825    1.239513    1.303356
 C   -0.964845    1.704515    3.165528
 C   -1.323143    0.687489   -0.560221
 N   -2.347618    0.038683   -1.150971
 N   -0.331695    0.790621   -1.436520
 C    0.898461    1.520033   -1.143354
 C    0.018524    1.329638    3.932327
 C    1.050713    0.903209    4.651536
 C   -0.654674    0.222883   -2.746199
 H    0.143498   -0.456843   -3.070128
 C   -1.963912   -0.513486   -2.454127
 H   -2.744095   -0.328612   -3.204790
 C   -3.566265   -0.276070   -0.520102
 C   -4.283653   -1.412318   -0.901395
 C   -4.074356    0.556237    0.484597
 C   -5.477256   -1.748668   -0.254425
 C   -5.256312    0.231626    1.150385
 C   -5.946259   -0.926510    0.773681
 H   -6.876359   -1.186961    1.286622
 B    2.597317   -0.988766   -0.510723
 H   -1.802269   -1.599001   -2.364443
 H   -0.780505    1.022890   -3.493878
 H    1.100602    1.334571   -0.081524
 C    0.722527    3.016943   -1.319341
 C    0.571146    3.598157   -2.584548
 C    0.682610    3.844697   -0.191761
 C    0.379260    4.972810   -2.716516
 H    0.603509    2.978048   -3.483578
 C    0.493204    5.220360   -0.320567
 H    0.791304    3.402448    0.802840
 C    0.339552    5.788054   -1.584734
 H    0.261123    5.410857   -3.710090
 H    0.464140    5.849831    0.571670
 H    0.188992    6.864626   -1.689828
 C    2.095607    0.970163   -1.926391
 H    2.975049    1.548641   -1.586970
 H    1.965958    1.195620   -2.999748
 O    2.279684   -0.392260   -1.794536
 H   -1.716764    2.346356    3.655291
 H    1.967128    1.497205    4.739020
 H    0.990948   -0.021381    5.236133
 O    1.312859   -1.393464    0.202612
 C    0.424515   -2.262619   -0.280972
 C    0.631012   -2.998942   -1.461745
 C   -0.770668   -2.460111    0.433256
 C   -0.332506   -3.907229   -1.896960
 H    1.556051   -2.861276   -2.020326
 C   -1.723297   -3.372494   -0.010216
 H   -0.943625   -1.870850    1.337994
 C   -1.514653   -4.104693   -1.181230
 H   -0.151604   -4.470926   -2.815957
 H   -2.646284   -3.501798    0.559791
 H   -2.263574   -4.818892   -1.529803
Na    1.634795   -0.206231    2.148438
 C   -5.788037    1.144749    2.224368
 H   -6.219677    2.056893    1.782556
 H   -6.574351    0.655534    2.815561
 H   -4.986938    1.460700    2.908732
 C   -6.213540   -3.001996   -0.650978
 H   -7.190120   -3.071987   -0.153039
 H   -6.378072   -3.039483   -1.738302
 H   -5.632023   -3.897875   -0.380537
 H   -3.551531    1.482163    0.736377
 H   -3.899348   -2.069178   -1.683006
 O    3.524365   -2.081184   -0.688877
 O    3.224218   -0.087812    0.475153
 C    4.547330   -1.992537    0.278809
 C    4.593097   -0.451600    0.591523
 C    5.094298   -0.102061    1.987404
 C    5.396846    0.333138   -0.450219
 C    5.844283   -2.545736   -0.303242
 C    4.148839   -2.829044    1.502705
 H    6.079045   -2.073119   -1.265729
 H    5.742552   -3.627785   -0.473885
 H    6.687998   -2.386907    0.386310
 H    3.225597   -2.449985    1.963156
 H    4.939333   -2.860071    2.266899
 H    3.947174   -3.857884    1.170473
 H    4.466280   -0.548244    2.770784
 H    5.092195    0.989578    2.127503
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 H    6.124097   -0.461090    2.134953
 H    5.075546    0.075229   -1.469390
 H    6.477260    0.148174   -0.361823
 H    5.220843    1.408388   -0.296041
84
Figure_S15-9_9d(Naborate)-Cu-allenyl_05 / electronic energy: -3556.59701117 a.u. / lowest freq: 13.81 cm-1
 H   -2.290956   -0.219092    3.771425
 C   -1.542055   -0.620520    3.066779
Cu   -1.617169    0.027328    1.242204
 H    1.896846    2.336508    4.120856
 C   -0.716270   -1.484742    3.582877
 H    1.053819    0.362462    2.873524
 C    2.410422    2.014327    3.211189
 C    0.181788   -2.353144    4.029706
 C    1.937936    0.900241    2.522921
 H   -0.021182   -3.429615    4.044658
 H    1.131641   -2.011379    4.455845
 H    3.885238    3.601092    3.278400
 C    3.518755    2.722669    2.743271
Na    0.632564   -2.332437    1.272400
 C    2.570126    0.460437    1.344960
 C    4.151355    2.285458    1.579185
 O    2.054508   -0.606849    0.728389
 C    3.695952    1.166119    0.883437
 H    5.024379    2.823096    1.199835
 H    4.205485    0.812404   -0.012327
 N   -2.979158    0.482760   -1.303631
 C   -1.842647    0.649773   -0.590157
 N   -0.954466    1.265204   -1.362671
 C    0.407125    1.590284   -0.949649
 C   -1.501833    1.645155   -2.667542
 H   -0.816256    1.377545   -3.481697
 C   -2.804532    0.848202   -2.712179
 H   -3.658739    1.434081   -3.076166
 C   -4.161471   -0.108921   -0.810106
 C   -4.967788   -0.880703   -1.655628
 C   -4.539199    0.083096    0.520102
 C   -6.126990   -1.486897   -1.167767
 C   -5.681581   -0.537481    1.035066
 C   -6.463666   -1.317853    0.181734
 H   -7.364722   -1.799984    0.571701
 B    2.292127   -1.158157   -0.679634
 H   -2.708771   -0.056055   -3.334232
 H   -1.672455    2.732884   -2.700200
 H    0.486372    1.204715    0.073845
 C    0.662582    3.083328   -0.905589
 C    0.848763    3.843214   -2.067545
 C    0.750795    3.722083    0.335824
 C    1.100846    5.212754   -1.987693
 H    0.805509    3.367508   -3.050146
 C    1.009400    5.089189    0.418911
 H    0.638498    3.133352    1.249754
 C    1.180992    5.839579   -0.744198
 H    1.242796    5.790757   -2.903532
 H    1.084977    5.567733    1.397839
 H    1.383331    6.911114   -0.681545
 C    1.444372    0.827188   -1.787633
 H    2.439583    1.226305   -1.524050
 H    1.298655    1.059373   -2.859290
 O    1.351941   -0.542055   -1.596919
 C   -6.047644   -0.339894    2.482587
 H   -6.193144    0.727472    2.708699
 H   -6.972572   -0.872603    2.741847
 H   -5.244691   -0.705294    3.141187
 C   -7.004749   -2.314519   -2.070531
 H   -7.200971   -3.303645   -1.630603
 H   -7.980464   -1.826558   -2.221103
 H   -6.545415   -2.462975   -3.057334
 H   -3.944253    0.736640    1.162315
 H   -4.687712   -1.027719   -2.700266
 O    1.976949   -2.587939   -0.592515
 O    3.685434   -1.077200   -1.057843
 C    3.189855   -3.319722   -0.689611
 C    4.093823   -2.346192   -1.528682
 C    5.589678   -2.513354   -1.287329
 C    3.801718   -2.439479   -3.031811
 C    2.918676   -4.661758   -1.357916
 C    3.749959   -3.545696    0.720186
 H    2.384368   -4.531210   -2.307905
 H    2.298839   -5.292730   -0.702355
 H    3.859361   -5.199330   -1.553443
 H    3.966411   -2.586559    1.211915
 H    4.667391   -4.152118    0.708726
 H    3.005895   -4.086834    1.325660
 H    5.851333   -2.289415   -0.244721
 H    6.151185   -1.821525   -1.932908
 H    5.916856   -3.538244   -1.521962
 H    2.722420   -2.368118   -3.225441
 H    4.184743   -3.372356   -3.472015
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 H    4.293209   -1.593317   -3.534723
84
Figure_S15-9_9d(Naborate)-Cu-allenyl_06 / electronic energy: -3556.60439142 a.u. / lowest freq: 19.97 cm-1
 H   -1.883550    2.200903    4.067178
Cu   -0.798297    1.561921    1.704095
 C   -1.340298    1.390722    3.553391
 C   -1.195239    0.292923    4.236973
 C   -1.008538   -0.860737    4.869381
 H   -1.748298   -1.666429    4.811728
 H   -0.148620   -1.013063    5.531913
Na    0.807960   -1.289977    2.798307
 N   -1.103958    1.363300   -1.223858
 C   -0.287791    1.595794   -0.173074
 N    0.964797    1.594213   -0.612327
 C    2.132450    1.788812    0.232908
 C    1.087441    1.322583   -2.043617
 H    1.746513    0.459615   -2.212459
 C   -0.359788    1.017900   -2.438308
 H   -0.710922    1.611506   -3.294176
 C   -2.507869    1.251229   -1.152409
 C   -3.200686    0.541822   -2.134142
 C   -3.221544    1.847570   -0.104974
 C   -4.587393    0.379455   -2.052140
 C   -4.600423    1.681556    0.004994
 C   -5.273461    0.940955   -0.974659
 H   -6.355366    0.802182   -0.893748
 H   -0.498857   -0.048844   -2.669060
 H    1.502245    2.200272   -2.563567
 H    1.726238    2.021464    1.229540
 C    2.923886    2.993998   -0.252885
 C    4.154298    2.883938   -0.906931
 C    2.369388    4.268013   -0.073624
 C    4.819402    4.023618   -1.365152
 H    4.609593    1.905298   -1.069332
 C    3.028307    5.405508   -0.531040
 H    1.402861    4.363150    0.429743
 C    4.259552    5.285357   -1.179418
 H    5.781076    3.919795   -1.872467
 H    2.581411    6.390688   -0.380254
 H    4.779463    6.175833   -1.539413
 C    2.950179    0.501244    0.378719
 H    3.854541    0.753081    0.960879
 H    3.292542    0.157135   -0.612558
 O    2.252414   -0.503575    1.028224
 C   -5.343379    2.319762    1.150334
 H   -6.336334    1.868708    1.285713
 H   -4.785298    2.213321    2.092236
 H   -5.488068    3.397708    0.974052
 C   -5.304427   -0.411539   -3.113853
 H   -6.367901   -0.545072   -2.872445
 H   -5.238611    0.090462   -4.091870
 H   -4.849399   -1.407460   -3.226716
 H   -2.663749    0.063961   -2.953899
 H   -2.694063    2.447633    0.639358
 B    1.515947   -1.568158    0.308743
 O    1.717258   -2.806455    1.070331
 O    1.944819   -1.843527   -1.032095
 C    2.274145   -3.805245    0.237857
 C    2.794749   -2.980433   -1.011410
 C    4.243072   -2.506836   -0.836733
 H    4.483919   -1.798173   -1.643395
 H    4.376419   -1.989288    0.123399
 H    4.959307   -3.339637   -0.888298
 C    2.664584   -3.714111   -2.341694
 H    3.246335   -4.648528   -2.336639
 H    1.617423   -3.956995   -2.564904
 H    3.047455   -3.078198   -3.153990
 C    3.380349   -4.538878    0.994405
 H    3.898435   -5.257978    0.341359
 H    2.942963   -5.099587    1.834294
 H    4.121044   -3.840096    1.404218
 C    1.177428   -4.812836   -0.123160
 H    0.756551   -5.223801    0.806952
 H    0.358713   -4.334233   -0.675862
 H    1.567904   -5.650402   -0.720065
 H   -2.155721   -1.084778    1.675523
 O    0.091845   -1.136143    0.456419
 C   -2.193619   -1.604182    0.713811
 C   -1.013432   -1.697478   -0.044219
 C   -3.387073   -2.135864    0.236858
 C   -1.068019   -2.319017   -1.302282
 C   -3.432839   -2.778734   -1.001645
 H   -0.155661   -2.371415   -1.896136
 C   -2.268580   -2.858715   -1.764360
 H   -4.369303   -3.200021   -1.373137
 H   -2.290820   -3.346245   -2.742798
 H   -4.294654   -2.041567    0.838106
84
Figure_S15-9_9d(Naborate)-Cu-allenyl_07 / electronic energy: -3556.59700883 a.u. / lowest freq: 14.20 cm-1
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Cu   -1.615307    0.015206    1.240734
 C   -1.536126   -0.634821    3.064377
 C   -1.846416    0.640390   -0.590150
 N   -2.983976    0.474046   -1.302375
 N   -0.959596    1.257194   -1.363024
 C    0.400737    1.587233   -0.949505
 C   -0.707551   -1.497613    3.578344
 C    0.193673   -2.363870    4.022897
 C   -1.508859    1.638831   -2.666576
 H   -0.823982    1.373279   -3.481996
 C   -2.810852    0.840841   -2.710666
 H   -3.665952    1.426216   -3.073425
 C   -4.165256   -0.120036   -0.809331
 C   -4.980014   -0.876006   -1.656921
 C   -4.535929    0.061712    0.526735
 C   -6.142463   -1.481179   -1.168138
 C   -5.678818   -0.553738    1.040242
 C   -6.472228   -1.321287    0.181599
 H   -7.377119   -1.796012    0.571113
 B    2.300694   -1.150745   -0.682078
 H   -2.715050   -0.062974   -3.333443
 H   -1.680563    2.726453   -2.697094
 H    0.481595    1.200073    0.073260
 C    0.648588    3.081497   -0.902438
 C    0.836600    3.843562   -2.062652
 C    0.726552    3.719474    0.340059
 C    1.080708    5.214391   -1.980135
 H    0.801301    3.368510   -3.045883
 C    0.977084    5.087907    0.425842
 H    0.612982    3.129119    1.252802
 C    1.150741    5.840390   -0.735620
 H    1.224361    5.794093   -2.894633
 H    1.044856    5.565921    1.405591
 H    1.346989    6.912924   -0.670806
 C    1.441384    0.830476   -1.788948
 H    2.434645    1.234962   -1.526246
 H    1.293233    1.062333   -2.860331
 O    1.356886   -0.539408   -1.598952
 H   -2.285410   -0.236411    3.770318
 H    1.142876   -2.019710    4.448571
 H   -0.005959   -3.440979    4.036523
 O    2.059790   -0.602004    0.726353
 C    2.568071    0.468125    1.344058
 C    3.688811    1.182607    0.883661
 C    1.932660    0.901690    2.522581
 C    4.135954    2.304195    1.581267
 H    4.201165    0.834185   -0.012580
 C    2.396805    2.018109    3.212597
 H    1.052450    0.357057    2.872233
 C    3.500089    2.735081    2.745923
 H    5.005093    2.848768    1.202884
 H    1.880750    2.335114    4.122684
 H    3.860151    3.615342    3.282399
Na    0.644070   -2.334939    1.266556
 C   -6.042290   -0.363094    2.489431
 H   -6.191403    0.702816    2.720143
 H   -6.964830   -0.900018    2.748553
 H   -5.236789   -0.728263    3.144934
 C   -6.998159   -2.320829   -2.081086
 H   -7.992784   -2.496391   -1.648945
 H   -7.127130   -1.840284   -3.061925
 H   -6.531678   -3.303216   -2.257157
 H   -3.935906    0.708756    1.170796
 H   -4.709260   -1.012576   -2.705682
 O    1.993483   -2.582289   -0.595935
 O    3.693522   -1.061640   -1.059755
 C    3.210674   -3.307090   -0.691088
 C    4.110258   -2.328512   -1.529075
 C    5.606700   -2.486435   -1.285089
 C    3.821353   -2.424410   -3.032636
 C    2.948020   -4.650825   -1.359422
 C    3.770085   -3.529842    0.719500
 H    2.414311   -4.523590   -2.310183
 H    2.330716   -5.284938   -0.704506
 H    3.891924   -5.183293   -1.553374
 H    3.980209   -2.569566    1.211744
 H    4.691192   -4.130682    0.709103
 H    3.028544   -4.075617    1.323896
 H    5.865208   -2.260493   -0.242123
 H    6.164983   -1.791348   -1.929961
 H    5.940647   -3.509335   -1.518836
 H    2.742001   -2.359676   -3.228329
 H    4.210624   -3.355294   -3.471585
 H    4.308720   -1.575684   -3.535227
116
Figure_S15-9_PA-9b(Naborate)-ts(1,6major)_01 / electronic energy: -4398.56325172 a.u. / lowest freq: -433.67 cm-1
 H    5.797940    2.532949    0.596683
 H    6.963864    3.051104   -1.899424
 H    4.704182    2.588892   -1.456197
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H	9.243414	2.365363	-2.578522
C	7.185485	1.992191	-2.058303
C	4.820159	1.501774	-1.468964
C	8.469503	1.607186	-2.439232
C	6.169159	1.042761	-1.874278
C	8.764441	0.259393	-2.641663
H	9.770085	-0.046006	-2.938646
C	6.480921	-0.310027	-2.079656
C	7.763505	-0.696598	-2.459469
H	5.717070	-1.074501	-1.933309
H	7.983070	-1.755376	-2.614234
H	2.438478	2.469411	-1.445404
C	2.401070	1.384218	-1.570359
C	3.656844	0.768668	-1.698867
H	3.714699	-0.294662	-1.919598
Cu	1.507608	0.800125	0.251881
H	2.320983	1.584188	2.613719
C	2.816334	1.503532	1.645373
C	4.036234	1.601539	1.319164
C	5.249099	1.594260	0.710811
H	5.864106	0.693390	0.802860
N	-1.026655	0.400537	1.792347
C	0.187997	-0.034738	1.493140
N	0.505244	-1.020444	2.363082
C	-1.679766	1.539683	1.163268
O	-1.098164	1.745558	-2.486599
C	-0.002847	1.892539	-1.972662
C	1.067162	0.888066	-1.849207
C	0.755689	-0.473962	-2.291986
O	-0.325745	-0.878846	-2.688079
Na	-2.439204	-0.111997	-2.458558
C	-1.659965	-0.334294	2.892038
H	-2.474603	-0.953758	2.485630
C	-0.497912	-1.172478	3.423451
H	-0.106956	-0.783907	4.377396
C	1.709463	-1.750512	2.359546
C	2.216392	-2.261967	3.557834
C	2.402592	-1.972775	1.164723
C	3.428201	-2.959665	3.579132
C	3.622301	-2.650087	1.169806
C	4.126227	-3.133691	2.381732
H	5.082603	-3.664722	2.390182
H	-0.759283	-2.231265	3.562096
H	-2.057864	0.362722	3.643188
O	1.789937	-1.322322	-2.201774
O	0.325697	3.069818	-1.413527
C	-0.638959	4.110192	-1.475433
H	-1.559434	3.823064	-0.946855
H	-0.182540	4.974211	-0.981411
H	-0.884938	4.353105	-2.518214
C	1.538111	-2.676445	-2.555045
H	0.794126	-3.118315	-1.877999
H	2.495572	-3.197444	-2.453929
H	1.173497	-2.751001	-3.588143
H	-1.107974	1.729853	0.247704
C	-1.567424	2.770362	2.048398
C	-2.580522	3.161824	2.929091
C	-0.381326	3.515127	2.011813
C	-2.408999	4.272196	3.758101
H	-3.518394	2.604533	2.977122
C	-0.207111	4.621762	2.838485
H	0.414178	3.218507	1.322020
C	-1.223161	5.002934	3.716930
H	-3.209278	4.565736	4.440857
H	0.725013	5.189431	2.795241
H	-1.090477	5.870677	4.366709
C	-3.102147	1.195727	0.726247
H	-3.565954	2.126491	0.344385
H	-3.711022	0.880817	1.592180
O	-3.071367	0.214200	-0.250899
C	4.369762	-2.887830	-0.115225
H	5.448935	-2.721817	0.015765
H	4.236634	-3.924519	-0.463539
H	4.009647	-2.218049	-0.906763
C	3.966447	-3.521524	4.869366
H	5.054835	-3.382583	4.941202
H	3.500524	-3.046144	5.743557
H	3.770177	-4.603731	4.934819
H	1.681928	-2.101669	4.495436
H	1.987152	-1.622060	0.218058
B	-3.955752	-0.968938	-0.157641
O	-3.561335	-1.948622	0.837021
O	-3.801069	-1.636254	-1.455632
C	-2.944746	-3.043413	0.190100
C	-3.614876	-3.023493	-1.233659
C	-2.741031	-3.593031	-2.346054
H	-3.280017	-3.546882	-3.304995
H	-1.805361	-3.026327	-2.451580
H	-2.492660	-4.647672	-2.150344

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 C   -4.985543   -3.707657   -1.243293
 H   -4.900788   -4.800419   -1.148349
 H   -5.616383   -3.327717   -0.427397
 H   -5.487906   -3.481155   -2.195588
 C   -1.430980   -2.807110    0.117846
 H   -0.903506   -3.665260   -0.325062
 H   -1.042361   -2.669058    1.135456
 H   -1.191603   -1.904243   -0.461136
 C   -3.214393   -4.312965    0.990678
 H   -2.697577   -4.255947    1.960973
 H   -4.286877   -4.439776    1.186406
 H   -2.843171   -5.203759    0.460490
 H   -4.610150    1.252894   -1.676818
 O   -5.347213   -0.579939    0.160886
 C   -5.680666    1.082496   -1.571193
 C   -6.139906    0.144820   -0.625528
 C   -6.584975    1.809712   -2.344734
 C   -7.531013   -0.022198   -0.484538
 C   -7.960883    1.633784   -2.200219
 H   -7.887528   -0.748057    0.249610
 C   -8.424465    0.712031   -1.258077
 H   -8.661643    2.208738   -2.809070
 H   -9.498682    0.558890   -1.125271
 H   -6.201335    2.532592   -3.069896
116
Figure_S15-9_PA-9b(Naborate)-ts(1,6major)_02 / electronic energy: -4398.56128250 a.u. / lowest freq: -438.38 cm-1
 H    5.740831    2.642307    0.738122
 H    7.367429    2.508999   -1.628147
 H    5.048800    2.181854   -1.437421
 H    9.696529    1.673001   -1.690672
 C    7.567459    1.449991   -1.443307
 C    5.117458    1.126736   -1.159469
 C    8.879319    0.980316   -1.477446
 C    6.495819    0.584356   -1.178781
 C    9.146540   -0.367690   -1.241496
 H   10.173221   -0.739227   -1.267111
 C    6.779959   -0.768923   -0.939499
 C    8.089838   -1.239378   -0.971176
 H    5.970473   -1.464352   -0.714922
 H    8.287337   -2.296914   -0.781998
 H    2.818028    2.057773   -1.831034
 C    2.756510    0.975858   -1.689168
 C    3.986890    0.353713   -1.420069
 H    4.040234   -0.730950   -1.359180
Cu    1.514966    0.858241    0.010365
 H    1.907128    2.209168    2.218633
 C    2.571226    1.893500    1.413089
 C    3.833666    1.914699    1.313034
 C    5.137472    1.760319    0.970054
 H    5.682339    0.912378    1.397191
 N   -1.281228    0.828615    1.073422
 C   -0.048199    0.350254    1.140821
 N    0.056906   -0.374441    2.278202
 C   -1.764048    1.749812    0.054646
 O   -0.502443    1.078368   -3.303184
 C    0.493805    1.356053   -2.658715
 C    1.478820    0.419939   -2.090695
 C    1.197889   -1.011740   -2.235007
 O    0.196990   -1.510579   -2.723499
Na   -1.903678   -0.729760   -3.108470
 C   -2.145066    0.375437    2.167366
 H   -2.865043   -0.357331    1.770559
 C   -1.136613   -0.258074    3.124024
 H   -0.927245    0.384467    3.994397
 C    1.210192   -1.064392    2.697710
 C    1.454609   -1.248317    4.059280
 C    2.110594   -1.580959    1.756544
 C    2.610504   -1.909598    4.493641
 C    3.273038   -2.227357    2.170291
 C    3.513664   -2.382403    3.542040
 H    4.423112   -2.892913    3.871477
 H   -1.453577   -1.244964    3.490096
 H   -2.683100    1.222637    2.615392
 O    2.159042   -1.802145   -1.734622
 O    0.774269    2.639375   -2.373461
 C   -0.124672    3.623865   -2.862596
 H   -1.124919    3.490190   -2.425610
 H    0.288419    4.589225   -2.552124
 H   -0.202149    3.574928   -3.957224
 C    1.930031   -3.203862   -1.793704
 H    1.049678   -3.476947   -1.195686
 H    2.827099   -3.674200   -1.378134
 H    1.776350   -3.531844   -2.830388
 H   -1.015002    1.709891   -0.743953
 C   -1.796823    3.168376    0.599100
 C   -2.955401    3.750460    1.123122
 C   -0.604036    3.903017    0.620352
 C   -2.919267    5.039282    1.659580
 H   -3.901324    3.204417    1.118960
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 C   -0.565290    5.187532    1.155572
 H    0.306174    3.456247    0.209573
 C   -1.726450    5.759455    1.679136
 H   -3.831927    5.480659    2.065860
 H    0.374341    5.744281    1.162545
 H   -1.700114    6.766362    2.101341
 C   -3.080185    1.262940   -0.546990
 H   -3.429698    2.035290   -1.258655
 H   -3.851134    1.199147    0.240327
 O   -2.883843    0.042965   -1.172485
 C    4.237545   -2.787741    1.159589
 H    5.280110   -2.599423    1.454520
 H    4.115938   -3.878256    1.060523
 H    4.071049   -2.340281    0.170895
 C    2.865391   -2.080667    5.968700
 H    3.780311   -2.659212    6.154906
 H    2.976137   -1.103485    6.463834
 H    2.026078   -2.598839    6.457088
 H    0.754976   -0.861727    4.802429
 H    1.898455   -1.489394    0.689653
 B   -3.833387   -1.077878   -0.997761
 O   -3.700102   -1.785379    0.267737
 O   -3.447942   -2.047800   -2.024889
 C   -2.979940   -2.983456    0.053307
 C   -3.341762   -3.331815   -1.435724
 C   -2.272169   -4.131756   -2.171377
 H   -2.608168   -4.348224   -3.197256
 H   -1.327296   -3.574420   -2.232817
 H   -2.083379   -5.093154   -1.668857
 C   -4.696392   -4.037627   -1.552213
 H   -4.655256   -5.072048   -1.179762
 H   -5.469565   -3.490341   -0.994357
 H   -4.993460   -4.062628   -2.611110
 C   -1.480130   -2.720018    0.235107
 H   -0.892056   -3.645487    0.143415
 H   -1.307944   -2.316958    1.241897
 H   -1.108471   -1.986478   -0.493860
 C   -3.432687   -4.023496    1.071992
 H   -3.127021   -3.710373    2.082171
 H   -4.524532   -4.136395    1.069052
 H   -2.974559   -5.003800    0.868263
 H   -7.291010    0.617109   -2.079715
 O   -5.211882   -0.593709   -1.252438
 C   -7.217816    0.582980   -0.990259
 C   -6.104790   -0.067289   -0.420708
 C   -8.192673    1.170252   -0.189819
 C   -6.014359   -0.116087    0.985398
 C   -8.090846    1.130336    1.202997
 H   -5.176046   -0.643144    1.438560
 C   -6.996278    0.481582    1.775132
 H   -8.854693    1.593720    1.830927
 H   -6.901291    0.430238    2.863394
 H   -9.043724    1.668706   -0.661684
116
Figure_S15-9_PA-9b(Naborate)-ts(1,6major)_03 / electronic energy: -4398.56061938 a.u. / lowest freq: -437.49 cm-1
 H   -5.772804   -1.897057    1.824301
 H   -6.914458   -3.679267   -0.126138
 H   -4.678540   -2.974901    0.081395
 H   -9.181570   -3.499135   -1.107567
 C   -7.149904   -2.850022   -0.798831
 C   -4.811750   -2.053691   -0.491961
 C   -8.426063   -2.748535   -1.349980
 C   -6.156861   -1.904619   -1.095228
 C   -8.736773   -1.693615   -2.207400
 H   -9.735671   -1.610627   -2.640925
 C   -6.484684   -0.847100   -1.957606
 C   -7.759232   -0.743009   -2.507389
 H   -5.738545   -0.089302   -2.198583
 H   -7.992231    0.088069   -3.176878
 H   -2.407045   -2.789892    0.055832
 C   -2.392316   -1.934690   -0.624763
 C   -3.658753   -1.517226   -1.064423
 H   -3.735771   -0.732155   -1.813092
Cu   -1.544134   -0.441988    0.614496
 H   -2.409025    0.178506    3.006488
 C   -2.878296   -0.299249    2.145600
 C   -4.082413   -0.623509    1.923066
 C   -5.277762   -1.013499    1.411708
 H   -5.944324   -0.240405    1.016792
 N    0.941471    0.665500    1.780606
 C   -0.216759    0.933540    1.196045
 N   -0.424972    2.269526    1.269333
 C    1.499411   -0.671198    1.937257
 O    1.125028   -2.629577   -1.232616
 C    0.027161   -2.524334   -0.715073
 C   -1.065418   -1.621240   -1.117279
 C   -0.775484   -0.659679   -2.186450
 O    0.308891   -0.458692   -2.708427
Na    2.425153   -0.928815   -2.061494
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 C    1.640938    1.847156    2.288961
 H    2.576534    1.996057    1.725980
 C    0.612106    2.951962    2.052947
 H    0.190094    3.331668    2.995972
 C   -1.565046    2.958447    0.809906
 C   -1.847774    4.233603    1.311289
 C   -2.424354    2.395263   -0.142604
 C   -2.989652    4.930975    0.900817
 C   -3.580901    3.062921   -0.541550
 C   -3.854889    4.330080   -0.013607
 H   -4.758969    4.858846   -0.329084
 H    1.019108    3.805988    1.492402
 H    1.880617    1.719118    3.354487
 O   -1.838423    0.067905   -2.558950
 O   -0.284405   -3.269378    0.359552
 C    0.708935   -4.164206    0.838542
 H    1.616019   -3.618468    1.137026
 H    0.271150   -4.661292    1.710325
 H    0.974374   -4.903439    0.070664
 C   -1.610435    1.090870   -3.519260
 H   -0.915231    1.844853   -3.123482
 H   -2.586912    1.547852   -3.711463
 H   -1.199262    0.671924   -4.447168
 H    0.928230   -1.298670    1.244274
 C    1.269653   -1.205687    3.339932
 C    2.179223   -0.995231    4.382043
 C    0.086234   -1.904633    3.609626
 C    1.908491   -1.470132    5.666200
 H    3.114135   -0.460773    4.200981
 C   -0.187566   -2.377049    4.891097
 H   -0.629644   -2.078826    2.801351
 C    0.725033   -2.159850    5.924451
 H    2.630456   -1.300353    6.467934
 H   -1.116916   -2.918020    5.082095
 H    0.515319   -2.532080    6.929593
 C    2.953711   -0.704684    1.472485
 H    3.330520   -1.737443    1.617957
 H    3.579651   -0.055185    2.110281
 O    3.013274   -0.305636    0.149292
 C   -4.534699    2.422332   -1.514407
 H   -5.473617    2.144028   -1.010205
 H   -4.794476    3.107195   -2.335153
 H   -4.104124    1.509212   -1.945747
 C   -3.263800    6.316540    1.425661
 H   -4.342452    6.493835    1.541396
 H   -2.780121    6.483958    2.398127
 H   -2.878923    7.077882    0.728083
 H   -1.186745    4.700651    2.041625
 H   -2.193833    1.430641   -0.595265
 B    4.184048    0.466204   -0.311711
 O    4.319898    1.737197    0.371756
 O    3.928376    0.788263   -1.723242
 C    4.449032    2.754864   -0.604624
 C    3.622878    2.172240   -1.805788
 C    2.112679    2.362772   -1.606634
 H    1.566159    1.767070   -2.353151
 H    1.806000    2.007750   -0.613111
 H    1.808071    3.413382   -1.722853
 C    4.032994    2.696227   -3.175637
 H    3.913055    3.789173   -3.232195
 H    5.077178    2.444363   -3.401773
 H    3.397146    2.246579   -3.953685
 C    3.906084    4.065895   -0.048563
 H    3.904842    4.851230   -0.819778
 H    4.536801    4.407452    0.785834
 H    2.881762    3.948231    0.327181
 C    5.932334    2.925409   -0.956285
 H    6.492388    3.118081   -0.029410
 H    6.334049    2.009536   -1.411607
 H    6.099040    3.768070   -1.643930
 H    3.836549   -2.463375   -0.445621
 O    5.431966   -0.318752   -0.154046
 C    4.785946   -2.495794   -0.981157
 C    5.682121   -1.413361   -0.877357
 C    5.109345   -3.613903   -1.750846
 C    6.914136   -1.509417   -1.549548
 C    6.330261   -3.694860   -2.419770
 H    7.613731   -0.675111   -1.462770
 C    7.232773   -2.634582   -2.305204
 H    6.579807   -4.574564   -3.016730
 H    8.197663   -2.681651   -2.816704
 H    4.392029   -4.436394   -1.816269
116
Figure_S15-9_PA-9b(Naborate)-ts(1,6major)_04 / electronic energy: -4398.56064928 a.u. / lowest freq: -431.71 cm-1
 H   -5.600828    3.180922    0.402947
 H   -7.564720    1.530238    2.046290
 H   -5.198214    1.663359    2.060578
 H   -9.690264    0.481019    1.327931
 C   -7.545200    0.688037    1.349338
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C	-5.060237	0.870714	1.321636
C	-8.741640	0.098077	0.944799
C	-6.311735	0.215500	0.878104
C	-8.727767	-0.975405	0.054773
H	-9.663754	-1.437235	-0.266559
C	-6.311700	-0.865595	-0.017256
C	-7.506075	-1.453460	-0.424221
H	-5.368491	-1.240772	-0.420126
H	-7.483486	-2.289808	-1.127146
H	-2.881952	1.729538	2.454202
C	-2.715988	0.759644	1.978537
C	-3.842434	0.188089	1.362212
H	-3.749144	-0.775429	0.865091
Cu	-1.531746	1.068320	0.291757
H	-1.747281	3.222907	-1.171766
C	-2.473475	2.646438	-0.597217
C	-3.732238	2.711022	-0.487311
C	-5.044880	2.480199	-0.226096
H	-5.634537	1.960647	-0.987089
N	1.135816	0.925224	-1.055007
C	-0.125975	0.518050	-0.988660
N	-0.380391	-0.258071	-2.052079
C	1.767249	1.772319	-0.050480
O	0.628753	0.700294	3.430124
C	-0.432188	1.041822	2.934092
C	-1.413129	0.186996	2.251222
C	-1.072193	-1.229349	2.085395
O	-0.024344	-1.766004	2.413010
Na	2.069652	-0.961646	2.816525
C	1.855640	0.385693	-2.216057
H	2.619981	-0.328935	-1.872378
C	0.732261	-0.301013	-3.005832
H	0.458749	0.243079	-3.924224
C	-1.645887	-0.862161	-2.296778
C	-2.721960	-0.076862	-2.704302
C	-1.804613	-2.233217	-2.096556
C	-3.980673	-0.651579	-2.901197
C	-3.050782	-2.833900	-2.292333
C	-4.123610	-2.027020	-2.690793
H	-5.106039	-2.486896	-2.838132
H	0.977936	-1.335606	-3.285532
H	2.336648	1.192125	-2.787822
O	-2.042252	-1.947535	1.512228
O	-0.790604	2.337908	2.943308
C	0.104022	3.250745	3.561278
H	1.082428	3.239619	3.059540
H	-0.356831	4.238998	3.459272
H	0.245179	3.006689	4.623234
C	-1.795711	-3.330040	1.315046
H	-0.914325	-3.482948	0.678086
H	-2.690015	-3.728217	0.823812
H	-1.634047	-3.839187	2.275378
H	1.123783	1.695831	0.837159
C	1.789763	3.224866	-0.488359
C	2.759558	3.722853	-1.366730
C	0.787930	4.089502	-0.032410
C	2.718220	5.052192	-1.787957
H	3.562237	3.074592	-1.726575
C	0.744801	5.418369	-0.450696
H	0.026749	3.711108	0.655684
C	1.710219	5.902554	-1.333759
H	3.481009	5.425301	-2.474884
H	-0.045307	6.077733	-0.084715
H	1.679297	6.942967	-1.664658
C	3.135528	1.228363	0.355623
H	3.578494	1.945870	1.072632
H	3.807708	1.217264	-0.520253
O	2.989607	-0.033057	0.910487
C	-3.245866	-4.312131	-2.076681
H	-4.076042	-4.504777	-1.380022
H	-3.492594	-4.817987	-3.022934
H	-2.340659	-4.783353	-1.669676
C	-5.151122	0.186285	-3.343668
H	-6.052238	-0.050549	-2.758337
H	-4.938645	1.258586	-3.232191
H	-5.388373	-0.000913	-4.402893
H	-2.575476	0.995200	-2.844576
H	-0.948085	-2.825360	-1.767296
B	3.973274	-1.107884	0.655338
O	3.808364	-1.781239	-0.626033
O	3.674804	-2.126434	1.665437
C	3.168433	-3.024252	-0.418245
C	3.613425	-3.396324	1.041766
C	2.622308	-4.274674	1.797764
H	3.012712	-4.494465	2.803380
H	1.649352	-3.775837	1.909416
H	2.468500	-5.233771	1.279309
C	5.007834	-4.029308	1.075898
H	5.005779	-5.052068	0.670699

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 H    5.722429   -3.422374    0.502025
 H    5.355042   -4.070573    2.118864
 C    1.650030   -2.838345   -0.524726
 H    1.116538   -3.796486   -0.429924
 H    1.417058   -2.421934   -1.513233
 H    1.270743   -2.143058    0.236786
 C    3.629233   -4.008343   -1.487909
 H    3.255630   -3.687765   -2.472504
 H    4.724489   -4.055751   -1.542005
 H    3.240134   -5.019304   -1.290362
 H    7.539109    0.467442    1.591736
 O    5.343035   -0.579292    0.857927
 C    7.373242    0.529929    0.513798
 C    6.187541   -0.026920   -0.006304
 C    8.302654    1.145335   -0.318583
 C    5.977176    0.046510   -1.398570
 C    8.082748    1.226454   -1.695826
 H    5.083309   -0.410415   -1.821151
 C    6.915850    0.670081   -2.220362
 H    8.810768    1.712369   -2.348765
 H    6.728259    0.715992   -3.296759
 H    9.210982    1.570982    0.116305
116
Figure_S15-9_PA-9b(Naborate)-ts(1,6major)_O5 / electronic energy: -4398.55507914 a.u. / lowest freq: -437.49 cm-1
Na   -2.788311   -1.959483   -0.913315
 H    5.865899    1.199277   -2.441072
 C    5.370185    1.017247   -1.484050
 H    6.020929    0.679093   -0.670764
 H    6.721140   -0.759321   -3.794938
 H    8.854563   -2.000231   -3.642901
 C    6.865875   -1.488106   -2.992643
 C    8.068393   -2.184988   -2.907473
 H    4.442718   -0.466520   -3.179797
 C    4.571616   -0.936530   -2.201266
 C    5.833977   -1.701685   -2.064718
 C    8.266356   -3.117523   -1.888780
 H    9.208955   -3.664309   -1.817368
 C    6.042545   -2.653304   -1.055112
 C    7.245988   -3.349547   -0.965972
 H    5.256188   -2.863636   -0.329557
 H    7.384246   -4.085885   -0.170998
 C    4.266281    1.737720   -1.156925
 C    3.111142    2.135170   -0.828219
 H    2.212079   -0.164914   -2.889396
 C    3.395060   -1.259963   -1.524400
 O    0.103778    0.515694   -3.158183
 C    2.169275   -0.718964   -1.948364
 H    3.425637   -1.882632   -0.632313
 C    0.817242   -0.988893   -1.505611
 C   -0.272336   -0.498837   -2.368742
 O    1.488231   -2.225774    0.377559
 H    2.744896    3.104392   -0.487206
Cu    1.686418    0.709521   -0.495032
 C    0.780610    1.482870    1.113879
 N    1.457514    2.028324    2.141439
 N   -0.497358    1.827662    1.228953
 C   -1.553068    1.359825    0.349558
 O   -1.420572   -0.907853   -2.400813
 O   -0.660387   -2.325311   -0.169527
 C   -0.773462    2.680030    2.388147
 H   -1.431805    2.160138    3.099920
 C    0.630191    2.924230    2.957726
 H    0.947748    3.969575    2.826771
 C    2.828615    1.799287    2.390777
 C    3.645847    2.830932    2.846830
 C    3.365081    0.527231    2.159680
 C    5.016625    2.614193    3.037901
 C    4.727241    0.295727    2.329271
 C    5.541596    1.350383    2.764391
 H    6.612548    1.175116    2.902225
 H    0.716843    2.668555    4.022730
 H   -1.273727    3.606269    2.070723
 C    0.456058   -1.900054   -0.417273
 C   -0.888999    1.064914   -4.014641
 H   -1.232826    0.316144   -4.741940
 H   -0.409251    1.902477   -4.531726
 H   -1.747231    1.427802   -3.431670
 C    1.192171   -3.033119    1.509237
 H    0.445103   -2.547480    2.153006
 H    2.138737   -3.154534    2.047358
 H    0.804958   -4.014123    1.200609
 H   -1.105661    0.535963   -0.221867
 C   -1.992051    2.431170   -0.641133
 C   -1.019607    3.218316   -1.271218
 C   -3.336117    2.619484   -0.983051
 C   -1.375238    4.170146   -2.223820
 H    0.035472    3.077807   -1.024116
 C   -3.690741    3.572657   -1.939784
 H   -4.117267    2.014275   -0.515517
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 C   -2.716184    4.349383   -2.564299
 H   -0.600042    4.769782   -2.706246
 H   -4.744511    3.709360   -2.194940
 H   -3.000064    5.093012   -3.312159
 C   -2.676844    0.710215    1.159725
 H   -3.354288    1.479618    1.576455
 H   -2.211186    0.183002    2.014628
 O   -3.354618   -0.175063    0.338230
 C    5.318482   -1.062134    2.062394
 H    6.078002   -1.013028    1.267136
 H    5.813041   -1.464136    2.959698
 H    4.547363   -1.779108    1.748238
 C    5.894857    3.732386    3.536009
 H    6.959106    3.507222    3.382863
 H    5.666485    4.678068    3.022968
 H    5.738776    3.900183    4.613598
 H    3.228027    3.823505    3.028115
 H    2.708151   -0.281530    1.831861
 B   -4.752598   -0.542003    0.641787
 O   -5.124297   -1.568355   -0.348365
 O   -5.668431    0.556803    0.439370
 C   -6.013642   -0.984160   -1.286170
 C   -6.698654    0.151379   -0.438528
 C   -7.158333    1.351657   -1.259258
 H   -7.896907    1.053897   -2.019553
 H   -7.628958    2.094664   -0.598000
 H   -6.311196    1.835399   -1.763541
 C   -7.870897   -0.380081    0.395625
 H   -8.744838   -0.631410   -0.223965
 H   -7.570823   -1.271739    0.964491
 H   -8.168720    0.396284    1.115584
 C   -5.197429   -0.426571   -2.460119
 H   -5.836729    0.019362   -3.236002
 H   -4.474926    0.327191   -2.117464
 H   -4.636722   -1.248484   -2.932774
 C   -6.975225   -2.049857   -1.800491
 H   -6.425451   -2.794732   -2.396002
 H   -7.467957   -2.574971   -0.971986
 H   -7.748402   -1.605365   -2.446170
 H   -2.603065   -4.981676    1.820806
 H   -1.381215   -4.494405    3.940131
 C   -2.789705   -4.047907    2.357779
 C   -2.107294   -3.780587    3.545134
 C   -3.718374   -3.141909    1.847436
 C   -2.376948   -2.591379    4.226542
 H   -1.861026   -2.370688    5.164769
 C   -3.970780   -1.927397    2.511361
 C   -3.295705   -1.675925    3.719064
 O   -4.829858   -1.015180    2.046121
 H   -3.502267   -0.737865    4.239447
 H   -4.276149   -3.360901    0.934962
116
Figure_S15-9_PA-9b(Naborate)-ts(1,6major)_06 / electronic energy: -4398.56485118 a.u. / lowest freq: -458.95 cm-1
 H    5.796405    2.467817    0.910039
 H    7.503943    2.213729   -1.164601
 H    5.154911    2.026391   -1.258632
 H    9.769252    1.215640   -1.157831
 C    7.617688    1.129653   -1.077338
 C    5.135874    0.971060   -0.972846
 C    8.893008    0.568901   -1.073514
 C    6.471498    0.326538   -0.972670
 C    9.050148   -0.812509   -0.962140
 H   10.048069   -1.255947   -0.956168
 C    6.645112   -1.061884   -0.870038
 C    7.919083   -1.624285   -0.862692
 H    5.776731   -1.717023   -0.794790
 H    8.029692   -2.707785   -0.778855
 H    2.931414    2.081150   -1.684336
 C    2.784560    1.004889   -1.562118
 C    3.953803    0.286233   -1.263602
 H    3.913219   -0.798594   -1.190840
Cu    1.528896    0.864995    0.127591
 H    1.926541    2.191397    2.352636
 C    2.602757    1.838887    1.573340
 C    3.864678    1.812733    1.481560
 C    5.162726    1.604886    1.132972
 H    5.680873    0.749818    1.579646
 N   -1.077007    1.162626    1.433162
 C   -0.067952    0.333651    1.190110
 N   -0.221366   -0.761109    1.956700
 C   -1.309776    2.386166    0.679636
 O   -0.427885    1.390676   -3.206708
 C    0.555783    1.577513   -2.513395
 C    1.473157    0.557816   -1.981068
 C    1.061749   -0.845030   -2.098506
 O   -0.015718   -1.250126   -2.507949
Na   -2.038359   -0.139291   -2.651255
 C   -2.001609    0.676230    2.458526
 H   -3.026195    0.617789    2.065303
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 C   -1.430491   -0.706274    2.786046
 H   -1.163123   -0.822132    3.846577
 C    0.613924   -1.900508    1.927420
 C    1.995787   -1.758990    1.757174
 C    0.061447   -3.174245    2.073354
 C    2.822459   -2.878563    1.695529
 C    0.879288   -4.310677    2.035925
 C    2.251811   -4.149397    1.837868
 H    2.895330   -5.033332    1.795185
 H   -2.130137   -1.505318    2.513551
 H   -1.991122    1.352196    3.327538
 O    1.987804   -1.701819   -1.657644
 O    0.890650    2.825787   -2.137965
 C    0.044451    3.878650   -2.575277
 H   -0.982144    3.727521   -2.211846
 H    0.461949    4.797681   -2.150352
 H    0.028366    3.941933   -3.672077
 C    1.619732   -3.067892   -1.538355
 H    0.869955   -3.193281   -0.743204
 H    2.534850   -3.602356   -1.261926
 H    1.222232   -3.455542   -2.486120
 H   -0.579997    2.355794   -0.139997
 C   -1.021843    3.630720    1.497550
 C   -1.912838    4.105757    2.468010
 C    0.174722    4.325562    1.285552
 C   -1.605896    5.241706    3.217362
 H   -2.861096    3.591965    2.642727
 C    0.483904    5.460812    2.033004
 H    0.876197    3.964227    0.528417
 C   -0.406363    5.920725    3.003375
 H   -2.310946    5.599446    3.970960
 H    1.424868    5.986530    1.856685
 H   -0.167221    6.810378    3.590233
 C   -2.700531    2.398438    0.028390
 H   -2.799883    3.377277   -0.476675
 H   -3.489263    2.368551    0.801242
 O   -2.868538    1.376889   -0.887072
 C    0.272698   -5.677346    2.217415
 H    0.936727   -6.466649    1.838394
 H    0.087785   -5.880509    3.284562
 H   -0.693846   -5.751587    1.699004
 C    4.305615   -2.720000    1.490767
 H    4.645809   -3.297767    0.617059
 H    4.576437   -1.666890    1.331969
 H    4.870414   -3.089597    2.360471
 H    2.434932   -0.762329    1.687644
 H   -1.017474   -3.300033    2.183335
 B   -3.644284    0.155178   -0.598214
 O   -4.289829   -0.241107   -1.857639
 O   -4.703318    0.287965    0.365887
 C   -5.692104   -0.309092   -1.684289
 C   -5.921250    0.484151   -0.333340
 C   -6.119404    1.987687   -0.565917
 H   -6.090337    2.502278    0.406233
 H   -5.315600    2.397918   -1.192811
 H   -7.086088    2.207646   -1.041881
 C   -7.067940   -0.049426    0.517693
 H   -8.024274    0.008892   -0.024282
 H   -6.894818   -1.092779    0.812019
 H   -7.158837    0.551951    1.434764
 C   -6.382794    0.318287   -2.893275
 H   -7.471528    0.380589   -2.741636
 H   -6.200698   -0.299663   -3.785688
 H   -5.997870    1.325935   -3.096452
 C   -6.102758   -1.782198   -1.587408
 H   -5.739752   -2.307122   -2.483814
 H   -5.651640   -2.265206   -0.710794
 H   -7.195160   -1.903687   -1.536996
 H   -4.344897   -1.793494    1.527945
 O   -2.605691   -0.852831   -0.236964
 C   -3.766810   -2.555605    1.004007
 C   -2.851824   -2.143117    0.019906
 C   -3.935497   -3.911293    1.282546
 C   -2.121735   -3.120733   -0.673456
 C   -3.206300   -4.880193    0.590799
 H   -1.400275   -2.791583   -1.423937
 C   -2.299354   -4.472400   -0.389221
 H   -3.344853   -5.940670    0.811941
 H   -1.716349   -5.216372   -0.938560
 H   -4.651631   -4.213814    2.050934
116
Figure_S15-9_PA-9b(Naborate)-ts(1,6major)_07 / electronic energy: -4398.56096625 a.u. / lowest freq: -450.65 cm-1
 H   -5.831829   -1.844022    1.262390
 H   -7.331535   -2.328229   -0.695857
 H   -4.945847   -2.415660   -0.797657
 H   -9.479622   -1.313068   -1.383208
 C   -7.334258   -1.351630   -1.187738
 C   -4.851234   -1.342452   -0.983644
 C   -8.544671   -0.781248   -1.573262
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C	-6.114432	-0.694868	-1.416217
C	-8.563579	0.464411	-2.201412
H	-9.510824	0.916004	-2.503609
C	-6.149226	0.549965	-2.063119
C	-7.359143	1.123990	-2.446990
H	-5.221236	1.078741	-2.283310
H	-7.358921	2.094294	-2.948590
H	-2.681904	-2.753649	-0.918314
C	-2.463794	-1.727450	-1.225811
C	-3.589504	-0.902604	-1.384130
H	-3.456535	0.111295	-1.756122
Cu	-1.359363	-0.992629	0.395879
H	-2.069438	-1.312727	2.898413
C	-2.636697	-1.273084	1.968281
C	-3.876034	-1.179541	1.732007
C	-5.111818	-1.024781	1.186944
H	-5.547820	-0.020305	1.181799
N	1.296189	-0.690609	1.674157
C	0.137311	-0.118779	1.380790
N	0.063346	1.052025	2.050020
C	1.739315	-1.963931	1.133619
O	0.787746	-2.891420	-2.348348
C	-0.233098	-2.727088	-1.704455
C	-1.100703	-1.539213	-1.683385
C	-0.645075	-0.367972	-2.441653
O	0.301494	-0.323219	-3.206641
Na	2.349627	-1.304323	-3.024697
C	2.151689	0.121820	2.536977
H	3.027946	0.477347	1.975194
C	1.216065	1.265965	2.931947
H	0.908069	1.197448	3.986982
C	-1.015599	1.953740	2.009800
C	-1.191829	2.875146	3.045033
C	-1.903956	1.960751	0.927765
C	-2.259050	3.780483	3.023435
C	-2.990987	2.831116	0.904896
C	-3.158651	3.739615	1.957378
H	-4.000894	4.437054	1.937148
H	1.656897	2.257287	2.754176
H	2.497743	-0.464082	3.400838
O	-1.376458	0.734518	-2.215300
O	-0.663216	-3.686657	-0.862597
C	0.115179	-4.869356	-0.775133
H	1.118307	-4.648864	-0.381352
H	-0.415633	-5.529465	-0.081018
H	0.213525	-5.350833	-1.757784
C	-0.972705	1.916697	-2.893344
H	0.088937	2.125595	-2.707294
H	-1.593601	2.724407	-2.489872
H	-1.136783	1.819031	-3.975600
H	0.957537	-2.253585	0.422896
C	1.779646	-3.022347	2.221769
C	2.951161	-3.366186	2.902706
C	0.581118	-3.653797	2.579330
C	2.925175	-4.324483	3.918169
H	3.898054	-2.886724	2.645591
C	0.552152	-4.609130	3.591609
H	-0.339361	-3.389353	2.049830
C	1.727947	-4.947776	4.264621
H	3.848851	-4.583765	4.440284
H	-0.390295	-5.094882	3.853828
H	1.709705	-5.699025	5.057058
C	3.029305	-1.820155	0.322154
H	3.335487	-2.840430	0.023918
H	3.847873	-1.417004	0.944677
O	2.836841	-1.037026	-0.801299
C	-3.979292	2.769332	-0.228247
H	-4.745869	2.003434	-0.028611
H	-4.497151	3.727799	-0.372201
H	-3.487310	2.494621	-1.172264
C	-2.409704	4.788658	4.133228
H	-2.302948	4.314714	5.120323
H	-1.632749	5.566274	4.060478
H	-3.388156	5.286633	4.094804
H	-0.495850	2.902683	3.884454
H	-1.732237	1.304843	0.072737
B	3.377022	0.336307	-0.913081
O	3.621275	0.538672	-2.354788
O	4.663810	0.516818	-0.274414
C	4.961729	0.945056	-2.548283
C	5.674874	0.394596	-1.256825
C	6.063278	-1.083867	-1.393510
H	6.365522	-1.462623	-0.405621
H	5.209332	-1.684687	-1.737070
H	6.902815	-1.229092	-2.089352
C	6.894576	1.200267	-0.824298
H	7.661891	1.208198	-1.613656
H	6.625480	2.238137	-0.587830
H	7.338158	0.750220	0.076726

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 C    5.486025    0.353976   -3.853380
 H    6.560946    0.556224   -3.979131
 H    4.956406    0.804342   -4.706810
 H    5.331758   -0.733357   -3.893596
 C    5.002064    2.475134   -2.630951
 H    4.311208    2.802728   -3.421932
 H    4.671465    2.929316   -1.686382
 H    6.007520    2.851948   -2.871609
 H    4.406176    2.460270    0.767464
 O    2.319507    1.232462   -0.403477
 C    3.494459    3.050883    0.689449
 C    2.376238    2.481401    0.048780
 C    3.416048    4.338025    1.222665
 C    1.202586    3.251709   -0.042433
 C    2.240988    5.086710    1.143754
 H    0.330532    2.799499   -0.514673
 C    1.131949    4.527798    0.504009
 H    2.188350    6.087850    1.576844
 H    0.193557    5.084885    0.437220
 H    4.295056    4.758441    1.719171
116
Figure_S15-9_PA-9b(Naborate)-ts(1,6major)_08 / electronic energy: -4398.56213541 a.u. / lowest freq: -466.03 cm-1
 H   -5.354416   -3.216702    0.841375
 C   -8.454198   -2.224031   -1.753864
 H   -9.978381   -0.703317   -1.952683
 H   -6.747166   -3.517086   -1.511738
 C   -8.920171   -0.909645   -1.778875
 C   -7.103508   -2.483266   -1.530443
 C   -8.020317    0.139035   -1.581839
 C   -6.187720   -1.439332   -1.329911
 H   -8.372867    1.172888   -1.601731
 C   -6.670587   -0.122515   -1.360770
 H   -4.516695   -2.816254   -1.277209
 C   -4.759615   -1.765842   -1.093722
 H   -5.984986    0.711307   -1.208251
 C   -4.947379   -2.218500    1.026709
 C   -3.699598   -2.105008    1.559560
 C   -2.486293   -1.842723    1.806133
 C   -3.719971   -0.860186   -1.322299
Cu   -1.446383   -0.808515    0.375336
 H   -2.294848   -2.414275   -1.441120
 C   -2.396252   -1.324287   -1.414060
 C   -1.171485   -0.630049   -1.738680
 C   -0.037576   -1.476747   -2.159186
 C   -1.040371    0.802408   -2.012067
 O    0.748207   -1.229718   -3.052561
 O   -0.036412    1.360309   -2.430467
Na    2.056816    0.618181   -3.145304
 H    1.143057   -4.259061   -1.024700
 O    0.047027   -2.620306   -1.466535
 C    1.128875   -3.482559   -1.797523
 H    2.072350   -2.919681   -1.802269
 H    0.973692   -3.939338   -2.785495
 H   -5.688262   -1.463430    1.309349
 H   -3.913151    0.210720   -1.360466
 O   -2.137122    1.507864   -1.714640
 C   -2.033151    2.921725   -1.780388
 H   -1.684176    3.246564   -2.769910
 N    0.968960   -0.435687    1.977970
 N   -0.188791    1.399717    2.007696
 C   -0.129912    0.147122    1.514253
 C    1.441613   -1.731329    1.508626
 H   -9.147169   -3.053894   -1.910037
 H   -1.878110   -1.950040    2.704628
 C    1.788792    0.440376    2.813683
 H    2.794696    0.548153    2.383091
 C    1.014331    1.759214    2.768111
 H    0.739383    2.134556    3.764334
 C   -1.231929    2.322354    1.796027
 C   -2.528553    1.890360    1.494680
 C   -0.976832    3.691923    1.916739
 C   -3.548758    2.811747    1.264461
 C   -1.989568    4.630494    1.698193
 C   -3.269470    4.178671    1.368644
 H   -4.068505    4.905781    1.195566
 H    1.581112    2.539139    2.242530
 H    1.878643    0.030663    3.830783
 H   -1.341966    3.290406   -1.007396
 H   -3.038263    3.310189   -1.585748
 H    0.679131   -2.066211    0.792726
 C    1.529352   -2.760281    2.617803
 C    2.556697   -2.737568    3.569567
 C    0.558043   -3.764772    2.703910
 C    2.602302   -3.687156    4.589740
 H    3.336746   -1.974610    3.518493
 C    0.603090   -4.718000    3.720572
 H   -0.245405   -3.796136    1.962711
 C    1.625198   -4.679339    4.668764
 H    3.408346   -3.653326    5.325927
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 H   -0.163468   -5.494300    3.770708
 H    1.662474   -5.424636    5.466180
 C    2.743561   -1.564206    0.720562
 H    2.969840   -2.542395    0.251208
 H    3.592023   -1.346969    1.394813
 O    2.555162   -0.550018   -0.194881
 C   -1.689753    6.105007    1.778356
 H   -1.563503    6.531306    0.769928
 H   -2.509285    6.654662    2.263729
 H   -0.763655    6.298707    2.337384
 C   -4.926627    2.339450    0.884735
 H   -5.123720    2.552546   -0.178816
 H   -5.039129    1.256798    1.036445
 H   -5.705799    2.854239    1.465819
 H   -2.755177    0.823672    1.457527
 H    0.025157    4.042456    2.162994
 B    3.659880    0.003379   -0.945292
 O    3.864489   -0.614111   -2.268656
 O    4.934361   -0.110497   -0.274225
 C    5.177891   -1.126102   -2.357625
 C    5.941126   -0.309834   -1.246770
 C    7.109340   -1.053543   -0.609763
 H    7.598051   -0.408805    0.136084
 H    6.771149   -1.964885   -0.099775
 H    7.861038   -1.330439   -1.364971
 C    6.423968    1.054872   -1.756458
 H    7.255903    0.958929   -2.469823
 H    5.603626    1.606362   -2.236339
 H    6.773684    1.649725   -0.899445
 C    5.137501   -2.627248   -2.048184
 H    6.118819   -3.107555   -2.178305
 H    4.425422   -3.110579   -2.733759
 H    4.795019   -2.805156   -1.018752
 C    5.713394   -0.916898   -3.770565
 H    5.144279   -1.537416   -4.479678
 H    5.615092    0.131562   -4.082291
 H    6.773552   -1.205537   -3.842442
 H    4.736141    1.891880    0.820452
 O    3.207809    1.409292   -1.290866
 C    3.939797    2.617926    0.656272
 C    3.058950    2.410194   -0.422138
 C    3.801938    3.743376    1.467483
 C    2.019878    3.336016   -0.630528
 C    2.793999    4.681332    1.233172
 H    1.307068    3.143205   -1.435256
 C    1.902849    4.462674    0.179729
 H    2.699075    5.566004    1.866541
 H    1.094381    5.174370   -0.007765
 H    4.503181    3.892690    2.292937
116
Figure_S15-9_PA-9b(Naborate)-ts(1,6major)_09 / electronic energy: -4398.56071055 a.u. / lowest freq: -403.07 cm-1
 C   -1.406877    1.844433   -2.080887
 H   -2.294799    2.192140   -1.545881
 C   -0.182486    2.722316   -1.838677
 H    0.105444    3.323113   -2.711957
 C    0.332854    0.514266   -1.255826
 C    2.224423    2.066242   -1.496545
 C    2.627895    3.328472   -1.063645
 C    3.177737    1.152505   -1.962483
 C    3.985628    3.675460   -1.049111
 C    4.530911    1.481665   -1.968046
 C    4.922035    2.744252   -1.498834
 H    5.983761    3.008536   -1.501748
Cu    1.323328   -0.979937   -0.350220
 N   -0.968192    0.552912   -1.529963
 N    0.852880    1.731381   -1.524687
 C    2.173334   -1.441959    1.547332
 C    0.862893   -0.890911    1.800286
 B   -4.327693    0.976694   -0.090502
 H   -0.335843    3.401787   -0.984151
 H   -1.645067    1.736481   -3.150536
 H    2.226250   -2.525081    1.674612
 C    0.596727    0.528681    2.047706
 C   -0.217740   -1.841301    2.098801
 O    1.654592    1.318138    1.833121
 O   -0.458380    1.015642    2.425626
 O   -1.392522   -1.570145    2.308432
 O    0.187833   -3.116277    2.124438
 C   -0.768652   -4.104452    2.470537
 H   -1.198754   -3.904358    3.461562
 H   -0.228812   -5.057092    2.479179
 H   -1.583908   -4.148896    1.734628
 C    1.474965    2.707469    2.048354
 H    0.702488    3.107787    1.376541
 H    2.440896    3.173234    1.826088
 H    1.184202    2.910013    3.088310
 C   -1.867766   -0.573943   -1.282258
 H   -2.004418   -0.680215   -0.195992
 C   -1.290829   -1.873244   -1.805288
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 C   -1.306909   -3.011849   -0.998342
 C   -0.826895   -1.982887   -3.121326
 C   -0.854846   -4.239091   -1.483683
 H   -1.697103   -2.926678    0.017531
 C   -0.386404   -3.208795   -3.614237
 H   -0.798276   -1.097843   -3.762213
 C   -0.395256   -4.341029   -2.794749
 H   -0.864632   -5.117176   -0.834111
 H   -0.025387   -3.282673   -4.642418
 H   -0.038913   -5.298456   -3.180506
 C   -3.266488   -0.404370   -1.912759
 H   -3.765310   -1.379149   -1.750819
 H   -3.135097   -0.306060   -3.005687
 O   -4.048826    0.646488   -1.478436
 C    3.409240   -0.804259    1.353609
 H    3.441407    0.271820    1.199491
 C    4.589495   -1.547420    1.307171
 H    4.549660   -2.552181    1.732458
 C    5.926932   -0.915725    1.339845
 C    7.044448   -1.684707    1.700363
 C    6.126874    0.437057    1.023949
 C    8.318759   -1.123885    1.744245
 H    6.908689   -2.741258    1.946771
 C    7.400336    0.998224    1.065680
 H    5.283741    1.062155    0.724353
 C    8.503126    0.221961    1.425814
 H    9.173262   -1.741718    2.029507
 H    7.531683    2.053147    0.813506
 H    9.500758    0.664887    1.459515
 C    5.556466    0.515669   -2.498591
 H    5.086377   -0.412650   -2.850773
 H    6.114810    0.957935   -3.337786
 H    6.290076    0.258297   -1.718748
 C    4.408984    5.029821   -0.542461
 H    5.484423    5.196792   -0.691095
 H    3.862907    5.835069   -1.056795
 H    4.197583    5.131357    0.533794
 H    1.887340    4.053402   -0.720000
 H    2.852868    0.184031   -2.343496
 C    2.376379   -2.285125   -1.497220
 H    1.726459   -2.575453   -2.325111
 C    3.582213   -2.547346   -1.218792
 C    4.827554   -2.612121   -0.685135
 H    5.163914   -3.540711   -0.215509
 H    5.614758   -1.982405   -1.108151
Na   -2.586713    0.357566    2.161736
 H   -6.547795   -0.485721   -0.635785
 C   -6.160230   -1.416015   -0.218159
 O   -4.298645   -0.254722    0.774965
 C   -4.982345   -1.382181    0.544667
 C   -4.488469   -2.576161    1.096520
 H   -3.565389   -2.535045    1.681272
 C   -5.153444   -3.780031    0.879190
 H   -4.751390   -4.700380    1.311094
 H   -7.727187   -2.643933   -1.029798
 C   -6.812678   -2.629594   -0.430986
 C   -6.319131   -3.817739    0.110982
 H   -6.837427   -4.763061   -0.062474
 O   -3.289871    1.860208    0.497655
 O   -5.557377    1.723602    0.029034
 C   -5.248739    3.093447    0.167810
 C   -3.887787    3.059341    0.960899
 C   -5.092947    3.721486   -1.224825
 C   -6.388372    3.791055    0.903552
 H   -4.262891    3.259279   -1.776675
 C   -2.952186    4.228898    0.671752
 C   -4.103866    2.949733    2.476315
 H   -4.930256    4.808333   -1.172392
 H   -6.015242    3.534925   -1.794412
 H   -7.291425    3.784713    0.274825
 H   -6.136730    4.839795    1.125596
 H   -6.630797    3.278761    1.843784
 H   -2.691535    4.279364   -0.393648
 H   -3.410752    5.186625    0.962617
 H   -2.019908    4.107305    1.244272
 H   -3.132207    2.814206    2.978842
 H   -4.556135    3.857253    2.900636
 H   -4.754996    2.095740    2.716480
116
Figure_S15-9_PA-9b(Naborate)-ts(1,6major)_10 / electronic energy: -4398.56065632 a.u. / lowest freq: -402.77 cm-1
 C    1.404445    1.842430    2.083772
 H    2.290958    2.192644    1.547997
 C    0.178071    2.718922    1.845294
 H   -0.111136    3.314996    2.721394
 C   -0.333492    0.511590    1.255895
 C   -2.227806    2.059006    1.500194
 C   -2.634436    3.320786    1.064813
 C   -3.177905    1.145418    1.969258
 C   -3.991476    3.665354    1.052108
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C	-4.532638	1.473195	1.977644
C	-4.925998	2.733639	1.508728
H	-5.987859	2.997690	1.516070
Cu	-1.322460	-0.981103	0.346809
N	0.967311	0.551172	1.531036
N	-0.855322	1.727328	1.526661
C	-2.172031	-1.438848	-1.551427
C	-0.861311	-0.888023	-1.803442
B	4.327384	0.979212	0.093260
H	0.330081	3.402829	0.994091
H	1.644712	1.732966	3.152776
H	-2.225690	-2.521677	-1.680905
C	-0.594236	0.531724	-2.049033
C	0.219110	-1.838508	-2.102584
O	-1.651233	1.322023	-1.833234
O	0.461194	1.018216	-2.426685
O	1.394134	-1.567623	-2.311222
O	-0.186944	-3.113297	-2.129836
C	0.769385	-4.101391	-2.476600
H	1.199160	-3.900934	-3.467698
H	0.229493	-5.053999	-2.485450
H	1.584903	-4.146118	-1.741005
C	-1.469410	2.711434	-2.046655
H	-0.697292	3.109778	-1.373234
H	-2.434815	3.178578	-1.825235
H	-1.176691	2.914736	-3.085901
C	1.868061	-0.574356	1.281728
H	2.005363	-0.678644	0.195353
C	1.292002	-1.875108	1.802142
C	1.309240	-3.012186	0.993072
C	0.827584	-1.987580	3.117762
C	0.857861	-4.240660	1.475927
H	1.699685	-2.924807	-0.022521
C	0.387771	-3.214732	3.608196
H	0.798068	-1.103784	3.760325
C	0.397776	-4.345420	2.786593
H	0.868499	-5.117485	0.824671
H	0.026354	-3.290794	4.636076
H	0.041954	-5.303832	3.170384
C	3.266264	-0.404619	1.913235
H	3.765927	-1.378793	1.750281
H	3.134219	-0.307893	3.006226
O	4.047932	0.647458	1.480689
C	-3.407485	-0.800663	-1.355980
H	-3.438813	0.275179	-1.199801
C	-4.588212	-1.543149	-1.310626
H	-4.549323	-2.546907	-1.738351
C	-5.925275	-0.910613	-1.340303
C	-7.043296	-1.677194	-1.704303
C	-6.124340	0.440652	-1.017513
C	-8.317309	-1.115430	-1.744985
H	-6.908195	-2.732588	-1.955972
C	-7.397489	1.002713	-1.055925
H	-5.280690	1.063542	-0.714863
C	-8.500824	0.228880	-1.419656
H	-9.172270	-1.731338	-2.033023
H	-7.528241	2.056387	-0.798233
H	-9.498238	0.672486	-1.450666
C	-5.555304	0.505725	2.511301
H	-5.083302	-0.422715	2.860593
H	-6.111011	0.946485	3.353015
H	-6.291377	0.248702	1.733633
C	-4.430567	5.005344	0.520780
H	-5.377722	5.327546	0.975473
H	-3.674534	5.780878	0.709239
H	-4.587475	4.957005	-0.569168
H	-1.894841	4.045592	0.719227
H	-2.850920	0.178357	2.352093
C	-2.374771	-2.288923	1.491245
H	-1.724529	-2.581139	2.318206
C	-3.580840	-2.549893	1.212725
C	-4.826420	-2.612582	0.679442
H	-5.163719	-3.539747	0.207682
H	-5.612943	-1.983154	1.104135
Na	2.588740	0.359691	-2.160758
H	6.548155	-0.481978	0.639395
C	6.161970	-1.412149	0.220223
O	4.300258	-0.251493	-0.773388
C	4.984834	-1.378540	-0.543770
C	4.492677	-2.572346	-1.097543
H	3.570152	-2.531537	-1.683203
C	5.158605	-3.775827	-0.880980
H	4.757880	-4.696060	-1.314352
H	7.729291	-2.639509	1.032004
C	6.815393	-2.625340	0.432254
C	6.323555	-3.813312	-0.111650
H	6.842573	-4.758345	0.061218
O	3.289020	1.862035	-0.494925
O	5.556328	1.727547	-0.024739

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 C    5.246241    3.097164   -0.162615
 C    3.886018    3.062133   -0.956870
 C    5.088557    3.723846    1.230420
 C    6.385688    3.796645   -0.896861
 H    4.258400    3.260373    1.781063
 C    2.948847    4.230451   -0.667780
 C    4.103578    2.953809   -2.472183
 H    4.924901    4.810590    1.178795
 H    6.010481    3.537626    1.800715
 H    7.288204    3.790912   -0.267357
 H    6.133009    4.845246   -1.118386
 H    6.629490    3.285273   -1.837237
 H    2.687043    4.279829    0.397392
 H    3.406662    5.188902   -0.957438
 H    2.017274    4.108276   -1.241324
 H    3.132519    2.817573   -2.975674
 H    4.555187    3.862159   -2.895439
 H    4.755918    2.100746   -2.712449
51
Figure_S15-9_9d-Cu-allenyl / electronic energy: -2677.36469942 a.u. / lowest freq: 18.91 cm-1
 C   -0.949725   -2.111091   -0.745708
 H   -1.456710   -2.283710   -1.705397
 C    0.561005   -2.346837   -0.831595
 H    0.890390   -3.232260   -0.270668
 C    0.165570   -0.172304   -0.062012
 C    2.489588   -0.947618   -0.009125
 C    3.411595   -1.770382   -0.661262
 C    2.949352    0.031053    0.882181
 C    4.786704   -1.603717   -0.456366
 C    4.314605    0.217353    1.092648
 C    5.223765   -0.605927    0.415840
 H    6.296282   -0.467228    0.579491
Cu    0.319303    1.720856    0.321210
 N   -1.018985   -0.701736   -0.358187
 N    1.108117   -1.120853   -0.238640
 H   -1.611031    2.294197   -1.821534
 H    0.899252   -2.452084   -1.873899
 H   -1.438768   -2.738242    0.015197
 C   -2.263181    0.059952   -0.389790
 H   -2.079760    0.941851    0.244418
 C   -3.394832   -0.734034    0.234210
 C   -4.274734   -1.509681   -0.527751
 C   -3.538962   -0.723986    1.626854
 C   -5.279826   -2.255582    0.089569
 H   -4.183468   -1.543227   -1.615414
 C   -4.540821   -1.467687    2.245898
 H   -2.855877   -0.121511    2.231908
 C   -5.415255   -2.236764    1.476429
 H   -5.958977   -2.855647   -0.519831
 H   -4.643075   -1.444096    3.332974
 H   -6.203316   -2.819047    1.958824
 C   -2.550525    0.591965   -1.802286
 H   -3.536244    1.092393   -1.782965
 H   -2.627040   -0.245072   -2.514744
 O   -1.535632    1.430876   -2.265600
 C    4.800481    1.257189    2.068770
 H    4.053326    2.049530    2.216065
 H    5.002982    0.802287    3.051711
 H    5.735078    1.721832    1.723578
 C    5.770329   -2.464765   -1.205878
 H    6.734464   -2.524069   -0.682115
 H    5.386771   -3.485941   -1.343318
 H    5.962508   -2.048637   -2.207961
 H    3.073111   -2.542835   -1.353500
 H    2.231718    0.647662    1.427342
 C    0.056509    3.624341    0.493740
 H    0.571009    4.357231    1.130573
 C   -0.918418    4.038216   -0.261867
 C   -1.925600    4.342938   -1.074928
 H   -2.962524    4.334227   -0.721718
 H   -1.744517    4.692912   -2.096941
83
Figure_S15-9_PA-9b-ts(1,6major)_01 / electronic energy: -3519.31528051 a.u. / lowest freq: -465.34 cm-1
 C    3.034515    2.602950    0.387172
 H    3.544892    2.951927   -0.520229
 C    1.692551    3.314894    0.614999
 H    1.658274    3.874150    1.560695
 C    1.323993    1.008726    0.402695
 C   -0.640733    2.364519    0.904516
 C   -1.369351    3.334313    0.220290
 C   -1.271565    1.542913    1.842780
 C   -2.744001    3.474562    0.444986
 C   -2.640900    1.659177    2.077962
 C   -3.361611    2.630826    1.371193
 H   -4.436203    2.732299    1.550886
Cu    0.311656   -0.682535    0.106216
 N    2.626678    1.205870    0.227952
 N    0.745043    2.195348    0.651104
 C   -0.807356   -1.657947   -1.438614
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 C    0.241365   -0.898350   -2.063450
 H    3.271968    0.521313   -2.632356
 H    1.449883    4.010548   -0.202024
 H    3.716239    2.713074    1.244396
 H   -0.616595   -2.730673   -1.357833
 C    0.012583    0.497569   -2.477931
 C    1.496096   -1.585721   -2.394531
 O    1.133758    1.155007   -2.804177
 O   -1.067028    1.056467   -2.486036
 O    2.451956   -1.137450   -3.005954
 O    1.540268   -2.841084   -1.907341
 C    2.727582   -3.578121   -2.143943
 H    2.912116   -3.696572   -3.220727
 H    2.573941   -4.557894   -1.678846
 H    3.597076   -3.081254   -1.689021
 C    1.012938    2.537030   -3.072941
 H    0.418744    2.719086   -3.979971
 H    2.035989    2.904559   -3.207104
 H    0.530836    3.054274   -2.230657
 C    3.553798    0.128474   -0.091281
 H    2.925633   -0.662466   -0.518856
 C    4.207746   -0.448107    1.150490
 C    5.238571    0.215036    1.827142
 C    3.744133   -1.666450    1.660464
 C    5.785024   -0.324995    2.991349
 H    5.628772    1.162590    1.447550
 C    4.288228   -2.208711    2.823681
 H    2.941421   -2.195317    1.138605
 C    5.310411   -1.536666    3.493619
 H    6.589545    0.203626    3.507443
 H    3.911863   -3.159602    3.207307
 H    5.740155   -1.958774    4.404572
 C    4.554100    0.539275   -1.179592
 H    5.129696   -0.369498   -1.441788
 H    5.281557    1.263853   -0.778216
 O    3.946771    1.132520   -2.282164
 C   -2.076818   -1.224287   -1.027548
 H   -2.325214   -0.166624   -1.112352
 C   -2.998431   -2.123955   -0.475851
 H   -2.840657   -3.178936   -0.712229
 C   -4.415808   -1.748131   -0.260387
 C   -5.405040   -2.741835   -0.248424
 C   -4.806801   -0.416897   -0.047889
 C   -6.744101   -2.418714   -0.034267
 H   -5.119263   -3.784755   -0.410434
 C   -6.143316   -0.093621    0.169106
 H   -4.056534    0.376272   -0.032972
 C   -7.119385   -1.092107    0.177277
 H   -7.498733   -3.208356   -0.032379
 H   -6.423680    0.949203    0.335937
 H   -8.167634   -0.837758    0.348211
 C   -3.327689    0.776603    3.086135
 H   -2.655665   -0.015017    3.445491
 H   -3.664371    1.360079    3.957379
 H   -4.218533    0.301248    2.647674
 C   -3.539811    4.484284   -0.339826
 H   -4.522224    4.665264    0.117499
 H   -3.009465    5.444943   -0.412637
 H   -3.709068    4.125240   -1.367406
 H   -0.877238    3.972405   -0.516841
 H   -0.683356    0.805049    2.389476
 C   -0.084798   -1.773153    1.767661
 H    0.738167   -1.717067    2.481522
 C   -1.244705   -2.273912    1.824499
 C   -2.541372   -2.633669    1.613644
 H   -2.783260   -3.693567    1.493511
 H   -3.315183   -2.030353    2.097322
83
Figure_S15-9_PA-9b-ts(1,6major)_02 / electronic energy: -3519.31441637 a.u. / lowest freq: -439.92 cm-1
 C   -2.736778    2.980363   -0.100816
 H   -3.290936    3.283679    0.795415
 C   -1.325690    3.576136   -0.149421
 H   -1.204588    4.344022   -0.925176
 C   -1.184069    1.246358   -0.307451
 C    0.887946    2.481105   -0.706873
 C    1.678369    3.409484   -0.031224
 C    1.463842    1.634344   -1.660251
 C    3.057121    3.474558   -0.272037
 C    2.831896    1.686408   -1.919360
 C    3.616634    2.608887   -1.213322
 H    4.691530    2.657028   -1.411590
Cu   -0.444180   -0.604290   -0.219012
 N   -2.455482    1.544289   -0.059072
 N   -0.501014    2.398433   -0.448224
 C    0.435762   -1.900086    1.218416
 C   -0.632618   -1.219439    1.898582
 H   -3.184290    0.995915    2.637551
 H   -1.037244    4.013654    0.819465
 H   -3.325204    3.232437   -0.997558
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 H    0.218940   -2.945195    0.984524
 C   -0.517462    0.086993    2.556672
 C   -1.904101   -1.944340    2.087930
 O    0.733423    0.574841    2.556386
 O   -1.424964    0.733899    3.049959
 O   -2.845490   -1.597053    2.769282
 O   -1.957551   -3.086945    1.367753
 C   -3.142634   -3.855330    1.487274
 H   -3.335951   -4.122765    2.535440
 H   -2.981264   -4.760066    0.891056
 H   -4.010171   -3.301152    1.099118
 C    0.907953    1.887994    3.057037
 H    0.235117    2.591313    2.546699
 H    1.951759    2.153360    2.854963
 H    0.707939    1.929800    4.137041
 C   -3.455591    0.510997    0.186955
 H   -2.900711   -0.299747    0.670800
 C   -4.041833   -0.044591   -1.094581
 C   -4.879407    0.718366   -1.916774
 C   -3.715293   -1.347158   -1.486729
 C   -5.374389    0.189689   -3.108165
 H   -5.151130    1.737819   -1.631291
 C   -4.211455   -1.879969   -2.676226
 H   -3.057242   -1.949712   -0.853606
 C   -5.041715   -1.110684   -3.490551
 H   -6.024979    0.796875   -3.741363
 H   -3.946926   -2.899249   -2.966012
 H   -5.432321   -1.524624   -4.422711
 C   -4.511278    0.957082    1.201807
 H   -5.131194    0.064881    1.414832
 H   -5.184746    1.708522    0.755021
 O   -3.958882    1.517221    2.349744
 C    1.739897   -1.471776    0.916535
 H    2.024453   -0.441405    1.120700
 C    2.666245   -2.339930    0.327314
 H    2.472099   -3.408456    0.441140
 C    4.097715   -1.979969    0.209306
 C    5.064789   -2.992382    0.123656
 C    4.527600   -0.644509    0.167979
 C    6.418320   -2.683106    0.003386
 H    4.748429   -4.038722    0.151984
 C    5.879017   -0.334526    0.045129
 H    3.798470    0.167014    0.209303
 C    6.831970   -1.351384   -0.037876
 H    7.155027   -3.487132   -0.058777
 H    6.188947    0.712717    0.008848
 H    7.891900   -1.107581   -0.136669
 C    3.453643    0.784503   -2.952253
 H    2.718755    0.074429   -3.356039
 H    3.862651    1.368923   -3.790931
 H    4.286178    0.210218   -2.517492
 C    3.913745    4.435523    0.510591
 H    4.889948    4.588341    0.030316
 H    3.423661    5.414093    0.618524
 H    4.098158    4.049088    1.525977
 H    1.233087    4.080990    0.705571
 H    0.832392    0.935985   -2.209739
 C   -0.075076   -1.564201   -1.970953
 H   -0.883180   -1.376076   -2.679607
 C    1.038597   -2.156753   -2.060294
 C    2.286944   -2.654392   -1.852506
 H    2.428016   -3.737762   -1.801674
 H    3.137313   -2.087412   -2.242056
83
Figure_S15-9_PA-9b-ts(1,6major)_O3 / electronic energy: -3519.31189147 a.u. / lowest freq: -467.94 cm-1
 C   -3.976361    1.354508   -0.568416
 H   -4.627860    1.502537    0.301363
 C   -3.092496    2.572081   -0.850211
 H   -3.321589    3.058229   -1.808424
 C   -1.725989    0.712724   -0.465939
 C   -0.599486    2.800845   -1.070907
 C   -0.726658    4.191540   -1.113607
 C    0.668798    2.225615   -1.222340
 C    0.402109    5.008860   -1.256547
 C    1.804903    3.021304   -1.336824
 C    1.660198    4.414752   -1.352122
 H    2.548064    5.045593   -1.449256
Cu   -0.182296   -0.477893   -0.052127
 N   -2.981651    0.318268   -0.279402
 N   -1.740982    1.998222   -0.867239
 C    1.225957   -1.069610    1.462714
 C    0.296434   -0.102188    1.984524
 H   -3.554070   -0.084617    2.493840
 H   -3.170620    3.324975   -0.051257
 H   -4.597084    1.072655   -1.432922
 H    0.939438   -2.111539    1.626861
 C    0.671149    1.328824    2.049965
 C   -0.914731   -0.588386    2.658957
 O   -0.356499    2.164352    2.227716
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 O    1.808264    1.740744    1.930127
 O   -1.823254    0.078644    3.124858
 O   -0.971097   -1.937176    2.707128
 C   -2.033792   -2.521156    3.441096
 H   -1.937818   -2.292136    4.512137
 H   -1.954917   -3.601835    3.281909
 H   -3.012194   -2.162365    3.094852
 C   -0.035532    3.542873    2.306289
 H    0.582401    3.752549    3.191823
 H   -0.991738    4.072137    2.385126
 H    0.504816    3.872453    1.407734
 C   -3.319294   -1.026353    0.150636
 H   -2.463293   -1.374183    0.749726
 C   -3.469359   -2.017112   -0.992433
 C   -3.468843   -3.386952   -0.702236
 C   -3.571919   -1.614116   -2.326252
 C   -3.580887   -4.331600   -1.719336
 H   -3.357420   -3.723097    0.332269
 C   -3.683010   -2.558993   -3.347456
 H   -3.540295   -0.553998   -2.583063
 C   -3.691057   -3.919843   -3.048055
 H   -3.570250   -5.395877   -1.474554
 H   -3.758125   -2.225188   -4.384612
 H   -3.772486   -4.659261   -3.847401
 C   -4.548219   -1.013557    1.072578
 H   -4.694914   -2.046923    1.439191
 H   -5.447187   -0.764725    0.484668
 O   -4.452476   -0.090220    2.114251
 C    2.500341   -0.874524    0.909290
 H    2.880615    0.140232    0.800819
 C    3.232428   -1.965060    0.430161
 H    2.900836   -2.946675    0.780563
 C    4.685837   -1.888716    0.143992
 C    5.460735   -3.056044    0.206519
 C    5.324305   -0.686954   -0.199014
 C    6.829535   -3.025904   -0.055404
 H    4.980406   -4.003066    0.467582
 C    6.691211   -0.655159   -0.461688
 H    4.746859    0.236038   -0.267823
 C    7.451768   -1.823991   -0.390677
 H    7.412246   -3.948004    0.004019
 H    7.167752    0.292004   -0.724441
 H    8.524145   -1.796269   -0.595674
 C    3.165662    2.383082   -1.401271
 H    3.114491    1.370988   -1.828094
 H    3.867888    2.980780   -1.999153
 H    3.579910    2.295757   -0.383510
 C    0.239906    6.506498   -1.281708
 H    1.201470    7.012477   -1.441986
 H   -0.448343    6.816462   -2.082721
 H   -0.181880    6.872237   -0.332577
 H   -1.704213    4.664935   -1.016169
 H    0.783663    1.140691   -1.263436
 C    0.136172   -1.690672   -1.638628
 H   -0.731428   -1.733308   -2.298901
 C    1.305884   -2.167076   -1.725879
 C    2.615940   -2.513350   -1.587720
 H    2.866229   -3.567487   -1.437644
 H    3.352152   -1.937594   -2.157643
83
Figure_S15-9_PA-9b-ts(1,6major)_04 / electronic energy: -3519.31309758 a.u. / lowest freq: -455.22 cm-1
 C    2.826531    2.804131   -0.405111
 H    3.267875    2.896141   -1.405534
 C    1.445247    3.467928   -0.312313
 H    1.390389    4.249264    0.459319
 C    1.228641    1.169463    0.102230
 C   -0.804097    2.509523    0.329667
 C   -1.575513    3.392121   -0.423527
 C   -1.384013    1.807942    1.392908
 C   -2.941478    3.548432   -0.154337
 C   -2.738683    1.954365    1.683552
 C   -3.507285    2.822185    0.894791
 H   -4.571965    2.943245    1.115569
Cu    0.414502   -0.642231    0.234408
 N    2.516252    1.397458   -0.135304
 N    0.572403    2.341669    0.044317
 C   -0.592157   -2.031673   -1.017543
 C    0.452751   -1.441032   -1.810352
 H    3.235105    0.101526   -2.714521
 H    1.140958    3.910764   -1.271539
 H    3.539462    3.197478    0.335801
 H   -0.378136   -3.051496   -0.688928
 C    0.317622   -0.225835   -2.629474
 C    1.712194   -2.191823   -1.956624
 O   -0.892566    0.354220   -2.515087
 O    1.166708    0.256216   -3.350295
 O    2.731666   -1.805867   -2.500948
 O    1.672767   -3.402052   -1.372860
 C    2.872310   -4.156513   -1.386325
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 H     3.197778   -4.362090   -2.415645
 H     2.647821   -5.095466   -0.868830
 H     3.678130   -3.622998   -0.861224
 C    -1.090682    1.548088   -3.248384
 H    -0.337903    2.302363   -2.978402
 H    -2.091434    1.906613   -2.982699
 H    -1.028231    1.362741   -4.330264
 C     3.513082    0.344237   -0.145263
 H     2.957784   -0.581477   -0.353067
 C     4.206707    0.166454    1.197589
 C     3.886997    0.956322    2.306308
 C     5.169991   -0.840437    1.353256
 C     4.522883    0.759707    3.533080
 H     3.120737    1.728822    2.223661
 C     5.805759   -1.038487    2.576956
 H     5.420543   -1.492649    0.513212
 C     5.487904   -0.235149    3.672765
 H     4.256005    1.389109    4.385010
 H     6.552046   -1.829926    2.675506
 H     5.985007   -0.390404    4.632616
 C     4.503864    0.536569   -1.309062
 H     5.136524   -0.367757   -1.362604
 H     5.176375    1.380256   -1.079063
 O     3.873050    0.812607   -2.515947
 C    -1.873534   -1.551831   -0.697643
 H    -2.156754   -0.544555   -0.996913
 C    -2.770154   -2.336904    0.037176
 H    -2.581803   -3.412730    0.040644
 C    -4.196529   -1.962382    0.176513
 C    -5.151070   -2.955801    0.440202
 C    -4.634564   -0.633707    0.062670
 C    -6.499872   -2.635899    0.583248
 H    -4.828041   -3.996049    0.535961
 C    -5.981423   -0.312651    0.207791
 H    -3.914778    0.166599   -0.120763
 C    -6.921663   -1.311128    0.468566
 H    -7.226148   -3.426109    0.786336
 H    -6.297868    0.729455    0.118975
 H    -7.977787   -1.058239    0.583840
 C    -3.361344    1.218456    2.840384
 H    -2.633835    0.556285    3.329786
 H    -3.744324    1.923682    3.594079
 H    -4.211602    0.605768    2.503117
 C    -3.777456    4.463300   -1.011122
 H    -4.765735    4.639915   -0.565236
 H    -3.284708    5.436099   -1.155493
 H    -3.933361    4.025597   -2.010099
 H    -1.124850    3.952651   -1.244921
 H    -0.765532    1.150041    2.003893
 C     0.108771   -1.367783    2.103924
 H     0.947794   -1.116528    2.754652
 C    -1.017308   -1.907128    2.304998
 C    -2.289622   -2.380371    2.208866
 H    -2.465977   -3.455115    2.309010
 H    -3.100551   -1.737141    2.562776
83
Figure_S15-9_PA-9b-ts(1,6major)_05 / electronic energy: -3519.31462563 a.u. / lowest freq: -460.87 cm-1
 C     2.924243    2.689380    0.047145
 H     3.274692    2.896331   -0.973731
 C     1.587210    3.373715    0.359440
 H     1.582695    3.877731    1.338476
 C     1.274970    1.051882    0.300819
 C    -0.733473    2.395459    0.637051
 C    -1.497232    3.250428   -0.152595
 C    -1.327590    1.683134    1.682394
 C    -2.870037    3.390320    0.080624
 C    -2.695122    1.799532    1.928577
 C    -3.449691    2.661012    1.121383
 H    -4.523062    2.761602    1.308732
Cu     0.320818   -0.689263    0.163577
 N     2.580475    1.267521    0.157418
 N     0.655149    2.239422    0.381980
 C    -0.794994   -1.799385   -1.282294
 C     0.246978   -1.087729   -1.971877
 H     3.255528    0.316958   -2.615629
 H     1.304582    4.111090   -0.404353
 H     3.717609    2.965745    0.756236
 H    -0.599291   -2.861579   -1.119262
 C     0.008884    0.269070   -2.497557
 C     1.501640   -1.798241   -2.257261
 O     1.122293    0.898412   -2.896229
 O    -1.073645    0.820335   -2.542524
 O     2.489032   -1.367038   -2.831073
 O     1.503222   -3.055324   -1.778264
 C     2.689695   -3.808311   -1.959614
 H     2.908163   -3.949598   -3.027405
 H     2.510634   -4.777620   -1.481934
 H     3.548499   -3.310765   -1.486482
 C     0.992094    2.248403   -3.293186
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H	0.312664	2.351029	-4.151110
H	2.001797	2.578895	-3.559551
H	0.604430	2.858769	-2.464301
C	3.542280	0.200317	-0.038512
H	2.955816	-0.668145	-0.373528
C	4.260269	-0.202907	1.240878
C	4.056913	0.466739	2.451020
C	5.136425	-1.297053	1.222371
C	4.724575	0.066172	3.609605
H	3.355655	1.301721	2.499299
C	5.803622	-1.698631	2.377175
H	5.292503	-1.854902	0.295687
C	5.603307	-1.014462	3.576855
H	4.550246	0.601812	4.545397
H	6.480631	-2.554987	2.341009
H	6.124043	-1.328808	4.483815
C	4.529088	0.544804	-1.171843
H	5.154360	-0.348556	-1.351825
H	5.211351	1.340561	-0.828962
O	3.902501	0.990413	-2.330508
C	-2.063436	-1.339477	-0.895008
H	-2.320936	-0.294734	-1.068166
C	-2.970141	-2.196182	-0.258231
H	-2.796788	-3.266058	-0.396583
C	-4.391638	-1.824935	-0.066547
C	-5.364043	-2.829194	0.044332
C	-4.803980	-0.486486	0.024423
C	-6.707095	-2.509388	0.237174
H	-5.061391	-3.877804	-0.023513
C	-6.144335	-0.166139	0.220336
H	-4.067019	0.316439	-0.039378
C	-7.103613	-1.175156	0.327765
H	-7.448657	-3.307491	0.316883
H	-6.441429	0.882977	0.292422
H	-8.154957	-0.923098	0.482248
C	-3.348487	1.031660	3.047003
H	-2.657778	0.296299	3.482604
H	-3.678735	1.708686	3.850313
H	-4.239373	0.496510	2.683734
C	-3.703303	4.274211	-0.810061
H	-4.697336	4.456354	-0.379160
H	-3.216031	5.245742	-0.978838
H	-3.844782	3.803397	-1.795822
H	-1.031779	3.791501	-0.979166
H	-0.713052	1.028077	2.301426
C	-0.039794	-1.633788	1.917222
H	0.797813	-1.519194	2.606701
C	-1.198984	-2.125711	2.035958
C	-2.498488	-2.500196	1.875505
H	-2.745063	-3.565611	1.854801
H	-3.266870	-1.850848	2.305375