Versatile Homoallylic Boronates by Chemo-, S_N2'-, Diastereo- and Enantioselective Catalytic Sequence of Cu–H Addition to Vinyl–B(pin)/Allylic Substitution

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SUPPORTING INFORMATION

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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). ^1H NMR spectra were recorded on Varian Unity INOVA 400 (400 MHz), 500 (500 MHz), or 600 (600 MHz) spectrometers. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 7.26 ppm). Data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, pent = pentet, m = multiplet, br = broad, app = apparent), and coupling constants (Hz). ^{13}C NMR spectra were recorded on Varian Unity INOVA 400 (100 MHz), 500 (125 MHz), or 600 (150 MHz) spectrometers with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 77.16 ppm). High-resolution mass spectrometry was performed on a JEOL AccuTOF DART (positive mode) at the Mass Spectrometry Facility, Boston College. Enantiomeric ratios were determined by HPLC analysis (high-performance liquid chromatography) with a Shimadzu chromatograph [Chiral Technologies Chiralcel AZ-H (4.6 x 250 mm), Chiral Technologies Chiralcel OC-H (4.6 x 250 mm), Chiral Technologies Chiralcel OD-H (4.6 x 250 mm), Chiral Technologies Chiralcel OJ-H (4.6 x 250 mm), Chiral Technologies Chiralcel OZ-H (4.6 x 250 mm), or Chiral Technologies Chiralpak AD-H (4.6 x 250 mm)] in comparison with authentic racemic materials. Specific rotations were measured on a Rudolph Research Analytical Autopol IV Polarimeter. Melting points were measured on a Thomas Hoover capillary melting point apparatus and are uncorrected.

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

■ **Reagents:**

***N*-Bromosuccinimide (NBS):** purchased from Alfa Aesar and recrystallized from H_2O.

Buffer solution pH = 7.0 (20 ºC): purchased from Aldrich and used as received.

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

Chiral imidazolinium salt (imid-1): prepared according to previously reported procedure.[1]

Chiral imidazolinium salt (imid-2): prepared according to previously reported procedure.[2]

Chiral imidazolinium salt (imid-3): prepared according to previously reported procedure.[3]

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[1] X. Li, F. Meng, S. Torker, Y. Shi, A. H. Hoveyda, *Angew. Chem. Int. Ed.* **2016**, *55*, 9997–10002.

[2] M. K. Brown, T. L. May, C. A. Baxter, H. Hoveyda, *Angew. Chem. Int. Ed.* **2007**, *119*, 1115–1118.

[3] B. Jung, A. H. Hoveyda, *J. Am. Chem. Soc*. **2012,** *134,* 1490–1493.

Chiral phosphine ligand (phos-1): purchased from Strem and used as received.

Chiral phosphine ligand (phos-2): purchased from Strem and used as received.

Chiral phosphine ligand (phos-3): purchased from Strem and used as received.

Chiral phosphine ligand (phos-4): purchased from Strem and used as received.

Chiral phosphine ligand (phos-5): purchased from Strem and used as received.

Chiral phosphine ligand (phos-6): purchased from Strem and used as received.

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

Furan: purchased from Aldrich and purified by washing with aqueous 5% KOH, dried with Na_2SO_4, then distilled over KOH under reduced pressure prior to use.

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

Poly(methylhydrosiloxane) (PMHS): purchased from Alfa Aesar and used as received.

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

Sodium perborate tetrahydrate ($NaBO_3•4H_2O$): purchased from Aldrich and used as received.

4,4,5,5-Tetramethyl-2-vinyl-1,3,2-dioxaborolane: purchased from Combi-blocks and distilled over CaH_2 under reduced pressure prior to use.

Triethylamine (Et_3N): purchased from Aldrich and used as received.

■ **Preparation of Allylic Phosphates:** Allylic alcohols were synthesized from the corresponding ester by a two-step Horner-Wadsworth-Emmons olefin synthesis/dibal–H reduction sequence. Subsequently, allylic alcohols were converted to the corresponding allylic phosphates based on established methods.[4],[5] The following substrates were prepared according to the above sequence. Characterization data matched those reported previously.

(*E*)-Diethyl 3-phenylprop-2-enyl phosphate (1a)[6]

(*E*)-Diethyl (3-(2-fluorophenyl)allyl) phosphate (1b)[3]

(*E*)-3-(2-Bromophenyl)allyl diethyl phosphate (1c)[3]

(*E*)-Diethyl (3-(2-methoxyphenyl)allyl) phosphate (1d)[7]

(*E*)-Diethyl (3-(*o*-tolyl)allyl) phosphate (1e)[7]

(*E*)-Diethyl (3-(naphthalen-2-yl)allyl) phosphate (1f)[8]

(*E*)-3-(3-Bromophenyl)allyl diethyl phosphate (1g)[7]

(*E*)-Diethyl (3-(3-methoxyphenyl)allyl) phosphate (1h)[9]

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[4] Y. Shi, B. Jung, S. Torker, A. H. Hoveyda, *J. Am. Chem. Soc*. **2015,** *137,* 8948–8964.

[5] Y. Shi, A. H. Hoveyda, *Angew. Chem. Int. Ed.* **2016**, *55*, 3455–3458.

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[7] K. Akiyama, F. Gao, A. H. Hoveyda, *Angew. Chem. Int. Ed.* **2010**, *49,* 429–433.

[8] M. A. Kacprzynski, A. H. Hoveyda, *J. Am. Chem. Soc*. **2004,** *126,* 10676–10681.

[9] L. B. Delvos, D. J. Vyas, M. Oestreich, *Angew. Chem. Int. Ed.* **2013**, *52,* 4650–4653.

(*E*)-3-(4-Chlorophenyl)allyl diethyl phosphate (1i)[7]

(*E*)-3-(4-Bromophenyl)allyl diethyl phosphate (1j)[10]

(*E*)-Diethyl (3-(4-(trifluoromethyl)phenyl)allyl) phosphate (1k)[3]

(*E*)-Diethyl (3-(4-nitrophenyl)allyl) phosphate (1l)[11]

(*E*)-Diethyl (3-(pyridin-3-yl)allyl) phosphate (1-4)[4]

(*E*)-Diethyl (5-phenylpent-2-en-1-yl) phosphate (1-8)[7]

(*E*)-3-Cyclohexylallyl diethyl phosphate (1-9)[7]

(*E*)-But-2-en-1-yl diethyl phosphate (1-10)[12]

(*E*)-3-(Benzo[*b*]thiophen-3-yl)allyl diethyl phosphate (1-5): IR (neat): 2983 (w), 1655 (w), 1510 (w), 1259 (s), 1164 (w), 1002 (s), 957 (s), 851 (m), 756 (s), 729 (s), 669 (w), 523 (m), 421 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.91 (1H, d, J = 8.0 Hz), 7.87 (1H, d, J = 8.0 Hz), 7.48 (1H, s), 7.44–7.38 (2H, m), 6.96 (1H, d, J = 15.2 Hz), 6.44–6.36 (1H, m), 4.77 (1H, dd, J = 7.6, 1.6 Hz), 4.75 (1H, dd, J = 8.4, 1.2 Hz), 4.16 (4H, m), 1.36 (6H, t, J = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.5 137.6, 132.9, 126.2, 125.3 (d, J_{CP} = 6.8 Hz), 124.7, 124.5, 123.4, 123.0, 122.0, 68.1 (d, J_{CP} = 5.3 Hz), 64.0 (d, J_{CP} = 5.3 Hz), 16.3(d, J_{CP} = 6.8 Hz); HRMS (DART): Calcd for $C_{15}H_{19}O_4PS$ $[M]^+$: 326.0742; Found: 326.0747.

Diethyl ((2*E*,4*E*)-5-phenylpenta-2,4-dien-1-yl) phosphate (1-6): IR (neat): 2983 (w), 1976 (w), 1449 (w), 1260 (m), 1165 (w), 1017 (s), 965 (s), 851 (m), 749 (m), 693 (m), 507 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.41–7.39 (2H, m), 7.34–7.30 (2H, m), 7.25–7.22 (1H, m), 6.77 (1H, dd, J = 15.6, 10.8 Hz), 6.60 (1H, d, J = 15.6 Hz), 6.48 (1H, dd, J = 15.2, 10.4 Hz), 5.90 (1H, dt, J = 15.2, 6.4 Hz), 4.64 (1H, dd, J = 6.4, 1.2 Hz), 4.62 (1H, dd, J = 6.8, 1.2 Hz), 4.13 (4H, m), 1.35 (6H, td, J = 7.2, 0.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.0, 134.4, 134.3, 128.8, 128.0, 127.6, 127.3 (d, J_{CP} = 6.1 Hz), 126.7, 67.8 (d, J_{CP} = 5.3 Hz), 63.9 (d, J_{CP} = 6.1 Hz), 16.3 (d, J_{CP} = 6.8 Hz).

(*E*)-Diethyl (5-phenylpent-2-en-4-yn-1-yl) phosphate (1-7): IR (neat): 2983 (w), 1490 (w), 1443 (w), 1262 (s), 1004 (s), 950 (s), 846 (m), 800 (m), 755 (s), 690 (s), 582 (w), 527 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.44–7.42 (2H, m), 7.32– 7.31 (3H, m), 6.26 (1H, dt, J = 15.6, 5.6 Hz), 6.02 (1H, dt, J = 15.6, 1.6 Hz), 4.63 (1H, dd, J = 6.0, 1.6 Hz), 4.61 (1H, dd, J = 6.0, 1.6 Hz), 4.17–4.10 (4H, m), 1.35 (6H, t, J = 6.8); ^{13}C NMR (100 MHz, $CDCl_3$): δ 136.6, 136.56, 131.7, 128.5 (d, J_{CP} = 11.4 Hz), 123.1, 113.3, 91.3, 86.8, 66.9 (d, J_{CP} = 5.3 Hz), 64.1 (d, J_{CP} = 6.0 Hz), 16.3 (d, J_{CP} = 6.1 Hz); HRMS (DART): Calcd for $C_{15}H_{20}O_4P$ $[M+H]^+$: 295.1099; Found: 295.1098

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[10] Z.-Q. Zhang, B. Zhang, X. Lu, J.-H. Liu, X.-Y. Lu, B. Xiao, Y. Fu, *Org. Lett.* **2016,** *18,* 952–955.

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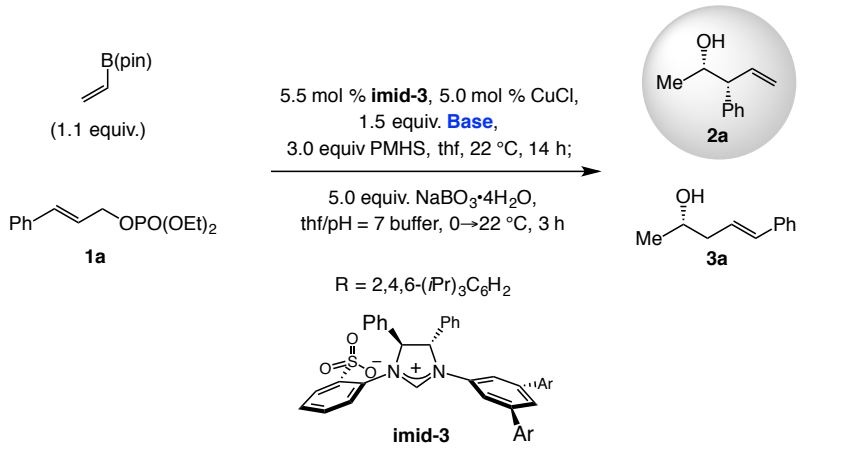
■ Examining the Influence of Base



NaOMe
35% conv., 71:29 **2a**:**3a**,
9% yield (**2a**), 97:3 d.r. (**2a**),
95:5 e.r. (**2a**, major diast.),
59:41 e.r. (**2a**, minor diast.)

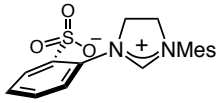
NaO*t*Bu
83% conv., 94:6 **2a**:**3a**,
59% yield (**2a**), 94:6 d.r. (**2a**),
94:6 e.r. (**2a**, major diast.),
77:23 e.r. (**2a**, minor diast.)

LiO*t*Bu
95% conv., 95:5 **2a**:**3a**,
66% yield (**2a**), 96:4 d.r. (**2a**),
95:5 e.r. (**2a**, major diast.),
75:25 e.r. (**2a**, minor diast.)

KO*t*Bu & KOMe
<2% conv.

NaOPh
<10% conv.

■ **Representative Procedure:** In an N_2-filled glove box, an oven-dried 2-dram vial with magnetic stir bar was charged with CuCl (0.5 mg, 0.005 mmol), **imid-3** (4.70 mg, 0.0055 mmol), LiO*t*Bu (12 mg, 0.15 mmol), and freshly distilled tetrahydrofuran (thf, 0.5 mL). The mixture was premixed for 1 h before PMHS (18 mg, 0.30 mmol) and additional thf (0.5 mL) were added. The solution immediately turned dark red. After 1 min, vinyl boronic acid pinacol ester (17 mg, 0.11 mmol), allylic phosphate (27 mg, 0.10 mmol), and thf (0.5 mL) were added. The vial was sealed with electrical tape before removal from the glove box, and the resulting mixture was allowed to stir at 22 °C for 14 h. The mixture was passed through a short plug of basified silica gel (4 cm x 1 cm, 1% of triethylamine) and eluted with Et_2O. Removal of the volatiles *in vacuo* afforded bright yellow oil. To the oil was added thf (1.0 mL), pH = 7.0 buffer solution (1.0 mL), and $NaBO_3$•$4H_2O$ (77 mg, 0.50 mmol) at 0 ºC. The mixture was then allowed to stir at 22 ºC for 3 h after which it was washed with Et_2O (3 x 1.0 mL) and the combined organic layers were passed through a short plug of $MgSO_4$, concentrated and purified by silica gel chromatography (hexanes:Et_2O = 10:5, R_f = 0.2) to afford the desired product as colorless oil (10.7 mg, 0066 mmol, 66% yield). The racemic sample was prepared by the same procedure except through the use of 10 mol % **imid-4** and CuCl.

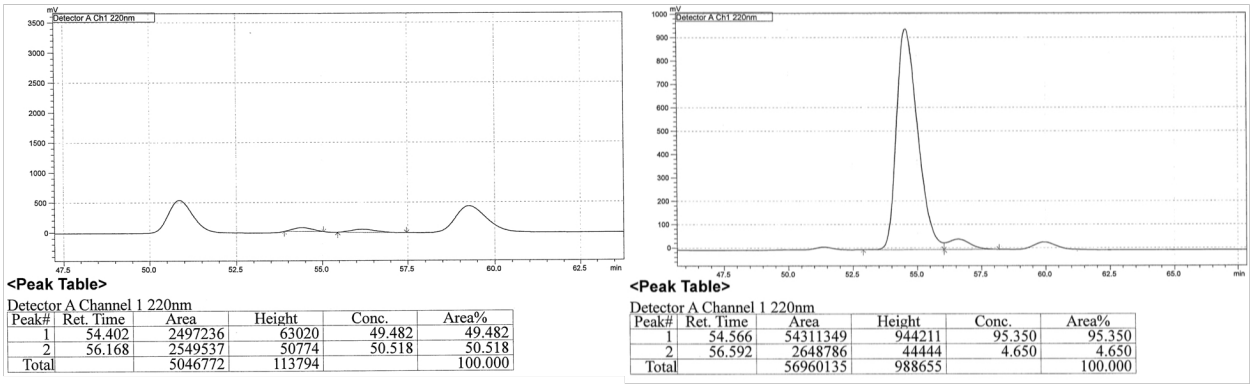


imid-4

(2*S*,3*R*)-3-Phenylpent-4-en-2-ol (2a): IR (neat): 3407 (br s) 2972 (w), 2924 (w), 1638 (w), 1493 (w), 1268 (w), 1116 (m), 1056 (m), 993 (m), 757 (m), 700 (s), 672 (m), 530 (m) cm^{-1}; ^1H NMR

(400 MHz, $CDCl_3$): δ 7.40–7.33 (2H, m), 7.27–7.24 (3H, m), 6.09–6.00 (1H, m), 5.16–5.11 (2H, m), 4.07–4.03 (1H, m), 3.25 (1H, t, J = 8.2 Hz), 1.47 (1H, br), 1.24 (3H, dd, J = 6.0, 0.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.0, 138.5, 129.0, 128.6, 127.1, 117.1, 70.6, 59.1, 20.9; HRMS (DART): Calcd for $C_{11}H_{13}$ $[M+H–H_2O]^+$: 145.1017; Found: 145.1013; Specific rotation: $[\alpha]_D^{20}$ –65.02 (*c* 0.61, $CHCl_3$) for a >98% S_N2', 96:4 d.r., and 95:5 e.r. sample. Enantiomeric purity of **2a** 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, 0.3 mL/min, 220 nm).

Enantiomeric purity of the major diastereomers



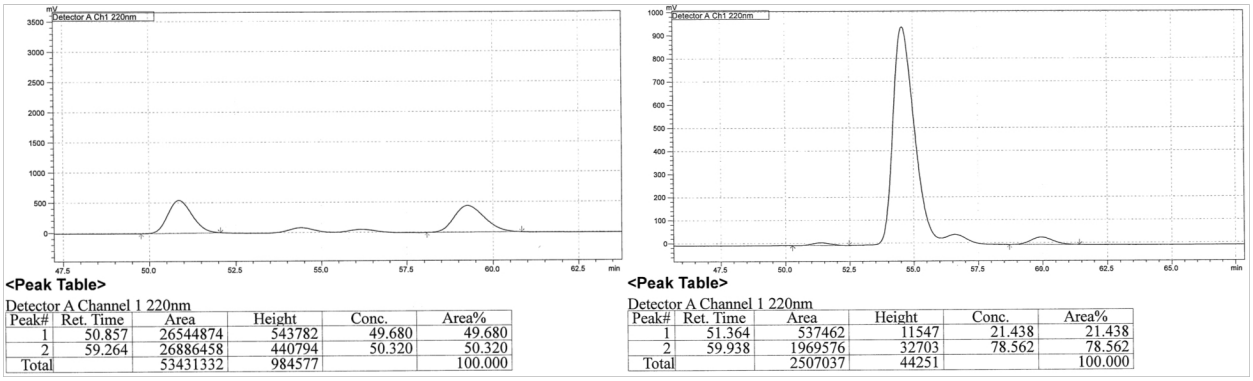
<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	54.402	2497236	63020	49.482	49.482
2	56.168	2549537	50774	50.518	50.518
Total		5046772	113794		100.000

<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	54.566	54311349	944211	95.350	95.350
2	56.592	2648786	44444	4.650	4.650
Total		56960135	988655		100.000

Enantiomeric purity of the minor diastereomers



<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	50.857	26544874	543782	49.680	49.680
2	59.264	26886458	440794	50.320	50.320
Total		53431332	984577		100.000

<Peak Table>
Detector A Channel 1 220nm

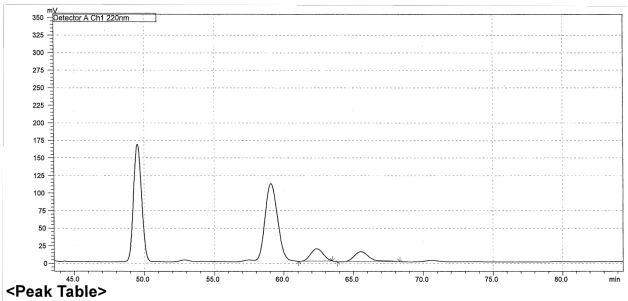
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	51.364	537462	11547	21.438	21.438
2	59.938	1969576	32703	78.562	78.562
Total		2507037	44251		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	54.402	2497236	49.482	1	54.566	54311349	95.350
2	56.168	2549537	50.518	2	56.592	2648786	4.650
1	50.857	26544874	49.680	1	51.364	537462	21.438
2	59.264	26886458	50.320	2	59.938	1969576	78.562

(2*S*,3*R*)-3-(2-Fluorophenyl)pent-4-en-2-ol (2b): IR (CH_2Cl_2): 3209 (br s), 2925 (m), 1638 (w), 1490 (m), 1454 (m), 1375 (m), 1119 (s), 1058 (s), 800 (w), 753 (s), 603 (w), 401 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.34–7.29 (1H, m), 7.25–7.20 (1H, m), 7.15–7.11 (1H, m), 7.08–7.03 (1H, m), 6.11–6.02 (1H, m), 5.18–5.14 (2H, m), 4.18–4.12 (1H, m), 3.62 (1H, t, J = 8.4 Hz), 1.45 (1H, d, J = 4.4 Hz), 1.24 (3H, d, J = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.1 (d, J_{CF} = 244.4 Hz), 137.3, 129.9 (d, J_{CF} = 4.6 Hz), 128.4 (d, J_{CF} = 8.4 Hz), 127.9 (d, J_{CF} = 14.4 Hz), 124.4 (d, J_{CF} = 3.0 Hz), 117.6, 115.9 (d, J_{CF} = 22.8 Hz), 69.8, 51.9, 21.2; HRMS (DART): Calcd

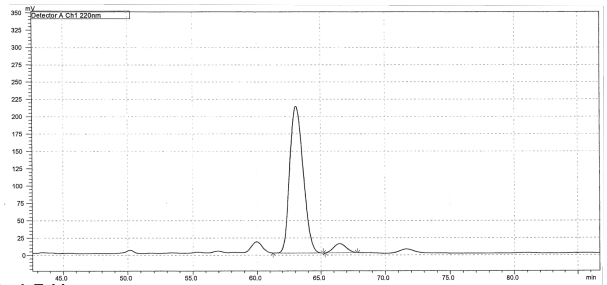
for $C_{11}H_{12}F$ $[M+H–H_2O]^+$: 163.0929; Found: 163.0923; Specific rotation: $[\alpha]_D^{20}$ –44.30 (*c* 0.46, $CHCl_3$) for a >98% S_N2', 93:7 d.r., and 95:5 e.r. sample. Enantiomeric purity of **2b** was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; chiralcel AD–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 220 nm).

Enantiomeric purity of the major diastereomers



<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	62.348	1098734	17525	51.093	51.093
2	65.523	1051722	14048	48.907	48.907
Total		2150456	31573		100.000



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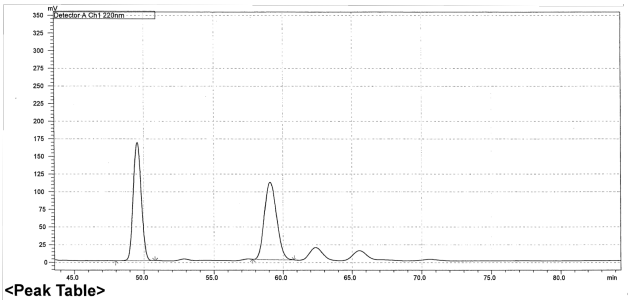
Detector A Channel 1 220nm

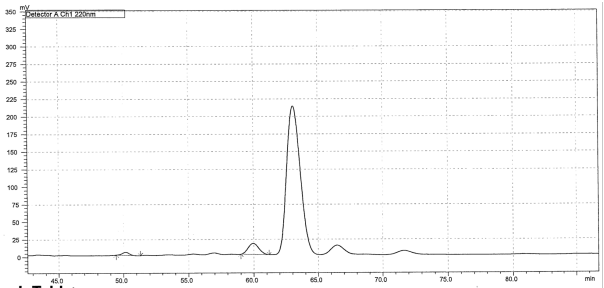
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	63.066	15535438	211889	94.606	94.606
2	66.463	885722	13001	5.394	5.394
Total		16421161	224890		100.000

Enantiomeric purity of the minor diastereomers



<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	49.520	6685853	167293	49.674	49.674
2	59.073	6773530	109558	50.326	50.326
Total		13459383	276851		100.000



<Peak Table>
Detector A Channel 1 220nm

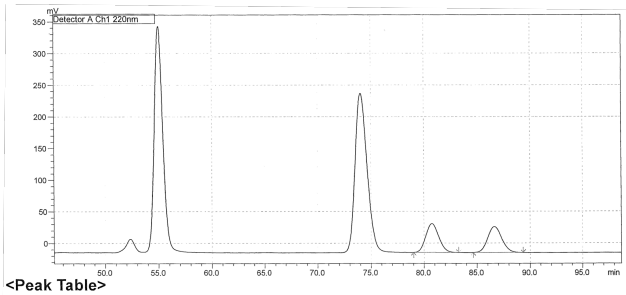
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	50.158	153821	4256	14.670	14.670
2	59.953	894747	15541	85.330	85.330
Total		1048568	19797		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	62.348	1098734	51.093	1	63.066	15535438	94.606
2	65.523	1051722	48.907	2	66.463	885722	5.394
1	49.520	6685853	49.674	1	50.158	153821	14.670
2	59.073	6773530	50.326	2	59.953	894747	85.330

(2*S*,3*R*)-3-(2-Bromophenyl)pent-4-en-2-ol (2c): IR (CH_2Cl_2): 3419 (br s), 2974 (w), 1637 (w), 1437 (m), 1266 (m), 1107 (s), 1020 (s), 993 (m), 816 (w), 422 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.59 (1H, dd, *J* = 7.6, 0.8 Hz), 7.38 (1H, dd, *J* = 7.6, 1.6 Hz), 7.33–7.29 (1H, m), 7.12–7.01 (1H, m), 6.03–5.94 (1H, m), 5.19–5.14 (2H, m), 4.21–4.13 (1H, m), 3.95 (1H, t, *J* = 7.6 Hz), 1.46 (1H, d, *J* = 4.4 Hz), 1.27 (3H, d, *J* = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.1, 137.5, 133.5, 129.2, 128.3, 127.8, 126.0, 117.9, 70.2, 56.4, 21.0; HRMS (DART): Calcd for $C_{11}H_{12}Br$ $[M+H–H_2O]^+$: 223.0122; Found: 223.0122; Specific rotation: $[\alpha]_D^{20}$ –20.07 (*c* 1.12, $CHCl_3$) for a >98% S_N2', 90:10 d.r., and 98:2 e.r. sample. Enantiomeric purity of **2c** was determined by HPLC analysis in comparison with authentic racemic material (98:2 e.r. shown;

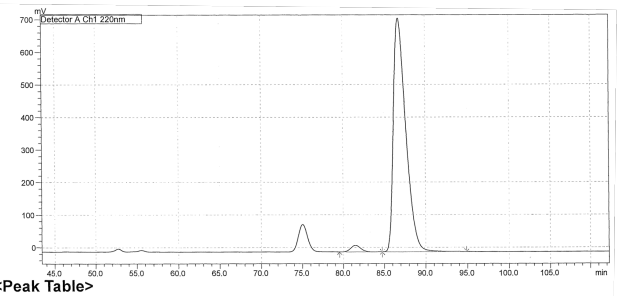
chiralcel OD–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 220 nm).

Enantiomeric purity of the major diastereomers



<Peak Table>
Detector A Channel 1 220nm

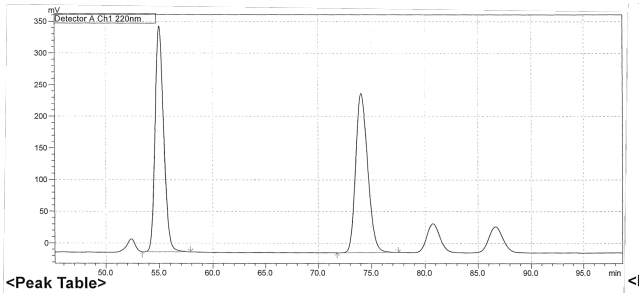
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	80.743	3892381	45554	50.593	50.593
2	86.625	3801200	40914	49.407	49.407
Total		7693582	86469		100.000



<Peak Table>
Detector A Channel 1 220nm

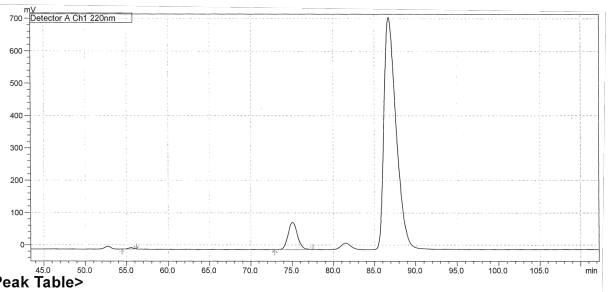
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	81.459	1735145	20275	2.279	2.279
2	86.755	74391917	718863	97.721	97.721
Total		76127062	739137		100.000

Enantiomeric purity of the minor diastereomers



<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	55.004	19766804	356754	49.918	49.918
2	74.047	19832077	251709	50.082	50.082
Total		39598882	608463		100.000



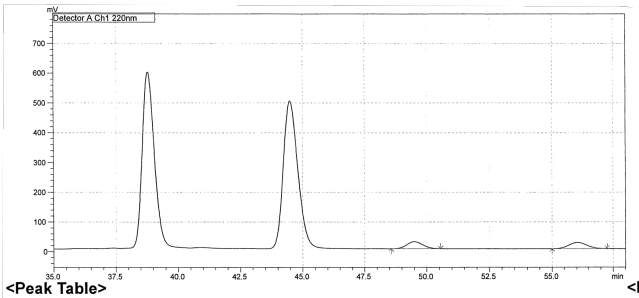
<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	55.505	188295	4070	2.759	2.759
2	75.029	6637342	84243	97.241	97.241
Total		6825637	88313		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	80.743	3892381	50.593	1	81.459	1735145	2.279
2	86.625	3801200	49.407	2	86.755	74391917	97.721
1	55.004	19766804	49.918	1	55.505	188295	2.759
2	74.047	19832077	50.082	2	75.029	6637342	97.241

(2*S*,3*R*)-3-(2-Methoxyphenyl)pent-4-en-2-ol (2d): IR (CH_2Cl_2): 3423 (br s), 2926 (w), 1637 (w), 1491 (m), 1463 (m), 1170 (s), 1120 (m), 1026 (s), 915 (m), 879 (w), 579 (m), 400 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.26–7.21 (2H, m), 6.98–6.94 (1H, m), 6.09 (1H, d, J = 8.4 Hz), 6.15–6.06 (1H, m), 5.15–5.08 (1H, m), 4.19–4.11 (1H, m), 3.83 (3H, s), 3.74 (1H, t, J = 8.0 Hz), 1.70 (1H, d, J = 4.4 Hz), 1.22 (3H, d, J = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 1.57.5, 138.2, 129.2, 128.0, 121.1, 116.8, 111.2, 69.8, 55.6, 52.5, 21.1; HRMS (DART): Calcd for $C_{12}H_{15}O$ $[M+H–H_2O]^+$: 175.1123; Found: 175.1123; Specific rotation: $[\alpha]_D^{20}$ –36.14 (*c* 1.16, $CHCl_3$) for a >98% S_N2', 92:8 d.r., and 98:2 e.r. sample. Enantiomeric purity of **2d** was determined by HPLC analysis in comparison with authentic racemic material (98:2 e.r. shown; chiralcel OD–H column, 98:2 hexanes:*i*PrOH, 0.3 mL/min, 220 nm).

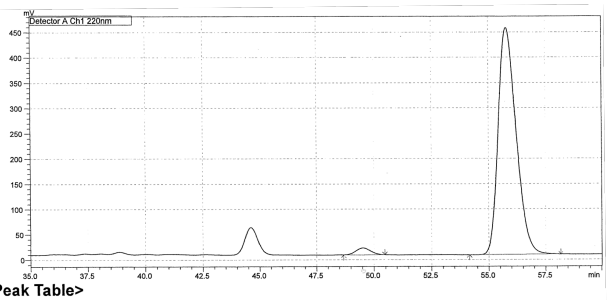
Enantiomeric purity of the major diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	49.501	1076980	23844	49.410	49.410
2	56.029	1102695	21125	50.590	50.590
Total		2179675	44969		100.000

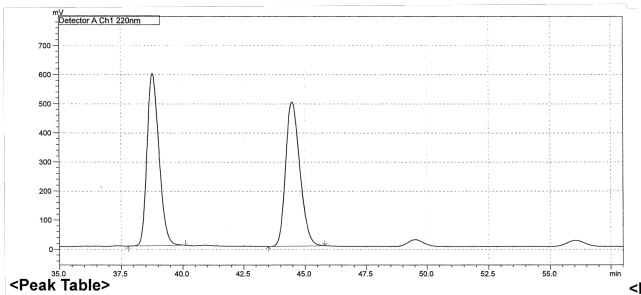


<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	49.523	604502	13609	2.394	2.394
2	55.777	24650974	448868	97.606	97.606
Total		25255476	462477		100.000

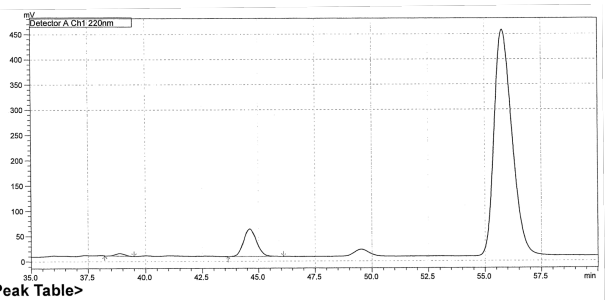
Enantiomeric purity of the minor diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	38.789	20061008	591772	49.921	49.921
2	44.487	20124475	495872	50.079	50.079
Total		40185484	1087645		100.000



<Peak Table>

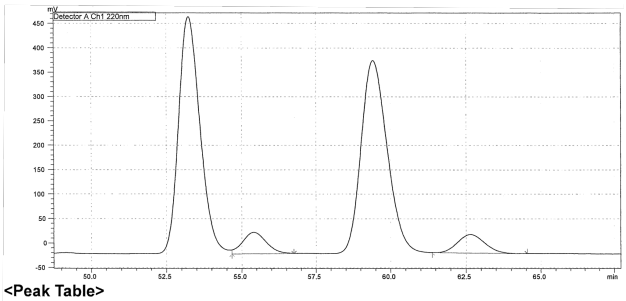
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	38.871	135564	4644	5.796	5.796
2	44.608	2203203	54500	94.204	94.204
Total		2338767	59145		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	49.501	1076980	49.410	1	49.523	604502	2.394
2	56.029	1102695	50.590	2	55.777	24650974	97.606
1	38.789	20061008	49.921	1	38.871	135564	5.796
2	44.487	20124475	50.079	2	44.608	2203203	94.204

(2*S*,3*R*)-3-(*o*-Tolyl)pent-4-en-2-ol (2e): IR (CH_2Cl_2): 3424 (br s), 2955 (m), 2854 (m), 1636 (w), 1490 (m), 1460 (m), 1118 (s), 1057 (s), 992 (m), 914 (s), 880 (m), 753 (s), 633 (m), 547 (m), 408 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.30–7.12 (4H, m), 5.97–5.88 (1H, m), 5.10–5.05 (2H, m), 4.12 (1H, pent, J = 6.7 Hz), 3.55 (1H, t, J = 8.6 Hz), 2.36 (3H, s), 1.56 (1H, br), 1.30 (3H, d, J = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.6, 138.5, 137.4, 137.1, 131.1, 126.7, 126.7, 116.8, 70.3, 54.3, 20.9, 20.0; HRMS (DART): Calcd for $C_{12}H_{15}$ $[M+H–H_2O]^+$: 159.1174; Found: 159.1172; Specific rotation: $[\alpha]_D^{20}$ –44.38 (*c* 0.73, $CHCl_3$) for a >98% S_N2', 90:10 d.r., and 97:3 e.r. sample. Enantiomeric purity of **2e** was determined by HPLC analysis in comparison with authentic racemic material (97:3 e.r. shown; chiralcel OD–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 220 nm).

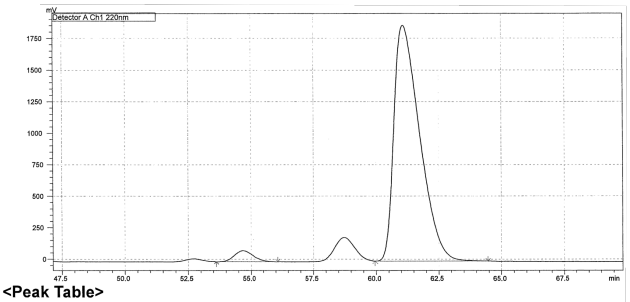
Enantiomeric purity of the major diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	55.405	2454587	44017	50.940	50.940
2	62.644	2364037	37886	49.060	49.060
Total		4818624	81902		100.000

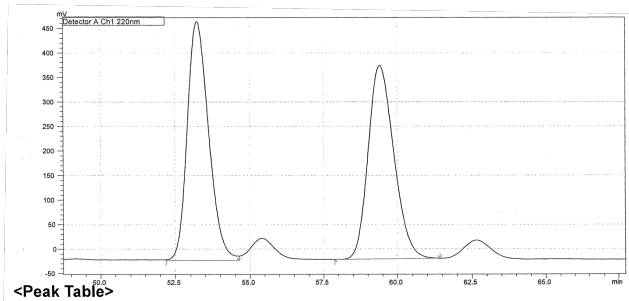


<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	54.676	4534962	86504	3.287	3.287
2	61.089	133439314	1866785	96.713	96.713
Total		137974276	1953288		100.000

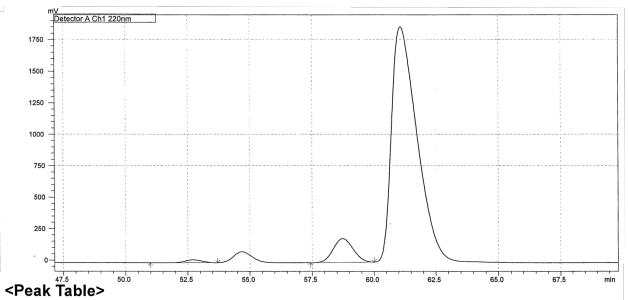
Enantiomeric purity of the minor diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	53.235	24253929	487018	50.354	50.354
2	59.415	23912636	394898	49.646	49.646
Total		48166565	881916		100.000



<Peak Table>

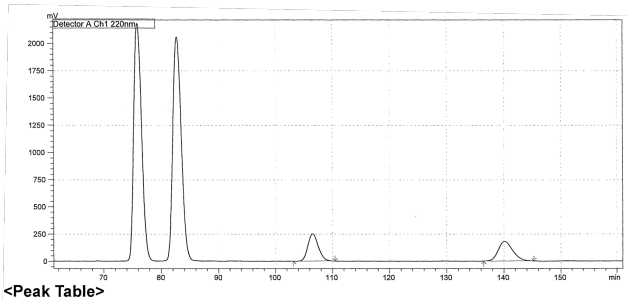
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	52.708	1038401	22865	8.963	8.963
2	58.731	10546819	188976	91.037	91.037
Total		11585221	211841		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	55.405	2454587	50.940	1	54.676	4534962	3.287
2	62.644	2364037	49.060	2	61.089	133439314	96.713
1	53.235	24253929	50.354	1	52.708	22865	8.963
2	59.415	23912636	49.646	2	58.731	188976	91.037

(2*S*,3*R*)-3-(Naphthalen-2-yl)pent-4-en-2-ol (2f): IR (CH_2Cl_2): 3423 (br s), 2971 (w), 1634 (w), 1599 (w), 1507 (w), 1370 (m), 1113 (s), 1056 (m), 1018 (m), 916 (s), 855 (m), 815 (s), 685 (m), 476 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.85–7.81 (3H, m), 7.72 (1H, s), 7.51–7.44 (2H, m), 7.41 (1H, dd, *J* = 8.4, 1.6 Hz), 6.18–6.09 (1H, m), 5.20–5.16 (2H, m), 4.21–4.14 (1H, m), 3.43 (1H, t, *J* = 8.0 Hz), 1.52 (1H, d, *J* = 3.6 Hz), 1.29 (3H, d, *J* = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 138. 5, 138.4, 133.7, 132.7, 128.7, 127.8, 127.79, 127.4, 126.6, 126.3, 125.9, 117.3, 70.5, 59.2, 20.9; HRMS (DART): Calcd for $C_{15}H_{15}$ $[M+H–H_2O]^+$: 195.1174; Found: 195.1174; Specific rotation: $[\alpha]_D^{20}$ –73.27 (*c* 1.35, $CHCl_3$) for a >98% S_N2', 95:5 d.r., and 95:5 e.r. sample. Enantiomeric purity of **2f** was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; chiralcel AD–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 220 nm).

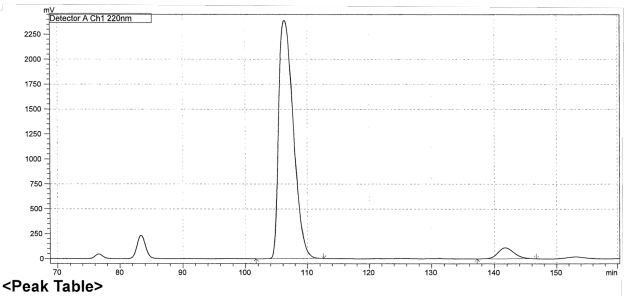
Enantiomeric purity of the major diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	106.504	31890262	250665	50.004	50.004
2	140.112	31884760	179534	49.996	49.996
Total		63775022	430199		100.000

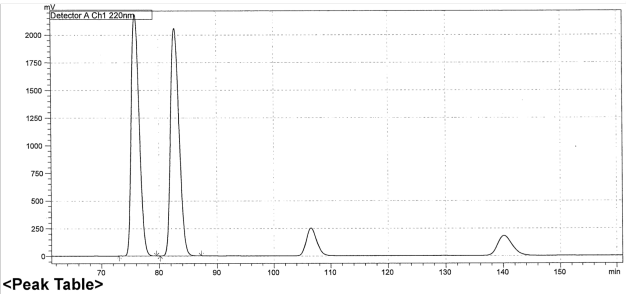


<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	106.315	392512518	2388461	95.218	95.218
2	141.696	19714745	109509	4.782	4.782
Total		412227263	2497969		100.000

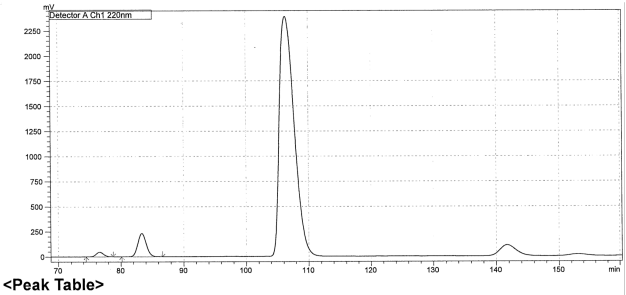
Enantiomeric purity of the minor diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	75.906	208858929	2181643	49.489	49.489
2	82.734	213168273	2056619	50.511	50.511
Total		422027201	4238262		100.000



<Peak Table>

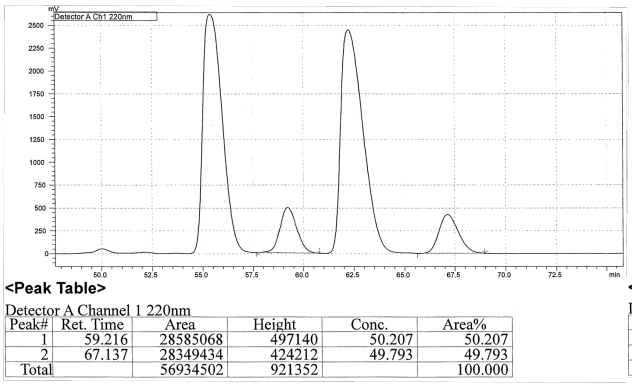
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	76.574	3771038	44981	14.834	14.834
2	83.358	21650989	231891	85.166	85.166
Total		25422028	276872		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	106.504	31890262	50.004	1	106.315	392512518	95.218
2	140.112	31884760	49.996	2	141.696	19714745	4.782
1	75.906	208858929	49.489	1	76.574	3771038	14.834
2	82.734	213168273	50.511	2	83.358	21650989	85.166

(2*S*,3*R*)-3-(3-Bromophenyl)pent-4-en-2-ol (2g): IR (CH_2Cl_2): 3386 (br s), 2924 (m), 1638 (w), 1592 (m), 1566 (m), 1474 (m), 1427 (w), 1193 (s), 1072 (s), 919 (s), 779 (s), 438 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.42–7.36 (2H, m), 7.24–7.18 (2H, m), 5.99 (1H, ddd J = 17.2, 10.8, 8.8 Hz), 5.18–5.11 (2H, m), 4.09–4.01 (1H, m), 3.22 (1H, t, J = 8.0 Hz), 1.47 (1H, br), 1.23 (3H, d, J = 6.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 143.5, 137.9, 131.6, 130.4, 130.2, 127.3, 123.0, 117.6, 70.5, 58.6, 21.0; HRMS (DART): Calcd for $C_{11}H_{12}Br$ $[M+H–H_2O]^+$: 223.0122; Found: 223.0128; Specific rotation: $[\alpha]_D^{20}$ –52.90 (*c* 2.60, $CHCl_3$) for a >98% S_N2', 94:6 d.r., and 96:4 e.r. sample. Enantiomeric purity of **2g** was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; chiralcel OD–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 220 nm).

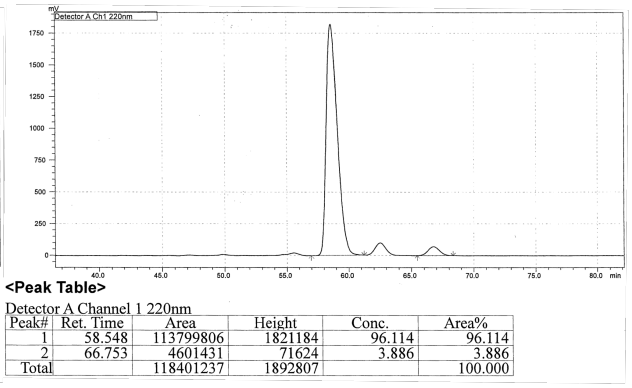
Enantiomeric purity of the major diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	59.216	28585068	497140	50.207	50.207
2	67.137	28349434	424212	49.793	49.793
Total		56934502	921352		100.000

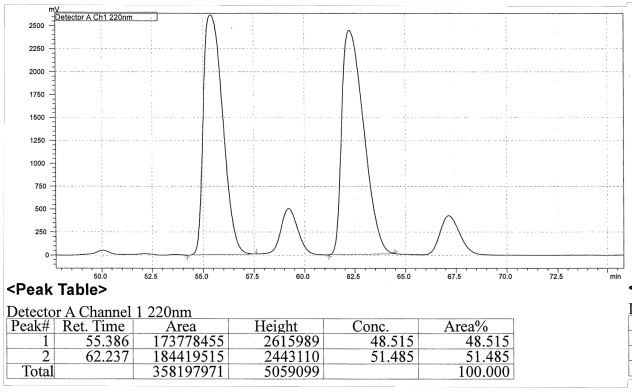


<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	58.548	113799806	1821184	96.114	96.114
2	66.753	4601431	71624	3.886	3.886
Total		118401237	1892807		100.000

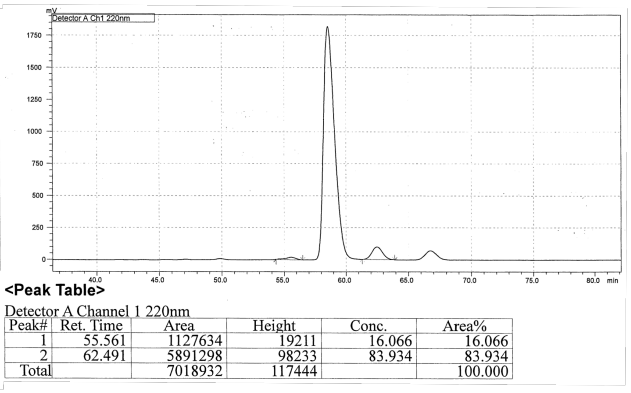
Enantiomeric purity of the minor diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	55.386	173778455	2615989	48.515	48.515
2	62.237	184419515	2443110	51.485	51.485
Total		358197971	5059099		100.000



<Peak Table>

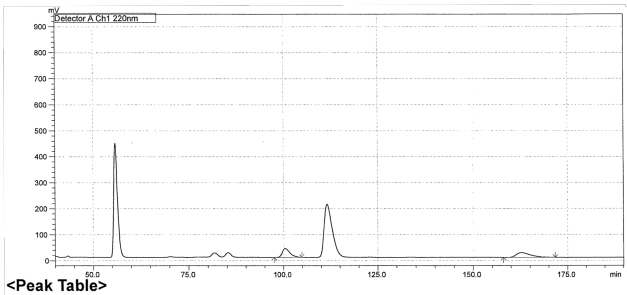
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	55.561	1127634	19211	16.066	16.066
2	62.491	5891298	98233	83.934	83.934
Total		7018932	117444		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	59.216	28585068	50.207	1	58.548	113799806	96.114
2	67.137	28349434	49.793	2	66.753	4601431	3.886
1	55.386	173778455	48.515	1	55.561	1127634	16.066
2	62.237	184419515	51.485	2	62.491	5891298	83.934

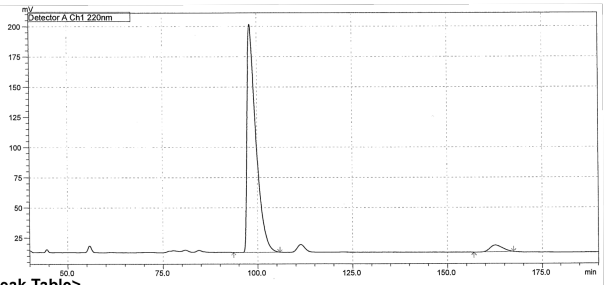
(2*S*,3*R*)-3-(3-Methoxyphenyl)pent-4-en-2-ol (2h): IR (CH_2Cl_2): 3402 (br s), 2974 (w), 1599 (m), 1488 (m), 1155 (m), 1118 (s), 1043 (s), 995 (m), 916 (m), 849 (w), 594 (m), 410 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.29–7.25 (1H, m), 6.89–6.84 (1H, m), 6.81–6.78 (2H, m), 6.01 (1H, ddd, J = 17.2, 10.4, 8.4 Hz), 5.16–5.11 (2H, m), 4.08–3.99 (1H, m), 3.81 (3H, s), 3.21 (1H, t, J = 8.4 Hz), 1.50 (1H, d, J = 3.6 Hz), 1.24 (3H, d, J = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.1, 142.7, 138.4, 130.0, 120.7, 117.1, 114.4, 112.3, 70.6, 59.3, 55.3, 20.8; HRMS (DART): Calcd for $C_{12}H_{15}O$ $[M+H–H_2O]^+$: 175.1123; Found: 175.1129; Specific rotation: $[\alpha]_D^{20}$ –47.84 (*c* 1.30, $CHCl_3$) for a >98% S_N2', 95:5 d.r., and 96:4 e.r. sample. Enantiomeric purity of **2h** was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; chiralcel AD–H column, 98:2 hexanes:*i*PrOH, 0.3 mL/min, 220 nm).

Enantiomeric purity of the major diastereomers



<Peak Table>
Detector A Channel 1 220nm

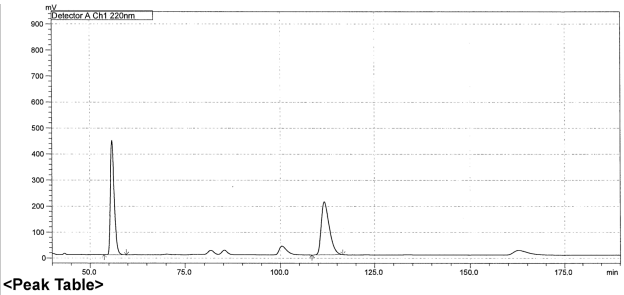
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	100.366	4735579	33805	49.828	49.828
2	162.668	4768358	18136	50.172	50.172
Total		9503937	51940		100.000



<Peak Table>
Detector A Channel 1 220nm

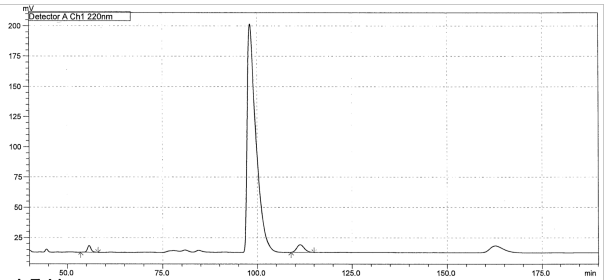
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	98.096	30598073	188770	96.031	96.031
2	162.526	1264504	5485	3.969	3.969
Total		31862577	194255		100.000

Enantiomeric purity of the minor diastereomers



<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	55.854	30827488	439133	50.306	50.306
2	111.656	30452064	203900	49.694	49.694
Total		61279552	643033		100.000



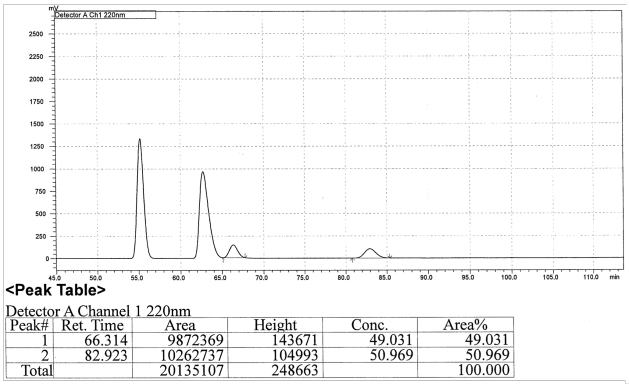
<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	55.718	374425	5598	29.247	29.247
2	111.289	905812	6416	70.753	70.753
Total		1280238	12015		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	100.366	4735579	49.828	1	98.096	30598073	96.031
2	162.668	4768358	50.172	2	162.526	1264504	3.969
1	55.854	30827488	50.306	1	55.718	374425	29.247
2	111.656	30452064	49.694	2	111.289	905812	70.753

(2*S*,3*R*)-3-(4-Chlorophenyl)pent-4-en-2-ol (2i): IR (CH_2Cl_2): 3399 (br s), 2973 (w), 1637 (w), 1490 (s), 1374 (m), 1090 (s), 992 (s), 918 (s), 818 (s), 626 (m),530 (s), 412 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.33–7.26 (2H, m), 7.21–7.19 (2H, m), 6.0 (1H, ddd, J = 16.8, 10.4, 8.4 Hz), 5.16–5.09 (2H, m), 4.08–4.00 (1H, m), 3.24 (1H, t, J = 8.0 Hz), 1.42 (1H, d, J = 4.0 Hz), 1.22 (3H, d, J = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.5, 138.1, 132.8, 130.0, 129.0, 117.4, 70.5, 58.2, 21.0; HRMS (DART): Calcd for $C_{11}H_{12}Cl$ $[M+H–H_2O]^+$: 179.0628; Found: 179.0634; Specific rotation: $[\alpha]_D^{20}$ –70.10 (*c* 1.73, $CHCl_3$) for a >98% S_N2', 95:5 d.r., and 95:5 e.r. sample. Enantiomeric purity of **2i** was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; chiralcel AD–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 220 nm).

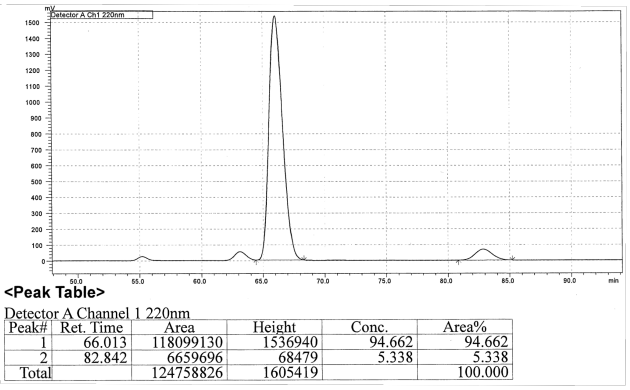
Enantiomeric purity of the major diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	66.314	9872369	143671	49.031	49.031
2	82.923	10262737	104993	50.969	50.969
Total		20135107	248663		100.000

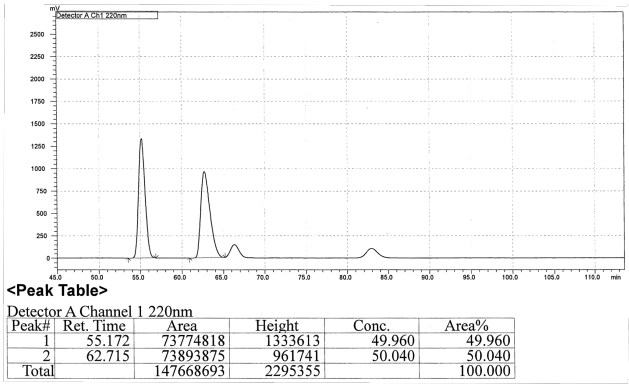


<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	66.013	118099130	1536940	94.662	94.662
2	82.842	6659696	68479	5.338	5.338
Total		124758826	1605419		100.000

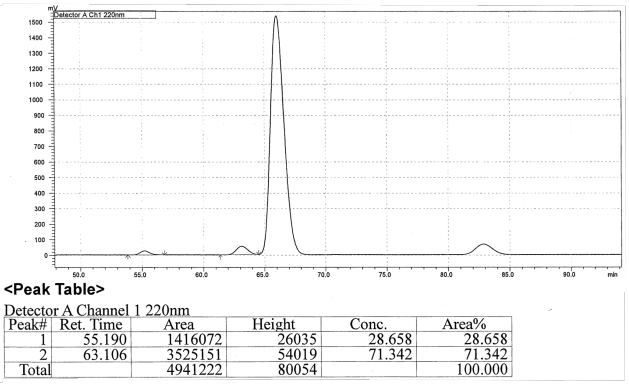
Enantiomeric purity of the minor diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	55.172	73774818	1333613	49.960	49.960
2	62.715	73893875	961741	50.040	50.040
Total		147668693	2295355		100.000



<Peak Table>

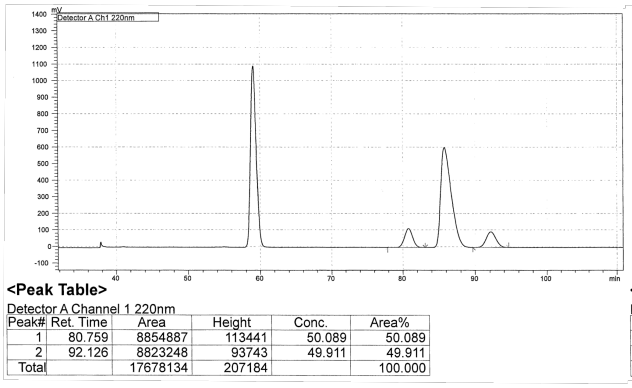
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	55.190	1416072	26035	28.658	28.658
2	63.106	3525151	54019	71.342	71.342
Total		4941222	80054		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	66.314	9872369	49.031	1	66.013	118099130	94.662
2	82.923	10262737	50.969	2	82.842	6659696	5.338
1	55.172	73774818	49.960	1	55.190	1416072	28.658
2	62.715	73893875	50.040	2	63.106	3525151	71.342

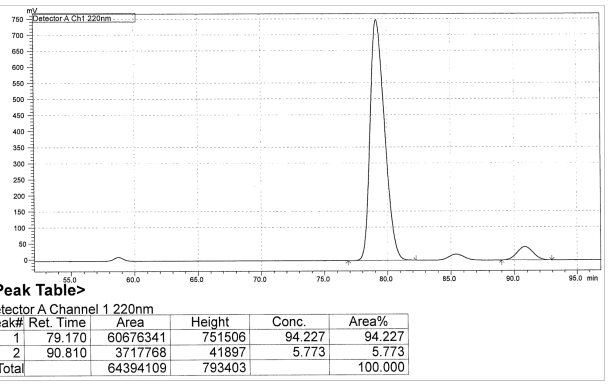
(2*S*,3*R*)-3-(4-Bromophenyl)pent-4-en-2-ol (2j): White solid; m.p. = 46–47 ºC; IR (CH_2Cl_2): 3400 (br s), 3078 (w), 2973 (w), 1637 (w), 1590 (s), 1487 (m), 1193 (s), 1117 (s), 1072 (s), 1010 (m), 918 (s), 617 (m), 527 (s), 412 (m) cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ 7.47 (2H, d, J = 7.8 Hz), 7.14 (2H, d, J = 8.4 Hz), 5.99 (1H, ddd, J = 16.8, 10.8, 9.0 Hz), 5.16–5.10 (2H, m), 4.06–4.01 (1H, m), 3.22 (1H, t, J = 8.4 Hz), 1.42 (1H, d, J = 3.6 Hz), 1.22 (3H, d, J = 6.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.1, 138.0, 132.0, 130.4, 120.9, 117.5, 70.5, 58.2, 21.0; HRMS (DART): Calcd for $C_{11}H_{12}Br$ $[M+H–H_2O]^+$: 223.0122; Found: 223.0123; Specific rotation: $[\alpha]_D^{20}$ –64.88 (*c* 1.55, $CHCl_3$) for a >98% S_N2', 95:5 d.r., and 94:6 e.r. sample. Enantiomeric purity of **2j** was determined by HPLC analysis in comparison with authentic racemic material (94:6 e.r. shown; chiralcel AZ–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 220 nm).

Enantiomeric purity of the major diastereomers



<Peak Table>
Detector A Channel 1 220nm

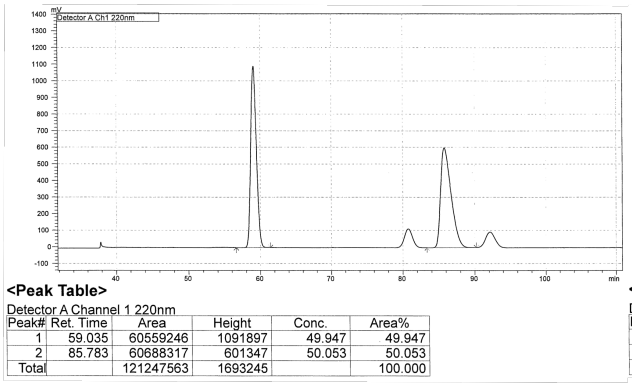
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	80.759	8854887	113441	50.089	50.089
2	92.126	8823248	93743	49.911	49.911
Total		17678134	207184		100.000



<Peak Table>
Detector A Channel 1 220nm

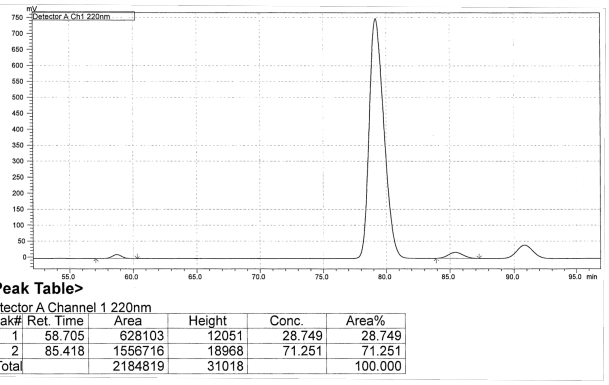
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	79.170	60676341	751506	94.227	94.227
2	90.810	3717768	41897	5.773	5.773
Total		64394109	793403		100.000

Enantiomeric purity of the minor diastereomers



<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	59.035	60559246	1091897	49.947	49.947
2	85.783	60688317	601347	50.053	50.053
Total		121247563	1693245		100.000



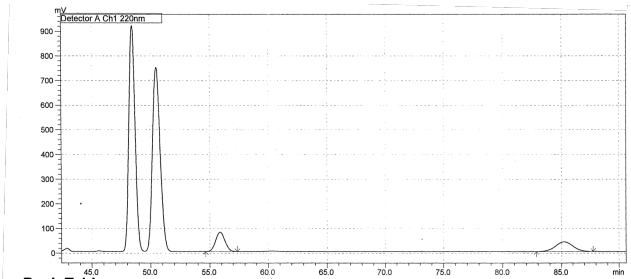
<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	58.705	628103	12051	28.749	28.749
2	85.418	1556716	18968	71.251	71.251
Total		2184819	31018		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	80.759	8854887	50.089	1	79.170	60676341	94.227
2	92.126	8823248	49.911	2	90.810	41897	5.773
1	59.035	60559246	49.947	1	58.705	628103	28.749
2	87.783	60688317	50.053	2	85.418	1556716	71.251

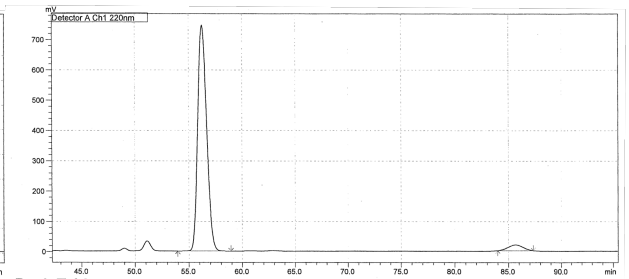
(2*S*,3*R*)-3-(4-(Trifluoromethyl)phenyl)pent-4-en-2-ol (2k): IR (CH_2Cl_2): 3412 (br, s), 2977 (w), 1638 (w), 1323 (s), 1162 (m), 1118 (s), 1066 (s), 1018 (m), 921 (m), 835 (m), 405 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.60 (2H, d, J = 8.0 Hz), 7.39 (2H, d, J = 8.8 Hz), 6.04 (1H, ddd, J = 16.8, 10.4, 8.8 Hz), 5.19–5.12 (2H, m), 4.14–4.07 (1H, m), 3.34 (1H, t, J = 8.0 Hz), 1.42 (1H, br), 1.24 (3H, d, J = 6.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.3, 137.8, 129.1 (q, J_{CF} = 31.9 Hz), 129.0, 125.7 (q, J_{CF} = 3.8 Hz), 124.3 (q, J_{CF} = 270.2 Hz), 117.8, 70.5, 58.6, 21.2; HRMS (DART): Calcd for $C_{12}H_{12}F_3$ $[M+H–H_2O]^+$: 213.0891; Found: 213.0900; Specific rotation: $[\alpha]_D^{20}$ –50.53 (*c* 1.67, $CHCl_3$) for a >98% S_N2', 95:5 d.r., and 96:4 e.r. sample. Enantiomeric purity of **2k** was determined by HPLC analysis in comparison with authentic racemic material (96:4 e.r. shown; chiralcel AD–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 220 nm).

Enantiomeric purity of the major diastereomers



<Peak Table>
Detector A Channel 1 220nm

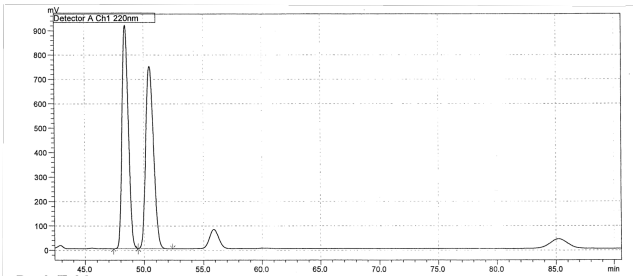
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	55.882	4306390	78757	50.641	50.641
2	85.208	4197368	39471	49.359	49.359
Total		8503758	118228		100.000



<Peak Table>
Detector A Channel 1 220nm

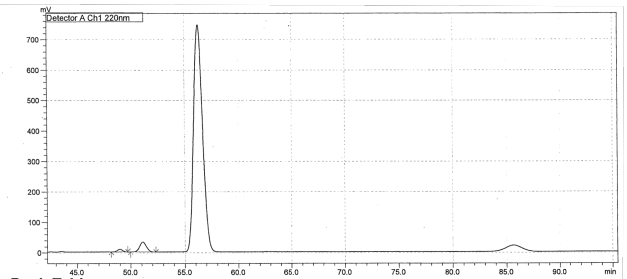
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	56.241	43337839	745578	95.817	95.817
2	85.646	1892198	19245	4.183	4.183
Total		45230037	764823		100.000

Enantiomeric purity of the minor diastereomers



<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	48.426	33828664	915978	49.672	49.672
2	50.475	34275705	746951	50.328	50.328
Total		68104370	1662929		100.000



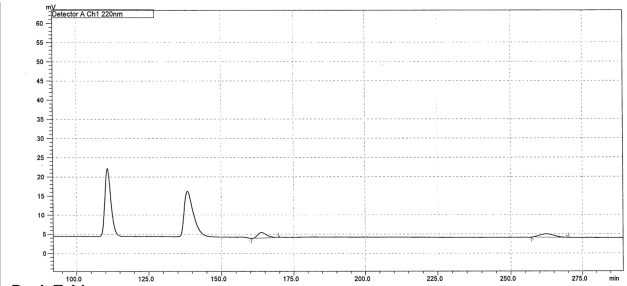
<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	48.976	297865	8638	17.357	17.357
2	51.105	1418264	32384	82.643	82.643
Total		1716129	41022		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	55.882	4306390	50.641	1	56.241	43337839	95.817
2	85.208	4197368	49.359	2	85.646	1892198	4.183
1	48.426	33828664	49.672	1	48.976	297865	17.357
2	50.275	34275705	50.328	2	51.105	1418264	82.643

(2*S*,3*R*)-3-(4-Nitrophenyl)pent-4-en-2-ol (2l): IR (CH_2Cl_2): 3431 (br s), 2924 (w),1638 (m), 1517 (s), 1457 (w), 1343 (s), 1108 (s), 1055 (s), 922 (m), 846 (m), 661 (m), 522 (m), 402 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.20 (2H, d, J = 8.8 Hz), 7.45 (2H, d, J = 8.8 Hz), 6.03 (1H, ddd, J = 16.8, 10.8, 8.8 Hz), 5.23–5.12 (2H, m), 4.14 (1H, pent, J = 6.0 Hz), 3.40 (1H, t, J = 8.0 Hz), 1.23 (1H, br), 1.24 (3H, d, J = 6.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.0, 147.0, 137.3, 129.6, 123.9, 118.3, 70.5, 58.4, 21.4; HRMS (DART): Calcd for $C_{11}H_{14}NO_3$ $[M+H]^+$: 208.0974; Found: 208.0973; Specific rotation: $[\alpha]_D^{20}$ –48.57 (*c* 1.97, $CHCl_3$) for a >98% S_N2', 93:7 d.r., and 95:5 e.r. sample. Enantiomeric purity of **2l** was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; chiralcel AD–H column, 98:2 hexanes:*i*PrOH, 0.3 mL/min, 220 nm).

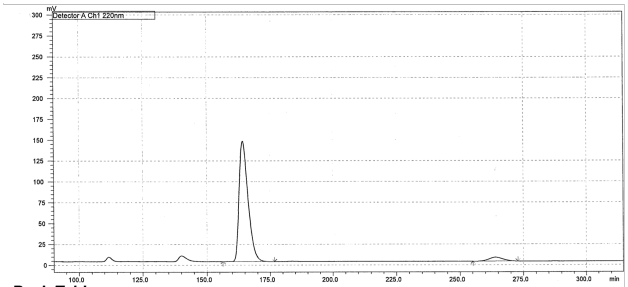
Enantiomeric purity of the major diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	163.790	318540	1479	50.220	50.220
2	262.444	315751	907	49.780	49.780
Total		634291	2386		100.000

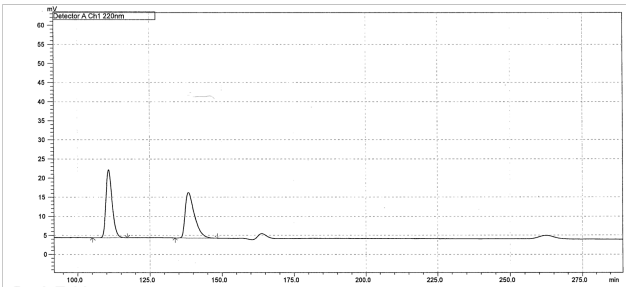


<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	164.250	35426562	144444	95.017	95.017
2	263.980	1857942	4773	4.983	4.983
Total		37284504	149217		100.000

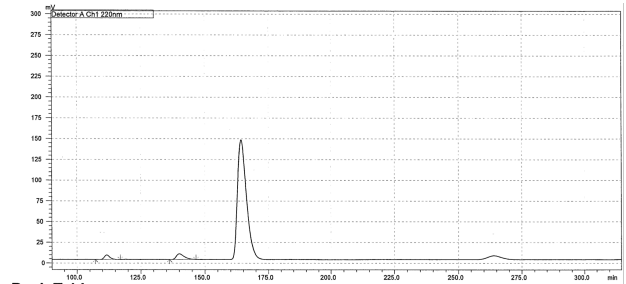
Enantiomeric purity of the minor diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	110.793	2640525	17737	49.848	49.848
2	138.390	2656616	11908	50.152	50.152
Total		5297141	29645		100.000



<Peak Table>

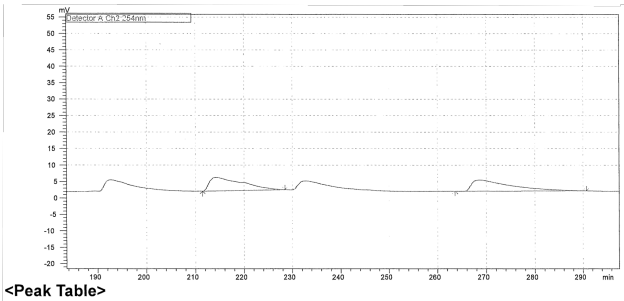
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	111.597	809379	5466	35.568	35.568
2	140.009	1466230	6879	64.432	64.432
Total		2275609	12344		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	163.790	318540	50.220	1	164.250	35426562	95.017
2	262.444	315751	49.780	2	263.980	1857942	4.983
1	110.793	2640525	49.848	1	111.597	809379	35.568
2	138.390	2656616	50.152	2	140.009	1466230	64.432

(2*S*,3*R*)-3-(Pyridin-3-yl)pent-4-en-2-ol (4): Following the representative procedure except 7.5 mol % **imid-3** and 7.0 mol % CuCl were used. IR (CH_2Cl_2): 3232 (br s), 2923 (m), 1577 (w), 1427 (m), 1373 (m), 1312 (w), 1119 (s), 1029 (m), 918 (s), 802 (m), 714 (s), 402 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.51–8.48 (2H, m), 7.61 (1H, dt, J = 7.6, 2.0 Hz), 7.28–7.25 (2H, m), 6.06 (1H, ddd, J = 16.8, 10.4, 8.4 Hz), 5.21–5.12 (2H, m), 4.11 (1H, pent, J = 6.8 Hz), 3.30 (1H, t, J = 7.6 Hz), 1.63 (1H, br), 1.22 (3H, d, J = 6.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.4, 148.4, 137.7, 136.5, 136.2, 123.6, 118.0, 70.4, 55.8, 21.3; HRMS (DART): Calcd for $C_{10}H_{14}NO$ $[M+H]^+$: 164.1075; Found: 164.1073; Specific rotation: $[\alpha]_D^{20}$ –43.32 (*c* 0.42, $CHCl_3$) for a 96% S_N2', 92:8 d.r., and 93:7 e.r. sample. Enantiomeric purity of **4** was determined by HPLC analysis in comparison with authentic racemic material (93:7 e.r. shown; chiralcel OZ–H column, 97:3 hexanes:*i*PrOH, 0.3 mL/min, 254 nm).

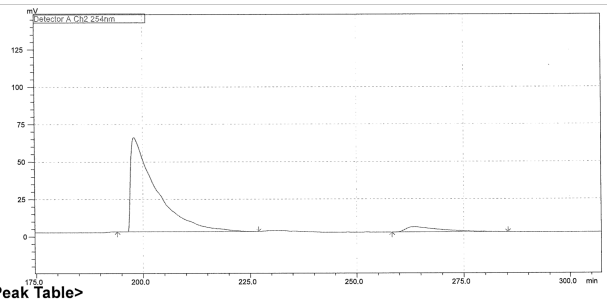
Enantiomeric purity of the major diastereomers



<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	214.158	1921177	4097	50.393	50.393
2	268.479	1891182	3393	49.607	49.607
Total		3812358	7490		100.000



<Peak Table>

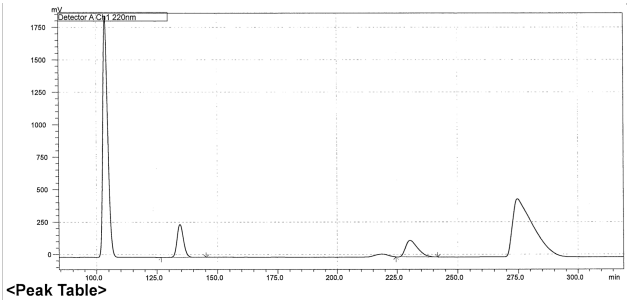
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	197.925	25868140	62908	93.180	93.180
2	263.432	1893233	3423	6.820	6.820
Total		27761373	66331		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	214.158	1921177	50.393	1	197.925	25868140	93.180
2	268.479	1891182	49.607	2	263.432	1893233	6.820

(2*S*,3*R*)-3-(Benzo[*b*]thiophen-3-yl)pent-4-en-2-ol (5): IR (CH_2Cl_2): 3429 (br s), 2974 (w), 1637 (w), 1426 (m), 1392 (w), 1116 (m), 1063 (m), 871 (m), 760 (s), 599 (w), 425 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.89–7.87 (1H, m), 7.82 (1H, dd, J = 6.4, 1.2 Hz), 7.14–7.34 (2H, m), 7.33 (1H, s), 7.26 (1H, s), 6.15–6.06 (1H, m), 5.21–5.17 (2H, m), 4.26 (1H, pent, J = 6.4 Hz), 3.81 (1H, t, J = 7.6 Hz), 1.71 (1H, br), 1.28 (3H, d, J = 6.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.7, 138.9, 137.2, 135.3, 124.6, 124.2, 123.1, 122.7, 122.2, 117.7, 70.0, 52.0, 20.9; HRMS (DART): Calcd for $C_{13}H_{13}S$ $[M+H–H_2O]^+$: 201.0738; Found: 201.0738; Specific rotation: $[\alpha]_D^{20}$ –20.61 (*c* 1.82, $CHCl_3$) for a >98% S_N2', 91:9 d.r., and 95:5 e.r. sample. Enantiomeric purity of **5** was determined by HPLC analysis in comparison with authentic racemic material (95:5 e.r. shown; chiralcel AD–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 220 nm).

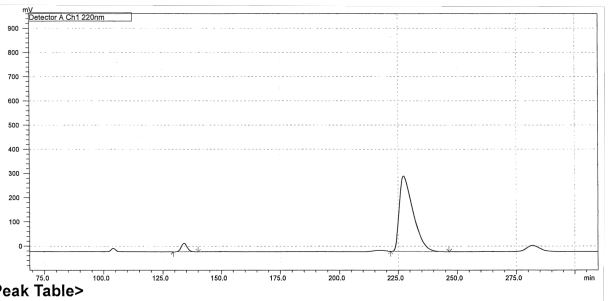
Enantiomeric purity of the major diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	134.537	46490882	253966	50.812	50.812
2	230.390	45004239	128962	49.188	49.188
Total		91495121	382928		100.000

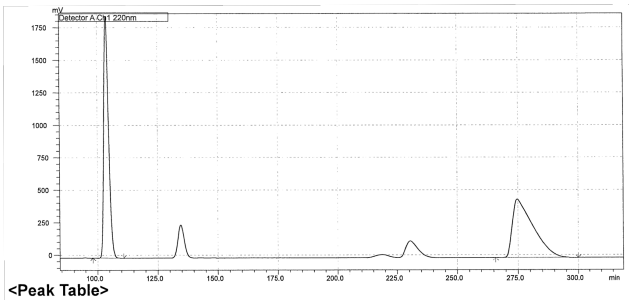


<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	133.993	6142996	34919	4.597	4.597
2	227.344	127481162	311851	95.403	95.403
Total		133624158	346770		100.000

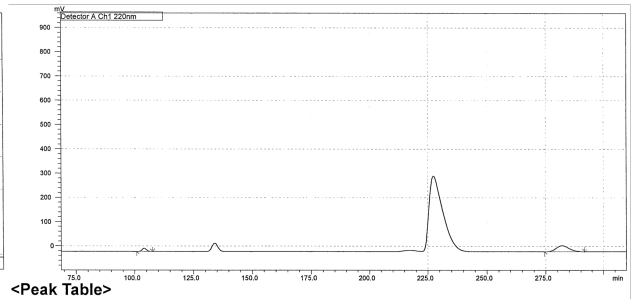
Enantiomeric purity of the minor diastereomers



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	103.675	267438465	1857474	49.975	49.975
2	274.662	267701211	448953	50.025	50.025
Total		535139676	2306427		100.000



<Peak Table>

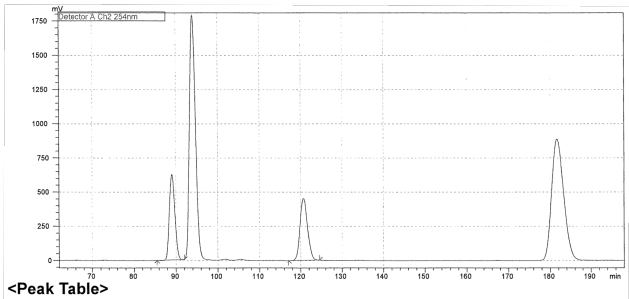
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	103.999	1728472	13379	15.230	15.230
2	281.890	9620797	24958	84.770	84.770
Total		11349269	38337		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	134.537	46490882	50.812	1	133.993	6142996	4.597
2	230.390	45004239	49.188	2	227.344	127481162	95.403
1	103.675	267438465	49.975	1	103.999	1728472	15.230
2	274.662	267701211	50.025	2	281.890	9620797	84.770

(2*S*,3*R*,*E*)-5-Phenyl-3-vinylpent-4-en-2-ol (6): Following the representative procedure except 7.5 mol % **imid-3** and 7.0 mol % CuCl were used. IR (CH_2Cl_2): 3377 (br s), 2972 (w), 1636 (w), 1599 (w), 1449 (m), 1373 (w), 1119 (s), 1072 (s), 996 (s), 915 (s), 865 (m), 607 (m), 517 (m) cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 7.40–7.37 (2H, m), 7.32 (2H, t, J = 7.0 Hz), 7.23 (1H, t, J = 7.0 Hz), 6.50 (1H, d, J = 16.0 Hz), 6.21 (1H, dd, J = 16.0, 8.5 Hz), 5.88 (1H, ddd, J = 17.5, 10.5, 8.0 Hz), 5.20–5.17 (2H, m), 3.83 (1H, pent, J = 6.0 Hz), 2.91 (1H, q, J = 8.0 Hz), 1.73 (1H, br), 1.23 (3H, d, J = 6.0 Hz);^{13}C NMR (100 MHz, $CDCl_3$): δ 137.6, 137.2, 133.0, 128.7, 128.5, 127.6, 126.4, 117.3, 69.9, 55.8, 20.5; HRMS (DART): Calcd for $C_{13}H_{15}$ $[M+H–H_2O]^+$: 171.1174; Found: 171.1183; Specific rotation: $[\alpha]_D^{20}$ –60.33 (*c* 1.15, $CHCl_3$) for a >98:2 S_N2', 90:10 d.r., and 92:8 e.r. sample. Enantiomeric purity of **6** was determined by HPLC analysis in comparison with authentic racemic material (92:8 e.r. shown; chiralcel OD–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 254 nm).

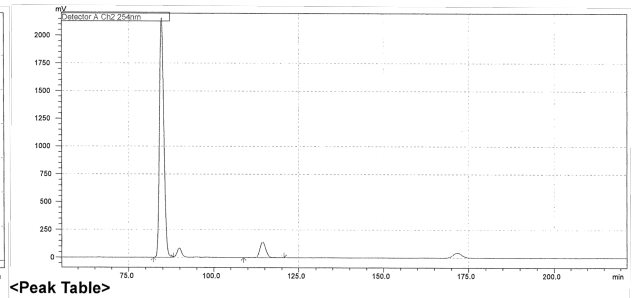
Enantiomeric purity of the major diastereomers



<Peak Table>

Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	89.082	55911504	625821	49.674	49.674
2	120.692	56644252	452282	50.326	50.326
Total		112555757	1078103		100.000

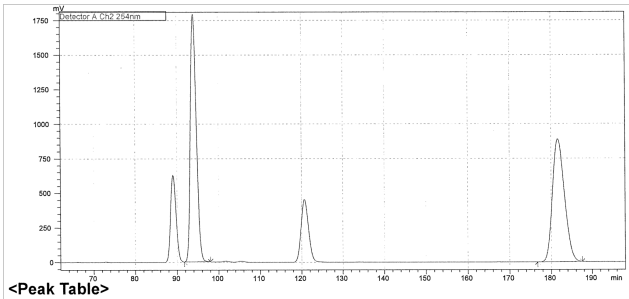


<Peak Table>

Detector A Channel 2 254nm

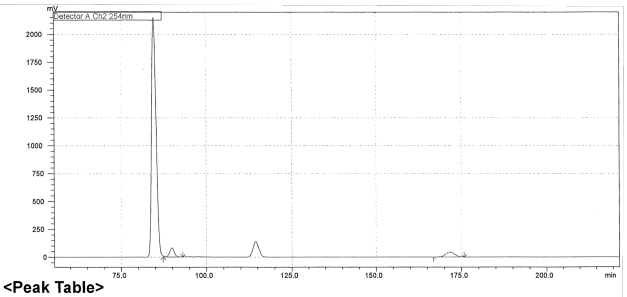
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	84.609	195678063	2154765	92.103	92.103
2	114.405	16777727	140555	7.897	7.897
Total		212455790	2295320		100.000

Enantiomeric purity of the minor diastereomers



<Peak Table>
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	93.997	178674606	1790176	49.880	49.880
2	181.639	179532462	886824	50.120	50.120
Total		358207068	2677000		100.000



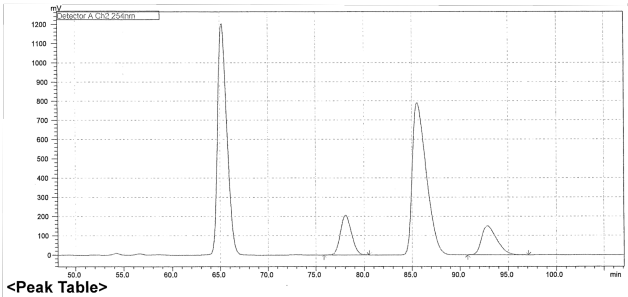
<Peak Table>
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	89.829	7853360	81506	49.388	49.388
2	171.676	8047969	44063	50.612	50.612
Total		15901329	125568		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	89.082	55911504	49.674	1	84.609	195678063	92.103
2	120.692	56644252	50.326	2	114.405	16777727	7.897
1	93.997	178674606	49.880	1	89.829	7853360	49.388
2	181.639	179532462	50.120	2	171.676	8047969	50.612

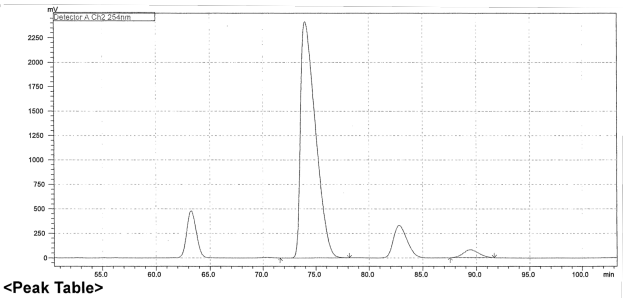
(2*S*,3*R*)-3-(Phenylethynyl)pent-4-en-2-ol (7): IR (CH_2Cl_2): 3399 (br s), 2975 (w), 1639 (w), 1598 (w), 1490 (m), 1443 (m), 1115 (s), 1070 (s), 921 (s), 825 (m), 597 (m), 469 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.47–7.43 (2H, m), 7.33–7.30 (3H, m), 5.91 (1H, ddd, J = 20.8, 10, 6.4 Hz), 5.43–5.47 (1H, m), 5.31–5.28 (1H, m), 3.93–3.88 (1H, m), 3.38–3.35 (1H, m), 1.99 (1H, d, J = 2.0 Hz), 1.34 (3H, d, J = 6.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.5, 131.9, 128.4, 128.3, 123.2, 118.2, 86.7, 86.2, 69.9, 45.4, 20.7; HRMS (DART): Calcd for $C_{11}H_{15}O$ $[M+H]^+$: 187.1123; Found: 187.1131; Specific rotation: $[\alpha]_D^{20}$ –82.21 (*c* 0.85, $CHCl_3$) for a >98% S_N2', 93:7 d.r., and 91:9 e.r. sample. Enantiomeric purity of **7** was determined by HPLC analysis in comparison with authentic racemic material (97:3 e.r. shown; chiralcel AZ–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 254 nm).

Enantiomeric purity of the major diastereomers



<Peak Table>
Detector A Channel 2 254nm

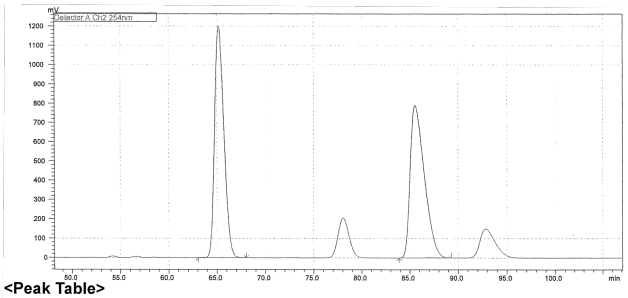
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	78.052	16615430	206893	50.119	50.119
2	92.829	16536389	150750	49.881	49.881
Total		33151819	357643		100.000



<Peak Table>
Detector A Channel 2 254nm

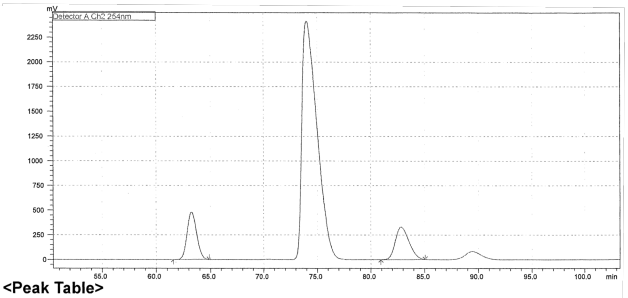
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	74.007	235964984	2414322	96.619	96.619
2	89.420	8256356	80432	3.381	3.381
Total		244221340	2494754		100.000

Enantiomeric purity of the minor diastereomers



<Peak Table>
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	65.189	80801160	1203861	49.993	49.993
2	85.567	80822719	790731	50.007	50.007
Total		161623879	1994592		100.000



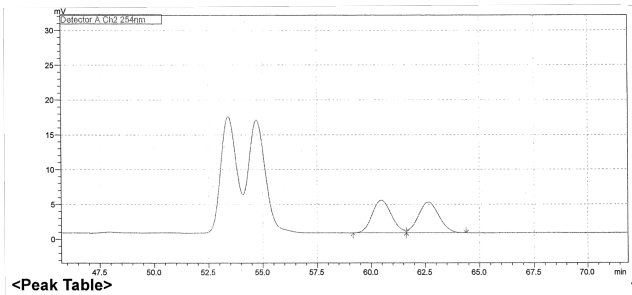
<Peak Table>
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	63.246	29463954	480871	50.300	50.300
2	82.812	29112280	329933	49.700	49.700
Total		58576234	810805		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	78.052	16615430	50.119	1	74.007	235964984	96.619
2	92.829	16536389	49.881	2	89.420	8256356	3.381
1	65.189	80801160	49.993	1	63.246	480871	50.300
2	85.567	80822719	50.007	2	82.812	329933	49.700

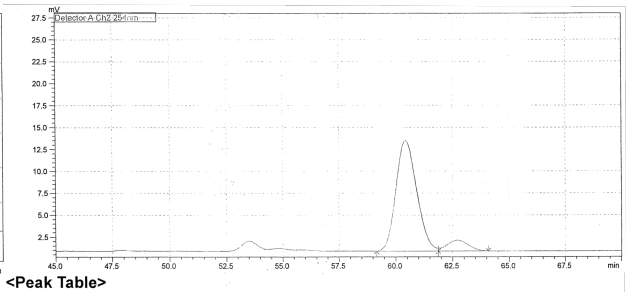
(2*S*,3*S*)-3-Phenethylpent-4-en-2-ol (8): IR (CH_2Cl_2): 3358 (br s), 2923 (w), 1639 (w), 1496 (m), 1374 (w), 1122 (s), 1053 (m), 998 (m), 913 (s), 697 (s), 413 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.30–7.27 (2H, m), 7.20–7.16 (3H, m), 5.66 (1H, ddd, *J* = 17.2, 10.4, 9.2 Hz), 5.23 (1H, dd, *J* = 10.0, 2.0 Hz), 5.15 (1H, ddd, *J* = 17.2, 2.0, 0.8 Hz), 3.75–3.67 (1H, m), 2.71 (1H, ddd, *J* = 14.0, 10.0, 4.4 Hz), 2.51 (1H, ddd, *J* = 13.6, 10.0, 7.2 Hz), 2.17–2.10 (1H, m), 1.92–1.84 (1H, m), 1.62–1.52 (1H, m), 1.45 (1H, d, *J* = 7.6 Hz), 1.15 (3H, d, *J* = 6.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.5, 138.4, 128.6, 128.5, 125.9, 118.4, 70.3, 51.4, 33.7, 32.4, 20.2; HRMS (DART): Calcd for $C_{13}H_{17}$ $[M+H–H_2O]^+$: 173.1330; Found: 173.1329; Specific rotation: $[\alpha]_D^{20}$ –6.29 (*c* 2.50, $CHCl_3$) for a >98% S_N2', 92:8 d.r., and 91:9 e.r. sample. Enantiomeric purity of **8** was determined by HPLC analysis in comparison with authentic racemic material (91:9 e.r. shown; chiralcel AD–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 254 nm).

Enantiomeric purity of the major diastereomers



<Peak Table>
Detector A Channel 2 254nm

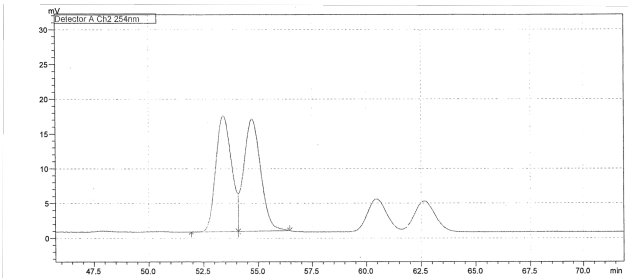
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	60.459	292381	4701	50.242	50.242
2	62.663	289564	4403	49.758	49.758
Total		581945	9104		100.000



<Peak Table>
Detector A Channel 2 254nm

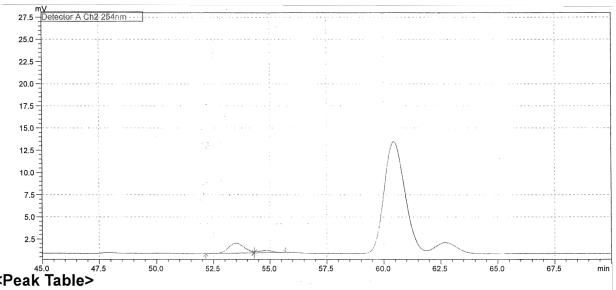
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	60.443	803668	12613	90.809	90.809
2	62.693	81343	1253	9.191	9.191
Total		885012	13866		100.000

Enantiomeric purity of the minor diastereomers



<Peak Table>
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	53.416	834260	16669	48.791	48.791
2	54.720	875598	16122	51.209	51.209
Total		1709858	32792		100.000



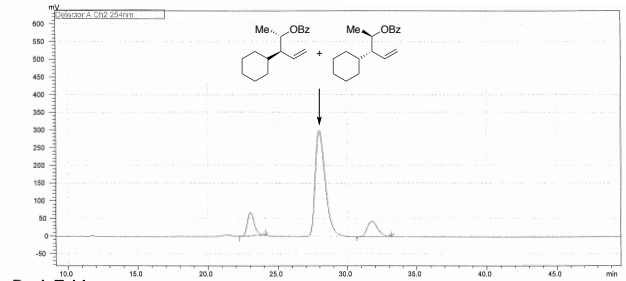
<Peak Table>
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	53.476	53606	1108	84.024	84.024
2	54.788	10193	226	15.976	15.976
Total		63799	1334		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	60.459	292381	50.242	1	60.443	803668	90.809
2	62.663	289564	49.758	2	62.693	81343	9.191
1	53.416	834260	48.791	1	53.476	53606	84.024
2	54.720	875598	51.209	2	54.788	10193	15.976

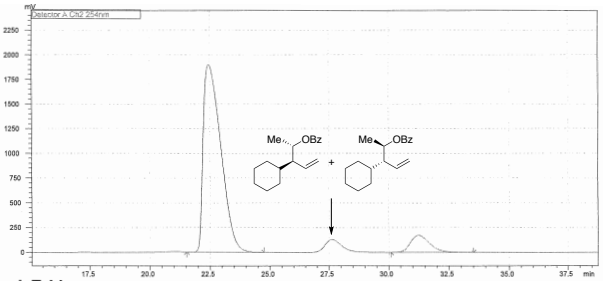
(2*S*,3*R*)-3-Cyclohexylpent-4-en-2-ol (9): Following the representative procedure except 7.5 mol % **imid-3** and 7.0 mol % CuCl were used. IR (CH_2Cl_2): 3377 (br s), 2967 (m), 2922 (s), 2852 (m), 1449 (m), 1420 (w), 1118 (s), 1057 (s), 1001 (m), 956 (w), 910 (s), 872 (w), 838 (w), 768 (s), 507 (w), 407 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 5.56 (1H, dt, J = 16.8, 10.0 Hz), 5.17 (1H, dd, J = 10.0, 2.4 Hz), 5.06 (1H, dd, J = 16.8, 2.0 Hz), 3.92–3.87 (1H, m), 1.94–1.88 (1H, m), 1.74–1.71 (3H, m), 1.66–1.60 (2H, m), 1.50–1.41 (2H, m), 1.31–1.20 (3H, m), 1.10 (3H, d, J = 6.0 Hz), 0.99–0.84 (1H, m);^{13}C NMR (100 MHz, $CDCl_3$): δ 137.1, 118.8, 66.8, 57.9, 37.9m, 31.4, 30.3, 26.7, 26.6, 26.5, 20.0; HRMS (DART): Calcd for $C_{11}H_{19}$ $[M+H–H_2O]^+$: 151.1487; Found: 151.1491; Specific rotation: $[\alpha]_D^{20}$ –9.83 (*c* 0.55, $CHCl_3$) for a >98% S_N2', 93:7 d.r., and 91:9 e.r. sample. Enantiomeric purity of **9** was determined by HPLC analysis of the product from *p*-bromobenzoylation[13] in comparison with authentic racemic material (91:9 e.r. shown; chiralcel AD–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 254 nm).

Enantiomeric purity of the major diastereomers



<Peak Table>
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	23.031	2275091	65643	50.212	50.212
2	31.762	2255881	43492	49.788	49.788
Total		4530972	109135		100.000



<Peak Table>
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	22.453	96662248	1899556	91.048	91.048
2	31.232	9503542	172352	8.952	8.952
Total		106165790	2071908		100.000

[13] W. Rao, M. J. Koh, P. Kothandaraman, P. W. H. Chan, *J. Am. Chem. Soc*. **2012,** *134,* 10811–10814.

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	23.031	2275091	50.212	1	22.453	96662248	91.048
2	31.762	2255881	49.788	2	31.232	9503542	8.952

■ **Gram Scale Reaction with (*E*)-But-2-en-1-yl diethyl phosphate (2*S*,3*S*)-3-methylpent-4-en-2-ol (10):** In a N_2-filled glove box, a flame-dried 100 mL round-bottom flask equipped with a stir bar was charged with CuCl (9.9 mg, 0.10 mmol), imidazolinium ligand (107.4 mg, 0.125 mmol), and Li*O*t*Bu (600 mg, 7.50 mmol). The flask was sealed with a septum and electrical tape before removal from the glove box. Freshly distilled thf (10 mL) was added and the resulting solution was allowed to stir for 1 h under N_2 at 22 °C. A solution of PMHS (902.3 mg, 15.0 mmol) in thf (5 mL) was added to the mixture at 0 °C, causing the solution to turn yellow brown immediately. After 1 min, a solution of vinyl boronic acid pinacol ester (847mg, 5.50 mmol) and (*E*)-but-2-en-1-yl diethyl phosphate (1041 mg, 5.0 mmol) in thf (10 mL) was added by syringe. The resulting mixture was allowed to stir at 22 °C for 14 h after which the mixture was passed through a short plug of silica gel (4x4 cm, 1% of triethylamine) and eluted with Et_2O. Removal of the volatiles *in vacuo* afforded bright yellow oil. To the oil was added thf (10 mL), pH 7.0 buffer solution (10 mL), and $NaBO_3$•$4H_2O$ (3846 mg, 25.0 mmol) at 0 ºC. After complete addition, the mixture was allowed to stir at 22 ºC for 3 h. The mixture was washed with Et_2O (3 x 10 mL), and the combined organic layers were dried over $MgSO_4$. Carefully concentrated (product is volatile) mixture was purified by silica gel chromatography (hexanes:Et_2O = 10:5, R_f = 0.2) to afford the desired product as clear oil (275 mg, 2.746 mmol, 55% yield). Spectroscopic data match those reported previously.[14] ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.83–5.74 (1H, m), 5.12–5.07 (2H, m), 3.73–3.64 (1H, m), 2.27–2.20 (1H, m), 1.50 (1H, br), 1.15 (3H, d, *J* = 6.4 Hz), 1.03 (3H, d, *J* = 6.8 Hz); Specific rotation: $[\alpha]_D^{20}$ –19.05 (c 4.43, $CHCl_3$) for a >98% S_N2', 92:8 d.r., and 93:7 e.r. sample. Based on reported optical rotation values $[\alpha]_D$ –35.2 (c 1.6, $CHCl_3$)[14] and $[\alpha]_D$ –19.56 (neat),[15] the absolute stereochemistry of the major enantiomer is assigned to be (2*S*,3*S*). The diastereoselectivity was determined by ^{1}H NMR spectra after *p*-methoxybenzylation of the alcohol.[16] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27 (2H, d, *J* = 8.8 Hz), 6.87 (2H, d, *J* = 8.0 Hz), 5.82 (1H, ddd, *J* = 17.2, 10.0, 7.2 Hz), 5.05 (1H, d, *J* = 11.6 Hz), 5.01 (1H, d, *J* = 4.8 Hz), 4.52 (1H, d, *J* = 11.6 Hz), 4.40 (1H, d, *J* = 11.6 Hz), 3.80 (3H, s), 3.35 (1H, pent, *J* = 6.4 Hz), 2.41–2.33 (1H, m), 1.12 (3H, d, *J* = 6.4 Hz), 1.04 (3H, d, *J* = 7.2 Hz). Enantiomeric purity of **10** was determined by HPLC analysis of the corresponding *p*-methoxybenzyl ether[16] in comparison with authentic racemic material (93:7

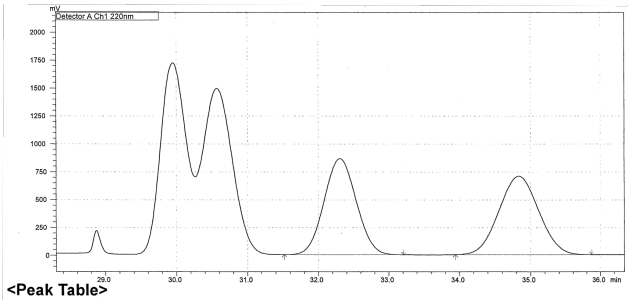
[14] R. Tannert, L.-G. Milroy, B. Ellinger, T-S. Hu, H-D. Arndt, H. Waldmann, *J. Am. Chem. Soc*. **2010,** *132,* 3063–3077.

[15] H. C. Brown, K. S. Bhat, *J. Am. Chem. Soc*. **1986,** *108,* 293–294.

[16] U. Eggert, R. Diestel, F. Sasse, R. Jansen, B. Kunze, M. Kalesse, *Angew. Chem. Int. Ed.* **2008**, *47,* 6478–6482.

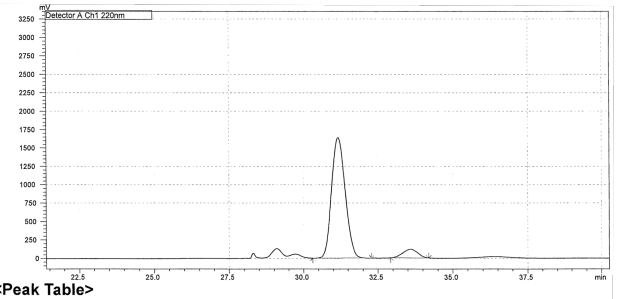
e.r. shown; chiralcel OJ–H column, 99:1 hexanes:*i*PrOH, 0.3 mL/min, 220 nm).

Enantiomeric purity of the major isomers



<Peak Table>
Detector A Channel 1 220nm

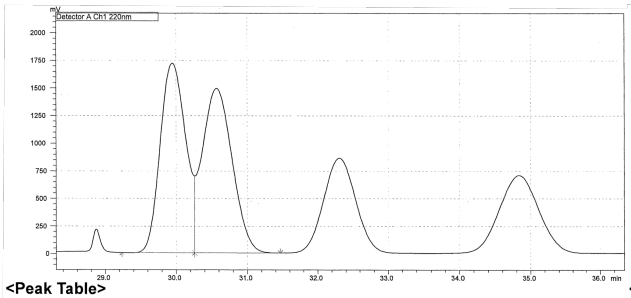
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	32.306	27352504	861994	50.024	50.024
2	34.835	27326687	705214	49.976	49.976
Total		54679191	1567207		100.000



<Peak Table>
Detector A Channel 1 220nm

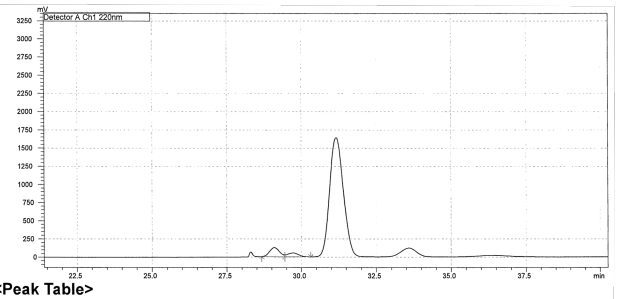
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	31.169	52308708	1638017	92.774	92.774
2	33.586	4074216	117164	7.226	7.226
Total		56382924	1755181		100.000

Enantiomeric purity of the minor isomers



<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	29.948	42912130	1718245	49.685	49.685
2	30.569	43456870	1490743	50.315	50.315
Total		86368999	3208988		100.000



<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	29.090	2912130	126958	68.995	68.995
2	29.713	1308670	52532	31.005	31.005
Total		4220800	179490		100.000

Peak #	Retention time	Area	Area %	Peak #	Retention time	Area	Area %
1	32.306	27352504	50.024	1	31.169	52308798	92.774
2	34.835	27326687	49.976	2	33.586	4074216	7.226
1	29.948	42912130	49.685	1	29.090	2912130	68.995
2	30.569	43456870	50.315	2	29.713	1308670	31.005

■ C–B(pin) to C–furyl Conversion

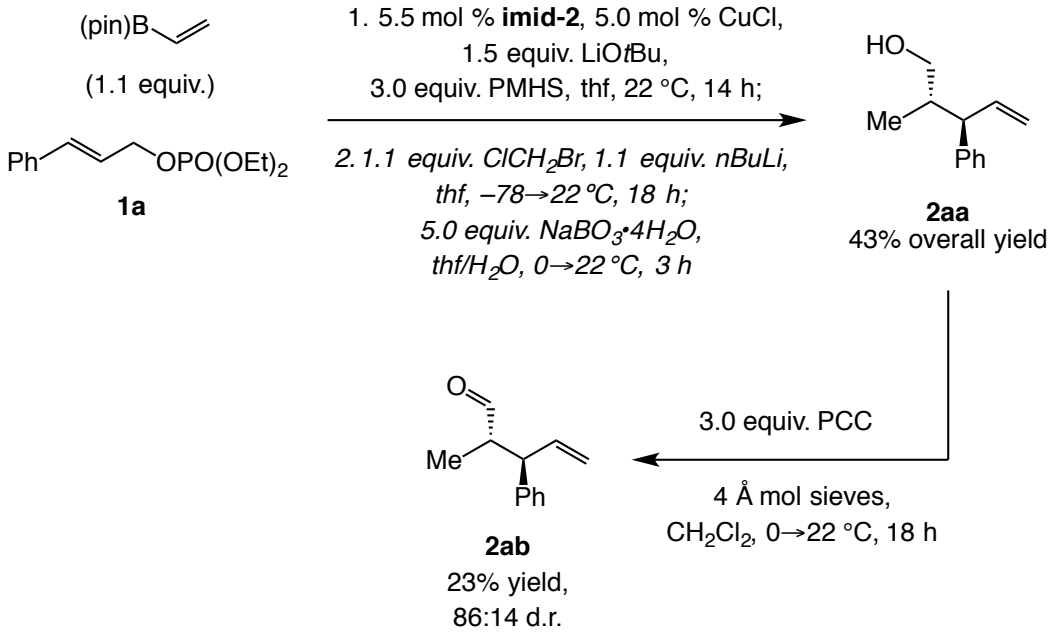
2-((2*S*,3*S*)-3-Phenethylpent-4-en-2-yl)furan (12): The secondary boron compound (0.35 mmol, precursor to alcohol **8**) was converted to **12** by a reported procedure[17] except 1.5 equiv. furan, 1.5 equiv. *n*-BuLi, and 1.5 equiv. NBS were used. IR (neat): 3026 (w), 2933 (w), 1640 (w), 1496 (m), 1454 (m), 1148 (m), 1117 (w), 1030 (s), 914 (s), 793 (m), 598 (m), 497 (m) cm^{-1}; ^1H NMR (400, MHz $CDCl_3$): δ 7.30–7.23 (3H, m), 7.18–7.16 (1H, m), 7.11 (2H, d, *J* = 7.6 Hz), 6.27 (1H, dd, *J* = 3.2, 2.0 Hz), 5.95 (1H, d, *J* = 2.8 Hz), 5.60 (1H, ddd, *J* = 16.8, 10.0, 9.2 Hz), 5.10 (1H, dd, *J* = 10.4, 2.0 Hz), 5.02–4.97 (2H, m), 2.81 (1H, pent, *J* = 6.8 Hz), 2.66 (1H, ddd, *J* = 13.6, 10.8, 5.2 Hz), 2.44 (1H, ddd, *J* = 14.0, 10.0, 6.4 Hz), 1.71–1.62 (1H, m), 1.51–1.44 (1H, m), 1.19 (3H, d, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.3, 142.7, 140.7, 140.4, 128.5, 128.4, 125.7, 116.6, 110.0, 104.9, 48.7, 37.6, 34.1, 33.8, 16.4; HRMS $[M+H]^+$ Found for $C_{17}H_{21}O$:

[17] A. Bonet, M. Odachowski, D. Leonori, S. Essafi, V. K. Aggarwal, *Nature Chem.* **2014,** *6,* 584–589.

241.1601; Specific rotation: $[\alpha]_D^{20}$ –2.31 (*c* 6.67, $CHCl_3$).

■ **Assignment of Absolute Configuration of the Major Isomer from imid-2**

The absolute configuration of the major isomer from **imid-2** was assigned by comparing the optical rotation of corresponding aldehyde **2ab** after homologation and oxidations.



2-Methyl-3-phenylpent-4-en-1-ol (2aa): The secondary boron compound was prepared from the representative procedure except **imid-2** was used (0.3 mmol scale). After purification, the sample was homologated by the reported procedure[18] and oxidized to give the final product (43% overall yield after flash column chromatography). ^{1}H NMR data match those reported previously.[19] ^{1}H NMR (400, MHz $CDCl_3$): δ 7.32–7.17 (5H, m), 6.11–6.01 (1H, m), 5.14–5.04 (2H, m), 3.71–3.67 (1H, m), 3.60–3.56 (1H, m), 3.17 (1H, t, *J* = 9.6 Hz), 2.08–2.01 (1H, m), 1.51 (1H, br), 0.80 (3H, dd, *J* = 7.2, 1.2 Hz).

(2*S*,3*R*)-2-Methyl-3-phenylpent-4-enal (2ab): Prepared from **S2** according to the reported procedure.[20] Spectroscopic data match those reported previously.[21] ^{1}H NMR (400, MHz $CDCl_3$): δ 9.71–9.69 (1H, m), 7.36–7.18 (5H, m), 6.08–5.98 (1H, m), 5.14–5.09 (2H, m), 3.53 (1H, t, *J* = 9.0 Hz), 2.83–2.75 (1H, m), 0.94–0.92 (3H, m); Specific rotation: $[\alpha]_D^{20}$ +22.79 (c 0.63, $CHCl_3$) for a >98% S_N2', 86:14 d.r., and 87:13 e.r. sample. Based on reported optical rotation values $[\alpha]_D^{26}$ +57.4 (c 1.0, $CHCl_3$)[21], the absolute stereochemistry of the major enantiomer is assigned to be (2*S*,3*R*).

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[18] T. Ohmura, H. Furukawa, M. Suginome, *J. Am. Chem. Soc*. **2006,** *128,* 13366–13367.

[19] a) E. E. Kwan, J. R. Scheerer, D. A. Evans, *J. Org. Chem.* **2013,** *78,* 175–203; b) B. D. Kelly, J. M. Allen, R. E. Tundel, T. H. Lambert, *Org. Lett.* **2009,** *11,* 1381–1383.

[20] C. H. Oh, J. H. Hong, *Bull. Korean Chem. Soc.* **2005,** *26,* 1520–1524.

[21] S. Krautwald, M. A. Schafroth, D. Sarlah, E. M. Carreira, *J. Am. Chem. Soc*. **2014,** *136,* 3020–3023.

■ Density Functional Theory (DFT)/ONIOM Calculations

DFT/OMIOM computations[22] were performed with the Gaussian 09 suite of programs.[23] Geometries were optimized by the following ONIOM[24] method: M06L/Def2SVP:UFF (see Scheme S2 for definition of the boundaries; in cases where explicit thf molecules have been used in the simulations, only the oxygen atom has been modeled with the higher level). The effect of a polar reaction medium (tetrahydrofuran, THF) was approximated by means of an integral equation formalism variant of the polarizable continuum model (IEFPCM).[25] Stationary points were probed through vibrational analysis and Gibbs free energy corrections were performed under standard conditions (298.15 K, 1.0 atm). Intrinsic reaction coordinate (IRC) calculations have been performed starting from selected transition states (**ts**) employing the L(ocal) Q(uadratic) A(approximation) method, followed by subsequent optimization to obtain structures and energies for educt (**ed**) and product (**prod**) on either side of the transition state.[26] We furthermore probed the performance of various density functionals through single point energy calculations at the geometries optimized at the levels described above by means of the SMD solvation model[27] with THF as solvent and the larger Def2TZVPP[28] basis set. Since the correct density functional is not known we tested several state of the art approaches that have been

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

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

[24] L. W. Chung, W. M. C. Sameera, R. Ramozzi, A. J. Page, M. Hatanaka, G. P. Petrova, T. V. Harris, X. Li, Z. Ke, F. Liu, H.-B. Li, L. Ding, K. Morokuma, *Chem. Rev.* **2015,** *115,* 5678–5769.

[25] G. Scalmani, M. J. Frisch, *Chem. Phys.* **2010***, 132,* 114110.

[26] a) M. Page, J. W. McIver Jr., *Phys.* **1988,** *88,* 922–935; b) M. Page, C. Doubleday Jr., J. W. McIver Jr., *J. Chem. Phys.* **1990,** *93,* 5634–5642.

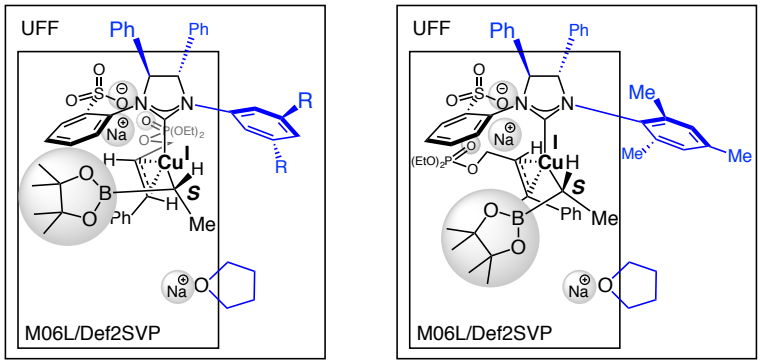
[27] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B.* **2009.** *113,* 6378–6396.

[28] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297–3305.

[29] For selected examples highlighting the importance of including treatment of dispersion interactions in modeling olefin metathesis reactions promoted by Ru carbene complexes, see: a) S. Torker, D. Merki, P. Chen, *J. Am. Chem. Soc.* **2008,** *130,* 4808–4814; b) Y. Minenkov, G. Occhipinti, A. Singstad, V. R. Jensen, *Dalton Trans.* 2012. 41, 5526–5541; c) Y. Minenkov, G. Occhipinti, V. R. Jensen, *Organometallics* **2013,** *32,* 2099–2111; d) S. Torker, R. K. M. Khan, A. H. Hoveyda, *J. Am. Chem. Soc.* **2014,** *136,* 3439–3455; e) R. K. M. Khan, S. Torker, A. H. Hoveyda, *J. Am. Chem. Soc.* **2014,** *136,* 14337–14340; f) S. Torker, M. J. Koh, R. K. M. Khan, A. H. Hoveyda, *Organometallics,* **2016,** *35,* 543–562; g) M. S. Mikus, S. Torker, A. H. Hoveyda, *Angew. Chem., Int. Ed.* **2016,** *55,* 4997–5002; For modeling allyl addition to CF_3-ketones, see: h) K.-A. Lee, D. L. Silverio, S. Torker, D. W. Robbins, F. Haeffner, A. H. Hoveyda, *Nature Chem.* **2016,** *8,* 768–777.

developed over the past decade:[22],[29] ωB97XD,[30] M06, [31] MN12SX,[32] MN12L,[32] M06L,[31] BP86-D3BJ[1b],[33] and PBE0-D3BJ[1b],[34] (Figures S1–S9). Electronic and Gibbs free energies for Figures S4–S9 are provided in S53 to S76 and the entries that have been used to construct Figures S1–S3 are highlighted with grey background. A file for convenient viewing of computed geometries with the program Mercury 3.3 is appended as separate "coordinates.xyz" file in S77 to S374.[35]

Scheme S1. ONIOM boundaries used in the simulations (two layers)



major product with ligand derived from **imid-3**

R = 2,6-(*i*-Pr)$_2$-C$_6$H$_3$

major product with ligand derived from **imid-2**

Nomenclature

The following modes for Cu-H addition with ligands derived from imid-3 and imid-2 have been investigated (Scheme S2). Modes S1 and S2 lead to the *S*-configuration at the carbon center that is directly bound to Cu after Cu-H addition, whereas modes R1 and R2 will generate the carbon stereogenic center with *R*-configuration. In modes S1 and R1 one of the oxygen atoms on the Bpin moiety, which is situated in the rear, is coordinated to the sodium counterion that is bound to the ligand's sulfonate group. In contrast, the Bpin group is facing towards the front in modes of addition S2 and R2. The modes for Cu-H addition shown in Scheme 2a have further been reinvestigated with either two or three explicit thf molecules bound to the metal center in order to test the stability of the O^{Bpin}→Na coordination in presence of a coordinating solvent (tetrahydrofuran). See below for a detailed discussion.

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[31] Y. Zhao, D. G. Truhlar, *Acc. Chem. Res.* **2008,** *41,* 157–167.

[32] R. Peverati, D. G. Truhlar, . *Phys. Chem. Chem. Phys.* **2013***, 14,* 16187–16191.

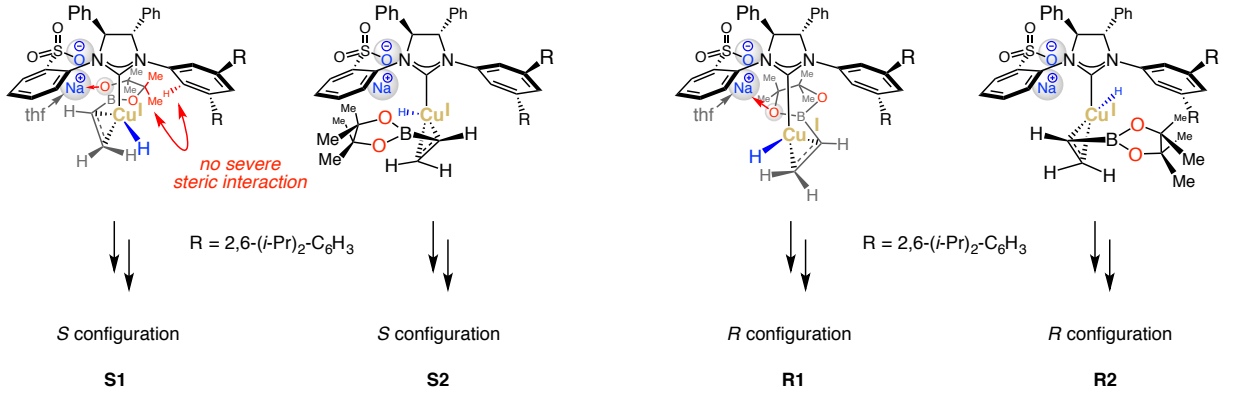
B, **1986***, 33,* 8800–8802.

[34] C. Adamo, V. Barone, *J. Chem. Phys.* **1999,** *110,* 6158–6169.

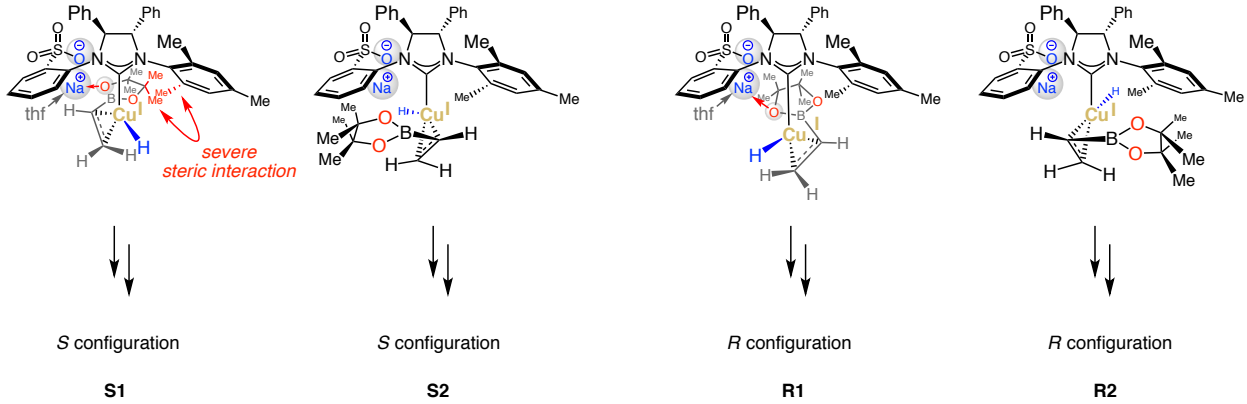
[35] D. L. Lichtenberger, J. A. Gladysz, *Organometallics,* **2014,** *33,* 835−835. The "coordinates.xyz" file can be generated by copying all the coordinates in S77–S330 into a text file without empty lines and changing the extension to ".xyz".

Scheme S2. Investigated modes of Cu-H addition with ligands derived from **imid-3** (a) and **imid-2** (b)

a Cu-H addition with **imid-3**

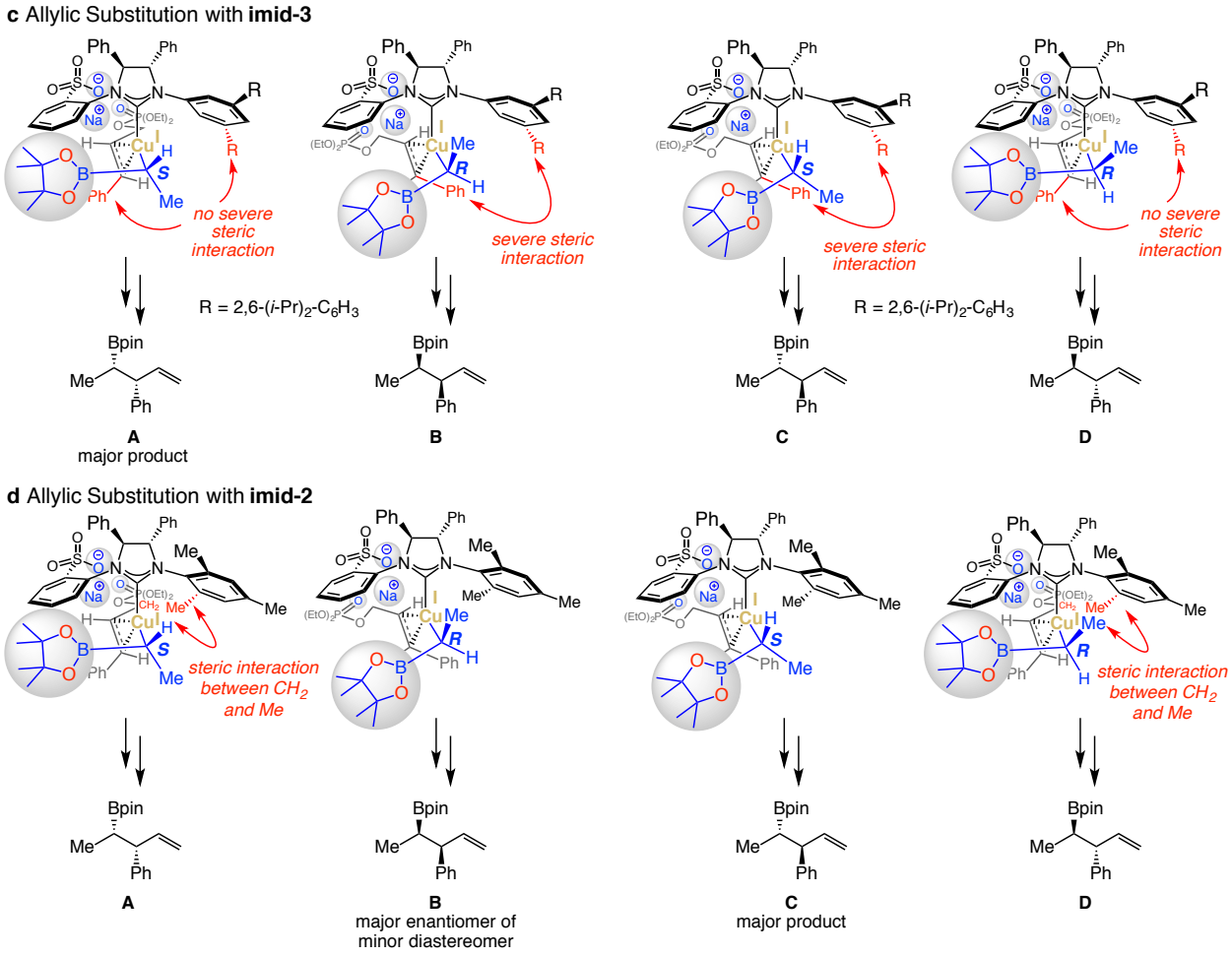


b Cu-H addition with **imid-2**



Additionally, all investigated modes for allylic substitution with ligands derived from **imid-3** and **imid-2** are displayed in Scheme 3. Here, **A** and **B** denote the pathways leading to the two enantiomers of the first diastereomer, whereas nomenclature **C** and **D** is used for the two enantiomers of the opposite diastereomer. Mode of allylic substitution **A** leads to the major product when the NHC ligand derived from **imid-3** is involved (Scheme 3a). Furthermore, mode **C** yields the major product when the reaction is performed with **imid-2** and mode **B** leads to the major enantiomer of the minor diastereomer under the same conditions (Scheme 3b).

Scheme S3. Investigated modes of allylic substitution (AS) with ligands derived from **imid-3** (a) and **imid-2** (b)



Stereochemical model with Cu–NHC complex derived from imid-3 (cf. Figure S1-1)

The pathways leading to the major (**A**) and minor enantiomer (**B**) of the major diastereomer at the MN12SX/Def2TZVPP$_{THF(SMD)}$//M06L/Def2SVP:UFF$_{THF}$ level are shown in Figure S1-1. For the corresponding free energy diagrams with other density functional, see Figure S1-2. For a complete picture containing all possible modes for Cu-H addition and allylic substitution (including investigation of several conformers), see Figures S4-1 and S7-1 or Figures S4-2 and S7-2, respectively. As seen in Figure S1-1, mode of Cu-H addition **S1** (9.6 kcal/mol relative to the Cu-H species), wherein a coordination between the Bpin moiety and the Na counterion is established, is significantly more favored compared to the mode of addition **R2**, which leads to the opposite stereochemistry (*R*-configuration) while a O^{Bpin}→Na interaction is absent (20.0 kcal/mol). Such a large energy difference (10.4 kcal/mol) should preclude generation of even trace amounts of products that originate from the *R*-configured Cu-alkyl species and suggests that this model system represents a rather simplified version of the true mechanism (see below for further discussion of models with explicit thf molecules). Following Cu-H addition, the major

product (**A**) is generated through the allylic substitution transition state to generate a π-allyl species (with a relative free energy of 6.5 kcal/mol).[36] In agreement with the experimental results Cu-H addition is likely irreversible as supported by the lower energy for allylic substitution (6.5 kcal/mol; Figure S1-1) compared to the transition state for Cu-H addition (9.6 kcal/mol; Figure S1-1). Further in agreement with the experimental results are the higher calculated free energies for allylic substitution that lead to minor products **B**, **C** and **D** (8.5–9.1 kcal/mol; cf. Figures S1-1 and S7-1). The herein proposed model for AS with the NHC ligand derived form **imid-3** supports a previous model for nucleophilic addition of propargyl groups to allyl electrophiles, and we refer here to this earlier work for a much more detailed mechanistic discussion.[37],[38]

Stereochemical model with Cu–NHC complex derived from imid-2 (cf. Figure S2-1)

The most critical pathways leading to the major product (C) and the major enantiomer of the minor diastereomer (B) at the MN12SX/Def2TZVPP$_{THF(SMD)}$//M06L/Def2SVP:UFF$_{THF}$ level are shown in Figure S2-1. For the corresponding free energy diagrams with other density functional, see Figure S2-2. For a complete picture containing all possible modes for Cu-H addition and allylic substitution (including investigation of several conformers), see Figures S8-1 and S9-1 or Figures S8-2 and S9-2, respectively. As seen in Figure S2-1, and similar to the reaction promoted by the NHC ligand derived from imid-3, mode of Cu-H addition S1 (8.6 kcal/mol relative to the Cu-H species), wherein the a coordination between the Bpin moiety and the Na counterion is established, is significantly more favored compared to the mode of addition R2, which leads to the opposite stereochemistry (*R*-configuration), while a $O^{Bpin}\rightarrow$Na interaction is absent (17.9 kcal/mol). Again, such a large energy difference (9.3 kcal/mol) should preclude generation of even trace amounts of products that originate from the *R*-configured Cu-alkyl species, which contradicts the experimental observation that significant amounts of allylic substitution product B are isolated. Nonetheless, the energy difference between modes of addition S1 and R2 (9.3 kcal/mol) is slightly smaller than in the case when imid-3 is involved (10.4 kcal/mol). This likely originates from a significant steric interaction between the Bpin moiety and the ortho methyl group on the mesityl group of the NHC (mode S1 in Scheme S2b). Following Cu-H addition, the major product (C) is generated through allylic substitution transition state with a relative free energy of 1.5 kcal/mol (Figure S2-1). In agreement with the previous case (cf. Figure S1-1) as well as the experimental results, Cu-H addition is likely irreversible as supported by the lower energy for allylic substitution (1.5 kcal/mol) compared to Cu-H addition (8.6 kcal/mol). Further in agreement with the experimental results are the higher calculated free energies for AS that

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[36] For general mechanistic considerations regarding nucleophilic reaction promoted by Cu(I) species, see: N. Yoshikai, E. Nakamura, *Chem. Rev.* **2012,** *112,* 2339–2372.

[37] Y. Shi, B. Jung, S. Torker, A. H. Hoveyda, *J. Am. Chem. Soc.* **2015,** *137,* 8948–8964.

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

lead to minor products A, B and D (4.4–6.7 kcal/mol; cf. Figures S2-1 and S9-1). The herein proposed model for AS with the NHC ligand derived from imid-2 supports a previous model for nucleophilic addition of vinyl groups to allyl electrophiles, and we refer here to this earlier work for a much more detailed mechanistic discussion.[37],[38]

The effect of a coordinating reaction medium (thf) on the stability of intramolecular chelate intercations (cf. Figure S3-1)

Modeling reactions that involve charged species including counterions, etc. can be quite challenging and the use of solvation models such as PCM or SMD will face certain limitations. For example, relying solely on a continuum model will underestimate the distances between the metal center and the heteroatoms that are included in the simulation. The $O^{Bpin}\rightarrow$Na distance in mode of addition **S1** without explicit thf molecules is 2.30 Å, whereas the same distance elongates to 2.59 Å when 3 thf molecules are added. Furthermore, one of the largest sources of error relates to the loss entropy that occurs when thf molecules are being bound to the Na counterion. The estimated gas phase corrections to the free energy (ΔG_{corr} ~15 kcal/mol which corresponds to dilute conditions at 1 atm or 0.05 M) will certainly be significantly overestimated for solvent molecules (as discussed below, 5–9 kcal/mol instead of 15 kcal/mol for ΔG_{corr} will be more realistic). It is also very unlikely that the simplified model without thf molecules is a true representation of the actual experiment since it precludes formation of products that arise from the *R*-configured Cu-alkyl species. To address the above issues, we have performed the following additional calculations depicted in Figure S3-1. There, mode of addition **S1** with 0, 2 and 3 thf molecules is compared to mode of addition **R2** with also 0, 2 and 3 thf molecules. The top grey curve uses gas phase entropies for thf molecules, which renders binding of thf unfavorable. Additionally we have included scenarios wherein the gas phase free energy correction per thf molecule (~15 kcal/mol) is overestimated by 4, 6 and 8 kcal/mol, respectively (black, blue and green curves). The same analysis has been performed with all other investigated functionals (cf. Figure S3-2). For the inclusion of 2 or 3 thf molecules in all other modes of Cu-H addition (**S2** and **R1**), see Figures S5 and S6, respectively.

The following analysis should severe as guidance to Figure S3-1: The gas phase free energies for Cu-H addition mode **S1** with 2 thf molecules and mode **R2** with 3 thf molecules are 18.9 and 33.9 kcal/mol, respectively (Figure S3-1). This corresponds to a difference of 15.0 kcal/mol. This means that in order to significantly disrupt the $O^{Bpin}\rightarrow$Na interaction (i.e., favoring path **R2** with 3 thf molecules), the gas phase correction to the free energy has to be overestimated by more than 15 kcal/mol, otherwise binding of a third thf molecule will be entropically disfavored. In order to allow for some formation of the *R*-configured Cu-alkyl species through pathway **R2**, the gas phase entropy likely has to be overestimated by about 12 kcal/mol with functional MN12SX and to a lesser degree with functionals ωB97XD (ca. 8 kcal/mol), M06 (ca. 8 kcal/mol) or MN12L (ca. 6 kcal/mol). In other words: applying an overestimation of 12 kcal/mol per thf molecule to mode **S1** with 2 thf molecules leads to a free energy of –5.1 kcal/mol (= 18.9 – 2 x 12.0; cf. Figure S3-1). The same procedure applied to mode **R2** with 3 thf molecules yields a free

energy of −2.1 kcal/mol (33.9 – 3 x 12.0; cf. Figure S3-1). Only under these conditions, generation of the *R*-configured Cu-alkyl species can become competitive (ΔΔG between modes **S1** and **R2** will be close to 3 kcal/mol or below; = −2.1 – (−5.1) kcal/mol). Please note that the free energies after removal of the overestimated portion of the entropy are actually not negative, since additional thf molecules have not been included in the ground state Cu-H species, which would also experience a lowering in energy.

Figures of Free Energy Surfaces

Free Energy Surface for Cu-H Addition/Allylic Substitution with ligand derived from imid-3

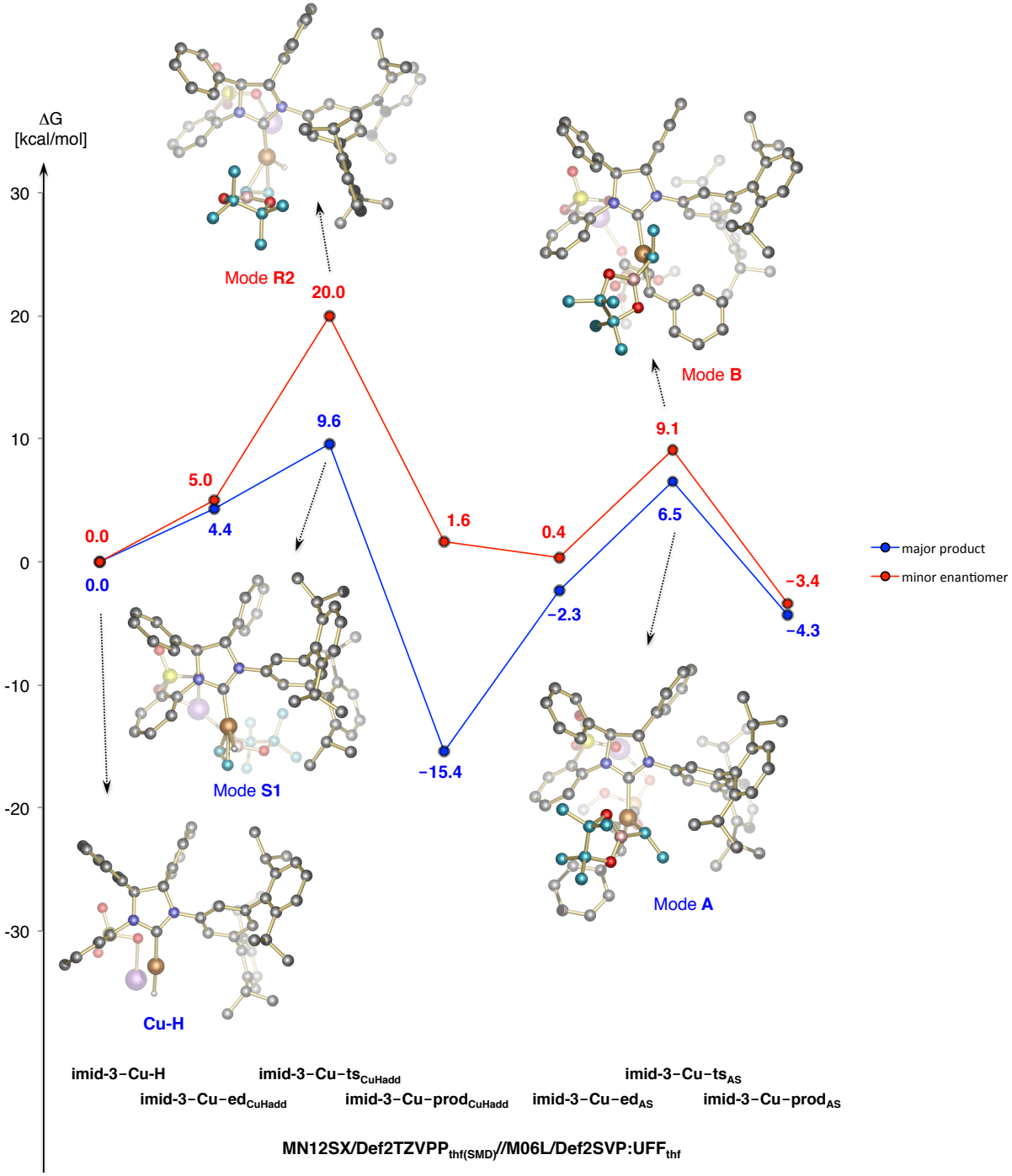

Figure S1-1. Free energy surfaces for Cu-H addition (CuHadd) and allylic substitution (AS) with NHC ligand derived from **imid-3** at the MN12SX/DefTZVPP$_{THF(SMD)}$//M06L/Def2SVP:UFF$_{THF}$ level (only lowest conformers for most critical pathways shown). For all other pathways including several conformers, see Figures S4-1 and S7-1.

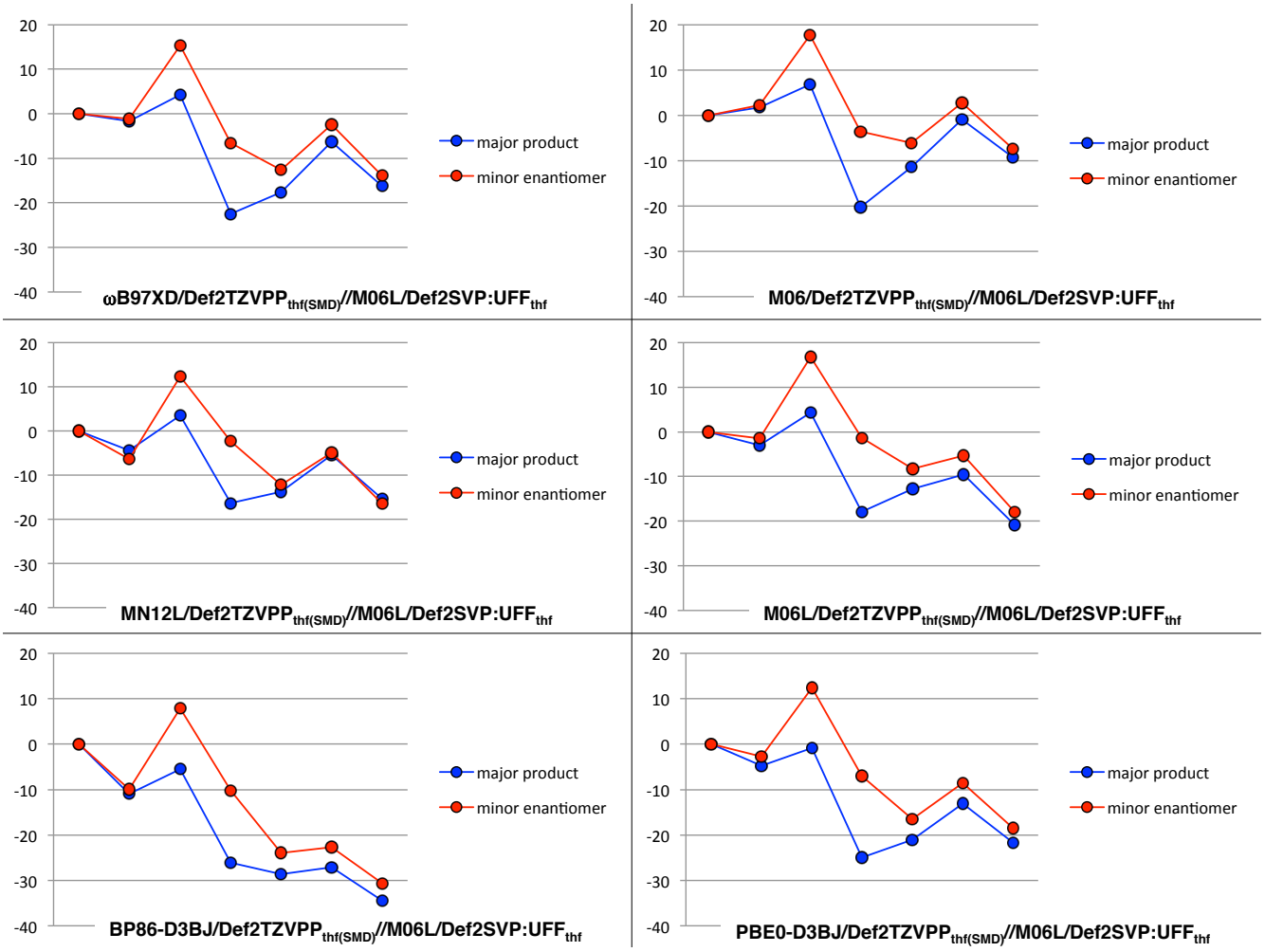

Figure S1-2. Free energy surfaces for Cu-H addition (CuHadd) and allylic substitution (AS) with NHC ligand derived from **imid-3** with various density functionals after optimization with M06L/Def2SVP:UFF$_{THF}$ (only lowest conformers for most critical pathways shown; cf. Figure S1-1). For all other pathways including several conformers, see Figures S4-2 and S7-2.

Free Energy Surface for Cu-H Addition/Allylic Substitution with ligand derived from imid-2

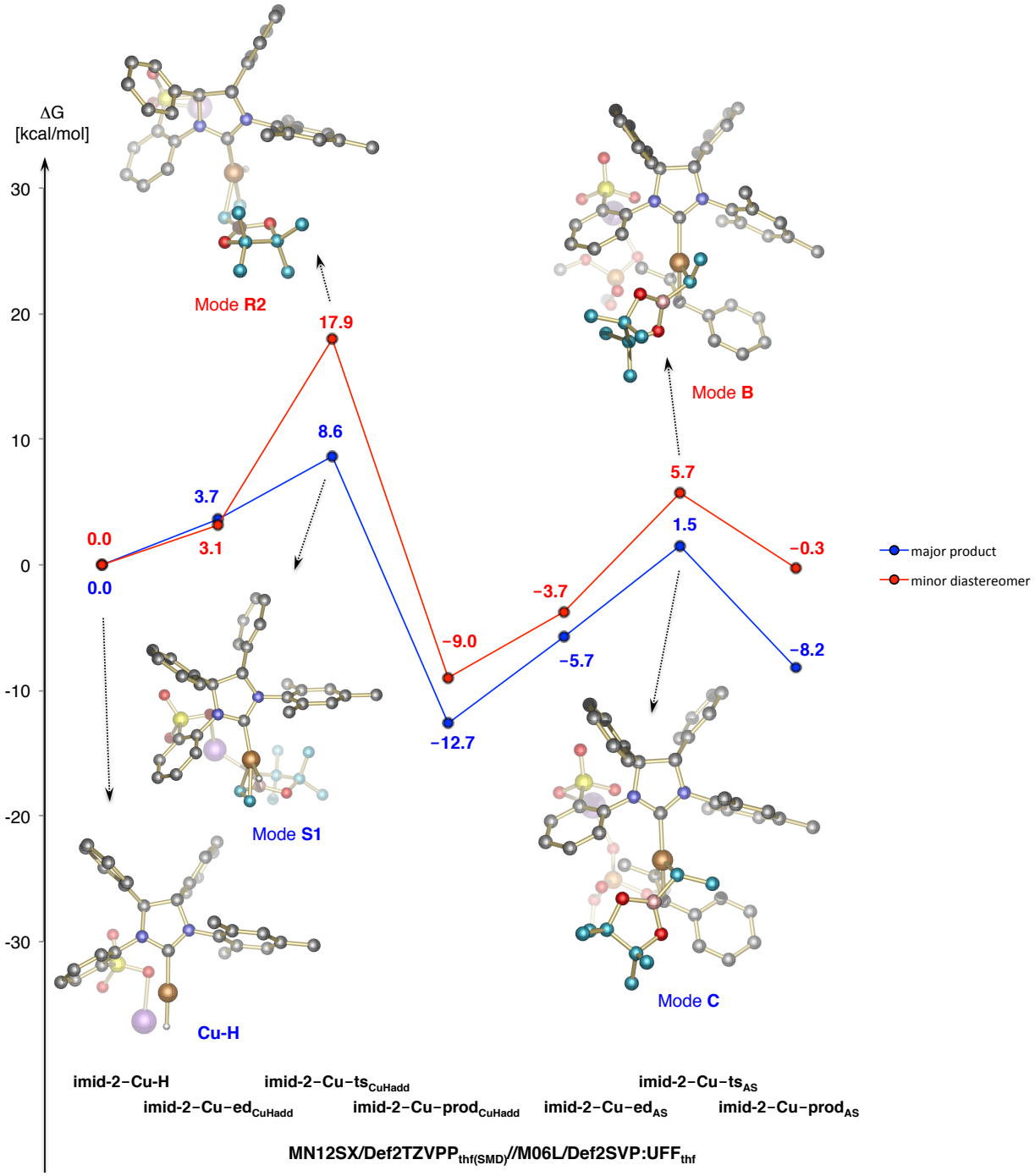

Figure S2-1. Free energy surfaces for Cu-H addition (CuHadd) and allylic substitution (AS) with NHC ligand derived from **imid-2** at the MN12SX/DefTZVPP$_{THF(SMD)}$//M06L/Def2SVP:UFF$_{THF}$ level (only lowest conformers for most critical pathways shown). For all other pathways including several conformers, see Figures S8-1 and S9-1.

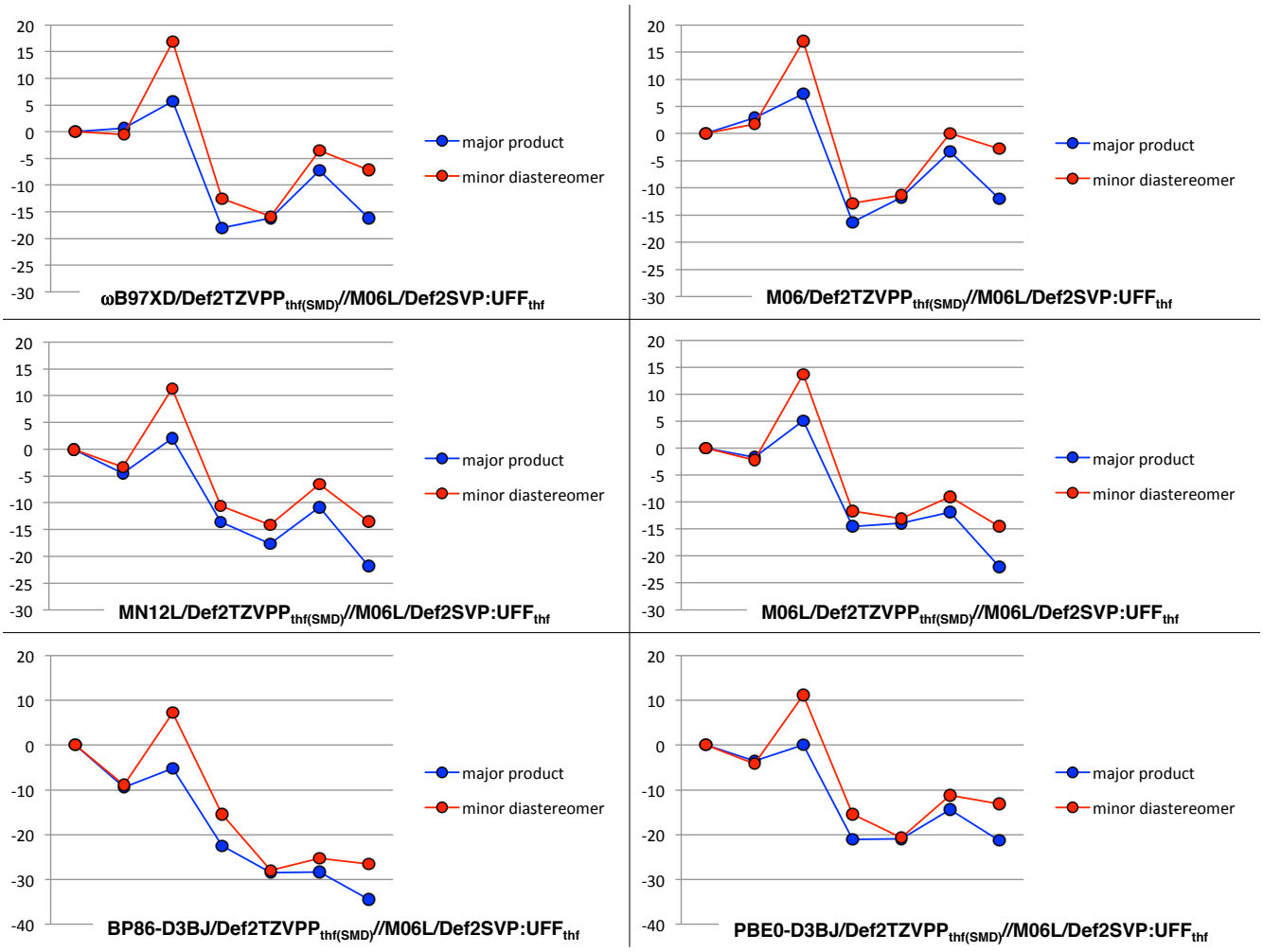

Figure S2-2. Free energy surfaces for Cu-H addition (CuHadd) and allylic substitution (AS) with NHC ligand derived from **imid-2** with various density functionals after optimization with M06L/Def2SVP:UFF$_{THF}$ (only lowest conformers for most critical pathways shown; cf. Figure S2-1). For all other pathways including several conformers, see Figures S8-2 and S9-2.

Detailed Investigation of the O^{Bpin}→Metal Coordination

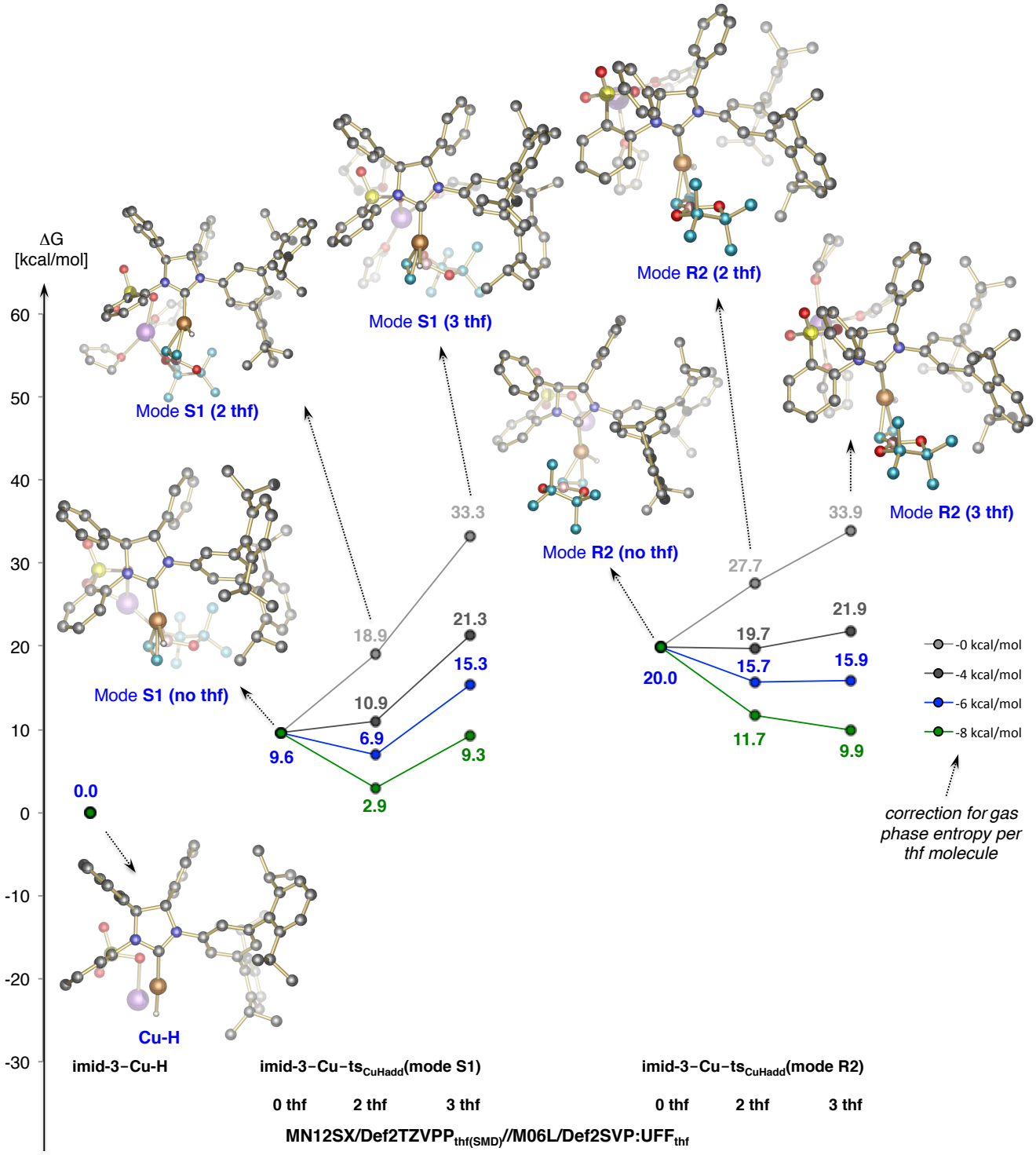

Figure S3-1. Free energies for Cu-H addition (CuHadd) with NHC ligand derived from **imid-3** at the MN12SX/DefTZVPP$_{THF(SMD)}$//M06L/Def2SVP:UFF$_{THF}$ level with varying number of thf molcules coordinated to the Na counterion (only lowest conformers for pathways **S1** and **R2** shown). For all other pathways including several conformers, see Figures S4-1, S5-1 and S6-1.

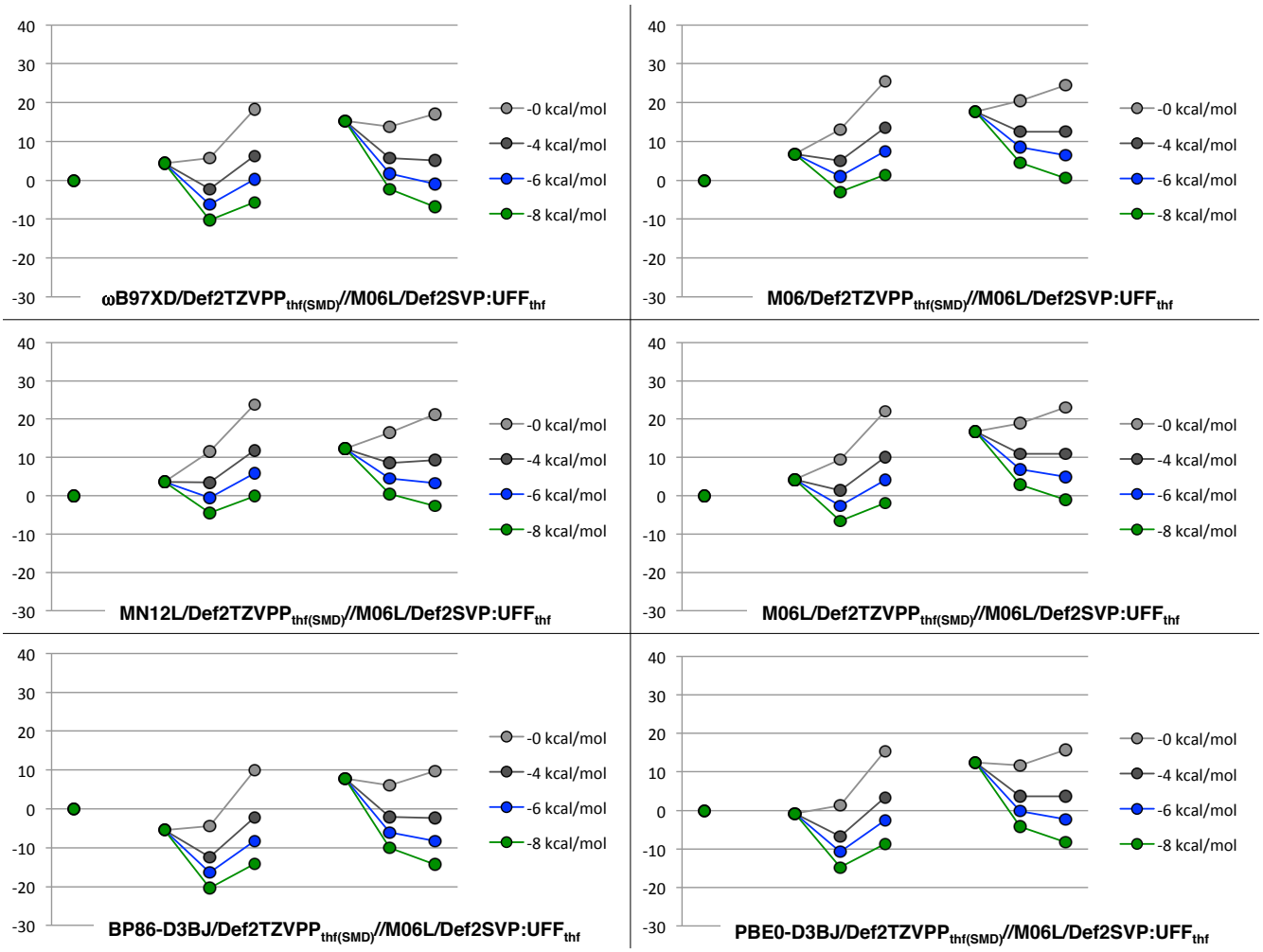

Figure S3-2. Free energies for Cu-H addition (CuHadd) with NHC ligand derived from **imid-3** with various density functionals after optimization with M06L/Def2SVP:UFF$_{THF}$ with varying number of thf molcules coordinated to the Na counterion (only lowest conformers for pathways **S1** and **R2** shown; cf. Figure S3-1). For all other pathways including several conformers, see Figures S4-2, S5-2 and S6-2.

Several Pathways and Conformers for Cu-H Addition (model without explicit thf molecules) with ligand derived from imid-3

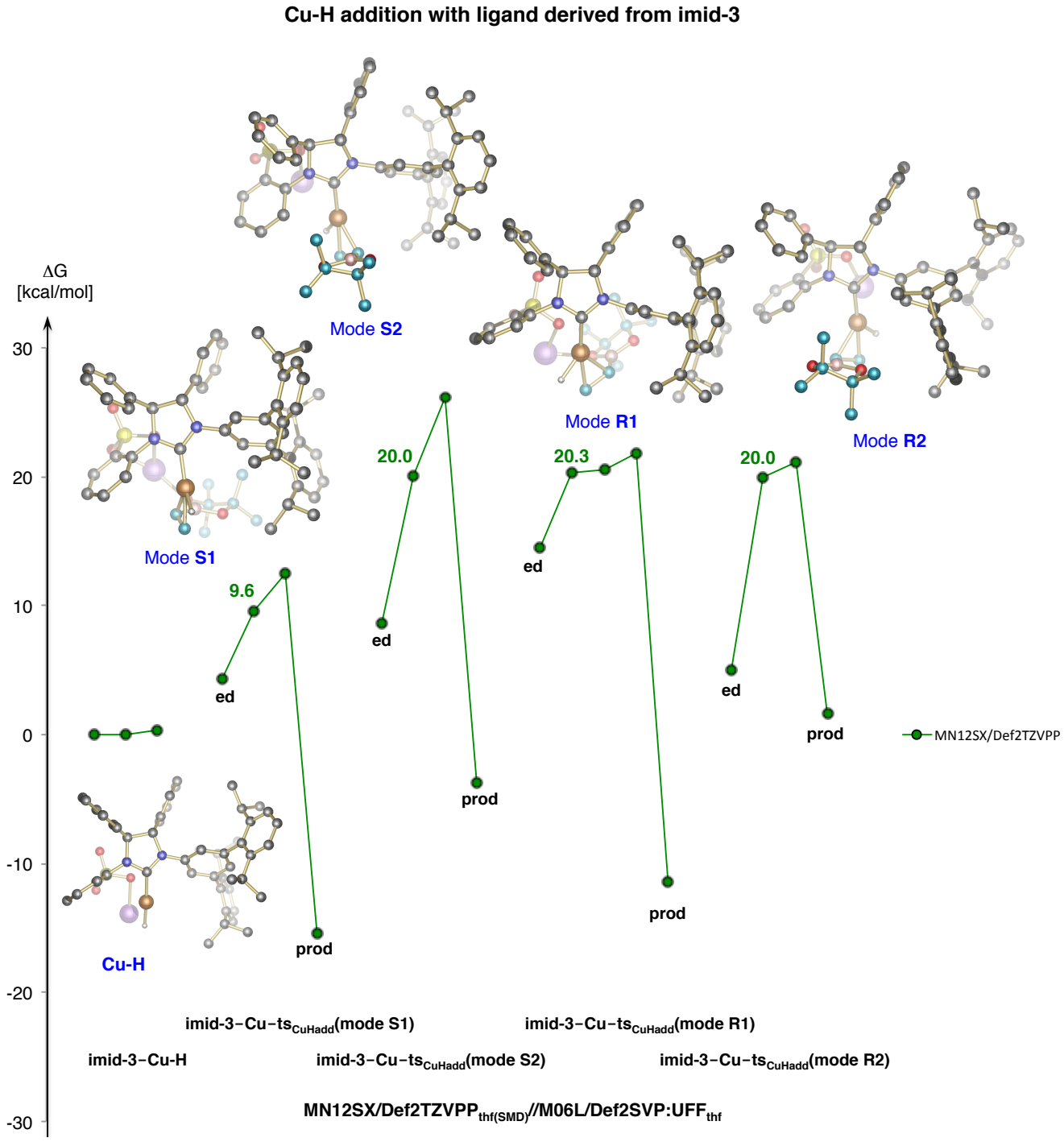

Figure S4-1. Free energy surfaces for Cu-H addition (CuHadd) with NHC ligand derived from **imid-3** at the MN12SX/DefTZVPP$_{THF(SMD)}$//M06L/Def2SVP:UFF$_{THF}$ level (all pathways **S1**, **S2**, **R1** and **R2** shown, including one **ed** and **prod** for each mode of addition).

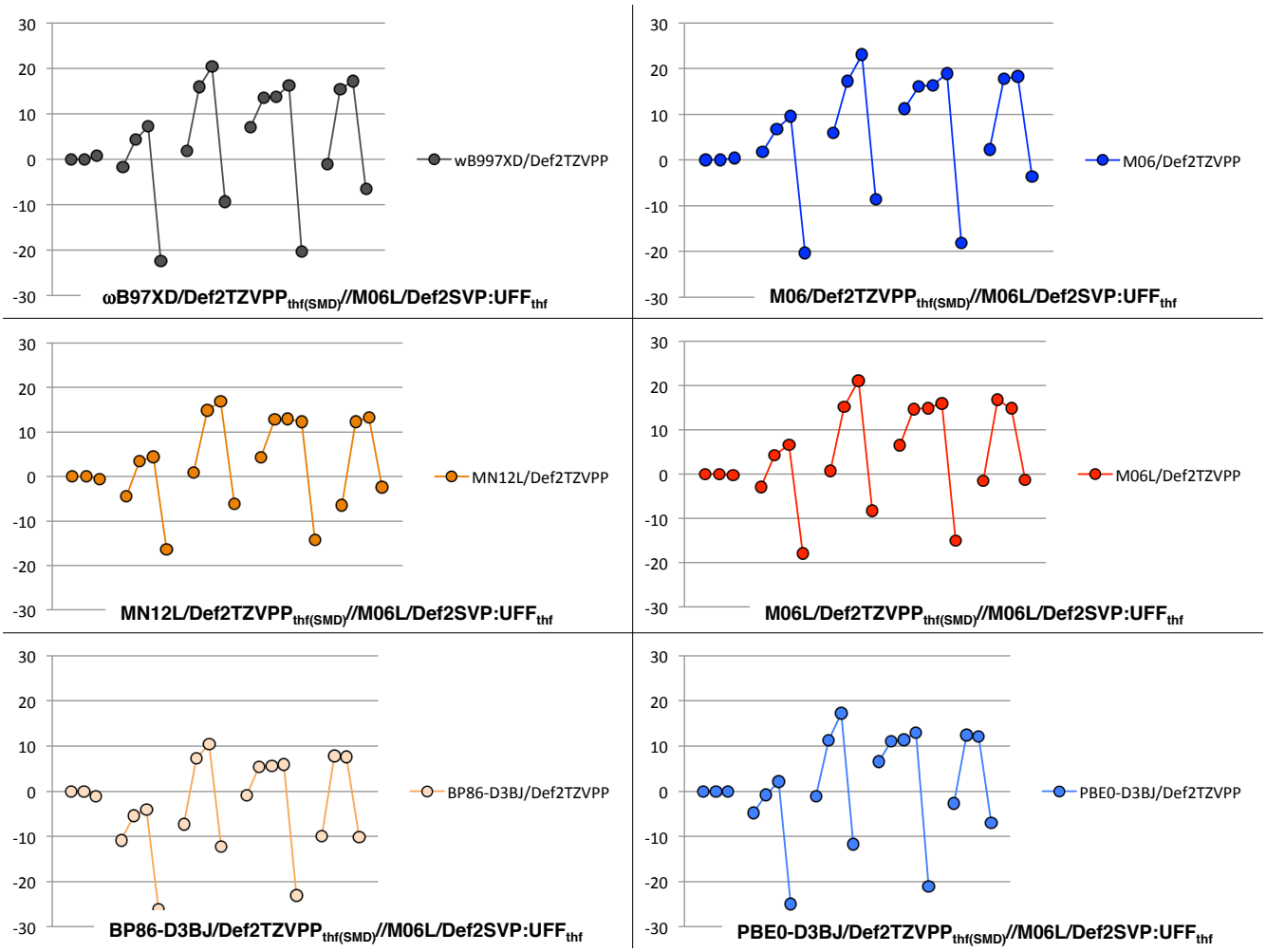

Figure S4-2. Free energy surfaces for Cu-H addition (CuHadd) with NHC ligand derived from **imid-3** with various density functionals after optimization with M06L/Def2SVP:UFF$_{THF}$ (all pathways **S1**, **S2**, **R1** and **R2** shown, including one **ed** and **prod** for each mode of addition; cf. Figure S4-1).

Several Pathways and Conformers for Cu-H Addition (model with 2 explicit thf molecules) with ligand derived from imid-3

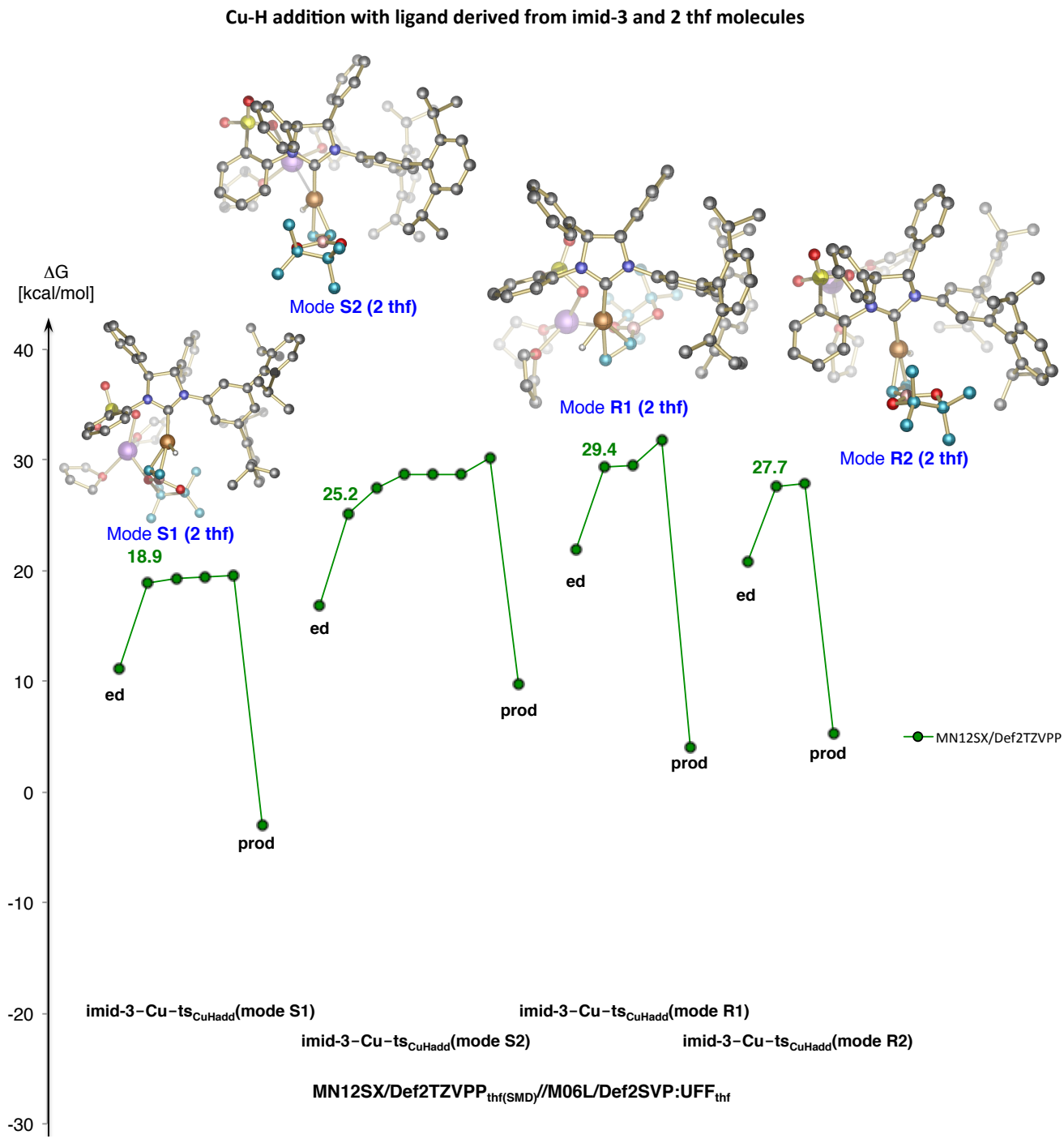

Figure S5-1. Free energy surfaces for Cu-H addition (CuHadd) with NHC ligand derived from **imid-3** with two explicit thf molecules coordinated to the Na counterion at the MN12SX/DefTZVPP$_{THF(SMD)}$//M06L/Def2SVP:UFF$_{THF}$ level (all pathways **S1**, **S2**, **R1** and **R2** shown, including one **ed** and **prod** for each mode of addition).

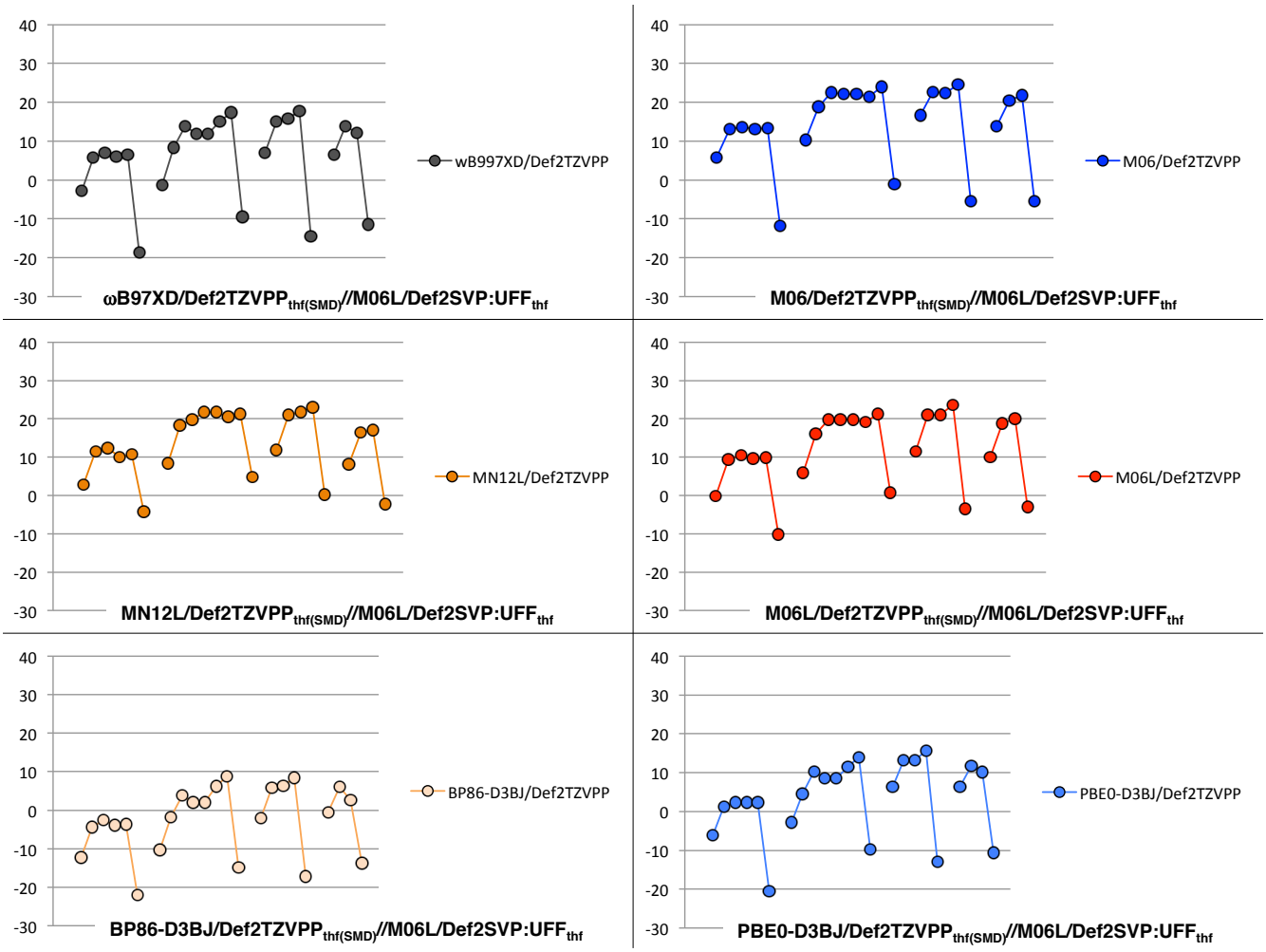

Figure S5-2. Free energy surfaces for Cu-H addition (CuHadd) with NHC ligand derived from **imid-3** with two explicit thf molecules coordinated to the Na counterion with various density functionals after optimization with M06L/Def2SVP:UFF$_{THF}$ (all pathways **S1**, **S2**, **R1** and **R2** shown, including one **ed** and **prod** for each mode of addition; cf. Figure S5-1).

Several Pathways and Conformers for Cu-H Addition (model with 3 explicit thf molecules) with ligand derived from imid-3

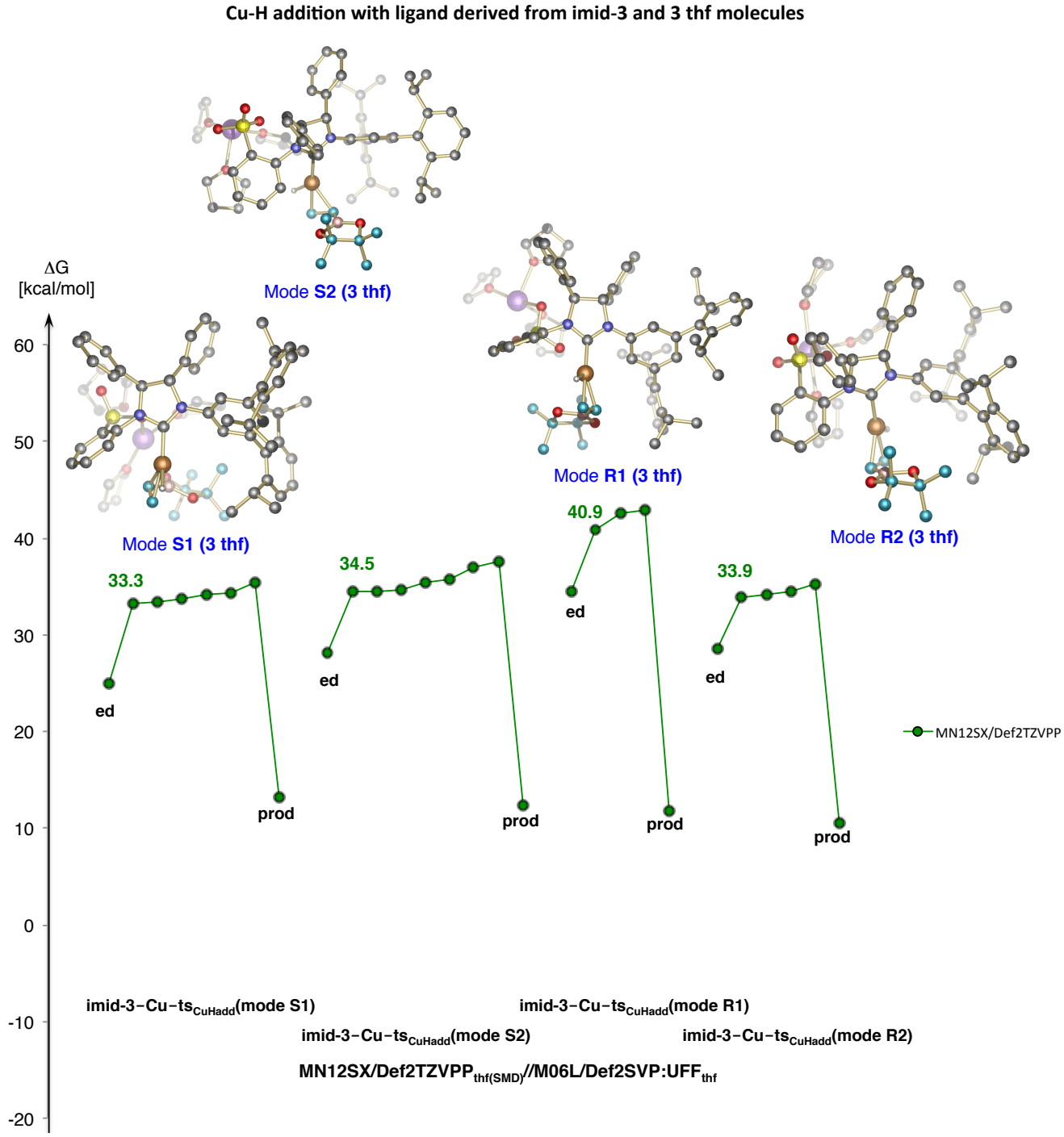

Figure S6-1. Free energy surfaces for Cu-H addition (CuHadd) with NHC ligand derived from **imid-3** with three explicit thf molecules coordinated to the Na counterion at the MN12SX/DefTZVPP$_{THF(SMD)}$//M06L/Def2SVP:UFF$_{THF}$ level (all pathways **S1**, **S2**, **R1** and **R2** shown, including one **ed** and **prod** for each mode of addition).

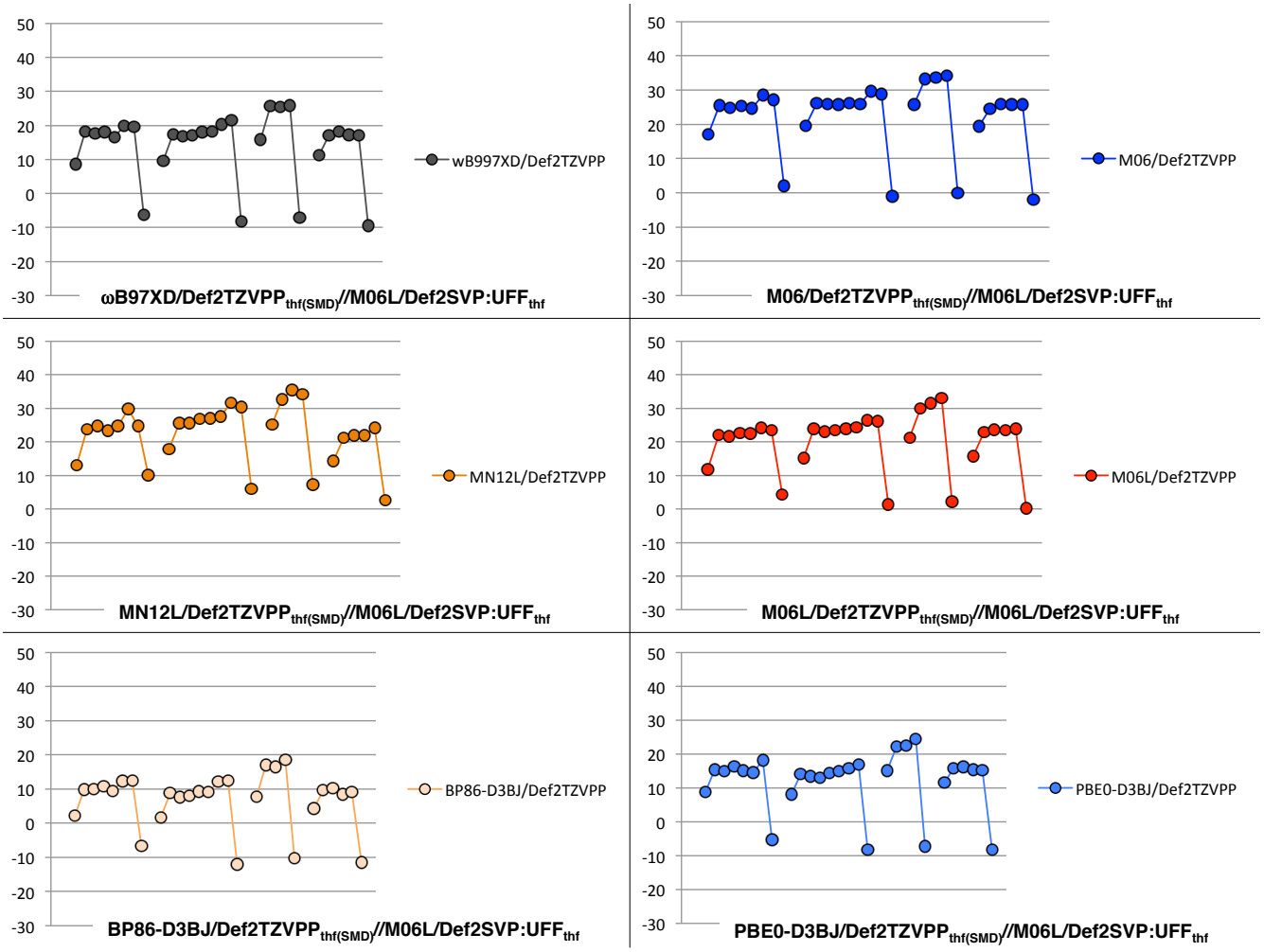

Figure S6-2. Free energy surfaces for Cu-H addition (CuHadd) with NHC ligand derived from **imid-3** with three explicit thf molecules coordinated to the Na counterion with various density functionals after optimization with M06L/Def2SVP:UFF$_{THF}$ (all pathways **S1**, **S2**, **R1** and **R2** shown, including one **ed** and **prod** for each mode of addition; cf. Figure S6-1).

Several Pathways and Conformers for Allylic Substitution with ligand derived from imid-3

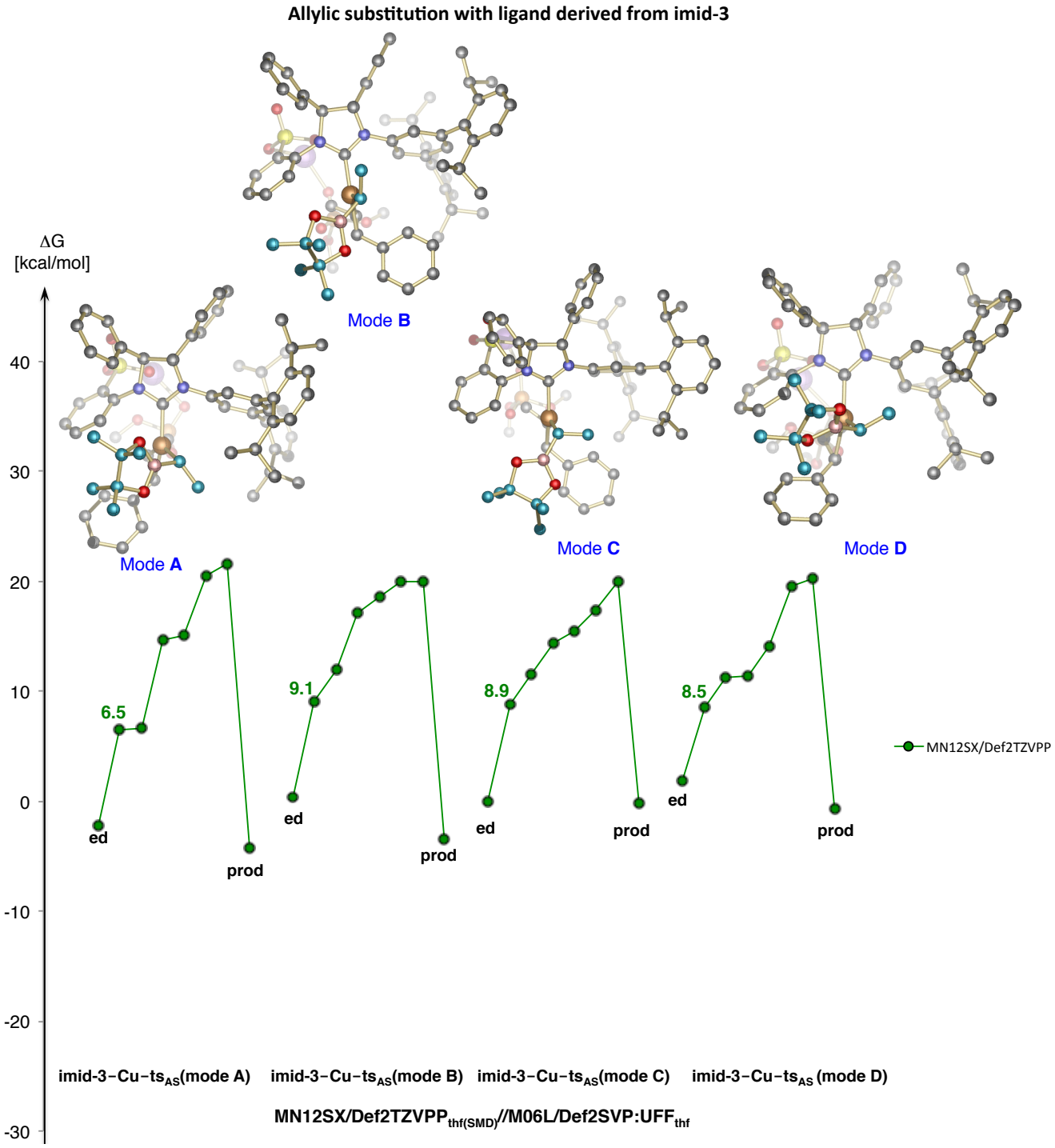

Figure S7-1. Free energy surfaces for allylic substitution (AS) with NHC ligand derived from **imid-3** at the MN12SX/DefTZVPP$_{THF(SMD)}$//M06L/Def2SVP:UFF$_{THF}$ level (all pathways **A**, **B**, **C** and **D** shown, including one **ed** and **prod** for each mode of addition).

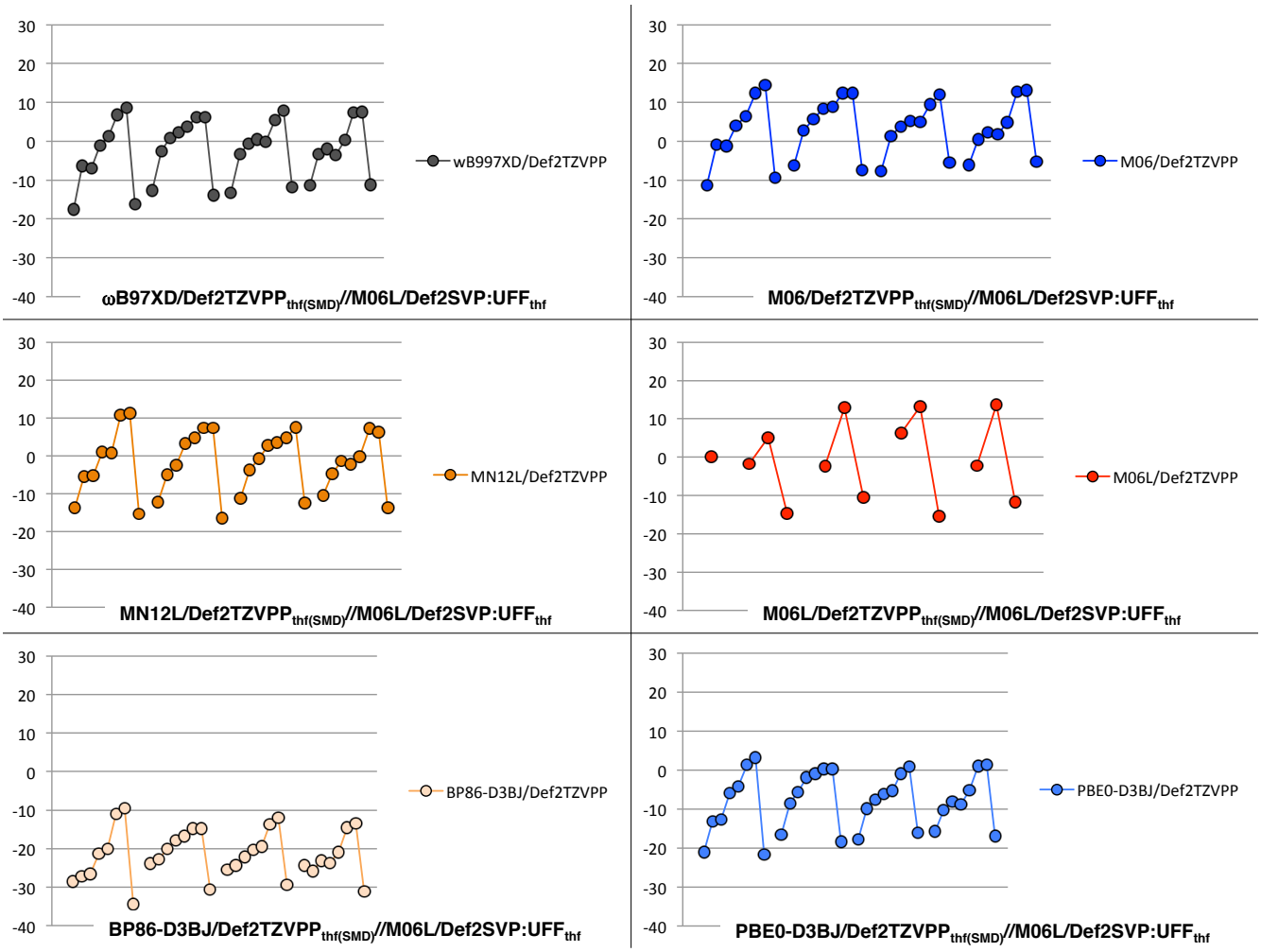

Figure S7-2. Free energy surfaces for allylic substitution (AS) with NHC ligand derived from **imid-3** with various density functionals after optimization with M06L/Def2SVP:UFF$_{THF}$ (all pathways **A**, **B**, **C** and **D** shown, including one **ed** and **prod** for each mode of addition; cf. Figure S7-1).

Several Pathways and Conformers for Cu-H Addition (model without explicit thf molecules) with ligand derived from imid-2

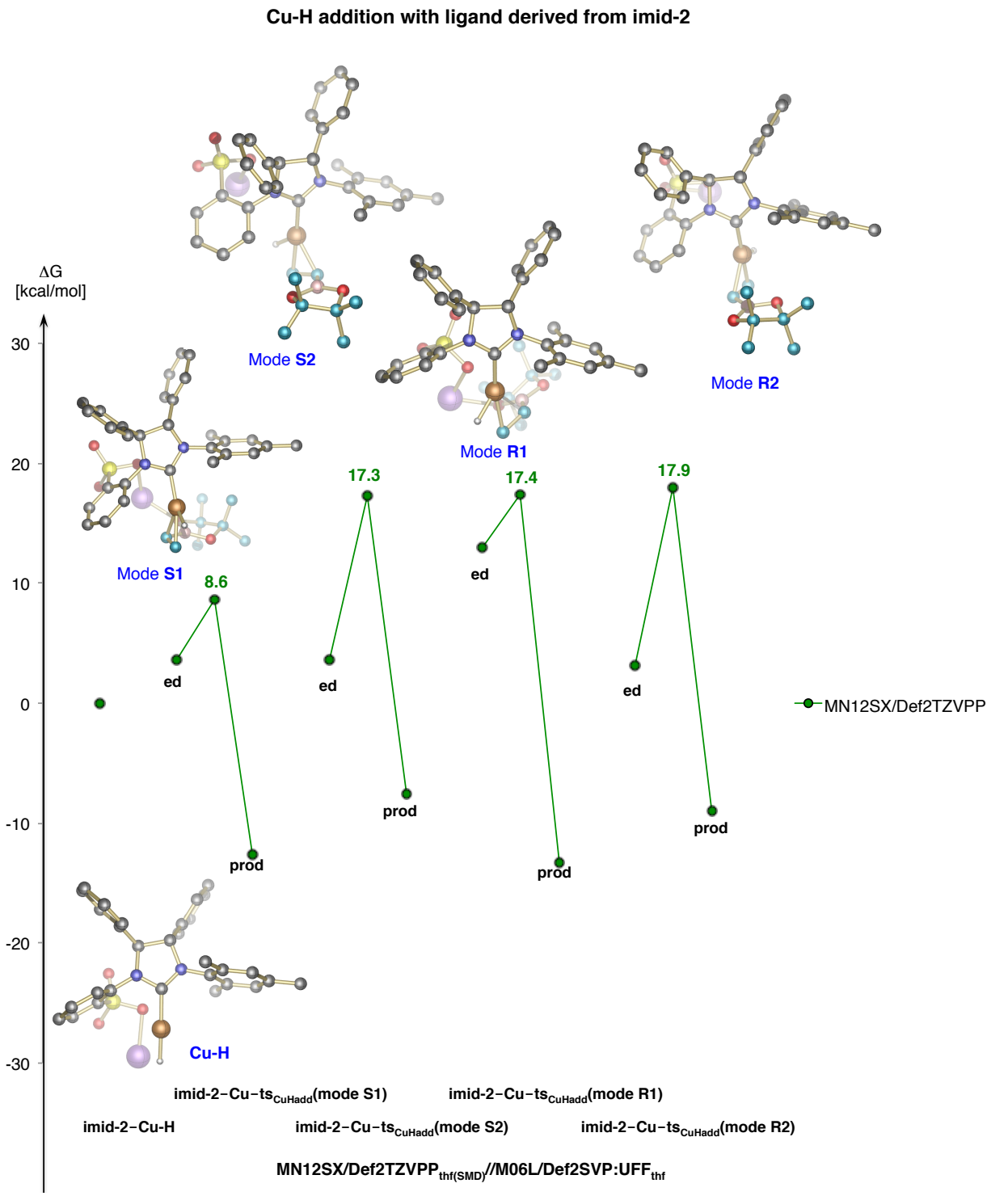

Figure S8-1. Free energy surfaces for Cu-H addition (CuHadd) with NHC ligand derived from **imid-2** at the MN12SX/DefTZVPP$_{THF(SMD)}$//M06L/Def2SVP:UFF$_{THF}$ level (all pathways **S1**, **S2**, **R1** and **R2** shown, including one **ed** and **prod** for each mode of addition).

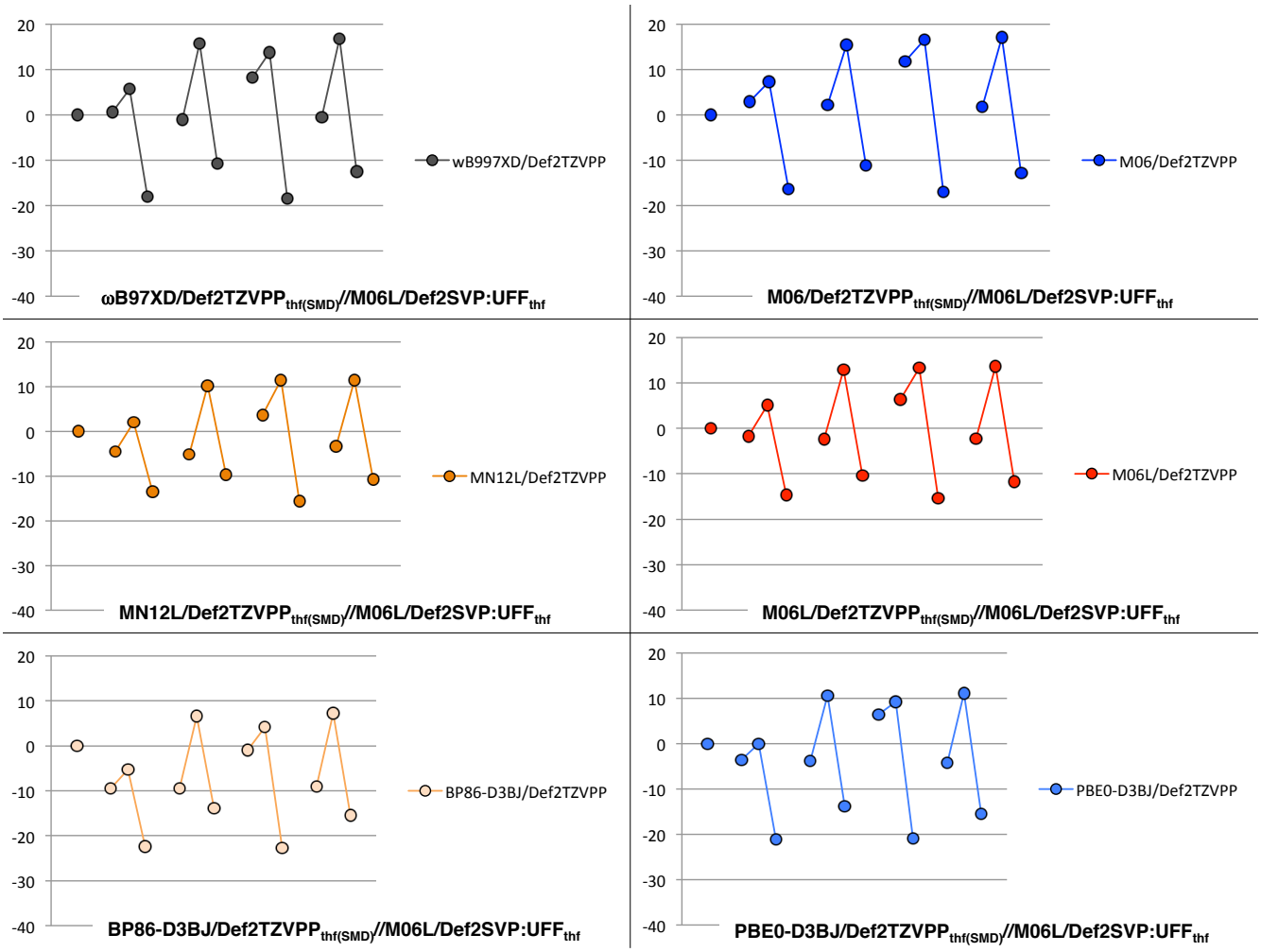

Figure S8-2. Free energy surfaces for Cu-H addition (CuHadd) with NHC ligand derived from **imid-2** with various density functionals after optimization with M06L/Def2SVP:UFF$_{THF}$ (all pathways **S1**, **S2**, **R1** and **R2** shown, including one **ed** and **prod** for each mode of addition; cf. Figure S8-1).

Several Pathways and Conformers for Cu-H Allylic Substitution with ligand derived from imid-2

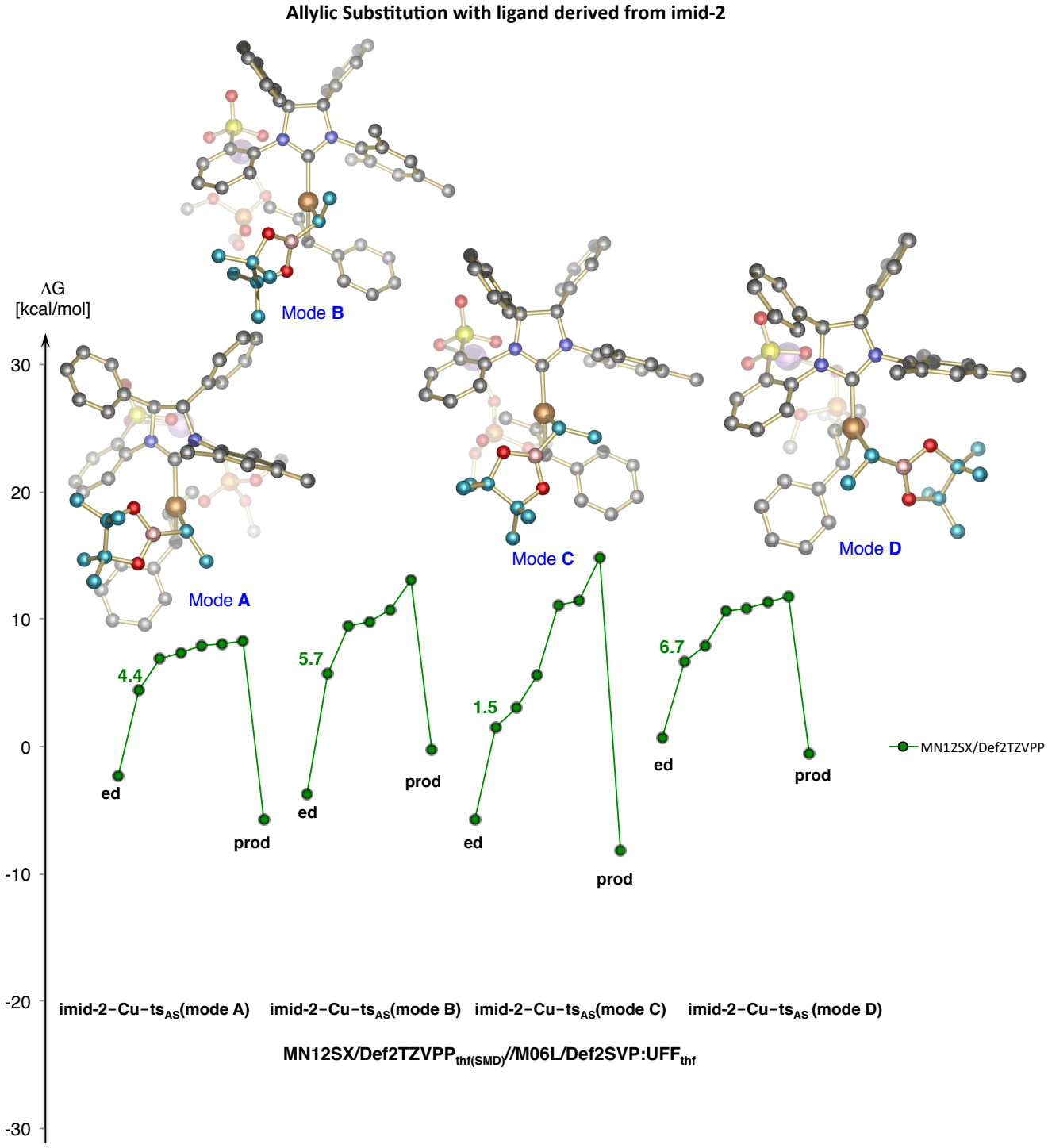

Figure S9-1. Free energy surfaces for allylic substitution (AS) with NHC ligand derived from **imid-2** at the MN12SX/DefTZVPP$_{THF(SMD)}$//M06L/Def2SVP:UFF$_{THF}$ level (all pathways **A**, **B**, **C** and **D** shown, including one **ed** and **prod** for each mode of addition).

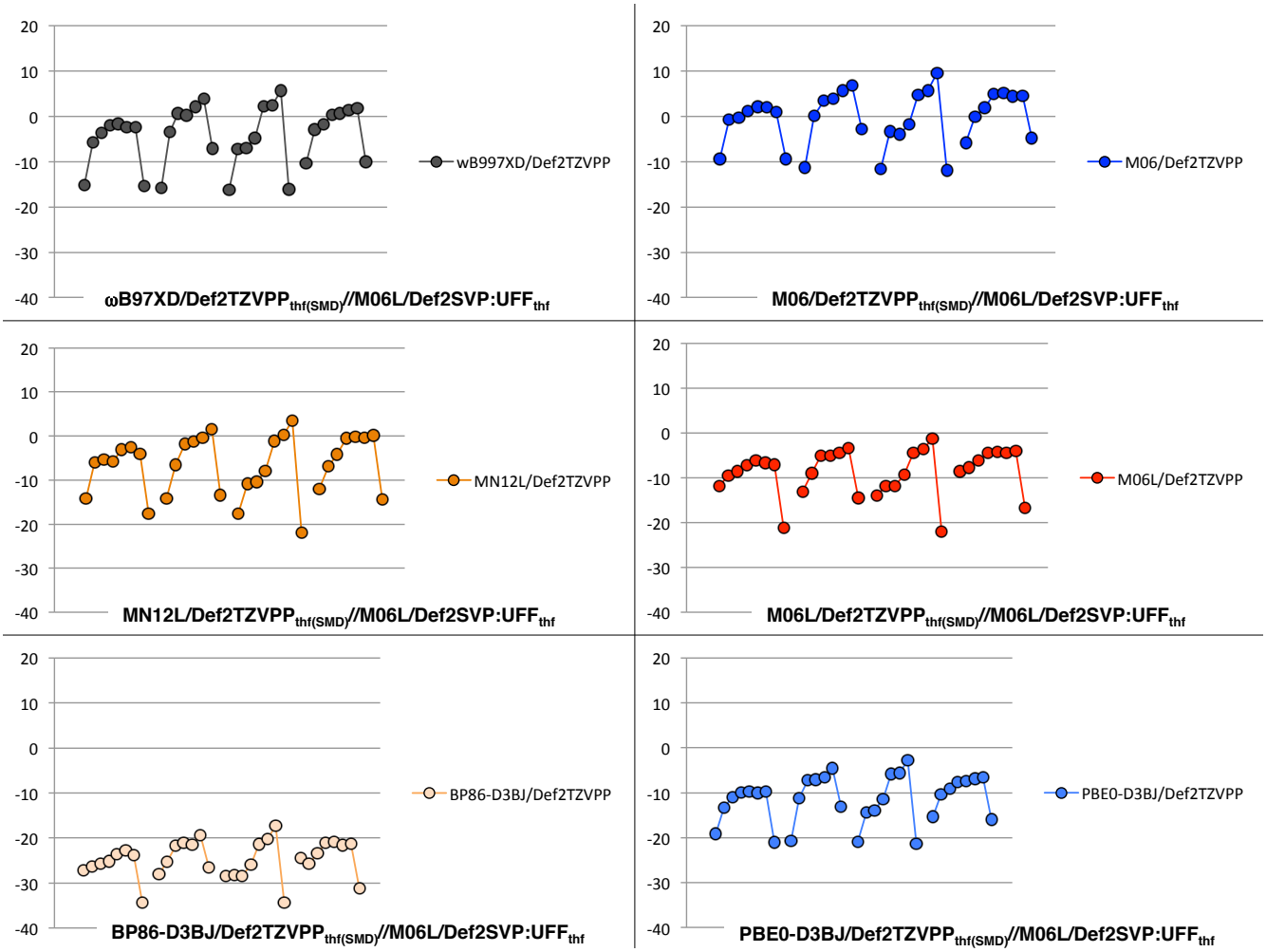

Figure S9-2. Free energy surfaces for allylic substitution (AS) with NHC ligand derived from **imid-2** with various density functionals after optimization with M06L/Def2SVP:UFF$_{THF}$ (all pathways **A**, **B**, **C** and **D** shown, including one **ed** and **prod** for each mode of addition; cf. Figure S9-1)

■ Energies and Gibbs Free Energies

Optimization in Figure S4-1 with M06L/Def2SVP:UFF in THF

structure	M06L/Def2SVP:UFF in THF					
	E(sum) [hartree]	ΔE [kcal/mol]	G(sum) [hartree]	ΔG [kcal/mol]	ΔG_{Corr} [kcal/mol]	Freq [cm^{-1}]
Figure_S4_imid-3-Cu-H_01	-3372.87604070	0.0	-3371.801994	0.0	0.0	6.4
Figure_S4_imid-3-Cu-H_02	-3372.87604072	0.0	-3371.801993	0.0	0.0	6.4
Figure_S4_imid-3-Cu-H_03	-3372.87648077	-0.3	-3371.801495	0.3	0.6	13.8
Figure_S4_imid-3_modeS1_ed(CuHadd)	-3372.92134984	-28.4	-3371.817018	-9.4	19.0	11.9
Figure_S4_imid-3_modeS1_ts(CuHadd)_01	-3372.90750384	-19.7	-3371.805433	-2.2	17.6	-764.6
Figure_S4_imid-3_modeS1_ts(CuHadd)_02	-3372.91008226	-21.4	-3371.807454	-3.4	17.9	-788.9
Figure_S4_imid-3_modeS1_prod(CuHadd)	-3372.94563861	-43.7	-3371.842069	-25.1	18.5	10.9
Figure_S4_imid-3_modeS2_ed(CuHadd)	-3372.91713925	-25.8	-3371.813870	-7.5	18.3	13.6
Figure_S4_imid-3_modeS2_ts(CuHadd)_01	-3372.89612623	-12.6	-3371.797742	2.7	15.3	-736.2
Figure_S4_imid-3_modeS2_ts(CuHadd)_02	-3372.89780518	-13.7	-3371.792077	6.2	19.9	-779.5
Figure_S4_imid-3_modeS2_prod(CuHadd)	-3372.94310094	-42.1	-3371.839636	-23.6	18.5	11.7
Figure_S4_imid-3_modeR1_ed(CuHadd)	-3372.91815406	-26.4	-3371.810018	-5.0	21.4	13.0
Figure_S4_imid-3_modeR1_ts(CuHadd)_01	-3372.90096062	-15.6	-3371.795685	4.0	19.6	-843.8
Figure_S4_imid-3_modeR1_ts(CuHadd)_02	-3372.90095394	-15.6	-3371.795444	4.1	19.7	-824.3
Figure_S4_imid-3_modeR1_ts(CuHadd)_03	-3372.90075002	-15.5	-3371.794146	4.9	20.4	-693.0
Figure_S4_imid-3_modeR1_prod(CuHadd)	-3372.94544671	-43.6	-3371.837078	-22.0	21.5	6.1
Figure_S4_imid-3_modeR2_ed(CuHadd)	-3372.92183666	-28.7	-3371.820055	-11.3	17.4	4.0
Figure_S4_imid-3_modeR2_ts(CuHadd)_01	-3372.89617832	-12.6	-3371.794160	4.9	17.6	-766.6
Figure_S4_imid-3_modeR2_ts(CuHadd)_02	-3372.90217399	-16.4	-3371.801482	0.3	16.7	-659.5
Figure_S4_imid-3_modeR2_prod(CuHadd)	-3372.93517459	-37.1	-3371.828484	-16.6	20.5	12.9

E(sum) . electronic energy in hartree with M06L/Def2SVP:UFF after mass balance
G(sum) . sum of electronic and thermal free energies with M06L/Def2SVP:UFF after mass balance
ΔE … relative electronic energy in kcal/mol with M06L/Def2SVP:UFF
ΔG … relative free energy in kcal/mol with M06L/Def2SVP:UFF
ΔG_{corr} thermal correction to free energy in kcal/mol obtained with M06L/Def2SVP:UFF ($\Delta G = \Delta E + \Delta G_{corr}$)
Freq … lowest frequency

Optimization in Figure S5-1 with M06L/Def2SVP:UFF in THF

structure	M06L/Def2SVP:UFF in THF					
	E(sum) [hartree]	ΔE [kcal/mol]	G(sum) [hartree]	ΔG [kcal/mol]	ΔG_{Corr} [kcal/mol]	Freq [cm^{-1}]
Figure_S5_imid-3_modeS1_ed(CuHadd)	-3372.96983691	-58.9	-3371.824750	-14.3	44.6	7.1
Figure_S5_imid-3_modeS1_ts(CuHadd)_01	-3372.95731868	-51.0	-3371.812120	-6.4	44.6	-746.1
Figure_S5_imid-3_modeS1_ts(CuHadd)_02	-3372.95441057	-49.2	-3371.809702	-4.8	44.3	-772.9
Figure_S5_imid-3_modeS1_ts(CuHadd)_03	-3372.95743357	-51.1	-3371.809861	-4.9	46.1	-768.5
Figure_S5_imid-3_modeS1_ts(CuHadd)_04	-3372.95684576	-50.7	-3371.809313	-4.6	46.1	-755.6
Figure_S5_imid-3_modeS1_prod(CuHadd)	-3372.99485508	-74.6	-3371.845701	-27.4	47.1	7.9
Figure_S5_imid-3_modeS2_ed(CuHadd)	-3372.96785239	-57.6	-3371.819818	-11.2	46.4	11.2
Figure_S5_imid-3_modeS2_ts(CuHadd)_01	-3372.94965474	-46.2	-3371.804630	-1.7	44.5	-769.5
Figure_S5_imid-3_modeS2_ts(CuHadd)_02	-3372.94855407	-45.5	-3371.800692	0.8	46.3	-714.5
Figure_S5_imid-3_modeS2_ts(CuHadd)_03	-3372.94887049	-45.7	-3371.798967	1.9	47.6	-756.6
Figure_S5_imid-3_modeS2_ts(CuHadd)_04	-3372.94887049	-45.7	-3371.798967	1.9	47.6	-756.5
Figure_S5_imid-3_modeS2_ts(CuHadd)_05	-3372.95090653	-47.0	-3371.803222	-0.8	46.2	-635.7
Figure_S5_imid-3_modeS2_ts(CuHadd)_06	-3372.94902570	-45.8	-3371.800566	0.9	46.7	-742.2
Figure_S5_imid-3_modeS2_prod(CuHadd)	-3372.99141382	-72.4	-3371.834389	-20.3	52.1	-53.6
Figure_S5_imid-3_modeR1_ed(CuHadd)	-3372.96280021	-54.4	-3371.811507	-6.0	48.5	9.7
Figure_S5_imid-3_modeR1_ts(CuHadd)_01	-3372.94795883	-45.1	-3371.797412	2.9	48.0	-747.2
Figure_S5_imid-3_modeR1_ts(CuHadd)_02	-3372.94707794	-44.6	-3371.797514	2.8	47.4	-740.2
Figure_S5_imid-3_modeR1_ts(CuHadd)_03	-3372.94609965	-44.0	-3371.793883	5.1	49.1	-756.9
Figure_S5_imid-3_modeR1_prod(CuHadd)	-3372.98999087	-71.5	-3371.834823	-20.6	50.9	13.8
Figure_S5_imid-3_modeR2_ed(CuHadd)	-3372.96474072	-55.7	-3371.811179	-5.8	49.9	15.6
Figure_S5_imid-3_modeR2_ts(CuHadd)_01	-3372.95069423	-46.8	-3371.800619	0.9	47.7	-778.2
Figure_S5_imid-3_modeR2_ts(CuHadd)_02	-3372.94792114	-45.1	-3371.797717	2.7	47.8	-758.4
Figure_S5_imid-3_modeR2_prod(CuHadd)	-3372.99344822	-73.7	-3371.839408	-23.5	50.2	15.4

E(sum) . electronic energy in hartree with M06L/Def2SVP:UFF after mass balance
G(sum) . sum of electronic and thermal free energies with M06L/Def2SVP:UFF after mass balance
ΔE … relative electronic energy in kcal/mol with M06L/Def2SVP:UFF
ΔG … relative free energy in kcal/mol with M06L/Def2SVP:UFF
ΔG_{corr} thermal correction to free energy in kcal/mol obtained with M06L/Def2SVP:UFF ($\Delta G = \Delta E + \Delta G_{corr}$)
Freq … lowest frequency

Optimization in Figure S6-1 with M06L/Def2SVP:UFF in THF

structure	M06L/Def2SVP:UFF in THF					
	E(sum) [hartree]	ΔE [kcal/mol]	G(sum) [hartree]	ΔG [kcal/mol]	ΔG_{Corr} [kcal/mol]	Freq [cm^{-1}]
Figure_S6_imid-3_modeS1_ed(CuHadd)	-3372.98714806	-69.7	-3371.812933	-6.9	62.9	11.5
Figure_S6_imid-3_modeS1_ts(CuHadd)_01	-3372.97105366	-59.6	-3371.798094	2.4	62.1	-771.3
Figure_S6_imid-3_modeS1_ts(CuHadd)_02	-3372.96872652	-58.2	-3371.796391	3.5	61.7	-745.5
Figure_S6_imid-3_modeS1_ts(CuHadd)_03	-3372.97189669	-60.2	-3371.798564	2.2	62.3	-744.2
Figure_S6_imid-3_modeS1_ts(CuHadd)_04	-3372.97187659	-60.1	-3371.797372	2.9	63.0	-759.1
Figure_S6_imid-3_modeS1_ts(CuHadd)_05	-3372.95756504	-51.2	-3371.795935	3.8	55.0	-675.0
Figure_S6_imid-3_modeS1_ts(CuHadd)_06	-3372.96535034	-56.0	-3371.793440	5.4	61.4	-759.3
Figure_S6_imid-3_modeS1_prod(CuHadd)	-3373.00820663	-82.9	-3371.829477	-17.2	65.7	8.0
Figure_S6_imid-3_modeS2_ed(CuHadd)	-3372.98795076	-70.2	-3371.812327	-6.5	63.7	14.9
Figure_S6_imid-3_modeS2_ts(CuHadd)_01	-3372.97248273	-60.5	-3371.802731	-0.5	60.1	-697.0
Figure_S6_imid-3_modeS2_ts(CuHadd)_02	-3372.97452925	-61.8	-3371.802671	-0.4	61.4	-684.8
Figure_S6_imid-3_modeS2_ts(CuHadd)_03	-3372.97308258	-60.9	-3371.802807	-0.5	60.4	-639.9
Figure_S6_imid-3_modeS2_ts(CuHadd)_04	-3372.97274485	-60.7	-3371.800939	0.7	61.3	-703.6
Figure_S6_imid-3_modeS2_ts(CuHadd)_05	-3372.97287149	-60.8	-3371.800618	0.9	61.6	-736.0
Figure_S6_imid-3_modeS2_ts(CuHadd)_06	-3372.96215852	-54.0	-3371.791787	6.4	60.4	-668.7
Figure_S6_imid-3_modeS2_ts(CuHadd)_07	-3372.96784920	-57.6	-3371.797960	2.5	60.1	-591.3
Figure_S6_imid-3_modeS2_prod(CuHadd)	-3373.02006953	-90.4	-3371.841768	-25.0	65.4	15.9
Figure_S6_imid-3_modeR1_ed(CuHadd)	-3372.98019796	-65.4	-3371.805303	-2.1	63.3	12.7
Figure_S6_imid-3_modeR1_ts(CuHadd)_01	-3372.96279015	-54.4	-3371.789314	8.0	62.4	-707.7
Figure_S6_imid-3_modeR1_ts(CuHadd)_02	-3372.96494953	-55.8	-3371.790600	7.1	62.9	-688.9
Figure_S6_imid-3_modeR1_ts(CuHadd)_03	-3372.96084190	-53.2	-3371.788960	8.2	61.4	-758.5
Figure_S6_imid-3_modeR1_prod(CuHadd)	-3373.01344700	-86.2	-3371.838634	-23.0	63.2	12.3
Figure_S6_imid-3_modeR2_ed(CuHadd)	-3372.98864943	-70.7	-3371.809261	-4.6	66.1	16.3
Figure_S6_imid-3_modeR2_ts(CuHadd)_01	-3372.97410523	-61.5	-3371.800273	1.1	62.6	-754.1
Figure_S6_imid-3_modeR2_ts(CuHadd)_02	-3372.97127491	-59.8	-3371.797599	2.8	62.5	-764.5
Figure_S6_imid-3_modeR2_ts(CuHadd)_03	-3372.97355227	-61.2	-3371.800637	0.9	62.0	-733.8
Figure_S6_imid-3_modeR2_ts(CuHadd)_04	-3372.97327826	-61.0	-3371.799712	1.4	62.4	-727.1
Figure_S6_imid-3_modeR2_prod(CuHadd)	-3373.01571161	-87.6	-3371.838321	-22.8	64.8	17.1

E(sum) . electronic energy in hartree with M06L/Def2SVP:UFF after mass balance
G(sum) . sum of electronic and thermal free energies with M06L/Def2SVP:UFF after mass balance
ΔE … relative electronic energy in kcal/mol with M06L/Def2SVP:UFF
ΔG … relative free energy in kcal/mol with M06L/Def2SVP:UFF
ΔG_{corr} thermal correction to free energy in kcal/mol obtained with M06L/Def2SVP:UFF ($\Delta G = \Delta E + \Delta G_{corr}$)
Freq … lowest frequency

Optimization in Figure S7-1 with M06L/Def2SVP:UFF in THF

structure	M06L/Def2SVP:UFF in THF					
	E(sum) [hartree]	ΔE [kcal/mol]	G(sum) [hartree]	ΔG [kcal/mol]	ΔG_{Corr} [kcal/mol]	Freq [cm^{-1}]
Figure_S7_imid-3_modeA_ed(AS)	-3372.99177203	-72.6	-3371.852923	-32.0	40.7	14.0
Figure_S7_imid-3_modeA_ts(AS)_01	-3372.97722854	-63.5	-3371.842482	-25.4	38.1	-257.3
Figure_S7_imid-3_modeA_ts(AS)_02	-3372.97943620	-64.9	-3371.844368	-26.6	38.3	-262.8
Figure_S7_imid-3_modeA_ts(AS)_03	-3372.97768242	-63.8	-3371.839196	-23.3	40.4	-178.3
Figure_S7_imid-3_modeA_ts(AS)_04	-3372.97591088	-62.7	-3371.837131	-22.0	40.6	-265.0
Figure_S7_imid-3_modeA_ts(AS)_05	-3372.97336700	-61.1	-3371.834971	-20.7	40.4	-255.6
Figure_S7_imid-3_modeA_ts(AS)_06	-3372.96940761	-58.6	-3371.829779	-17.4	41.2	-260.5
Figure_S7_imid-3_modeA_prod(AS)	-3372.98772048	-70.1	-3371.853773	-32.5	37.6	11.3
Figure_S7_imid-3_modeB_ed(AS)	-3372.98797496	-70.2	-3371.848116	-28.9	41.3	17.8
Figure_S7_imid-3_modeB_ts(AS)_01	-3372.97437306	-61.7	-3371.838078	-22.6	39.1	-268.4
Figure_S7_imid-3_modeB_ts(AS)_02	-3372.97024971	-59.1	-3371.831245	-18.4	40.8	-273.5
Figure_S7_imid-3_modeB_ts(AS)_03	-3372.96769186	-57.5	-3371.826211	-15.2	42.3	-229.9
Figure_S7_imid-3_modeB_ts(AS)_04	-3372.96529896	-56.0	-3371.822632	-13.0	43.1	-260.2
Figure_S7_imid-3_modeB_ts(AS)_05	-3372.96535873	-56.0	-3371.826363	-15.3	40.8	-253.8
Figure_S7_imid-3_modeB_ts(AS)_06	-3372.96535888	-56.0	-3371.826362	-15.3	40.8	-253.8
Figure_S7_imid-3_modeB_prod(AS)	-3372.98442740	-68.0	-3371.847842	-28.8	39.2	17.1
Figure_S7_imid-3_modeC_ed(AS)	-3372.98850883	-70.6	-3371.850057	-30.2	40.4	15.1
Figure_S7_imid-3_modeC_ts(AS)_01	-3372.97470009	-61.9	-3371.839481	-23.5	38.4	-264.9
Figure_S7_imid-3_modeC_ts(AS)_02	-3372.97092575	-59.5	-3371.833855	-20.0	39.5	-279.7
Figure_S7_imid-3_modeC_ts(AS)_03	-3372.96857306	-58.1	-3371.835302	-20.9	37.2	-266.3
Figure_S7_imid-3_modeC_ts(AS)_04	-3372.97545969	-62.4	-3371.837262	-22.1	40.3	-272.3
Figure_S7_imid-3_modeC_ts(AS)_05	-3372.97394834	-61.4	-3371.836163	-21.4	40.0	-266.7
Figure_S7_imid-3_modeC_ts(AS)_06	-3372.97024299	-59.1	-3371.830962	-18.2	40.9	-278.3
Figure_S7_imid-3_modeC_prod(AS)	-3372.98335742	-67.3	-3371.846253	-27.8	39.6	17.4
Figure_S7_imid-3_modeD_ed(AS)	-3372.98897190	-70.9	-3371.848982	-29.5	41.4	12.4
Figure_S7_imid-3_modeD_ts(AS)_01	-3372.97572877	-62.6	-3371.840756	-24.3	38.2	-259.2
Figure_S7_imid-3_modeD_ts(AS)_02	-3372.97692514	-63.3	-3371.840767	-24.3	39.0	-275.8
Figure_S7_imid-3_modeD_ts(AS)_03	-3372.98320274	-67.2	-3371.843558	-26.1	41.2	-273.1
Figure_S7_imid-3_modeD_ts(AS)_04	-3372.97873553	-64.4	-3371.837227	-22.1	42.3	-270.7
Figure_S7_imid-3_modeD_ts(AS)_05	-3372.97501365	-62.1	-3371.838720	-23.0	39.1	-217.0
Figure_S7_imid-3_modeD_ts(AS)_06	-3372.97091627	-59.5	-3371.830554	-17.9	41.6	-246.6
Figure_S7_imid-3_modeD_prod(AS)	-3372.98661582	-69.4	-3371.850909	-30.7	38.7	10.9

E(sum) . electronic energy in hartree with M06L/Def2SVP:UFF after mass balance
G(sum) . sum of electronic and thermal free energies with M06L/Def2SVP:UFF after mass balance
ΔE … relative electronic energy in kcal/mol with M06L/Def2SVP:UFF
ΔG … relative free energy in kcal/mol with M06L/Def2SVP:UFF
ΔG_{corr} thermal correction to free energy in kcal/mol obtained with M06L/Def2SVP:UFF ($\Delta G = \Delta E + \Delta G_{corr}$)
Freq … lowest frequency

Optimization in Figure S8-1 with M06L/Def2SVP:UFF in THF

structure	M06L/Def2SVP:UFF in THF					
	E(sum) [hartree]	ΔE [kcal/mol]	G(sum) [hartree]	ΔG [kcal/mol]	ΔG_{Corr} [kcal/mol]	Freq [cm^{-1}]
Figure_S8_imid-2-Cu-H	-3372.94728108	0.0	-3372.286789	0.0	0.0	26.4
Figure_S8_imid-2_modeS1_ed(CuHadd)	-3372.98529559	-23.9	-3372.295676	-5.6	18.3	19.8
Figure_S8_imid-2_modeS1_ts(CuHadd)	-3372.97337225	-16.4	-3372.286669	0.1	16.4	-704.0
Figure_S8_imid-2_modeS1_prod(CuHadd)	-3373.01685232	-43.7	-3372.327143	-25.3	18.3	16.5
Figure_S8_imid-2_modeS2_ed(CuHadd)	-3372.98629061	-24.5	-3372.299901	-8.2	16.3	19.7
Figure_S8_imid-2_modeS2_ts(CuHadd)	-3372.96595014	-11.7	-3372.281787	3.1	14.9	-778.0
Figure_S8_imid-2_modeS2_prod(CuHadd)	-3373.00940304	-39.0	-3372.322528	-22.4	16.6	15.0
Figure_S8_imid-2_modeR1_ed(CuHadd)	-3372.98177770	-21.6	-3372.290055	-2.0	19.6	19.4
Figure_S8_imid-2_modeR1_ts(CuHadd)	-3372.96598463	-11.7	-3372.278183	5.4	17.1	-740.1
Figure_S8_imid-2_modeR1_prod(CuHadd)	-3373.01751384	-44.1	-3372.325868	-24.5	19.5	20.3
Figure_S8_imid-2_modeR2_ed(CuHadd)	-3372.98152932	-21.5	-3372.297081	-6.5	15.0	17.4
Figure_S8_imid-2_modeR2_ts(CuHadd)	-3372.96517948	-11.2	-3372.282077	3.0	14.2	-710.2
Figure_S8_imid-2_modeR2_prod(CuHadd)	-3373.00912849	-38.8	-3372.323251	-22.9	15.9	15.6

E(sum) . electronic energy in hartree with M06L/Def2SVP:UFF after mass balance
G(sum) . sum of electronic and thermal free energies with M06L/Def2SVP:UFF after mass balance
ΔE … relative electronic energy in kcal/mol with M06L/Def2SVP:UFF
ΔG … relative free energy in kcal/mol with M06L/Def2SVP:UFF
ΔG_{corr} thermal correction to free energy in kcal/mol obtained with M06L/Def2SVP:UFF ($\Delta G = \Delta E + \Delta G_{corr}$)
Freq … lowest frequency

Optimization in Figure S9-1 with M06L/Def2SVP:UFF in THF

structure	M06L/Def2SVP:UFF in THF					
	E(sum) [hartree]	ΔE [kcal/mol]	G(sum) [hartree]	ΔG [kcal/mol]	ΔG_{Corr} [kcal/mol]	Freq [cm^{-1}]
Figure_S9_imid-2_modeA_ed(AS)	-3373.05577416	-68.1	-3372.333077	-29.0	39.0	-7.0
Figure_S9_imid-2_modeA_ts(AS)_01	-3373.04236717	-59.7	-3372.325870	-24.5	35.1	-256.8
Figure_S9_imid-2_modeA_ts(AS)_02	-3373.04350747	-60.4	-3372.322609	-22.5	37.9	-238.2
Figure_S9_imid-2_modeA_ts(AS)_03	-3373.04282244	-60.0	-3372.322037	-22.1	37.8	-239.1
Figure_S9_imid-2_modeA_ts(AS)_04	-3373.04211773	-59.5	-3372.323485	-23.0	36.5	-253.2
Figure_S9_imid-2_modeA_ts(AS)_05	-3373.03951562	-57.9	-3372.319903	-20.8	37.1	-254.6
Figure_S9_imid-2_modeA_ts(AS)_06	-3373.04075075	-58.7	-3372.318540	-19.9	38.7	-237.8
Figure_S9_imid-2_modeA_prod(AS)	-3373.05268811	-66.1	-3372.334750	-30.1	36.0	10.6
Figure_S9_imid-2_modeB_ed(AS)	-3373.05031071	-64.7	-3372.331306	-27.9	36.7	15.9
Figure_S9_imid-2_modeB_ts(AS)_01	-3373.03616694	-55.8	-3372.318918	-20.2	35.6	-220.8
Figure_S9_imid-2_modeB_ts(AS)_02	-3373.03927418	-57.7	-3372.319290	-20.4	37.3	-251.1
Figure_S9_imid-2_modeB_ts(AS)_03	-3373.04153325	-59.1	-3372.322171	-22.2	36.9	-267.6
Figure_S9_imid-2_modeB_ts(AS)_04	-3373.03662678	-56.1	-3372.316049	-18.4	37.7	-234.0
Figure_S9_imid-2_modeB_ts(AS)_05	-3373.04013757	-58.3	-3372.318263	-19.8	38.5	-188.3
Figure_S9_imid-2_modeB_prod(AS)	-3373.04693774	-62.5	-3372.326930	-25.2	37.3	16.0
Figure_S9_imid-2_modeC_ed(AS)	-3373.05670770	-68.7	-3372.335213	-30.4	38.3	15.8
Figure_S9_imid-2_modeC_ts(AS)_01	-3373.04232375	-59.6	-3372.326187	-24.7	34.9	-218.5
Figure_S9_imid-2_modeC_ts(AS)_02	-3373.04306643	-60.1	-3372.324855	-23.9	36.2	-249.7
Figure_S9_imid-2_modeC_ts(AS)_03	-3373.04323129	-60.2	-3372.321732	-21.9	38.3	-237.1
Figure_S9_imid-2_modeC_ts(AS)_04	-3373.03388548	-54.3	-3372.314883	-17.6	36.7	-226.8
Figure_S9_imid-2_modeC_ts(AS)_05	-3373.03470396	-54.9	-3372.316610	-18.7	36.1	-206.1
Figure_S9_imid-2_modeC_ts(AS)_06	-3373.03413600	-54.5	-3372.313809	-17.0	37.5	-226.5
Figure_S9_imid-2_modeC_prod(AS)	-3373.05244613	-66.0	-3372.332970	-29.0	37.0	-8.9
Figure_S9_imid-2_modeD_ed(AS)	-3373.05975930	-70.6	-3372.334884	-30.2	40.4	-8.4
Figure_S9_imid-2_modeD_ts(AS)_01	-3373.04766133	-63.0	-3372.329248	-26.6	36.3	-255.5
Figure_S9_imid-2_modeD_ts(AS)_02	-3373.04766477	-63.0	-3372.327501	-25.5	37.4	-265.7
Figure_S9_imid-2_modeD_ts(AS)_03	-3373.03925149	-57.7	-3372.320304	-21.0	36.7	-260.3
Figure_S9_imid-2_modeD_ts(AS)_04	-3373.03926580	-57.7	-3372.319991	-20.8	36.9	-259.9
Figure_S9_imid-2_modeD_ts(AS)_05	-3373.03918846	-57.7	-3372.318375	-19.8	37.9	-260.1
Figure_S9_imid-2_modeD_ts(AS)_06	-3373.03914741	-57.6	-3372.317884	-19.5	38.1	-264.3
Figure_S9_imid-2_modeD_prod(AS)	-3373.05877766	-70.0	-3372.337640	-31.9	38.1	20.3

E(sum) . electronic energy in hartree with M06L/Def2SVP:UFF after mass balance
G(sum) . sum of electronic and thermal free energies with M06L/Def2SVP:UFF after mass balance
ΔE … relative electronic energy in kcal/mol with M06L/Def2SVP:UFF
ΔG … relative free energy in kcal/mol with M06L/Def2SVP:UFF
ΔG_{corr} thermal correction to free energy in kcal/mol obtained with M06L/Def2SVP:UFF ($\Delta G = \Delta E + \Delta G_{corr}$)
Freq … lowest frequency

Single point energies in Figure S4-1 with M06, ωB97XD and MN12SX

ωB97XD/Def2TZVPP thf(SMD)			M06/Def2TZVPP thf(SMD)			MN12SX/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-5001.82121551	0.0	0.00	-5000.53870244	0.0	0.00	-5000.05232062	0.0	0.00
-5001.82121555	0.0	0.00	-5000.53870255	0.0	0.00	-5000.05232071	0.0	0.00
-5001.82098875	0.1	0.73	-5000.53892004	-0.1	0.45	-5000.05261586	-0.2	0.40
-5001.85420131	-20.7	-1.69	-5000.56615354	-17.2	1.78	-5000.07565975	-14.6	4.36
-5001.84235753	-13.3	4.32	-5000.55588917	-10.8	6.80	-5000.06502681	-8.0	9.61
-5001.83826060	-10.7	7.24	-5000.55207254	-8.4	9.55	-5000.06094247	-5.4	12.52
-5001.88654787	-41.0	-22.47	-5000.60060473	-38.8	-20.32	-5000.10641699	-33.9	-15.42
-5001.84739895	-16.4	1.91	-5000.55843620	-12.4	5.95	-5000.06785505	-9.7	8.59
-5001.82025552	0.6	15.87	-5000.53546938	2.0	17.30	-5000.04472667	4.8	20.04
-5001.82042276	0.5	20.38	-5000.53365008	3.2	23.05	-5000.04235609	6.3	26.13
-5001.86551949	-27.8	-9.34	-5000.58187843	-27.1	-8.63	-5000.08776603	-22.2	-3.78
-5001.84396144	-14.3	7.12	-5000.55493224	-10.2	11.21	-5000.06340609	-7.0	14.44
-5001.83100260	-6.1	13.45	-5000.54430496	-3.5	16.08	-5000.05125485	0.7	20.27
-5001.83064705	-5.9	13.83	-5000.54412501	-3.4	16.34	-5000.05102277	0.8	20.56
-5001.82777988	-4.1	16.31	-5000.54116291	-1.5	18.89	-5000.05010490	1.4	21.82
-5001.88776926	-41.8	-20.23	-5000.60191567	-39.7	-18.13	-5000.10487202	-33.0	-11.44
-5001.85069729	-18.5	-1.10	-5000.56285576	-15.2	2.25	-5000.07210990	-12.4	4.99
-5001.82468955	-2.2	15.37	-5000.53845200	0.2	17.71	-5000.04845940	2.4	19.98
-5001.82054702	0.4	17.14	-5000.53623012	1.6	18.27	-5000.04537794	4.4	21.08
-5001.86435892	-27.1	-6.59	-5000.57709700	-24.1	-3.61	-5000.08238668	-18.9	1.62

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

Single point energies in Figure S4-1 with MN12L and M06L

MN12L/Def2TZVPP thf(SMD)			M06L/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-4999.36375350	0.0	0.00	-5002.20546124	0.0	0.00
-4999.36375360	0.0	0.00	-5002.20546135	0.0	0.00
-4999.36571598	-1.2	-0.64	-5002.20674708	-0.8	-0.22
-4999.40113075	-23.5	-4.45	-5002.24055608	-22.0	-3.02
-4999.38614054	-14.0	3.54	-5002.22668371	-13.3	4.27
-4999.38537478	-13.6	4.37	-5002.22341690	-11.3	6.67
-4999.41932121	-34.9	-16.34	-5002.26353003	-36.4	-17.91
-4999.39152843	-17.4	0.91	-5002.23349172	-17.6	0.75
-4999.36451058	-0.5	14.80	-5002.20552764	0.0	15.23
-4999.36841543	-2.9	16.96	-5002.20344110	1.3	21.15
-4999.40307283	-24.7	-6.21	-5002.24802840	-26.7	-8.25
-4999.39112388	-17.2	4.22	-5002.22912291	-14.8	6.54
-4999.37451967	-6.8	12.84	-5002.21323276	-4.9	14.72
-4999.37468867	-6.9	12.88	-5002.21312903	-4.8	14.93
-4999.37670889	-8.1	12.30	-5002.21255861	-4.5	15.98
-4999.42074872	-35.8	-14.23	-5002.26380660	-36.6	-15.07
-4999.40175916	-23.8	-6.44	-5002.23558096	-18.9	-1.50
-4999.37212158	-5.3	12.30	-5002.20666361	-0.8	16.80
-4999.36925353	-3.5	13.27	-5002.20858968	-2.0	14.76
-4999.40025537	-22.9	-2.42	-5002.24021261	-21.8	-1.32

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

Single point energies in Figure S4-1 with BP86-D3BJ and PBE0-D3BJ

BP86-D3BJ/Def2TZVPP thf(SMD)			PBE0-D3BJ/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-5003.23606760	0.0	0.00	-4999.03162587	0.0	0.00
-5003.23606773	0.0	0.00	-4999.03162595	0.0	0.00
-5003.23870982	-1.7	-1.07	-4999.03267207	-0.7	-0.07
-5003.28370254	-29.9	-10.89	-4999.06949506	-23.8	-4.76
-5003.27279223	-23.0	-5.46	-4999.06094770	-18.4	-0.81
-5003.27118420	-22.0	-4.10	-4999.05686443	-15.8	2.10
-5003.30724589	-44.7	-26.14	-4999.10089685	-43.5	-24.94
-5003.27687124	-25.6	-7.27	-4999.06262564	-19.5	-1.12
-5003.24872569	-7.9	7.33	-4999.03804854	-4.0	11.24
-5003.25129684	-9.6	10.32	-4999.03585653	-2.7	17.23
-5003.28501637	-30.7	-12.26	-4999.07974126	-30.2	-11.73
-5003.27162920	-22.3	-0.92	-4999.05530433	-14.9	6.53
-5003.25863665	-14.2	5.43	-4999.04525034	-8.5	11.05
-5003.25851836	-14.1	5.66	-4999.04492637	-8.3	11.40
-5003.25924190	-14.5	5.89	-4999.04358706	-7.5	12.92
-5003.30720647	-44.6	-23.10	-4999.09944526	-42.6	-21.02
-5003.27961941	-27.3	-9.93	-4999.06377437	-20.2	-2.77
-5003.25154561	-9.7	7.84	-4999.03987709	-5.2	12.37
-5003.25069813	-9.2	7.54	-4999.03896516	-4.6	12.11
-5003.28488909	-30.6	-10.15	-4999.07548417	-27.5	-7.04

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

Single point energies in Figure S5-1 with M06, ωB97XD and MN12SX

ωB97XD/Def2TZVPP thf(SMD)			M06/Def2TZVPP thf(SMD)			MN12SX/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-5001.89690063	-47.5	-2.91	-5000.60063002	-38.9	5.72	-5000.10559372	-33.4	11.15
-5001.88317149	-38.9	5.77	-5000.58907855	-31.6	13.04	-5000.09328282	-25.7	18.94
-5001.88073907	-37.4	6.99	-5000.58754011	-30.6	13.69	-5000.09212051	-25.0	19.37
-5001.88519355	-40.1	5.99	-5000.59139458	-33.1	13.07	-5000.09495389	-26.8	19.39
-5001.88425843	-39.6	6.55	-5000.59083536	-32.7	13.40	-5000.09459295	-26.5	19.59
-5001.92592484	-65.7	-18.58	-5000.63278273	-59.0	-11.91	-5000.13236209	-50.2	-3.10
-5001.89705277	-47.6	-1.16	-5000.59633723	-36.2	10.26	-5000.09945292	-29.6	16.85
-5001.87895937	-36.2	8.30	-5000.57954155	-25.6	18.91	-5000.08310464	-19.3	25.22
-5001.87292563	-32.4	13.87	-5000.57669406	-23.8	22.48	-5000.08238553	-18.9	27.45
-5001.87802123	-35.6	11.95	-5000.57940466	-25.5	22.06	-5000.08246550	-18.9	28.68
-5001.87802116	-35.6	11.95	-5000.57940460	-25.5	22.06	-5000.08246539	-18.9	28.68
-5001.87090248	-31.2	15.03	-5000.57805701	-24.7	21.51	-5000.08021031	-17.5	28.71
-5001.86789209	-29.3	17.40	-5000.57491075	-22.7	23.97	-5000.07868294	-16.5	30.15
-5001.91928551	-61.5	-9.47	-5000.62336707	-53.1	-1.06	-5000.11983857	-42.4	9.70
-5001.88735084	-41.5	6.97	-5000.58950576	-31.9	16.59	-5000.09473871	-26.6	21.86
-5001.87370218	-32.9	15.07	-5000.57895696	-25.3	22.74	-5000.08194272	-18.6	29.42
-5001.87167302	-31.7	15.73	-5000.57848193	-25.0	22.43	-5000.08072393	-17.8	29.56
-5001.87107373	-31.3	17.77	-5000.57763144	-24.4	24.62	-5000.07979264	-17.2	31.81
-5001.92538477	-65.4	-14.46	-5000.62870724	-56.5	-5.57	-5000.12701476	-46.9	4.03
-5001.89030693	-43.4	6.54	-5000.59609964	-36.0	13.88	-5000.09877087	-29.1	20.75
-5001.87527608	-33.9	13.79	-5000.58204333	-27.2	20.51	-5000.08428425	-20.1	27.65
-5001.87801833	-35.6	12.15	-5000.58007548	-26.0	21.83	-5000.08399835	-19.9	27.91
-5001.91943372	-61.6	-11.44	-5000.62737282	-55.6	-5.44	-5000.12386257	-44.9	5.30

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

Single point energies in Figure S5-1 with MN12L and M06L

MN12L/Def2TZVPP thf(SMD)			M06L/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-4999.43022220	-41.7	2.87	-5002.27672779	-44.7	-0.14
-4999.41662374	-33.2	11.47	-5002.26165490	-35.3	9.39
-4999.41457818	-31.9	12.45	-5002.25947297	-33.9	10.45
-4999.42127194	-36.1	10.04	-5002.26379922	-36.6	9.53
-4999.41996552	-35.3	10.84	-5002.26318508	-36.2	9.89
-4999.44564233	-51.4	-4.26	-5002.29670133	-57.3	-10.12
-4999.42441786	-38.1	8.36	-5002.27008231	-40.6	5.88
-4999.40559770	-26.3	18.28	-5002.25081486	-28.5	16.08
-4999.40596839	-26.5	19.83	-5002.24786516	-26.6	19.71
-4999.40495083	-25.9	21.75	-5002.24986609	-27.9	19.74
-4999.40495072	-25.9	21.75	-5002.24986606	-27.9	19.74
-4999.40470597	-25.7	20.51	-5002.24867526	-27.1	19.09
-4999.40436310	-25.5	21.21	-5002.24589592	-25.4	21.32
-4999.43908241	-47.3	4.80	-5002.28730320	-51.4	0.71
-4999.42214888	-36.6	11.83	-5002.26439619	-37.0	11.49
-4999.40694520	-27.1	20.90	-5002.24862959	-27.1	20.92
-4999.40454929	-25.6	21.79	-5002.24731663	-26.3	21.12
-4999.40528230	-26.1	22.99	-5002.24589762	-25.4	23.68
-4999.44449801	-50.7	0.24	-5002.29214136	-54.4	-3.49
-4999.43045895	-41.9	8.04	-5002.26894155	-39.8	10.06
-4999.41351382	-31.2	16.48	-5002.25140464	-28.8	18.88
-4999.41283694	-30.8	16.99	-5002.24965773	-27.7	20.06
-4999.44727611	-52.4	-2.21	-5002.29026729	-53.2	-3.02

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

Single point energies in Figure S5-1 with BP86-D3BJ and PBE0-D3BJ

BP86-D3BJ/Def2TZVPP thf(SMD)			PBE0-D3BJ/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-5003.32653379	-56.8	-12.19	-4999.11232192	-50.6	-6.06
-5003.31422568	-49.0	-4.40	-4999.10075213	-43.4	1.27
-5003.31080573	-46.9	-2.56	-4999.09854764	-42.0	2.35
-5003.31587175	-50.1	-3.94	-4999.10151706	-43.9	2.28
-5003.31544925	-49.8	-3.70	-4999.10130513	-43.7	2.39
-5003.34636078	-69.2	-22.08	-4999.13943130	-67.6	-20.52
-5003.32643032	-56.7	-10.28	-4999.11000934	-49.2	-2.76
-5003.31000976	-46.4	-1.86	-4999.09541891	-40.0	4.51
-5003.30379792	-42.5	3.82	-4999.08898209	-36.0	10.33
-5003.30867404	-45.6	2.04	-4999.09386713	-39.1	8.54
-5003.30867402	-45.6	2.04	-4999.09386705	-39.1	8.54
-5003.29989215	-40.1	6.16	-4999.08707099	-34.8	11.42
-5003.29625575	-37.8	8.93	-4999.08366227	-32.7	14.04
-5003.34278418	-67.0	-14.90	-4999.13009244	-61.8	-9.72
-5003.31650420	-50.5	-2.00	-4999.09888093	-42.2	6.27
-5003.30326347	-42.2	5.84	-4999.08723017	-34.9	13.11
-5003.30146274	-41.0	6.35	-4999.08594713	-34.1	13.30
-5003.30076205	-40.6	8.46	-4999.08491826	-33.4	15.61
-5003.34450863	-68.0	-17.14	-4999.13339101	-63.9	-12.95
-5003.31645990	-50.4	-0.55	-4999.10114463	-43.6	6.27
-5003.30256345	-41.7	5.98	-4999.08895484	-36.0	11.73
-5003.30806778	-45.2	2.61	-4999.09154851	-37.6	10.19
-5003.33784827	-63.9	-13.67	-4999.12857705	-60.8	-10.64

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

Single point energies in Figure S6-1 with M06, ωB97XD and MN12SX

ωB97XD/Def2TZVPP thf(SMD)			M06/Def2TZVPP thf(SMD)			MN12SX/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-5001.90756306	-54.2	8.67	-5000.61152952	-45.7	17.16	-5000.11270746	-37.9	24.96
-5001.89097513	-43.8	18.29	-5000.59700350	-36.6	25.48	-5000.09819516	-28.8	33.28
-5001.89162436	-44.2	17.49	-5000.59733181	-36.8	24.89	-5000.09734228	-28.3	33.43
-5001.89161389	-44.2	18.13	-5000.59761706	-37.0	25.33	-5000.09786587	-28.6	33.72
-5001.89520041	-46.4	16.61	-5000.59982652	-38.4	24.68	-5000.09823198	-28.8	34.23
-5001.87691485	-35.0	20.01	-5000.58100226	-26.5	28.42	-5000.08524528	-20.7	34.30
-5001.88794185	-41.9	19.54	-5000.59320708	-34.2	27.21	-5000.09377249	-26.0	35.40
-5001.93569830	-71.8	-6.15	-5000.64023440	-63.7	1.98	-5000.13592968	-52.5	13.22
-5001.90739707	-54.1	9.66	-5000.60891668	-44.1	19.68	-5000.10901535	-35.6	28.16
-5001.88906798	-42.6	17.48	-5000.59281238	-34.0	26.10	-5000.09306514	-25.6	34.49
-5001.89204537	-44.4	16.93	-5000.59514852	-35.4	25.96	-5000.09514509	-26.9	34.50
-5001.89034576	-43.4	17.00	-5000.59378523	-34.6	25.82	-5000.09341887	-25.8	34.60
-5001.89024095	-43.3	18.03	-5000.59465875	-35.1	26.23	-5000.09368986	-26.0	35.39
-5001.89042672	-43.4	18.20	-5000.59560887	-35.7	25.92	-5000.09358993	-25.9	35.73
-5001.88526542	-40.2	20.25	-5000.58777713	-30.8	29.65	-5000.08975900	-23.5	36.95
-5001.88261103	-38.5	21.62	-5000.58848502	-31.2	28.90	-5000.08823436	-22.5	37.61
-5001.93858249	-73.6	-8.23	-5000.64464256	-66.5	-1.06	-5000.13678295	-53.0	12.42
-5001.89675026	-47.4	15.88	-5000.59837063	-37.4	25.84	-5000.09814646	-28.8	34.53
-5001.87985739	-36.8	25.59	-5000.58532226	-29.3	33.14	-5000.08661401	-21.5	40.87
-5001.88079839	-37.4	25.55	-5000.58533214	-29.3	33.68	-5000.08466438	-20.3	42.64
-5001.87787201	-35.6	25.84	-5000.58195117	-27.1	34.25	-5000.08179746	-18.5	42.90
-5001.93330735	-70.3	-7.11	-5000.63939255	-63.2	0.05	-5000.13424345	-51.4	11.82
-5001.90859131	-54.8	11.27	-5000.61292570	-46.6	19.53	-5000.11219734	-37.6	28.53
-5001.89375686	-45.5	17.10	-5000.59948731	-38.1	24.47	-5000.09813921	-28.8	33.86
-5001.89182495	-44.3	18.21	-5000.59695368	-36.6	25.97	-5000.09739206	-28.3	34.24
-5001.89251303	-44.7	17.30	-5000.59646611	-36.2	25.79	-5000.09622155	-27.5	34.49
-5001.89347739	-45.3	17.10	-5000.59704844	-36.6	25.84	-5000.09573575	-27.2	35.21
-5001.93962729	-74.3	-9.46	-5000.64523542	-66.9	-2.00	-5000.13897620	-54.4	10.47

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

Single point energies in Figure S6-1 with MN12L and M06L

MN12L/Def2TZVPP thf(SMD)			M06L/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-4999.44324736	-49.9	12.97	-5002.28667419	-51.0	11.89
-4999.42468038	-38.2	23.84	-5002.26930978	-40.1	22.00
-4999.42278821	-37.0	24.63	-5002.26922483	-40.0	21.66
-4999.42594177	-39.0	23.28	-5002.26869367	-39.7	22.62
-4999.42490314	-38.4	24.67	-5002.27015537	-40.6	22.44
-4999.40386740	-25.2	29.79	-5002.25468844	-30.9	24.07
-4999.42236135	-36.8	24.63	-5002.26607281	-38.0	23.38
-4999.45241764	-55.6	10.05	-5002.30341873	-61.5	4.22
-4999.43689770	-45.9	17.84	-5002.28293304	-48.6	15.13
-4999.41889055	-34.6	25.46	-5002.26296681	-36.1	23.97
-4999.42072532	-35.8	25.63	-5002.26652615	-38.3	23.06
-4999.41722302	-33.6	26.83	-5002.26443861	-37.0	23.38
-4999.41833120	-34.2	27.10	-5002.26503463	-37.4	23.96
-4999.41798604	-34.0	27.59	-5002.26482651	-37.3	24.37
-4999.40969098	-28.8	31.62	-5002.25975093	-34.1	26.38
-4999.41139831	-29.9	30.24	-5002.25956881	-34.0	26.19
-4999.45840033	-59.4	6.03	-5002.30743946	-64.0	1.43
-4999.42454335	-38.1	25.14	-5002.27248111	-42.1	21.23
-4999.41117998	-29.8	32.63	-5002.25715206	-32.4	29.96
-4999.40762530	-27.5	35.41	-5002.25552834	-31.4	31.52
-4999.40715046	-27.2	34.16	-5002.25054135	-28.3	33.10
-4999.45292779	-56.0	7.27	-5002.30278869	-61.1	2.16
-4999.44622142	-51.7	14.35	-5002.28582307	-50.4	15.68
-4999.42967533	-41.4	21.25	-5002.26860884	-39.6	22.99
-4999.42853585	-40.7	21.87	-5002.26748335	-38.9	23.60
-4999.42764377	-40.1	21.95	-5002.26693637	-38.6	23.46
-4999.42478391	-38.3	24.15	-5002.26676596	-38.5	23.98
-4999.46304380	-62.3	2.54	-5002.30861920	-64.7	0.12

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

Single point energies in Figure S6-1 with BP86-D3BJ and PBE0-D3BJ

BP86-D3BJ/Def2TZVPP thf(SMD)			PBE0-D3BJ/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-5003.33272675	-60.7	2.20	-4999.11783551	-54.1	8.76
-5003.31935363	-52.3	9.81	-4999.10604625	-46.7	15.37
-5003.31838903	-51.7	10.02	-4999.10622652	-46.8	14.86
-5003.31814674	-51.5	10.80	-4999.10483853	-45.9	16.36
-5003.32149682	-53.6	9.43	-4999.10799872	-47.9	15.11
-5003.30409805	-42.7	12.27	-4999.09596840	-40.4	14.58
-5003.31396298	-48.9	12.53	-4999.10062486	-43.3	18.11
-5003.35134178	-72.3	-6.65	-4999.14472951	-71.0	-5.28
-5003.33489796	-62.0	1.72	-4999.12018845	-55.6	8.17
-5003.31769084	-51.2	8.84	-4999.10488992	-46.0	14.08
-5003.32160111	-53.7	7.70	-4999.10815566	-48.0	13.35
-5003.31967663	-52.5	7.92	-4999.10720565	-47.4	12.96
-5003.31903510	-52.1	9.28	-4999.10650574	-47.0	14.36
-5003.31960494	-52.4	9.21	-4999.10622579	-46.8	14.81
-5003.31291734	-48.2	12.22	-4999.10298189	-44.8	15.67
-5003.31189330	-47.6	12.56	-4999.10039342	-43.2	16.99
-5003.35952671	-77.5	-12.05	-4999.14915449	-73.8	-8.33
-5003.32437687	-55.4	7.87	-4999.10842087	-48.2	15.09
-5003.30829520	-45.3	17.07	-4999.09577432	-40.3	22.14
-5003.31004206	-46.4	16.52	-4999.09612729	-40.5	22.47
-5003.30440346	-42.9	18.51	-4999.09070689	-37.1	24.32
-5003.35311027	-73.4	-10.21	-4999.14391782	-70.5	-7.23
-5003.33472962	-61.9	4.19	-4999.11845580	-54.5	11.62
-5003.32043250	-52.9	9.68	-4999.10634116	-46.9	15.73
-5003.31939614	-52.3	10.23	-4999.10533565	-46.3	16.26
-5003.32154248	-53.6	8.40	-4999.10596654	-46.6	15.39
-5003.32110947	-53.4	9.08	-4999.10687767	-47.2	15.23
-5003.35772807	-76.3	-11.49	-4999.14812239	-73.1	-8.25

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

Single point energies in Figure S7-1 with M06, ωB97XD and MN12SX

ωB97XD/Def2TZVPP thf(SMD)			M06/Def2TZVPP thf(SMD)			MN12SX/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-5001.91401352	-58.2	-17.57	-5000.62159518	-52.0	-11.35	-5000.12075468	-42.9	-2.28
-5001.89200821	-44.4	-6.33	-5000.60087750	-39.0	-0.93	-5000.10266440	-31.6	6.50
-5001.89336983	-45.3	-6.99	-5000.60158736	-39.5	-1.17	-5000.10286012	-31.7	6.58
-5001.88725593	-41.4	-1.00	-5000.59672776	-36.4	4.03	-5000.09332767	-25.7	14.70
-5001.88375074	-39.2	1.38	-5000.59317950	-34.2	6.44	-5000.09306834	-25.6	15.05
-5001.87485435	-33.7	6.72	-5000.58319990	-27.9	12.46	-5000.08395132	-19.8	20.53
-5001.87288221	-32.4	8.73	-5000.58127611	-26.7	14.44	-5000.08346240	-19.5	21.61
-5001.90695014	-53.8	-16.21	-5000.61335548	-46.8	-9.26	-5000.11905804	-41.9	-4.29
-5001.90721479	-54.0	-12.67	-5000.61432785	-47.5	-6.16	-5000.11748710	-40.9	0.41
-5001.88736765	-41.5	-2.45	-5000.59649869	-36.3	2.79	-5000.10014186	-30.0	9.05
-5001.88486751	-39.9	0.82	-5000.59455563	-35.0	5.71	-5000.09823032	-28.8	11.95
-5001.88490390	-40.0	2.35	-5000.59264603	-33.9	8.47	-5000.09254001	-25.2	17.08
-5001.88402858	-39.4	3.64	-5000.59321917	-34.2	8.85	-5000.09127240	-24.4	18.62
-5001.87619367	-34.5	6.26	-5000.58382935	-28.3	12.44	-5000.08553047	-20.8	19.92
-5001.87619419	-34.5	6.26	-5000.58382950	-28.3	12.44	-5000.08553052	-20.8	19.92
-5001.90597418	-53.2	-13.94	-5000.61298941	-46.6	-7.37	-5000.12030774	-42.7	-3.42
-5001.90690216	-53.8	-13.35	-5000.61535263	-48.1	-7.68	-5000.11668422	-40.4	0.03
-5001.88759507	-41.7	-3.27	-5000.59771895	-37.0	1.35	-5000.09939277	-29.5	8.85
-5001.88520982	-40.2	-0.61	-5000.59555335	-35.7	3.87	-5000.09702547	-28.1	11.50
-5001.87981464	-36.8	0.39	-5000.58972896	-32.0	5.14	-5000.08855108	-22.7	14.43
-5001.88568060	-40.5	-0.20	-5000.59476301	-35.2	5.08	-5000.09174479	-24.7	15.52
-5001.87629984	-34.6	5.43	-5000.58744726	-30.6	9.41	-5000.08842520	-22.7	17.34
-5001.87377449	-33.0	7.95	-5000.58471424	-28.9	12.06	-5000.08581791	-21.0	19.92
-5001.90304888	-51.4	-11.78	-5000.61057733	-45.1	-5.53	-5000.11571549	-39.8	-0.21
-5001.90525279	-52.7	-11.35	-5000.61440297	-47.5	-6.12	-5000.11530437	-39.5	1.86
-5001.88737952	-41.5	-3.29	-5000.59895736	-37.8	0.42	-5000.09969520	-29.7	8.50
-5001.88638833	-40.9	-1.92	-5000.59697868	-36.6	2.41	-5000.09642232	-27.7	11.30
-5001.89240732	-44.7	-3.51	-5000.60154249	-39.4	1.73	-5000.09971593	-29.7	11.42
-5001.88811836	-42.0	0.35	-5000.59849388	-37.5	4.81	-5000.09727701	-28.2	14.12
-5001.87174813	-31.7	7.35	-5000.58073001	-26.4	12.69	-5000.08340206	-19.5	19.56
-5001.87543932	-34.0	7.59	-5000.58419738	-28.5	13.07	-5000.08631114	-21.3	20.28
-5001.90067856	-49.9	-11.17	-5000.60859558	-43.9	-5.17	-5000.11505035	-39.4	-0.67

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

Single point energies in Figure S7-1 with MN12L and M06L

MN12L/Def2TZVPP thf(SMD)			M06L/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-4999.45045198	-54.4	-13.74	-5002.29056710	-53.4	-12.74
-4999.43323393	-43.6	-5.51	-5002.28134722	-47.6	-9.53
-4999.43327250	-43.6	-5.33	-5002.28102398	-47.4	-9.12
-4999.42644752	-39.3	1.10	-5002.27561188	-44.0	-3.58
-4999.42729841	-39.9	0.75	-5002.27365878	-42.8	-2.17
-4999.41102718	-29.7	10.72	-5002.25987186	-34.1	6.24
-4999.41158870	-30.0	11.14	-5002.25865131	-33.4	7.78
-4999.44805976	-52.9	-15.31	-5002.29849977	-58.4	-20.79
-4999.44899822	-53.5	-12.19	-5002.28447389	-49.6	-8.28
-4999.43390756	-44.0	-4.96	-5002.27622563	-44.4	-5.34
-4999.43252042	-43.2	-2.39	-5002.27476723	-43.5	-2.73
-4999.42578358	-38.9	3.39	-5002.27096322	-41.1	1.21
-4999.42493778	-38.4	4.67	-5002.27054141	-40.8	2.22
-4999.41698036	-33.4	7.36	-5002.26449727	-37.0	3.71
-4999.41697953	-33.4	7.36	-5002.26449728	-37.0	3.71
-4999.45251584	-55.7	-16.46	-5002.29649161	-57.1	-17.88
-4999.44595938	-51.6	-11.17	-5002.28489594	-49.8	-9.43
-4999.43075826	-42.0	-3.66	-5002.27643069	-44.5	-6.15
-4999.42809323	-40.4	-0.83	-5002.27484589	-43.5	-3.99
-4999.41867136	-34.5	2.70	-5002.26747332	-38.9	-1.75
-4999.42225924	-36.7	3.54	-5002.27108304	-41.2	-0.92
-4999.41966643	-35.1	4.91	-5002.26540188	-37.6	2.38
-4999.41695287	-33.4	7.55	-5002.26371842	-36.6	4.38
-4999.44657711	-52.0	-12.40	-5002.29268166	-54.7	-15.16
-4999.44630590	-51.8	-10.42	-5002.28678838	-51.0	-9.65
-4999.43221323	-43.0	-4.73	-5002.27964484	-46.6	-8.32
-4999.42797896	-40.3	-1.33	-5002.27624296	-44.4	-5.44
-4999.43300918	-43.5	-2.30	-5002.27917764	-46.3	-5.09
-4999.43156116	-42.5	-0.22	-5002.27629585	-44.4	-2.12
-4999.41452961	-31.9	7.20	-5002.26066528	-34.6	4.42
-4999.41986531	-35.2	6.40	-5002.26472398	-37.2	4.43
-4999.44725825	-52.4	-13.71	-5002.29500558	-56.2	-17.50

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

Single point energies in Figure S7-1 with BP86-D3BJ and PBE0-D3BJ

BP86-D3BJ/Def2TZVPP thf(SMD)			PBE0-D3BJ/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-5003.34634733	-69.2	-28.54	-4999.12994117	-61.7	-21.03
-5003.34001039	-65.2	-27.14	-4999.11324574	-51.2	-13.13
-5003.33946796	-64.9	-26.59	-4999.11288511	-51.0	-12.70
-5003.33451434	-61.8	-21.34	-4999.10545583	-46.3	-5.89
-5003.33279040	-60.7	-20.07	-4999.10288820	-44.7	-4.10
-5003.31777379	-51.3	-10.89	-4999.09385376	-39.0	1.33
-5003.31681965	-50.7	-9.52	-4999.09209862	-37.9	3.21
-5003.35077723	-72.0	-34.39	-4999.12606032	-59.3	-21.67
-5003.33992291	-65.2	-23.87	-4999.12365755	-57.8	-16.45
-5003.33450577	-61.8	-22.71	-4999.10743784	-47.6	-8.51
-5003.33298756	-60.8	-20.06	-4999.10544459	-46.3	-5.56
-5003.33187843	-60.1	-17.81	-4999.10224063	-44.3	-2.00
-5003.33147462	-59.9	-16.81	-4999.10176089	-44.0	-0.95
-5003.32457524	-55.5	-14.78	-4999.09616684	-40.5	0.26
-5003.32457511	-55.5	-14.78	-4999.09616709	-40.5	0.26
-5003.34732200	-69.8	-30.57	-4999.12358887	-57.7	-18.46
-5003.34112130	-65.9	-25.51	-4999.12450974	-58.3	-17.87
-5003.33591961	-62.7	-24.27	-4999.10846961	-48.2	-9.83
-5003.33439094	-61.7	-22.15	-4999.10697898	-47.3	-7.74
-5003.32773732	-57.5	-20.36	-4999.10069300	-43.3	-6.18
-5003.33112944	-59.7	-19.40	-4999.10428364	-45.6	-5.34
-5003.32156149	-53.6	-13.65	-4999.09683535	-40.9	-0.92
-5003.32031854	-52.9	-11.93	-4999.09541379	-40.0	0.91
-5003.34601555	-69.0	-29.42	-4999.12026813	-55.6	-16.05
-5003.34072850	-65.7	-24.30	-4999.12270057	-57.2	-15.77
-5003.33808022	-64.0	-25.78	-4999.10906595	-48.6	-10.36
-5003.33515433	-62.2	-23.20	-4999.10668236	-47.1	-8.12
-5003.33948776	-64.9	-23.73	-4999.11125458	-50.0	-8.80
-5003.33687881	-63.3	-20.93	-4999.10744956	-47.6	-5.25
-5003.32134219	-53.5	-14.45	-4999.09229341	-38.1	0.99
-5003.32387222	-55.1	-13.48	-4999.09563723	-40.2	1.45
-5003.34750142	-69.9	-31.23	-4999.12032439	-55.7	-16.97

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

Single point energies in Figure S8-1 with M06, ωB97XD and MN12SX

ωB97XD/Def2TZVPP thf(SMD)			M06/Def2TZVPP thf(SMD)			MN12SX/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-4185.83520838	0.0	0.00	-4184.95773520	0.0	0.00	-4184.53426963	0.0	0.00
-4185.86333861	-17.7	0.63	-4184.98217787	-15.3	2.94	-4184.55757620	-14.6	3.65
-4185.85228895	-10.7	5.73	-4184.97235717	-9.2	7.27	-4184.54680228	-7.9	8.58
-4185.89314905	-36.4	-18.02	-4185.01294873	-34.6	-16.31	-4184.58364982	-31.0	-12.65
-4185.86270919	-17.3	-1.01	-4184.98034692	-14.2	2.06	-4184.55438564	-12.6	3.63
-4185.83361800	1.0	15.85	-4184.95681452	0.6	15.43	-4184.53041341	2.4	17.27
-4185.87886607	-27.4	-10.84	-4185.00187771	-27.7	-11.14	-4184.57271902	-24.1	-7.57
-4185.85346603	-11.5	8.14	-4184.97019390	-7.8	11.78	-4184.54494436	-6.7	12.90
-4185.84059218	-3.4	13.76	-4184.95875623	-0.6	16.50	-4184.53377163	0.3	17.45
-4185.89592491	-38.1	-18.55	-4185.01590174	-36.5	-16.95	-4184.58672060	-32.9	-13.36
-4185.85998646	-15.5	-0.52	-4184.97887995	-13.3	1.76	-4184.55328899	-11.9	3.10
-4185.83097315	2.7	16.85	-4184.95326745	2.8	16.99	-4184.52831716	3.7	17.92
-4185.88049731	-28.4	-12.49	-4185.00356216	-28.8	-12.83	-4184.57404651	-25.0	-9.03

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

Single point energies in Figure S8-1 with MN12L and M06L

MN12L/Def2TZVPP thf(SMD)			M06L/Def2TZVPP thf(SMD)			
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	
-4184.01094594	0.0	0.00	-4186.09250778	0.0	0.00	
-4184.04726833	-22.8	-4.51	-4186.12432860	-20.0	-1.69	
-4184.03391579	-14.4	2.03	-4186.11065577	-11.4	5.06	
-4184.06177213	-31.9	-13.56	-4186.14496921	-32.9	-14.59	
-4184.04501935	-21.4	-5.13	-4186.12212055	-18.6	-2.33	
-4184.01840665	-4.7	10.17	-4186.09560297	-1.9	12.91	
-4184.05266478	-26.2	-9.62	-4186.13546539	-27.0	-10.40	
-4184.03624698	-15.9	3.72	-4186.11368646	-13.3	6.31	
-4184.01991279	-5.6	11.51	-4186.09871474	-3.9	13.24	
-4184.06712841	-35.3	-15.71	-4186.14818972	-34.9	-15.39	
-4184.04024668	-18.4	-3.35	-4186.12004934	-17.3	-2.25	
-4184.01549497	-2.9	11.33	-4186.09335726	-0.5	13.66	
-4184.05328443	-26.6	-10.64	-4186.13646950	-27.6	-11.66	

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

Single point energies in Figure S8-1 with BP86-D3BJ and PBE0-D3BJ

BP86-D3BJ/Def2TZVPP thf(SMD)			PBE0-D3BJ/Def2TZVPP thf(SMD)			
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	
-4186.92335169	0.0	0.00	-4183.72992118	0.0	0.00	
-4186.96758681	-27.8	-9.48	-4183.76475091	-21.9	-3.58	
-4186.95792492	-21.7	-5.25	-4183.75612906	-16.4	0.00	
-4186.98829815	-40.8	-22.42	-4183.79270230	-39.4	-21.06	
-4186.96428178	-25.7	-9.43	-4183.76179524	-20.0	-3.75	
-4186.93653475	-8.3	6.58	-4183.73662648	-4.2	10.65	
-4186.97183042	-30.4	-13.87	-4183.77825545	-30.3	-13.77	
-4186.95617983	-20.6	-1.00	-4183.75079342	-13.1	6.50	
-4186.94394492	-12.9	4.21	-4183.74258571	-7.9	9.19	
-4186.99071675	-42.3	-22.72	-4183.79422407	-40.4	-20.80	
-4186.96154509	-24.0	-8.93	-4183.76055032	-19.2	-4.19	
-4186.93451756	-7.0	7.18	-4183.73483976	-3.1	11.10	
-4186.97334117	-31.4	-15.44	-4183.77985079	-31.3	-15.40	

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

Single point energies in Figure S9-1 with M06, ωB97XD and MN12SX

ωB97XD/Def2TZVPP thf(SMD)			M06/Def2TZVPP thf(SMD)			MN12SX/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-4185.92171926	-54.3	-15.25	-4185.03498110	-48.5	-9.44	-4184.60015296	-41.3	-2.31
-4185.90038859	-40.9	-5.76	-4185.01509906	-36.0	-0.85	-4184.58327663	-30.8	4.39
-4185.90157186	-41.6	-3.74	-4185.01864356	-38.2	-0.31	-4184.58369802	-31.0	6.89
-4185.89866784	-39.8	-1.99	-4185.01630605	-36.8	1.08	-4184.58288901	-30.5	7.33
-4185.89604164	-38.2	-1.69	-4185.01254212	-34.4	2.09	-4184.57973748	-28.5	7.95
-4185.89815480	-39.5	-2.40	-4185.01362404	-35.1	2.03	-4184.58052780	-29.0	8.07
-4185.90076506	-41.1	-2.41	-4185.01789493	-37.8	0.98	-4184.58284024	-30.5	8.25
-4185.91709026	-51.4	-15.33	-4185.03022477	-45.5	-9.44	-4184.60075568	-41.7	-5.67
-4185.91904030	-52.6	-15.89	-4185.03424931	-48.0	-11.30	-4184.59868998	-40.4	-3.71
-4185.89749842	-39.1	-3.47	-4185.01445143	-35.6	0.03	-4184.58195169	-29.9	5.69
-4185.89377166	-36.7	0.58	-4185.01179198	-33.9	3.41	-4184.57863802	-27.8	9.49
-4185.89382294	-36.8	0.16	-4185.01049410	-33.1	3.83	-4184.57749404	-27.1	9.82
-4185.89191524	-35.6	2.12	-4185.00876976	-32.0	5.68	-4184.57724870	-27.0	10.73
-4185.89038023	-34.6	3.90	-4185.00827409	-31.7	6.80	-4184.57481848	-25.4	13.07
-4185.90608215	-44.5	-7.13	-4185.02178790	-40.2	-2.85	-4184.59423608	-37.6	-0.28
-4185.92207329	-54.5	-16.23	-4185.03741919	-50.0	-11.72	-4184.60434920	-44.0	-5.70
-4185.90245788	-42.2	-7.28	-4185.01871942	-38.3	-3.35	-4184.58748665	-33.4	1.52
-4185.90410980	-43.2	-7.02	-4185.02180702	-40.2	-3.99	-4184.58719147	-33.2	3.01
-4185.90386126	-43.1	-4.80	-4185.02155512	-40.0	-1.76	-4184.58629730	-32.6	5.63
-4185.89009821	-34.4	2.27	-4185.00865158	-32.0	4.77	-4184.57519078	-25.7	11.04
-4185.88899596	-33.8	2.39	-4185.00638611	-30.5	5.62	-4184.57357003	-24.7	11.48
-4185.88601198	-31.9	5.67	-4185.00234305	-28.0	9.56	-4184.57044026	-22.7	14.85
-4185.91996338	-53.2	-16.17	-4185.03576633	-49.0	-11.95	-4184.60627563	-45.2	-8.17
-4185.91627494	-50.9	-10.47	-4185.03138800	-46.2	-5.82	-4184.59759881	-39.7	0.66
-4185.89787854	-39.3	-2.98	-4185.01570942	-36.4	-0.03	-4184.58151705	-29.6	6.70
-4185.89769025	-39.2	-1.76	-4185.01452972	-35.6	1.81	-4184.58124791	-29.5	7.97
-4185.89310331	-36.3	0.35	-4185.00836763	-31.8	4.91	-4184.57586085	-26.1	10.58
-4185.89307773	-36.3	0.57	-4185.00829593	-31.7	5.16	-4184.57578884	-26.1	10.83
-4185.89329561	-36.5	1.40	-4185.01105036	-33.5	4.40	-4184.57649793	-26.5	11.35
-4185.89332600	-36.5	1.67	-4185.01133488	-33.6	4.50	-4184.57628632	-26.4	11.77
-4185.91179512	-48.1	-10.00	-4185.02618419	-43.0	-4.90	-4184.59587831	-38.7	-0.60

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

Single point energies in Figure S9-1 with MN12L and M06L

MN12L/Def2TZVPP thf(SMD)			M06L/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-4184.09578035	-53.2	-14.20	-4186.17355491	-50.9	-11.82
-4184.07651221	-41.1	-6.00	-4186.16363468	-44.6	-9.49
-4184.07982685	-43.2	-5.32	-4186.16654711	-46.5	-8.55
-4184.08040263	-43.6	-5.75	-4186.16427291	-45.0	-7.20
-4184.07406790	-39.6	-3.13	-4186.16052199	-42.7	-6.20
-4184.07418697	-39.7	-2.59	-4186.16218559	-43.7	-6.62
-4184.07898340	-42.7	-3.97	-4186.16556321	-45.8	-7.11
-4184.09646558	-53.7	-17.62	-4186.18370773	-57.2	-21.18
-4184.09204378	-50.9	-14.17	-4186.17185800	-49.8	-13.08
-4184.07815797	-42.2	-6.56	-4186.16358453	-44.6	-8.99
-4184.07335961	-39.2	-1.83	-4186.16003122	-42.4	-5.04
-4184.07182372	-38.2	-1.26	-4186.15947407	-42.0	-5.08
-4184.07162081	-38.1	-0.37	-4186.15947164	-42.0	-4.32
-4184.06989610	-37.0	1.53	-4186.15930698	-41.9	-3.40
-4184.09188701	-50.8	-13.44	-4186.17518565	-51.9	-14.53
-4184.10006582	-55.9	-17.64	-4186.17570698	-52.2	-13.93
-4184.08383455	-45.7	-10.82	-4186.16707273	-46.8	-11.87
-4184.08530996	-46.7	-10.44	-4186.16897149	-48.0	-11.76
-4184.08453602	-46.2	-7.90	-4186.16834953	-47.6	-9.31
-4184.07139308	-37.9	-1.22	-4186.15800743	-41.1	-4.39
-4184.06815500	-35.9	0.25	-4186.15579507	-39.7	-3.57
-4184.06513221	-34.0	3.54	-4186.15440790	-38.8	-1.30
-4184.10474359	-58.9	-21.85	-4186.18657732	-59.0	-22.02
-4184.09450871	-52.4	-12.04	-4186.17065932	-49.0	-8.64
-4184.07992575	-43.3	-6.94	-4186.16276283	-44.1	-7.74
-4184.07714197	-41.5	-4.09	-4186.16202185	-43.6	-6.18
-4184.07023436	-37.2	-0.52	-4186.15815813	-41.2	-4.51
-4184.07018213	-37.2	-0.28	-4186.15812478	-41.2	-4.29
-4184.07189557	-38.2	-0.39	-4186.15970809	-42.2	-4.32
-4184.07148535	-38.0	0.15	-4186.15968428	-42.2	-4.02
-4184.09451422	-52.4	-14.38	-4186.17983140	-54.8	-16.74

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

Single point energies in Figure S9-1 with BP86-D3BJ and PBE0-D3BJ

BP86-D3BJ/Def2TZVPP thf(SMD)			PBE0-D3BJ/Def2TZVPP thf(SMD)		
E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]	E_{sp} [hartree]	ΔE_{sp} [kcal/mol]	ΔG_{sp} [kcal/mol]
-4187.02900925	-66.3	-27.27	-4183.82254398	-58.1	-19.09
-4187.02131940	-61.5	-26.33	-4183.80715459	-48.5	-13.32
-4187.02472903	-63.6	-25.71	-4183.80787586	-48.9	-11.01
-4187.02371300	-63.0	-25.14	-4183.80608925	-47.8	-9.96
-4187.01902633	-60.0	-23.55	-4183.80350648	-46.2	-9.69
-4187.01875073	-59.9	-22.77	-4183.80502074	-47.1	-10.03
-4187.02299426	-62.5	-23.80	-4183.80700581	-48.4	-9.64
-4187.03554089	-70.4	-34.35	-4183.82083167	-57.0	-21.00
-4187.02643817	-64.7	-27.97	-4183.82140071	-57.4	-20.69
-4187.02045819	-60.9	-25.32	-4183.80445544	-46.8	-11.16
-4187.01745246	-59.0	-21.72	-4183.80093560	-44.6	-7.23
-4187.01578837	-58.0	-21.06	-4183.80010592	-44.0	-7.10
-4187.01756687	-59.1	-21.42	-4183.80053039	-44.3	-6.60
-4187.01549952	-57.8	-19.31	-4183.79862949	-43.1	-4.60
-4187.02511932	-63.9	-26.51	-4183.81031186	-50.4	-13.10
-4187.02974379	-66.8	-28.48	-4183.82425684	-59.2	-20.92
-4187.02408361	-63.2	-28.29	-4183.80853130	-49.3	-14.41
-4187.02631708	-64.6	-28.39	-4183.80978345	-50.1	-13.89
-4187.02569743	-64.2	-25.94	-4183.80914504	-49.7	-11.43
-4187.01581894	-58.0	-21.31	-4183.79772735	-42.5	-5.83
-4187.01322132	-56.4	-20.25	-4183.79640673	-41.7	-5.57
-4187.01069847	-54.8	-17.26	-4183.79415606	-40.3	-2.76
-4187.03718045	-71.4	-34.42	-4183.82288955	-58.3	-21.33
-4187.02655059	-64.8	-24.36	-4183.81871413	-55.7	-15.32
-4187.02224289	-62.1	-25.71	-4183.80419929	-46.6	-10.26
-4187.02028190	-60.8	-23.38	-4183.80420674	-46.6	-9.17
-4187.01544982	-57.8	-21.11	-4183.80044444	-44.3	-7.57
-4187.01544077	-57.8	-20.90	-4183.80038728	-44.2	-7.33
-4187.01816059	-59.5	-21.64	-4183.80127233	-44.8	-6.92
-4187.01790821	-59.3	-21.20	-4183.80117513	-44.7	-6.58
-4187.03362563	-69.2	-31.14	-4183.81599402	-54.0	-15.96

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

■ Coordinates after optimization with M06L/Def2SVP:UFF

```
26
vinylBpin / electronic energy: -488.860054406 a.u. / lowest freq: 64.97 cm-1
 B   1.230595  -0.336224   0.080649
 O   0.272206  -1.259835   0.408633
 O   0.702073   0.864867  -0.320149
 C  -1.009372  -0.710335   0.003398
 C  -0.716625   0.827511  -0.017968
 C  -2.065795  -1.136809   0.998019
 C  -1.312568  -1.271413  -1.375920
 C  -0.895891   1.478674   1.343519
 C  -1.468588   1.598127  -1.080028
 H  -0.366786   0.923678   2.130675
 H  -1.955351   1.547746   1.625181
 H  -0.486706   2.497284   1.318067
 H  -1.222125   1.253144  -2.091114
 H  -1.220055   2.666226  -1.021534
 H  -2.554339   1.501095  -0.937099
 H  -0.559001  -0.960329  -2.112718
 H  -2.298858  -0.950115  -1.737432
 H  -1.309099  -2.368613  -1.334618
 H  -3.031269  -0.664045   0.767247
 H  -1.791842  -0.873923   2.026745
 H  -2.209474  -2.224761   0.956151
 H   4.759177   0.082437  -0.084499
 C   3.685593   0.292150  -0.133096
 C   2.750540  -0.623311   0.156155
 H   3.082869  -1.625350   0.455959
 H   3.411892   1.308818  -0.436603
31
allyl_phosphate / electronic energy: -1069.76845592 a.u. / lowest freq: 24.13 cm-1
 C   1.569815   1.313754  -0.235460
 C   2.758927   0.483151  -0.061425
 C   3.934544   0.817484  -0.756391
 C   2.776526  -0.661179   0.758822
 C   5.088790   0.049018  -0.630371
 C   3.928702  -1.428471   0.884204
 C   5.091024  -1.077222   0.191897
 H   5.990834   0.328856  -1.179519
 H   3.921220  -2.313697   1.524509
 H   5.993453  -1.684683   0.291460
 C   0.409603   1.218745   0.436196
 C  -0.779996   2.057528   0.141576
 H  -1.199382   2.508570   1.055281
 H  -0.543590   2.864083  -0.563649
 H   1.872747  -0.959455   1.296652
 H   0.283663   0.468915   1.227052
 P  -2.518293   0.083112   0.299582
 O  -1.597223  -1.223791   0.069553
 O  -2.775544   0.276407   1.744310
 O  -3.778564  -0.099167  -0.684519
 O  -1.825775   1.289185  -0.505208
 H   1.653091   2.092060  -1.005339
 H   3.934746   1.698752  -1.404080
 C  -1.098572  -1.545632  -1.224636
 H  -0.704933  -2.566496  -1.177106
 H  -1.892732  -1.501951  -1.984148
 H  -0.288130  -0.859683  -1.513302
 C  -4.746738  -1.095503  -0.365930
 H  -5.574656  -0.977809  -1.071638
 H  -4.326645  -2.106670  -0.471986
 H  -5.124202  -0.968594   0.658098
13
thf / electronic energy: -76.339715260087 a.u. / lowest freq: 27.33 cm-1
 O   0.000025  -1.225546  -0.212974
 C   1.109558  -0.458776   0.113122
 H   1.412272  -0.676586   1.161824
 H   1.954309  -0.722409  -0.558305
 C  -1.109537  -0.458822   0.113131
 H  -1.954287  -0.722499  -0.558278
 H  -1.412224  -0.676633   1.161841
 C  -0.751551   1.007103  -0.038813
 H  -1.140164   1.404849  -1.002354
 H  -1.158790   1.606421   0.804749
 C   0.751507   1.007136  -0.038799
 H   1.158701   1.606454   0.804786
 H   1.140120   1.404924  -1.002322
113
Figure_S4_imid-3-Cu-H_01 / electronic energy: -2884.015986291803 a.u. / lowest freq: 6.42 cm-1
 C   2.926015   1.508514   0.341065
 H   3.299473   1.041555   1.269943
 C   1.416947   1.807489   0.392609
```

H	1.144219	2.688402	-0.213874
C	1.786994	-0.140666	-0.892011
C	4.188301	-0.137746	-1.164701
C	4.753290	0.331057	-2.353122
C	4.808206	-1.196242	-0.477631
C	5.925545	-0.225439	-2.856687
H	4.244808	1.132814	-2.891730
C	5.982306	-1.752685	-0.990776
C	6.542180	-1.269752	-2.171553
H	6.350378	0.152785	-3.788728
H	6.446018	-2.578858	-0.448947
H	7.460401	-1.717031	-2.558286
C	-0.511639	0.292304	-0.306024
C	-1.442613	1.288039	-0.641091
C	-0.966955	-0.988770	0.040575
C	-2.813441	1.001782	-0.637856
C	-2.339608	-1.265819	0.068372
C	-3.260782	-0.272926	-0.278425
H	-4.323182	-0.487889	-0.256442
S	4.191474	-1.847559	1.088771
O	4.832043	-3.187479	1.212202
O	2.709339	-2.010074	0.930214
O	4.579280	-0.862194	2.111851
Cu	1.817155	-1.982425	-1.471365
C	3.768402	2.709962	-0.001863
C	4.758929	3.153557	0.891944
C	3.589384	3.395237	-1.218327
C	5.552586	4.260099	0.575007
H	4.919046	2.643961	1.833988
C	4.386160	4.500166	-1.531136
H	2.839019	3.068884	-1.927570
C	5.366691	4.932604	-0.635229
H	6.313263	4.595650	1.267990
H	4.244528	5.020119	-2.469731
H	5.983160	5.788084	-0.879181
C	0.900602	1.985993	1.798252
C	0.363904	3.221206	2.201465
C	0.926061	0.919461	2.717149
C	-0.130746	3.386808	3.498391
H	0.328781	4.057414	1.514337
C	0.425334	1.089009	4.010660
H	1.327014	-0.043924	2.430392
C	-0.104327	2.320964	4.400666
H	-0.537870	4.342168	3.803053
H	0.450505	0.265418	4.711860
H	-0.491834	2.450597	5.402814
N	2.979789	0.468349	-0.711892
N	0.869409	0.592970	-0.247225
H	-0.257794	-1.754380	0.331464
H	-1.105552	2.281165	-0.910151
C	-2.823027	-2.583429	0.517363
C	-3.126207	-3.593223	-0.437293
C	-3.028782	-2.824117	1.904746
C	-3.628453	-4.826435	0.016882
C	-3.525820	-4.076834	2.308427
C	-3.820745	-5.063729	1.373802
H	-3.878372	-5.613092	-0.682758
H	-3.697594	-4.292474	3.354763
H	-4.207988	-6.019230	1.703751
C	-3.791394	2.042404	-1.002420
C	-4.343051	2.881654	0.005103
C	-4.215249	2.173070	-2.354275
C	-5.310161	3.835364	-0.362349
C	-5.181012	3.145695	-2.671045
C	-5.719236	3.965764	-1.685227
H	-5.759310	4.482073	0.379743
H	-5.529086	3.268499	-3.688214
H	-6.464955	4.705157	-1.947938
C	-3.667902	1.279269	-3.468049
H	-2.902539	0.576986	-3.079857
C	-2.966652	2.107359	-4.551896
H	-2.175527	2.738751	-4.093533
H	-2.485777	1.433352	-5.292795
H	-3.684182	2.762210	-5.089360
C	-4.776863	0.407017	-4.068384
H	-5.270852	-0.182026	-3.266147
H	-5.541579	1.025409	-4.583909
H	-4.344853	-0.305213	-4.803635
C	-3.936017	2.763428	1.474688
H	-3.142114	2.001118	1.612632
C	-5.119223	2.305745	2.335179
H	-4.784357	2.129209	3.379819
H	-5.926758	3.067894	2.346890
H	-5.529259	1.352448	1.938062
C	-3.348628	4.079468	1.998821
H	-2.992610	3.945385	3.042072
H	-2.484179	4.384906	1.371194
H	-4.103670	4.892968	1.993655

C -2.750166 -1.757683 2.966332
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C -2.937294 -3.374560 -1.938671
H -2.495753 -2.378466 -2.145922
C -1.961063 -4.397619 -2.532875
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H -2.378656 -5.425618 -2.496458
H -1.746344 -4.145489 -3.593393
C -4.283923 -3.405403 -2.670680
H -4.754738 -4.408979 -2.604950
H -4.972834 -2.654928 -2.227039
H -4.140374 -3.151592 -3.742810
C -1.674089 -2.224333 3.953816
H -2.010347 -3.111068 4.530779
H -0.742961 -2.481515 3.404755
H -1.439922 -1.410408 4.672120
C -4.037285 -1.358814 3.697982
H -4.804224 -1.031937 2.963468
H -4.443488 -2.205345 4.290607
H -3.835801 -0.510686 4.387010
Na 2.806457 -4.337068 0.315215
H 1.904808 -3.499469 -1.869644
113
Figure_S4_imid-3-Cu-H_02 / electronic energy: -2884.015986317998 a.u. / lowest freq: 6.42 cm-1
C 2.926014 1.508517 0.341064
H 3.299470 1.041560 1.269943
C 1.416946 1.807493 0.392605
H 1.144219 2.688406 -0.213880
C 1.786996 -0.140663 -0.892014
C 4.188303 -0.137745 -1.164697
C 4.753296 0.331055 -2.353117
C 4.808206 -1.196239 -0.477623
C 5.925552 -0.225443 -2.856678
H 4.244815 1.132811 -2.891729
C 5.982308 -1.752683 -0.990763
C 6.542185 -1.269753 -2.171540
H 6.350387 0.152780 -3.788719
H 6.446018 -2.578855 -0.448931
H 7.460407 -1.717033 -2.558269
C -0.511639 0.292306 -0.306028
C -0.966952 -0.988771 0.040565
C -1.442615 1.288041 -0.641088
C -2.339604 -1.265822 0.068363
C -2.813443 1.001782 -0.637851
C -3.260781 -0.272928 -0.278427
H -4.323180 -0.487893 -0.256443
S 4.191470 -1.847553 1.088779
O 4.832037 -3.187474 1.212213
O 2.709334 -2.010067 0.930219
O 4.579274 -0.862188 2.111859
Cu 1.817156 -1.982423 -1.471365
C 3.768402 2.709965 -0.001864
C 4.758927 3.153561 0.891945
C 3.589387 3.395239 -1.218329
C 5.552585 4.260102 0.575009
H 4.919042 2.643966 1.833990
C 4.386164 4.500168 -1.531137
H 2.839024 3.068885 -1.927573
C 5.366693 4.932606 -0.635229
H 6.313261 4.595654 1.267994
H 4.244535 5.020119 -2.469733
H 5.983163 5.788086 -0.879180
C 0.900598 1.985998 1.798246
C 0.363898 3.221211 2.201457
C 0.926056 0.919467 2.717143
C -0.130756 3.386812 3.498381
H 0.328775 4.057418 1.514328
C 0.425325 1.089014 4.010653
H 1.327010 -0.043919 2.430387
C -0.104339 2.320969 4.400657
H -0.537882 4.342172 3.803041
H 0.450493 0.265424 4.711853
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C -4.343064 2.881639 0.005125
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C -5.310174 3.835351 -0.362320
C -5.181010 3.145714 -2.671024
C -5.719242 3.965768 -1.685199
H -5.759330 4.482048 0.379779
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C -3.126202 -3.593224 -0.437316

C	-3.028771	-2.824135	1.904728
C	-3.628446	-4.826439	0.016852
C	-3.525806	-4.076855	2.308402
C	-3.820732	-5.063743	1.373771
H	-3.878366	-5.613092	-0.682793
H	-3.697576	-4.292502	3.354737
H	-4.207974	-6.019247	1.703714
C	-2.750151	-1.757708	2.966321
H	-2.359754	-0.825475	2.509999
C	-1.674069	-2.224364	3.953796
H	-0.742944	-2.481542	3.404729
H	-1.439898	-1.410443	4.672104
H	-2.010324	-3.111103	4.530755
C	-4.037267	-1.358846	3.697980
H	-4.804210	-1.031964	2.963472
H	-4.443467	-2.205382	4.290600
H	-3.835781	-0.510723	4.387013
C	-2.937292	-3.374550	-1.938693
H	-2.495751	-2.378455	-2.145938
C	-4.283924	-3.405387	-2.670698
H	-4.140377	-3.151570	-3.742828
H	-4.754739	-4.408963	-2.604973
H	-4.972833	-2.654914	-2.227051
C	-1.961064	-4.397605	-2.532907
H	-1.746348	-4.145468	-3.593424
H	-1.003145	-4.378126	-1.970814
H	-2.378657	-5.425604	-2.496497
C	-3.667891	1.279302	-3.468044
H	-2.902528	0.577016	-3.079857
C	-3.936038	2.763394	1.474711
H	-3.142135	2.001084	1.612650
C	-3.348655	4.079428	1.998865
H	-2.484204	4.384876	1.371247
H	-4.103699	4.892926	1.993706
H	-2.992642	3.945331	3.042116
C	-5.119248	2.305697	2.335189
H	-5.926786	3.067844	2.346906
H	-5.529280	1.352405	1.938056
H	-4.784389	2.129147	3.379828
C	-2.966637	2.107408	-4.551877
H	-3.684166	2.762265	-5.089336
H	-2.175516	2.738796	-4.093502
H	-2.485756	1.433412	-5.292782
C	-4.776846	0.407056	-4.068397
H	-5.270837	-0.182000	-3.266170
H	-5.541562	1.025452	-4.583917
H	-4.344831	-0.305163	-4.803655
Na	2.806453	-4.337063	0.315221
H	1.904804	-3.499468	-1.869641

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Figure_S4_imid-3-Cu-H_03 / electronic energy: -2884.016426363786 a.u. / lowest freq: 13.84 cm-1

C	-2.937124	-1.629721	0.161149
H	-3.308068	-1.253393	1.131131
C	-1.424472	-1.924910	0.178573
H	-1.156948	-2.791409	-0.449930
C	-1.816713	0.091785	-0.994282
C	-4.229195	0.187005	-1.082788
C	-4.947921	-0.168595	-2.227402
C	-4.715125	1.219647	-0.259681
C	-6.136583	0.477929	-2.556545
H	-4.548112	-0.953636	-2.872222
C	-5.907353	1.862861	-0.597405
C	-6.618328	1.495581	-1.737258
H	-6.680560	0.188399	-3.457964
H	-6.267016	2.663842	0.050250
H	-7.548307	2.011436	-1.985823
C	0.497268	-0.353381	-0.442720
C	0.894569	0.972123	-0.199655
C	1.482171	-1.345392	-0.592274
C	2.250647	1.299062	-0.093644
C	2.840918	-1.012547	-0.502153
C	3.222629	0.308388	-0.250610
H	4.273019	0.562052	-0.162697
S	-3.918715	1.739996	1.278794
O	-4.517292	3.073445	1.570489
O	-2.459604	1.904360	0.977851
O	-4.217799	0.683991	2.260059
Cu	-1.819914	1.963943	-1.475440
C	-3.769133	-2.803491	-0.286426
C	-4.736328	-3.351733	0.574003
C	-3.598808	-3.361225	-1.567516
C	-5.515796	-4.436493	0.160859
H	-4.887753	-2.941940	1.564858
C	-4.381106	-4.444988	-1.976234
H	-2.865174	-2.952170	-2.251089
C	-5.338528	-4.982568	-1.112767
H	-6.258155	-4.853871	0.828795
H	-4.245712	-4.867366	-2.963483

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C -0.898701 -2.140969 1.576880
C -0.437166 -3.409740 1.968256
C -0.856980 -1.082995 2.505073
C 0.049876 -3.615870 3.262211
H -0.458398 -4.241372 1.275104
C -0.355017 -1.290705 3.792438
H -1.203168 -0.096622 2.229479
C 0.096677 -2.556468 4.171412
H 0.400590 -4.596294 3.557417
H -0.318963 -0.470735 4.497591
H 0.483581 -2.716631 5.169358
N -3.012910 -0.501870 -0.794819
N -0.879776 -0.696465 -0.446557
H 1.197721 -2.373883 -0.775082
H 0.152163 1.742936 -0.039176
C 3.878767 -2.049079 -0.651855
C 4.419693 -2.681284 0.502500
C 4.400391 -2.347537 -1.941363
C 5.483740 -3.587959 0.342769
C 5.453441 -3.274220 -2.049232
C 5.987670 -3.883581 -0.919172
H 5.935941 -4.067693 1.200534
H 5.878683 -3.518324 -3.013784
H 6.805638 -4.585204 -1.021537
C 2.652557 2.675181 0.247294
C 3.063576 3.571522 -0.777772
C 2.629093 3.101022 1.604999
C 3.442590 4.878966 -0.422406
C 3.002889 4.423256 1.906543
C 3.406699 5.298175 0.903431
H 3.765520 5.585025 -1.176098
H 2.988704 4.782587 2.927094
H 3.696442 6.310097 1.156141
C 2.218771 2.165538 2.744723
H 1.986860 1.148432 2.368920
C 0.943800 2.664448 3.434162
H 0.126376 2.765736 2.688644
H 0.618286 1.935683 4.206562
H 1.108635 3.646760 3.924740
C 3.359380 1.982662 3.753467
H 4.277072 1.639503 3.229494
H 3.582223 2.929307 4.288922
H 3.081841 1.211963 4.504273
C 3.102898 3.159857 -2.250025
H 2.753483 2.116071 -2.384598
C 4.535210 3.201896 -2.795280
H 4.558699 2.807067 -3.833604
H 4.933295 4.238445 -2.803039
H 5.197250 2.566137 -2.168999
C 2.162552 4.027993 -3.095375
H 2.128693 3.646317 -4.138265
H 1.133089 3.988038 -2.678748
H 2.500513 5.085198 -3.121011
C 3.874898 -1.670003 -3.207424
H 3.029999 -0.989774 -2.977374
C 3.902965 -2.380701 1.910297
H 3.005498 -1.729226 1.876333
C 3.460732 -3.659302 2.633513
H 2.719329 -4.208076 2.014416
H 4.320783 -4.328554 2.843188
H 2.984701 -3.399445 3.602741
C 4.956803 -1.623995 2.725852
H 5.862115 -2.247034 2.886271
H 5.249994 -0.693293 2.194399
H 4.540573 -1.339658 3.716069
C 3.325635 -2.699024 -4.203355
H 4.131247 -3.355118 -4.594505
H 2.554503 -3.329105 -3.710435
H 2.850607 -2.179196 -5.062723
C 4.958135 -0.797472 -3.852639
H 5.335274 -0.056221 -3.115607
H 5.809560 -1.412738 -4.212599
H 4.534727 -0.240956 -4.716008
Na -2.607474 4.258453 0.457739
H -1.861473 3.502791 -1.792123
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Figure_S4_imid-3_modeS1_ed(CuHadd) / electronic energy: -3372.921349842059 a.u. / lowest freq: 11.86 cm-1
C -1.910181 -2.643302 0.668179
H -2.569047 -2.440681 1.523400
C -0.428825 -2.298818 0.948923
H 0.227997 -3.171972 0.811051
C -1.211337 -0.929097 -0.819408
C -3.461465 -1.722077 -1.154995
C -3.376351 -1.897839 -2.543890
C -4.727901 -1.573274 -0.565166
C -4.518252 -1.932742 -3.336494
H -2.384873 -2.009361 -2.991843

C	-5.871677	-1.638699	-1.366746
C	-5.775011	-1.821504	-2.743373
H	-4.423419	-2.064189	-4.416460
H	-6.844429	-1.508550	-0.889169
H	-6.680598	-1.864353	-3.351995
C	1.129432	-0.705244	-0.248368
C	2.267071	-1.521261	-0.345293
C	1.283207	0.687173	-0.198146
C	3.545257	-0.951449	-0.381140
C	2.564695	1.255648	-0.205768
C	3.693176	0.436474	-0.309934
H	4.684139	0.876165	-0.307283
S	-4.953348	-1.147926	1.168695
O	-6.298522	-0.498184	1.216323
O	-3.887320	-0.138823	1.447807
O	-4.851738	-2.387662	1.955744
Cu	-1.439098	0.347256	-2.318869
C	-2.095449	-4.074589	0.220506
C	-2.870870	-4.964190	0.984847
C	-1.495103	-4.538529	-0.965865
C	-3.050376	-6.285726	0.565321
H	-3.332238	-4.640365	1.908536
C	-1.678150	-5.860307	-1.381266
H	-0.888219	-3.875579	-1.569705
C	-2.456316	-6.732932	-0.617208
H	-3.649433	-6.964226	1.158815
H	-1.216099	-6.208153	-2.296073
H	-2.596871	-7.756384	-0.939972
C	-0.195624	-1.727226	2.327258
C	0.622571	-2.406542	3.246802
C	-0.742273	-0.482284	2.690929
C	0.888866	-1.850270	4.501653
H	1.060225	-3.363270	2.991920
C	-0.477075	0.067910	3.947352
H	-1.355018	0.071855	1.994094
C	0.340201	-0.614094	4.851362
H	1.523859	-2.376767	5.202291
H	-0.896714	1.028957	4.215544
H	0.550928	-0.183146	5.821487
N	-2.247688	-1.698529	-0.426606
N	-0.149289	-1.288652	-0.088515
H	0.410665	1.318965	-0.100412
H	2.162888	-2.598403	-0.381717
C	2.733263	2.708000	-0.024381
C	2.665157	3.577964	-1.147029
C	2.975382	3.234050	1.276776
C	2.798458	4.962896	-0.940094
C	3.106126	4.626401	1.429591
C	3.008695	5.478123	0.334460
H	2.747227	5.653531	-1.771416
H	3.291551	5.060964	2.402886
H	3.110721	6.546810	0.472835
C	4.740378	-1.812174	-0.442804
C	5.280451	-2.361428	0.753839
C	5.371039	-2.062053	-1.693262
C	6.441009	-3.152616	0.672580
C	6.534343	-2.852803	-1.719887
C	7.058489	-3.392616	-0.550251
H	6.879988	-3.583377	1.562844
H	7.044261	-3.055025	-2.652568
H	7.953655	-3.999903	-0.591414
C	4.828399	-1.493700	-3.005121
H	3.888654	-0.928811	-2.839110
C	4.473958	-2.612280	-3.993168
H	3.770002	-3.328708	-3.517984
H	3.978186	-2.183209	-4.890121
H	5.379213	-3.162708	-4.324847
C	5.818823	-0.501028	-3.624728
H	6.051826	0.305216	-2.896346
H	6.763478	-1.005338	-3.918660
H	5.372929	-0.031978	-4.527859
C	4.651368	-2.104941	2.124649
H	3.745600	-1.470781	2.040933
C	5.615284	-1.340965	3.039944
H	5.103226	-1.067880	3.987489
H	6.508560	-1.952677	3.286215
H	5.946394	-0.404188	2.542920
C	4.191609	-3.414492	2.776391
H	3.662299	-3.199523	3.728930
H	3.488653	-3.946713	2.100264
H	5.051689	-4.080337	2.998381
C	3.122334	2.334144	2.506934
H	2.966845	1.267489	2.247435
C	2.481906	3.053087	-2.571099
H	2.384911	1.948555	-2.581525
C	1.196565	3.597937	-3.202273
H	0.333031	3.358968	-2.550070
H	1.247608	4.697767	-3.344267

H 1.025678 3.122014 -4.191435
C 3.704120 3.376036 -3.438818
H 3.825004 4.471501 -3.574037
H 4.622721 2.967178 -2.965559
H 3.594064 2.907680 -4.440312
C 2.071279 2.657674 3.575363
H 2.188934 3.690318 3.964567
H 1.053988 2.544215 3.150064
H 2.165062 1.950053 4.426749
C 4.539019 2.428610 3.084933
H 5.285499 2.184991 2.298798
H 4.747006 3.446962 3.475737
H 4.661027 1.700661 3.915364
C -3.033472 1.643101 -2.021138
C -2.449277 1.739994 -3.304060
H -1.786052 2.575577 -3.549741
B -2.759472 2.684080 -0.929658
O -1.677600 3.528101 -0.918659
O -3.633970 2.969818 0.120521
C -1.712161 4.294343 0.305730
C -3.225995 4.252144 0.678750
C -0.847049 3.572507 1.321105
H 0.170273 3.490459 0.924654
H -0.790867 4.118567 2.272239
H -1.218789 2.558010 1.522911
C -1.163872 5.676718 0.029708
H -1.246830 6.318355 0.918280
H -0.100492 5.610109 -0.234546
H -1.683471 6.167206 -0.801905
C -4.034021 5.325082 -0.030262
H -3.823824 6.323785 0.375772
H -3.822322 5.340877 -1.108247
H -5.107224 5.133018 0.099887
C -3.504134 4.260924 2.166176
H -3.087500 3.378984 2.669725
H -3.069303 5.154413 2.636459
H -4.584497 4.297704 2.367229
Na -5.311640 1.704798 1.224120
H -2.916887 1.262052 -4.171788
H -3.927202 1.012054 -1.921644
H -0.421684 -0.031021 -3.475427
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Figure_S4_imid-3_modeS1_ts(CuHadd)_01 / electronic energy: -3372.907503843620 a.u. / lowest freq: -764.65 cm-1
C -1.848808 -2.810909 0.514021
H -2.468142 -2.597214 1.397725
C -0.345704 -2.529292 0.748385
H 0.287594 -3.351189 0.375204
C -1.190936 -0.949593 -0.799985
C -3.415529 -1.764292 -1.237351
C -3.369705 -1.887729 -2.632964
C -4.656497 -1.570356 -0.609900
C -4.531390 -1.841738 -3.395889
H -2.395048 -2.026502 -3.107690
C -5.821816 -1.552353 -1.381924
C -5.766272 -1.693323 -2.765765
H -4.471188 -1.938217 -4.481991
H -6.775223 -1.390929 -0.875569
H -6.687235 -1.673119 -3.352188
C 1.130886 -0.691082 -0.187446
C 2.286568 -1.448974 -0.435075
C 1.245635 0.689633 0.023793
C 3.543888 -0.833190 -0.458222
C 2.506853 1.300879 0.022303
C 3.653491 0.539972 -0.222276
H 4.629013 1.012953 -0.217425
S -4.806341 -1.204624 1.145735
O -6.099247 -0.462453 1.253923
O -3.662178 -0.291099 1.443939
O -4.777083 -2.485288 1.870762
Cu -1.565878 0.469732 -2.029573
C -2.110196 -4.221845 0.046654
C -2.867578 -5.102979 0.838127
C -1.602031 -4.675456 -1.185632
C -3.119459 -6.406849 0.400849
H -3.259428 -4.785458 1.795806
C -1.857335 -5.979496 -1.618726
H -1.012084 -4.017354 -1.811492
C -2.616510 -6.844202 -0.826884
H -3.704237 -7.079170 1.015230
H -1.466452 -6.319605 -2.568939
H -2.813280 -7.853822 -1.163541
C -0.009503 -2.268149 2.195660
C 0.847408 -3.137799 2.892823
C -0.512036 -1.130591 2.855106
C 1.190734 -2.875249 4.222600
H 1.252625 -4.017284 2.408496
C -0.167647 -0.873849 4.184519
H -1.156957 -0.435064 2.335117

C	0.685172	-1.743813	4.867240
H	1.850610	-3.548927	4.753551
H	-0.557419	0.003881	4.683479
H	0.954666	-1.540963	5.895586
N	-2.185187	-1.826297	-0.538373
N	-0.128438	-1.324203	-0.071478
H	0.360452	1.274962	0.235163
H	2.214348	-2.515098	-0.608015
C	2.637788	2.731920	0.343491
C	2.664868	3.696275	-0.701258
C	2.734733	3.143637	1.702372
C	2.752782	5.058856	-0.362800
C	2.819698	4.518486	1.988341
C	2.821499	5.462159	0.966555
H	2.769548	5.819578	-1.132025
H	2.889129	4.867468	3.010116
H	2.886377	6.515597	1.206728
C	4.758681	-1.630369	-0.706802
C	5.384857	-2.322733	0.367082
C	5.327848	-1.666392	-2.010421
C	6.571899	-3.034382	0.113603
C	6.517785	-2.389488	-2.210962
C	7.128752	-3.065621	-1.160447
H	7.078943	-3.565242	0.908491
H	6.982220	-2.430116	-3.187424
H	8.044544	-3.615934	-1.334508
C	4.692158	-0.938159	-3.195688
H	3.741951	-0.447433	-2.902446
C	4.326400	-1.915364	-4.320071
H	3.676602	-2.724326	-3.922645
H	3.766766	-1.382631	-5.118502
H	5.232094	-2.370242	-4.773123
C	5.608374	0.178522	-3.709297
H	5.856594	0.875393	-2.880275
H	6.550841	-0.234323	-4.126881
H	5.093111	0.757919	-4.505079
C	4.821875	-2.299943	1.789319
H	3.875854	-1.723755	1.839781
C	5.789608	-1.604057	2.753406
H	5.325433	-1.514047	3.758933
H	6.738353	-2.172413	2.852427
H	6.018365	-0.580472	2.386163
C	4.479787	-3.714392	2.273352
H	3.992109	-3.667170	3.269761
H	3.774400	-4.197001	1.563423
H	5.389474	-4.344282	2.361965
C	2.764114	2.139731	2.857160
H	2.696736	1.096476	2.487178
C	2.611426	3.297791	-2.176424
H	2.541125	2.197160	-2.292708
C	1.367933	3.874152	-2.861420
H	0.459114	3.543139	-2.319843
H	1.392167	4.983842	-2.882149
H	1.301387	3.503011	-3.906433
C	3.891350	3.718719	-2.908219
H	3.988784	4.824076	-2.947583
H	4.779413	3.296764	-2.390702
H	3.880189	3.328939	-3.948619
C	1.566225	2.331717	3.794437
H	1.573769	3.337906	4.262975
H	0.619832	2.202245	3.228554
H	1.590655	1.569909	4.602435
C	4.087560	2.224302	3.626921
H	4.941052	2.088184	2.928455
H	4.193822	3.202752	4.140846
H	4.135525	1.418474	4.390505
C	-3.060345	1.901064	-2.094941
C	-2.266659	1.839052	-3.307658
H	-1.586177	2.673661	-3.509571
B	-2.821216	2.920671	-1.013028
O	-1.756228	3.806353	-0.968794
O	-3.694598	3.162204	0.070159
C	-1.806263	4.511509	0.284717
C	-3.323435	4.447830	0.631965
C	-0.957276	3.743175	1.282505
H	0.057640	3.654492	0.881715
H	-0.891135	4.253741	2.253160
H	-1.346010	2.727642	1.447212
C	-1.257014	5.906602	0.083968
H	-1.355600	6.506438	1.000039
H	-0.189314	5.855838	-0.167859
H	-1.765991	6.432908	-0.732541
C	-4.131379	5.512424	-0.091871
H	-3.946900	6.513735	0.321013
H	-3.893629	5.533213	-1.164401
H	-5.204152	5.301074	0.011733
C	-3.635548	4.457476	2.112781
H	-3.191304	3.602390	2.638964

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 H  -3.253935   5.373694   2.585694
 H  -4.722172   4.442488   2.283633
Na  -4.978731   1.667202   1.264137
 H  -2.749957   1.482600  -4.224123
 H  -4.002648   1.337325  -2.096727
 H  -1.054121   0.701116  -3.516117
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Figure_S4_imid-3_modeS1_ts(CuHadd)_02 / electronic energy: -3372.910082259358 a.u. / lowest freq: -788.91 cm-1
 C  -2.602455   2.142530  -0.274179
 H  -3.277499   2.022524  -1.135555
 C  -1.110293   2.170345  -0.682407
 H  -0.565685   3.018857  -0.234733
 C  -1.520795   0.244176   0.627004
 C  -3.843717   0.458529   1.207583
 C  -3.807467   0.383097   2.605865
 C  -5.001397   0.050736   0.527250
 C  -4.905341  -0.077511   3.324807
 H  -2.891990   0.690801   3.116646
 C  -6.107257  -0.391370   1.258733
 C  -6.065712  -0.453253   2.648508
 H  -4.856593  -0.131313   4.414350
 H  -6.992686  -0.718290   0.710626
 H  -6.937889  -0.805656   3.203268
 C   0.805050   0.676310   0.108031
 C   1.286053   0.190121   1.340696
 C   1.733153   0.945534  -0.915573
 C   2.657976  -0.006712   1.545263
 C   3.104503   0.750411  -0.709029
 C   3.565226   0.275910   0.521166
 H   4.628062   0.139705   0.685658
 S  -5.096687  -0.034515  -1.267374
 O  -6.101664  -1.105836  -1.532511
 O  -3.739734  -0.481809  -1.701861
 O  -5.479680   1.304684  -1.745669
Cu  -1.551665  -1.390350   1.629925
 C  -3.015190   3.353540   0.525883
 C  -4.021216   4.210796   0.047365
 C  -2.408784   3.635125   1.765153
 C  -4.412703   5.326140   0.794185
 H  -4.502588   4.018820  -0.903097
 C  -2.804054   4.750907   2.507988
 H  -1.632867   2.988399   2.156155
 C  -3.805323   5.595723   2.023183
 H  -5.188031   5.981935   0.419713
 H  -2.334273   4.960034   3.460361
 H  -4.110533   6.459352   2.599715
 C  -0.948425   2.229935  -2.181508
 C  -0.554688   3.431833  -2.796050
 C  -1.164894   1.093666  -2.982736
 C  -0.373731   3.491949  -4.180936
 H  -0.383232   4.322039  -2.203615
 C  -0.981670   1.157641  -4.366447
 H  -1.448559   0.153131  -2.536428
 C  -0.586195   2.355812  -4.965421
 H  -0.065926   4.419687  -4.645627
 H  -1.140541   0.275708  -4.973493
 H  -0.442621   2.403497  -6.037064
 N  -2.676536   0.923704   0.546825
 N  -0.587392   0.910020  -0.089071
 H   1.410136   1.302950  -1.879648
 H   0.602994  -0.004586   2.157439
 C   4.069738   1.093866  -1.772124
 C   4.617751   0.071931  -2.597734
 C   4.462505   2.449498  -1.959120
 C   5.551098   0.427574  -3.588604
 C   5.391089   2.753789  -2.971188
 C   5.928668   1.752953  -3.772612
 H   5.991078  -0.325124  -4.229463
 H   5.708989   3.774016  -3.141317
 H   6.645448   2.006780  -4.543073
 C   3.155407  -0.459423   2.858347
 C   3.325481   0.481327   3.913016
 C   3.487209  -1.828312   3.061630
 C   3.811407   0.029244   5.153455
 C   3.984532  -2.226540   4.316095
 C   4.138729  -1.307997   5.348545
 H   3.947634   0.716824   5.977788
 H   4.253737  -3.257879   4.502266
 H   4.517995  -1.635137   6.308206
 C   3.316761  -2.879547   1.964615
 H   2.884954  -2.433574   1.046732
 C   2.339825  -3.978504   2.398656
 H   1.377386  -3.521613   2.708078
 H   2.141721  -4.670396   1.553251
 H   2.744917  -4.571336   3.245201
 C   4.669013  -3.474033   1.555992
 H   5.364350  -2.661359   1.256273
 H   5.125558  -4.047415   2.390091
```

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 H   4.537646  -4.156384   0.689073
 C   3.011236   1.968138   3.737374
 H   2.659616   2.187163   2.709169
 C   4.265007   2.828193   3.939060
 H   4.038524   3.890555   3.705318
 H   4.632013   2.770129   4.985266
 H   5.071254   2.488375   3.253968
 C   1.880575   2.407484   4.675275
 H   1.602105   3.462731   4.467100
 H   0.983070   1.773788   4.508753
 H   2.185410   2.327850   5.739961
 C   3.916705   3.583998  -1.090309
 H   3.205192   3.203693  -0.330255
 C   4.221283  -1.396605  -2.448649
 H   3.463386  -1.525796  -1.651916
 C   3.579819  -1.931574  -3.735240
 H   2.727639  -1.283575  -4.032608
 H   4.311942  -1.965937  -4.569036
 H   3.193614  -2.959411  -3.567731
 C   5.422829  -2.253430  -2.034556
 H   6.192852  -2.281239  -2.834038
 H   5.880338  -1.841921  -1.109785
 H   5.093115  -3.293791  -1.826020
 C   3.134584   4.597136  -1.934827
 H   3.801283   5.133282  -2.642490
 H   2.342621   4.075749  -2.513110
 H   2.646269   5.345993  -1.275244
 C   5.039919   4.268715  -0.302057
 H   5.592292   3.516011   0.300604
 H   5.753870   4.783452  -0.978798
 H   4.611286   5.021212   0.394045
 C  -2.502936  -3.206068   1.307433
 C  -1.903250  -3.105315   2.619761
 H  -0.996945  -3.688477   2.809998
 B  -1.700381  -3.574727   0.088025
 O  -0.336560  -3.848081   0.097329
 O  -2.212125  -3.674841  -1.219449
 C   0.119518  -3.754043  -1.265859
 C  -1.149260  -4.180003  -2.066469
 C   0.483319  -2.299545  -1.506147
 H   1.252480  -2.009805  -0.778911
 H   0.877640  -2.120460  -2.514765
 H  -0.388430  -1.647885  -1.351672
 C   1.321073  -4.649666  -1.468313
 H   1.584805  -4.712364  -2.533888
 H   2.193369  -4.247083  -0.936274
 H   1.140626  -5.666183  -1.098150
 C  -1.303719  -5.689023  -2.148659
 H  -0.566243  -6.135533  -2.829641
 H  -1.186299  -6.156091  -1.161054
 H  -2.303487  -5.941616  -2.527169
 C  -1.267392  -3.546942  -3.436060
 H  -1.319035  -2.452121  -3.377860
 H  -0.407067  -3.814901  -4.066288
 H  -2.170542  -3.903816  -3.952521
Na  -4.220291  -2.739823  -1.881390
 H  -2.565094  -3.090074   3.492202
 H  -3.582780  -3.018750   1.237186
 H  -1.160872  -1.678271   3.145601
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Figure_S4_imid-3_modeS1_prod(CuHadd) / electronic energy: -3372.945638609404 a.u. / lowest freq: 10.95 cm-1
 C  -1.577608  -3.104569   0.314876
 H  -2.089302  -2.980738   1.282672
 C  -0.069863  -2.791586   0.389955
 H   0.524497  -3.481619  -0.232322
 C  -1.167777  -1.035443  -0.749425
 C  -3.363526  -1.952697  -1.134399
 C  -3.482274  -1.971761  -2.529759
 C  -4.518928  -1.838321  -0.346954
 C  -4.729806  -1.900480  -3.139781
 H  -2.570026  -2.046465  -3.126295
 C  -5.770179  -1.783365  -0.967795
 C  -5.880411  -1.824214  -2.354383
 H  -4.803081  -1.912009  -4.229118
 H  -6.655933  -1.674050  -0.339511
 H  -6.865938  -1.777669  -2.822498
 C   1.181733  -0.668567  -0.269414
 C   2.413687  -1.299535  -0.521415
 C   1.161434   0.713009  -0.016780
 C   3.603477  -0.562288  -0.513399
 C   2.358193   1.444145   0.011702
 C   3.574616   0.806591  -0.242607
 H   4.499232   1.372253  -0.214639
 S  -4.446928  -1.569433   1.431649
 O  -5.710847  -0.831577   1.728869
 O  -3.266243  -0.669889   1.620109
 O  -4.329152  -2.881433   2.087546
Cu  -2.021613   0.571211  -1.428490
```

C	-1.869400	-4.475209	-0.241542
C	-2.517117	-5.437904	0.552042
C	-1.505052	-4.808830	-1.559862
C	-2.797889	-6.706450	0.035584
H	-2.802354	-5.210319	1.571147
C	-1.788714	-6.077992	-2.071865
H	-1.005590	-4.084326	-2.191088
C	-2.434980	-7.025997	-1.275097
H	-3.296884	-7.442577	0.652475
H	-1.507702	-6.326340	-3.087116
H	-2.653756	-8.008481	-1.672915
C	0.457847	-2.811233	1.802570
C	1.367599	-3.804634	2.203802
C	0.069118	-1.825276	2.729709
C	1.873928	-3.813336	3.506815
H	1.685088	-4.573249	1.510289
C	0.588319	-1.830964	4.027019
H	-0.624091	-1.044897	2.443779
C	1.489878	-2.824370	4.415551
H	2.572056	-4.582965	3.809588
H	0.291530	-1.064648	4.731230
H	1.890740	-2.828224	5.420812
N	-2.055799	-2.036701	-0.587336
N	-0.013097	-1.430578	-0.191871
H	0.224899	1.207281	0.206118
H	2.456507	-2.361337	-0.723954
C	2.356962	2.871588	0.375157
C	2.413783	3.864867	-0.641856
C	2.329438	3.250697	1.746695
C	2.435648	5.220396	-0.264687
C	2.337222	4.619713	2.070967
C	2.391713	5.589950	1.075617
H	2.474450	6.001698	-1.012177
H	2.306158	4.943400	3.102908
H	2.399201	6.638161	1.345444
C	4.895526	-1.225912	-0.764538
C	5.668224	-1.708042	0.328585
C	5.397430	-1.319441	-2.092311
C	6.933425	-2.266514	0.069730
C	6.663700	-1.896376	-2.299406
C	7.420101	-2.362692	-1.229567
H	7.555711	-2.625787	0.878588
H	7.078297	-1.977122	-3.295602
H	8.395873	-2.795951	-1.408371
C	4.615932	-0.790479	-3.295596
H	3.628792	-0.389487	-2.988335
C	4.319519	-1.908769	-4.302523
H	3.794873	-2.746373	-3.794790
H	3.660175	-1.526501	-5.110949
H	5.251657	-2.295023	-4.765585
C	5.357078	0.374103	-3.962970
H	5.556331	1.172868	-3.216601
H	6.321912	0.040330	-4.399669
H	4.733541	0.807416	-4.774068
C	5.179354	-1.611122	1.774752
H	4.143570	-1.216984	1.823045
C	6.046937	-0.636913	2.579254
H	5.628797	-0.508648	3.600684
H	7.090234	-1.007248	2.667035
H	6.058180	0.357425	2.083386
C	5.131337	-2.989810	2.445163
H	4.678232	-2.902679	3.455540
H	4.508286	-3.683575	1.841195
H	6.146563	-3.423448	2.559247
C	2.304080	2.218625	2.876520
H	2.338686	1.184064	2.479315
C	2.421911	3.506437	-2.127910
H	2.389259	2.407988	-2.276398
C	1.179900	4.061815	-2.835548
H	0.262678	3.693984	-2.329101
H	1.172809	5.171982	-2.831028
H	1.155017	3.714086	-3.890387
C	3.709649	3.987981	-2.806341
H	3.772653	5.096478	-2.812181
H	4.594233	3.579119	-2.272500
H	3.743245	3.627756	-3.856883
C	1.006694	2.317257	3.687319
H	0.915004	3.305556	4.184766
H	0.131864	2.165674	3.020438
H	0.984134	1.526448	4.467180
C	3.534823	2.355232	3.781305
H	4.461671	2.299546	3.171052
H	3.524848	3.317019	4.335735
H	3.557440	1.524982	4.519443
C	-3.255239	1.954973	-2.125134
C	-2.841043	2.279738	-3.553339
H	-1.857340	2.773640	-3.592592
B	-3.122011	3.027047	-1.072468

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O  -2.286002   4.135933  -1.144736
O  -3.819667   3.047367   0.165821
C  -2.198262   4.711800   0.170056
C  -3.576405   4.335177   0.782693
C  -1.055204   4.019313   0.889948
H  -0.161326   4.104913   0.266308
H  -0.837333   4.465573   1.869938
H  -1.262768   2.948910   1.030081
C  -1.935216   6.195607   0.047115
H  -1.955943   6.684954   1.031804
H  -0.941103   6.365937  -0.388878
H  -2.672601   6.686660  -0.599743
C  -4.687527   5.275653   0.346747
H  -4.593980   6.262134   0.821640
H  -4.684510   5.417620  -0.742704
H  -5.663421   4.858363   0.630350
C  -3.570678   4.174976   2.289278
H  -2.872489   3.394954   2.623122
H  -3.275856   5.113791   2.779662
H  -4.575112   3.925795   2.663383
Na -4.565031   1.298466   1.418545
H  -3.541577   2.964312  -4.069705
H  -4.228845   1.431147  -2.082194
H  -2.762184   1.388394  -4.199685
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Figure_S4_imid-3_modeS2_ed(CuHadd) / electronic energy: -3372.917139250770 a.u. / lowest freq: 13.57 cm-1
C   2.659037  -1.133880   1.494163
H   3.060245  -2.148254   1.348373
C   1.134120  -1.134541   1.754544
H   0.852398  -0.518466   2.623543
C   1.567799  -0.105588  -0.332828
C   3.955673  -0.226555  -0.518387
C   4.307517   1.079266  -0.877489
C   4.749811  -1.298704  -0.953398
C   5.464689   1.332758  -1.604863
H   3.644285   1.895605  -0.584577
C   5.923863  -1.031937  -1.664372
C   6.293597   0.273559  -1.974731
H   5.718602   2.359658  -1.877858
H   6.522720  -1.875433  -2.013710
H   7.213178   0.460263  -2.533402
C  -0.769006  -0.292658   0.261490
C  -1.659267  -0.008151   1.310196
C  -1.280515  -0.480683  -1.034766
C  -3.036179   0.063719   1.071460
C  -2.660398  -0.417897  -1.271287
C  -3.536142  -0.146149  -0.216127
H  -4.605546  -0.122000  -0.391428
S   4.224463  -3.024415  -0.845807
O   4.777468  -3.633033  -2.084843
O   2.729888  -2.970728  -0.905525
O   4.752549  -3.573216   0.415501
Cu  1.525291   0.645396  -2.168510
C   3.447655  -0.424305   2.565739
C   4.499516  -1.081939   3.226939
C   3.157779   0.910404   2.902619
C   5.248608  -0.413767   4.200585
H   4.743825  -2.109280   2.988160
C   3.909933   1.575525   3.874100
H   2.342440   1.429784   2.417827
C   4.955686   0.914153   4.522312
H   6.058336  -0.925424   4.704534
H   3.680449   2.603213   4.124815
H   5.537722   1.429683   5.275186
C   0.594005  -2.527873   1.981963
C   0.607051  -3.059977   3.283009
C   0.089767  -3.317575   0.928799
C   0.107988  -4.342000   3.530128
H   1.001033  -2.478894   4.107788
C  -0.415925  -4.595457   1.182760
H   0.086118  -2.954013  -0.089346
C  -0.407401  -5.107186   2.481756
H   0.116102  -4.740340   4.536361
H  -0.811199  -5.191668   0.370892
H  -0.798755  -6.097331   2.675879
N   2.755318  -0.407760   0.211947
N   0.612433  -0.492971   0.522259
H  -0.614472  -0.737191  -1.849404
H  -1.294105   0.139857   2.317522
C  -3.201189  -0.730823  -2.608868
C  -3.700347   0.311658  -3.440830
C  -3.259806  -2.084846  -3.047940
C  -4.244022  -0.022743  -4.694547
C  -3.785503  -2.361766  -4.323131
C  -4.274137  -1.342074  -5.132160
H  -4.646523   0.742717  -5.344727
H  -3.834744  -3.377730  -4.692201
H  -4.687754  -1.577536  -6.104428
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C	-3.967581	0.294908	2.189133
C	-4.428965	-0.806380	2.962991
C	-4.416953	1.612754	2.478785
C	-5.334894	-0.564504	4.011830
C	-5.323691	1.801828	3.537731
C	-5.774779	0.724670	4.293330
H	-5.709883	-1.379022	4.617432
H	-5.688620	2.790473	3.783203
H	-6.473224	0.890325	5.103595
C	-3.947172	2.826475	1.676046
H	-3.230368	2.530864	0.882938
C	-3.199753	3.824236	2.568627
H	-2.351241	3.316383	3.075182
H	-2.791417	4.652609	1.952214
H	-3.870094	4.260336	3.338632
C	-5.121635	3.500373	0.956929
H	-5.660214	2.756329	0.332287
H	-5.836013	3.945821	1.680867
H	-4.747027	4.306372	0.290175
C	-3.981240	-2.242709	2.682851
H	-3.264839	-2.285564	1.837398
C	-5.168513	-3.120714	2.270481
H	-4.810155	-4.130327	1.975526
H	-5.894943	-3.234093	3.102497
H	-5.686860	-2.669924	1.397021
C	-3.243967	-2.838773	3.887767
H	-2.868892	-3.853752	3.638445
H	-2.372755	-2.201339	4.151232
H	-3.911227	-2.921984	4.770950
C	-2.797992	-3.250519	-2.169327
H	-2.451496	-2.897833	-1.177813
C	-3.676068	1.779600	-3.012889
H	-3.137431	1.905477	-2.051968
C	-2.927773	2.651949	-4.030117
H	-1.937759	2.206976	-4.259605
H	-3.499456	2.754325	-4.976232
H	-2.764362	3.667604	-3.610225
C	-5.098461	2.303329	-2.785718
H	-5.682454	2.299856	-3.730399
H	-5.621994	1.668647	-2.039471
H	-5.063572	3.342488	-2.394135
C	-1.608662	-3.981373	-2.803147
H	-1.891859	-4.451197	-3.768400
H	-0.775981	-3.267565	-2.979439
H	-1.241536	-4.776455	-2.120159
C	-3.950849	-4.218834	-1.876352
H	-4.804938	-3.666346	-1.428936
H	-4.295112	-4.730747	-2.799320
H	-3.621337	-4.991781	-1.149140
C	0.440483	2.390258	-2.217434
C	1.049403	2.129222	-3.451326
H	1.983628	2.633318	-3.726676
B	0.970403	3.350645	-1.139987
O	2.103715	4.121421	-1.275796
O	0.305469	3.591314	0.040030
C	2.278267	4.878507	-0.051212
C	0.848005	4.814047	0.593111
C	3.329779	4.167719	0.779982
H	4.266766	4.094559	0.210914
H	3.546262	4.701140	1.715334
H	3.008719	3.149974	1.032835
C	2.745315	6.274495	-0.403384
H	2.799580	6.906583	0.494607
H	3.750383	6.236534	-0.844427
H	2.081240	6.760938	-1.127347
C	-0.057220	5.942969	0.125663
H	0.248956	6.912679	0.541153
H	-0.063770	6.025684	-0.970046
H	-1.086896	5.744731	0.450085
C	0.841531	4.718970	2.103142
H	1.357105	3.819752	2.460681
H	1.328237	5.596199	2.553036
H	-0.189958	4.684320	2.476447
Na	2.384574	-2.733726	-3.166685
H	0.491258	1.709277	-4.292819
H	-0.596609	2.053877	-2.089521
H	2.208435	-0.369621	-3.205592

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Figure_S4_imid-3_modeS2_ts(CuHadd)_01 / electronic energy: -3372.896126228521 a.u. / lowest freq: -736.24 cm-1

C	2.439088	-1.676187	1.378705
H	2.657417	-2.705158	1.053479
C	0.943375	-1.457967	1.701738
H	0.799796	-0.779283	2.560465
C	1.466658	-0.340104	-0.308979
C	3.856795	-0.513696	-0.431264
C	4.213988	0.828414	-0.607110
C	4.680625	-1.518725	-0.962378
C	5.402625	1.175608	-1.239295

H	3.532279	1.602717	-0.248156
C	5.888440	-1.160601	-1.569962
C	6.261973	0.174813	-1.692996
H	5.653583	2.231523	-1.368951
H	6.509886	-1.953040	-1.991539
H	7.207924	0.432359	-2.174403
C	-0.871747	-0.442648	0.230868
C	-1.638076	0.196557	1.216589
C	-1.469841	-0.804004	-0.984770
C	-2.992716	0.469822	0.986966
C	-2.829560	-0.552880	-1.203135
C	-3.588281	0.089003	-0.219878
H	-4.642358	0.279091	-0.387588
S	4.145817	-3.234684	-1.124042
O	4.839291	-3.701324	-2.355620
O	2.670501	-3.130265	-1.361512
O	4.505594	-3.951071	0.110174
Cu	1.487606	0.792058	-1.843877
C	3.348839	-1.296500	2.519225
C	4.154140	-2.267824	3.138822
C	3.413433	0.034264	2.972312
C	5.010930	-1.912223	4.185135
H	4.118306	-3.300516	2.816730
C	4.272463	0.385889	4.016689
H	2.799890	0.797469	2.513870
C	5.071455	-0.586597	4.622489
H	5.628578	-2.665265	4.657214
H	4.318417	1.412727	4.355883
H	5.736240	-0.313467	5.431710
C	0.198466	-2.744411	1.955625
C	-0.336345	-3.012526	3.227911
C	0.005222	-3.680750	0.922751
C	-1.043590	-4.195779	3.461833
H	-0.205768	-2.308266	4.040016
C	-0.703552	-4.860954	1.161273
H	0.391713	-3.491397	-0.069228
C	-1.229344	-5.117744	2.429181
H	-1.448801	-4.397815	4.444781
H	-0.845656	-5.576392	0.361978
H	-1.779437	-6.031685	2.611891
N	2.628031	-0.776435	0.220329
N	0.476192	-0.785184	0.477198
H	-0.888900	-1.321230	-1.739302
H	-1.186218	0.482102	2.158241
C	-3.482839	-1.026510	-2.435997
C	-3.587274	-0.165662	-3.563247
C	-4.043605	-2.333864	-2.478345
C	-4.250643	-0.632295	-4.712962
C	-4.695448	-2.753624	-3.652256
C	-4.794689	-1.911606	-4.754707
H	-4.354810	-0.001345	-5.585784
H	-5.139037	-3.738454	-3.716538
H	-5.303017	-2.251665	-5.647887
C	-3.802703	1.141236	2.019361
C	-4.374722	0.381812	3.078025
C	-4.051755	2.539104	1.925532
C	-5.184229	1.039222	4.022668
C	-4.872148	3.148040	2.892613
C	-5.427605	2.405217	3.928693
H	-5.641267	0.491441	4.836179
H	-5.089785	4.206916	2.845743
H	-6.057022	2.891785	4.662792
C	-3.465343	3.396353	0.802704
H	-2.807583	2.797082	0.140749
C	-2.582007	4.518030	1.361136
H	-1.794339	4.087112	2.015237
H	-2.085924	5.059472	0.527617
H	-3.175688	5.250599	1.946774
C	-4.574100	3.960597	-0.092872
H	-5.202756	3.132237	-0.483931
H	-5.220768	4.669652	0.465819
H	-4.128586	4.495504	-0.958816
C	-4.159332	-1.127131	3.207055
H	-3.491038	-1.509349	2.409014
C	-5.481083	-1.887535	3.047755
H	-5.291843	-2.982453	3.044789
H	-6.183375	-1.653381	3.875323
H	-5.958806	-1.617363	2.081556
C	-3.475611	-1.478157	4.534010
H	-3.264022	-2.567121	4.575322
H	-2.511482	-0.932469	4.618654
H	-4.115684	-1.216987	5.402428
C	-3.978939	-3.286755	-1.282476
H	-3.422811	-2.835468	-0.435792
C	-3.015789	1.252241	-3.558729
H	-2.503757	1.474378	-2.600509
C	-1.957390	1.427900	-4.654695
H	-1.154472	0.670199	-4.529309

H -2.399469 1.320404 -5.667193
H -1.498649 2.436913 -4.582204
C -4.131297 2.294867 -3.695964
H -4.629280 2.224218 -4.685917
H -4.890862 2.143486 -2.899461
H -3.711751 3.317578 -3.583987
C -3.227055 -4.575415 -1.636333
H -3.758883 -5.153643 -2.420507
H -2.205297 -4.330099 -1.997587
H -3.131976 -5.217966 -0.735354
C -5.382532 -3.594310 -0.747785
H -5.908259 -2.647550 -0.498782
H -5.983954 -4.155471 -1.493652
H -5.311617 -4.203408 0.178860
C 0.867979 2.711249 -2.270975
C 1.629752 2.123255 -3.352141
H 2.667682 2.459354 -3.476783
B 1.429176 3.582712 -1.171500
O 2.782114 3.850206 -0.951184
O 0.631260 4.277533 -0.267800
C 2.879186 4.612875 0.270971
C 1.462328 5.266477 0.365393
C 3.129009 3.641962 1.414721
H 4.064861 3.091429 1.246808
H 3.222609 4.158753 2.379813
H 2.308555 2.913278 1.494462
C 4.023094 5.596360 0.152402
H 4.061750 6.260538 1.028190
H 4.981871 5.061945 0.099022
H 3.936248 6.217613 -0.747382
C 1.356361 6.543973 -0.454658
H 1.911237 7.374750 0.003435
H 1.737330 6.397470 -1.475314
H 0.301659 6.841574 -0.529353
C 0.977746 5.507914 1.779012
H 0.860938 4.570000 2.335896
H 1.680929 6.150793 2.328567
H 0.005190 6.017805 1.769610
Na 2.636377 -2.677026 -3.609013
H 1.137835 1.988786 -4.321142
H -0.223937 2.683870 -2.374204
H 2.020231 0.564049 -3.351297
139
Figure_S4_imid-3_modeS2_ts(CuHadd)_02 / electronic energy: -3372.897805175084 a.u. / lowest freq: -779.49 cm-1
C 2.401260 -1.918754 1.049481
H 2.908302 -2.878444 0.875470
C 0.860478 -2.046981 1.134384
H 0.449913 -1.568364 2.040020
C 1.417552 -0.683434 -0.712547
C 3.821542 -0.578584 -0.625222
C 3.951490 0.808534 -0.770804
C 4.887781 -1.412452 -1.004523
C 5.125403 1.372842 -1.258070
H 3.113057 1.450863 -0.489870
C 6.072832 -0.832489 -1.466658
C 6.201385 0.549277 -1.586430
H 5.188922 2.458034 -1.370684
H 6.882512 -1.497885 -1.772657
H 7.134599 0.978065 -1.958003
C -0.894764 -0.741190 -0.090927
C -1.110114 0.599827 0.267694
C -1.990570 -1.563970 -0.377258
C -2.415130 1.100340 0.390361
C -3.293777 -1.060215 -0.283477
C -3.504862 0.263998 0.117069
H -4.515687 0.633770 0.238838
S 4.753406 -3.213980 -1.092967
O 5.811050 -3.623800 -2.036694
O 3.372768 -3.427402 -1.637530
O 4.912765 -3.736795 0.278406
Cu 1.379247 0.558769 -2.147556
C 2.993366 -1.245889 2.264223
C 3.928568 -1.918235 3.069507
C 2.620149 0.068051 2.602778
C 4.482875 -1.284500 4.186237
H 4.227285 -2.932321 2.837696
C 3.176604 0.698232 3.718277
H 1.897346 0.600247 2.000023
C 4.108524 0.022611 4.509449
H 5.202998 -1.807648 4.801977
H 2.884374 1.709943 3.968897
H 4.539210 0.510879 5.373985
C 0.397724 -3.481174 1.101635
C -0.119469 -4.081125 2.263598
C 0.490400 -4.243658 -0.076853
C -0.529650 -5.417508 2.246422
H -0.198979 -3.518556 3.185501
C 0.069688 -5.576405 -0.091895

H	0.872651	-3.802142	-0.986603
C	-0.438460	-6.163526	1.069105
H	-0.925422	-5.872730	3.145034
H	0.137626	-6.154193	-1.004476
H	-0.762963	-7.195906	1.056198
N	2.576955	-1.067631	-0.147847
N	0.407024	-1.290674	-0.053966
H	-1.832721	-2.599541	-0.651600
H	-0.267132	1.230125	0.522989
C	-4.447992	-1.936791	-0.557825
C	-5.047350	-1.938846	-1.848315
C	-4.969749	-2.766896	0.473426
C	-6.153268	-2.776683	-2.081593
C	-6.083158	-3.579702	0.192149
C	-6.663756	-3.584389	-1.071360
H	-6.630132	-2.805334	-3.052499
H	-6.508543	-4.218115	0.955249
H	-7.518052	-4.219091	-1.269198
C	-2.647184	2.463242	0.920842
C	-2.399684	2.736231	2.298942
C	-3.163791	3.489845	0.075516
C	-2.635988	4.033857	2.787734
C	-3.422783	4.757823	0.627774
C	-3.150753	5.026416	1.963265
H	-2.440128	4.279327	3.823090
H	-3.836601	5.552192	0.021284
H	-3.343040	6.013330	2.364178
C	-3.470844	3.257137	-1.404517
H	-3.090850	2.268851	-1.734935
C	-2.783199	4.295248	-2.304934
H	-1.710460	4.386004	-2.045689
H	-2.857593	3.980938	-3.367939
H	-3.254173	5.295731	-2.207709
C	-4.984588	3.259456	-1.647363
H	-5.476659	2.493718	-1.012177
H	-5.425023	4.251550	-1.411610
H	-5.200106	3.020732	-2.710635
C	-1.922794	1.659926	3.277934
H	-1.848279	0.669952	2.787328
C	-2.921766	1.465340	4.426200
H	-2.614766	0.601159	5.053531
H	-2.976188	2.364264	5.075193
H	-3.932824	1.252794	4.016976
C	-0.522901	1.983614	3.812198
H	-0.157433	1.153541	4.453888
H	0.185255	2.100816	2.966123
H	-0.525590	2.919077	4.410256
C	-4.363599	-2.799739	1.876762
H	-3.478280	-2.136051	1.948606
C	-4.528429	-1.061853	-2.988057
H	-3.668371	-0.443778	-2.659367
C	-4.014987	-1.917273	-4.152324
H	-3.236191	-2.621835	-3.789444
H	-4.837170	-2.499307	-4.619412
H	-3.559223	-1.267069	-4.929449
C	-5.603608	-0.075455	-3.460141
H	-6.448819	-0.602723	-3.950394
H	-5.995012	0.500825	-2.595302
H	-5.167691	0.642045	-4.187883
C	-3.866161	-4.206254	2.230355
H	-4.709955	-4.919643	2.337957
H	-3.184256	-4.575334	1.435091
H	-3.304178	-4.180872	3.188436
C	-5.362017	-2.286862	2.920889
H	-5.701215	-1.264180	2.649069
H	-6.247613	-2.952751	2.993620
H	-4.876048	-2.236194	3.918774
C	0.593388	2.428110	-2.470053
C	1.372622	1.963968	-3.598824
H	2.366606	2.407043	-3.743157
B	1.107667	3.338119	-1.375070
O	2.435166	3.741206	-1.224600
O	0.294242	3.942059	-0.423450
C	2.511300	4.544975	-0.025752
C	1.038378	5.042120	0.126010
C	2.919413	3.640555	1.126045
H	3.885417	3.162785	0.913656
H	3.026089	4.198707	2.066465
H	2.171066	2.851380	1.283380
C	3.532131	5.642649	-0.230871
H	3.540230	6.335298	0.623428
H	4.540793	5.215710	-0.321071
H	3.330854	6.221001	-1.140866
C	0.742630	6.262463	-0.734570
H	1.217594	7.172266	-0.341104
H	1.083264	6.115288	-1.769372
H	-0.342805	6.429771	-0.760758
C	0.600295	5.291900	1.552208

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 H   0.604652   4.374013   2.150216
 H   1.256926   6.026257   2.040822
 H  -0.418208   5.699440   1.569017
Na   2.333343  -2.430849  -3.328527
 H   0.860331   1.813181  -4.555303
 H  -0.492291   2.292025  -2.547587
 H   1.911444   0.464626  -3.659957
139
Figure_S4_imid-3_modeS2_prod(CuHadd) / electronic energy: -3372.943100938274 a.u. / lowest freq: 11.70 cm-1
 C   2.702533  -1.593922   1.219470
 H   3.218536  -2.428134   0.724161
 C   1.173444  -1.804520   1.324039
 H   0.818821  -1.730454   2.364249
 C   1.601913   0.107008  -0.005591
 C   4.002965   0.283001   0.043627
 C   4.099631   1.635888   0.401846
 C   5.083910  -0.327445  -0.615426
 C   5.251978   2.367295   0.135446
 H   3.250161   2.108603   0.902254
 C   6.242027   0.414567  -0.867123
 C   6.334327   1.750975  -0.489949
 H   5.299880   3.418925   0.426160
 H   7.063697  -0.074590  -1.392604
 H   7.247650   2.312634  -0.697147
 C  -0.735057  -0.480710   0.260942
 C  -1.705767  -0.825711   1.218270
 C  -1.155208  -0.051334  -1.011593
 C  -3.068591  -0.764292   0.901902
 C  -2.518562  -0.009900  -1.332394
 C  -3.472175  -0.360720  -0.372916
 H  -4.526049  -0.346796  -0.626353
 S   5.031009  -2.010511  -1.248782
 O   6.068407  -2.043593  -2.324107
 O   3.671449  -2.167620  -1.848614
 O   5.309925  -2.910673  -0.116872
Cu   1.513033   1.754408  -1.009423
 C   3.343999  -1.333866   2.562037
 C   4.320245  -2.210832   3.066528
 C   2.977207  -0.208757   3.325134
 C   4.923682  -1.960667   4.302797
 H   4.612908  -3.090403   2.508161
 C   3.584008   0.037791   4.559384
 H   2.222679   0.476896   2.962491
 C   4.557635  -0.836690   5.047465
 H   5.675382  -2.639590   4.684178
 H   3.298633   0.907110   5.137584
 H   5.026650  -0.644900   6.003825
 C   0.732408  -3.131217   0.753493
 C   0.302320  -4.157705   1.612361
 C   0.741280  -3.361700  -0.635299
 C  -0.104804  -5.389765   1.092707
 H   0.286505  -4.007898   2.684689
 C   0.323361  -4.591944  -1.150142
 H   1.057892  -2.586098  -1.319850
 C  -0.099385  -5.605094  -0.287178
 H  -0.432741  -6.175788   1.760557
 H   0.329255  -4.761482  -2.218515
 H  -0.422438  -6.557263  -0.687495
 N   2.795970  -0.394638   0.355616
 N   0.646353  -0.662326   0.540476
 H  -0.425218   0.183418  -1.776517
 H  -1.409519  -1.157028   2.204774
 C  -2.954631   0.306242  -2.706375
 C  -3.518590   1.579442  -3.000046
 C  -2.880339  -0.692935  -3.718677
 C  -4.017825   1.818181  -4.293681
 C  -3.362081  -0.391198  -5.005618
 C  -3.929971   0.846783  -5.284446
 H  -4.478333   2.764596  -4.543754
 H  -3.316786  -1.125265  -5.799290
 H  -4.310636   1.053437  -6.276523
 C  -4.083361  -1.172449   1.891876
 C  -4.576753  -2.507279   1.890852
 C  -4.602068  -0.219744   2.812403
 C  -5.586018  -2.857633   2.806566
 C  -5.595421  -0.625469   3.722017
 C  -6.081838  -1.928137   3.714391
 H  -5.997335  -3.858218   2.820786
 H  -6.008158   0.073137   4.437917
 H  -6.854288  -2.218618   4.414931
 C  -4.124651   1.231520   2.833778
 H  -3.358697   1.406568   2.054515
 C  -3.460125   1.575522   4.172041
 H  -2.624083   0.871210   4.371024
 H  -3.044249   2.604736   4.138106
 H  -4.186602   1.519124   5.009702
 C  -5.271152   2.199618   2.517971
 H  -5.740400   1.927181   1.548391
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H  -6.046672   2.180490   3.312178
H  -4.880689   3.236343   2.433393
C  -4.060128  -3.564664   0.913698
H  -3.220428  -3.172554   0.303990
C  -5.155888  -3.973534  -0.076705
H  -4.743784  -4.677285  -0.831370
H  -6.003068  -4.468221   0.443757
H  -5.535958  -3.076789  -0.611575
C  -3.501918  -4.786948   1.653209
H  -3.038251  -5.488176   0.927281
H  -2.723220  -4.468157   2.378584
H  -4.299550  -5.333315   2.198210
C  -2.319776  -2.091264  -3.448246
H  -2.004103  -2.204714  -2.392133
C  -3.609443   2.688760  -1.952154
H  -3.073609   2.402563  -1.023891
C  -2.938883   3.980032  -2.439234
H  -1.899290   3.769406  -2.767515
H  -3.496241   4.437313  -3.282922
H  -2.902649   4.719931  -1.613228
C  -5.067093   2.945171  -1.555208
H  -5.655517   3.323694  -2.417804
H  -5.531963   2.005334  -1.188489
H  -5.112326   3.695120  -0.736527
C  -1.070054  -2.356288  -4.295884
H  -1.309241  -2.354785  -5.380010
H  -0.304344  -1.576914  -4.093901
H  -0.635240  -3.344115  -4.035597
C  -3.384456  -3.171056  -3.677476
H  -4.286560  -2.948465  -3.068241
H  -3.677110  -3.230769  -4.746736
H  -2.992673  -4.162748  -3.364636
C   1.531944   3.501583  -1.950171
C   2.922457   3.920381  -2.385175
H   3.596286   4.040211  -1.521683
B   0.936142   4.038147  -0.665832
O   1.668462   4.513643   0.437379
O  -0.431387   4.028587  -0.362389
C   0.786366   4.499743   1.572417
C  -0.617542   4.671530   0.902452
C   0.933445   3.144628   2.252853
H   1.978317   3.003522   2.565236
H   0.303261   3.052227   3.148900
H   0.672512   2.329746   1.557782
C   1.176884   5.610554   2.523916
H   0.465944   5.684730   3.360230
H   2.171432   5.415447   2.948924
H   1.215947   6.583480   2.018491
C  -0.955824   6.132847   0.644809
H  -1.172128   6.677131   1.575133
H  -0.132428   6.647154   0.129463
H  -1.844608   6.199317   0.003861
C  -1.751456   3.983255   1.632060
H  -1.573135   2.903884   1.702393
H  -1.879246   4.382625   2.648867
H  -2.696849   4.130031   1.091850
Na  4.500036  -2.206091  -4.097946
H   2.940439   4.891668  -2.917213
H   0.807585   3.450826  -2.779996
H   3.420954   3.200812  -3.059211
139
Figure_S4_imid-3_modeR1_ed(CuHadd) / electronic energy: -3372.918154055547 a.u. / lowest freq: 13.02 cm-1
C  -2.842116  -1.600754   1.226396
H  -3.412973  -0.862402   1.812809
C  -1.338878  -1.588601   1.552203
H  -0.880990  -2.588237   1.451714
C  -1.675630  -0.554906  -0.540209
C  -4.047714  -0.989363  -0.931013
C  -4.495452  -2.080989  -1.676886
C  -4.796390   0.198405  -0.945848
C  -5.673509  -2.008536  -2.414181
H  -3.889214  -2.987443  -1.706471
C  -5.973072   0.270456  -1.690700
C  -6.417680  -0.831076  -2.418525
H  -6.000657  -2.871623  -2.997504
H  -6.532251   1.207714  -1.690791
H  -7.342269  -0.764617  -2.995862
C   0.580627  -0.728240   0.206720
C   1.118377  -1.744423  -0.594312
C   1.432633   0.226500   0.777810
C   2.497205  -1.816227  -0.813145
C   2.815609   0.182846   0.527689
C   3.345602  -0.858631  -0.247105
H   4.414147  -0.921218  -0.413792
S  -4.243013   1.662788  -0.068867
O  -5.175592   2.751336  -0.473421
O  -2.874082   1.949300  -0.621577
O  -4.247240   1.325053   1.363904
```

Cu	-1.504687	0.530577	-2.226251
C	-3.472731	-2.964645	1.364372
C	-4.566933	-3.149211	2.227898
C	-2.983808	-4.067143	0.637117
C	-5.159872	-4.408594	2.358921
H	-4.963305	-2.319667	2.800078
C	-3.580354	-5.323831	0.771316
H	-2.149073	-3.951251	-0.043116
C	-4.667323	-5.494675	1.631521
H	-6.002463	-4.542352	3.024943
H	-3.201066	-6.165102	0.205808
H	-5.128626	-6.468399	1.733739
C	-1.051013	-1.057467	2.932176
C	-0.473374	-1.892225	3.905318
C	-1.400503	0.258070	3.282936
C	-0.274361	-1.425313	5.207923
H	-0.194502	-2.910346	3.663582
C	-1.194149	0.723630	4.583914
H	-1.849395	0.914834	2.552732
C	-0.639768	-0.120360	5.548550
H	0.163322	-2.075688	5.954064
H	-1.469885	1.737039	4.845199
H	-0.482703	0.239911	6.556877
N	-2.842568	-1.114372	-0.175057
N	-0.805799	-0.711487	0.483012
H	1.022718	0.993482	1.420785
H	0.464549	-2.495295	-1.022674
C	3.717598	1.218338	1.086811
C	4.345703	2.167354	0.223241
C	3.995721	1.244272	2.484717
C	5.213060	3.124855	0.780323
C	4.855673	2.237354	2.989954
C	5.452049	3.165462	2.147158
H	5.715395	3.849046	0.152973
H	5.087113	2.285604	4.045717
H	6.119569	3.913466	2.555532
C	3.052274	-2.921018	-1.616086
C	3.336492	-4.170462	-0.997491
C	3.251430	-2.753525	-3.014716
C	3.806932	-5.230200	-1.794231
C	3.720545	-3.845248	-3.768148
C	3.995273	-5.066592	-3.162372
H	4.025365	-6.195725	-1.357351
H	3.871512	-3.756206	-4.835877
H	4.354395	-5.895085	-3.759399
C	2.954123	-1.433336	-3.726208
H	2.644565	-0.650535	-3.004999
C	1.790008	-1.591204	-4.710612
H	0.888521	-1.957492	-4.174057
H	1.544940	-0.610226	-5.170505
H	2.042557	-2.306689	-5.521400
C	4.201816	-0.886109	-4.430583
H	5.047761	-0.827772	-3.713223
H	4.500172	-1.529080	-5.284947
H	4.000844	0.135988	-4.817028
C	3.134947	-4.400127	0.501238
H	2.794087	-3.474364	1.007695
C	4.450300	-4.789534	1.187233
H	4.303283	-4.842693	2.287269
H	4.814265	-5.777504	0.835184
H	5.227416	-4.023145	0.978908
C	2.045830	-5.449090	0.754627
H	1.850216	-5.538970	1.844607
H	1.100526	-5.140610	0.258311
H	2.347785	-6.445010	0.367363
C	3.436813	0.201892	3.453079
H	2.789874	-0.531174	2.932088
C	4.134325	2.171840	-1.292011
H	3.347636	1.450270	-1.584441
C	3.654778	3.538806	-1.798942
H	2.805407	3.895531	-1.186887
H	4.464199	4.297283	-1.756922
H	3.312388	3.453485	-2.852533
C	5.416467	1.749711	-2.018908
H	6.241951	2.466656	-1.823945
H	5.733893	0.741080	-1.680590
H	5.237845	1.710179	-3.114215
C	2.564999	0.860567	4.527909
H	3.147339	1.576200	5.144491
H	1.719742	1.401059	4.050642
H	2.153111	0.084733	5.204949
C	4.564906	-0.621415	4.087821
H	5.192870	-1.079237	3.293527
H	5.208230	0.007011	4.738936
H	4.136757	-1.440712	4.704341
C	0.111068	1.827332	-2.215977
C	-0.537009	1.763391	-3.464750
H	-0.135729	1.159918	-4.284973

B -0.104649 2.953198 -1.200760
O 0.623258 3.082282 -0.046470
O -0.988409 4.019951 -1.369662
C 0.072610 4.161274 0.732287
C -0.679161 5.009836 -0.350722
C -0.864180 3.542055 1.755209
H -0.288253 2.862318 2.396540
H -1.321822 4.299851 2.406034
H -1.660479 2.962725 1.267344
C 1.207854 4.883188 1.427666
H 0.834606 5.741020 2.005376
H 1.703819 4.198387 2.128956
H 1.967699 5.245499 0.725294
C 0.198435 6.061837 -1.006954
H 0.448052 6.873754 -0.310504
H 1.135919 5.630966 -1.381264
H -0.330206 6.503717 -1.862382
C -1.973352 5.628188 0.134467
H -2.684587 4.869151 0.486221
H -1.789112 6.321326 0.967318
H -2.446492 6.213597 -0.667916
Na -3.301253 3.694794 -2.015835
H -1.181509 2.584155 -3.802489
H 0.974727 1.168627 -2.063994
H -2.529753 -0.018440 -3.317941
139
Figure_S4_imid-3_modeR1_ts(CuHadd)_01 / electronic energy: -3372.900960619068 a.u. / lowest freq: -843.80 cm-1
C -2.393461 -2.396715 0.918817
H -2.969236 -1.825301 1.664766
C -0.871097 -2.249494 1.101119
H -0.323551 -3.166166 0.820906
C -1.557638 -0.930440 -0.738412
C -3.850880 -1.705405 -1.074997
C -4.082541 -2.677989 -2.051423
C -4.855546 -0.760754 -0.808827
C -5.294879 -2.734289 -2.733749
H -3.286588 -3.385614 -2.289470
C -6.069323 -0.818931 -1.493349
C -6.295278 -1.808761 -2.447719
H -5.451945 -3.501139 -3.494973
H -6.829877 -0.068735 -1.269264
H -7.250857 -1.847601 -2.975061
C 0.763171 -0.776687 -0.122004
C 1.692604 -1.703594 -0.611084
C 1.190308 0.509287 0.230958
C 3.041900 -1.353163 -0.729778
C 2.541378 0.870367 0.100534
C 3.465157 -0.068816 -0.373594
H 4.515477 0.189386 -0.439605
S -4.566551 0.596946 0.323799
O -5.751006 1.492995 0.195544
O -3.357647 1.286586 -0.242794
O -4.358364 0.018404 1.660621
Cu -1.792506 0.554861 -1.965650
C -2.861263 -3.830818 0.902085
C -3.829883 -4.264921 1.824473
C -2.346204 -4.751491 -0.030308
C -4.273814 -5.590618 1.812763
H -4.243430 -3.578939 2.553230
C -2.793964 -6.075445 -0.038619
H -1.603985 -4.442614 -0.755683
C -3.756704 -6.494917 0.882191
H -5.019852 -5.916868 2.525823
H -2.395033 -6.776233 -0.760497
H -4.102347 -7.520521 0.874459
C -0.476672 -1.848419 2.498947
C 0.352121 -2.684481 3.267465
C -0.902996 -0.621619 3.041707
C 0.735650 -2.306151 4.557116
H 0.700972 -3.629523 2.870992
C -0.521853 -0.250558 4.333367
H -1.526151 0.047782 2.462393
C 0.294064 -1.093703 5.091886
H 1.374651 -2.954378 5.142670
H -0.853010 0.694682 4.743597
H 0.591429 -0.803126 6.091101
N -2.601316 -1.714024 -0.384939
N -0.566292 -1.179336 0.135312
H 0.482471 1.199691 0.659292
H 1.373078 -2.706719 -0.866687
C 3.017043 2.208139 0.520415
C 3.355418 3.185916 -0.461986
C 3.269557 2.470826 1.899074
C 3.914482 4.406531 -0.042891
C 3.845021 3.703749 2.260321
C 4.146586 4.662554 1.301834
H 4.198653 5.162221 -0.762780
H 4.088954 3.923977 3.290131

H 4.590647 5.603073 1.601909
C 4.028000 -2.362027 -1.155091
C 4.605895 -3.233497 -0.189905
C 4.385316 -2.474930 -2.527010
C 5.519084 -4.212494 -0.621949
C 5.303605 -3.470328 -2.908258
C 5.860687 -4.327845 -1.965344
H 5.973215 -4.894883 0.084421
H 5.592402 -3.588344 -3.944376
H 6.564928 -5.087969 -2.278485
C 3.798989 -1.554760 -3.597948
H 3.111387 -0.807523 -3.151840
C 2.965422 -2.349500 -4.610003
H 2.172443 -2.920850 -4.081343
H 2.474118 -1.656209 -5.325804
H 3.597387 -3.058764 -5.184946
C 4.899130 -0.749136 -4.300082
H 5.511306 -0.207286 -3.548176
H 5.564413 -1.407664 -4.897066
H 4.443991 0.000439 -4.982291
C 4.267661 -3.137225 1.299497
H 3.556665 -2.309950 1.499414
C 5.516221 -2.824021 2.133025
H 5.230224 -2.641295 3.191084
H 6.242053 -3.663682 2.105704
H 6.010560 -1.907626 1.745312
C 3.579060 -4.414842 1.792997
H 3.270567 -4.294876 2.853637
H 2.668199 -4.611137 1.187420
H 4.256098 -5.291869 1.721138
C 3.040947 1.416463 2.984407
H 2.424397 0.578865 2.601664
C 3.193843 2.929875 -1.960689
H 2.617215 2.000144 -2.138440
C 2.416617 4.057598 -2.657968
H 1.499701 4.309075 -2.088844
H 3.031664 4.976593 -2.755506
H 2.116673 3.734296 -3.677670
C 4.561877 2.732089 -2.623445
H 5.175288 3.655683 -2.555383
H 5.111014 1.904355 -2.128055
H 4.431733 2.469511 -3.695077
C 2.274846 1.978449 4.191384
H 2.880302 2.715162 4.757945
H 1.334858 2.463719 3.859536
H 2.016374 1.156107 4.889353
C 4.376604 0.808396 3.423713
H 4.901957 0.375057 2.545765
H 5.029276 1.577570 3.889041
H 4.202665 -0.006444 4.158844
C -0.771041 2.347718 -2.224579
C -1.707498 2.074929 -3.294490
H -1.310416 1.870251 -4.295074
B -1.039030 3.238934 -1.043755
O -0.114813 3.532068 -0.049997
O -2.232395 3.965819 -0.815911
C -0.798632 4.209508 1.010483
C -1.959115 4.915184 0.242941
C -1.314066 3.162173 1.988586
H -0.472837 2.559790 2.351697
H -1.796967 3.618943 2.864279
H -2.028920 2.479120 1.507372
C 0.172398 5.147234 1.696065
H -0.336930 5.775525 2.441240
H 0.942433 4.567697 2.222446
H 0.684116 5.801259 0.979457
C -1.517127 6.214043 -0.411575
H -1.337666 7.005702 0.329255
H -0.594618 6.068712 -0.990909
H -2.295837 6.568896 -1.100647
C -3.217030 5.124572 1.059372
H -3.625966 4.177880 1.438822
H -3.020693 5.769723 1.927640
H -3.992754 5.624834 0.459892
Na -4.406813 3.196905 -1.084985
H -2.596601 2.716117 -3.362088
H 0.251610 1.984509 -2.370656
H -2.569818 0.676423 -3.365360
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Figure_S4_imid-3_modeR1_ts(CuHadd)_02 / electronic energy: -3372.900953941339 a.u. / lowest freq: -824.32 cm-1
C -2.352671 -2.451423 0.904926
H -2.934195 -1.902815 1.663326
C -0.831638 -2.282134 1.083950
H -0.270637 -3.190354 0.803103
C -1.544676 -0.956079 -0.742577
C -3.840508 -1.747041 -1.055506
C -4.085839 -2.720394 -2.027995
C -4.849136 -0.813517 -0.763903

C	-5.314691	-2.790473	-2.678881
H	-3.288388	-3.418689	-2.287553
C	-6.079741	-0.886123	-1.416189
C	-6.319296	-1.879080	-2.364048
H	-5.481774	-3.558134	-3.437151
H	-6.842900	-0.144845	-1.171985
H	-7.288652	-1.930639	-2.864468
C	0.778212	-0.776948	-0.133487
C	1.176963	0.518739	0.218589
C	1.729735	-1.686032	-0.613619
C	2.521417	0.906658	0.096078
C	3.072173	-1.308022	-0.725832
C	3.466818	-0.014417	-0.370628
H	4.512052	0.265027	-0.430964
S	-4.534811	0.561617	0.340538
O	-5.742151	1.432175	0.267550
O	-3.375308	1.268532	-0.302909
O	-4.238441	0.006697	1.670259
Cu	-1.799935	0.526767	-1.967703
C	-2.795444	-3.893217	0.865987
C	-3.754468	-4.359094	1.782865
C	-2.265969	-4.789605	-0.081905
C	-4.174861	-5.692118	1.750634
H	-4.178784	-3.692244	2.523101
C	-2.690183	-6.120998	-0.110672
H	-1.531149	-4.455804	-0.803807
C	-3.643552	-6.572138	0.804892
H	-4.913668	-6.042912	2.459553
H	-2.280367	-6.802938	-0.844409
H	-3.970988	-7.603460	0.781291
C	-0.441880	-1.876137	2.481646
C	0.395169	-2.702598	3.251489
C	-0.883308	-0.654476	3.023450
C	0.771844	-2.319937	4.541888
H	0.755167	-3.643730	2.855730
C	-0.509842	-0.279479	4.316146
H	-1.512699	0.007279	2.442052
C	0.314626	-1.113022	5.076109
H	1.417244	-2.960728	5.128606
H	-0.853347	0.661511	4.725968
H	0.606333	-0.819275	6.076062
N	-2.579557	-1.750830	-0.386240
N	-0.543640	-1.207257	0.118892
H	1.432677	-2.696427	-0.867673
H	0.453122	1.195907	0.641625
C	4.081571	-2.297072	-1.143026
C	4.671541	-3.154483	-0.172566
C	4.450239	-2.404568	-2.512393
C	5.607216	-4.115367	-0.597113
C	5.391382	-3.381339	-2.885999
C	5.959738	-4.225838	-1.938090
H	6.070819	-4.787070	0.113331
H	5.689511	-3.494778	-3.919984
H	6.681527	-4.971753	-2.245388
C	2.968470	2.253634	0.518126
C	3.291972	3.237898	-0.462726
C	3.211575	2.520486	1.897708
C	3.826914	4.468515	-0.041414
C	3.763178	3.763650	2.261199
C	4.049984	4.728254	1.304073
H	4.099302	5.229661	-0.760109
H	4.000014	3.987962	3.291761
H	4.475634	5.676696	1.605893
C	2.998860	1.461764	2.981985
H	2.398561	0.613382	2.597019
C	2.219340	2.009373	4.187013
H	1.270075	2.474665	3.852927
H	1.976874	1.182854	4.885724
H	2.808392	2.758965	4.753901
C	4.344025	0.877878	3.424993
H	4.880146	0.455377	2.548304
H	4.980882	1.658411	3.893311
H	4.182716	0.059104	4.158632
C	3.139542	2.979782	-1.961944
H	2.580385	2.039786	-2.141743
C	4.512891	2.807262	-2.620704
H	4.390732	2.542698	-3.692786
H	5.109134	3.741878	-2.550519
H	5.075539	1.989545	-2.123845
C	2.344004	4.093790	-2.660605
H	2.051624	3.765359	-3.680849
H	1.421971	4.329339	-2.092765
H	2.943121	5.023366	-2.757081
C	3.852604	-1.497911	-3.588599
H	3.146406	-0.764695	-3.148321
C	4.322911	-3.061890	1.314668
H	3.595120	-2.247931	1.508865
C	3.656178	-4.351610	1.806609

H 2.752275 -4.565902 1.196726
H 4.350070 -5.215739 1.739369
H 3.340191 -4.236073 2.865527
C 5.560383 -2.723306 2.154832
H 6.301863 -3.549372 2.134249
H 6.040008 -1.798937 1.767591
H 5.264619 -2.543181 3.210649
C 3.043067 -2.310794 -4.605734
H 3.693792 -3.007171 -5.175474
H 2.258461 -2.898140 -4.082144
H 2.542510 -1.628540 -5.325718
C 4.940839 -0.670330 -4.283736
H 5.536311 -0.115255 -3.528081
H 5.623867 -1.315512 -4.875231
H 4.475198 0.069050 -4.969971
C -0.814931 2.340463 -2.233844
C -1.742192 2.042753 -3.304739
H -1.337750 1.845696 -4.303912
B -1.103312 3.223256 -1.051152
O -0.188117 3.521552 -0.050374
O -2.305826 3.935605 -0.826331
C -0.886323 4.180022 1.012166
C -2.053586 4.875587 0.245721
C -1.390494 3.117882 1.980362
H -0.541769 2.525524 2.342827
H -1.883919 3.561706 2.856922
H -2.093086 2.427073 1.492218
C 0.068117 5.126660 1.709179
H -0.452927 5.741880 2.457226
H 0.844462 4.554371 2.234142
H 0.573133 5.793454 0.999573
C -1.629345 6.189518 -0.390341
H -1.467575 6.975286 0.360774
H -0.701157 6.066330 -0.965655
H -2.409762 6.539479 -1.079996
C -3.319062 5.055208 1.058046
H -3.719985 4.096660 1.416526
H -3.134528 5.685267 1.939880
H -4.095751 5.560190 0.463548
Na -4.474915 3.142711 -1.114197
H -2.646645 2.661775 -3.376334
H 0.215679 1.999011 -2.376399
H -2.567431 0.622846 -3.374029

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Figure_S4_imid-3_modeR1_ts(CuHadd)_03 / electronic energy: -3372.900750020183 a.u. / lowest freq: -693.02 cm-1

C -2.817490 2.191578 -0.529698
H -3.475611 2.007654 -1.393014
C -1.319261 2.159884 -0.903386
H -0.776529 3.052216 -0.550494
C -1.801091 0.333990 0.531738
C -4.197919 0.599000 0.896356
C -4.670156 1.159650 2.085475
C -4.968155 -0.382920 0.254432
C -5.890384 0.761208 2.626447
H -4.056909 1.896667 2.607008
C -6.187626 -0.780581 0.798778
C -6.652784 -0.209335 1.981321
H -6.238265 1.206150 3.561025
H -6.761229 -1.550905 0.280705
H -7.609814 -0.527895 2.400045
C 0.563557 0.727182 0.102749
C 1.556114 1.252306 -0.748196
C 0.980846 0.046276 1.266473
C 2.913830 1.137181 -0.430846
C 2.343378 -0.071136 1.586733
C 3.305237 0.485088 0.738843
H 4.354463 0.440963 1.004562
S -4.414811 -1.162455 -1.262474
O -5.354709 -2.293604 -1.503209
O -3.048394 -1.703111 -0.951355
O -4.432944 -0.104469 -2.286930
Cu -1.871381 -1.455440 1.344108
C -3.224236 3.470025 0.162131
C -4.257035 4.263234 -0.367293
C -2.581464 3.883973 1.344680
C -4.639032 5.445481 0.274071
H -4.768171 3.968204 -1.275194
C -2.967246 5.066354 1.981993
H -1.787324 3.286564 1.775621
C -3.995039 5.846660 1.447210
H -5.435356 6.051084 -0.138916
H -2.469986 5.376838 2.891783
H -4.292851 6.762003 1.942021
C -1.121524 2.034137 -2.396054
C -0.621389 3.122029 -3.135148
C -1.411837 0.833668 -3.065875
C -0.397248 2.999902 -4.509770
H -0.396851 4.062023 -2.646972

C	-1.184830	0.713836	-4.439228
H	-1.804294	-0.010800	-2.523822
C	-0.675366	1.795594	-5.160769
H	-0.005218	3.838872	-5.069957
H	-1.402430	-0.219085	-4.943077
H	-0.498497	1.701579	-6.224344
N	-2.941162	1.026080	0.369829
N	-0.824293	0.965310	-0.154266
H	0.251812	-0.328514	1.970536
H	1.296492	1.785475	-1.646615
C	2.762950	-0.671946	2.873679
C	2.517565	0.025661	4.093497
C	3.457697	-1.918071	2.896127
C	2.921575	-0.562239	5.305914
C	3.883720	-2.435369	4.133487
C	3.601558	-1.773499	5.322000
H	2.732196	-0.068940	6.250153
H	4.435264	-3.364486	4.185339
H	3.924045	-2.197526	6.264376
C	3.924477	1.793447	-1.283590
C	4.618615	1.045698	-2.275183
C	4.173908	3.187160	-1.135457
C	5.537634	1.711077	-3.107296
C	5.099855	3.806131	-1.994829
C	5.772321	3.074345	-2.967143
H	6.074523	1.174704	-3.878555
H	5.304681	4.865688	-1.916322
H	6.480623	3.568756	-3.619583
C	3.463864	4.033339	-0.077111
H	2.798487	3.411977	0.555659
C	2.566039	5.089598	-0.731564
H	1.840661	4.597772	-1.414399
H	1.991826	5.636470	0.046577
H	3.164509	5.824319	-1.310354
C	4.466911	4.678110	0.887710
H	5.116451	3.896417	1.336866
H	5.105307	5.424637	0.370449
H	3.925171	5.191804	1.710636
C	4.379370	-0.448810	-2.482986
H	3.667461	-0.844816	-1.732973
C	5.671355	-1.253719	-2.295233
H	5.448645	-2.341723	-2.325505
H	6.410150	-1.026586	-3.092005
H	6.123289	-1.020334	-1.307650
C	3.754873	-0.714891	-3.858463
H	3.521370	-1.794256	-3.972272
H	2.807179	-0.143327	-3.960419
H	4.443468	-0.418560	-4.677453
C	3.772525	-2.706354	1.623470
H	3.262249	-2.259499	0.747072
C	1.865652	1.410229	4.131787
H	1.663013	1.790761	3.111823
C	0.513410	1.361925	4.852814
H	-0.147271	0.609659	4.371228
H	0.638039	1.097104	5.923937
H	0.013050	2.351962	4.789817
C	2.796583	2.449472	4.770638
H	2.964739	2.238131	5.847356
H	3.776094	2.454191	4.245850
H	2.351761	3.463669	4.680083
C	3.272556	-4.156687	1.711790
H	3.877173	-4.754195	2.425475
H	2.213116	-4.181333	2.039450
H	3.342228	-4.642075	0.715108
C	5.275386	-2.674637	1.323384
H	5.628949	-1.625516	1.243638
H	5.852942	-3.184365	2.123606
H	5.481035	-3.183714	0.357487
C	-0.612821	-3.088402	1.670409
C	-1.909814	-3.233471	2.289787
H	-1.960402	-3.289473	3.381868
B	-0.258662	-3.457954	0.260026
O	1.003504	-3.294669	-0.292514
O	-1.125583	-4.055943	-0.685809
C	0.889751	-3.456202	-1.709977
C	-0.324448	-4.429939	-1.834757
C	0.574212	-2.087395	-2.291370
H	1.359496	-1.379289	-2.000001
H	0.513922	-2.093468	-3.388355
H	-0.377802	-1.718477	-1.885819
C	2.196937	-3.996141	-2.245833
H	2.153325	-4.151524	-3.333456
H	3.002978	-3.281234	-2.037296
H	2.472842	-4.944145	-1.768850
C	0.074690	-5.885588	-1.659184
H	0.639957	-6.260446	-2.523992
H	0.690804	-6.022659	-0.759666
H	-0.823290	-6.509651	-1.551798

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C  -1.146323  -4.243310  -3.093972
H  -1.590199  -3.240465  -3.145881
H  -0.525523  -4.385803  -3.990345
H  -1.957668  -4.985092  -3.153640
Na  -3.422707  -3.961952  -0.885826
H  -2.618955  -3.940280   1.838162
H   0.195663  -2.719604   2.312972
H  -3.024280  -1.954015   2.350442
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Figure_S4_imid-3_modeR1_prod(CuHadd) / electronic energy: -3372.945446709363 a.u. / lowest freq: 6.10 cm-1
C   1.666549   2.991780   0.719367
H   2.307062   2.833228   1.600024
C   0.205816   2.529047   0.938592
H  -0.518421   3.338143   0.754282
C   1.197461   1.170769  -0.733560
C   3.384734   2.180504  -0.996420
C   3.413787   2.710479  -2.290453
C   4.591021   1.816344  -0.379433
C   4.622496   2.917892  -2.949189
H   2.467239   2.965085  -2.772672
C   5.801555   2.045580  -1.035626
C   5.821637   2.608635  -2.309593
H   4.625418   3.332352  -3.959375
H   6.725762   1.749954  -0.535499
H   6.775724   2.785865  -2.810647
C  -1.141651   0.748539  -0.254593
C  -2.353509   1.435956  -0.418661
C  -1.150056  -0.651594  -0.162962
C  -3.562947   0.734292  -0.478669
C  -2.364928  -1.351362  -0.176545
C  -3.567981  -0.657302  -0.347653
H  -4.507483  -1.197765  -0.367184
S   4.592062   0.853529   1.137862
O   5.995498   0.355950   1.262433
O   3.677677  -0.287920   0.820761
O   4.147538   1.723113   2.239133
Cu   1.830815  -0.392645  -1.655276
C   1.770408   4.429310   0.268590
C   2.547568   5.344857   0.999627
C   1.111503   4.868382  -0.895565
C   2.662235   6.671859   0.574367
H   3.068365   5.032851   1.896342
C   1.229834   6.195703  -1.316766
H   0.510573   4.181338  -1.478319
C   2.004482   7.096826  -0.582575
H   3.263203   7.370894   1.141487
H   0.721870   6.525270  -2.213835
H   2.095766   8.124210  -0.910516
C  -0.039738   1.960224   2.316780
C  -0.978574   2.559726   3.174118
C   0.609994   0.782948   2.733825
C  -1.270306   1.985884   4.415313
H  -1.492588   3.465283   2.879061
C   0.314192   0.211644   3.973883
H   1.326731   0.295195   2.088616
C  -0.627168   0.811333   4.813362
H  -2.000201   2.449150   5.066439
H   0.808218  -0.701701   4.279454
H  -0.859547   0.364953   5.771483
N   2.127616   2.062682  -0.341434
N   0.061576   1.473856  -0.086557
H  -0.219942  -1.185606  -0.035491
H  -2.358460   2.515952  -0.498934
C  -2.399604  -2.809237   0.051862
C  -2.372218  -3.701258  -1.056512
C  -2.619577  -3.309444   1.368262
C  -2.571574  -5.074709  -0.826488
C  -2.831198  -4.689434   1.541367
C  -2.797674  -5.559454   0.457024
H  -2.581968  -5.777955  -1.648255
H  -3.040815  -5.100194   2.519454
H  -2.963851  -6.617926   0.611003
C  -4.833689   1.462532  -0.656431
C  -5.476585   2.055699   0.466390
C  -5.411726   1.575021  -1.952278
C  -6.676496   2.762605   0.265590
C  -6.616306   2.287025  -2.098499
C  -7.236930   2.874782  -1.001926
H  -7.188357   3.230611   1.096102
H  -7.081753   2.392782  -3.069607
H  -8.162038   3.420848  -1.135388
C  -4.764551   0.952732  -3.190264
H  -3.825481   0.423655  -2.930236
C  -4.372999   2.029103  -4.209922
H  -3.710407   2.781362  -3.730608
H  -3.818807   1.567853  -5.055248
H  -5.267728   2.545058  -4.617395
C  -5.682998  -0.099653  -3.823423
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H -5.977153 -0.853466 -3.062259
H -6.600844 0.364356 -4.241794
H -5.149507 -0.625170 -4.644206
C -4.910357 1.945091 1.882731
H -3.983105 1.336607 1.899332
C -5.894525 1.234795 2.820528
H -5.413009 1.047854 3.804277
H -6.806703 1.845198 2.987742
H -6.192562 0.256082 2.388265
C -4.528601 3.325374 2.429769
H -4.052512 3.220676 3.427750
H -3.802564 3.815194 1.746034
H -5.419947 3.978899 2.535042
C -2.724159 -2.380374 2.580884
H -2.348909 -1.366347 2.330463
C -2.215196 -3.202511 -2.493392
H -1.943814 -2.127034 -2.510665
C -1.085654 -3.929375 -3.235905
H -0.152258 -3.894052 -2.640491
H -1.343638 -4.990337 -3.434940
H -0.892641 -3.431936 -4.210397
C -3.539348 -3.332642 -3.253407
H -3.837412 -4.397780 -3.356022
H -4.341199 -2.787441 -2.711722
H -3.443027 -2.889840 -4.267783
C -1.868780 -2.856767 3.765239
H -2.287526 -3.773798 4.229205
H -0.830646 -3.064699 3.439878
H -1.833278 -2.066380 4.545071
C -4.187765 -2.221442 3.004521
H -4.792780 -1.849569 2.151055
H -4.609666 -3.191202 3.344680
H -4.268058 -1.485571 3.833039
C 2.582862 -2.026191 -2.473397
C 3.888113 -1.769564 -3.208343
H 4.342274 -2.673895 -3.660418
B 2.593883 -2.901535 -1.237698
O 1.485771 -3.527580 -0.674576
O 3.744905 -3.204312 -0.467774
C 1.848821 -4.007211 0.628776
C 3.380306 -4.244084 0.473257
C 1.537286 -2.908144 1.632658
H 0.470491 -2.664709 1.568353
H 1.743732 -3.218815 2.666724
H 2.108489 -1.993387 1.418452
C 1.050969 -5.254420 0.938933
H 1.385623 -5.713779 1.880387
H -0.008713 -4.997786 1.055591
H 1.127048 -6.001690 0.139703
C 3.702623 -5.578488 -0.180278
H 3.510236 -6.422782 0.496245
H 3.107837 -5.726329 -1.092485
H 4.764494 -5.608053 -0.460356
C 4.169213 -4.074309 1.754998
H 4.071398 -3.061869 2.171163
H 3.816658 -4.779225 2.521604
H 5.237114 -4.289617 1.596322
Na 5.401566 -1.733125 0.131327
H 4.666274 -1.347570 -2.547295
H 1.764303 -2.315922 -3.156116
H 3.788104 -1.038877 -4.028072
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Figure_S4_imid-3_modeR2_ed(CuHadd) / electronic energy: -3372.921836660248 a.u. / lowest freq: 3.97 cm-1
C 2.242230 -2.208189 1.100301
H 2.332332 -3.170969 0.568378
C 0.787132 -1.866490 1.437320
H 0.712311 -1.139929 2.266003
C 1.433823 -0.682658 -0.479896
C 3.839553 -1.040328 -0.510489
C 4.806321 -0.263843 0.133588
C 4.176866 -1.688652 -1.710494
C 6.090733 -0.137371 -0.384613
H 4.529073 0.282485 1.034835
C 5.470132 -1.559982 -2.223880
C 6.427857 -0.796295 -1.564153
H 6.822617 0.486799 0.132039
H 5.710061 -2.078363 -3.153880
H 7.434390 -0.709866 -1.978786
C -0.876539 -0.526284 0.113627
C -2.020511 -1.240159 -0.265534
C -0.990281 0.827654 0.464712
C -3.271599 -0.609274 -0.281961
C -2.242552 1.455500 0.462499
C -3.381944 0.734467 0.089975
H -4.353398 1.215420 0.097301
S 3.010657 -2.579209 -2.750031
O 2.331005 -1.498784 -3.542356
O 2.020158 -3.259871 -1.865110

O	3.825092	-3.489173	-3.568844
Cu	1.252941	0.404364	-2.134455
C	3.169235	-2.178456	2.289378
C	3.937733	-3.312235	2.607365
C	3.286784	-1.028690	3.093072
C	4.806857	-3.293593	3.702455
H	3.867331	-4.211317	2.007913
C	4.158250	-1.013747	4.185235
H	2.713167	-0.140281	2.869287
C	4.917653	-2.145383	4.490181
H	5.395764	-4.170110	3.939805
H	4.245701	-0.123295	4.794261
H	5.592141	-2.132541	5.336512
C	-0.052120	-3.075710	1.762520
C	-0.631881	-3.204220	3.037706
C	-0.257192	-4.096000	0.815376
C	-1.386938	-4.335117	3.361092
H	-0.492938	-2.434714	3.786892
C	-1.018636	-5.221825	1.141223
H	0.166948	-4.019738	-0.175439
C	-1.578071	-5.344284	2.414832
H	-1.826505	-4.427923	4.345726
H	-1.173351	-6.000845	0.406067
H	-2.166855	-6.216958	2.665903
N	2.550576	-1.158742	0.094417
N	0.373665	-1.183150	0.193436
H	-0.112375	1.379039	0.773769
H	-1.940327	-2.282059	-0.546838
C	-2.374623	2.855560	0.910580
C	-2.328009	3.160177	2.301031
C	-2.581926	3.894143	-0.041274
C	-2.459449	4.500932	2.706180
C	-2.745684	5.213417	0.419397
C	-2.672381	5.511540	1.775452
H	-2.413938	4.769125	3.753388
H	-2.920477	6.024253	-0.275214
H	-2.785522	6.535213	2.108542
C	-4.481023	-1.358294	-0.670677
C	-4.906203	-1.364410	-2.028398
C	-5.253307	-2.021989	0.322910
C	-6.091352	-2.043572	-2.365298
C	-6.441284	-2.670171	-0.062065
C	-6.848894	-2.684969	-1.391482
H	-6.442440	-2.068817	-3.388516
H	-7.062293	-3.168229	0.670649
H	-7.763572	-3.193186	-1.668776
C	-4.844459	-2.033439	1.796189
H	-3.851082	-1.561433	1.940156
C	-4.706529	-3.465532	2.327490
H	-4.035369	-4.050948	1.664344
H	-4.266427	-3.450422	3.347293
H	-5.690539	-3.976148	2.382575
C	-5.832441	-1.223456	2.642581
H	-5.898663	-0.184115	2.254897
H	-6.844758	-1.679868	2.624009
H	-5.483014	-1.177508	3.696280
C	-4.126916	-0.642710	-3.127915
H	-3.222209	-0.149014	-2.720165
C	-4.968481	0.472606	-3.759841
H	-4.348127	1.061908	-4.468597
H	-5.837449	0.058663	-4.313333
H	-5.339956	1.159980	-2.970309
C	-3.628031	-1.628614	-4.190584
H	-2.989118	-1.099600	-4.929610
H	-3.017495	-2.423201	-3.710612
H	-4.473408	-2.101390	-4.733250
C	-2.636779	3.623227	-1.545342
H	-2.416920	2.559444	-1.767829
C	-2.166289	2.076590	3.369562
H	-2.129190	1.065633	2.917096
C	-0.850690	2.249379	4.137791
H	0.006564	2.217804	3.432900
H	-0.828986	3.212446	4.689778
H	-0.724260	1.421171	4.867425
C	-3.366842	2.053085	4.324281
H	-3.421754	2.981729	4.930093
H	-4.309031	1.942382	3.745496
H	-3.284243	1.188242	5.016949
C	-1.576586	4.433177	-2.303077
H	-1.791548	5.521516	-2.266077
H	-0.574968	4.251499	-1.864315
H	-1.549071	4.119209	-3.368426
C	-4.038509	3.903129	-2.098598
H	-4.791481	3.302057	-1.545574
H	-4.299507	4.978496	-2.005106
H	-4.088080	3.619345	-3.171605
C	2.804624	1.726096	-2.399638
C	1.840416	1.836197	-3.413935

H 1.994343 1.379531 -4.396909
B 2.759360 2.620160 -1.150160
O 3.796883 2.798775 -0.259542
O 1.658426 3.383562 -0.824393
C 3.295066 3.608512 0.832758
C 2.081050 4.340468 0.169802
C 2.869277 2.661198 1.941743
H 3.736614 2.079233 2.281774
H 2.474419 3.200886 2.813305
H 2.099889 1.957461 1.593382
C 4.398325 4.524588 1.314293
H 4.026692 5.212177 2.088008
H 5.213987 3.936124 1.755985
H 4.821462 5.122271 0.497891
C 2.491074 5.602113 -0.573190
H 2.758149 6.415529 0.115217
H 3.347158 5.416748 -1.236878
H 1.652422 5.944776 -1.194003
C 0.929549 4.629885 1.104980
H 0.494616 3.710132 1.509845
H 1.251810 5.260367 1.945882
H 0.138646 5.169309 0.569338
Na 0.115110 -2.214699 -3.073179
H 1.091942 2.634898 -3.378931
H 3.691808 1.110040 -2.595290
H -0.206239 0.032097 -2.733340
139
Figure_S4_imid-3_modeR2_ts(CuHadd)_01 / electronic energy: -3372.896178322465 a.u. / lowest freq: -766.58 cm-1
C 2.447560 -1.850732 1.216380
H 2.605068 -2.851607 0.777565
C 0.977220 -1.588084 1.577363
H 0.882291 -0.814334 2.361385
C 1.477494 -0.480073 -0.420372
C 3.884581 -0.643929 -0.523153
C 4.580244 0.536975 -0.250201
C 4.403808 -1.553913 -1.456081
C 5.795675 0.804493 -0.869712
H 4.133776 1.260380 0.434014
C 5.626654 -1.277501 -2.075860
C 6.324450 -0.110456 -1.780542
H 6.321424 1.736525 -0.650780
H 6.014521 -1.987192 -2.809639
H 7.277676 0.090817 -2.274567
C -0.843110 -0.552072 0.172861
C -1.846575 -1.418899 -0.277353
C -1.168461 0.766169 0.519869
C -3.173911 -0.979415 -0.354084
C -2.498860 1.204959 0.456453
C -3.500732 0.326106 0.027216
H -4.531494 0.658538 -0.014521
S 3.594873 -3.095277 -1.921120
O 3.889848 -3.230505 -3.378144
O 2.128918 -2.892482 -1.720861
O 4.184312 -4.132241 -1.058602
Cu 1.464776 0.616056 -1.979732
C 3.401197 -1.634017 2.362419
C 4.211330 -2.690524 2.813705
C 3.509761 -0.376280 2.984527
C 5.109157 -2.492174 3.867114
H 4.149847 -3.667870 2.351350
C 4.409592 -0.182038 4.035745
H 2.901470 0.453730 2.652562
C 5.208495 -1.239294 4.477346
H 5.729387 -3.310346 4.209653
H 4.488019 0.789096 4.507154
H 5.904998 -1.087667 5.291762
C 0.230663 -2.825950 2.004699
C -0.343896 -2.891203 3.286929
C 0.098497 -3.929857 1.141959
C -1.021681 -4.041440 3.700860
H -0.263528 -2.055095 3.970476
C -0.581039 -5.077316 1.559973
H 0.514770 -3.901403 0.144746
C -1.135023 -5.135671 2.840582
H -1.459746 -4.084307 4.689589
H -0.679306 -5.921443 0.889856
H -1.662379 -6.024371 3.162142
N 2.642398 -0.858330 0.141833
N 0.481271 -1.020723 0.308561
H -0.393266 1.434474 0.869961
H -1.597535 -2.432102 -0.566482
C -2.855457 2.573512 0.884085
C -2.842903 2.909220 2.268868
C -3.236619 3.549174 -0.082514
C -3.176488 4.221063 2.652010
C -3.604173 4.833665 0.359090
C -3.559851 5.166387 1.707957
H -3.159003 4.514495 3.693263

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H  -3.913930   5.593661  -0.345827
H  -3.828846   6.165751   2.025130
C  -4.231623  -1.886199  -0.837366
C  -4.522367  -1.957742  -2.228323
C  -4.990649  -2.650713   0.091641
C  -5.564020  -2.798376  -2.661366
C  -6.036615  -3.459337  -0.389687
C  -6.313092  -3.535232  -1.750471
H  -5.809618  -2.877926  -3.712199
H  -6.645752  -4.039126   0.291074
H  -7.117823  -4.168143  -2.102095
C  -4.713683  -2.610488   1.594604
H  -3.812601  -2.003822   1.819335
C  -4.421995  -4.011398   2.146947
H  -3.626446  -4.497257   1.543573
H  -4.069872  -3.938735   3.198090
H  -5.327622  -4.652998   2.128035
C  -5.875696  -1.952163   2.346115
H  -6.053839  -0.930657   1.946582
H  -6.808178  -2.546563   2.243095
H  -5.629193  -1.863125   3.425822
C  -3.750863  -1.138876  -3.263835
H  -2.972122  -0.513239  -2.782433
C  -4.678601  -0.164660  -3.999856
H  -4.082181   0.510301  -4.650390
H  -5.412298  -0.705903  -4.633521
H  -5.230702   0.459500  -3.265518
C  -3.011675  -2.050795  -4.250064
H  -2.382398  -1.440900  -4.932979
H  -2.346830  -2.747250  -3.695544
H  -3.722616  -2.643518  -4.863301
C  -3.258823   3.251219  -1.583079
H  -2.873119   2.233768  -1.795166
C  -2.507338   1.885846   3.356287
H  -2.333952   0.880244   2.924722
C  -1.217781   2.266512   4.093385
H  -0.377092   2.345943   3.372214
H  -1.328718   3.234607   4.625621
H  -0.958421   1.482353   4.836435
C  -3.674373   1.710367   4.336795
H  -3.850213   2.632847   4.928745
H  -4.601852   1.455191   3.780363
H  -3.455782   0.880040   5.042041
C  -2.347445   4.208287  -2.362632
H  -2.730270   5.249776  -2.335137
H  -1.325385   4.191435  -1.935159
H  -2.281778   3.888840  -3.424747
C  -4.691125   3.298366  -2.127400
H  -5.332973   2.582605  -1.571027
H  -5.123671   4.316687  -2.032117
H  -4.700269   3.011402  -3.200569
C   2.543225   2.268691  -2.599865
C   1.536828   1.877970  -3.565647
H   1.870220   1.588235  -4.568133
B   2.296567   3.144637  -1.397819
O   3.300957   3.610302  -0.545645
O   1.048686   3.636920  -1.007698
C   2.654312   4.259492   0.564020
C   1.290126   4.691732  -0.058823
C   2.480498   3.226541   1.668289
H   3.465244   2.840436   1.967645
H   2.007004   3.649944   2.565140
H   1.870669   2.378044   1.323318
C   3.517643   5.405786   1.044719
H   3.007381   5.978598   1.832970
H   4.457907   5.024378   1.466395
H   3.772329   6.093710   0.229239
C   1.395477   5.993851  -0.839527
H   1.518499   6.863134  -0.178071
H   2.241206   5.972265  -1.541230
H   0.477574   6.141188  -1.424835
C   0.144948   4.766266   0.925823
H  -0.073687   3.790257   1.371985
H   0.367227   5.473505   1.738136
H  -0.763014   5.119544   0.421926
Na  1.598694  -2.355337  -3.920572
H   0.624696   2.486810  -3.613651
H   3.564063   1.907318  -2.780539
H   0.752318   0.513276  -3.425487
139
Figure_S4_imid-3_modeR2_ts(CuHadd)_02 / electronic energy: -3372.902173985523 a.u. / lowest freq: -659.52 cm-1
C  -2.705361  -1.470468  -1.252734
H  -3.162198  -2.333798  -0.746261
C  -1.177020  -1.613839  -1.427496
H  -0.859584  -1.428990  -2.466738
C  -1.620462   0.175890   0.064010
C  -4.036275   0.316618  -0.004573
C  -4.234957   1.642042  -0.411332
```

C	-5.052130	-0.343336	0.707065
C	-5.429873	2.299473	-0.141378
H	-3.426369	2.153626	-0.938831
C	-6.254179	0.323220	0.965596
C	-6.449306	1.633066	0.538535
H	-5.562053	3.333356	-0.468611
H	-7.026892	-0.202384	1.529350
H	-7.395302	2.137351	0.747954
C	0.730659	-0.370737	-0.277117
C	1.694071	-0.659521	-1.262478
C	1.164025	-0.028627	1.015959
C	3.060585	-0.629512	-0.953242
C	2.529550	-0.009927	1.326937
C	3.475113	-0.303415	0.340553
H	4.530687	-0.308350	0.587271
S	-4.864067	-2.005561	1.367877
O	-5.838791	-2.072880	2.499801
O	-3.467642	-2.076443	1.893388
O	-5.154210	-2.943074	0.269220
Cu	-1.600432	1.533010	1.412843
C	-3.423612	-1.220733	-2.557541
C	-4.405453	-2.118063	-3.013320
C	-3.129688	-0.081469	-3.329361
C	-5.082924	-1.874983	-4.212109
H	-4.647635	-3.006489	-2.444792
C	-3.809783	0.158359	-4.526120
H	-2.374694	0.619224	-3.001154
C	-4.786732	-0.737273	-4.966928
H	-5.838498	-2.569456	-4.555988
H	-3.579061	1.038969	-5.111551
H	-5.313088	-0.550728	-5.894031
C	-0.684085	-2.977076	-1.002468
C	-0.274361	-3.910099	-1.970666
C	-0.635700	-3.338263	0.357718
C	0.167549	-5.179288	-1.586148
H	-0.304275	-3.659605	-3.023722
C	-0.179084	-4.603217	0.737395
H	-0.939954	-2.638322	1.124443
C	0.220282	-5.523738	-0.233570
H	0.478334	-5.893581	-2.337526
H	-0.138225	-4.871816	1.784633
H	0.571818	-6.503732	0.061849
N	-2.808303	-0.300508	-0.357744
N	-0.654544	-0.535849	-0.554088
H	0.444208	0.151748	1.802396
H	1.389051	-0.929268	-2.264899
C	2.972504	0.220794	2.715327
C	3.517887	1.480435	3.090186
C	2.897022	-0.836909	3.665869
C	3.989963	1.651081	4.404558
C	3.353026	-0.604407	4.976257
C	3.898268	0.622965	5.336206
H	4.431126	2.588215	4.717052
H	3.302282	-1.383224	5.725717
H	4.257835	0.777232	6.345527
C	4.067236	-0.998783	-1.969564
C	4.587930	-2.323339	-2.001573
C	4.557667	-0.018700	-2.877531
C	5.600282	-2.632508	-2.928847
C	5.550902	-0.385439	-3.803526
C	6.067896	-1.675742	-3.822709
H	6.034606	-3.622716	-2.964779
H	5.941273	0.335201	-4.510114
H	6.841492	-1.935488	-4.533982
C	4.051975	1.421729	-2.867393
H	3.294214	1.562765	-2.076611
C	3.363111	1.776792	-4.190345
H	2.541228	1.057199	-4.393719
H	2.923370	2.794900	-4.130562
H	4.080567	1.754077	-5.037332
C	5.180299	2.408550	-2.544400
H	5.663872	2.129375	-1.583585
H	5.948526	2.420642	-3.345788
H	4.767832	3.434741	-2.437396
C	4.094697	-3.414847	-1.050584
H	3.235407	-3.060698	-0.444760
C	5.193181	-3.808133	-0.057186
H	4.798790	-4.545478	0.674429
H	6.063778	-4.258016	-0.579764
H	5.534370	-2.911980	0.504057
C	3.584066	-4.640403	-1.818993
H	3.115794	-5.359895	-1.114280
H	2.820355	-4.329876	-2.563403
H	4.408068	-5.163904	-2.346911
C	2.356322	-2.222556	3.305052
H	2.074288	-2.281312	2.234828
C	3.614655	2.648068	2.108603
H	3.127004	2.397535	1.145197

C 2.882740 3.888809 2.636440
H 1.828055 3.635178 2.872307
H 3.369296 4.293434 3.548066
H 2.885092 4.685812 1.864495
C 5.077378 2.969018 1.783275
H 5.620539 3.321119 2.685707
H 5.585239 2.063497 1.387605
H 5.129277 3.761039 1.005646
C 1.084167 -2.539455 4.099469
H 1.292238 -2.594900 5.188677
H 0.319748 -1.753903 3.917775
H 0.663297 -3.513716 3.772677
C 3.421563 -3.306996 3.508942
H 4.343774 -3.042004 2.949018
H 3.674943 -3.429529 4.582833
H 3.050357 -4.280608 3.122807
C -2.203444 3.504964 1.648890
C -1.654425 2.948448 2.860601
H -2.297517 2.880254 3.743755
B -1.369378 3.945557 0.473066
O -1.877728 4.440702 -0.728820
O 0.026605 3.906925 0.450811
C -0.792960 4.432314 -1.676732
C 0.458121 4.573105 -0.748146
C -0.831139 3.092694 -2.398084
H -1.798365 2.987071 -2.908843
H -0.041121 3.002002 -3.156704
H -0.728187 2.257919 -1.687852
C -0.979090 5.566333 -2.661362
H -0.119963 5.638252 -3.344465
H -1.876051 5.395011 -3.272203
H -1.099440 6.532216 -2.155904
C 0.755011 6.022694 -0.396655
H 1.157202 6.578816 -1.255314
H -0.147713 6.541217 -0.044163
H 1.499853 6.063789 0.408362
C 1.694394 3.879038 -1.271568
H 1.525747 2.797575 -1.327861
H 1.966569 4.246956 -2.271313
H 2.552083 4.054299 -0.609294
Na -4.164515 -2.084585 4.168242
H -0.628039 3.224445 3.130149
H -3.296469 3.511574 1.559499
H -1.346906 1.324939 2.982086
139
Figure_S4_imid-3_modeR2_prod(CuHadd) / electronic energy: -3372.935174585896 a.u. / lowest freq: 12.93 cm-1
C 2.173987 -2.141745 1.320699
H 2.678648 -3.112068 1.215956
C 0.637269 -2.241499 1.218571
H 0.134443 -1.942558 2.151517
C 1.431024 -0.716607 -0.411046
C 3.837158 -0.931298 -0.193396
C 4.187981 0.412916 -0.027807
C 4.796033 -1.838769 -0.676607
C 5.478452 0.857504 -0.299133
H 3.426190 1.116870 0.312361
C 6.096181 -1.388963 -0.918009
C 6.443934 -0.053608 -0.721930
H 5.715673 1.916528 -0.175737
H 6.824202 -2.109446 -1.294370
H 7.466296 0.275947 -0.920195
C -0.946531 -0.659993 0.030788
C -2.064869 -1.465462 -0.231080
C -1.129096 0.712525 0.271285
C -3.351884 -0.915974 -0.219485
C -2.421326 1.258688 0.311217
C -3.529706 0.440519 0.065738
H -4.530371 0.853617 0.116731
S 4.383575 -3.518314 -1.213660
O 5.637415 -4.072106 -1.757407
O 3.351936 -3.274877 -2.273370
O 3.848353 -4.250675 -0.048825
Cu 1.714200 0.733330 -1.659907
C 2.641298 -1.449570 2.581695
C 3.557401 -2.085604 3.437250
C 2.192496 -0.153591 2.904047
C 4.014884 -1.438511 4.589360
H 3.923012 -3.079514 3.211333
C 2.654673 0.489864 4.054770
H 1.488151 0.360017 2.263981
C 3.564993 -0.152030 4.897177
H 4.721554 -1.933935 5.242499
H 2.308343 1.487508 4.292018
H 3.922577 0.347621 5.788137
C 0.173421 -3.626340 0.838392
C -0.572654 -4.396338 1.748338
C 0.470253 -4.163906 -0.426838
C -1.009321 -5.677633 1.398423

H	-0.818001	-4.006939	2.728584
C	0.030198	-5.444195	-0.773346
H	1.028355	-3.585892	-1.148572
C	-0.709084	-6.200805	0.138619
H	-1.584121	-6.263736	2.103792
H	0.259666	-5.848309	-1.750760
H	-1.050534	-7.191689	-0.131350
N	2.505807	-1.318229	0.132408
N	0.335585	-1.247067	0.159237
H	-0.276721	1.339566	0.496614
H	-1.942637	-2.521320	-0.431199
C	-2.631356	2.665950	0.712216
C	-2.494104	3.039483	2.080981
C	-3.040117	3.632443	-0.251591
C	-2.735423	4.376191	2.447429
C	-3.307427	4.946156	0.175418
C	-3.144268	5.313229	1.506045
H	-2.625469	4.696499	3.475024
H	-3.639276	5.699601	-0.526357
H	-3.340718	6.332944	1.811394
C	-4.527016	-1.774962	-0.456121
C	-5.065601	-1.896147	-1.767179
C	-5.136437	-2.458125	0.633224
C	-6.201926	-2.702545	-1.961866
C	-6.278212	-3.242722	0.388407
C	-6.799920	-3.364449	-0.894943
H	-6.635787	-2.818000	-2.946401
H	-6.772353	-3.766801	1.195866
H	-7.677210	-3.975691	-1.063905
C	-4.596952	-2.357734	2.060641
H	-3.669178	-1.751610	2.097745
C	-4.218613	-3.738699	2.610511
H	-3.542863	-4.256696	1.898346
H	-3.685846	-3.629251	3.579300
H	-5.117018	-4.369985	2.774369
C	-5.601639	-1.652994	2.979002
H	-5.847894	-0.649474	2.570126
H	-6.538185	-2.241439	3.077885
H	-5.161701	-1.515794	3.990021
C	-4.452384	-1.175381	-2.967934
H	-3.571947	-0.571897	-2.667092
C	-5.449488	-0.189364	-3.588635
H	-4.947899	0.413687	-4.375501
H	-6.309994	-0.720017	-4.047671
H	-5.830463	0.504700	-2.809705
C	-3.942487	-2.176479	-4.011474
H	-3.417057	-1.638342	-4.829230
H	-3.222442	-2.879900	-3.540822
H	-4.777414	-2.759006	-4.454637
C	-3.217307	3.286643	-1.730507
H	-2.874261	2.252999	-1.940562
C	-2.124804	2.032387	3.172638
H	-2.014423	1.010418	2.760279
C	-0.776985	2.383305	3.813028
H	0.008844	2.436695	3.031415
H	-0.822940	3.357452	4.343581
H	-0.484915	1.597120	4.541673
C	-3.230396	1.926808	4.230896
H	-3.338821	2.873278	4.800813
H	-4.199368	1.685002	3.743460
H	-2.992548	1.112330	4.948288
C	-2.371977	4.197670	-2.630887
H	-2.754112	5.239818	-2.631187
H	-1.319849	4.205191	-2.284223
H	-2.390838	3.820695	-3.675834
C	-4.696034	3.350688	-2.129250
H	-5.295542	2.679166	-1.478965
H	-5.091545	4.384273	-2.035360
H	-4.821414	3.017927	-3.181763
C	2.151276	2.231779	-2.857986
C	1.161606	2.472781	-3.987446
H	1.384656	3.378949	-4.583338
B	2.156577	3.220126	-1.698912
O	3.247532	3.490009	-0.863285
O	1.048385	3.963836	-1.300690
C	2.770726	4.271853	0.249052
C	1.484284	4.938522	-0.342020
C	2.449445	3.316625	1.388783
H	3.356292	2.776367	1.694577
H	2.065631	3.840044	2.275446
H	1.698761	2.576869	1.073622
C	3.849939	5.246365	0.671275
H	3.484568	5.924297	1.456870
H	4.715051	4.703629	1.077184
H	4.202941	5.854399	-0.170369
C	1.788006	6.221794	-1.101970
H	2.061505	7.046308	-0.428687
H	2.606483	6.079120	-1.821671

H 0.896264 6.527160 -1.666165
C 0.376167 5.174679 0.660564
H 0.012840 4.233673 1.088951
H 0.711437 5.823755 1.482465
H -0.472422 5.669689 0.170550
Na 2.769586 -1.683965 -3.674549
H 0.136855 2.610495 -3.609808
H 3.178156 2.038580 -3.219316
H 1.106243 1.643564 -4.712428
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Figure_S5_imid-3_modeS1_ed(CuHadd) / electronic energy: -3525.649267433137 a.u. / lowest freq: 7.11 cm-1
C 0.412352 3.294450 0.389998
H 1.144496 3.134611 1.195081
C -0.967154 2.677321 0.700485
H -1.791609 3.360722 0.437461
C 0.039224 1.460491 -1.063838
C 2.013664 2.766584 -1.538968
C 1.863467 3.044694 -2.903583
C 3.303759 2.726059 -0.985502
C 2.971137 3.291276 -3.708836
H 0.852552 3.058913 -3.320761
C 4.407977 2.999116 -1.796353
C 4.248387 3.285029 -3.149464
H 2.832742 3.499140 -4.772095
H 5.401609 2.949506 -1.347865
H 5.123823 3.491305 -3.768826
C -2.072789 0.598946 -0.259745
C -3.398756 1.064473 -0.235319
C -1.830485 -0.782686 -0.238029
C -4.465563 0.158950 -0.181279
C -2.900245 -1.685961 -0.161822
C -4.214834 -1.214283 -0.139503
H -5.040433 -1.913954 -0.072955
S 3.620828 2.185074 0.701525
O 5.025894 1.684565 0.669100
O 2.664887 1.055999 0.909405
O 3.410007 3.340832 1.590161
Cu 0.400649 0.410241 -2.702562
C 0.333686 4.765678 0.064666
C 0.966683 5.710087 0.891559
C -0.371329 5.213533 -1.068877
C 0.901370 7.072956 0.586281
H 1.506399 5.395245 1.775292
C -0.432923 6.576837 -1.370205
H -0.869530 4.506011 -1.720022
C 0.203577 7.505873 -0.543907
H 1.391345 7.794258 1.227428
H -0.974475 6.913026 -2.244905
H 0.154620 8.561360 -0.778324
C -1.111355 2.264629 2.144147
C -2.011360 2.940019 2.986689
C -0.359252 1.195580 2.665336
C -2.149401 2.557162 4.324292
H -2.603190 3.765612 2.611646
C -0.503219 0.814713 4.001922
H 0.328181 0.650744 2.033780
C -1.398551 1.493788 4.830622
H -2.839669 3.085511 4.968944
H 0.079429 -0.006964 4.395988
H -1.509180 1.197291 5.865560
N 0.840628 2.507381 -0.787396
N -0.990117 1.510473 -0.206108
H -0.812046 -1.149387 -0.227595
H -3.607297 2.126171 -0.253984
C -2.647803 -3.130665 -0.031451
C -2.640073 -3.959236 -1.187480
C -2.409857 -3.691865 1.254918
C -2.364733 -5.330477 -1.035728
C -2.133512 -5.067964 1.352113
C -2.107018 -5.873440 0.218563
H -2.346431 -5.988988 -1.894026
H -1.938416 -5.526324 2.312573
H -1.892052 -6.930005 0.313849
C -5.856566 0.644134 -0.136563
C -6.460440 0.949278 1.115077
C -6.612762 0.737220 -1.337956
C -7.812336 1.338752 1.137781
C -7.960560 1.133077 -1.261849
C -8.549663 1.431154 -0.037842
H -8.307609 1.564048 2.072978
H -8.567259 1.204306 -2.154945
H -9.589574 1.729326 0.000816
C -6.012763 0.400102 -2.703597
H -4.936244 0.148096 -2.617351
C -6.085348 1.599197 -3.657355
H -5.604740 2.485108 -3.189689
H -5.543149 1.367885 -4.599125
H -7.135750 1.851618 -3.912984

C	-6.692045	-0.832720	-3.311155
H	-6.620879	-1.689237	-2.606868
H	-7.762530	-0.635077	-3.530522
H	-6.184322	-1.120251	-4.256667
C	-5.697007	0.836067	2.435865
H	-4.635340	0.564185	2.265655
C	-6.283854	-0.275119	3.313743
H	-5.663396	-0.407322	4.225996
H	-7.322882	-0.035954	3.624147
H	-6.286061	-1.236189	2.755932
C	-5.671239	2.175205	3.182949
H	-5.047906	2.086214	4.097276
H	-5.229696	2.962107	2.534755
H	-6.690185	2.489982	3.490256
C	-2.451725	-2.849460	2.531926
H	-2.702805	-1.792145	2.310518
C	-2.927836	-3.408308	-2.584481
H	-3.121859	-2.316913	-2.553336
C	-1.724185	-3.595405	-3.515120
H	-0.832987	-3.100979	-3.077948
H	-1.498279	-4.670091	-3.677491
H	-1.928289	-3.125967	-4.501041
C	-4.190038	-4.045108	-3.178029
H	-4.046774	-5.131122	-3.359545
H	-5.046648	-3.905392	-2.484255
H	-4.444382	-3.557160	-4.143282
C	-1.084619	-2.822432	3.225024
H	-0.755881	-3.841629	3.516910
H	-0.326805	-2.378033	2.546417
H	-1.134764	-2.196591	4.140893
C	-3.545425	-3.345447	3.485566
H	-4.523371	-3.373165	2.958791
H	-3.314498	-4.360143	3.872498
H	-3.638886	-2.652919	4.349506
C	2.270724	-0.488001	-2.842663
C	1.516068	-0.530238	-4.037682
H	1.015109	-1.457202	-4.337335
B	2.397138	-1.734525	-1.964808
O	1.553826	-2.814638	-2.059899
O	3.431088	-1.979258	-1.057584
C	1.932496	-3.765398	-1.039130
C	3.433586	-3.420856	-0.819279
C	1.095731	-3.465310	0.189789
H	0.041262	-3.507521	-0.093396
H	1.260898	-4.192428	0.995993
H	1.298001	-2.456842	0.578657
C	1.663570	-5.162549	-1.548464
H	2.022163	-5.917647	-0.834628
H	0.584001	-5.313073	-1.679208
H	2.144145	-5.343672	-2.517444
C	4.337622	-4.048662	-1.865200
H	4.412640	-5.135512	-1.727452
H	3.972757	-3.855933	-2.883516
H	5.350983	-3.635257	-1.783165
C	3.947515	-3.707254	0.572302
H	3.384838	-3.169319	1.343822
H	3.872046	-4.781825	0.791358
H	5.006130	-3.426910	0.659868
Na	4.291372	-0.596233	0.566307
H	1.718176	0.165978	-4.858979
H	3.013529	0.313947	-2.736389
H	-0.822217	0.691844	-3.674542
O	6.467374	-1.332810	0.168822
O	4.100602	-1.087567	2.810304
C	6.860083	-1.150202	-1.149726
H	7.494003	-2.008022	-1.466710
H	5.964942	-1.110006	-1.805682
C	7.432687	-0.723945	0.961657
H	6.946423	-0.276827	1.854392
H	8.159328	-1.491797	1.307333
C	8.141765	0.350656	0.154329
H	7.876578	1.366401	0.521414
H	9.244379	0.214193	0.204493
C	7.638639	0.142888	-1.245364
H	8.472647	0.059940	-1.975913
H	6.962737	0.974936	-1.540489
C	4.819716	-1.887107	3.685902
H	5.516909	-2.536526	3.115369
H	5.414639	-1.239715	4.367543
C	2.834771	-0.896700	3.356736
H	2.736909	0.153399	3.707734
H	2.074021	-1.076403	2.568488
C	2.618847	-1.866044	4.507100
H	2.557483	-1.312183	5.469881
H	1.698247	-2.472968	4.366148
C	3.845172	-2.725361	4.478392
H	4.225073	-2.944119	5.499925
H	3.634321	-3.674937	3.938200

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Figure_S5_imid-3_modeS1_ts(CuHadd)_01 / electronic energy: -3525.636749203804 a.u. / lowest freq: -746.07 cm-1

C	0.329402	3.358227	0.292017
H	1.047647	3.226651	1.115305
C	-1.045318	2.725779	0.592883
H	-1.874406	3.388373	0.293176
C	0.022810	1.468829	-1.105391
C	1.976518	2.798172	-1.592298
C	1.850746	3.029953	-2.968230
C	3.255895	2.786133	-1.013877
C	2.971461	3.258327	-3.760330
H	0.848060	3.023875	-3.403735
C	4.373739	3.038577	-1.812949
C	4.238197	3.278001	-3.177320
H	2.852024	3.432083	-4.831983
H	5.359076	3.008332	-1.344436
H	5.123920	3.468387	-3.787155
C	-2.095293	0.591868	-0.312260
C	-3.431257	1.026761	-0.251808
C	-1.823733	-0.785553	-0.313741
C	-4.476834	0.098215	-0.186513
C	-2.873333	-1.712052	-0.229281
C	-4.196689	-1.269304	-0.173178
H	-5.005778	-1.987296	-0.099252
S	3.544268	2.321790	0.701019
O	4.937021	1.788705	0.702430
O	2.558918	1.231073	0.960459
O	3.352786	3.529557	1.523347
Cu	0.661359	0.315555	-2.503662
C	0.233305	4.820399	-0.067076
C	0.832919	5.792619	0.752206
C	-0.454747	5.231958	-1.224519
C	0.751565	7.147421	0.416498
H	1.358625	5.505202	1.653531
C	-0.532534	6.587375	-1.556301
H	-0.927201	4.502315	-1.870473
C	0.070802	7.544405	-0.737040
H	1.215815	7.890305	1.052123
H	-1.060906	6.895739	-2.449122
H	0.009335	8.593719	-0.995037
C	-1.211966	2.357103	2.046496
C	-2.098563	3.081870	2.861556
C	-0.499143	1.278470	2.603231
C	-2.263506	2.737234	4.206379
H	-2.660096	3.915576	2.458801
C	-0.673451	0.932968	3.945859
H	0.178580	0.696369	1.994335
C	-1.555230	1.661402	4.746931
H	-2.945332	3.302110	4.828764
H	-0.125182	0.100156	4.365652
H	-1.689190	1.392828	5.786717
N	0.789010	2.554107	-0.856795
N	-1.032865	1.529680	-0.275880
H	-0.798248	-1.133069	-0.329893
H	-3.665649	2.082943	-0.250926
C	-2.589789	-3.152997	-0.128420
C	-2.538725	-3.951709	-1.303854
C	-2.355298	-3.738095	1.147583
C	-2.225824	-5.317868	-1.181009
C	-2.041564	-5.107871	1.216478
C	-1.975179	-5.884602	0.064398
H	-2.167515	-5.952430	-2.055423
H	-1.843727	-5.582494	2.168434
H	-1.729209	-6.936147	0.137521
C	-5.875473	0.553774	-0.095935
C	-6.464958	0.779978	1.179126
C	-6.650969	0.699552	-1.279441
C	-7.822537	1.144137	1.242613
C	-8.003502	1.068521	-1.162504
C	-8.578827	1.288821	0.084392
H	-8.307091	1.309262	2.195812
H	-8.624626	1.178693	-2.041618
H	-9.622652	1.566980	0.154191
C	-6.066695	0.445607	-2.669621
H	-4.985671	0.204826	-2.612396
C	-6.170492	1.693484	-3.555517
H	-5.695149	2.559681	-3.047239
H	-5.639578	1.521744	-4.516278
H	-7.228128	1.943872	-3.781636
C	-6.737123	-0.762740	-3.333642
H	-6.638032	-1.656381	-2.680497
H	-7.814667	-0.571842	-3.522264
H	-6.242892	-0.987554	-4.302997
C	-5.678929	0.609162	2.480422
H	-4.614739	0.369486	2.279612
C	-6.230907	-0.560743	3.302741
H	-5.593701	-0.731952	4.196738
H	-7.269116	-0.359453	3.641499

H -6.224677 -1.488626 2.691490
C -5.667052 1.904245 3.301776
H -5.024962 1.776747 4.198758
H -5.253877 2.735979 2.691971
H -6.686398 2.179098 3.644053
C -2.429176 -2.924938 2.441823
H -2.721395 -1.873963 2.242144
C -2.801348 -3.369632 -2.692867
H -3.052423 -2.290950 -2.635310
C -1.552039 -3.466310 -3.575329
H -0.707415 -2.940429 -3.084271
H -1.263698 -4.523115 -3.756138
H -1.738260 -2.978064 -4.555658
C -4.005871 -4.045354 -3.359186
H -3.802121 -5.115587 -3.573030
H -4.895214 -3.971973 -2.697019
H -4.245766 -3.535429 -4.316756
C -1.062603 -2.859068 3.132366
H -0.700887 -3.870148 3.413947
H -0.321359 -2.385322 2.455271
H -1.130536 -2.241236 4.052801
C -3.500833 -3.481545 3.387102
H -4.476917 -3.541946 2.859795
H -3.227831 -4.491563 3.758370
H -3.622328 -2.807523 4.262073
C 2.473054 -0.648534 -2.830061
C 1.617484 -0.607170 -3.999789
H 1.171544 -1.552265 -4.329269
B 2.577926 -1.885887 -1.978573
O 1.778087 -3.009515 -2.125535
O 3.532773 -2.098744 -0.965404
C 2.059443 -3.891660 -1.023604
C 3.530814 -3.522285 -0.680371
C 1.111504 -3.522746 0.103883
H 0.090906 -3.560681 -0.284952
H 1.180279 -4.210956 0.957326
H 1.291904 -2.498456 0.462138
C 1.841409 -5.320616 -1.465864
H 2.136239 -6.028617 -0.677842
H 0.778269 -5.489209 -1.684290
H 2.408052 -5.557036 -2.374891
C 4.533237 -4.180257 -1.613480
H 4.610833 -5.259818 -1.425185
H 4.259012 -4.034346 -2.667568
H 5.528842 -3.744363 -1.455849
C 3.916806 -3.755998 0.762285
H 3.289818 -3.183286 1.455583
H 3.819955 -4.821068 1.017984
H 4.963343 -3.466897 0.930224
Na 4.149671 -0.497896 0.552636
H 1.923179 0.017393 -4.846579
H 3.234324 0.138694 -2.743070
H 0.114357 0.171461 -3.989161
O 6.373836 -1.233599 0.382397
O 3.951547 -0.982789 2.798269
C 6.859605 -1.115855 -0.912350
H 7.520823 -1.982133 -1.137252
H 6.015565 -1.117554 -1.633814
C 7.270534 -0.569424 1.212337
H 6.706773 -0.031807 2.003873
H 7.934347 -1.314058 1.703569
C 8.091779 0.413435 0.392552
H 7.896040 1.463074 0.703454
H 9.177072 0.192185 0.494691
C 7.634496 0.176861 -1.016669
H 8.489700 0.084338 -1.720982
H 6.961034 0.998193 -1.346285
C 4.686105 -1.709504 3.723194
H 5.405727 -2.371518 3.197281
H 5.257954 -1.006877 4.368965
C 2.679071 -0.791795 3.328697
H 2.555587 0.273480 3.620786
H 1.926749 -1.032795 2.548284
C 2.481021 -1.699279 4.531658
H 2.398963 -1.093200 5.460886
H 1.577838 -2.337441 4.421531
C 3.729347 -2.526238 4.558356
H 4.108737 -2.675475 5.592543
H 3.546682 -3.510655 4.073015
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Figure_S5_imid-3_modeS1_ts(CuHadd)_02 / electronic energy: -3525.633841086988 a.u. / lowest freq: -772.94 cm-1
C 0.148808 3.382703 0.334870
H 0.949640 3.239316 1.076543
C -1.163391 2.668386 0.724609
H -2.048503 3.287128 0.499409
C -0.182357 1.530937 -1.102220
C 1.594248 3.014904 -1.763885
C 1.270763 3.273668 -3.102550

C	2.936024	3.084811	-1.357732
C	2.255531	3.613899	-4.024056
H	0.222679	3.201269	-3.403033
C	3.916627	3.445293	-2.285670
C	3.583005	3.715651	-3.610328
H	1.982477	3.809744	-5.063242
H	4.956151	3.473454	-1.954161
H	4.364177	3.991158	-4.322110
C	-2.161461	0.507635	-0.168412
C	-3.514285	0.882514	-0.110041
C	-1.824389	-0.853721	-0.153272
C	-4.515331	-0.092836	-0.028864
C	-2.828147	-1.827374	-0.050612
C	-4.171031	-1.445984	0.007427
H	-4.945465	-2.200046	0.092011
S	3.470785	2.593442	0.287452
O	4.895999	2.189223	0.102872
O	2.622942	1.410476	0.614987
O	3.278530	3.752478	1.176583
Cu	0.384140	0.418430	-2.556794
C	-0.044089	4.856039	0.075404
C	0.579158	5.808568	0.900190
C	-0.850055	5.298365	-0.990986
C	0.406958	7.174606	0.657210
H	1.193352	5.497107	1.735167
C	-1.018315	6.664995	-1.230397
H	-1.344482	4.584393	-1.637957
C	-0.389499	7.602497	-0.407750
H	0.890335	7.902124	1.296351
H	-1.636781	6.997213	-2.054115
H	-0.521164	8.660493	-0.594043
C	-1.201163	2.259076	2.175461
C	-2.132033	2.840481	3.053649
C	-0.326062	1.271446	2.663697
C	-2.180200	2.444884	4.393984
H	-2.819790	3.599986	2.703513
C	-0.379172	0.877685	4.003068
H	0.386493	0.799407	2.002120
C	-1.306653	1.462859	4.867609
H	-2.896408	2.899457	5.065989
H	0.297454	0.117447	4.370340
H	-1.348034	1.156046	5.904626
N	0.528957	2.661456	-0.897073
N	-1.143612	1.490930	-0.165298
H	-0.782950	-1.150455	-0.174530
H	-3.794722	1.927545	-0.128485
C	-2.473905	-3.251928	0.061350
C	-2.465608	-4.076509	-1.097599
C	-2.127459	-3.794592	1.330604
C	-2.081060	-5.423474	-0.967077
C	-1.742804	-5.145800	1.406549
C	-1.717601	-5.946626	0.269484
H	-2.055338	-6.076997	-1.829012
H	-1.458598	-5.587423	2.352488
H	-1.417513	-6.983636	0.347923
C	-5.934269	0.298958	0.041179
C	-6.528856	0.585146	1.301534
C	-6.719104	0.331592	-1.144978
C	-7.900654	0.894520	1.348559
C	-8.086415	0.646862	-1.044644
C	-8.666713	0.925930	0.188091
H	-8.388116	1.105528	2.291186
H	-8.714265	0.671432	-1.925564
H	-9.721356	1.163129	0.245332
C	-6.126845	0.019460	-2.520070
H	-5.036257	-0.170274	-2.453481
C	-6.285986	1.206091	-3.478913
H	-5.846373	2.120669	-3.026275
H	-5.750942	0.999243	-4.430446
H	-7.353944	1.397612	-3.713907
C	-6.745661	-1.254137	-3.107724
H	-6.612977	-2.100344	-2.399935
H	-7.829405	-1.119282	-3.308686
H	-6.239549	-1.518650	-4.060804
C	-5.731300	0.540488	2.606142
H	-4.660622	0.321737	2.416880
C	-6.237034	-0.581629	3.519939
H	-5.591155	-0.659073	4.420754
H	-7.280889	-0.393420	3.848604
H	-6.197312	-1.553557	2.982593
C	-5.761405	1.895061	3.324607
H	-5.108870	1.862059	4.222298
H	-5.383163	2.691034	2.648046
H	-6.788335	2.158432	3.653247
C	-2.159724	-2.956251	2.610498
H	-2.522013	-1.927406	2.410034
C	-2.855958	-3.544277	-2.477019
H	-3.142519	-2.474165	-2.428445

C	-1.677339	-3.620324	-3.453851
H	-0.818406	-3.048715	-3.047039
H	-1.362286	-4.670202	-3.629993
H	-1.959815	-3.168332	-4.428590
C	-4.080911	-4.283510	-3.028578
H	-3.851391	-5.350841	-3.230725
H	-4.917688	-4.226050	-2.299838
H	-4.415459	-3.810194	-3.976511
C	-0.755786	-2.802772	3.205999
H	-0.317452	-3.787746	3.470717
H	-0.091623	-2.295133	2.475337
H	-0.796693	-2.179092	4.123889
C	-3.135941	-3.545034	3.636375
H	-4.140977	-3.664656	3.177721
H	-2.787523	-4.531815	4.006957
H	-3.233180	-2.858953	4.505022
C	2.198097	-0.485255	-3.002743
C	1.251906	-0.508105	-4.102625
H	0.818629	-1.479054	-4.367641
B	2.430585	-1.702920	-2.146615
O	1.666310	-2.857047	-2.201742
O	3.501422	-1.870651	-1.242030
C	2.120857	-3.737972	-1.158664
C	3.602066	-3.296941	-0.986708
C	1.293926	-3.440236	0.079900
H	0.237127	-3.532024	-0.184626
H	1.501471	-4.134392	0.905618
H	1.460125	-2.412835	0.434367
C	1.927912	-5.170118	-1.603664
H	2.344117	-5.873286	-0.867884
H	0.857092	-5.390904	-1.706995
H	2.401716	-5.362227	-2.574247
C	4.511499	-3.884422	-2.053271
H	4.698291	-4.953826	-1.884491
H	4.080735	-3.764880	-3.057183
H	5.480153	-3.367197	-2.042152
C	4.162020	-3.544166	0.394817
H	3.591076	-3.019569	1.167196
H	4.144861	-4.619283	0.624716
H	5.205293	-3.208739	0.469183
Na	4.338072	-0.159242	0.040520
H	1.470156	0.096356	-4.990120
H	2.936873	0.327370	-3.001740
H	-0.263028	0.214801	-3.993680
O	6.680110	-0.609972	0.106946
O	4.238259	-0.747217	2.319085
C	7.339774	0.353211	0.859612
H	7.611912	1.210648	0.204590
H	6.670049	0.723739	1.663686
C	7.662680	-1.461256	-0.376828
H	7.241558	-2.474879	-0.534858
H	8.033252	-1.078916	-1.354177
C	8.791661	-1.512504	0.633508
H	8.699841	-2.419944	1.270613
H	9.781687	-1.507615	0.127383
C	8.585667	-0.271442	1.457815
H	9.454041	0.418490	1.378024
H	8.414964	-0.537117	2.524586
C	5.118192	-1.366504	3.194676
H	5.893513	-1.915372	2.619261
H	5.622680	-0.593367	3.815658
C	3.007217	-0.697682	2.958609
H	2.907378	0.272932	3.492995
H	2.197395	-0.773763	2.204530
C	2.914853	-1.854648	3.935041
H	2.499157	-1.518887	4.910159
H	2.279836	-2.667595	3.519206
C	4.336880	-2.321829	4.074686
H	4.682409	-2.266000	5.130048
H	4.440723	-3.364887	3.701832

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Figure_S5_imid-3_modeS1_ts(CuHadd)_03 / electronic energy: -3525.636864088099 a.u. / lowest freq: -768.46 cm-1

C	0.573259	3.187724	-0.017448
H	1.263637	3.093949	0.833309
C	-0.858506	2.713917	0.317940
H	-1.622896	3.404596	-0.076612
C	0.118282	1.190580	-1.207412
C	2.194788	2.268326	-1.788630
C	2.103526	2.310243	-3.185980
C	3.464157	2.242178	-1.187667
C	3.246104	2.339285	-3.979215
H	1.107936	2.315903	-3.638111
C	4.605912	2.300959	-1.991278
C	4.504508	2.352139	-3.378502
H	3.150796	2.364113	-5.066878
H	5.581465	2.268070	-1.502508
H	5.408748	2.387567	-3.989818
C	-2.063405	0.580848	-0.360643

C	-3.360711	1.113637	-0.442905
C	-1.898770	-0.795013	-0.139413
C	-4.477314	0.281073	-0.300754
C	-3.018496	-1.621919	0.025675
C	-4.305156	-1.084395	-0.061669
H	-5.170106	-1.724499	0.071084
S	3.694481	1.992067	0.579287
O	5.060444	1.403054	0.695177
O	2.654198	0.986623	0.944725
O	3.546424	3.304443	1.232904
Cu	0.604398	-0.183695	-2.448710
C	0.610502	4.600999	-0.543292
C	1.264879	5.610916	0.183364
C	-0.008639	4.929361	-1.764407
C	1.307044	6.919680	-0.306628
H	1.737450	5.389729	1.131531
C	0.037064	6.238956	-2.250412
H	-0.522888	4.170062	-2.340475
C	0.695358	7.233169	-1.522856
H	1.813246	7.691883	0.258084
H	-0.438282	6.482985	-3.191624
H	0.729573	8.246949	-1.900318
C	-1.080719	2.527851	1.798558
C	-1.947917	3.386257	2.496519
C	-0.442169	1.486270	2.497457
C	-2.165563	3.209188	3.866159
H	-2.453708	4.194518	1.983242
C	-0.668225	1.309789	3.864881
H	0.219232	0.803692	1.981473
C	-1.529165	2.170116	4.548984
H	-2.830539	3.877074	4.398123
H	-0.174088	0.506576	4.394886
H	-1.702277	2.032432	5.608366
N	0.982556	2.218162	-1.056303
N	-0.933976	1.433144	-0.409393
H	-0.903096	-1.210751	-0.047756
H	-3.507951	2.171927	-0.615214
C	-2.848822	-3.047038	0.354620
C	-2.845263	-4.020729	-0.682052
C	-2.689507	-3.444051	1.712115
C	-2.657994	-5.372676	-0.340882
C	-2.503887	-4.808607	2.000632
C	-2.484159	-5.757941	0.984220
H	-2.643786	-6.138761	-1.104817
H	-2.374170	-5.145490	3.020581
H	-2.337959	-6.802779	1.226201
C	-5.838474	0.840823	-0.374489
C	-6.463168	1.341205	0.801665
C	-6.544914	0.824411	-1.609147
C	-7.786360	1.812216	0.717610
C	-7.865498	1.308235	-1.640996
C	-8.475360	1.796845	-0.490510
H	-8.296659	2.187761	1.594671
H	-8.434564	1.302114	-2.561290
H	-9.493758	2.161213	-0.534250
C	-5.920446	0.281609	-2.895339
H	-4.868225	-0.027668	-2.730966
C	-5.874087	1.355441	-3.989633
H	-5.348128	2.258537	-3.612295
H	-5.317239	0.973907	-4.872133
H	-6.894378	1.643564	-4.318931
C	-6.661257	-0.970475	-3.378995
H	-6.675668	-1.736015	-2.573699
H	-7.706517	-0.732876	-3.668926
H	-6.140380	-1.405035	-4.258954
C	-5.752512	1.356907	2.156254
H	-4.707628	0.995622	2.067531
C	-6.443882	0.414938	3.148491
H	-5.862818	0.365256	4.094281
H	-7.472238	0.762127	3.383095
H	-6.497465	-0.609896	2.722321
C	-5.656579	2.779912	2.719894
H	-5.071728	2.774304	3.663643
H	-5.138702	3.441099	1.992546
H	-6.660448	3.199741	2.938630
C	-2.722877	-2.437626	2.864544
H	-2.891054	-1.405621	2.494883
C	-3.034895	-3.643549	-2.151422
H	-3.164641	-2.548744	-2.271537
C	-1.800792	-4.014809	-2.980865
H	-0.901295	-3.533551	-2.545716
H	-1.644530	-5.113605	-3.007718
H	-1.917900	-3.649562	-4.023505
C	-4.303089	-4.284612	-2.727112
H	-4.218335	-5.391316	-2.756468
H	-5.182430	-4.006427	-2.107410
H	-4.479083	-3.917286	-3.760851
C	-1.385336	-2.404181	3.613837

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H  -1.140895  -3.393370   4.053993
H  -0.571269  -2.104667   2.920726
H  -1.428845  -1.658589   4.435536
C  -3.885184  -2.732188   3.820442
H  -4.841238  -2.765760   3.255183
H  -3.741402  -3.700169   4.344872
H  -3.963715  -1.927514   4.582691
C   2.318523  -1.323030  -2.648984
C   1.430391  -1.422544  -3.790343
H   0.902757  -2.372020  -3.934769
B   2.356528  -2.364395  -1.562964
O   1.524234  -3.471364  -1.503322
O   3.297274  -2.408495  -0.512354
C   1.793077  -4.164240  -0.271132
C   3.271195  -3.762768   0.008979
C   0.843759  -3.612545   0.778243
H  -0.177273  -3.705242   0.397090
H   0.902545  -4.158573   1.729811
H   1.032656  -2.546992   0.972817
C   1.560894  -5.644100  -0.479153
H   1.847392  -6.219494   0.413088
H   0.496139  -5.834813  -0.671135
H   2.128607  -6.026891  -1.336183
C   4.267027  -4.583741  -0.793607
H   4.324884  -5.618958  -0.430096
H   3.998058  -4.607993  -1.858904
H   5.265937  -4.137335  -0.702795
C   3.653337  -3.756157   1.472858
H   3.023791  -3.087109   2.071990
H   3.556981  -4.765175   1.898585
H   4.702725  -3.453526   1.604579
Na  4.205574  -0.833273   0.919123
H   1.758781  -0.994064  -4.744043
H   3.118780  -0.574671  -2.713046
H   0.020128  -0.533041  -3.887464
O   6.252443  -1.564866  -0.131745
O   4.080726  -0.924266   3.291924
C   6.059761  -1.200542  -1.461645
H   5.798070  -2.094914  -2.065399
H   5.216710  -0.481149  -1.515253
C   7.426829  -0.966527   0.314513
H   7.225807  -0.398235   1.246381
H   8.167921  -1.762900   0.542542
C   7.975101  -0.046198  -0.756979
H   7.661543   1.002439  -0.558603
H   9.083291  -0.102676  -0.825470
C   7.316366  -0.552589  -1.997286
H   7.959977  -1.316750  -2.486922
H   7.088130   0.268281  -2.711645
C   2.838960  -0.596511   3.821958
H   2.060004  -0.688883   3.036302
H   2.590987  -1.308344   4.640257
C   5.016268  -0.167130   3.982552
H   5.381626  -0.746136   4.859750
H   5.880004   0.051292   3.320912
C   4.361470   1.121682   4.437502
H   4.668327   1.381302   5.474214
H   4.627029   1.954721   3.750351
C   2.891206   0.822359   4.356905
H   2.408802   0.887240   5.356686
H   2.389812   1.525505   3.657382
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Figure_S5_imid-3_modeS1_ts(CuHadd)_04 / electronic energy: -3525.636276276343 a.u. / lowest freq: -755.58 cm-1
C   0.475132   3.228426  -0.052348
H   1.163908   3.133791   0.799832
C  -0.947150   2.725293   0.271073
H  -1.722217   3.389971  -0.146994
C   0.076313   1.217872  -1.237866
C   2.114565   2.357822  -1.831967
C   2.022568   2.412029  -3.228572
C   3.383348   2.346768  -1.230378
C   3.165181   2.467858  -4.020476
H   1.027163   2.405252  -3.680712
C   4.524729   2.429497  -2.031879
C   4.422892   2.493485  -3.418581
H   3.070393   2.502713  -5.107898
H   5.499979   2.409492  -1.542287
H   5.326789   2.549025  -4.028902
C  -2.085096   0.545246  -0.378814
C  -3.399019   1.041743  -0.427214
C  -1.878152  -0.828136  -0.177641
C  -4.488694   0.176431  -0.273837
C  -2.971061  -1.688169  -0.001423
C  -4.273753  -1.186569  -0.057818
H  -5.117601  -1.852217   0.084768
S   3.613720   2.093136   0.535184
O   4.983920   1.513511   0.650926
O   2.580857   1.078570   0.898917
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O	3.454349	3.402921	1.191034
Cu	0.620532	-0.138479	-2.478501
C	0.490391	4.648931	-0.558724
C	1.119591	5.660397	0.187733
C	-0.124839	4.983040	-1.780206
C	1.141068	6.976613	-0.283206
H	1.588093	5.434462	1.136881
C	-0.099856	6.300130	-2.247154
H	-0.619965	4.222589	-2.371303
C	0.533562	7.295989	-1.499992
H	1.627839	7.749996	0.296773
H	-0.572032	6.548716	-3.188764
H	0.551668	8.315564	-1.862668
C	-1.184390	2.559276	1.751570
C	-2.075652	3.412901	2.424355
C	-0.536469	1.540500	2.475140
C	-2.308660	3.253141	3.793522
H	-2.588964	4.203595	1.891563
C	-0.779373	1.379742	3.841668
H	0.145163	0.863081	1.978695
C	-1.664575	2.235184	4.500661
H	-2.993499	3.916491	4.305659
H	-0.279716	0.592593	4.390377
H	-1.850865	2.109899	5.559344
N	0.903299	2.277785	-1.099977
N	-0.980707	1.430356	-0.436039
H	-0.869911	-1.216967	-0.108569
H	-3.580870	2.097366	-0.580960
C	-2.755464	-3.110782	0.310336
C	-2.734889	-4.073016	-0.736700
C	-2.564438	-3.516182	1.661276
C	-2.502864	-5.422178	-0.412220
C	-2.332500	-4.877109	1.932839
C	-2.299497	-5.815357	0.906421
H	-2.473770	-6.179378	-1.184548
H	-2.175425	-5.219550	2.947074
H	-2.117487	-6.857510	1.135318
C	-5.865711	0.700180	-0.305678
C	-6.495196	1.110103	0.902552
C	-6.580040	0.740845	-1.535074
C	-7.831198	1.548823	0.855117
C	-7.912642	1.191730	-1.530101
C	-8.527485	1.590979	-0.348180
H	-8.345287	1.854934	1.756603
H	-8.487425	1.228226	-2.446132
H	-9.555335	1.930228	-0.363908
C	-5.951790	0.291545	-2.854929
H	-4.892682	-0.005711	-2.714540
C	-5.934388	1.431867	-3.880580
H	-5.424053	2.320338	-3.450679
H	-5.376039	1.117381	-4.788199
H	-6.962565	1.718972	-4.185379
C	-6.668736	-0.943933	-3.411932
H	-6.659786	-1.758945	-2.656523
H	-7.721129	-0.712224	-3.679946
H	-6.145307	-1.310353	-4.320902
C	-5.774601	1.063680	2.251200
H	-4.719331	0.742868	2.133226
C	-6.428701	0.039797	3.185760
H	-5.839044	-0.051365	4.123070
H	-7.465420	0.339291	3.447767
H	-6.454476	-0.957075	2.695637
C	-5.718805	2.450387	2.903751
H	-5.121766	2.404097	3.838987
H	-5.232819	3.174019	2.214845
H	-6.733132	2.821066	3.159843
C	-2.608032	-2.522026	2.824084
H	-2.822829	-1.493844	2.468301
C	-2.946535	-3.685236	-2.200254
H	-3.115672	-2.594353	-2.306315
C	-1.704200	-4.002479	-3.039971
H	-0.820529	-3.491071	-2.605952
H	-1.506966	-5.094381	-3.077117
H	-1.841247	-3.633089	-4.078710
C	-4.194658	-4.363205	-2.777597
H	-4.072138	-5.465901	-2.820264
H	-5.080151	-4.122120	-2.151056
H	-4.388040	-3.990547	-3.806315
C	-1.255105	-2.445980	3.541919
H	-0.965518	-3.429333	3.967722
H	-0.469110	-2.112749	2.832218
H	-1.304691	-1.707641	4.369878
C	-3.735633	-2.867283	3.804363
H	-4.702295	-2.936086	3.260915
H	-3.541917	-3.831284	4.319901
H	-3.828067	-2.070298	4.573069
C	2.368741	-1.227530	-2.688775
C	1.488654	-1.331009	-3.835609

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 H   0.987374  -2.291793  -3.998221
 B   2.437088  -2.295759  -1.630143
 O   1.639740  -3.429231  -1.597702
 O   3.371585  -2.329827  -0.576110
 C   1.910197  -4.125429  -0.367363
 C   3.372220  -3.686548  -0.060188
 C   0.930492  -3.607179   0.670650
 H  -0.080288  -3.719052   0.268733
 H   0.985005  -4.160433   1.618277
 H   1.090920  -2.539476   0.877926
 C   1.718888  -5.608990  -0.590100
 H   2.010726  -6.184588   0.300257
 H   0.661210  -5.824843  -0.794358
 H   2.303868  -5.970468  -1.444730
 C   4.403213  -4.480742  -0.844386
 H   4.469868  -5.517766  -0.487643
 H   4.162787  -4.500916  -1.916510
 H   5.391168  -4.018702  -0.720880
 C   3.729807  -3.670334   1.409858
 H   3.072113  -3.018146   1.997856
 H   3.654689  -4.681364   1.835269
 H   4.767705  -3.335623   1.552441
Na   4.138815  -0.718106   0.898867
 H   1.806184  -0.875696  -4.780493
 H   3.155506  -0.462934  -2.734356
 H   0.047330  -0.478105  -3.923436
 O   6.232731  -1.509087   0.081914
 O   4.001018  -0.814428   3.266355
 C   6.230552  -1.094503  -1.249410
 H   6.110214  -1.983998  -1.903596
 H   5.370994  -0.414584  -1.427250
 C   7.419726  -1.078868   0.661509
 H   7.219453  -0.166498   1.263600
 H   7.815223  -1.868154   1.335385
 C   8.416952  -0.767537  -0.429714
 H   9.101919   0.059540  -0.142163
 H   9.002356  -1.679632  -0.681467
 C   7.534696  -0.391434  -1.575399
 H   7.956627  -0.729423  -2.546939
 H   7.382637   0.710224  -1.593730
 C   2.758366  -0.492984   3.797820
 H   1.977300  -0.597743   3.015832
 H   2.519042  -1.200121   4.622778
 C   4.932929  -0.048049   3.951531
 H   5.305425  -0.621343   4.829454
 H   5.792749   0.174009   3.286011
 C   4.269957   1.237669   4.403969
 H   4.573244   1.499514   5.441177
 H   4.532368   2.071763   3.716911
 C   2.801336   0.930399   4.320927
 H   2.314646   1.001619   5.318178
 H   2.299317   1.624757   3.613071
165
Figure_S5_imid-3_modeS1_prod(CuHadd) / electronic energy: -3525.674285600661 a.u. / lowest freq: 7.85 cm-1
 C   0.109390   3.509837   0.278317
 H   0.823751   3.466564   1.115804
 C  -1.225575   2.794015   0.584878
 H  -2.092893   3.389142   0.255904
 C  -0.009939   1.519783  -0.998260
 C   1.843645   2.969076  -1.536879
 C   1.727948   3.285372  -2.895343
 C   3.116068   2.934892  -0.946043
 C   2.854813   3.578568  -3.656630
 H   0.731954   3.292457  -3.344196
 C   4.241533   3.242592  -1.712499
 C   4.115159   3.571554  -3.059683
 H   2.746634   3.815811  -4.717063
 H   5.222317   3.185958  -1.237164
 H   5.004841   3.806821  -3.647571
 C  -2.122276   0.569784  -0.272001
 C  -3.479626   0.937793  -0.289774
 C  -1.784206  -0.792799  -0.220053
 C  -4.480783  -0.039020  -0.246166
 C  -2.791876  -1.768143  -0.159378
 C  -4.136032  -1.389387  -0.176670
 H  -4.912661  -2.144051  -0.121554
 S   3.359653   2.305144   0.718354
 O   4.794294   1.905674   0.756420
 O   2.469727   1.103029   0.766727
 O   2.997195   3.370851   1.670177
Cu   1.105255   0.238087  -1.937223
 C  -0.070536   4.942601  -0.156856
 C   0.505305   5.986304   0.588413
 C  -0.800972   5.254388  -1.319234
 C   0.352018   7.314431   0.179161
 H   1.072369   5.774565   1.486075
 C  -0.950604   6.583532  -1.724582
 H  -1.250021   4.467433  -1.912495
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C	-0.374806	7.612831	-0.976061
H	0.797843	8.112973	0.757955
H	-1.512348	6.815401	-2.620166
H	-0.491443	8.641611	-1.291350
C	-1.384039	2.455403	2.047045
C	-2.389528	3.071180	2.812242
C	-0.550121	1.499240	2.658201
C	-2.552189	2.741058	4.161165
H	-3.047638	3.806938	2.367191
C	-0.721584	1.167118	4.004375
H	0.221132	0.999911	2.088975
C	-1.722129	1.787414	4.755539
H	-3.325553	3.222605	4.745346
H	-0.079512	0.427377	4.464647
H	-1.854138	1.529547	5.798288
N	0.650430	2.680583	-0.817512
N	-1.112530	1.565507	-0.234880
H	-0.743779	-1.090237	-0.179545
H	-3.766244	1.979672	-0.339508
C	-2.449772	-3.192530	-0.007456
C	-2.413524	-4.042105	-1.147976
C	-2.167690	-3.716056	1.285287
C	-2.071115	-5.395708	-0.973651
C	-1.819736	-5.073933	1.405038
C	-1.771318	-5.900482	0.287343
H	-2.025580	-6.067939	-1.820231
H	-1.585158	-5.501282	2.370956
H	-1.501282	-6.942621	0.399697
C	-5.902623	0.348714	-0.245947
C	-6.571689	0.584654	0.987259
C	-6.617141	0.421619	-1.473820
C	-7.946104	0.884921	0.965481
C	-7.989266	0.730441	-1.442339
C	-8.642575	0.959665	-0.236120
H	-8.489888	1.054987	1.885271
H	-8.564650	0.785932	-2.357035
H	-9.700226	1.190247	-0.231997
C	-5.945872	0.153621	-2.821479
H	-4.861289	-0.041715	-2.697640
C	-6.048496	1.371766	-3.747827
H	-5.634142	2.269383	-3.240673
H	-5.460428	1.194812	-4.673735
H	-7.101152	1.574370	-4.036495
C	-6.529945	-1.098528	-3.486016
H	-6.439657	-1.967808	-2.799777
H	-7.599877	-0.954515	-3.745947
H	-5.968825	-1.333096	-4.415846
C	-5.851375	0.492179	2.333655
H	-4.767398	0.300441	2.197894
C	-6.390197	-0.679252	3.162504
H	-5.797510	-0.789853	4.095838
H	-7.454988	-0.521990	3.435783
H	-6.301984	-1.623878	2.583940
C	-5.947356	1.810145	3.112013
H	-5.345907	1.743644	4.043108
H	-5.546586	2.643771	2.496590
H	-6.995573	2.041152	3.394299
C	-2.234518	-2.850862	2.545302
H	-2.554016	-1.815836	2.308205
C	-2.713667	-3.526323	-2.555351
H	-2.963938	-2.446104	-2.542474
C	-1.487752	-3.662904	-3.465483
H	-0.625644	-3.130062	-3.013388
H	-1.212810	-4.727452	-3.619429
H	-1.695416	-3.205524	-4.456369
C	-3.932824	-4.235618	-3.156420
H	-3.731146	-5.314803	-3.322104
H	-4.804756	-4.131935	-2.475551
H	-4.198872	-3.773584	-4.131233
C	-0.856094	-2.727881	3.202184
H	-0.482783	-3.714308	3.548838
H	-0.131543	-2.303040	2.476503
H	-0.910801	-2.044289	4.075964
C	-3.274964	-3.388448	3.535317
H	-4.261677	-3.483384	3.033286
H	-2.977202	-4.379579	3.937207
H	-3.387752	-2.683960	4.387178
C	2.482212	-0.751529	-2.965765
C	1.919286	-0.939211	-4.368754
H	1.040013	-1.602727	-4.369220
B	2.672903	-1.975929	-2.104684
O	1.953113	-3.161980	-2.220697
O	3.609594	-2.098967	-1.044113
C	2.214397	-3.945135	-1.044380
C	3.657871	-3.501220	-0.683139
C	1.219908	-3.515062	0.021566
H	0.215649	-3.587713	-0.403478
H	1.261552	-4.144630	0.921158

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 H   1.377012  -2.467258   0.318579
 C   2.050302  -5.411002  -1.375541
 H   2.339850  -6.045607  -0.525316
 H   0.999299  -5.628539  -1.610465
 H   2.651440  -5.700705  -2.246297
 C   4.707002  -4.173997  -1.553667
 H   4.822879  -5.236434  -1.297193
 H   4.450069  -4.104353  -2.619775
 H   5.681276  -3.689463  -1.405387
 C   4.013740  -3.649682   0.779288
 H   3.363199  -3.052442   1.429470
 H   3.928027  -4.701306   1.089524
 H   5.052127  -3.335589   0.955414
Na   4.157703  -0.440982   0.468840
 H   2.640204  -1.395571  -5.075406
 H   3.361765  -0.080357  -2.954163
 H   1.591891   0.002713  -4.842794
 O   6.411594  -1.084154   0.308935
 O   3.988808  -0.851969   2.749139
 C   6.879096  -0.964107  -0.992364
 H   7.614625  -1.774050  -1.196132
 H   6.036111  -1.063477  -1.707783
 C   7.267341  -0.336698   1.110413
 H   6.682477   0.148055   1.920063
 H   8.014777  -1.014119   1.578741
 C   7.963580   0.715437   0.261719
 H   7.641773   1.740980   0.546828
 H   9.067767   0.630586   0.364765
 C   7.533183   0.390318  -1.139262
 H   8.395259   0.352525  -1.840231
 H   6.788164   1.135210  -1.495929
 C   4.763861  -1.526019   3.681088
 H   5.474871  -2.202993   3.162862
 H   5.347327  -0.787162   4.273891
 C   2.730070  -0.656879   3.310997
 H   2.590048   0.421143   3.542643
 H   1.958228  -0.960472   2.572921
 C   2.594357  -1.493010   4.572834
 H   2.556396  -0.833691   5.468096
 H   1.690477  -2.138378   4.546115
 C   3.846651  -2.313349   4.585176
 H   4.266466  -2.419206   5.609018
 H   3.651005  -3.316744   4.145727
165
Figure_S5_imid-3_modeS2_ed(CuHadd) / electronic energy: -3525.647282907852 a.u. / lowest freq: 11.24 cm-1
 C   1.784386   0.998893   2.406401
 H   2.390942   0.270403   2.960597
 C   0.269908   0.667579   2.410006
 H  -0.341883   1.521455   2.742969
 C   1.071845   0.573414   0.183629
 C   3.393038   1.172882   0.373314
 C   3.402135   2.036091  -0.732449
 C   4.602939   0.574813   0.778159
 C   4.575252   2.324159  -1.419513
 H   2.460791   2.491607  -1.049289
 C   5.779904   0.898434   0.096292
 C   5.778303   1.767402  -0.990549
 H   4.540722   2.989515  -2.285486
 H   6.701034   0.409543   0.418555
 H   6.711440   1.990807  -1.511915
 C  -1.252247   0.037031   0.479714
 C  -2.383851   0.812676   0.761368
 C  -1.395082  -1.165580  -0.229389
 C  -3.650685   0.386250   0.346184
 C  -2.665896  -1.602690  -0.627617
 C  -3.791214  -0.822275  -0.343188
 H  -4.776572  -1.164856  -0.638219
 S   4.735779  -0.716046   2.044031
 O   6.022482  -1.384093   1.773041
 O   3.551043  -1.589891   1.762201
 O   4.655951  -0.045007   3.355466
Cu   1.205157   0.390391  -1.782974
 C   2.065928   2.387991   2.926121
 C   2.849366   2.574398   4.078784
 C   1.531142   3.515908   2.276676
 C   3.117209   3.862485   4.551710
 H   3.244029   1.726282   4.621187
 C   1.802749   4.802152   2.752075
 H   0.897040   3.394667   1.408070
 C   2.598889   4.975478   3.886039
 H   3.723836   3.997436   5.437846
 H   1.393834   5.665532   2.244562
 H   2.807097   5.971788   4.253996
 C  -0.079210  -0.535432   3.251879
 C  -0.917574  -0.394591   4.372087
 C   0.397705  -1.815128   2.914003
 C  -1.265927  -1.510092   5.139339
 H  -1.304163   0.577175   4.651973
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C	0.059438	-2.924484	3.692433
H	1.017735	-1.956668	2.041057
C	-0.775674	-2.773545	4.801477
H	-1.915093	-1.394259	5.997544
H	0.436848	-3.903933	3.429417
H	-1.044889	-3.636009	5.397238
N	2.127957	0.895084	0.959681
N	0.011832	0.419548	0.980926
H	-0.526868	-1.781723	-0.419846
H	-2.282378	1.740648	1.310627
C	-2.843802	-2.922796	-1.263040
C	-2.923442	-3.027865	-2.679950
C	-3.051226	-4.072844	-0.449645
C	-3.215941	-4.279711	-3.252287
C	-3.337288	-5.301886	-1.072009
C	-3.415011	-5.401351	-2.456084
H	-3.309552	-4.391166	-4.324110
H	-3.515802	-6.192340	-0.484155
H	-3.642649	-6.354632	-2.915599
C	-4.843350	1.187279	0.672531
C	-5.442125	1.074419	1.958431
C	-5.398042	2.062794	-0.301777
C	-6.577030	1.853952	2.247567
C	-6.534758	2.819531	0.036123
C	-7.113132	2.716251	1.296873
H	-7.057465	1.793208	3.215211
H	-6.981293	3.496161	-0.680583
H	-7.987874	3.306609	1.537909
C	-4.799473	2.205042	-1.701905
H	-3.908111	1.557431	-1.826851
C	-4.314431	3.636230	-1.954783
H	-3.598751	3.938628	-1.160800
H	-3.791322	3.689164	-2.933470
H	-5.160551	4.354827	-1.969251
C	-5.799396	1.762861	-2.776887
H	-6.154084	0.732026	-2.563285
H	-6.676215	2.442910	-2.816555
H	-5.309498	1.761550	-3.774129
C	-4.902240	0.122034	3.027564
H	-4.013725	-0.432470	2.663134
C	-5.939824	-0.946765	3.391194
H	-5.492175	-1.690046	4.085355
H	-6.828110	-0.497001	3.882519
H	-6.267482	-1.483390	2.475121
C	-4.441063	0.890910	4.271271
H	-3.976412	0.192395	4.999345
H	-3.682211	1.650785	3.986025
H	-5.291731	1.400615	4.770291
C	-3.019320	-4.007384	1.078319
H	-2.743252	-2.993799	1.433776
C	-2.755666	-1.815388	-3.594805
H	-2.436086	-0.923859	-3.017592
C	-1.665019	-2.046598	-4.649417
H	-0.706404	-2.309841	-4.154600
H	-1.941037	-2.857953	-5.354097
H	-1.511440	-1.120396	-5.242687
C	-4.088725	-1.450928	-4.257079
H	-4.430372	-2.258110	-4.939240
H	-4.864775	-1.286186	-3.479640
H	-3.980149	-0.512793	-4.842315
C	-1.960992	-4.954233	1.655409
H	-2.182712	-6.014259	1.413723
H	-0.963588	-4.691277	1.246909
H	-1.923838	-4.853823	2.760540
C	-4.403459	-4.302122	1.667334
H	-5.154226	-3.606273	1.235142
H	-4.716301	-5.346444	1.456051
H	-4.388351	-4.152961	2.768326
C	-0.140173	1.661420	-2.702283
C	0.646110	0.957943	-3.625959
H	1.502183	1.448730	-4.103773
B	0.105531	3.142751	-2.358612
O	1.177424	3.859532	-2.844360
O	-0.752720	3.915881	-1.615564
C	1.098945	5.205601	-2.309413
C	-0.400252	5.301445	-1.849386
C	2.082031	5.303021	-1.157846
H	3.095556	5.071402	-1.511540
H	2.100908	6.311688	-0.723785
H	1.838756	4.593479	-0.358828
C	1.484478	6.180778	-3.401530
H	1.363522	7.218721	-3.059629
H	2.539164	6.041520	-3.674390
H	0.883015	6.044141	-4.307832
C	-1.316199	5.815833	-2.948247
H	-1.123511	6.873184	-3.174013
H	-1.199964	5.239098	-3.876129
H	-2.361745	5.731865	-2.627306

C	-0.623747	6.081971	-0.573323
H	-0.090673	5.639144	0.274996
H	-0.291410	7.123837	-0.685102
H	-1.693199	6.096861	-0.324566
Na	2.786243	-1.923363	-0.306437
H	0.278580	0.073710	-4.149987
H	-1.120302	1.238772	-2.441585
H	2.150827	-0.816323	-2.210648
O	4.511993	-2.664090	-1.613363
O	1.388223	-3.757433	-0.430435
C	5.031432	-1.756508	-2.529908
H	4.670016	-2.026150	-3.546131
H	4.673858	-0.733580	-2.289412
C	5.540419	-3.501509	-1.194411
H	5.704806	-3.349905	-0.106969
H	5.247331	-4.560475	-1.358542
C	6.808467	-3.180100	-1.959273
H	7.705571	-3.202039	-1.302873
H	6.937646	-3.895134	-2.801943
C	6.542420	-1.808819	-2.488281
H	6.933150	-1.045750	-1.780502
H	6.990435	-1.657358	-3.494341
C	1.029363	-4.089710	-1.729198
H	0.217467	-3.418342	-2.078122
H	1.908406	-3.958006	-2.398629
C	1.835646	-4.925803	0.172601
H	2.943861	-4.977110	0.092559
H	1.564897	-4.912347	1.249441
C	1.200485	-6.119137	-0.519564
H	0.432970	-6.593640	0.130799
H	1.972723	-6.871411	-0.792445
C	0.564922	-5.529418	-1.746420
H	0.894698	-6.048739	-2.672436
H	-0.541737	-5.575502	-1.665090

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Figure_S5_imid-3_modeS2_ts(CuHadd)_01 / electronic energy: -3525.629085258236 a.u. / lowest freq: -769.55 cm-1

C	1.691595	0.440110	2.732392
H	2.232837	-0.387712	3.211027
C	0.159449	0.209654	2.635551
H	-0.411922	1.038846	3.083066
C	1.049811	0.400857	0.447349
C	3.392484	0.820846	0.822150
C	3.491988	1.888842	-0.081122
C	4.550911	0.088195	1.147196
C	4.711264	2.252847	-0.640866
H	2.588966	2.451028	-0.333836
C	5.774459	0.483227	0.598365
C	5.865302	1.559190	-0.281440
H	4.746017	3.085347	-1.348349
H	6.656142	-0.109123	0.848824
H	6.834440	1.838780	-0.700341
C	-1.315836	0.009642	0.581832
C	-2.396739	0.826930	0.935412
C	-1.510275	-1.048191	-0.317866
C	-3.664876	0.588120	0.393366
C	-2.784188	-1.301809	-0.840756
C	-3.859217	-0.478319	-0.490633
H	-4.847234	-0.677967	-0.889643
S	4.541880	-1.460010	2.092865
O	5.861942	-2.066492	1.842279
O	3.415204	-2.226979	1.469114
O	4.287499	-1.116079	3.506148
Cu	1.231698	0.638243	-1.438716
C	2.036664	1.733257	3.432286
C	2.823141	1.729042	4.597698
C	1.583043	2.963208	2.920707
C	3.161369	2.931700	5.226089
H	3.173162	0.798328	5.024240
C	1.925256	4.162838	3.549693
H	0.960549	2.988096	2.036988
C	2.716085	4.147426	4.700765
H	3.769322	2.920891	6.121475
H	1.575578	5.103950	3.145120
H	2.980274	5.076926	5.188199
C	-0.299859	-1.085508	3.259615
C	-1.243170	-1.072702	4.302964
C	0.164474	-2.322003	2.775451
C	-1.705273	-2.271791	4.853129
H	-1.628203	-0.136371	4.686797
C	-0.291296	-3.517636	3.336531
H	0.867536	-2.359968	1.956055
C	-1.228047	-3.493082	4.372070
H	-2.435060	-2.253757	5.652177
H	0.072538	-4.464707	2.960281
H	-1.587379	-4.420603	4.798498
N	2.093955	0.503590	1.301405
N	-0.053002	0.204034	1.180602
H	-0.682516	-1.698288	-0.571871

H	-2.254489	1.644388	1.631673
C	-3.013951	-2.473361	-1.705053
C	-2.973007	-2.333620	-3.119661
C	-3.327513	-3.731664	-1.119212
C	-3.248845	-3.456888	-3.920508
C	-3.597989	-4.823780	-1.963858
C	-3.554678	-4.685891	-3.346741
H	-3.235127	-3.383615	-4.999878
H	-3.845737	-5.793307	-1.552439
H	-3.765011	-5.538408	-3.979709
C	-4.805585	1.434077	0.783264
C	-5.532828	1.137277	1.969399
C	-5.188553	2.530899	-0.037562
C	-6.629703	1.948860	2.311788
C	-6.297539	3.307572	0.344512
C	-7.005552	3.019348	1.506770
H	-7.205480	1.751203	3.206368
H	-6.620863	4.144557	-0.260281
H	-7.855126	3.629812	1.784893
C	-4.437234	2.886708	-1.321665
H	-3.571874	2.211825	-1.480969
C	-3.854698	4.303611	-1.252313
H	-3.209150	4.404071	-0.353602
H	-3.232712	4.501618	-2.151015
H	-4.656032	5.070475	-1.207710
C	-5.338357	2.719045	-2.550425
H	-5.750347	1.687596	-2.579504
H	-6.180384	3.442727	-2.534026
H	-4.750057	2.882516	-3.478730
C	-5.167206	-0.041232	2.874411
H	-4.287289	-0.591848	2.484404
C	-6.306484	-1.065406	2.936592
H	-5.983432	-1.958470	3.513434
H	-7.207561	-0.638098	3.424681
H	-6.574341	-1.395942	1.910080
C	-4.775892	0.438421	4.277128
H	-4.423182	-0.420127	4.887693
H	-3.948373	1.176649	4.206990
H	-5.635898	0.909164	4.798039
C	-3.398553	-3.929906	0.396096
H	-3.158547	-2.992837	0.938352
C	-2.654327	-1.000251	-3.794708
H	-2.414521	-0.220054	-3.044450
C	-1.418328	-1.113485	-4.695185
H	-0.558421	-1.502554	-4.109383
H	-1.602406	-1.789791	-5.555819
H	-1.146819	-0.112534	-5.092979
C	-3.863900	-0.480187	-4.579520
H	-4.112940	-1.153065	-5.427083
H	-4.746184	-0.404767	-3.908411
H	-3.648929	0.532538	-4.982880
C	-2.368949	-4.962648	0.868572
H	-2.556692	-5.960561	0.420516
H	-1.347604	-4.627308	0.590276
H	-2.411905	-5.064468	1.973478
C	-4.814967	-4.318499	0.835807
H	-5.543887	-3.560571	0.476674
H	-5.102587	-5.313826	0.436586
H	-4.872510	-4.353549	1.944926
C	0.431481	1.866867	-2.884628
C	1.466515	1.007328	-3.410285
H	2.454146	1.453774	-3.586025
B	0.645352	3.285302	-2.405998
O	1.878078	3.930633	-2.319948
O	-0.393525	4.137340	-2.055635
C	1.650851	5.233441	-1.737788
C	0.134406	5.475443	-2.044667
C	1.918337	5.129925	-0.245913
H	2.947897	4.790395	-0.066766
H	1.791897	6.095362	0.263320
H	1.231885	4.408768	0.217877
C	2.592203	6.229615	-2.379716
H	2.382924	7.251085	-2.029718
H	3.633029	5.995417	-2.115796
H	2.513788	6.218358	-3.473663
C	-0.093137	6.061102	-3.430556
H	0.220228	7.112607	-3.492935
H	0.450311	5.493776	-4.199408
H	-1.163352	6.012456	-3.672981
C	-0.597593	6.292892	-1.001418
H	-0.602680	5.796981	-0.023068
H	-0.138535	7.285422	-0.884435
H	-1.642476	6.445546	-1.303132
Na	2.575344	-1.967118	-0.561637
H	1.213989	0.288296	-4.195131
H	-0.603489	1.542576	-3.048906
H	2.036846	-0.220459	-2.528691
O	4.324563	-2.251752	-2.002178

O 1.187102 -3.762926 -0.841443
C 4.840665 -1.191430 -2.740099
H 4.413641 -1.228505 -3.765718
H 4.543506 -0.230175 -2.271874
C 5.360429 -3.135404 -1.720202
H 5.585419 -3.089041 -0.634252
H 5.045641 -4.171116 -1.969503
C 6.586777 -2.748965 -2.518000
H 7.524091 -2.908911 -1.941907
H 6.620545 -3.326101 -3.468703
C 6.349436 -1.302699 -2.805133
H 6.814950 -0.676809 -2.012642
H 6.744832 -1.007844 -3.801410
C 0.701869 -4.101420 -2.096101
H -0.137458 -3.427174 -2.367438
H 1.512277 -3.976540 -2.848213
C 1.666820 -4.931378 -0.263516
H 2.765498 -4.994347 -0.426766
H 1.476381 -4.905156 0.830152
C 0.970115 -6.125066 -0.892461
H 0.261290 -6.594308 -0.175022
H 1.713279 -6.881248 -1.228099
C 0.231840 -5.539510 -2.062039
H 0.477011 -6.066278 -3.009877
H -0.863728 -5.582122 -1.883982
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Figure_S5_imid-3_modeS2_ts(CuHadd)_02 / electronic energy: -3525.627984592980 a.u. / lowest freq: -714.49 cm-1
C 2.067313 1.324238 2.350164
H 2.765913 0.557224 2.715921
C 0.584706 0.915595 2.519800
H -0.043610 1.762610 2.844524
C 1.132439 0.897140 0.224459
C 3.347756 1.803129 0.157477
C 3.175528 2.798178 -0.812814
C 4.604994 1.192908 0.301234
C 4.238188 3.221999 -1.603076
H 2.180767 3.227279 -0.951265
C 5.672668 1.644835 -0.480312
C 5.501434 2.660342 -1.418095
H 4.069514 3.992629 -2.359766
H 6.637060 1.145538 -0.367866
H 6.349000 2.991367 -2.022194
C -1.039957 0.013064 0.763331
C -2.224909 0.500172 1.335358
C -1.104162 -1.053333 -0.147536
C -3.457568 -0.075083 1.002465
C -2.334559 -1.645377 -0.461971
C -3.510672 -1.153711 0.113681
H -4.463231 -1.614078 -0.122202
S 4.868639 -0.293192 1.296068
O 6.033221 -0.953927 0.666058
O 3.598775 -1.063183 1.103671
O 5.079625 0.138067 2.691044
Cu 1.088867 0.890985 -1.679740
C 2.385551 2.650101 2.993659
C 3.300446 2.722755 4.058385
C 1.776568 3.832777 2.535060
C 3.606691 3.955246 4.643658
H 3.773746 1.827687 4.440588
C 2.086841 5.062673 3.120979
H 1.062930 3.799182 1.723770
C 3.002431 5.124263 4.174063
H 4.312729 4.003800 5.462547
H 1.616603 5.967691 2.758499
H 3.241714 6.077185 4.627996
C 0.402782 -0.231747 3.481159
C -0.204940 -0.014797 4.729937
C 0.827891 -1.530811 3.144634
C -0.377989 -1.074612 5.624928
H -0.541819 0.974409 5.013919
C 0.649441 -2.587525 4.041535
H 1.284579 -1.727495 2.184465
C 0.045950 -2.360037 5.280178
H -0.844620 -0.899375 6.585613
H 0.980743 -3.583009 3.777855
H -0.092049 -3.179516 5.973484
N 2.195569 1.402370 0.879254
N 0.216492 0.545477 1.140137
H -0.192171 -1.457180 -0.568667
H -2.195607 1.327309 2.032895
C -2.384041 -2.835005 -1.334848
C -2.828090 -2.718068 -2.682803
C -2.004721 -4.106068 -0.816228
C -2.876328 -3.874293 -3.483061
C -2.033572 -5.223408 -1.670490
C -2.467596 -5.106360 -2.985728
H -3.223653 -3.825036 -4.506417
H -1.732180 -6.199735 -1.314738

H	-2.495621	-5.980561	-3.623390
C	-4.701358	0.449177	1.594020
C	-5.138607	-0.023476	2.862626
C	-5.469400	1.415324	0.886054
C	-6.334901	0.486472	3.399807
C	-6.653743	1.900060	1.470294
C	-7.078370	1.439690	2.712045
H	-6.701311	0.143342	4.358324
H	-7.260381	2.636844	0.960386
H	-7.995307	1.821005	3.142895
C	-5.054460	1.933800	-0.491812
H	-4.110243	1.462350	-0.831821
C	-4.782561	3.441785	-0.459975
H	-4.003683	3.671119	0.298516
H	-4.411387	3.776886	-1.451369
H	-5.702258	4.014654	-0.218195
C	-6.105936	1.585233	-1.552088
H	-6.305192	0.492520	-1.542940
H	-7.058524	2.125455	-1.369117
H	-5.733502	1.861605	-2.561743
C	-4.362108	-1.081054	3.648884
H	-3.431981	-1.374016	3.120526
C	-5.183981	-2.366369	3.800276
H	-4.571863	-3.153768	4.290115
H	-6.092955	-2.193681	4.414238
H	-5.489947	-2.739757	2.799372
C	-3.919168	-0.544776	5.015445
H	-3.292791	-1.301261	5.533650
H	-3.314098	0.377471	4.882253
H	-4.790420	-0.314180	5.663354
C	-1.587246	-4.301082	0.643101
H	-1.671434	-3.356692	1.217615
C	-3.270921	-1.383539	-3.283879
H	-3.103125	-0.550130	-2.571977
C	-2.461694	-1.030549	-4.539192
H	-1.376587	-1.056726	-4.312101
H	-2.670982	-1.734060	-5.371682
H	-2.718324	-0.004467	-4.879356
C	-4.772643	-1.399072	-3.589824
H	-5.014490	-2.148109	-4.373297
H	-5.344549	-1.645541	-2.669940
H	-5.099672	-0.398406	-3.944529
C	-0.120996	-4.732533	0.741265
H	0.051417	-5.703503	0.231360
H	0.526826	-3.959605	0.278265
H	0.175317	-4.837951	1.805602
C	-2.506883	-5.298245	1.359321
H	-3.566046	-4.978269	1.256545
H	-2.396360	-6.322242	0.945116
H	-2.260045	-5.331213	2.442255
C	-0.148423	1.701706	-3.114915
C	1.009640	1.046133	-3.685282
H	1.811297	1.685606	-4.076975
B	-0.251704	3.173917	-2.790739
O	0.791822	4.098449	-2.864926
O	-1.443322	3.796112	-2.429018
C	0.296131	5.354764	-2.355064
C	-1.245683	5.214207	-2.573852
C	0.650924	5.436683	-0.879182
H	1.740009	5.379647	-0.747807
H	0.314697	6.379768	-0.426690
H	0.189861	4.607296	-0.323253
C	0.942449	6.488279	-3.121475
H	0.518417	7.458214	-2.822566
H	2.021519	6.520333	-2.915960
H	0.811729	6.374883	-4.204584
C	-1.666292	5.590706	-3.986812
H	-1.610986	6.674803	-4.158856
H	-1.038317	5.090618	-4.737707
H	-2.704763	5.274276	-4.153570
C	-2.093441	5.949420	-1.557315
H	-1.957514	5.546525	-0.546196
H	-1.844807	7.020640	-1.539539
H	-3.158269	5.864713	-1.811544
Na	3.183538	-1.799278	-0.991210
H	0.850032	0.175333	-4.330414
H	-1.078649	1.121643	-3.092486
H	2.016846	0.173622	-2.771507
O	2.296113	-2.845992	-2.906120
O	3.225119	-3.955322	-0.181769
C	0.928276	-3.037269	-3.037899
H	0.570201	-3.740377	-2.258717
H	0.407665	-2.064283	-2.904088
C	2.816432	-2.655415	-4.182341
H	3.132745	-1.596504	-4.299382
H	3.711037	-3.302893	-4.303824
C	1.770388	-3.015682	-5.224980
H	1.425063	-2.100459	-5.755152

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H   2.158965  -3.752128  -5.961911
C   0.654068  -3.593786  -4.413395
H  -0.341177  -3.285646  -4.797397
H   0.727583  -4.703741  -4.393912
C   3.268098  -5.139830  -0.910043
H   2.248696  -5.364560  -1.290323
H   3.947761  -5.018350  -1.780422
C   3.564807  -4.238339   1.136201
H   4.590645  -3.858168   1.333697
H   2.858821  -3.727347   1.823675
C   3.518146  -5.733808   1.354618
H   2.512739  -6.035236   1.723049
H   4.301303  -6.073580   2.066687
C   3.742883  -6.271516  -0.020956
H   4.827626  -6.456847  -0.185314
H   3.167732  -7.206630  -0.196946
165
Figure_S5_imid-3_modeS2_ts(CuHadd)_03 / electronic energy: -3525.628301013297 a.u. / lowest freq: -756.56 cm-1
C   1.766908   0.294954   2.779292
H   2.115560  -0.659505   3.199906
C   0.225923   0.376995   2.642655
H  -0.166033   1.359869   2.955871
C   1.183870   0.309676   0.483048
C   3.546675   0.444804   0.907564
C   3.852051   1.480694   0.015318
C   4.539370  -0.495673   1.235679
C   5.129399   1.618866  -0.516409
H   3.062133   2.182874  -0.262855
C   5.827416  -0.329314   0.717109
C   6.130947   0.723752  -0.143099
H   5.333901   2.431625  -1.217999
H   6.579211  -1.080387   0.967039
H   7.142739   0.825946  -0.541327
C  -1.211875   0.181092   0.556933
C  -2.178772   1.162255   0.815411
C  -1.526318  -0.900895  -0.276756
C  -3.453166   1.059973   0.244130
C  -2.808822  -1.016270  -0.825302
C  -3.768479  -0.031284  -0.572029
H  -4.763701  -0.124256  -0.991769
S   4.202156  -2.018182   2.154501
O   5.285775  -2.940154   1.761684
O   2.860600  -2.440103   1.634858
O   4.175189  -1.667627   3.587634
Cu  1.482031   0.454847  -1.398851
C   2.338939   1.438887   3.579088
C   2.994158   1.199123   4.799469
C   2.225378   2.762191   3.114747
C   3.537221   2.260449   5.530331
H   3.080689   0.194122   5.190833
C   2.771359   3.819846   3.846347
H   1.713429   2.970760   2.186174
C   3.428715   3.569071   5.052930
H   4.041625   2.068081   6.468411
H   2.683428   4.833776   3.477807
H   3.850616   4.388809   5.619849
C  -0.502583  -0.706324   3.398025
C  -1.389128  -0.370845   4.436671
C  -0.344300  -2.059675   3.046377
C  -2.098153  -1.369542   5.110846
H  -1.536521   0.662923   4.722983
C  -1.051190  -3.054534   3.726928
H   0.313249  -2.341641   2.235755
C  -1.929814  -2.709859   4.756054
H  -2.779870  -1.103902   5.908291
H  -0.923899  -4.093208   3.451952
H  -2.481239  -3.481346   5.277595
N   2.205701   0.366371   1.363196
N   0.047948   0.233897   1.189933
H  -0.789453  -1.673965  -0.458254
H  -1.944551   2.000427   1.460011
C  -3.177100  -2.211368  -1.603667
C  -2.968412  -2.238339  -3.009830
C  -3.771407  -3.324513  -0.945766
C  -3.355661  -3.383162  -3.730287
C  -4.146000  -4.443086  -1.712015
C  -3.934877  -4.471132  -3.086203
H  -3.215709  -3.436046  -4.801838
H  -4.603689  -5.305064  -1.244902
H  -4.227047  -5.342491  -3.658053
C  -4.476973   2.082151   0.523266
C  -5.255134   2.000180   1.711654
C  -4.715132   3.121248  -0.418828
C  -6.258072   2.961978   1.931945
C  -5.736974   4.052058  -0.157073
C  -6.494915   3.972837   1.006401
H  -6.871201   2.927355   2.822836
H  -5.953159   4.847549  -0.857948
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H	-7.275510	4.699757	1.190970
C	-3.900760	3.252940	-1.706948
H	-3.098707	2.488392	-1.755141
C	-3.187097	4.608194	-1.779402
H	-2.568815	4.757610	-0.868586
H	-2.516130	4.636778	-2.664314
H	-3.910668	5.445535	-1.865111
C	-4.783071	3.025998	-2.939576
H	-5.282483	2.035837	-2.870090
H	-5.559019	3.815294	-3.029335
H	-4.160731	3.034979	-3.859995
C	-5.049810	0.890613	2.744813
H	-4.227167	0.209250	2.447489
C	-6.299376	0.010467	2.865571
H	-6.095624	-0.848055	3.540907
H	-7.158688	0.583223	3.273419
H	-6.575687	-0.393011	1.867860
C	-4.646800	1.469631	4.106274
H	-4.421943	0.647044	4.817591
H	-3.733711	2.093165	3.996664
H	-5.458480	2.091474	4.538481
C	-4.026226	-3.337935	0.563244
H	-3.675257	-2.400708	1.040803
C	-2.352934	-1.058858	-3.762195
H	-2.082028	-0.237835	-3.067896
C	-1.051790	-1.465263	-4.464687
H	-0.325723	-1.857365	-3.720525
H	-1.231570	-2.241701	-5.237098
H	-0.599429	-0.581496	-4.961906
C	-3.354072	-0.458468	-4.756079
H	-3.601561	-1.179113	-5.563771
H	-4.288872	-0.174431	-4.226702
H	-2.927908	0.457420	-5.218770
C	-3.251223	-4.468942	1.248414
H	-3.586327	-5.465714	0.893156
H	-2.166245	-4.356929	1.042500
H	-3.401259	-4.420999	2.348010
C	-5.525713	-3.430660	0.868477
H	-6.067484	-2.606130	0.357350
H	-5.946424	-4.401621	0.532265
H	-5.698035	-3.331398	1.961689
C	0.904730	1.711089	-2.932231
C	1.888646	0.740951	-3.352501
H	2.926024	1.083671	-3.461687
B	1.216285	3.116745	-2.469713
O	2.493361	3.633678	-2.249448
O	0.241897	4.085846	-2.266202
C	2.332805	4.955296	-1.689433
C	0.909073	5.358547	-2.194921
C	2.379332	4.829224	-0.175284
H	3.336187	4.390250	0.138907
H	2.283621	5.804012	0.322830
H	1.566087	4.181410	0.182928
C	3.453983	5.843374	-2.183782
H	3.301258	6.883868	-1.861427
H	4.416622	5.507357	-1.773847
H	3.533331	5.830151	-3.277566
C	0.936133	5.939361	-3.600886
H	1.377163	6.945809	-3.621052
H	1.508585	5.299451	-4.287210
H	-0.090291	6.010659	-3.985246
C	0.147606	6.275980	-1.262157
H	-0.048386	5.801934	-0.292731
H	0.705836	7.207153	-1.085995
H	-0.820280	6.550026	-1.702854
Na	2.249101	-2.470818	-0.499340
H	1.624109	0.024081	-4.135404
H	-0.139796	1.482197	-3.179105
H	2.281518	-0.512342	-2.391983
O	3.798221	-3.028603	-2.158982
O	0.626454	-4.078766	-0.519140
C	3.360224	-3.164588	-3.473949
H	3.402049	-4.239366	-3.753185
H	2.305304	-2.824402	-3.555608
C	4.898548	-2.178847	-2.158854
H	4.577490	-1.173690	-1.812152
H	5.671962	-2.564313	-1.461314
C	5.451467	-2.080394	-3.560888
H	5.881587	-1.075996	-3.766818
H	6.221097	-2.867351	-3.722769
C	4.248394	-2.357344	-4.401952
H	3.748122	-1.402909	-4.677657
H	4.511341	-2.924133	-5.321566
C	0.056743	-4.596112	-1.674105
H	-0.674342	-3.871312	-2.087561
H	0.855402	-4.762775	-2.429432
C	0.787166	-5.122462	0.387228
H	1.870160	-5.288677	0.571311

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 H   0.311339  -4.838047   1.348985
 C   0.143119  -6.385832  -0.155882
 H  -0.525576  -6.862355   0.594115
 H   0.926244  -7.109016  -0.474392
 C  -0.625055  -5.902682  -1.344562
 H  -0.575454  -6.619438  -2.192776
 H  -1.684468  -5.721172  -1.065412
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Figure_S5_imid-3_modeS2_ts(CuHadd)_04 / electronic energy: -3525.628301013864 a.u. / lowest freq: -756.50 cm-1
 C   1.766908   0.294955   2.779292
 H   2.115559  -0.659505   3.199905
 C   0.225923   0.376996   2.642655
 H  -0.166032   1.359870   2.955871
 C   1.183871   0.309677   0.483048
 C   3.546675   0.444805   0.907564
 C   3.852051   1.480695   0.015318
 C   4.539370  -0.495672   1.235678
 C   5.129399   1.618867  -0.516410
 H   3.062133   2.182875  -0.262855
 C   5.827415  -0.329313   0.717108
 C   6.130947   0.723753  -0.143100
 H   5.333901   2.431626  -1.218000
 H   6.579210  -1.080387   0.967037
 H   7.142739   0.825947  -0.541328
 C  -1.211874   0.181093   0.556932
 C  -2.178773   1.162256   0.815411
 C  -1.526317  -0.900894  -0.276757
 C  -3.453166   1.059973   0.244130
 C  -2.808821  -1.016269  -0.825303
 C  -3.768478  -0.031283  -0.572029
 H  -4.763700  -0.124256  -0.991770
 S   4.202155  -2.018182   2.154500
 O   5.285775  -2.940154   1.761682
 O   2.860599  -2.440102   1.634856
 O   4.175189  -1.667627   3.587633
Cu   1.482031   0.454848  -1.398851
 C   2.338939   1.438887   3.579088
 C   2.994157   1.199122   4.799469
 C   2.225379   2.762190   3.114748
 C   3.537221   2.260447   5.530333
 H   3.080688   0.194120   5.190833
 C   2.771360   3.819845   3.846349
 H   1.713430   2.970760   2.186175
 C   3.428715   3.569070   5.052932
 H   4.041624   2.068078   6.468412
 H   2.683430   4.833776   3.477809
 H   3.850616   4.388806   5.619852
 C  -0.502583  -0.706322   3.398024
 C  -1.389128  -0.370844   4.436671
 C  -0.344301  -2.059674   3.046376
 C  -2.098153  -1.369541   5.110845
 H  -1.536520   0.662924   4.722983
 C  -1.051191  -3.054533   3.726926
 H   0.313248  -2.341639   2.235754
 C  -1.929815  -2.709857   4.756053
 H  -2.779870  -1.103901   5.908291
 H  -0.923900  -4.093207   3.451951
 H  -2.481240  -3.481344   5.277594
 N   2.205701   0.366372   1.363196
 N   0.047949   0.233899   1.189933
 H  -0.789452  -1.673964  -0.458255
 H  -1.944552   2.000428   1.460011
 C  -3.177098  -2.211367  -1.603669
 C  -2.968409  -2.238337  -3.009832
 C  -3.771405  -3.324512  -0.945769
 C  -3.355657  -3.383161  -3.730290
 C  -4.145997  -4.443085  -1.712019
 C  -3.934874  -4.471131  -3.086206
 H  -3.215705  -3.436044  -4.801840
 H  -4.603686  -5.305063  -1.244905
 H  -4.227043  -5.342490  -3.658056
 C  -4.476974   2.082150   0.523266
 C  -5.255136   2.000177   1.711654
 C  -4.715133   3.121248  -0.418826
 C  -6.258074   2.961975   1.931945
 C  -5.736975   4.052058  -0.157071
 C  -6.494917   3.972835   1.006402
 H  -6.871204   2.927350   2.822836
 H  -5.953160   4.847550  -0.857945
 H  -7.275512   4.699754   1.190972
 C  -3.900760   3.252942  -1.706946
 H  -3.098707   2.488394  -1.755140
 C  -3.187097   4.608196  -1.779397
 H  -2.568814   4.757610  -0.868581
 H  -2.516130   4.636781  -2.664309
 H  -3.910668   5.445537  -1.865104
 C  -4.783070   3.026002  -2.939575
 H  -5.282483   2.035842  -2.870091
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H	-5.559018	3.815299	-3.029333
H	-4.160730	3.034985	-3.859993
C	-5.049812	0.890609	2.744811
H	-4.227168	0.209247	2.447487
C	-6.299377	0.010463	2.865567
H	-6.095625	-0.848060	3.540902
H	-7.158690	0.583218	3.273416
H	-6.575688	-0.393014	1.867855
C	-4.646803	1.469625	4.106273
H	-4.421946	0.647038	4.817590
H	-3.733714	2.093160	3.996665
H	-5.458484	2.091468	4.538481
C	-4.026225	-3.337935	0.563242
H	-3.675258	-2.400708	1.040801
C	-2.352932	-1.058856	-3.762196
H	-2.082027	-0.237832	-3.067897
C	-1.051787	-1.465260	-4.464688
H	-0.325720	-1.857361	-3.720525
H	-1.231566	-2.241697	-5.237099
H	-0.599427	-0.581492	-4.961906
C	-3.354070	-0.458466	-4.756080
H	-3.601558	-1.179111	-5.563773
H	-4.288870	-0.174430	-4.226704
H	-2.927906	0.457423	-5.218771
C	-3.251222	-4.468942	1.248412
H	-3.586324	-5.465714	0.893153
H	-2.166244	-4.356928	1.042499
H	-3.401259	-4.420999	2.348008
C	-5.525712	-3.430661	0.868473
H	-6.067484	-2.606131	0.357346
H	-5.946423	-4.401622	0.532261
H	-5.698036	-3.331399	1.961685
C	0.904730	1.711090	-2.932231
C	1.888647	0.740952	-3.352501
H	2.926025	1.083673	-3.461686
B	1.216286	3.116746	-2.469713
O	2.493361	3.633679	-2.249448
O	0.241897	4.085847	-2.266199
C	2.332806	4.955297	-1.689432
C	0.909073	5.358547	-2.194919
C	2.379333	4.829224	-0.175283
H	3.336189	4.390250	0.138906
H	2.283623	5.804011	0.322831
H	1.566090	4.181410	0.182929
C	3.453983	5.843375	-2.183782
H	3.301258	6.883869	-1.861426
H	4.416622	5.507358	-1.773848
H	3.533330	5.830152	-3.277566
C	0.936131	5.939362	-3.600883
H	1.377161	6.945810	-3.621049
H	1.508583	5.299453	-4.287209
H	-0.090293	6.010660	-3.985243
C	0.147606	6.275980	-1.262154
H	-0.048384	5.801933	-0.292728
H	0.705837	7.207152	-1.085991
H	-0.820280	6.550026	-1.702850
Na	2.249099	-2.470821	-0.499341
H	1.624111	0.024083	-4.135405
H	-0.139796	1.482198	-3.179105
H	2.281518	-0.512341	-2.391984
O	3.798222	-3.028609	-2.158982
O	0.626453	-4.078768	-0.519137
C	3.360226	-3.164593	-3.473950
H	3.402057	-4.239370	-3.753188
H	2.305304	-2.824413	-3.555608
C	4.898545	-2.178847	-2.158853
H	4.577483	-1.173693	-1.812147
H	5.671961	-2.564313	-1.461314
C	5.451463	-2.080388	-3.560887
H	5.881577	-1.075987	-3.766814
H	6.221098	-2.867340	-3.722770
C	4.248392	-2.357342	-4.401951
H	3.748115	-1.402909	-4.677654
H	4.511341	-2.924128	-5.321566
C	0.056743	-4.596116	-1.674102
H	-0.674340	-3.871316	-2.087560
H	0.855403	-4.762781	-2.429428
C	0.787168	-5.122464	0.387231
H	1.870161	-5.288680	0.571309
H	0.311344	-4.838048	1.348990
C	0.143116	-6.385834	-0.155875
H	-0.525581	-6.862352	0.594123
H	0.926239	-7.109021	-0.474383
C	-0.625056	-5.902684	-1.344557
H	-0.575455	-6.619443	-2.192770
H	-1.684469	-5.721174	-1.065410

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Figure_S5_imid-3_modeS2_ts(CuHadd)_05 / electronic energy: -3525.630337045497 a.u. / lowest freq: -635.75 cm-1

C	1.501521	0.911246	2.707495
H	2.123668	0.194166	3.260423
C	0.013038	0.482229	2.615197
H	-0.667796	1.270811	2.975569
C	0.925954	0.581169	0.428175
C	3.183314	1.333591	0.802735
C	3.196679	2.302176	-0.211683
C	4.410503	0.810456	1.253927
C	4.389667	2.776090	-0.745557
H	2.244594	2.702836	-0.571275
C	5.604639	1.317826	0.732095
C	5.604025	2.303060	-0.251510
H	4.358670	3.526471	-1.539765
H	6.542121	0.884533	1.084470
H	6.549986	2.677955	-0.647818
C	-1.374421	-0.100291	0.575314
C	-2.564874	0.582762	0.854327
C	-1.406275	-1.247355	-0.229803
C	-3.778997	0.120590	0.333047
C	-2.623869	-1.725831	-0.728306
C	-3.809200	-1.036468	-0.452836
H	-4.753495	-1.408273	-0.833959
S	4.543215	-0.626834	2.336291
O	5.907618	-1.170947	2.073416
O	3.506379	-1.572465	1.822889
O	4.334373	-0.177886	3.723559
Cu	1.117384	0.660213	-1.468735
C	1.665711	2.287286	3.308673
C	2.422027	2.473561	4.478993
C	1.066171	3.405202	2.700201
C	2.591175	3.754231	5.014742
H	2.877159	1.631124	4.981829
C	1.239200	4.683544	3.236566
H	0.458540	3.280160	1.814989
C	2.004098	4.858599	4.391902
H	3.177298	3.890287	5.914392
H	0.777779	5.537525	2.757541
H	2.137149	5.848863	4.807878
C	-0.295146	-0.795551	3.356913
C	-1.237922	-0.800511	4.400578
C	0.314586	-2.006093	2.983394
C	-1.557024	-1.991955	5.058830
H	-1.731444	0.114801	4.702081
C	0.001350	-3.192420	3.650777
H	1.018329	-2.032414	2.165261
C	-0.936566	-3.186568	4.685618
H	-2.286715	-1.988937	5.858139
H	0.477856	-4.118790	3.357289
H	-1.185255	-4.108205	5.195500
N	1.919766	0.914662	1.282300
N	-0.161059	0.314309	1.165211
H	-0.492413	-1.791110	-0.425352
H	-2.549677	1.468714	1.477199
C	-2.670611	-2.988341	-1.488444
C	-2.630280	-2.965461	-2.909894
C	-2.803897	-4.225291	-0.796721
C	-2.722263	-4.181595	-3.611095
C	-2.893703	-5.413668	-1.544551
C	-2.848218	-5.389254	-2.933898
H	-2.705116	-4.199292	-4.692755
H	-3.009767	-6.370088	-1.052376
H	-2.920969	-6.314260	-3.491409
C	-5.032166	0.829358	0.642460
C	-5.730060	0.538287	1.847506
C	-5.551248	1.785040	-0.274520
C	-6.936989	1.211631	2.110120
C	-6.766081	2.425447	0.030668
C	-7.446800	2.142018	1.210286
H	-7.494683	1.013331	3.015942
H	-7.194277	3.150982	-0.648355
H	-8.379413	2.646568	1.428135
C	-4.834546	2.131258	-1.581087
H	-3.877424	1.578332	-1.672937
C	-4.464938	3.618858	-1.637674
H	-3.858249	3.891853	-0.748071
H	-3.861126	3.825749	-2.546839
H	-5.369647	4.261335	-1.667472
C	-5.678658	1.725235	-2.794524
H	-5.936840	0.646429	-2.731823
H	-6.616616	2.317125	-2.848593
H	-5.102883	1.889100	-3.730529
C	-5.216165	-0.490184	2.857432
H	-4.259034	-0.940340	2.524117
C	-6.198283	-1.658150	3.005720
H	-5.760817	-2.441479	3.661235
H	-7.159331	-1.323720	3.449931
H	-6.398909	-2.112228	2.011656
C	-4.924124	0.163424	4.213320

H -4.464743 -0.577882 4.901474
H -4.209137 1.003710 4.081775
H -5.852161 0.550110 4.684216
C -2.882877 -4.301145 0.729209
H -2.746167 -3.301830 1.190343
C -2.510676 -1.661790 -3.697814
H -2.395215 -0.793740 -3.018048
C -1.266587 -1.664446 -4.593951
H -0.363714 -1.882381 -3.985201
H -1.347312 -2.422697 -5.400492
H -1.139021 -0.667465 -5.066943
C -3.779687 -1.398270 -4.516019
H -3.920174 -2.171768 -5.300350
H -4.667306 -1.398258 -3.847761
H -3.716291 -0.403534 -5.006904
C -1.768650 -5.183690 1.305467
H -1.872503 -6.238838 0.977904
H -0.777739 -4.801481 0.982274
H -1.805284 -5.162939 2.415131
C -4.263160 -4.791780 1.180258
H -5.054295 -4.135997 0.757447
H -4.446096 -5.836100 0.849904
H -4.338049 -4.752366 2.288190
C 0.125268 1.671434 -2.972931
C 1.263249 0.922971 -3.450713
H 2.177307 1.485920 -3.680915
B 0.153410 3.136267 -2.605774
O 1.290126 3.945801 -2.619173
O -0.979172 3.872468 -2.276050
C 0.911374 5.245672 -2.120710
C -0.633735 5.264818 -2.377770
C 1.239943 5.290846 -0.638487
H 2.310279 5.100036 -0.482452
H 1.006688 6.267217 -0.191740
H 0.672185 4.522512 -0.097775
C 1.693250 6.305170 -2.867368
H 1.364317 7.314568 -2.579763
H 2.763060 6.224785 -2.628613
H 1.586841 6.204337 -3.954249
C -0.983589 5.717473 -3.788161
H -0.808569 6.793011 -3.931705
H -0.398552 5.170155 -4.540827
H -2.046588 5.518137 -3.980422
C -1.434534 6.050428 -1.360492
H -1.336237 5.629934 -0.352153
H -1.112959 7.101718 -1.330303
H -2.500430 6.037357 -1.625056
Na 5.012835 -2.929338 0.642636
H 1.110748 0.108491 -4.164106
H -0.856674 1.191427 -3.069804
H 2.041024 -0.175823 -2.456806
O 5.745516 -1.806398 -1.309220
O 3.263747 -3.986902 -0.512548
C 6.378731 -2.495723 -2.337973
H 7.417941 -2.117594 -2.450059
H 6.425508 -3.573258 -2.071265
C 4.810554 -0.960132 -1.888946
H 3.936759 -0.854636 -1.214055
H 5.267567 0.041582 -2.042479
C 4.391841 -1.545366 -3.216323
H 3.531825 -2.234846 -3.073378
H 4.126870 -0.753863 -3.950736
C 5.605493 -2.315116 -3.634475
H 5.327734 -3.292001 -4.087298
H 6.205360 -1.723586 -4.361046
C 1.983430 -3.452061 -0.423812
H 1.502026 -3.826413 0.505060
H 2.041234 -2.345376 -0.371991
C 3.253367 -4.982605 -1.483556
H 3.956224 -4.697873 -2.295145
H 3.602255 -5.939084 -1.039142
C 1.854227 -5.140985 -2.047024
H 1.349806 -6.015347 -1.578617
H 1.862492 -5.256732 -3.152775
C 1.176878 -3.877655 -1.629986
H 1.258434 -3.113532 -2.433745
H 0.109321 -4.048723 -1.376878
165
Figure_S5_imid-3_modeS2_ts(CuHadd)_06 / electronic energy: -3525.628456218441 a.u. / lowest freq: -742.23 cm-1
C 1.446742 1.114445 2.634073
H 2.161351 0.454040 3.144723
C 0.004318 0.541197 2.601184
H -0.738679 1.278276 2.948121
C 0.825776 0.683884 0.384632
C 2.973093 1.724257 0.639593
C 2.809570 2.679844 -0.374225
C 4.276597 1.339548 0.999632
C 3.901172 3.263603 -1.005793

H	1.795555	2.973275	-0.658722
C	5.368936	1.954497	0.379508
C	5.192051	2.913342	-0.613855
H	3.731804	3.998354	-1.797208
H	6.370318	1.628797	0.666840
H	6.061645	3.371637	-1.089657
C	-1.377132	-0.253384	0.621337
C	-2.628208	0.284322	0.953550
C	-1.311074	-1.379373	-0.209498
C	-3.800501	-0.301826	0.457717
C	-2.479684	-1.972924	-0.697882
C	-3.725897	-1.432251	-0.364841
H	-4.633733	-1.896076	-0.733178
S	4.637373	0.001235	2.145521
O	5.999265	-0.472824	1.761679
O	3.624135	-1.054780	1.844853
O	4.548799	0.559312	3.506119
Cu	1.002215	0.782540	-1.516100
C	1.502739	2.491865	3.249288
C	2.241243	2.722429	4.422955
C	0.811743	3.564671	2.657067
C	2.303718	4.004479	4.977974
H	2.762927	1.912255	4.914633
C	0.878371	4.844802	3.212636
H	0.218462	3.403387	1.768238
C	1.626432	5.065410	4.371332
H	2.876257	4.175021	5.880492
H	0.347634	5.664628	2.745914
H	1.676656	6.056860	4.802444
C	-0.154279	-0.724332	3.407446
C	-1.032793	-0.759938	4.504989
C	0.546831	-1.892351	3.057071
C	-1.198076	-1.937766	5.239988
H	-1.591336	0.121784	4.792820
C	0.389040	-3.062980	3.802767
H	1.207089	-1.898841	2.202188
C	-0.486350	-3.087722	4.890498
H	-1.876903	-1.958169	6.082651
H	0.942409	-3.953007	3.533314
H	-0.613304	-3.997825	5.462220
N	1.795461	1.166920	1.193168
N	-0.192226	0.292902	1.164841
H	-0.355363	-1.823997	-0.434738
H	-2.693724	1.153864	1.595569
C	-2.396164	-3.200435	-1.512756
C	-2.507302	-3.126197	-2.929742
C	-2.207033	-4.459911	-0.876703
C	-2.428858	-4.313849	-3.679810
C	-2.114763	-5.615448	-1.674222
C	-2.225709	-5.540201	-3.057766
H	-2.522680	-4.294930	-4.757507
H	-1.965923	-6.588087	-1.224282
H	-2.160519	-6.441868	-3.653162
C	-5.115814	0.250904	0.826818
C	-5.717964	-0.119592	2.061754
C	-5.787597	1.138052	-0.059850
C	-6.981087	0.408959	2.384959
C	-7.049909	1.637670	0.309208
C	-7.635992	1.277000	1.517814
H	-7.469325	0.145682	3.314012
H	-7.589893	2.311701	-0.342668
H	-8.608319	1.671617	1.783638
C	-5.183875	1.561614	-1.399787
H	-4.184810	1.105779	-1.552691
C	-4.964931	3.077863	-1.456628
H	-4.328487	3.400324	-0.604865
H	-4.446984	3.350102	-2.400819
H	-5.927666	3.629005	-1.415819
C	-6.052371	1.085627	-2.570076
H	-6.210198	-0.011842	-2.502473
H	-7.040884	1.591289	-2.570464
H	-5.544669	1.304437	-3.533779
C	-5.043651	-1.083763	3.039849
H	-4.055053	-1.415517	2.662831
C	-5.873519	-2.360711	3.217341
H	-5.322763	-3.086467	3.853432
H	-6.851184	-2.143668	3.696802
H	-6.053481	-2.835262	2.228762
C	-4.775105	-0.406169	4.388929
H	-4.203185	-1.090727	5.050672
H	-4.171492	0.514081	4.236399
H	-5.721791	-0.135407	4.901634
C	-2.123039	-4.601850	0.644219
H	-2.242566	-3.622046	1.149469
C	-2.716114	-1.801182	-3.662412
H	-2.687954	-0.946461	-2.956933
C	-1.599553	-1.543770	-4.682742
H	-0.609048	-1.631915	-4.190385

H -1.644731 -2.263984 -5.526131
H -1.693256 -0.517543 -5.097758
C -4.093185 -1.760542 -4.333797
H -4.172653 -2.526322 -5.134136
H -4.887419 -1.946411 -3.579678
H -4.268123 -0.759604 -4.783036
C -0.752870 -5.138246 1.074489
H -0.545494 -6.132172 0.626107
H 0.043616 -4.428028 0.765930
H -0.716196 -5.242339 2.179031
C -3.256485 -5.484930 1.180956
H -4.238079 -5.088410 0.843186
H -3.151357 -6.534152 0.833593
H -3.247329 -5.481041 2.292078
C -0.143917 1.604051 -3.019289
C 1.100011 1.044988 -3.501880
H 1.889619 1.750890 -3.788922
B -0.342965 3.065786 -2.696034
O 0.664739 4.031658 -2.736892
O -1.569898 3.640802 -2.378631
C 0.105418 5.268390 -2.251837
C -1.423389 5.066346 -2.513344
C 0.417874 5.369783 -0.767964
H 1.503378 5.320080 -0.606613
H 0.058637 6.311930 -0.331089
H -0.050329 4.539840 -0.221612
C 0.728059 6.423532 -3.006220
H 0.253497 7.376403 -2.729064
H 1.797610 6.503046 -2.766207
H 0.638113 6.297544 -4.092080
C -1.822302 5.431309 -3.935656
H -1.806200 6.517426 -4.103448
H -1.156108 4.959351 -4.671608
H -2.842507 5.073558 -4.129592
C -2.326505 5.763782 -1.518006
H -2.195286 5.370254 -0.502699
H -2.128533 6.845528 -1.498745
H -3.380410 5.628036 -1.794816
Na 5.129098 -2.615776 0.922737
H 1.068580 0.185069 -4.178265
H -1.033835 0.967000 -3.087297
H 2.117332 0.196861 -2.497848
O 3.386840 -3.362550 -0.511508
O 6.465921 -2.300457 -0.991620
C 2.823357 -4.504424 -1.071533
H 3.623137 -5.085169 -1.578949
H 2.388982 -5.136058 -0.267003
C 2.651496 -2.268616 -0.947740
H 1.920334 -1.992142 -0.161525
H 3.327848 -1.406106 -1.113887
C 1.937315 -2.640584 -2.226394
H 0.970021 -2.107718 -2.336523
H 2.584391 -2.421966 -3.103319
C 1.751390 -4.115886 -2.076910
H 0.740816 -4.333729 -1.667543
H 1.883066 -4.642904 -3.046975
C 6.617974 -3.264860 -1.976385
H 7.701715 -3.413514 -2.180563
H 6.189069 -4.227433 -1.625301
C 6.351627 -1.077160 -1.640317
H 5.643872 -0.432208 -1.082160
H 7.344370 -0.576110 -1.658063
C 5.844834 -1.303906 -3.054509
H 6.499667 -0.789898 -3.791896
H 4.800802 -0.937686 -3.168269
C 5.907914 -2.794774 -3.226879
H 4.884016 -3.224840 -3.268872
H 6.470806 -3.079914 -4.142271
165
Figure_S5_imid-3_modeS2_prod(CuHadd) / electronic energy: -3525.670844336381 a.u. / lowest freq: -53.58 cm-1
C 1.553959 -2.148920 -2.073044
H 2.216910 -1.792782 -2.874591
C 0.103515 -1.642290 -2.206101
H -0.603641 -2.462520 -2.400186
C 0.971130 -0.953270 -0.116855
C 3.253312 -1.774072 -0.204075
C 3.275016 -2.404484 1.049077
C 4.471270 -1.417702 -0.815525
C 4.477131 -2.703757 1.681481
H 2.324250 -2.666814 1.519812
C 5.671219 -1.756910 -0.183778
C 5.682409 -2.398759 1.051924
H 4.463581 -3.188939 2.659952
H 6.601887 -1.473804 -0.678247
H 6.633475 -2.647148 1.527836
C -1.377923 -0.471891 -0.505845
C -2.582329 -1.151836 -0.757385
C -1.422710 0.843111 -0.010808

C	-3.815015	-0.517945	-0.544974
C	-2.655210	1.477891	0.199749
C	-3.846375	0.794014	-0.063218
H	-4.797587	1.297458	0.068042
S	4.584352	-0.363537	-2.291005
O	5.997008	0.056271	-2.344096
O	3.647713	0.756228	-1.956609
O	4.144051	-1.164319	-3.452301
Cu	1.318601	-0.241665	1.645942
C	1.641983	-3.655444	-1.977240
C	2.415695	-4.379208	-2.901470
C	0.970872	-4.353499	-0.954093
C	2.516539	-5.770311	-2.803050
H	2.943161	-3.869168	-3.697429
C	1.076278	-5.743522	-0.859119
H	0.368817	-3.822619	-0.228533
C	1.848415	-6.451646	-1.782723
H	3.114702	-6.320452	-3.517871
H	0.559401	-6.271538	-0.068191
H	1.929102	-7.528342	-1.707877
C	-0.049605	-0.599479	-3.289417
C	-0.759934	-0.904600	-4.462895
C	0.508544	0.685112	-3.145449
C	-0.920777	0.058224	-5.463817
H	-1.185603	-1.889434	-4.606116
C	0.351615	1.641553	-4.151623
H	1.052626	0.952303	-2.250578
C	-0.367418	1.330789	-5.307368
H	-1.472660	-0.183638	-6.362824
H	0.783570	2.626459	-4.033427
H	-0.492968	2.075049	-6.082967
N	1.984286	-1.526824	-0.797606
N	-0.139878	-1.065938	-0.862874
H	-0.504020	1.393417	0.142579
H	-2.564861	-2.161318	-1.148181
C	-2.715420	2.907061	0.565096
C	-2.778349	3.294716	1.932820
C	-2.832871	3.888361	-0.460606
C	-2.977331	4.652741	2.244397
C	-3.019817	5.234146	-0.095219
C	-3.090308	5.608304	1.241327
H	-3.061032	4.979625	3.271973
H	-3.120448	6.003719	-0.848993
H	-3.242083	6.647833	1.502215
C	-5.082071	-1.191278	-0.906187
C	-5.488706	-1.256361	-2.270790
C	-5.930629	-1.713705	0.112180
C	-6.721369	-1.858594	-2.584947
C	-7.159050	-2.293071	-0.255887
C	-7.543323	-2.369399	-1.588476
H	-7.061997	-1.921509	-3.609962
H	-7.832665	-2.687089	0.493507
H	-8.492025	-2.820004	-1.850780
C	-5.560677	-1.655000	1.593132
H	-4.556348	-1.210933	1.732480
C	-5.493524	-3.059328	2.208052
H	-4.743309	-3.673944	1.666007
H	-5.189128	-2.994755	3.273531
H	-6.477347	-3.570995	2.166773
C	-6.536204	-0.761286	2.367787
H	-6.583604	0.244688	1.898669
H	-7.556720	-1.198694	2.383596
H	-6.188209	-0.638187	3.415864
C	-4.652780	-0.662574	-3.405718
H	-3.715025	-0.210822	-3.025037
C	-5.406328	0.472276	-4.110099
H	-4.738300	0.974243	-4.842584
H	-6.297650	0.091023	-4.651349
H	-5.734771	1.228254	-3.365691
C	-4.233110	-1.746895	-4.405669
H	-3.599594	-1.305161	-5.202654
H	-3.646014	-2.533560	-3.885135
H	-5.114044	-2.216768	-4.890412
C	-2.785799	3.525644	-1.946098
H	-2.612251	2.439990	-2.091747
C	-2.689957	2.277975	3.070017
H	-2.414282	1.276380	2.682224
C	-1.600894	2.655013	4.084825
H	-0.630355	2.797332	3.566918
H	-1.855242	3.585770	4.632468
H	-1.481071	1.845541	4.834410
C	-4.048692	2.120405	3.759993
H	-4.363166	3.069284	4.244116
H	-4.818139	1.824717	3.015488
H	-3.993723	1.326780	4.535463
C	-1.623679	4.231095	-2.653689
H	-1.742649	5.334396	-2.634963
H	-0.668411	3.963061	-2.158045

H	-1.569404	3.904446	-3.713890
C	-4.120494	3.840666	-2.630951
H	-4.949766	3.330626	-2.095707
H	-4.319054	4.933042	-2.643659
H	-4.105843	3.473230	-3.679378
C	1.865013	0.436706	3.434518
C	3.325999	0.288646	3.807352
H	3.673733	-0.750466	3.693294
B	0.864364	-0.609430	3.891545
O	1.170712	-1.919594	4.280742
O	-0.523352	-0.435389	3.825120
C	-0.039607	-2.692281	4.182771
C	-1.146736	-1.604590	4.373335
C	-0.079457	-3.308371	2.790162
H	0.809470	-3.936950	2.637463
H	-0.964666	-3.941112	2.635463
H	-0.079298	-2.521898	2.017176
C	-0.027663	-3.776966	5.238243
H	-0.977520	-4.331744	5.245439
H	0.776545	-4.497323	5.034507
H	0.138196	-3.366167	6.241712
C	-1.447615	-1.326435	5.838381
H	-1.987500	-2.157492	6.313875
H	-0.526668	-1.142730	6.409501
H	-2.075455	-0.428692	5.916299
C	-2.426095	-1.879047	3.615692
H	-2.257348	-1.897288	2.531406
H	-2.857152	-2.844580	3.916407
H	-3.169117	-1.098449	3.826327
Na	3.406335	1.412225	0.171209
H	3.540379	0.564774	4.857475
H	1.491239	1.469405	3.529007
H	4.010454	0.905950	3.199140
O	5.430090	2.342260	0.656782
O	1.968480	3.155827	-0.039246
C	6.364054	1.608488	1.378680
H	6.525332	2.100604	2.362496
H	5.974423	0.584818	1.556215
C	6.097852	3.017263	-0.360728
H	5.723639	2.650758	-1.339776
H	5.880453	4.104427	-0.290144
C	7.588988	2.769556	-0.251747
H	8.055231	2.599701	-1.246603
H	8.082654	3.627459	0.256529
C	7.664785	1.552063	0.609729
H	7.696482	0.638969	-0.023149
H	8.547205	1.575447	1.285450
C	1.378128	3.775296	1.054023
H	0.580609	3.124781	1.468045
H	2.148719	3.934372	1.840025
C	2.217580	4.124871	-1.006069
H	3.311904	4.202027	-1.179997
H	1.739242	3.812245	-1.957633
C	1.659091	5.461939	-0.553961
H	1.069141	5.956379	-1.356523
H	2.485614	6.131111	-0.227016
C	0.800467	5.099030	0.614835
H	0.847560	5.861378	1.422401
H	-0.249085	4.959791	0.283993

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Figure_S5_imid-3_modeR1_ed(CuHadd) / electronic energy: -3525.642230729441 a.u. / lowest freq: 9.73 cm-1

C	-0.010388	3.285454	-1.458643
H	-0.669470	3.088660	-2.319861
C	1.275271	2.438088	-1.485265
H	2.136809	2.969239	-1.044027
C	-0.179420	1.571465	0.156443
C	-1.959135	3.258477	0.172070
C	-1.976110	4.295195	1.107408
C	-3.179247	2.784188	-0.336022
C	-3.175191	4.869776	1.518438
H	-1.031726	4.633723	1.536808
C	-4.380071	3.366709	0.071687
C	-4.381274	4.411481	0.992402
H	-3.164136	5.674327	2.256568
H	-5.312612	2.974560	-0.338653
H	-5.326583	4.860359	1.305207
C	1.906711	0.447830	-0.103112
C	2.695093	0.847706	0.983032
C	2.144617	-0.790752	-0.711993
C	3.720935	0.020541	1.451424
C	3.146436	-1.644769	-0.219335
C	3.952132	-1.219697	0.846062
H	4.749001	-1.856146	1.211040
S	-3.248158	1.377779	-1.445539
O	-4.689744	1.015180	-1.546991
O	-2.508784	0.293420	-0.717039
O	-2.615519	1.795995	-2.708102
Cu	-1.110837	0.453279	1.528759

C	0.252941	4.766262	-1.341544
C	-0.235828	5.647578	-2.321944
C	0.982213	5.288691	-0.256245
C	-0.000500	7.021815	-2.217772
H	-0.799503	5.273349	-3.167438
C	1.214191	6.663264	-0.156338
H	1.361527	4.633008	0.517751
C	0.723625	7.529210	-1.136297
H	-0.380365	7.693996	-2.976267
H	1.772845	7.057366	0.682686
H	0.903830	8.593480	-1.057279
C	1.638716	1.980764	-2.873958
C	2.837990	2.408728	-3.470425
C	0.768356	1.156169	-3.607878
C	3.143699	2.040259	-4.784098
H	3.528919	3.041481	-2.927334
C	1.076404	0.790734	-4.920556
H	-0.154816	0.811104	-3.166131
C	2.258756	1.240727	-5.512041
H	4.064988	2.379018	-5.239878
H	0.397125	0.160315	-5.479525
H	2.496492	0.957822	-6.529232
N	-0.700711	2.739230	-0.263648
N	0.905013	1.310592	-0.602033
H	1.560532	-1.083044	-1.572422
H	2.519835	1.809714	1.450404
C	3.359311	-2.983616	-0.821695
C	3.040526	-4.165437	-0.083802
C	3.914161	-3.097837	-2.130094
C	3.261400	-5.420405	-0.680295
C	4.092278	-4.378664	-2.685535
C	3.766000	-5.522131	-1.969339
H	3.043442	-6.334665	-0.144624
H	4.508002	-4.500105	-3.676958
H	3.922295	-6.497836	-2.411395
C	4.555973	0.460250	2.583152
C	5.734578	1.219062	2.341243
C	4.159691	0.158085	3.915475
C	6.490531	1.665780	3.440439
C	4.944886	0.635180	4.980831
C	6.096703	1.377750	4.742976
H	7.390612	2.247850	3.292383
H	4.665986	0.433404	6.006655
H	6.688960	1.734501	5.575894
C	2.904982	-0.659783	4.224319
H	2.417967	-1.014142	3.293504
C	1.860468	0.191714	4.954299
H	1.610542	1.087002	4.345423
H	0.929202	-0.395024	5.105069
H	2.233448	0.523165	5.946335
C	3.246408	-1.922553	5.024890
H	4.048170	-2.492819	4.509575
H	3.588345	-1.671771	6.050900
H	2.350485	-2.574955	5.104121
C	6.198662	1.570952	0.927116
H	5.517389	1.144909	0.162819
C	7.581869	0.977500	0.633324
H	7.853649	1.155572	-0.429193
H	8.363245	1.434482	1.276181
H	7.567627	-0.119885	0.807285
C	6.187869	3.088011	0.704648
H	6.435840	3.318910	-0.353491
H	5.176169	3.494652	0.919297
H	6.927197	3.597089	1.358176
C	4.374227	-1.883433	-2.936494
H	4.196251	-0.938864	-2.385763
C	2.488366	-4.126991	1.342643
H	2.248927	-3.090551	1.646796
C	1.176298	-4.913812	1.471404
H	0.475993	-4.625917	0.665016
H	1.349285	-6.008806	1.413955
H	0.694362	-4.689122	2.447076
C	3.527419	-4.652432	2.340223
H	3.778898	-5.714412	2.134199
H	4.456890	-4.048394	2.279557
H	3.131909	-4.580291	3.375511
C	3.597729	-1.769742	-4.252928
H	3.772823	-2.648538	-4.907594
H	2.509827	-1.687521	-4.044914
H	3.923056	-0.863406	-4.803282
C	5.885993	-1.932566	-3.192388
H	6.430520	-2.027165	-2.228348
H	6.158799	-2.787569	-3.846078
H	6.218473	-0.994308	-3.686107
C	-0.704918	-1.568965	1.415815
C	-1.529440	-1.229176	2.507220
H	-1.125853	-1.139996	3.520656
B	-1.173177	-2.219258	0.110751

O -0.291863 -2.652614 -0.845786
O -2.485930 -2.562258 -0.213507
C -1.029060 -3.121658 -1.986976
C -2.439491 -3.435125 -1.376321
C -1.062362 -1.991380 -3.002075
H -0.033770 -1.731361 -3.282759
H -1.591951 -2.279852 -3.920353
H -1.541341 -1.095853 -2.584250
C -0.305532 -4.322972 -2.560508
H -0.860976 -4.755616 -3.405113
H 0.681528 -4.015316 -2.932131
H -0.146138 -5.108612 -1.812019
C -2.570945 -4.858653 -0.863459
H -2.578057 -5.587881 -1.685235
H -1.752746 -5.120736 -0.180142
H -3.514276 -4.965446 -0.310365
C -3.593483 -3.095845 -2.295686
H -3.610923 -2.029984 -2.559710
H -3.526374 -3.668937 -3.231442
H -4.554368 -3.350665 -1.829902
Na -4.272235 -0.972909 -0.031005
H -2.605959 -1.437159 2.477574
H 0.375031 -1.605286 1.607454
H -1.750254 1.470631 2.571910
O -5.231486 -0.143920 1.907101
O -6.350850 -1.874190 -0.501763
C -7.365709 -0.939150 -0.663562
H -7.019844 0.049237 -0.294014
H -7.607768 -0.844904 -1.745030
C -6.961701 -3.082446 -0.203258
H -7.164272 -3.635378 -1.147501
H -6.284914 -3.696517 0.428153
C -8.255978 -2.798016 0.527518
H -8.095414 -2.851723 1.626770
H -9.053193 -3.513547 0.229852
C -8.588546 -1.391398 0.116101
H -9.494939 -1.368061 -0.527897
H -8.750815 -0.748268 1.008955
C -5.783846 -1.006163 2.841914
H -5.542883 -2.055962 2.570985
H -6.889543 -0.884229 2.846078
C -4.962105 1.046993 2.569713
H -4.031362 1.488273 2.164791
H -5.794931 1.762079 2.390354
C -4.810049 0.772403 4.056530
H -3.758695 0.920263 4.386828
H -5.481182 1.434651 4.646399
C -5.215074 -0.666323 4.201294
H -4.324208 -1.298092 4.412463
H -5.972382 -0.803899 5.003585

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Figure_S5_imid-3_modeR1_ts(CuHadd)_01 / electronic energy: -3525.627389349992 a.u. / lowest freq: -747.21 cm-1

C 0.071600 3.362476 -1.115416
H -0.502012 3.140714 -2.029905
C 1.404970 2.594439 -1.049110
H 2.210426 3.187246 -0.582412
C -0.136835 1.595307 0.450149
C -1.960379 3.252198 0.407502
C -2.031117 4.198997 1.433515
C -3.146400 2.882078 -0.249169
C -3.241473 4.797330 1.775133
H -1.118404 4.458807 1.973187
C -4.355488 3.491528 0.083730
C -4.403701 4.460327 1.084249
H -3.272496 5.532088 2.582229
H -5.258639 3.174469 -0.441870
H -5.353682 4.936998 1.335710
C 1.999519 0.492431 0.211002
C 3.186029 0.884093 0.845683
C 1.832784 -0.844209 -0.175720
C 4.203707 -0.047658 1.078049
C 2.853475 -1.782258 0.051816
C 4.038203 -1.377297 0.678438
H 4.841300 -2.088800 0.830879
S -3.159696 1.499652 -1.385897
O -4.594509 1.212265 -1.661154
O -2.569518 0.391039 -0.559362
O -2.354372 1.866957 -2.561606
Cu -1.215829 0.328591 1.445477
C 0.232541 4.854920 -0.961852
C -0.244068 5.720487 -1.962221
C 0.846627 5.403849 0.179989
C -0.109644 7.105039 -1.822143
H -0.721831 5.326081 -2.850381
C 0.977860 6.788664 0.315728
H 1.214854 4.759982 0.968962
C 0.500415 7.638676 -0.684452
H -0.479889 7.764827 -2.596127

H	1.448159	7.202951	1.198073
H	0.602316	8.710860	-0.577583
C	1.870935	2.107060	-2.397304
C	3.085953	2.565616	-2.934817
C	1.113950	1.167526	-3.121875
C	3.532298	2.095859	-4.173346
H	3.687448	3.287674	-2.397860
C	1.558285	0.709187	-4.363972
H	0.184687	0.785409	-2.720359
C	2.767467	1.171702	-4.889061
H	4.470700	2.450681	-4.579389
H	0.969227	-0.012556	-4.914975
H	3.113937	0.810277	-5.848528
N	-0.681629	2.755690	0.012389
N	1.048780	1.467124	-0.168715
H	0.941377	-1.130887	-0.709131
H	3.330373	1.918553	1.132800
C	2.728844	-3.178903	-0.424423
C	2.434603	-4.223444	0.500954
C	3.059510	-3.498897	-1.774412
C	2.461825	-5.556660	0.053946
C	3.093339	-4.852039	-2.161625
C	2.780671	-5.863111	-1.262164
H	2.263075	-6.373725	0.734258
H	3.384811	-5.138938	-3.161951
H	2.812588	-6.896931	-1.581554
C	5.475463	0.387081	1.684177
C	6.504460	0.924344	0.860635
C	5.664309	0.286460	3.090521
C	7.695388	1.366083	1.465510
C	6.873540	0.742518	3.646638
C	7.874088	1.276412	2.841723
H	8.495812	1.784787	0.869818
H	7.046936	0.687748	4.713301
H	8.797353	1.622501	3.288507
C	4.594121	-0.293745	4.015417
H	3.709575	-0.635790	3.440433
C	4.080584	0.767297	4.995760
H	3.702869	1.649145	4.435044
H	3.243024	0.354860	5.598065
H	4.882572	1.098189	5.688829
C	5.115529	-1.528337	4.761467
H	5.516699	-2.268503	4.036988
H	5.918218	-1.258321	5.479391
H	4.287718	-2.008411	5.325929
C	6.358212	1.034777	-0.658268
H	5.384950	0.627318	-1.000363
C	7.433374	0.213335	-1.380444
H	7.232960	0.203630	-2.473317
H	8.446083	0.636710	-1.213720
H	7.418334	-0.835914	-1.015814
C	6.388682	2.499619	-1.109120
H	6.202856	2.564653	-2.202501
H	5.593165	3.072530	-0.586061
H	7.371449	2.968568	-0.892460
C	3.493549	-2.428842	-2.778805
H	3.199334	-1.419208	-2.427550
C	2.161631	-3.949743	1.979707
H	2.019293	-2.864244	2.155696
C	0.875517	-4.636033	2.466512
H	0.043876	-4.453559	1.756990
H	1.013118	-5.732612	2.571012
H	0.584073	-4.230383	3.458897
C	3.357747	-4.382119	2.835076
H	3.517546	-5.479556	2.770885
H	4.279489	-3.868863	2.490095
H	3.185282	-4.108539	3.897917
C	2.824924	-2.601052	-4.151958
H	3.198625	-3.500311	-4.683058
H	1.724662	-2.679346	-4.040751
H	3.050098	-1.724144	-4.793004
C	5.018668	-2.422275	-2.918038
H	5.489041	-2.262237	-1.924748
H	5.382060	-3.385785	-3.335048
H	5.338178	-1.596528	-3.589356
C	-1.203218	-1.746985	1.665332
C	-2.097022	-1.086976	2.589958
H	-1.872747	-1.133546	3.661430
B	-1.594495	-2.396723	0.365251
O	-0.700608	-3.052165	-0.472403
O	-2.905358	-2.506177	-0.153588
C	-1.361210	-3.287354	-1.721447
C	-2.850926	-3.415246	-1.279742
C	-1.134981	-2.072088	-2.611164
H	-0.057688	-1.897536	-2.719982
H	-1.552690	-2.214530	-3.617884
H	-1.576862	-1.166009	-2.171815
C	-0.786328	-4.534644	-2.357531

H -1.350441 -4.817395 -3.258351
H 0.253577 -4.357168 -2.660556
H -0.791126 -5.383912 -1.663015
C -3.189407 -4.802336 -0.758689
H -3.229366 -5.545199 -1.567706
H -2.450229 -5.139622 -0.018687
H -4.173620 -4.784326 -0.269862
C -3.844621 -2.982864 -2.337185
H -3.722748 -1.926597 -2.613034
H -3.715932 -3.580154 -3.251647
H -4.878662 -3.129204 -1.998613
Na -4.464258 -0.792512 -0.101227
H -3.175671 -1.191601 2.415498
H -0.180073 -1.914280 2.019510
H -2.154547 0.562109 2.718050
O -5.471098 0.088763 1.812447
O -6.591208 -1.530672 -0.693745
C -7.517115 -0.523164 -0.933004
H -7.128065 0.437777 -0.534727
H -7.664978 -0.414780 -2.030074
C -7.312335 -2.690329 -0.453393
H -7.474701 -3.228311 -1.413888
H -6.738394 -3.351987 0.229512
C -8.639622 -2.310936 0.167231
H -8.580139 -2.383111 1.275557
H -9.460018 -2.961546 -0.206752
C -8.828073 -0.880719 -0.254209
H -9.677689 -0.782573 -0.965074
H -9.007061 -0.230721 0.630408
C -6.195084 -0.734973 2.661227
H -6.036056 -1.796648 2.377257
H -7.278194 -0.499692 2.566631
C -5.156615 1.229740 2.539413
H -4.166977 1.610311 2.219351
H -5.917317 2.014960 2.334300
C -5.135581 0.888568 4.019259
H -4.095417 0.887132 4.412809
H -5.750571 1.612703 4.597358
C -5.727456 -0.491070 4.079604
H -4.947720 -1.233501 4.359624
H -6.573634 -0.545602 4.798728

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Figure_S5_imid-3_modeR1_ts(CuHadd)_02 / electronic energy: -3525.626508464365 a.u. / lowest freq: -740.18 cm-1

C -0.191458 3.336765 -1.058310
H -0.792985 3.085953 -1.947084
C 1.180991 2.641520 -1.058803
H 1.963501 3.259576 -0.585155
C -0.241144 1.536731 0.477896
C -2.146838 3.080961 0.557239
C -2.239889 4.031803 1.577735
C -3.331569 2.586151 -0.012800
C -3.477571 4.503310 2.008303
H -1.323165 4.389595 2.049924
C -4.569778 3.067709 0.411481
C -4.646222 4.032470 1.413656
H -3.525562 5.240729 2.812152
H -5.470125 2.657013 -0.049715
H -5.620176 4.405212 1.738257
C 1.931062 0.550033 0.127628
C 3.081515 1.005847 0.785452
C 1.866636 -0.780212 -0.309808
C 4.167676 0.147171 0.984692
C 2.949950 -1.650082 -0.097344
C 4.102055 -1.177143 0.542138
H 4.956864 -1.830361 0.671802
S -3.292263 1.205263 -1.152560
O -4.709611 0.889762 -1.466255
O -2.691671 0.108328 -0.314792
O -2.464634 1.592652 -2.305719
Cu -1.163584 0.207638 1.541976
C -0.105267 4.834480 -0.899147
C -0.670671 5.678299 -1.871375
C 0.528482 5.409851 0.218763
C -0.604101 7.067375 -1.727140
H -1.164855 5.263250 -2.740954
C 0.591631 6.798999 0.358826
H 0.964589 4.783020 0.986577
C 0.026121 7.627222 -0.613282
H -1.042463 7.710289 -2.479429
H 1.077501 7.233426 1.222873
H 0.075431 8.702775 -0.503067
C 1.640963 2.237964 -2.436180
C 2.808497 2.798035 -2.983481
C 0.928179 1.279936 -3.181295
C 3.248839 2.413064 -4.252938
H 3.377532 3.534141 -2.430168
C 1.364027 0.909320 -4.455334
H 0.041257 0.814086 -2.772740

C	2.524842	1.473224	-4.990186
H	4.150373	2.846312	-4.666364
H	0.807346	0.175468	-5.023642
H	2.865965	1.177826	-5.973865
N	-0.855004	2.681284	0.098521
N	0.908654	1.462950	-0.216781
H	1.003233	-1.112971	-0.865995
H	3.147185	2.037317	1.109819
C	2.923452	-3.042008	-0.601234
C	2.747881	-4.126926	0.308930
C	3.215391	-3.306409	-1.971745
C	2.836862	-5.443871	-0.176780
C	3.307538	-4.644317	-2.399894
C	3.103478	-5.695819	-1.515848
H	2.724790	-6.289017	0.488918
H	3.564386	-4.885233	-3.422005
H	3.181372	-6.717011	-1.866404
C	5.410007	0.659852	1.589691
C	6.388542	1.286636	0.768025
C	5.624271	0.536076	2.990299
C	7.557607	1.787786	1.369076
C	6.808150	1.057473	3.543507
C	7.760865	1.675296	2.740350
H	8.321548	2.270934	0.774255
H	6.999644	0.986916	4.606147
H	8.666187	2.068842	3.184554
C	4.608634	-0.139988	3.911498
H	3.741080	-0.525080	3.337745
C	4.038777	0.856669	4.927593
H	3.594906	1.726055	4.396704
H	3.239270	0.372234	5.528024
H	4.826362	1.221728	5.620024
C	5.222360	-1.356348	4.616018
H	5.662118	-2.047545	3.866053
H	6.015208	-1.052355	5.331289
H	4.436786	-1.906492	5.176891
C	6.212346	1.427004	-0.745598
H	5.254211	0.982554	-1.083668
C	7.312761	0.674267	-1.503041
H	7.102746	0.691638	-2.594052
H	8.308966	1.132720	-1.329489
H	7.342016	-0.386330	-1.173342
C	6.164085	2.901652	-1.162361
H	5.952383	2.982256	-2.250046
H	5.352868	3.423847	-0.611009
H	7.127721	3.412349	-0.954654
C	3.541392	-2.190143	-2.966511
H	3.283501	-1.196072	-2.549917
C	2.534945	-3.911368	1.807754
H	2.344904	-2.841377	2.026267
C	1.313023	-4.680024	2.334402
H	0.437153	-4.517598	1.676390
H	1.510939	-5.770844	2.391532
H	1.053814	-4.323080	3.354086
C	3.792715	-4.304601	2.590913
H	4.005233	-5.389796	2.485321
H	4.669257	-3.734291	2.218944
H	3.658822	-4.071754	3.668875
C	2.735752	-2.318865	-4.267540
H	3.022360	-3.222103	-4.843772
H	1.650661	-2.363022	-4.043942
H	2.924505	-1.438924	-4.916340
C	5.045000	-2.159786	-3.258940
H	5.612194	-2.038755	-2.311217
H	5.372669	-3.097328	-3.756589
H	5.288810	-1.300102	-3.919398
C	-0.927519	-1.850294	1.775863
C	-1.798127	-1.269630	2.772267
H	-1.476670	-1.276770	3.819720
B	-1.376637	-2.539519	0.516832
O	-0.507763	-3.099115	-0.411978
O	-2.715443	-2.813018	0.144280
C	-1.271958	-3.488162	-1.558311
C	-2.659901	-3.793624	-0.919318
C	-1.325731	-2.302739	-2.513429
H	-0.303133	-1.994251	-2.763620
H	-1.840591	-2.552321	-3.452321
H	-1.823172	-1.436817	-2.053947
C	-0.604067	-4.676883	-2.216161
H	-1.228503	-5.087762	-3.022928
H	0.352714	-4.371764	-2.660524
H	-0.395913	-5.476788	-1.494465
C	-2.709242	-5.170372	-0.274827
H	-2.736146	-5.973555	-1.024474
H	-1.838470	-5.334605	0.374995
H	-3.613279	-5.256517	0.343662
C	-3.838814	-3.601162	-1.848296
H	-3.898530	-2.574338	-2.234998

H -3.764792 -4.271575 -2.716602
H -4.781082 -3.845407 -1.335107
Na -4.468180 -1.221056 0.134677
H -2.871044 -1.482512 2.689668
H 0.135673 -1.912399 2.033224
H -2.013165 0.362837 2.889995
O -5.300714 -0.567415 2.213889
O -6.766569 -1.520096 -0.476071
C -7.048921 -1.777651 -1.812487
H -6.211433 -1.400721 -2.439196
H -7.144540 -2.872640 -1.971382
C -7.510313 -0.407489 -0.088022
H -8.161631 -0.694402 0.765340
H -6.829590 0.401572 0.249811
C -8.362786 0.076927 -1.245377
H -7.896139 0.970224 -1.716933
H -9.399641 0.318224 -0.924545
C -8.332442 -1.077347 -2.192718
H -9.201143 -1.747355 -2.006928
H -8.325524 -0.745483 -3.253738
C -5.843034 -1.473152 3.113559
H -5.533523 -2.503559 2.837229
H -6.953344 -1.413756 3.070770
C -5.118887 0.622400 2.906272
H -4.226902 1.148551 2.511085
H -6.005869 1.275549 2.749927
C -4.942003 0.315657 4.382460
H -3.881705 0.449422 4.690293
H -5.593880 0.970460 5.001298
C -5.350118 -1.125915 4.502851
H -4.471998 -1.755165 4.768461
H -6.152443 -1.263559 5.260208
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Figure_S5_imid-3_modeR1_ts(CuHadd)_03 / electronic energy: -3525.625530169199 a.u. / lowest freq: -756.87 cm-1
C -0.279975 3.246934 -1.097823
H -0.852358 2.932076 -1.985656
C 1.126176 2.628600 -1.053436
H 1.854952 3.287577 -0.549750
C -0.270789 1.473027 0.465255
C -2.239523 2.949093 0.499789
C -2.384092 3.920432 1.494831
C -3.397091 2.407909 -0.085070
C -3.644164 4.372803 1.879387
H -1.489250 4.313946 1.980587
C -4.657125 2.875291 0.287827
C -4.784037 3.864846 1.260371
H -3.731812 5.127759 2.663371
H -5.534967 2.432683 -0.186976
H -5.774910 4.225312 1.545331
C 1.943371 0.571623 0.148328
C 3.062947 1.079691 0.821636
C 1.943288 -0.762259 -0.280770
C 4.180949 0.268236 1.043984
C 3.058582 -1.584713 -0.047173
C 4.178991 -1.060012 0.607729
H 5.058325 -1.675813 0.755091
S -3.297961 0.970474 -1.149641
O -4.695007 0.609497 -1.493076
O -2.709085 -0.063568 -0.227105
O -2.435317 1.309100 -2.293396
Cu -1.139816 0.117930 1.540799
C -0.279541 4.751640 -0.989469
C -0.872995 5.528518 -2.000044
C 0.300772 5.399882 0.117524
C -0.886277 6.923270 -1.904052
H -1.327303 5.056734 -2.862413
C 0.284093 6.794390 0.209332
H 0.756465 4.825690 0.914468
C -0.308601 7.555620 -0.800588
H -1.345783 7.514271 -2.685722
H 0.729096 7.284896 1.065342
H -0.321098 8.635400 -0.727721
C 1.657312 2.256864 -2.414081
C 2.824892 2.865754 -2.906570
C 1.012535 1.282125 -3.198107
C 3.332104 2.511475 -4.159926
H 3.342586 3.616061 -2.322864
C 1.513424 0.943831 -4.457082
H 0.126803 0.780236 -2.833163
C 2.674580 1.554703 -4.936499
H 4.233539 2.981998 -4.530614
H 1.006919 0.198578 -5.056606
H 3.066856 1.283468 -5.907990
N -0.925241 2.590179 0.069672
N 0.887539 1.436415 -0.220844
H 1.103609 -1.133360 -0.846532
H 3.079886 2.114538 1.141278
C 3.098496 -2.978284 -0.546956

C	2.958776	-4.068278	0.363656
C	3.411689	-3.233423	-1.914685
C	3.099416	-5.381539	-0.119822
C	3.555436	-4.567584	-2.340460
C	3.383505	-5.624934	-1.456749
H	3.014363	-6.229551	0.546260
H	3.828847	-4.800124	-3.360218
H	3.501229	-6.642939	-1.805479
C	5.389030	0.833481	1.671111
C	6.363888	1.485529	0.864920
C	5.577446	0.727634	3.076907
C	7.504565	2.026462	1.485756
C	6.732346	1.290549	3.650275
C	7.682317	1.931124	2.861854
H	8.266146	2.527412	0.902755
H	6.903807	1.233750	4.717154
H	8.565770	2.355607	3.321341
C	4.565570	0.024795	3.982111
H	3.721585	-0.389887	3.394016
C	3.945222	1.007939	4.981686
H	3.485390	1.860787	4.437725
H	3.149260	0.501698	5.568687
H	4.707184	1.400257	5.687725
C	5.203245	-1.168394	4.704652
H	5.678554	-1.848990	3.966780
H	5.972505	-0.836282	5.433074
H	4.424607	-1.740262	5.253352
C	6.214752	1.609810	-0.652937
H	5.272906	1.142602	-1.005880
C	7.346199	0.874732	-1.381217
H	7.159696	0.880730	-2.476616
H	8.328889	1.354445	-1.188888
H	7.389613	-0.182860	-1.043516
C	6.143636	3.079575	-1.083790
H	5.946536	3.146322	-2.175119
H	5.314547	3.590575	-0.548868
H	7.093825	3.611290	-0.867248
C	3.706764	-2.107680	-2.908455
H	3.416754	-1.121722	-2.493741
C	2.729018	-3.860017	1.860961
H	2.499085	-2.797722	2.077698
C	1.533154	-4.673152	2.380927
H	0.657154	-4.548139	1.714868
H	1.772790	-5.755240	2.444521
H	1.251694	-4.322300	3.396799
C	3.995772	-4.206200	2.651896
H	4.249460	-5.282637	2.547545
H	4.852711	-3.603305	2.285534
H	3.846485	-3.978994	3.729052
C	2.911354	-2.262727	-4.212865
H	3.221880	-3.162115	-4.782575
H	1.826411	-2.330974	-3.994525
H	3.083322	-1.382592	-4.865962
C	5.209969	-2.030262	-3.194556
H	5.769196	-1.893329	-2.244279
H	5.568767	-2.956190	-3.692454
H	5.429721	-1.162270	-3.852604
C	-0.781375	-1.916726	1.818309
C	-1.665059	-1.366904	2.821092
H	-1.313534	-1.329024	3.858384
B	-1.213300	-2.627168	0.565391
O	-0.329903	-3.152332	-0.369867
O	-2.542703	-2.941715	0.198218
C	-1.081605	-3.532878	-1.526418
C	-2.468378	-3.878199	-0.902988
C	-1.156000	-2.330523	-2.458057
H	-0.140274	-2.008177	-2.718091
H	-1.681349	-2.565776	-3.394737
H	-1.656137	-1.479272	-1.974887
C	-0.385548	-4.694459	-2.203384
H	-0.990574	-5.094825	-3.030003
H	0.572973	-4.362434	-2.624176
H	-0.175616	-5.508770	-1.498579
C	-2.507247	-5.279400	-0.314474
H	-2.513821	-6.052718	-1.095530
H	-1.641638	-5.457091	0.338815
H	-3.416805	-5.402473	0.289592
C	-3.643782	-3.653637	-1.830042
H	-3.714746	-2.605923	-2.155030
H	-3.554992	-4.272246	-2.734697
H	-4.586945	-3.940230	-1.340217
Na	-4.418426	-1.480501	0.288808
H	-2.723158	-1.655006	2.779038
H	0.287531	-1.918346	2.057645
H	-1.976917	0.242554	2.902245
O	-5.159324	-0.877756	2.446049
O	-6.751930	-1.664681	-0.388132
C	-7.465689	-0.506161	-0.090692

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 H  -8.246730  -0.752868   0.660047
 H  -6.786194   0.253678   0.348644
 C  -6.992804  -1.986703  -1.720035
 H  -6.080771  -1.768049  -2.315530
 H  -7.219171  -3.070532  -1.808126
 C  -8.149437  -1.161883  -2.239225
 H  -9.104299  -1.717267  -2.105296
 H  -8.015867  -0.884365  -3.307466
 C  -8.121638   0.032727  -1.344984
 H  -7.492387   0.832434  -1.794499
 H  -9.143175   0.423176  -1.144760
 C  -4.883438   0.349281   3.031401
 H  -4.367271   1.005810   2.304521
 H  -4.217975   0.201100   3.911256
 C  -6.245526  -1.397964   3.138083
 H  -6.856701  -2.024288   2.455157
 H  -5.878304  -2.042354   3.967490
 C  -7.071649  -0.244969   3.687663
 H  -8.029707  -0.139142   3.133431
 H  -7.281802  -0.394626   4.769411
 C  -6.195525   0.958472   3.470248
 H  -6.610054   1.596559   2.658656
 H  -6.074576   1.557835   4.398704
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Figure_S5_imid-3_modeR1_prod(CuHadd) / electronic energy: -3525.669421393887 a.u. / lowest freq: 13.75 cm-1
 C  -0.012502   3.387771  -1.037975
 H  -0.558164   3.197892  -1.977180
 C   1.337211   2.652468  -0.975937
 H   2.116155   3.244643  -0.465810
 C  -0.222614   1.541802   0.431756
 C  -2.099316   3.157836   0.368134
 C  -2.244534   4.095226   1.396499
 C  -3.235577   2.793604  -0.376544
 C  -3.470298   4.711471   1.640585
 H  -1.372131   4.349968   2.001472
 C  -4.461137   3.411857  -0.129416
 C  -4.576864   4.388074   0.857979
 H  -3.555277   5.449025   2.441241
 H  -5.324996   3.102031  -0.720489
 H  -5.538023   4.876712   1.031300
 C   1.953361   0.513788   0.215892
 C   3.132084   0.909578   0.863496
 C   1.800819  -0.821191  -0.183260
 C   4.157724  -0.014852   1.091426
 C   2.833514  -1.748340   0.030107
 C   4.010789  -1.339142   0.667692
 H   4.822874  -2.042582   0.809871
 S  -3.180093   1.457995  -1.577558
 O  -4.599176   1.151452  -1.892723
 O  -2.564875   0.330739  -0.798298
 O  -2.362692   1.916392  -2.713856
Cu  -1.069692  -0.048963   1.140002
 C   0.106837   4.874214  -0.805853
 C  -0.366418   5.778058  -1.773305
 C   0.676817   5.378496   0.378729
 C  -0.271897   7.156460  -1.559161
 H  -0.811149   5.418162  -2.692701
 C   0.768311   6.757230   0.588402
 H   1.039937   4.703882   1.144095
 C   0.294629   7.645616  -0.379680
 H  -0.639470   7.846003  -2.308053
 H   1.204421   7.136895   1.503300
 H   0.365515   8.713039  -0.215445
 C   1.848515   2.233349  -2.331044
 C   3.061318   2.748991  -2.819984
 C   1.142154   1.295989  -3.107762
 C   3.556767   2.334509  -4.059646
 H   3.624107   3.471580  -2.243271
 C   1.635889   0.892206  -4.350230
 H   0.215838   0.870510  -2.746624
 C   2.843828   1.408705  -4.825021
 H   4.493643   2.732482  -4.427402
 H   1.086214   0.170597  -4.940629
 H   3.228872   1.088932  -5.784564
 N  -0.785839   2.706447   0.038196
 N   0.989239   1.481009  -0.151458
 H   0.910563  -1.114278  -0.714822
 H   3.262971   1.940397   1.168983
 C   2.737196  -3.131432  -0.488122
 C   2.417592  -4.202847   0.396316
 C   3.130337  -3.410740  -1.830045
 C   2.503058  -5.524516  -0.077583
 C   3.209364  -4.752352  -2.248336
 C   2.887107  -5.791970  -1.385198
 H   2.295613  -6.362264   0.574129
 H   3.545416  -5.006216  -3.243914
 H   2.958472  -6.816806  -1.726397
 C   5.416879   0.421764   1.723051
```

C	6.445052	1.000690	0.927097
C	5.593836	0.281633	3.127836
C	7.621650	1.444953	1.557741
C	6.788437	0.743242	3.710355
C	7.787466	1.318247	2.932552
H	8.420839	1.894772	0.983480
H	6.951576	0.660522	4.776833
H	8.699615	1.667311	3.399404
C	4.525890	-0.345748	4.024139
H	3.656709	-0.693238	3.429417
C	3.976457	0.678726	5.023607
H	3.583838	1.564673	4.479864
H	3.142580	0.232056	5.606307
H	4.762921	1.011663	5.733322
C	5.065991	-1.586456	4.746812
H	5.500108	-2.296244	4.011049
H	5.847954	-1.315599	5.486924
H	4.240940	-2.102672	5.282690
C	6.313623	1.152926	-0.589356
H	5.351861	0.737948	-0.954323
C	7.411865	0.372784	-1.322611
H	7.222934	0.390207	-2.417415
H	8.414457	0.810482	-1.133261
H	7.413716	-0.686343	-0.987590
C	6.323046	2.630857	-0.996321
H	6.147288	2.725290	-2.089135
H	5.512879	3.174390	-0.464565
H	7.295307	3.109874	-0.755604
C	3.570372	-2.306871	-2.794306
H	3.270358	-1.309329	-2.414244
C	2.058550	-3.965742	1.862810
H	1.835160	-2.892773	2.036701
C	0.799082	-4.739542	2.285942
H	-0.004652	-4.619147	1.532300
H	1.007184	-5.823345	2.406240
H	0.427955	-4.352764	3.259086
C	3.239876	-4.331027	2.767865
H	3.475701	-5.414239	2.695021
H	4.139868	-3.752477	2.473947
H	3.000506	-4.087316	3.824962
C	2.912798	-2.439151	-4.176732
H	3.288343	-3.325314	-4.728324
H	1.811580	-2.518915	-4.075991
H	3.143726	-1.544104	-4.790758
C	5.096629	-2.289996	-2.920734
H	5.557970	-2.166017	-1.918122
H	5.467800	-3.235301	-3.371061
H	5.418218	-1.438347	-3.557811
C	-1.511651	-1.896408	1.742910
C	-2.598261	-2.109568	2.784483
H	-2.692148	-3.162817	3.115048
B	-1.733601	-2.514373	0.374407
O	-0.767871	-3.012719	-0.488287
O	-3.009348	-2.651878	-0.212910
C	-1.357497	-3.244688	-1.776598
C	-2.878360	-3.412931	-1.432064
C	-1.085241	-2.029250	-2.650128
H	-0.002055	-1.876972	-2.732529
H	-1.478365	-2.161183	-3.668127
H	-1.520799	-1.118558	-2.219746
C	-0.719291	-4.476443	-2.386907
H	-1.216216	-4.756429	-3.327201
H	0.334611	-4.274639	-2.617942
H	-0.751789	-5.336209	-1.706510
C	-3.257684	-4.846934	-1.099529
H	-3.232978	-5.497674	-1.984760
H	-2.584324	-5.270939	-0.341448
H	-4.278247	-4.870492	-0.692190
C	-3.817020	-2.836532	-2.472916
H	-3.668562	-1.755305	-2.598975
H	-3.664226	-3.315766	-3.450883
H	-4.865059	-3.000973	-2.186814
Na	-4.326273	-0.819104	0.046573
H	-3.597290	-1.828096	2.413789
H	-0.521135	-2.174091	2.141297
H	-2.448060	-1.520206	3.704144
O	-5.029797	0.341877	1.946189
O	-6.458836	-1.473578	-0.431994
C	-7.392412	-0.504667	-0.772059
H	-7.023910	0.493505	-0.453372
H	-7.527328	-0.495999	-1.876358
C	-7.166987	-2.637889	-0.175147
H	-7.257395	-3.228531	-1.113837
H	-6.619575	-3.248317	0.574194
C	-8.539895	-2.261946	0.346033
H	-8.569050	-2.342552	1.455143
H	-9.326609	-2.911091	-0.096750
C	-8.702933	-0.828567	-0.079848

H -9.560496 -0.708068 -0.777374
H -8.848429 -0.173416 0.807343
C -6.067239 -0.140998 2.730263
H -6.370154 -1.146496 2.371401
H -6.939375 0.544756 2.647101
C -4.233352 1.137041 2.763276
H -3.164428 0.960093 2.519116
H -4.466089 2.202863 2.570029
C -4.506976 0.811185 4.222383
H -3.600935 0.410243 4.726255
H -4.858026 1.717920 4.762942
C -5.594421 -0.219641 4.163780
H -5.178594 -1.229611 4.374340
H -6.417144 0.004491 4.877115
165
Figure_S5_imid-3_modeR2_ed(CuHadd) / electronic energy: -3525.644171244942 a.u. / lowest freq: 15.57 cm-1
C -2.212307 -0.824856 2.232479
H -2.806118 0.076153 2.451495
C -0.699649 -0.598728 2.383860
H -0.162713 -1.536938 2.619960
C -1.227327 -0.647097 0.100653
C -3.483548 -1.527457 0.108814
C -3.419039 -2.741515 -0.581623
C -4.685587 -0.798694 0.112443
C -4.531916 -3.243537 -1.247953
H -2.472252 -3.285867 -0.593194
C -5.805723 -1.325152 -0.537984
C -5.735455 -2.540161 -1.213188
H -4.455926 -4.191163 -1.786403
H -6.727820 -0.741127 -0.533030
H -6.619575 -2.930471 -1.722115
C 0.955376 0.177684 0.637178
C 1.276987 1.531900 0.509404
C 1.941163 -0.793177 0.428840
C 2.580622 1.920940 0.184148
C 3.261237 -0.408926 0.144740
C 3.579025 0.952423 0.033114
H 4.595752 1.256561 -0.184929
S -4.863626 0.822783 0.875885
O -5.976230 1.474573 0.121545
O -3.578685 1.538462 0.622965
O -5.161171 0.580930 2.299252
Cu -0.833704 -0.529337 -1.824217
C -2.722345 -1.979685 3.054763
C -3.605062 -1.752696 4.124917
C -2.317153 -3.295407 2.773046
C -4.082234 -2.823870 4.886672
H -3.918846 -0.747796 4.376329
C -2.796141 -4.364135 3.534948
H -1.634899 -3.488204 1.959944
C -3.679912 -4.128762 4.590697
H -4.762629 -2.641708 5.708431
H -2.481602 -5.374302 3.306665
H -4.050460 -4.956641 5.181180
C -0.351048 0.453015 3.404943
C 0.468907 0.128505 4.500240
C -0.831114 1.769262 3.277906
C 0.783959 1.097083 5.457822
H 0.862252 -0.873788 4.617021
C -0.520624 2.731724 4.241333
H -1.445397 2.048379 2.433536
C 0.283087 2.395054 5.332843
H 1.414058 0.840009 6.299370
H -0.898120 3.740827 4.137891
H 0.526002 3.142839 6.076537
N -2.307834 -1.086314 0.771956
N -0.351170 -0.195788 1.014017
H 1.688341 -1.840627 0.525040
H 0.515463 2.279967 0.669083
C 4.322388 -1.431928 0.017416
C 4.728456 -2.176358 1.164419
C 4.945977 -1.671318 -1.243427
C 5.706425 -3.176013 1.013753
C 5.954515 -2.649457 -1.325683
C 6.314985 -3.402127 -0.214590
H 6.019431 -3.775456 1.858323
H 6.459678 -2.846684 -2.261749
H 7.079034 -4.163573 -0.304844
C 2.893271 3.346898 -0.028785
C 2.760595 3.913078 -1.328351
C 3.321094 4.154812 1.060723
C 3.049910 5.278038 -1.507019
C 3.620374 5.509342 0.824698
C 3.477141 6.063069 -0.442442
H 2.952234 5.741384 -2.479898
H 3.964113 6.148228 1.627304
H 3.703037 7.109645 -0.601676
C 3.472050 3.597788 2.475421

H	3.132976	2.542924	2.529098
C	2.601986	4.371508	3.473645
H	1.550423	4.398692	3.117247
H	2.626663	3.869933	4.464027
H	2.961781	5.413122	3.605951
C	4.942032	3.600089	2.908908
H	5.551301	3.020795	2.182278
H	5.341494	4.634554	2.969560
H	5.045437	3.121781	3.906398
C	2.320235	3.086250	-2.536835
H	2.148490	2.027354	-2.257728
C	3.407850	3.066577	-3.617367
H	3.136872	2.343744	-4.416509
H	3.537536	4.068266	-4.078425
H	4.375196	2.748734	-3.174079
C	0.989961	3.596937	-3.102049
H	0.654039	2.944718	-3.936191
H	0.212778	3.571172	-2.310750
H	1.082025	4.635590	-3.482928
C	4.563287	-0.903859	-2.511410
H	3.703496	-0.229616	-2.328673
C	4.164321	-1.904772	2.561932
H	3.474662	-1.037903	2.557454
C	3.354997	-3.102621	3.073630
H	2.531784	-3.337577	2.366647
H	3.996743	-4.001335	3.189201
H	2.901462	-2.862353	4.059012
C	5.275338	-1.527140	3.550842
H	5.956659	-2.382003	3.743763
H	5.867038	-0.676299	3.149978
H	4.830003	-1.212214	4.518972
C	4.110103	-1.847341	-3.632514
H	4.943180	-2.486112	-3.992690
H	3.290789	-2.496639	-3.270106
H	3.725810	-1.257958	-4.492439
C	5.724755	-0.021481	-2.984353
H	6.018512	0.685914	-2.180254
H	6.607960	-0.634858	-3.261522
H	5.417398	0.569854	-3.872857
C	-0.993886	-2.255371	-2.936977
C	-0.406236	-1.187297	-3.646665
H	-0.953608	-0.632452	-4.412496
B	-0.197719	-3.375763	-2.260583
O	-0.773866	-4.545108	-1.797129
O	1.172604	-3.380334	-2.103944
C	0.265780	-5.312085	-1.142664
C	1.560860	-4.739772	-1.804509
C	0.190330	-5.010705	0.343440
H	-0.797927	-5.303679	0.721877
H	0.943581	-5.570005	0.914902
H	0.336147	-3.938837	0.541906
C	0.025416	-6.784259	-1.395975
H	0.852086	-7.389643	-0.996717
H	-0.896777	-7.110638	-0.896556
H	-0.077415	-7.003897	-2.465177
C	1.886748	-5.418161	-3.126618
H	2.245089	-6.446378	-2.979654
H	1.010706	-5.451574	-3.789311
H	2.676661	-4.858819	-3.644350
C	2.775049	-4.731266	-0.903886
H	2.627127	-4.095056	-0.024640
H	3.013866	-5.747226	-0.558228
H	3.647911	-4.355725	-1.451486
Na	-4.558250	3.163514	-0.855547
H	0.683944	-1.135138	-3.751899
H	-2.073349	-2.412521	-3.068831
H	-0.477739	0.991914	-2.080398
O	-2.771205	4.642339	-0.705134
O	-3.996487	2.068220	-2.793991
C	-1.793351	4.115023	0.126693
H	-2.239660	3.890781	1.117565
H	-1.414042	3.168522	-0.316686
C	-2.140862	5.557381	-1.535732
H	-1.825647	5.049028	-2.472796
H	-2.850216	6.370078	-1.799859
C	-0.933605	6.122960	-0.814073
H	-1.172853	7.119323	-0.381322
H	-0.062311	6.212975	-1.499321
C	-0.673044	5.127295	0.279962
H	0.318761	4.646256	0.155454
H	-0.721171	5.618901	1.276632
C	-3.062185	2.518776	-3.716142
H	-2.047166	2.473747	-3.264963
H	-3.282872	3.574770	-3.979670
C	-4.143444	0.708103	-3.022295
H	-3.394105	0.148252	-2.419452
H	-5.161392	0.388015	-2.718147
C	-3.134758	1.641156	-4.952610

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 H  -2.117255   1.346710  -5.288686
 H  -3.659556   2.169494  -5.778875
 C  -3.932276   0.449046  -4.498894
 H  -4.911084   0.416880  -5.026574
 H  -3.387729  -0.504707  -4.667205
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Figure_S5_imid-3_modeR2_ts(CuHadd)_01 / electronic energy: -3525.630124745377 a.u. / lowest freq: -778.17 cm-1
 C  -2.207389  -0.680284   2.306579
 H  -2.776977   0.239876   2.508860
 C  -0.687147  -0.487563   2.455174
 H  -0.174131  -1.429392   2.726334
 C  -1.215554  -0.582695   0.171647
 C  -3.484055  -1.412612   0.187368
 C  -3.406245  -2.617917  -0.519531
 C  -4.688120  -0.688884   0.186212
 C  -4.514165  -3.122498  -1.191083
 H  -2.453130  -3.150191  -0.545935
 C  -5.805550  -1.221112  -0.465951
 C  -5.725306  -2.431687  -1.147550
 H  -4.425952  -4.062414  -1.741295
 H  -6.731210  -0.642670  -0.461523
 H  -6.606323  -2.826450  -1.658519
 C   0.991910   0.181540   0.687539
 C   1.342545   1.517253   0.481955
 C   1.953113  -0.822418   0.528646
 C   2.655314   1.859270   0.145079
 C   3.282906  -0.485152   0.227293
 C   3.633587   0.862701   0.054827
 H   4.656638   1.132734  -0.176864
 S  -4.863430   0.946404   0.918489
 O  -5.955487   1.593862   0.130726
 O  -3.567229   1.645892   0.669938
 O  -5.181823   0.740355   2.342237
Cu  -0.891406  -0.731373  -1.697535
 C  -2.744715  -1.805241   3.153400
 C  -3.637213  -1.536380   4.205755
 C  -2.355333  -3.134443   2.913584
 C  -4.141260  -2.579210   4.989143
 H  -3.937812  -0.520582   4.427150
 C  -2.861366  -4.174665   3.697200
 H  -1.661357  -3.360754   2.119166
 C  -3.755859  -3.897550   4.733509
 H  -4.829249  -2.364539   5.796612
 H  -2.558624  -5.195199   3.501386
 H  -4.147044  -4.703428   5.340880
 C  -0.311926   0.591219   3.438152
 C   0.504716   0.287565   4.541897
 C  -0.753911   1.914976   3.259717
 C   0.856458   1.285373   5.455790
 H   0.869964  -0.720110   4.697251
 C  -0.406705   2.907010   4.179710
 H  -1.364688   2.177846   2.407481
 C   0.396075   2.592230   5.278397
 H   1.485025   1.044580   6.303286
 H  -0.753870   3.922080   4.036055
 H   0.668533   3.363022   5.987564
 N  -2.312189  -0.970244   0.854476
 N  -0.324249  -0.137758   1.075548
 H   1.672162  -1.856615   0.673843
 H   0.595117   2.288299   0.589064
 C   4.314544  -1.542940   0.129285
 C   4.683980  -2.282319   1.292403
 C   4.941708  -1.826820  -1.121695
 C   5.625213  -3.320038   1.167422
 C   5.913573  -2.843223  -1.177406
 C   6.235037  -3.590145  -0.050997
 H   5.909202  -3.915615   2.024901
 H   6.420798  -3.074403  -2.104525
 H   6.971122  -4.380721  -0.121130
 C   2.987959   3.261104  -0.169644
 C   2.826431   3.740768  -1.500121
 C   3.428585   4.140301   0.857348
 C   3.097019   5.094163  -1.771296
 C   3.711412   5.479077   0.529178
 C   3.538692   5.949116  -0.767976
 H   2.968625   5.494822  -2.768130
 H   4.059089   6.172046   1.283863
 H   3.748666   6.985853  -0.997700
 C   3.595405   3.680228   2.304542
 H   3.285833   2.622071   2.426964
 C   2.703441   4.494100   3.249938
 H   1.651947   4.468038   2.893223
 H   2.739876   4.060326   4.271631
 H   3.034042   5.552034   3.310427
 C   5.064482   3.749912   2.736074
 H   5.690519   3.145274   2.045269
 H   5.435332   4.796651   2.734901
 H   5.179945   3.335692   3.760537
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C   2.359203   2.835352  -2.640698
H   2.243068   1.787156  -2.299395
C   3.389616   2.791564  -3.775690
H   3.109030   2.008927  -4.512877
H   3.450895   3.765466  -4.305091
H   4.391707   2.541460  -3.367560
C   0.983999   3.269975  -3.158079
H   0.635104   2.571337  -3.948292
H   0.247909   3.247537  -2.327267
H   1.017314   4.295333  -3.582699
C   4.603024  -1.067863  -2.407722
H   3.761977  -0.365240  -2.249765
C   4.121937  -1.965930   2.681172
H   3.462114  -1.076677   2.656811
C   3.271266  -3.127070   3.210397
H   2.453862  -3.359407   2.495818
H   3.885899  -4.039520   3.360602
H   2.809076  -2.848028   4.181453
C   5.239935  -1.607251   3.669335
H   5.892395  -2.480104   3.880641
H   5.860941  -0.783274   3.256903
H   4.800436  -1.261279   4.629504
C   4.136393  -2.012623  -3.521981
H   4.954512  -2.679925  -3.864173
H   3.294880  -2.632475  -3.160472
H   3.779006  -1.423851  -4.393916
C   5.799474  -0.230989  -2.876565
H   6.103959   0.480661  -2.080489
H   6.666608  -0.877184  -3.128894
H   5.525467   0.354139  -3.779857
C  -1.020570  -2.225502  -3.112228
C  -0.384700  -1.030084  -3.621300
H  -0.860088  -0.486038  -4.442614
B  -0.299991  -3.352322  -2.414943
O  -0.920000  -4.530399  -1.990926
O   1.066565  -3.385252  -2.138403
C   0.045030  -5.262960  -1.210110
C   1.397113  -4.742366  -1.790910
C  -0.143227  -4.863307   0.243969
H  -1.170991  -5.100354   0.552297
H   0.539996  -5.399773   0.917078
H   0.016651  -3.782347   0.377038
C  -0.191593  -6.746989  -1.388847
H   0.593242  -7.333512  -0.888930
H  -1.155144  -7.035778  -0.946916
H  -0.211804  -7.030408  -2.447988
C   1.789799  -5.469099  -3.069622
H   2.112021  -6.501121  -2.871835
H   0.953818  -5.501134  -3.782370
H   2.623847  -4.944995  -3.554344
C   2.548354  -4.750859  -0.808695
H   2.360348  -4.096037   0.049255
H   2.733911  -5.766803  -0.430429
H   3.468748  -4.409147  -1.298428
Na -4.457351   3.195988  -0.915775
H   0.705658  -1.051934  -3.740670
H  -2.097779  -2.335182  -3.296144
H  -0.343717   0.365178  -2.724616
O  -2.662392   4.693061  -0.778341
O  -3.887323   1.977330  -2.809739
C  -1.708046   4.201166   0.101391
H  -2.163289   4.082548   1.106726
H  -1.369740   3.204725  -0.255787
C  -1.992733   5.506437  -1.680906
H  -1.688805   4.904563  -2.564599
H  -2.669090   6.317539  -2.024493
C  -0.770559   6.089078  -1.000178
H  -0.981412   7.121981  -0.645342
H   0.104202   6.100671  -1.686754
C  -0.543186   5.172383   0.167543
H   0.425597   4.639474   0.073729
H  -0.559216   5.742239   1.122657
C  -2.975547   2.369954  -3.778247
H  -1.942801   2.215017  -3.396450
H  -3.112451   3.448690  -4.002558
C  -4.140383   0.631301  -3.034870
H  -3.429147   0.017391  -2.439108
H  -5.175432   0.391897  -2.714417
C  -3.211371   1.540193  -5.024068
H  -2.250171   1.246343  -5.498166
H  -3.828399   2.107935  -5.755104
C  -3.971362   0.346238  -4.515213
H  -4.962802   0.274761  -5.014516
H  -3.405854  -0.596453  -4.677717
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Figure_S5_imid-3_modeR2_ts(CuHadd)_02 / electronic energy: -3525.627351660013 a.u. / lowest freq: -758.39 cm-1
C  -2.263165  -0.433494   2.420016
H  -2.622097   0.568290   2.701650
```

C	-0.731726	-0.558027	2.487362
H	-0.408989	-1.606180	2.628534
C	-1.375243	-0.349424	0.246352
C	-3.756452	-0.709891	0.327341
C	-4.009189	-1.866098	-0.419511
C	-4.721972	0.309135	0.382701
C	-5.225091	-2.033363	-1.075385
H	-3.225445	-2.624064	-0.493593
C	-5.946073	0.121640	-0.266423
C	-6.203635	-1.042908	-0.984589
H	-5.404904	-2.940718	-1.656399
H	-6.680499	0.928310	-0.223487
H	-7.164472	-1.168799	-1.488765
C	0.954091	-0.004677	0.678599
C	1.480204	1.270535	0.450211
C	1.759444	-1.133384	0.495800
C	2.823905	1.422028	0.091342
C	3.114525	-0.988790	0.157955
C	3.649351	0.296548	-0.015453
H	4.695816	0.419163	-0.267384
S	-4.456717	1.895534	1.205261
O	-5.365794	2.832869	0.512270
O	-3.011692	2.208879	0.961171
O	-4.760079	1.671520	2.631961
Cu	-1.148461	-0.424610	-1.640004
C	-2.982948	-1.477583	3.232526
C	-3.761996	-1.098883	4.339758
C	-2.882796	-2.840351	2.904147
C	-4.434796	-2.065038	5.094210
H	-3.844175	-0.058109	4.625505
C	-3.556905	-3.803638	3.659109
H	-2.284376	-3.152009	2.062716
C	-4.333935	-3.416151	4.753194
H	-5.033115	-1.765980	5.945086
H	-3.475943	-4.850368	3.395894
H	-4.855380	-4.162594	5.338246
C	-0.093799	0.312560	3.538510
C	0.703232	-0.265580	4.542411
C	-0.256032	1.709927	3.516248
C	1.316730	0.537675	5.508012
H	0.852984	-1.337106	4.578510
C	0.350960	2.507903	4.489153
H	-0.848278	2.180947	2.744542
C	1.137778	1.922688	5.483723
H	1.930603	0.085543	6.276201
H	0.217446	3.581715	4.467254
H	1.612641	2.543064	6.232668
N	-2.488143	-0.601285	0.962344
N	-0.375818	-0.138853	1.123460
H	1.338493	-2.117236	0.650300
H	0.847646	2.142170	0.559555
C	3.978780	-2.184937	0.020912
C	4.246539	-3.001008	1.161237
C	4.539440	-2.532006	-1.246740
C	5.016261	-4.166895	0.997574
C	5.336842	-3.687972	-1.341597
C	5.555832	-4.501166	-0.237358
H	5.219851	-4.818124	1.837261
H	5.787277	-3.974866	-2.282381
H	6.158814	-5.394564	-0.337547
C	3.357354	2.760786	-0.220338
C	3.271944	3.261403	-1.550021
C	3.945894	3.552218	0.804315
C	3.779838	4.543668	-1.826104
C	4.455189	4.821452	0.472805
C	4.367468	5.310084	-0.825995
H	3.721014	4.958550	-2.823658
H	4.917145	5.446177	1.225726
H	4.755104	6.293512	-1.058882
C	4.029811	3.074572	2.253229
H	3.553823	2.080140	2.376142
C	3.274481	4.023517	3.192046
H	2.225975	4.143259	2.845198
H	3.257581	3.605334	4.220655
H	3.754919	5.023345	3.232181
C	5.488629	2.908193	2.693285
H	6.014688	2.213461	2.003845
H	6.021567	3.882365	2.698771
H	5.530187	2.477882	3.716778
C	2.642763	2.452979	-2.685906
H	2.341237	1.443302	-2.341529
C	3.641972	2.225273	-3.826606
H	3.227746	1.494473	-4.553962
H	3.862862	3.170125	-4.366112
H	4.590662	1.814783	-3.421558
C	1.364631	3.126197	-3.197353
H	0.891041	2.499317	-3.982826
H	0.640927	3.238883	-2.362988

H 1.579360 4.127431 -3.626590
C 4.314305 -1.697642 -2.511237
H 3.609297 -0.865234 -2.324972
C 3.758729 -2.639433 2.567004
H 3.232671 -1.664932 2.574941
C 2.760880 -3.680810 3.089552
H 1.905189 -3.777446 2.388414
H 3.241279 -4.674921 3.206396
H 2.363187 -3.364929 4.077331
C 4.933446 -2.467047 3.539151
H 5.459320 -3.428333 3.717072
H 5.657578 -1.729091 3.132047
H 4.564350 -2.086308 4.515716
C 3.673300 -2.522678 -3.633557
H 4.348078 -3.328990 -3.988617
H 2.729787 -2.973727 -3.274000
H 3.430175 -1.865993 -4.496313
C 5.629091 -1.068002 -2.988205
H 6.059359 -0.429979 -2.187610
H 6.371412 -1.846736 -3.262826
H 5.447344 -0.432508 -3.880445
C -1.520696 -1.831449 -3.097129
C -0.742031 -0.720344 -3.596525
H -1.170399 -0.089669 -4.381877
B -0.955758 -3.086215 -2.472526
O -1.740185 -4.171823 -2.084286
O 0.395329 -3.339397 -2.243254
C -0.881639 -5.085422 -1.372402
C 0.518771 -4.750493 -1.974527
C -0.968737 -4.738812 0.104271
H -2.010396 -4.844342 0.436675
H -0.350427 -5.400638 0.726589
H -0.651441 -3.700034 0.281267
C -1.351852 -6.503278 -1.614628
H -0.654639 -7.229717 -1.171841
H -2.336062 -6.662467 -1.152986
H -1.445819 -6.724042 -2.684808
C 0.749321 -5.461280 -3.300675
H 0.909120 -6.539734 -3.162461
H -0.103331 -5.325381 -3.980968
H 1.640756 -5.053613 -3.794464
C 1.681932 -4.997865 -1.038966
H 1.642845 -4.358673 -0.150200
H 1.697809 -6.045855 -0.705934
H 2.633338 -4.803911 -1.549925
Na -2.208023 2.678661 -1.054011
H 0.329676 -0.888077 -3.762185
H -2.605604 -1.790943 -3.260854
H -0.482597 0.601026 -2.680961
O -1.352433 4.754096 -0.605340
O -3.297777 2.175756 -3.001506
C -0.892628 5.748107 -1.459255
H -0.785745 5.332733 -2.483903
H -1.635798 6.575037 -1.493350
C -0.770980 4.993943 0.630815
H -1.415919 5.686930 1.215953
H -0.673789 4.042426 1.192210
C 0.589763 5.609231 0.396786
H 1.361056 4.811698 0.356289
H 0.847680 6.344571 1.189503
C 0.445442 6.259443 -0.950284
H 0.431044 7.367403 -0.856277
H 1.272074 5.955272 -1.627589
C -2.878774 2.621795 -4.249679
H -1.823731 2.310717 -4.407426
H -2.923612 3.731168 -4.283756
C -4.212304 1.145000 -3.187349
H -3.891446 0.257066 -2.605152
H -5.204290 1.475725 -2.811079
C -3.762423 2.024397 -5.322954
H -3.187826 1.775202 -6.241509
H -4.589696 2.726333 -5.569735
C -4.308783 0.802550 -4.659429
H -5.356909 0.598225 -4.968785
H -3.669611 -0.077167 -4.892084

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Figure_S5_imid-3_modeR2_prod(CuHadd) / electronic energy: -3525.672878743977 a.u. / lowest freq: 15.36 cm-1

C -2.424447 -0.326660 2.267369
H -3.000389 0.602048 2.392571
C -0.906562 -0.124203 2.458076
H -0.413732 -1.032856 2.851409
C -1.338191 -0.444123 0.176990
C -3.626870 -1.166767 0.134873
C -3.525809 -2.390092 -0.538862
C -4.813821 -0.424117 0.037586
C -4.599779 -2.899979 -1.260003
H -2.578289 -2.930199 -0.500322
C -5.897594 -0.957538 -0.667653

C	-5.800833	-2.192031	-1.304128
H	-4.491812	-3.852816	-1.783573
H	-6.808426	-0.360953	-0.743880
H	-6.656500	-2.587577	-1.855677
C	0.881687	0.249845	0.716830
C	1.351754	1.535343	0.446074
C	1.764735	-0.836220	0.674847
C	2.700921	1.746750	0.154960
C	3.136475	-0.625197	0.450170
C	3.601121	0.676402	0.204006
H	4.655196	0.856090	0.037870
S	-4.969695	1.262393	0.649886
O	-5.983196	1.884798	-0.253971
O	-3.630670	1.885579	0.428264
O	-5.375217	1.177371	2.062830
Cu	-0.939696	-1.052429	-1.598593
C	-2.993549	-1.401389	3.157893
C	-3.958436	-1.079977	4.128427
C	-2.570378	-2.737239	3.033582
C	-4.494985	-2.076926	4.949051
H	-4.292161	-0.058458	4.256271
C	-3.109485	-3.730970	3.854596
H	-1.823300	-3.006534	2.301555
C	-4.072473	-3.401436	4.811080
H	-5.237886	-1.821921	5.693681
H	-2.779485	-4.756424	3.749474
H	-4.489098	-4.171609	5.447190
C	-0.555939	1.050787	3.333532
C	0.221082	0.862769	4.490493
C	-0.973870	2.350605	2.996414
C	0.557107	1.951854	5.300188
H	0.569121	-0.124954	4.766839
C	-0.639963	3.435513	3.810409
H	-1.555725	2.522453	2.103122
C	0.121865	3.235952	4.963849
H	1.155513	1.799963	6.189100
H	-0.966420	4.432168	3.542914
H	0.383562	4.077859	5.591521
N	-2.479197	-0.713515	0.835220
N	-0.471918	0.067850	1.065287
H	1.393797	-1.831738	0.875443
H	0.670058	2.371254	0.467812
C	4.092307	-1.755716	0.556558
C	4.262537	-2.420172	1.809746
C	4.854909	-2.177941	-0.576881
C	5.121818	-3.531471	1.879587
C	5.742936	-3.260230	-0.431856
C	5.854840	-3.940178	0.773685
H	5.250350	-4.074258	2.806659
H	6.350335	-3.594040	-1.262324
H	6.528610	-4.783422	0.855884
C	3.157030	3.089288	-0.247603
C	3.106604	3.466639	-1.619508
C	3.613635	4.013393	0.731617
C	3.516227	4.762795	-1.981333
C	4.027097	5.292471	0.316130
C	3.973051	5.661241	-1.023557
H	3.486811	5.083905	-3.014174
H	4.389712	6.016701	1.033550
H	4.288395	6.652708	-1.322349
C	3.664665	3.662974	2.217970
H	3.268518	2.643603	2.403558
C	2.787005	4.613533	3.041118
H	1.754579	4.624731	2.631570
H	2.742830	4.269414	4.096190
H	3.187799	5.648634	3.030007
C	5.108731	3.661016	2.732028
H	5.724230	2.960442	2.127796
H	5.557820	4.675058	2.675785
H	5.135409	3.321642	3.789639
C	2.621941	2.510094	-2.711554
H	2.356601	1.519046	-2.290983
C	3.724229	2.244527	-3.743346
H	3.406979	1.437803	-4.438643
H	3.948119	3.154593	-4.338626
H	4.651399	1.914706	-3.229086
C	1.350256	3.037814	-3.386342
H	0.999715	2.319457	-4.157187
H	0.544398	3.151307	-2.632144
H	1.526494	4.018113	-3.876368
C	4.762512	-1.492449	-1.942695
H	3.939713	-0.751353	-1.960270
C	3.585521	-1.940628	3.097825
H	3.016303	-1.005472	2.932506
C	2.583626	-2.979430	3.617431
H	1.828805	-3.209499	2.836756
H	3.095713	-3.920794	3.908032
H	2.047733	-2.579814	4.504863

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C   4.619624  -1.587636   4.175682
H   5.164204  -2.488132   4.528853
H   5.353152  -0.856588   3.772910
H   4.113245  -1.123292   5.049067
C   4.444580  -2.488494  -3.066725
H   5.303177  -3.160241  -3.275226
H   3.570856  -3.107110  -2.792653
H   4.201001  -1.939233  -4.001428
C   6.059953  -0.736702  -2.257613
H   6.276263   0.009029  -1.465012
H   6.920855  -1.434698  -2.330209
H   5.963313  -0.198690  -3.224364
C  -0.309216  -1.922779  -3.248000
C   0.872264  -1.218031  -3.894915
H   1.263624  -1.741369  -4.789244
B  -0.002351  -3.173978  -2.443464
O  -0.911318  -4.190433  -2.102854
O   1.254884  -3.460195  -1.902205
C  -0.267245  -5.054378  -1.147357
C   1.246568  -4.822714  -1.460252
C  -0.635342  -4.577091   0.248819
H  -1.722319  -4.648610   0.391965
H  -0.162122  -5.182384   1.034681
H  -0.335735  -3.527146   0.392989
C  -0.748925  -6.473981  -1.359883
H  -0.201563  -7.177772  -0.715451
H  -1.816364  -6.555343  -1.111059
H  -0.625570  -6.792850  -2.401828
C   1.731256  -5.695630  -2.611191
H   1.796865  -6.754656  -2.323920
H   1.062767  -5.617456  -3.480287
H   2.731836  -5.373127  -2.927585
C   2.174760  -4.968070  -0.272692
H   1.958175  -4.230727   0.508594
H   2.102872  -5.972323   0.170016
H   3.215426  -4.819468  -0.589640
Na -4.228800   2.996647  -1.579536
H   1.721048  -1.147287  -3.197937
H  -1.183716  -2.032471  -3.912138
H   0.666099  -0.185194  -4.218749
O  -2.407688   4.472118  -1.466044
O  -3.190522   1.275411  -2.808663
C  -1.628882   4.165894  -0.355130
H  -2.245186   4.305294   0.558430
H  -1.314874   3.103660  -0.416512
C  -1.782941   5.498944  -2.162109
H  -1.274794   5.074998  -3.055568
H  -2.541155   6.235026  -2.503823
C  -0.768752   6.167023  -1.260564
H  -1.240656   7.018071  -0.721332
H   0.120578   6.519777  -1.827266
C  -0.419330   5.080515  -0.296682
H   0.490018   4.544839  -0.642274
H  -0.249378   5.477071   0.728216
C  -2.043727   1.565716  -3.534164
H  -1.171701   1.062647  -3.062677
H  -1.865460   2.660449  -3.522489
C  -3.725978   0.127673  -3.375953
H  -3.289241  -0.766185  -2.881150
H  -4.826178   0.115963  -3.227497
C  -2.239142   1.082403  -4.958797
H  -1.325425   0.580973  -5.342649
H  -2.503241   1.933155  -5.625012
C  -3.390890   0.121262  -4.853772
H  -4.256662   0.486863  -5.448870
H  -3.106189  -0.897781  -5.195243
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Figure_S6_imid-3_modeS1_ed(CuHadd) / electronic energy: -3602.006293842289 a.u. / lowest freq: 11.51 cm-1
C   0.109200   3.175353   0.027174
H   0.847763   2.955608   0.813148
C  -1.310449   2.690164   0.377864
H  -2.083297   3.390229   0.016144
C  -0.417262   1.287269  -1.297191
C   1.520312   2.494814  -2.035170
C   1.214490   2.624696  -3.396608
C   2.864951   2.471545  -1.635250
C   2.220120   2.737232  -4.350750
H   0.162003   2.621996  -3.692118
C   3.868678   2.606796  -2.598713
C   3.554627   2.741637  -3.948517
H   1.957912   2.827162  -5.407162
H   4.907722   2.567348  -2.267708
H   4.354296   2.838780  -4.685934
C  -2.511854   0.561247  -0.340318
C  -3.817947   1.074342  -0.259142
C  -2.315692  -0.825910  -0.272717
C  -4.910489   0.210540  -0.115361
C  -3.408390  -1.686909  -0.103283
```

C	-4.705049	-1.169453	-0.037792
H	-5.548292	-1.836335	0.101756
S	3.374564	2.150258	0.057911
O	4.788159	1.693467	-0.065868
O	2.501196	1.039012	0.539330
O	3.212824	3.417294	0.794712
Cu	-0.143056	0.046881	-2.824697
C	0.148687	4.644581	-0.310659
C	0.803956	5.549320	0.542671
C	-0.488443	5.135172	-1.466426
C	0.840229	6.912463	0.234327
H	1.278628	5.203698	1.451985
C	-0.448543	6.498620	-1.771024
H	-1.014253	4.461578	-2.131417
C	0.217425	7.386335	-0.922811
H	1.348538	7.602509	0.895304
H	-0.936131	6.867304	-2.664167
H	0.246356	8.442091	-1.159317
C	-1.501364	2.454758	1.854276
C	-2.369079	3.274101	2.596527
C	-0.839568	1.396036	2.502036
C	-2.565891	3.039720	3.960733
H	-2.893892	4.093512	2.121424
C	-1.046847	1.159226	3.863400
H	-0.179142	0.746015	1.945536
C	-1.909546	1.980516	4.592509
H	-3.234633	3.675134	4.526764
H	-0.541325	0.337460	4.352742
H	-2.070174	1.795893	5.646708
N	0.429565	2.325484	-1.146157
N	-1.396084	1.433183	-0.392839
H	-1.310912	-1.229362	-0.301674
H	-3.991907	2.141384	-0.303664
C	-3.185382	-3.130338	0.084382
C	-3.101085	-3.988734	-1.045112
C	-2.988643	-3.647741	1.395230
C	-2.762538	-5.339356	-0.845239
C	-2.651839	-5.005777	1.542766
C	-2.535206	-5.837290	0.433684
H	-2.664508	-6.014858	-1.684681
H	-2.468316	-5.426831	2.522313
H	-2.268589	-6.877894	0.566573
C	-6.276179	0.752790	-0.000352
C	-6.838729	1.003843	1.281676
C	-7.053275	0.982123	-1.166616
C	-8.168800	1.465896	1.359731
C	-8.369325	1.452818	-1.009543
C	-8.898920	1.682770	0.259198
H	-8.626900	1.651880	2.322453
H	-8.997384	1.636438	-1.871389
H	-9.917242	2.038624	0.353604
C	-6.513694	0.719159	-2.571842
H	-5.462076	0.368578	-2.537155
C	-6.504577	2.002637	-3.411117
H	-5.931412	2.795557	-2.884397
H	-6.014038	1.812975	-4.389769
H	-7.535231	2.369043	-3.601387
C	-7.309156	-0.391655	-3.267660
H	-7.296319	-1.312541	-2.645758
H	-8.363080	-0.086513	-3.438400
H	-6.848381	-0.631574	-4.249763
C	-6.052602	0.772263	2.572858
H	-5.008902	0.464782	2.357601
C	-6.673005	-0.363112	3.394367
H	-6.045620	-0.574067	4.286593
H	-7.696055	-0.099420	3.736297
H	-6.725061	-1.288364	2.781335
C	-5.945355	2.058438	3.401294
H	-5.287286	1.888243	4.279838
H	-5.502094	2.870082	2.785571
H	-6.938339	2.388133	3.771676
C	-3.110321	-2.769400	2.642439
H	-3.455426	-1.748272	2.383286
C	-3.356120	-3.484788	-2.465519
H	-3.689312	-2.426832	-2.459918
C	-2.071123	-3.524990	-3.296439
H	-1.298960	-2.897153	-2.807024
H	-1.686241	-4.561837	-3.396336
H	-2.257213	-3.114058	-4.311626
C	-4.483870	-4.270312	-3.147053
H	-4.191103	-5.325357	-3.329936
H	-5.395793	-4.252331	-2.512479
H	-4.733812	-3.803894	-4.124046
C	-1.751320	-2.595726	3.326360
H	-1.332467	-3.573121	3.645973
H	-1.041986	-2.106826	2.625874
H	-1.852708	-1.944311	4.220362
C	-4.156120	-3.322881	3.618628

H -5.125153 -3.467370 3.094702
H -3.832561 -4.291087 4.054499
H -4.316579 -2.603633 4.450052
C 1.752401 -0.793429 -2.843819
C 1.015695 -1.042300 -4.021254
H 0.559511 -2.023460 -4.188309
B 1.912688 -1.892229 -1.786406
O 1.076050 -2.983444 -1.724223
O 2.971420 -2.007093 -0.890330
C 1.511869 -3.807744 -0.621669
C 3.012221 -3.411246 -0.510784
C 0.709343 -3.392978 0.597365
H -0.356466 -3.499720 0.370758
H 0.932918 -4.015563 1.474384
H 0.892081 -2.339886 0.852228
C 1.262873 -5.258385 -0.966421
H 1.661742 -5.923429 -0.186951
H 0.184806 -5.447040 -1.047992
H 1.722376 -5.531915 -1.923678
C 3.876415 -4.130383 -1.532828
H 4.008924 -5.190977 -1.279494
H 3.445379 -4.068873 -2.541906
H 4.863780 -3.657334 -1.556265
C 3.603359 -3.543602 0.871456
H 3.081219 -2.915255 1.599665
H 3.554954 -4.585203 1.219803
H 4.664588 -3.253827 0.865697
Na 4.405932 -0.492982 0.803120
H 1.191453 -0.460315 -4.932720
H 2.462067 0.043670 -2.849369
H -1.421057 0.141734 -3.766554
O 6.269042 0.175130 2.302973
O 3.550933 -0.936461 3.011079
C 5.828798 1.260193 3.058281
H 4.768339 1.483782 2.817709
H 5.895403 0.995801 4.135457
C 7.440980 0.552446 1.655019
H 8.206610 -0.243205 1.774283
H 7.232411 0.682114 0.572501
C 7.943333 1.856676 2.232959
H 8.663528 1.656526 3.057244
H 8.417389 2.499250 1.459405
C 6.697001 2.468965 2.778919
H 6.219119 3.114602 2.009223
H 6.895306 3.060248 3.699293
C 2.225221 -0.753618 3.375419
H 2.126315 0.200493 3.938847
H 1.599414 -0.692569 2.463612
C 4.139353 -1.687268 4.019248
H 4.961834 -2.301289 3.594780
H 4.566623 -1.004916 4.786627
C 3.081280 -2.574992 4.642089
H 3.147186 -3.605211 4.227042
H 3.188133 -2.609558 5.748293
C 1.788575 -1.926680 4.232792
H 1.176099 -2.637918 3.638941
H 1.208477 -1.580432 5.115878
O 6.066163 -1.359570 -0.740085
C 7.214028 -2.127351 -0.886436
H 8.083130 -1.575434 -0.466554
H 7.096862 -3.076589 -0.321788
C 5.896623 -0.671128 -1.934169
H 6.447946 0.294138 -1.885919
H 4.821490 -0.453254 -2.097070
C 7.435955 -2.412978 -2.363233
H 8.475451 -2.152362 -2.660602
H 7.239828 -3.482620 -2.596690
C 6.440051 -1.525849 -3.056590
H 6.918196 -0.903419 -3.844007
H 5.623039 -2.135194 -3.502581
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Figure_S6_imid-3_modeS1_ts(CuHadd)_01 / electronic energy: -3601.990199443651 a.u. / lowest freq: -771.28 cm-1
C 0.056556 3.243639 -0.074260
H 0.843577 2.989099 0.653326
C -1.326000 2.710630 0.337505
H -2.134993 3.375356 -0.013420
C -0.460256 1.348313 -1.379081
C 1.342101 2.669848 -2.247809
C 0.953466 2.890921 -3.576445
C 2.705437 2.609390 -1.933268
C 1.900969 3.073956 -4.577968
H -0.114711 2.914127 -3.803970
C 3.651620 2.816481 -2.941682
C 3.257655 3.051820 -4.254991
H 1.578193 3.242470 -5.607674
H 4.709017 2.750936 -2.680381
H 4.012462 3.203725 -5.029633
C -2.474235 0.530736 -0.321066

C	-3.789761	1.006409	-0.174636
C	-2.242918	-0.853232	-0.313707
C	-4.854876	0.110637	-0.024242
C	-3.309430	-1.747229	-0.141784
C	-4.614191	-1.265006	-0.008903
H	-5.436247	-1.957490	0.132841
S	3.330906	2.207971	-0.298112
O	4.664602	1.602747	-0.573487
O	2.407516	1.194031	0.294878
O	3.365524	3.488110	0.434408
Cu	0.110060	0.107483	-2.720813
C	0.060129	4.727521	-0.337851
C	0.795182	5.589773	0.493817
C	-0.674152	5.271872	-1.408603
C	0.806043	6.966560	0.251235
H	1.354963	5.199165	1.334040
C	-0.659536	6.648860	-1.647646
H	-1.254138	4.629577	-2.059494
C	0.081142	7.495485	-0.819464
H	1.375517	7.624109	0.895238
H	-1.223154	7.059674	-2.475264
H	0.091097	8.561623	-1.005589
C	-1.456835	2.501453	1.824378
C	-2.301819	3.330861	2.581514
C	-0.767484	1.456674	2.468467
C	-2.453976	3.118453	3.954757
H	-2.844509	4.140913	2.110385
C	-0.937824	1.236875	3.838182
H	-0.116582	0.801124	1.905329
C	-1.778734	2.068269	4.581115
H	-3.106274	3.761261	4.531544
H	-0.422575	0.419119	4.323914
H	-1.908714	1.897725	5.641897
N	0.306592	2.459916	-1.300548
N	-1.384089	1.433261	-0.403708
H	-1.231010	-1.230547	-0.396682
H	-3.994755	2.068548	-0.176713
C	-3.052082	-3.192130	-0.022028
C	-2.985999	-4.002708	-1.188108
C	-2.825992	-3.762511	1.261960
C	-2.651120	-5.362155	-1.049625
C	-2.489784	-5.125942	1.347120
C	-2.400244	-5.912407	0.203180
H	-2.575059	-6.003952	-1.917353
H	-2.288002	-5.586791	2.304969
H	-2.136074	-6.958608	0.288430
C	-6.228954	0.612592	0.154905
C	-6.736393	0.853563	1.461528
C	-7.068640	0.809333	-0.973247
C	-8.074281	1.276716	1.601829
C	-8.390114	1.238386	-0.754637
C	-8.863746	1.462443	0.537121
H	-8.490351	1.455755	2.584755
H	-9.065318	1.394584	-1.585678
H	-9.886835	1.787437	0.679226
C	-6.588889	0.555219	-2.401680
H	-5.523120	0.248502	-2.416754
C	-6.673199	1.829528	-3.250841
H	-6.109486	2.650813	-2.758508
H	-6.221890	1.650367	-4.250146
H	-7.726024	2.151011	-3.395222
C	-7.371949	-0.593631	-3.047780
H	-7.288652	-1.507571	-2.421061
H	-8.445103	-0.333582	-3.165298
H	-6.952663	-0.823299	-4.050708
C	-5.883809	0.648356	2.714334
H	-4.844784	0.363469	2.450628
C	-6.436366	-0.496384	3.570660
H	-5.758427	-0.690910	4.429085
H	-7.445232	-0.252642	3.965446
H	-6.501494	-1.424842	2.963834
C	-5.768518	1.941917	3.529886
H	-5.065956	1.793106	4.377285
H	-5.374696	2.759817	2.889371
H	-6.750691	2.250383	3.944765
C	-2.916523	-2.935368	2.546293
H	-3.246455	-1.898171	2.335850
C	-3.258943	-3.440372	-2.582980
H	-3.552193	-2.371819	-2.533433
C	-1.999386	-3.497432	-3.453126
H	-1.183533	-2.929615	-2.961208
H	-1.665239	-4.543948	-3.614540
H	-2.195805	-3.030971	-4.442014
C	-4.432051	-4.163642	-3.256034
H	-4.185995	-5.225331	-3.467619
H	-5.328169	-4.123801	-2.600176
H	-4.684673	-3.665013	-4.216268
C	-1.545714	-2.812952	3.216811

H -1.159562 -3.806121 3.528793
H -0.826718 -2.349457 2.509598
H -1.614102 -2.160516 4.113494
C -3.957570 -3.513278 3.512955
H -4.937063 -3.614989 2.998562
H -3.646619 -4.507063 3.897566
H -4.090932 -2.830314 4.379086
C 1.965565 -0.793176 -2.966249
C 1.109691 -0.911239 -4.132549
H 0.716522 -1.907550 -4.364139
B 2.098068 -1.931782 -1.987922
O 1.290991 -3.062858 -2.052808
O 3.073969 -2.081789 -0.982963
C 1.639610 -3.914229 -0.951715
C 3.117421 -3.503715 -0.691978
C 0.736036 -3.551789 0.215676
H -0.304702 -3.627875 -0.113886
H 0.869045 -4.221727 1.076335
H 0.905632 -2.516185 0.543396
C 1.436575 -5.357078 -1.358017
H 1.782905 -6.044173 -0.572092
H 0.369069 -5.554506 -1.526259
H 1.968237 -5.596311 -2.287402
C 4.081762 -4.147377 -1.675543
H 4.194106 -5.224264 -1.488367
H 3.752548 -4.010598 -2.715194
H 5.069479 -3.683669 -1.564660
C 3.583199 -3.739662 0.723210
H 2.984091 -3.177436 1.444144
H 3.517972 -4.808095 0.975084
H 4.631103 -3.433162 0.838792
Na 4.162355 -0.420539 0.675342
H 1.393281 -0.365485 -5.039884
H 2.690777 0.029922 -2.955359
H -0.390946 -0.226946 -4.195106
O 5.556073 0.770503 2.355410
O 3.375123 -1.140703 2.839228
C 6.702267 1.411869 1.900734
H 7.569914 1.066693 2.504689
H 6.890402 1.148133 0.840021
C 4.841003 1.673801 3.138684
H 3.825117 1.798183 2.709462
H 4.732827 1.271609 4.168025
C 5.555541 3.011400 3.174875
H 4.853389 3.861142 3.031095
H 6.096722 3.129734 4.139884
C 6.532749 2.905812 2.050414
H 7.494954 3.409958 2.286786
H 6.097032 3.336167 1.122708
C 2.084789 -1.147105 3.343784
H 1.947670 -0.264357 4.006703
H 1.358345 -1.080469 2.508627
C 4.156665 -1.850545 3.742014
H 4.979780 -2.360947 3.198326
H 4.606677 -1.147340 4.476125
C 3.282306 -2.864328 4.457394
H 3.475937 -3.890535 4.073924
H 3.460633 -2.836071 5.554649
C 1.882593 -2.430243 4.122692
H 1.389768 -3.195217 3.484176
H 1.274270 -2.254415 5.036568
O 6.140170 -1.419483 -0.121595
C 7.287349 -2.024640 0.367231
H 7.952670 -1.251826 0.812561
H 7.019602 -2.756845 1.157884
C 6.413136 -1.050897 -1.434153
H 6.748098 0.008988 -1.457209
H 5.488879 -1.138526 -2.043683
C 7.982759 -2.717045 -0.783980
H 9.088408 -2.668197 -0.678172
H 7.655513 -3.778667 -0.844161
C 7.501721 -1.955526 -1.987380
H 8.324220 -1.352256 -2.430682
H 7.093603 -2.648145 -2.755947
178
Figure_S6_imid-3_modeS1_ts(CuHadd)_02 / electronic energy: -3601.987872299208 a.u. / lowest freq: -745.47 cm-1
C -0.174442 3.327335 -0.039451
H 0.580902 3.133492 0.737988
C -1.547899 2.729858 0.308055
H -2.375510 3.349585 -0.080695
C -0.539527 1.408276 -1.363673
C 1.283284 2.779296 -2.110826
C 0.983072 2.936816 -3.470267
C 2.625796 2.793617 -1.701078
C 1.991246 3.117547 -4.411756
H -0.066462 2.906581 -3.772526
C 3.631259 2.993773 -2.650427
C 3.321725 3.158924 -3.998017

H	1.734472	3.232599	-5.467145
H	4.668675	2.980552	-2.311410
H	4.122230	3.306621	-4.726183
C	-2.532067	0.474646	-0.362145
C	-3.881732	0.852438	-0.256604
C	-2.193871	-0.885697	-0.296777
C	-4.876912	-0.117521	-0.087133
C	-3.190244	-1.852401	-0.103983
C	-4.530437	-1.468604	-0.009684
H	-5.298687	-2.216993	0.148767
S	3.121162	2.434260	-0.011663
O	4.549765	2.024666	-0.115064
O	2.264977	1.283334	0.399741
O	2.903221	3.667803	0.767782
Cu	0.030037	0.193354	-2.723067
C	-0.240870	4.804655	-0.332455
C	0.369722	5.726216	0.535843
C	-0.926725	5.284052	-1.464758
C	0.309823	7.096990	0.267663
H	0.884126	5.387217	1.425748
C	-0.982834	6.655300	-1.729260
H	-1.415318	4.595766	-2.143075
C	-0.363450	7.561039	-0.864936
H	0.783339	7.800270	0.940430
H	-1.508059	7.015854	-2.604196
H	-0.408675	8.622684	-1.070504
C	-1.734054	2.523162	1.792049
C	-2.592434	3.379050	2.510484
C	-1.090169	1.520346	2.441648
C	-2.770388	3.189674	3.882667
H	-3.115178	4.186456	2.013037
C	-1.254072	1.316585	3.762951
H	-0.433922	0.854493	1.894791
C	-2.096376	2.143884	4.514515
H	-3.426822	3.839828	4.446192
H	-0.729626	0.506109	4.250808
H	-2.223805	1.974189	5.575698
N	0.190180	2.541330	-1.237369
N	-1.512872	1.455604	-0.437802
H	-1.153819	-1.185803	-0.343706
H	-4.164310	1.896113	-0.299834
C	-2.823436	-3.266312	0.079973
C	-2.749797	-4.134366	-1.043371
C	-2.513212	-3.749590	1.382037
C	-2.327112	-5.461682	-0.846690
C	-2.090707	-5.083897	1.525547
C	-1.995756	-5.925723	0.422192
H	-2.246483	-6.145531	-1.681279
H	-1.827494	-5.479007	2.497751
H	-1.665571	-6.948322	0.552033
C	-6.288558	0.281642	0.052841
C	-6.829204	0.527672	1.345690
C	-7.119183	0.365977	-1.098734
C	-8.195202	0.844912	1.459438
C	-8.477433	0.692595	-0.932322
C	-9.005882	0.928575	0.332365
H	-8.642757	1.023798	2.428129
H	-9.138962	0.758186	-1.786082
H	-10.054772	1.173409	0.440507
C	-6.586439	0.095227	-2.506271
H	-5.498526	-0.119120	-2.489079
C	-6.757998	1.321160	-3.411952
H	-6.280368	2.208223	-2.943297
H	-6.266625	1.140761	-4.391971
H	-7.830239	1.543433	-3.594713
C	-7.253030	-1.142826	-3.117501
H	-7.106235	-2.019489	-2.450460
H	-8.341452	-0.981818	-3.267327
H	-6.792263	-1.376675	-4.101102
C	-5.978672	0.434933	2.613919
H	-4.915913	0.229263	2.371992
C	-6.445632	-0.723733	3.501968
H	-5.764770	-0.834129	4.372990
H	-7.476193	-0.551856	3.878170
H	-6.426022	-1.673395	2.925444
C	-5.980963	1.759187	3.387378
H	-5.283720	1.694516	4.249568
H	-5.642074	2.584920	2.725782
H	-6.991493	2.001129	3.777470
C	-2.614947	-2.862129	2.624585
H	-3.014149	-1.858866	2.372092
C	-3.111434	-3.668383	-2.453757
H	-3.453313	-2.613298	-2.452258
C	-1.891222	-3.717481	-3.378532
H	-1.081071	-3.089914	-2.954832
H	-1.517586	-4.755581	-3.503030
H	-2.153087	-3.312515	-4.379336
C	-4.276098	-4.484458	-3.027629

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H  -3.988555  -5.545284  -3.184371
H  -5.144347  -4.443591  -2.335360
H  -4.592975  -4.059141  -4.003966
C  -1.235232  -2.623629   3.246344
H  -0.761716  -3.577574   3.559994
H  -0.576124  -2.115095   2.511565
H  -1.327486  -1.966711   4.136852
C  -3.591690  -3.449271   3.651071
H  -4.576132  -3.639189   3.172272
H  -3.208133  -4.399410   4.078191
H  -3.745690  -2.729216   4.483154
C   1.875187  -0.679865  -3.059564
C   0.961528  -0.826763  -4.176517
H   0.570541  -1.830779  -4.376689
B   2.104530  -1.779164  -2.056146
O   1.373782  -2.960685  -2.006516
O   3.151429  -1.819231  -1.116866
C   1.862359  -3.731577  -0.894007
C   3.323568  -3.215550  -0.772674
C   1.029101  -3.366274   0.323633
H  -0.027499  -3.508969   0.075716
H   1.261533  -3.996884   1.193681
H   1.168841  -2.313605   0.609553
C   1.729171  -5.202270  -1.220132
H   2.183888  -5.825219  -0.436093
H   0.668669  -5.479031  -1.292927
H   2.203476  -5.449461  -2.178119
C   4.254453  -3.836098  -1.802703
H   4.475954  -4.887315  -1.570896
H   3.824466  -3.789721  -2.813121
H   5.199956  -3.279245  -1.806819
C   3.927029  -3.324784   0.609078
H   3.355609  -2.748055   1.343076
H   3.955769  -4.370885   0.945673
H   4.961418  -2.953151   0.602729
Na  4.088161  -0.300526   0.513990
H   1.191171  -0.290969  -5.104791
H   2.575278   0.165745  -3.097309
H  -0.547645  -0.154384  -4.167093
O   5.767314  -0.040343   2.160063
O   2.776953  -0.849501   2.763773
C   6.144409  -0.916134   3.165371
H   5.559858  -0.696629   4.086019
H   5.934410  -1.960257   2.851019
C   6.582916   1.078222   2.275776
H   6.804392   1.482100   1.266077
H   6.049396   1.861996   2.857260
C   7.872948   0.683291   2.975943
H   8.737047   0.726406   2.276839
H   8.064326   1.348350   3.846590
C   7.621720  -0.728246   3.425174
H   7.866449  -0.870912   4.500274
H   8.210828  -1.439686   2.805064
C   2.620997   0.406244   3.343649
H   3.470277   1.062113   3.060706
H   1.686082   0.865689   2.965421
C   2.553005  -1.809494   3.746259
H   1.796886  -2.540230   3.390426
H   3.501709  -2.356176   3.935957
C   2.082292  -1.142364   5.021222
H   0.972579  -1.176876   5.083415
H   2.526388  -1.614069   5.924640
C   2.543864   0.266440   4.847466
H   1.832531   0.993966   5.295766
H   3.553839   0.396354   5.295501
O   6.009969  -0.920865  -0.837127
C   7.326098  -1.242046  -0.541695
H   7.842916  -0.348258  -0.127788
H   7.353097  -2.050170   0.219649
C   6.008984  -0.435550  -2.138835
H   6.136248   0.669397  -2.120227
H   5.039370  -0.666395  -2.626067
C   8.001653  -1.693136  -1.819725
H   9.051005  -1.329069  -1.869920
H   7.984241  -2.803126  -1.892405
C   7.149706  -1.085516  -2.900495
H   7.717517  -0.327997  -3.483900
H   6.765995  -1.874020  -3.584984
178
Figure_S6_imid-3_modeS1_ts(CuHadd)_03 / electronic energy: -3601.991042465432 a.u. / lowest freq: -744.17 cm-1
C   0.037342   3.228583  -0.022707
H   0.781092   3.007570   0.758681
C  -1.373436   2.721216   0.330870
H  -2.157112   3.395556  -0.057025
C  -0.446991   1.314262  -1.318832
C   1.452859   2.550584  -2.091985
C   1.146725   2.685211  -3.453135
C   2.797446   2.498646  -1.695655
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C	2.152464	2.778456	-4.409375
H	0.093955	2.706234	-3.744604
C	3.801928	2.614924	-2.660639
C	3.487628	2.756031	-4.009402
H	1.890636	2.876186	-5.465250
H	4.840561	2.554921	-2.331370
H	4.287521	2.837328	-4.748614
C	-2.519823	0.547798	-0.343565
C	-3.837685	1.033047	-0.284219
C	-2.294245	-0.833947	-0.259280
C	-4.912740	0.146949	-0.145300
C	-3.370252	-1.717204	-0.096237
C	-4.678470	-1.227415	-0.051876
H	-5.508783	-1.910995	0.084457
S	3.301725	2.186860	0.000430
O	4.710785	1.715218	-0.117992
O	2.416127	1.093077	0.496896
O	3.150374	3.466503	0.719207
Cu	0.079040	0.036517	-2.642081
C	0.059309	4.700870	-0.346206
C	0.714946	5.603123	0.509385
C	-0.590540	5.196219	-1.492789
C	0.736031	6.969444	0.214000
H	1.202183	5.252795	1.410217
C	-0.565841	6.562893	-1.784422
H	-1.114307	4.523876	-2.160749
C	0.098702	7.448648	-0.933000
H	1.244207	7.657695	0.876953
H	-1.063762	6.935536	-2.670190
H	0.115954	8.506846	-1.159522
C	-1.571815	2.521914	1.811912
C	-2.463490	3.342599	2.523708
C	-0.896753	1.493034	2.494229
C	-2.671782	3.138755	3.891102
H	-2.999144	4.138821	2.022017
C	-1.115783	1.286430	3.858725
H	-0.217559	0.840902	1.963179
C	-2.002660	2.108832	4.556908
H	-3.359787	3.774548	4.433124
H	-0.601001	0.486574	4.374394
H	-2.172474	1.947444	5.613481
N	0.357150	2.396568	-1.203565
N	-1.423109	1.442403	-0.403720
H	-1.280512	-1.215092	-0.270604
H	-4.034779	2.095338	-0.343457
C	-3.119397	-3.152899	0.114926
C	-3.023860	-4.030474	-0.998988
C	-2.914561	-3.643961	1.434480
C	-2.673683	-5.374350	-0.774289
C	-2.560714	-4.994700	1.606579
C	-2.438357	-5.845816	0.513132
H	-2.571696	-6.064771	-1.601067
H	-2.370574	-5.395192	2.593463
H	-2.160989	-6.881012	0.664907
C	-6.291010	0.660430	-0.052267
C	-6.870974	0.920891	1.220016
C	-7.061375	0.853401	-1.229458
C	-8.211034	1.356189	1.277879
C	-8.388584	1.298374	-1.092673
C	-8.935012	1.538699	0.167042
H	-8.681947	1.549041	2.233049
H	-9.011994	1.454035	-1.963356
H	-9.961414	1.874561	0.245906
C	-6.502171	0.579269	-2.624881
H	-5.443627	0.252153	-2.574188
C	-6.512013	1.848787	-3.485139
H	-5.961035	2.662263	-2.966118
H	-6.007874	1.653744	-4.455803
H	-7.548293	2.189895	-3.691236
C	-7.266438	-0.559749	-3.309941
H	-7.239946	-1.469902	-2.672845
H	-8.324919	-0.280368	-3.495908
H	-6.790673	-0.805579	-4.283412
C	-6.092457	0.727439	2.522062
H	-5.041106	0.436604	2.321600
C	-6.697938	-0.405386	3.358127
H	-6.074008	-0.589051	4.258798
H	-7.728631	-0.155573	3.687284
H	-6.727259	-1.341838	2.760773
C	-6.017779	2.029927	3.328220
H	-5.362533	1.889117	4.214100
H	-5.586910	2.839591	2.701224
H	-7.020159	2.345378	3.685536
C	-3.046839	-2.744491	2.665257
H	-3.404405	-1.732427	2.388011
C	-3.276635	-3.554586	-2.429131
H	-3.595421	-2.492299	-2.446713
C	-1.994826	-3.630110	-3.263086

H -1.206556 -3.017765 -2.780066
H -1.633825 -4.675912 -3.357866
H -2.174633 -3.221879 -4.280537
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H -4.139255 -5.406773 -3.238350
H -5.327691 -4.290802 -2.455641
H -4.657649 -3.901240 -4.079206
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H -1.266816 -3.507447 3.693820
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H 0.564613 -2.062050 -4.220919
B 2.041650 -1.989195 -1.868200
O 1.229166 -3.117120 -1.804707
O 3.054999 -2.061291 -0.894290
C 1.610597 -3.866349 -0.639936
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C 0.745296 -3.393910 0.516151
H -0.307495 -3.519605 0.241166
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H 1.751695 -5.952899 -0.068327
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H 1.903526 -5.665311 -1.820171
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H 4.149825 -5.242105 -1.131003
H 3.628182 -4.172234 -2.456490
H 4.998111 -3.708242 -1.426083
C 3.628408 -3.529298 0.938677
H 3.067687 -2.882016 1.620329
H 3.571514 -4.558857 1.320713
H 4.686919 -3.230045 0.972768
Na 4.320445 -0.460662 0.788796
H 1.260291 -0.575118 -4.989093
H 2.632203 -0.110169 -2.980781
H -0.481994 -0.337678 -4.086550
O 6.142866 0.299906 2.330301
O 3.456917 -0.867204 3.012100
C 5.667507 1.399951 3.041470
H 4.615013 1.608771 2.757307
H 5.696624 1.163445 4.126639
C 7.334386 0.671601 1.715712
H 8.099866 -0.116719 1.876949
H 7.162869 0.780441 0.624638
C 7.808793 1.989711 2.285248
H 8.494702 1.810236 3.142874
H 8.312286 2.617458 1.518140
C 6.538523 2.607531 2.765365
H 6.088431 3.229128 1.960268
H 6.696656 3.223981 3.676966
C 2.122592 -0.756220 3.372600
H 1.973107 0.187085 3.943005
H 1.495190 -0.721942 2.459922
C 4.084455 -1.576137 4.027862
H 4.931144 -2.158624 3.606559
H 4.485666 -0.864200 4.781933
C 3.073202 -2.502247 4.674079
H 3.210379 -3.544162 4.308639
H 3.163418 -2.480021 5.782153
C 1.748737 -1.955994 4.220854
H 1.216796 -2.713991 3.607698
H 1.112091 -1.655056 5.081307
O 6.133820 -1.317920 -0.636576
C 7.287706 -2.084892 -0.731305
H 8.142958 -1.518476 -0.302434
H 7.157781 -3.018834 -0.144334
C 5.982082 -0.677516 -1.859296
H 6.524144 0.294026 -1.837641
H 4.908800 -0.474931 -2.050186
C 7.552476 -2.410384 -2.193008
H 8.592215 -2.132156 -2.473205
H 7.389175 -3.491174 -2.398470
C 6.553845 -1.569434 -2.937282
H 7.033651 -0.973590 -3.744001
H 5.752310 -2.209761 -3.367632
178
Figure_S6_imid-3_modeS1_ts(CuHadd)_04 / electronic energy: -3601.991022371877 a.u. / lowest freq: -759.06 cm-1
C -0.134743 3.357697 0.249231
H 0.660428 3.259496 1.002786
C -1.446199 2.648583 0.655926
H -2.330633 3.283762 0.480842

C	-0.490867	1.504816	-1.185975
C	1.369341	2.923364	-1.785900
C	1.096540	3.209988	-3.129104
C	2.699552	2.953583	-1.334604
C	2.118226	3.552274	-4.009704
H	0.057794	3.159883	-3.466282
C	3.714787	3.327162	-2.217636
C	3.430677	3.632852	-3.546743
H	1.885020	3.769198	-5.054353
H	4.741775	3.335359	-1.847134
H	4.239368	3.916788	-4.223751
C	-2.500768	0.529924	-0.263612
C	-3.847679	0.922699	-0.209093
C	-2.179009	-0.834315	-0.218130
C	-4.860038	-0.038602	-0.103540
C	-3.192510	-1.793861	-0.086737
C	-4.531304	-1.395004	-0.038149
H	-5.314030	-2.137021	0.072526
S	3.164802	2.346502	0.294380
O	4.629158	2.079218	0.202738
O	2.399168	1.076276	0.432106
O	2.818153	3.390598	1.279941
Cu	-0.016024	0.361160	-2.637739
C	-0.334680	4.816980	-0.079222
C	0.317044	5.809622	0.673600
C	-1.165604	5.204796	-1.147637
C	0.142090	7.161354	0.362156
H	0.958363	5.540777	1.503169
C	-1.336520	6.557324	-1.455380
H	-1.677036	4.458950	-1.743500
C	-0.683097	7.534904	-0.701404
H	0.646817	7.919992	0.946249
H	-1.975421	6.847501	-2.279382
H	-0.816534	8.581918	-0.940887
C	-1.446663	2.193946	2.094641
C	-2.349040	2.755625	3.014930
C	-0.566718	1.185364	2.529857
C	-2.365731	2.320172	4.343493
H	-3.039314	3.530764	2.706612
C	-0.588987	0.753244	3.858204
H	0.126157	0.725396	1.838284
C	-1.488020	1.318579	4.764179
H	-3.060463	2.759254	5.047545
H	0.087937	-0.023381	4.185032
H	-1.504486	0.980400	5.792096
N	0.271813	2.593514	-0.950652
N	-1.472525	1.501122	-0.269975
H	-1.141237	-1.140653	-0.232919
H	-4.112647	1.971688	-0.243607
C	-2.855112	-3.217546	0.085254
C	-2.837873	-4.086882	-1.040246
C	-2.597066	-3.727765	1.389027
C	-2.541096	-5.447354	-0.840767
C	-2.282438	-5.091464	1.531808
C	-2.253626	-5.937620	0.428579
H	-2.530312	-6.138879	-1.672738
H	-2.073731	-5.511756	2.506704
H	-2.019263	-6.986134	0.560237
C	-6.272429	0.373628	-0.020574
C	-6.845894	0.709163	1.236945
C	-7.079968	0.389111	-1.188780
C	-8.213397	1.049841	1.288974
C	-8.435502	0.740458	-1.058197
C	-8.972265	1.065343	0.186570
H	-8.678094	1.301190	2.233553
H	-9.087470	0.758896	-1.921646
H	-10.019769	1.329340	0.261163
C	-6.528325	0.027017	-2.567260
H	-5.443514	-0.198582	-2.517049
C	-6.669705	1.197796	-3.547719
H	-6.184816	2.104801	-3.127196
H	-6.168770	0.951014	-4.508229
H	-7.736228	1.423831	-3.757650
C	-7.202915	-1.236626	-3.113604
H	-7.091914	-2.069303	-2.386471
H	-8.283778	-1.066143	-3.302732
H	-6.721435	-1.543385	-4.066772
C	-6.032890	0.688878	2.532181
H	-4.971822	0.431434	2.337472
C	-6.558150	-0.383236	3.493737
H	-5.898058	-0.451116	4.384970
H	-7.588624	-0.148797	3.834523
H	-6.561400	-1.373793	2.990300
C	-6.015426	2.069605	3.199103
H	-5.353016	2.051937	4.089907
H	-5.623212	2.828202	2.488435
H	-7.030533	2.374647	3.528556
C	-2.684892	-2.850124	2.640393

H	-2.953536	-1.805375	2.383311
C	-3.165290	-3.596030	-2.450730
H	-3.315766	-2.497199	-2.466459
C	-2.014686	-3.875310	-3.425011
H	-1.072549	-3.451544	-3.024456
H	-1.876280	-4.963943	-3.591751
H	-2.221479	-3.394811	-4.405130
C	-4.473859	-4.216433	-2.952762
H	-4.378959	-5.317244	-3.065025
H	-5.295135	-3.997751	-2.237155
H	-4.748360	-3.781949	-3.937814
C	-1.336526	-2.769880	3.364504
H	-0.986724	-3.771649	3.689784
H	-0.578338	-2.320826	2.691255
H	-1.424255	-2.122156	4.262463
C	-3.788610	-3.345311	3.582708
H	-4.753457	-3.409096	3.035319
H	-3.543947	-4.344448	4.000646
H	-3.917034	-2.632893	4.425718
C	1.743027	-0.595964	-3.164275
C	0.697793	-0.717828	-4.164046
H	0.217203	-1.696418	-4.276164
B	2.007675	-1.661929	-2.133833
O	1.161064	-2.744108	-1.917065
O	3.169191	-1.790826	-1.343717
C	1.714051	-3.539166	-0.856880
C	3.224659	-3.183005	-0.950370
C	1.096828	-3.075795	0.452752
H	0.007992	-3.176222	0.385485
H	1.433401	-3.682279	1.305879
H	1.327272	-2.019808	0.660089
C	1.389980	-4.994844	-1.113667
H	1.870962	-5.647009	-0.370116
H	0.306601	-5.155186	-1.046462
H	1.709479	-5.313177	-2.113728
C	3.933206	-3.946796	-2.057832
H	4.066532	-5.007589	-1.804218
H	3.380440	-3.885222	-3.005483
H	4.928095	-3.513569	-2.220462
C	3.985769	-3.314332	0.348298
H	3.582395	-2.650847	1.121700
H	3.934768	-4.343564	0.731012
H	5.048703	-3.074495	0.205204
Na	4.381261	-0.348248	0.319618
H	0.857359	-0.235537	-5.134944
H	2.483306	0.192016	-3.342307
H	-0.749149	0.066695	-4.021632
O	6.386433	-1.048682	1.475828
O	3.443598	-0.766527	2.818279
C	7.242787	0.025774	1.673429
H	8.234036	-0.205839	1.223602
H	6.833867	0.928470	1.175063
C	6.549305	-1.881051	2.574440
H	5.609746	-2.436037	2.770725
H	7.350282	-2.622183	2.356339
C	6.927856	-1.034486	3.773949
H	6.045381	-0.871003	4.429578
H	7.742449	-1.515115	4.358537
C	7.380877	0.263356	3.164502
H	8.433843	0.495830	3.435629
H	6.718550	1.096059	3.488526
C	2.782258	-1.673401	3.634596
H	1.724301	-1.759811	3.305590
H	3.256602	-2.673690	3.550727
C	3.290213	0.475956	3.419678
H	4.161377	1.118907	3.174271
H	2.370257	0.964343	3.034257
C	3.179144	0.281897	4.919294
H	4.145312	0.518483	5.416798
H	2.374768	0.921516	5.344374
C	2.853216	-1.178261	5.065247
H	3.664428	-1.702820	5.616831
H	1.884386	-1.330915	5.589265
O	6.131665	-0.256707	-1.372614
C	7.052143	-1.222099	-1.767469
H	8.075619	-0.891854	-1.487230
H	6.835146	-2.168888	-1.230309
C	5.617125	0.326581	-2.521281
H	6.185523	1.256092	-2.745604
H	4.555135	0.592637	-2.357659
C	6.958737	-1.442030	-3.268899
H	7.862243	-1.032847	-3.772969
H	6.844255	-2.517961	-3.524093
C	5.748945	-0.653438	-3.661106
H	5.884085	-0.137001	-4.636117
H	4.855580	-1.314810	-3.700084

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Figure_S6_imid-3_modeS1_ts(CuHadd)_05 / electronic energy: -3601.976710824634 a.u. / lowest freq: -675.01 cm-1

C	-0.373716	-3.132179	-0.725216
H	-1.294636	-3.169701	-0.127482
C	0.865836	-2.712756	0.101989
H	1.670695	-3.460956	0.024810
C	0.485385	-1.088454	-1.582302
C	-1.394666	-1.983794	-2.793037
C	-0.849178	-1.836946	-4.077723
C	-2.793333	-2.048101	-2.659288
C	-1.658388	-1.740123	-5.203871
H	0.239995	-1.805285	-4.175212
C	-3.598232	-1.960080	-3.798751
C	-3.043128	-1.805291	-5.065573
H	-1.201798	-1.621166	-6.189140
H	-4.680605	-1.993539	-3.663634
H	-3.693254	-1.735056	-5.940082
C	2.417397	-0.720281	-0.167941
C	3.624257	-1.379908	0.120416
C	2.335027	0.670578	0.016186
C	4.727709	-0.663253	0.596821
C	3.439351	1.383242	0.507719
C	4.633047	0.715596	0.793505
H	5.481560	1.265834	1.184509
S	-3.637438	-2.251773	-1.087238
O	-5.018953	-1.733193	-1.309880
O	-2.909100	-1.392496	-0.106950
O	-3.577288	-3.694848	-0.787966
Cu	0.580119	0.318138	-2.882159
C	-0.170423	-4.456401	-1.423875
C	-0.941578	-5.575347	-1.063775
C	0.807968	-4.596383	-2.427155
C	-0.753204	-6.801421	-1.708695
H	-1.680876	-5.505015	-0.276859
C	0.991935	-5.823882	-3.069500
H	1.427081	-3.754981	-2.711982
C	0.210203	-6.924918	-2.712609
H	-1.352093	-7.657739	-1.426745
H	1.742616	-5.921879	-3.842972
H	0.354756	-7.875243	-3.209983
C	0.558396	-2.481615	1.561930
C	1.111002	-3.322718	2.543881
C	-0.252592	-1.404648	1.963811
C	0.852428	-3.092395	3.898458
H	1.741976	-4.156746	2.263377
C	-0.504248	-1.175778	3.319602
H	-0.672501	-0.734409	1.227019
C	0.047903	-2.018541	4.286039
H	1.278533	-3.745723	4.648653
H	-1.122861	-0.342593	3.623539
H	-0.146999	-1.838916	5.335341
N	-0.486147	-2.025541	-1.705294
N	1.276347	-1.462445	-0.562623
H	1.402185	1.188030	-0.174706
H	3.712157	-2.449059	-0.020930
C	3.333406	2.823728	0.798352
C	3.801546	3.777700	-0.147339
C	2.800548	3.254198	2.046016
C	3.696120	5.145962	0.162084
C	2.703568	4.634314	2.301153
C	3.142685	5.566121	1.366847
H	4.044403	5.898476	-0.532920
H	2.292095	4.996574	3.233951
H	3.063600	6.623772	1.583022
C	5.981448	-1.361938	0.930270
C	6.164044	-1.920790	2.225217
C	7.032190	-1.434479	-0.022265
C	7.396312	-2.534655	2.530810
C	8.231660	-2.064826	0.354466
C	8.384844	-2.603640	1.631011
H	7.566454	-2.959504	3.511573
H	9.059736	-2.136580	-0.338419
H	9.319730	-3.080305	1.898026
C	6.904214	-0.841800	-1.425070
H	5.897152	-0.404971	-1.584058
C	7.069699	-1.921297	-2.501750
H	6.344611	-2.744924	-2.327045
H	6.868594	-1.489962	-3.505704
H	8.097923	-2.340095	-2.500718
C	7.903493	0.302533	-1.630613
H	7.767330	1.070361	-0.839225
H	8.950336	-0.066390	-1.597514
H	7.730446	0.786695	-2.615531
C	5.076893	-1.854576	3.298982
H	4.154750	-1.377224	2.909107
C	5.529072	-0.995610	4.485356
H	4.695681	-0.880319	5.211165
H	6.393119	-1.455814	5.009447
H	5.819802	0.016422	4.130270
C	4.661151	-3.257441	3.757996

H	3.811613	-3.186833	4.469493
H	4.334162	-3.860309	2.883954
H	5.496195	-3.782793	4.266646
C	2.343588	2.265795	3.120880
H	2.490937	1.216576	2.793752
C	4.436362	3.362619	-1.475152
H	4.423748	2.260560	-1.598367
C	3.656995	3.925999	-2.668707
H	2.597638	3.607635	-2.605790
H	3.699563	5.034834	-2.697454
H	4.078930	3.533526	-3.618538
C	5.909870	3.781781	-1.531958
H	6.014040	4.887348	-1.528964
H	6.455435	3.366654	-0.657620
H	6.383353	3.384769	-2.455369
C	0.845646	2.412953	3.403920
H	0.607676	3.411608	3.826236
H	0.277301	2.274874	2.461885
H	0.514525	1.637329	4.126681
C	3.167857	2.421705	4.404276
H	4.250039	2.320077	4.173569
H	2.991442	3.408995	4.880547
H	2.893690	1.626764	5.130622
C	-0.722896	1.704235	-3.699746
C	0.521090	1.587475	-4.433891
H	1.217456	2.431873	-4.383144
B	-0.965739	2.844040	-2.740579
O	0.034099	3.716729	-2.318176
O	-2.208077	3.231897	-2.233439
C	-0.544542	4.591961	-1.337487
C	-2.047198	4.580132	-1.750023
C	-0.319537	3.958797	0.026489
H	0.753490	3.786115	0.161155
H	-0.667447	4.596551	0.851328
H	-0.821923	2.983690	0.095225
C	0.127742	5.944757	-1.415971
H	-0.357362	6.667695	-0.743889
H	1.180285	5.863524	-1.114003
H	0.108428	6.350808	-2.434534
C	-2.334548	5.519782	-2.913071
H	-2.302709	6.575447	-2.608912
H	-1.613270	5.375122	-3.729450
H	-3.337556	5.312190	-3.309905
C	-3.015168	4.844114	-0.619395
H	-2.919042	4.103247	0.180432
H	-2.844237	5.838808	-0.182352
H	-4.049888	4.817521	-0.987467
Na	-4.816022	-0.227809	0.614033
H	0.494754	1.145681	-5.436983
H	-1.574325	1.121163	-4.073005
H	1.715106	0.502120	-3.992244
O	-6.227317	-1.582236	1.840725
O	-3.585523	0.571832	2.471810
C	-6.031776	-1.960846	3.164898
H	-4.948261	-2.131347	3.344512
H	-6.371966	-1.135800	3.826328
C	-6.888539	-2.621077	1.200159
H	-7.578660	-2.211223	0.432615
H	-6.143031	-3.276069	0.698777
C	-7.654893	-3.410729	2.233368
H	-8.664134	-2.965632	2.379141
H	-7.745946	-4.482301	1.951652
C	-6.825825	-3.221532	3.464834
H	-6.137720	-4.085218	3.600746
H	-7.462442	-3.103335	4.368859
C	-2.855698	1.630053	1.939587
H	-1.799388	1.315202	1.823832
H	-3.251003	1.886379	0.936296
C	-4.002893	0.936189	3.746849
H	-5.099273	1.118089	3.726926
H	-3.793165	0.110755	4.459874
C	-3.282098	2.196367	4.172663
H	-3.926197	2.854545	4.795313
H	-2.351459	1.936403	4.724858
C	-2.940974	2.825721	2.864060
H	-3.764593	3.500437	2.541463
H	-1.985185	3.390208	2.909079
O	-6.209012	1.588352	0.811333
C	-7.480813	1.380638	1.334551
H	-7.945868	0.516431	0.812413
H	-7.406074	1.139968	2.416384
C	-6.215398	2.786066	0.106339
H	-5.767036	2.632270	-0.898191
H	-5.598943	3.527449	0.658897
C	-8.323070	2.620813	1.125166
H	-9.379330	2.370627	0.884968
H	-8.280651	3.267655	2.029592
C	-7.635804	3.293207	-0.017834

H -8.078396 2.955852 -0.981355
H -7.689739 4.401004 0.058987
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Figure_S6_imid-3_modeS1_ts(CuHadd)_06 / electronic energy: -3601.984496122795 a.u. / lowest freq: -759.34 cm-1
C 0.085254 3.109095 -0.243743
H 0.902674 2.946550 0.474283
C -1.282265 2.607629 0.274658
H -2.099209 3.304760 0.019490
C -0.543037 1.174253 -1.453502
C 1.359452 2.329321 -2.359348
C 0.986554 2.380777 -3.709992
C 2.726280 2.332879 -2.033068
C 1.941642 2.444075 -4.719805
H -0.079272 2.368072 -3.951530
C 3.677026 2.426473 -3.051973
C 3.295549 2.482215 -4.389013
H 1.624370 2.476660 -5.764375
H 4.731054 2.417029 -2.769629
H 4.055567 2.545468 -5.170819
C -2.558321 0.490730 -0.310779
C -3.863100 1.004863 -0.237110
C -2.347605 -0.881271 -0.114441
C -4.942966 0.154148 0.030773
C -3.426454 -1.726159 0.179006
C -4.723011 -1.209393 0.242448
H -5.556107 -1.863302 0.474449
S 3.323972 2.098927 -0.355253
O 4.738592 1.646084 -0.508009
O 2.466594 1.010229 0.192140
O 3.190907 3.403119 0.321466
Cu -0.154876 -0.193812 -2.726696
C 0.048211 4.561249 -0.647541
C 0.750877 5.521974 0.100392
C -0.707920 4.979505 -1.759021
C 0.714710 6.869872 -0.268870
H 1.317603 5.232069 0.975968
C -0.740113 6.328048 -2.124797
H -1.270737 4.261094 -2.341987
C -0.027471 7.272238 -1.381926
H 1.259326 7.603661 0.311101
H -1.319743 6.641388 -2.983420
H -0.054632 8.316374 -1.665537
C -1.293317 2.355557 1.764213
C -2.080471 3.167721 2.605009
C -0.573899 1.336590 2.299766
C -2.109109 2.919769 3.979324
H -2.664734 3.984770 2.200615
C -0.594363 1.076762 3.621130
H 0.030037 0.705058 1.660022
C -1.360230 1.859946 4.491740
H -2.705199 3.538791 4.636949
H -0.008837 0.256915 4.016694
H -1.369836 1.646786 5.552670
N 0.313458 2.221628 -1.406451
N -1.454860 1.358214 -0.487124
H -1.341330 -1.278090 -0.141154
H -4.042662 2.062159 -0.384576
C -3.193657 -3.146535 0.489348
C -3.215162 -4.114842 -0.551581
C -2.943701 -3.543277 1.833278
C -2.946236 -5.458208 -0.232424
C -2.680884 -4.899348 2.100363
C -2.675102 -5.841259 1.076921
H -2.947669 -6.219933 -1.000847
H -2.480969 -5.235612 3.109116
H -2.468724 -6.879688 1.302107
C -6.312065 0.691643 0.120756
C -6.791886 1.204320 1.358076
C -7.169715 0.637584 -1.013007
C -8.123481 1.652374 1.434678
C -8.493602 1.095499 -0.883959
C -8.960951 1.598465 0.325528
H -8.524694 2.038439 2.362411
H -9.175738 1.058607 -1.723076
H -9.983762 1.943748 0.405816
C -6.702764 0.081721 -2.359125
H -5.629542 -0.195936 -2.327747
C -6.829383 1.130528 -3.471317
H -6.287419 2.056528 -3.182595
H -6.378383 0.743891 -4.410238
H -7.891619 1.382279 -3.672984
C -7.464482 -1.199688 -2.716984
H -7.348850 -1.948011 -1.903659
H -8.545591 -0.996022 -2.868185
H -7.053209 -1.639059 -3.650959
C -5.916296 1.257097 2.611400
H -4.887298 0.901259 2.400123
C -6.466361 0.333522 3.704363

H	-5.768013	0.308350	4.568238
H	-7.458790	0.679762	4.062409
H	-6.565700	-0.700782	3.310642
C	-5.766066	2.694036	3.125425
H	-5.068462	2.716487	3.988774
H	-5.349490	3.341016	2.323973
H	-6.739696	3.111236	3.456998
C	-2.964778	-2.546247	2.994395
H	-3.187411	-1.519060	2.640599
C	-3.535708	-3.743269	-1.999587
H	-3.724760	-2.655267	-2.102270
C	-2.356209	-4.056405	-2.925818
H	-1.450098	-3.532442	-2.561390
H	-2.150630	-5.146503	-2.968760
H	-2.572695	-3.697047	-3.954513
C	-4.815144	-4.439912	-2.477799
H	-4.683880	-5.541749	-2.518042
H	-5.655301	-4.201331	-1.790806
H	-5.087004	-4.080386	-3.493347
C	-1.599609	-2.464142	3.687216
H	-1.303736	-3.441922	4.121188
H	-0.826275	-2.141141	2.959567
H	-1.634089	-1.714423	4.506169
C	-4.072100	-2.893390	3.996568
H	-5.049960	-2.958360	3.472945
H	-3.869102	-3.860422	4.502992
H	-4.147282	-2.099609	4.770450
C	1.620913	-1.219577	-3.007712
C	0.648272	-1.464685	-4.056333
H	0.188113	-2.458719	-4.088800
B	1.806172	-2.163642	-1.847091
O	0.972013	-3.252864	-1.610935
O	2.874270	-2.162449	-0.935347
C	1.419280	-3.899971	-0.409250
C	2.919163	-3.489166	-0.364310
C	0.635784	-3.319800	0.755468
H	-0.432322	-3.461483	0.562587
H	0.872915	-3.817733	1.706240
H	0.819279	-2.241452	0.869423
C	1.165365	-5.387303	-0.528948
H	1.581349	-5.933130	0.330589
H	0.084828	-5.583214	-0.556479
H	1.599792	-5.802555	-1.446636
C	3.790428	-4.356610	-1.260460
H	3.910605	-5.369864	-0.851703
H	3.362797	-4.443157	-2.269440
H	4.785731	-3.901308	-1.347617
C	3.516962	-3.411654	1.021591
H	3.015612	-2.652777	1.639984
H	3.431537	-4.375330	1.544452
H	4.588261	-3.174467	0.952622
Na	4.403555	-0.479338	0.533798
H	0.870851	-1.092526	-5.063082
H	2.358197	-0.431087	-3.202077
H	-0.798403	-0.701282	-4.096667
O	4.327402	0.795117	2.707785
O	6.229578	-1.537616	2.027310
C	3.108969	0.782494	3.371359
H	2.361286	0.220512	2.774383
H	3.233330	0.267641	4.349611
C	4.939182	2.015940	2.978215
H	5.815862	1.850465	3.640303
H	5.307554	2.457328	2.029466
C	3.950224	2.958137	3.643884
H	4.244537	3.140190	4.701215
H	3.877940	3.927397	3.104031
C	2.657952	2.207112	3.589419
H	2.052210	2.552224	2.724615
H	2.073201	2.315459	4.528648
C	7.365908	-0.764732	2.247779
H	8.205967	-1.156204	1.635969
H	7.158439	0.278359	1.927335
C	5.795393	-2.023867	3.257102
H	4.696274	-1.898069	3.346616
H	6.029431	-3.109221	3.315673
C	6.495093	-1.285742	4.375870
H	5.873968	-0.430027	4.719502
H	6.720092	-1.954949	5.234662
C	7.739145	-0.790168	3.716755
H	8.027560	0.217472	4.087939
H	8.572247	-1.507852	3.887056
O	5.839428	-1.464531	-1.219536
C	5.323958	-1.083071	-2.457154
H	4.854482	-1.966095	-2.940719
H	4.546746	-0.307365	-2.311378
C	7.207699	-1.224328	-1.236728
H	7.742884	-2.068809	-0.753307
H	7.416345	-0.293340	-0.666372

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C   6.435099  -0.550995  -3.340426
H   6.351486  -0.924699  -4.384179
H   6.429740   0.561529  -3.335571
C   7.666402  -1.059522  -2.666812
H   7.954247  -2.047169  -3.090814
H   8.513434  -0.344522  -2.751827
178
Figure_S6_imid-3_modeS1_prod(CuHadd) / electronic energy: -3602.027352408956 a.u. / lowest freq: 8.03 cm-1
C  -0.309630   3.574231   0.231764
H   0.402455   3.714549   1.056636
C  -1.589750   2.817866   0.656909
H  -2.495784   3.412396   0.464252
C  -0.431779   1.517175  -0.951091
C   1.474984   2.905263  -1.481724
C   1.335871   3.265088  -2.827061
C   2.756559   2.835131  -0.918827
C   2.450720   3.576581  -3.599498
H   0.333934   3.291377  -3.262051
C   3.869274   3.169463  -1.692259
C   3.720821   3.544684  -3.025370
H   2.324597   3.848132  -4.649638
H   4.855930   3.104221  -1.229704
H   4.600810   3.799566  -3.619908
C  -2.573222   0.640544  -0.207753
C  -3.925663   1.022502  -0.195862
C  -2.246032  -0.722866  -0.120273
C  -4.934201   0.058599  -0.082732
C  -3.259400  -1.685528   0.005411
C  -4.600081  -1.292904   0.021113
H  -5.381209  -2.036499   0.133018
S   3.017586   2.130525   0.713138
O   4.498915   2.050200   0.852727
O   2.421533   0.765422   0.611260
O   2.366644   3.022266   1.692067
Cu  0.490881   0.247389  -2.080456
C  -0.596177   4.903092  -0.426697
C  -0.028000   6.082298   0.086438
C  -1.417941   4.980337  -1.567315
C  -0.278207   7.312781  -0.528497
H   0.611004   6.051125   0.960176
C  -1.664511   6.212723  -2.178611
H  -1.863932   4.085988  -1.984289
C  -1.095389   7.378062  -1.659708
H   0.163033   8.216399  -0.128200
H  -2.296371   6.263964  -3.055816
H  -1.287054   8.331623  -2.134444
C  -1.577450   2.405827   2.110364
C  -2.553271   2.897161   2.995625
C  -0.613554   1.500440   2.592439
C  -2.560223   2.493640   4.334392
H  -3.309665   3.591301   2.651859
C  -0.624817   1.100592   3.930970
H   0.139411   1.097771   1.930185
C  -1.598778   1.594389   4.800911
H  -3.311763   2.878491   5.011198
H   0.118814   0.403754   4.293385
H  -1.607891   1.280954   5.836745
N   0.299966   2.625239  -0.726757
N  -1.556634   1.628602  -0.225953
H  -1.207608  -1.028798  -0.096923
H  -4.200156   2.066715  -0.269352
C  -2.921129  -3.105261   0.207491
C  -2.956265  -4.011231  -0.888889
C  -2.576297  -3.568630   1.507957
C  -2.605621  -5.355760  -0.668097
C  -2.216560  -4.918712   1.672796
C  -2.227749  -5.797785   0.595216
H  -2.620241  -6.071492  -1.479341
H  -1.933780  -5.300999   2.644666
H  -1.952649  -6.834190   0.742880
C  -6.350445   0.462817  -0.032791
C  -6.959168   0.777316   1.213539
C  -7.129750   0.476295  -1.219802
C  -8.334326   1.089041   1.236660
C  -8.494019   0.802723  -1.118555
C  -9.066710   1.102768   0.116449
H  -8.826745   1.318716   2.172639
H  -9.125571   0.817675  -1.997095
H -10.120793   1.345044   0.168753
C  -6.539721   0.132442  -2.586861
H  -5.451975  -0.071464  -2.512681
C  -6.682317   1.304970  -3.565087
H  -6.226709   2.219788  -3.128989
H  -6.153609   1.073556  -4.514457
H  -7.748019   1.509721  -3.799520
C  -7.175823  -1.142043  -3.153697
H  -7.059969  -1.976804  -2.429637
H  -8.256431  -0.993984  -3.362222
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H	-6.669750	-1.432064	-4.099307
C	-6.175624	0.761430	2.526876
H	-5.100793	0.551592	2.350995
C	-6.680422	-0.351481	3.452027
H	-6.044875	-0.407808	4.361733
H	-7.730390	-0.169299	3.764340
H	-6.623915	-1.331167	2.930593
C	-6.226884	2.126391	3.224405
H	-5.574022	2.117371	4.122354
H	-5.861488	2.917867	2.535768
H	-7.257593	2.378865	3.549642
C	-2.604573	-2.651354	2.732256
H	-2.937177	-1.628080	2.464270
C	-3.368959	-3.572279	-2.293863
H	-3.578935	-2.483939	-2.328396
C	-2.243905	-3.814376	-3.305920
H	-1.317502	-3.316128	-2.957264
H	-2.041681	-4.897596	-3.439850
H	-2.519414	-3.383690	-4.292264
C	-4.662195	-4.271010	-2.728763
H	-4.513572	-5.366978	-2.828273
H	-5.463370	-4.082883	-1.982270
H	-5.000754	-3.869825	-3.708018
C	-1.206767	-2.497414	3.337307
H	-0.814209	-3.471215	3.697303
H	-0.513352	-2.083298	2.574880
H	-1.238086	-1.794972	4.196599
C	-3.608670	-3.151891	3.777775
H	-4.611350	-3.269905	3.313678
H	-3.293068	-4.125296	4.208476
H	-3.695903	-2.414160	4.604136
C	1.597782	-0.785381	-3.349702
C	0.792772	-1.081968	-4.605770
H	-0.089511	-1.705570	-4.393056
B	1.938783	-1.927650	-2.420741
O	1.195989	-3.110073	-2.326305
O	3.028321	-1.983612	-1.525796
C	1.660613	-3.819274	-1.169998
C	3.142277	-3.354654	-1.103942
C	0.863701	-3.328632	0.029394
H	-0.202769	-3.438051	-0.193103
H	1.079671	-3.906347	0.939008
H	1.056399	-2.264003	0.229628
C	1.455502	-5.303489	-1.378900
H	1.901851	-5.886549	-0.559787
H	0.382054	-5.536832	-1.407118
H	1.892378	-5.644524	-2.325723
C	4.017692	-4.089019	-2.109321
H	4.204532	-5.130522	-1.811324
H	3.561406	-4.092278	-3.108852
H	4.987332	-3.582048	-2.183903
C	3.764619	-3.413761	0.271544
H	3.220842	-2.794486	0.992696
H	3.779329	-4.443999	0.656766
H	4.810803	-3.070624	0.237980
Na	4.545143	-0.385804	0.689997
H	1.366369	-1.630348	-5.379736
H	2.461863	-0.128799	-3.554502
H	0.409210	-0.175208	-5.105285
O	6.614195	-0.005058	1.997001
O	3.877736	-1.258088	2.852411
C	6.363152	0.750549	3.141043
H	5.281433	0.990811	3.209224
H	6.645672	0.150155	4.032202
C	7.601127	0.647069	1.264732
H	8.355261	-0.089130	0.915324
H	7.137200	1.131490	0.379045
C	8.258562	1.698891	2.128709
H	9.138682	1.265784	2.654066
H	8.565860	2.589503	1.538425
C	7.183835	2.023896	3.111152
H	6.566276	2.869484	2.735640
H	7.600256	2.274249	4.111184
C	2.584117	-1.257927	3.355321
H	2.499965	-0.482027	4.147796
H	1.867230	-1.013847	2.544283
C	4.589553	-2.192593	3.592044
H	5.393372	-2.631285	2.963428
H	5.057798	-1.690744	4.467158
C	3.635250	-3.270937	4.062135
H	3.709870	-4.167191	3.407227
H	3.844701	-3.559293	5.115391
C	2.282699	-2.631589	3.924839
H	1.655724	-3.217846	3.220326
H	1.767079	-2.551097	4.906716
O	5.972090	-0.574818	-1.221652
C	7.003418	-1.375619	-1.699761
H	7.979686	-0.927383	-1.415592

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 H   6.932415  -2.378704  -1.228801
 C   5.457510   0.119242  -2.307546
 H   5.988385   1.092259  -2.403400
 H   4.379354   0.321506  -2.150219
 C   6.902919  -1.494091  -3.213513
 H   7.794620  -1.035954  -3.695835
 H   6.809283  -2.553241  -3.538160
 C   5.670247  -0.711202  -3.549860
 H   5.812070  -0.074463  -4.449966
 H   4.809451  -1.398109  -3.702885
178
Figure_S6_imid-3_modeS2_ed(CuHadd) / electronic energy: -3602.007096538227 a.u. / lowest freq: 14.86 cm-1
 C   1.094457   1.544452   2.251053
 H   1.994340   1.052576   2.644628
 C  -0.171068   0.653426   2.325904
 H  -1.019816   1.172764   2.800708
 C   0.334091   1.087360   0.050297
 C   2.243261   2.546015   0.167341
 C   1.799615   3.476116  -0.783774
 C   3.626217   2.434138   0.410214
 C   2.689097   4.302393  -1.460306
 H   0.727019   3.548841  -0.983219
 C   4.508077   3.290159  -0.256080
 C   4.051373   4.227291  -1.178751
 H   2.308679   5.008445  -2.202404
 H   5.576230   3.169999  -0.068098
 H   4.762075   4.878083  -1.692449
 C  -1.528477  -0.383332   0.451118
 C  -2.831425  -0.184256   0.925675
 C  -1.259437  -1.467012  -0.397700
 C  -3.855678  -1.066432   0.560475
 C  -2.277227  -2.366661  -0.739877
 C  -3.576379  -2.160550  -0.265244
 H  -4.364591  -2.858436  -0.523975
 S   4.366399   1.117803   1.400473
 O   5.777116   1.033772   0.924702
 O   3.605803  -0.101681   1.001098
 O   4.239520   1.493001   2.819907
Cu   0.234916   1.213274  -1.919588
 C   0.903631   2.870167   2.948067
 C   1.712542   3.225628   4.041890
 C  -0.095353   3.764132   2.520951
 C   1.543936   4.460834   4.674696
 H   2.466620   2.546261   4.414884
 C  -0.259120   4.999094   3.155197
 H  -0.750217   3.497163   1.701749
 C   0.562615   5.348857   4.228585
 H   2.172789   4.728250   5.514015
 H  -1.024477   5.685048   2.817768
 H   0.433870   6.304721   4.719640
 C   0.062012  -0.651367   3.047074
 C  -0.647986  -0.948796   4.223683
 C   0.973575  -1.599306   2.542363
 C  -0.436126  -2.167267   4.873000
 H  -1.359087  -0.244245   4.635856
 C   1.183455  -2.764840   3.175916
 H   1.509983  -1.394844   1.628517
 C   0.485438  -3.076547   4.348132
 H  -0.980269  -2.404269   5.777949
 H   1.894873  -3.474001   2.772982
 H   0.657569  -4.022084   4.845664
 N   1.259199   1.735811   0.785508
 N  -0.473732   0.442385   0.899790
 H  -0.250633  -1.638041  -0.743853
 H  -3.048401   0.649410   1.582168
 C  -1.974959  -3.574193  -1.532741
 C  -2.187262  -3.575594  -2.939680
 C  -1.549309  -4.763243  -0.874400
 C  -1.982319  -4.769302  -3.656050
 C  -1.359253  -5.930191  -1.637258
 C  -1.569477  -5.928773  -3.010844
 H  -2.155297  -4.812220  -4.723027
 H  -1.059451  -6.857209  -1.167279
 H  -1.422356  -6.838252  -3.579170
 C  -5.223624  -0.863132   1.068714
 C  -5.576656  -1.334797   2.363805
 C  -6.192002  -0.212339   0.254789
 C  -6.892711  -1.137728   2.820664
 C  -7.494642  -0.040587   0.757160
 C  -7.837245  -0.497200   2.025461
 H  -7.196168  -1.485810   3.799214
 H  -8.255377   0.449963   0.164231
 H  -8.845175  -0.356327   2.394278
 C  -5.861271   0.305531  -1.145652
 H  -4.800515   0.114315  -1.405545
 C  -6.045089   1.824303  -1.232029
 H  -5.451336   2.322048  -0.435878
 H  -5.685612   2.193044  -2.216646
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H	-7.111466	2.111019	-1.117219
C	-6.696131	-0.413729	-2.211572
H	-6.562333	-1.512629	-2.119345
H	-7.775341	-0.173882	-2.108425
H	-6.362522	-0.107445	-3.226153
C	-4.577566	-2.061811	3.266048
H	-3.583250	-2.145622	2.782138
C	-5.029635	-3.500197	3.544370
H	-4.242382	-4.042994	4.110320
H	-5.967686	-3.520939	4.138039
H	-5.197706	-4.036272	2.585779
C	-4.349299	-1.291429	4.572014
H	-3.559741	-1.789273	5.173990
H	-4.013859	-0.256394	4.346700
H	-5.275626	-1.245200	5.182072
C	-1.332817	-4.825062	0.638499
H	-1.435512	-3.822341	1.100952
C	-2.663075	-2.333516	-3.691488
H	-2.706170	-1.452220	-3.019216
C	-1.695133	-1.955478	-4.820334
H	-0.673764	-1.806540	-4.409715
H	-1.656123	-2.738078	-5.605993
H	-2.024495	-1.009475	-5.299701
C	-4.082847	-2.537610	-4.231313
H	-4.108153	-3.338750	-5.000067
H	-4.766754	-2.815358	-3.401245
H	-4.456169	-1.595939	-4.687642
C	0.083235	-5.302943	0.986408
H	0.257943	-6.346285	0.652049
H	0.835672	-4.640894	0.508692
H	0.233522	-5.269840	2.085801
C	-2.391070	-5.713074	1.301933
H	-3.407797	-5.344771	1.046384
H	-2.295677	-6.767942	0.967911
H	-2.279233	-5.678669	2.406920
C	-1.632197	1.881375	-2.488742
C	-0.772312	1.660401	-3.581676
H	-0.283156	2.509989	-4.072176
B	-1.940247	3.285352	-1.951262
O	-1.342470	4.429969	-2.439981
O	-2.895038	3.562201	-0.998672
C	-1.851835	5.560502	-1.692905
C	-3.165615	4.981736	-1.055891
C	-0.806743	5.940955	-0.659669
H	0.139685	6.184707	-1.161035
H	-1.112037	6.817694	-0.072257
H	-0.608808	5.117599	0.036048
C	-2.073053	6.713818	-2.649084
H	-2.536659	7.566575	-2.132459
H	-1.111619	7.054642	-3.056292
H	-2.713421	6.433487	-3.493923
C	-4.379602	5.171329	-1.951660
H	-4.660870	6.229671	-2.036064
H	-4.200086	4.782001	-2.963421
H	-5.237314	4.632357	-1.530383
C	-3.463610	5.477432	0.341722
H	-2.659282	5.228233	1.042289
H	-3.605066	6.567631	0.351868
H	-4.387544	5.016221	0.715800
Na	5.328346	-0.961924	-0.419410
H	-0.837325	0.761391	-4.197406
H	-2.306474	1.064464	-2.197011
H	1.508520	0.619018	-2.644656
O	3.859486	-2.441338	-1.374748
O	6.060873	-2.511812	1.182938
C	4.106003	-3.497118	-2.245381
H	4.672347	-3.113036	-3.120440
H	4.726923	-4.263339	-1.733948
C	2.483585	-2.280697	-1.264629
H	2.152744	-2.687980	-0.286379
H	2.226276	-1.202743	-1.302146
C	1.801673	-3.034005	-2.384359
H	0.830126	-3.463938	-2.064749
H	1.651621	-2.368084	-3.261868
C	2.794330	-4.100911	-2.707962
H	2.568854	-5.020112	-2.122370
H	2.805251	-4.336859	-3.794337
C	6.967289	-2.063296	2.134080
H	7.726265	-2.855720	2.318773
H	7.489380	-1.159924	1.753927
C	5.012540	-3.096936	1.881388
H	4.069130	-2.976013	1.311417
H	5.212558	-4.185010	1.999475
C	4.895893	-2.432598	3.239404
H	4.720117	-3.186453	4.037650
H	4.068405	-1.690219	3.242611
C	6.219386	-1.742928	3.414300
H	6.076146	-0.645260	3.518104

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 H   6.765023  -2.132096   4.301597
 O   5.695672   0.248443  -2.383048
 C   6.325006  -0.318411  -3.486301
 H   7.232727   0.272321  -3.736388
 H   6.641821  -1.351379  -3.227711
 C   4.527074   0.846821  -2.832366
 H   3.750051   0.772465  -2.045951
 H   4.721974   1.921877  -3.041011
 C   5.369757  -0.348357  -4.668716
 H   5.722865   0.342106  -5.466329
 H   5.261033  -1.374360  -5.083645
 C   4.079773   0.144077  -4.091157
 H   3.548174   0.834133  -4.781844
 H   3.425719  -0.716430  -3.834231
178
Figure_S6_imid-3_modeS2_ts(CuHadd)_01 / electronic energy: -3601.991628510991 a.u. / lowest freq: -696.99 cm-1
 C   0.547330   1.416976   2.779529
 H   1.380129   0.959508   3.331505
 C  -0.687667   0.485916   2.653824
 H  -1.605669   0.964068   3.032657
 C   0.147664   0.957924   0.485233
 C   1.967934   2.472472   0.912490
 C   1.624098   3.392085  -0.088579
 C   3.292618   2.450897   1.385565
 C   2.548283   4.303007  -0.585776
 H   0.598266   3.401336  -0.466613
 C   4.201485   3.402684   0.912055
 C   3.837806   4.332901  -0.057695
 H   2.240586   4.996582  -1.372833
 H   5.222599   3.368483   1.295924
 H   4.568360   5.062062  -0.414509
 C  -1.777692  -0.480473   0.578283
 C  -3.132539  -0.278881   0.870123
 C  -1.402791  -1.525939  -0.276306
 C  -4.104257  -1.118326   0.312440
 C  -2.370716  -2.384015  -0.811156
 C  -3.722984  -2.174943  -0.521780
 H  -4.474381  -2.839669  -0.932492
 S   3.949186   1.129562   2.421872
 O   5.414965   1.130091   2.144436
 O   3.316043  -0.110381   1.883340
 O   3.601205   1.433639   3.821604
Cu   0.365948   1.136810  -1.403903
 C   0.201793   2.748139   3.405049
 C   0.826555   3.166066   4.593085
 C  -0.747338   3.593076   2.800956
 C   0.521414   4.411269   5.151694
 H   1.545374   2.530266   5.091958
 C  -1.047806   4.837531   3.360246
 H  -1.256621   3.280852   1.900083
 C  -0.411624   5.247886   4.533876
 H   1.008470   4.727464   6.065056
 H  -1.775539   5.482244   2.884450
 H  -0.645320   6.211580   4.967510
 C  -0.515171  -0.843614   3.346620
 C  -1.394935  -1.227657   4.374411
 C   0.492579  -1.740822   2.940077
 C  -1.254746  -2.480242   4.976230
 H  -2.187054  -0.566942   4.703252
 C   0.629517  -2.941274   3.527199
 H   1.160990  -1.471733   2.135982
 C  -0.237455  -3.338558   4.551852
 H  -1.930771  -2.784465   5.764718
 H   1.412071  -3.613175   3.198339
 H  -0.122547  -4.311514   5.011657
 N   0.952136   1.598344   1.362678
 N  -0.789638   0.316363   1.196458
 H  -0.357502  -1.698692  -0.483229
 H  -3.432420   0.527533   1.527993
 C  -1.965990  -3.543241  -1.628212
 C  -1.974030  -3.451821  -3.047673
 C  -1.615954  -4.768121  -0.993090
 C  -1.639526  -4.590397  -3.803224
 C  -1.289346  -5.877828  -1.794035
 C  -1.298875  -5.786066  -3.181204
 H  -1.646923  -4.558607  -4.884681
 H  -1.034341  -6.828646  -1.345293
 H  -1.047136  -6.652011  -3.779978
 C  -5.527319  -0.908683   0.627516
 C  -6.079738  -1.470294   1.812007
 C  -6.345928  -0.155298  -0.259017
 C  -7.443727  -1.262967   2.086928
 C  -7.704920   0.020405   0.059144
 C  -8.243760  -0.526318   1.219352
 H  -7.896974  -1.676856   2.978067
 H  -8.357146   0.584276  -0.594714
 H  -9.291819  -0.379719   1.447104
 C  -5.796317   0.463378  -1.545811
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H	-4.712441	0.258810	-1.659300
C	-5.934251	1.990511	-1.533148
H	-5.432583	2.409111	-0.634362
H	-5.448081	2.421864	-2.434095
H	-6.999897	2.301481	-1.528858
C	-6.472977	-0.142497	-2.780929
H	-6.368426	-1.248465	-2.765437
H	-7.552109	0.116454	-2.817099
H	-5.987820	0.237831	-3.705339
C	-5.240891	-2.299196	2.787084
H	-4.188619	-2.380036	2.446472
C	-5.761668	-3.738257	2.879893
H	-5.080900	-4.348640	3.511297
H	-6.778590	-3.771887	3.324323
H	-5.794961	-4.194523	1.867258
C	-5.186562	-1.639415	4.170066
H	-4.496724	-2.203586	4.833435
H	-4.805803	-0.599604	4.078210
H	-6.189145	-1.615410	4.646299
C	-1.615709	-4.926256	0.528517
H	-1.835274	-3.964096	1.034263
C	-2.344739	-2.161144	-3.776413
H	-2.527261	-1.336456	-3.058416
C	-1.202404	-1.687186	-4.683376
H	-0.263753	-1.606873	-4.095827
H	-1.036950	-2.386991	-5.528904
H	-1.440307	-0.686571	-5.103063
C	-3.644400	-2.333985	-4.570111
H	-3.520909	-3.076067	-5.386979
H	-4.457586	-2.675174	-3.894340
H	-3.949597	-1.363334	-5.016370
C	-0.240572	-5.366863	1.045799
H	0.028758	-6.378828	0.678541
H	0.536693	-4.645490	0.716842
H	-0.244836	-5.394215	2.155872
C	-2.711152	-5.900410	0.976136
H	-3.698953	-5.557105	0.600311
H	-2.517151	-6.925576	0.595852
H	-2.758059	-5.937022	2.085699
C	-0.843412	1.765717	-2.958508
C	0.507825	1.471066	-3.375261
H	1.175306	2.322353	-3.562520
B	-1.355087	3.137773	-2.589866
O	-0.576067	4.292380	-2.500960
O	-2.696627	3.422528	-2.354072
C	-1.421861	5.355071	-2.013503
C	-2.849736	4.851768	-2.410385
C	-1.250154	5.436169	-0.505781
H	-0.196404	5.616250	-0.253123
H	-1.842511	6.250216	-0.065585
H	-1.561189	4.494069	-0.034231
C	-1.001131	6.654963	-2.665447
H	-1.680983	7.474190	-2.388899
H	0.008802	6.936017	-2.334756
H	-0.984315	6.576307	-3.759393
C	-3.214987	5.216092	-3.842041
H	-3.412724	6.291322	-3.955985
H	-2.415075	4.937980	-4.542927
H	-4.122051	4.670915	-4.136322
C	-3.952652	5.273301	-1.462181
H	-3.804705	4.861760	-0.456448
H	-4.008443	6.368866	-1.383475
H	-4.925489	4.918147	-1.827871
Na	5.214051	-0.873829	0.692601
H	0.680045	0.665920	-4.095437
H	-1.588983	0.976060	-3.112512
H	1.576710	0.706547	-2.345696
O	3.810776	-2.295950	-0.545110
O	6.974340	-2.247430	0.119461
C	2.436466	-2.123658	-0.666258
H	1.935221	-2.676925	0.155659
H	2.182514	-1.047357	-0.575026
C	4.241073	-3.115073	-1.583115
H	4.886905	-2.520530	-2.264418
H	4.840872	-3.954414	-1.172375
C	3.044694	-3.646443	-2.344248
H	3.233235	-3.688752	-3.439041
H	2.768798	-4.656135	-1.966084
C	1.974572	-2.664082	-2.002844
H	1.950029	-1.847375	-2.757510
H	0.978399	-3.151378	-1.936481
C	7.306951	-3.419024	0.785065
H	8.067491	-3.194582	1.565459
H	6.402986	-3.830428	1.282532
C	7.797440	-2.176126	-0.994823
H	7.283243	-1.622425	-1.807837
H	8.729569	-1.629130	-0.729740
C	8.121055	-3.585968	-1.443845

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H   9.178977  -3.668824  -1.775779
H   7.443044  -3.891811  -2.271224
C   7.857100  -4.416350  -0.218756
H   7.107860  -5.208874  -0.437729
H   8.792635  -4.882946   0.160412
O   5.540033   0.392031  -1.281097
C   4.358640   0.790153  -1.889751
H   3.900684  -0.077713  -2.407950
H   3.652644   1.153694  -1.114478
C   6.412860   1.470784  -1.329407
H   6.410006   1.990650  -0.348989
H   7.442250   1.098471  -1.517979
C   4.659272   1.888671  -2.884986
H   4.739348   1.465581  -3.910730
H   3.873248   2.674973  -2.865613
C   5.988879   2.420334  -2.435882
H   6.720744   2.405241  -3.273352
H   5.893512   3.457817  -2.048272
178
Figure_S6_imid-3_modeS2_ts(CuHadd)_02 / electronic energy: -3601.993675027721 a.u. / lowest freq: -684.78 cm-1
C   1.217977   1.000264   2.594864
H   2.096436   0.395219   2.856368
C  -0.093021   0.173890   2.543252
H  -0.903074   0.646953   3.123104
C   0.394882   0.980848   0.369470
C   2.342932   2.350064   0.700694
C   1.897804   3.443930  -0.055065
C   3.727616   2.169899   0.877561
C   2.791270   4.359492  -0.599946
H   0.823219   3.577385  -0.206612
C   4.615791   3.113908   0.352652
C   4.158476   4.210000  -0.374012
H   2.407927   5.194127  -1.192562
H   5.685338   2.941595   0.486168
H   4.871812   4.928980  -0.782428
C  -1.539799  -0.438783   0.548807
C  -2.813284  -0.294997   1.115951
C  -1.360836  -1.311936  -0.533291
C  -3.896503  -1.021422   0.606319
C  -2.436494  -2.063229  -1.021989
C  -3.706085  -1.911001  -0.456425
H  -4.539932  -2.493112  -0.832015
S   4.433199   0.670154   1.580313
O   5.818778   0.604349   1.029511
O   3.590717  -0.419186   1.004418
O   4.378858   0.788724   3.047626
Cu  0.293244   1.485735  -1.469814
C   1.118247   2.174275   3.538459
C   1.937026   2.248096   4.678794
C   0.196086   3.207798   3.294115
C   1.849808   3.345158   5.541592
H   2.636563   1.455556   4.907997
C   0.113036   4.303742   4.156583
H  -0.459346   3.157771   2.437035
C   0.941803   4.374025   5.278615
H   2.485185   3.396252   6.416310
H  -0.595974   5.096636   3.955989
H   0.876238   5.222294   5.947568
C   0.078780  -1.248470   3.017628
C  -0.626230  -1.711691   4.142543
C   0.913852  -2.143802   2.319253
C  -0.484913  -3.039821   4.551755
H  -1.281801  -1.052301   4.697128
C   1.049602  -3.419257   2.718581
H   1.448995  -1.809299   1.442759
C   0.356398  -3.895612   3.836819
H  -1.024034  -3.403923   5.416552
H   1.698565  -4.087930   2.168221
H   0.470753  -4.926377   4.146137
N   1.357254   1.460073   1.189773
N  -0.427000   0.225540   1.111697
H  -0.376849  -1.442101  -0.958459
H  -2.964408   0.378293   1.950543
C  -2.223166  -3.065099  -2.083212
C  -2.455546  -2.723182  -3.444173
C  -1.823288  -4.386875  -1.737121
C  -2.291211  -3.712841  -4.430520
C  -1.672252  -5.339693  -2.761330
C  -1.901415  -5.003110  -4.090475
H  -2.469805  -3.489239  -5.473940
H  -1.382651  -6.356793  -2.533098
H  -1.781765  -5.751019  -4.863819
C  -5.234468  -0.870860   1.203496
C  -5.590474  -1.638507   2.347079
C  -6.175351   0.020349   0.616705
C  -6.884698  -1.498013   2.880544
C  -7.457300   0.123305   1.186807
C  -7.804122  -0.626684   2.305766
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H	-7.191022	-2.070539	3.746107
H	-8.199445	0.786508	0.762285
H	-8.796023	-0.534476	2.729356
C	-5.839888	0.860204	-0.617150
H	-4.792516	0.696543	-0.942842
C	-5.953863	2.359896	-0.318981
H	-5.300905	2.626276	0.539718
H	-5.622380	2.946281	-1.202085
H	-6.998957	2.648734	-0.081188
C	-6.721266	0.464748	-1.807598
H	-6.628539	-0.625308	-2.001405
H	-7.788026	0.706901	-1.616958
H	-6.393690	1.007197	-2.720302
C	-4.618123	-2.621213	3.002551
H	-3.635082	-2.619513	2.489139
C	-5.139425	-4.059752	2.906281
H	-4.376465	-4.767387	3.295931
H	-6.073422	-4.190453	3.492324
H	-5.340399	-4.318960	1.844635
C	-4.333682	-2.231832	4.458176
H	-3.559460	-2.902981	4.886492
H	-3.952889	-1.189033	4.503228
H	-5.246963	-2.309591	5.084415
C	-1.576491	-4.810919	-0.288292
H	-1.685621	-3.953994	0.407124
C	-2.883983	-1.319303	-3.867432
H	-2.924452	-0.635263	-2.996032
C	-1.874904	-0.703200	-4.844455
H	-0.857037	-0.730458	-4.401125
H	-1.859431	-1.248370	-5.811165
H	-2.140700	0.355760	-5.048669
C	-4.294904	-1.333130	-4.466020
H	-4.325267	-1.915229	-5.411206
H	-5.008024	-1.783732	-3.742974
H	-4.627872	-0.294735	-4.678940
C	-0.146240	-5.329960	-0.093142
H	0.039524	-6.248761	-0.687043
H	0.584424	-4.551001	-0.396688
H	0.025502	-5.572113	0.976770
C	-2.607308	-5.853531	0.158873
H	-3.634743	-5.456393	0.012587
H	-2.500287	-6.797292	-0.416451
H	-2.475650	-6.080323	1.238636
C	-1.128355	2.379072	-2.676672
C	0.135364	2.169845	-3.346204
H	0.786159	3.043388	-3.482052
B	-1.548181	3.655491	-1.988572
O	-0.734309	4.772484	-1.785335
O	-2.839432	3.891582	-1.523312
C	-1.476342	5.705210	-0.972321
C	-2.954396	5.305719	-1.282362
C	-1.119414	5.443530	0.481774
H	-0.036161	5.548727	0.631210
H	-1.619664	6.144789	1.164140
H	-1.410915	4.422901	0.766992
C	-1.101249	7.116381	-1.369029
H	-1.722095	7.852721	-0.837794
H	-0.052451	7.318186	-1.110115
H	-1.216150	7.282004	-2.447534
C	-3.469337	5.946358	-2.563065
H	-3.657149	7.022440	-2.440194
H	-2.756527	5.813655	-3.389381
H	-4.414408	5.468386	-2.854466
C	-3.923901	5.546248	-0.144693
H	-3.683116	4.934246	0.733012
H	-3.919657	6.603564	0.158280
H	-4.947552	5.296654	-0.454538
Na	5.233997	-1.055366	-0.593591
H	0.172940	1.508575	-4.217005
H	-1.908487	1.629219	-2.855264
H	1.337086	1.244324	-2.650169
O	3.662555	-2.254077	-1.852276
O	5.788913	-2.990874	0.628866
C	2.303905	-1.987129	-1.728627
H	1.923707	-2.489571	-0.815021
H	2.142147	-0.894740	-1.622897
C	3.837477	-3.149866	-2.900877
H	4.408050	-2.645422	-3.709854
H	4.424119	-4.025163	-2.549118
C	2.487658	-3.594165	-3.426288
H	2.478737	-3.675773	-4.534977
H	2.201863	-4.568640	-2.970799
C	1.573802	-2.518108	-2.942783
H	1.475428	-1.721494	-3.712143
H	0.572397	-2.919613	-2.685055
C	6.754671	-2.857063	1.616144
H	7.386602	-3.772798	1.638158
H	7.404583	-1.985907	1.387178

C 4.677756 -3.562401 1.236943
H 3.753389 -3.185938 0.753431
H 4.714784 -4.666254 1.104332
C 4.681808 -3.207926 2.713221
H 4.491445 -4.109385 3.335880
H 3.914971 -2.434951 2.937588
C 6.062121 -2.664064 2.949296
H 6.013352 -1.583097 3.205047
H 6.587425 -3.216609 3.758602
O 5.517625 0.529032 -2.357926
C 6.104822 0.157189 -3.562583
H 7.036060 0.744848 -3.714801
H 6.375715 -0.919199 -3.513887
C 4.403337 1.297934 -2.662649
H 3.623885 1.148635 -1.888513
H 4.691061 2.372340 -2.674762
C 5.132566 0.398552 -4.706778
H 5.527223 1.183500 -5.389187
H 4.937232 -0.532880 -5.282178
C 3.892280 0.881584 -4.020802
H 3.417899 1.730001 -4.560333
H 3.168215 0.045970 -3.914925
178
Figure_S6_imid-3_modeS2_ts(CuHadd)_03 / electronic energy: -3601.992228363180 a.u. / lowest freq: -639.86 cm-1
C 1.110058 1.075844 2.667306
H 2.014056 0.520509 2.952804
C -0.149002 0.175498 2.571052
H -0.994817 0.582940 3.149220
C 0.342857 1.046613 0.422329
C 2.223898 2.491087 0.820544
C 1.753421 3.582915 0.077862
C 3.609101 2.361132 1.031976
C 2.622426 4.549095 -0.416303
H 0.678840 3.676229 -0.100194
C 4.470900 3.355263 0.558424
C 3.987558 4.451362 -0.151603
H 2.220814 5.382715 -0.998417
H 5.542806 3.222438 0.716339
H 4.681042 5.210607 -0.519377
C -1.522428 -0.471156 0.536270
C -2.811973 -0.412897 1.081308
C -1.273026 -1.310919 -0.558761
C -3.841333 -1.190852 0.538013
C -2.294192 -2.113920 -1.081389
C -3.580372 -2.047044 -0.536957
H -4.372341 -2.668217 -0.939634
S 4.358500 0.868975 1.707073
O 5.758701 0.880897 1.192297
O 3.579355 -0.239163 1.079657
O 4.264330 0.933127 3.176570
Cu 0.275327 1.577126 -1.411062
C 0.915668 2.238210 3.611039
C 1.721283 2.375155 4.755027
C -0.077420 3.201761 3.358122
C 1.548651 3.464614 5.614617
H 2.477924 1.638440 4.988752
C -0.245645 4.290367 4.217459
H -0.722370 3.102453 2.497155
C 0.568934 4.423345 5.344157
H 2.174097 3.564566 6.492269
H -1.009350 5.029010 4.010647
H 0.437517 5.265959 6.010556
C 0.099896 -1.246119 3.012053
C -0.588976 -1.778111 4.116521
C 0.993703 -2.072947 2.302320
C -0.373216 -3.105224 4.495482
H -1.288680 -1.172694 4.678709
C 1.201176 -3.346929 2.672926
H 1.513294 -1.688248 1.437219
C 0.525944 -3.891334 3.770941
H -0.899774 -3.522158 5.344033
H 1.890520 -3.962152 2.111771
H 0.697726 -4.921140 4.055993
N 1.264478 1.553735 1.270767
N -0.461938 0.245577 1.134747
H -0.275874 -1.374890 -0.968773
H -3.017197 0.234446 1.924883
C -2.006233 -3.076670 -2.161071
C -2.244275 -2.718920 -3.517096
C -1.535800 -4.381220 -1.838464
C -2.016961 -3.676967 -4.521951
C -1.325414 -5.302910 -2.880534
C -1.560785 -4.951162 -4.204661
H -2.198966 -3.441733 -5.562204
H -0.984476 -6.307918 -2.670546
H -1.394424 -5.675174 -4.991984
C -5.196342 -1.127088 1.111371
C -5.531881 -1.940905 2.228796

C	-6.170255	-0.267277	0.531849
C	-6.839555	-1.877596	2.743826
C	-7.464044	-0.240684	1.083498
C	-7.791305	-1.036454	2.176531
H	-7.130544	-2.486385	3.589720
H	-8.230258	0.398588	0.665029
H	-8.792740	-1.002996	2.586167
C	-5.856124	0.621730	-0.672887
H	-4.799485	0.510421	-0.990519
C	-6.035581	2.105729	-0.331509
H	-5.407666	2.371674	0.545779
H	-5.713871	2.732749	-1.190248
H	-7.095290	2.344122	-0.102321
C	-6.706466	0.226484	-1.885842
H	-6.567744	-0.852882	-2.109650
H	-7.784340	0.420456	-1.702938
H	-6.389792	0.808053	-2.778077
C	-4.521609	-2.889693	2.876887
H	-3.532874	-2.828311	2.378272
C	-4.970081	-4.349484	2.741411
H	-4.178057	-5.027602	3.125503
H	-5.903683	-4.539353	3.311671
H	-5.144849	-4.593771	1.671633
C	-4.276531	-2.519782	4.344670
H	-3.475086	-3.160882	4.769177
H	-3.949198	-1.460564	4.418191
H	-5.193245	-2.657124	4.955524
C	-1.278805	-4.821831	-0.396303
H	-1.426331	-3.982796	0.313586
C	-2.747716	-1.332518	-3.915394
H	-2.828499	-0.668527	-3.031254
C	-1.771295	-0.642133	-4.875951
H	-0.755049	-0.621702	-4.429107
H	-1.722740	-1.165841	-5.853345
H	-2.094422	0.404493	-5.060110
C	-4.153538	-1.412896	-4.520576
H	-4.148236	-1.978689	-5.476103
H	-4.843373	-1.915091	-3.809025
H	-4.542387	-0.390678	-4.716401
C	0.170429	-5.286209	-0.200455
H	0.394223	-6.191897	-0.801254
H	0.871630	-4.477335	-0.494293
H	0.347908	-5.531311	0.867861
C	-2.268576	-5.913917	0.024194
H	-3.310524	-5.554944	-0.118012
H	-2.121947	-6.839727	-0.571309
H	-2.131662	-6.158599	1.099381
C	-1.143661	2.423717	-2.651654
C	0.147339	2.277108	-3.284657
H	0.764659	3.178195	-3.396013
B	-1.641868	3.669093	-1.958672
O	-0.887123	4.820012	-1.720661
O	-2.953064	3.836160	-1.521504
C	-1.691026	5.705246	-0.913427
C	-3.141572	5.238183	-1.260050
C	-1.349741	5.443110	0.544519
H	-0.277364	5.607081	0.717860
H	-1.901602	6.104753	1.226605
H	-1.587375	4.403307	0.809242
C	-1.376202	7.137834	-1.285823
H	-2.043332	7.836753	-0.760198
H	-0.344069	7.386495	-1.001525
H	-1.475912	7.311263	-2.364625
C	-3.661702	5.874940	-2.540581
H	-3.900207	6.939404	-2.405352
H	-2.929101	5.786764	-3.355380
H	-4.578611	5.359374	-2.856643
C	-4.145140	5.411107	-0.139535
H	-3.894161	4.795486	0.732761
H	-4.198935	6.461814	0.181213
H	-5.148477	5.117483	-0.476190
Na	5.286469	-0.826782	-0.466071
H	0.238627	1.624330	-4.158058
H	-1.883058	1.641336	-2.860860
H	1.368348	1.400932	-2.559481
O	3.802657	-2.036035	-1.828633
O	5.797135	-2.794969	0.738520
C	4.037392	-2.759937	-2.991288
H	4.521413	-2.094630	-3.737696
H	4.724990	-3.604571	-2.774563
C	2.434624	-1.803369	-1.728960
H	2.046661	-2.343417	-0.840792
H	2.246106	-0.719797	-1.588586
C	1.738043	-2.305725	-2.976793
H	0.771536	-2.797936	-2.744772
H	1.574535	-1.468095	-3.689679
C	2.724254	-3.274981	-3.537313
H	2.520897	-4.295601	-3.142694

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 H   2.710477  -3.284886  -4.648861
 C   6.160261  -2.700160   2.079594
 H   7.259790  -2.839064   2.161337
 H   5.905565  -1.691761   2.467288
 C   4.881769  -3.834162   0.617050
 H   3.857068  -3.409519   0.550956
 H   5.088234  -4.412607  -0.308048
 C   4.987875  -4.725847   1.831425
 H   5.761161  -5.507813   1.662454
 H   4.016768  -5.200247   2.089375
 C   5.445781  -3.770476   2.883999
 H   4.567232  -3.332558   3.408678
 H   6.121403  -4.259839   3.618865
 O   5.557977   0.827437  -2.177219
 C   6.205856   0.597976  -3.386143
 H   7.099812   1.255290  -3.454913
 H   6.546624  -0.458555  -3.418211
 C   4.422570   1.573821  -2.458437
 H   3.628585   1.339051  -1.721043
 H   4.667240   2.656338  -2.384663
 C   5.253809   0.874890  -4.540062
 H   5.624469   1.728500  -5.149568
 H   5.124961  -0.018642  -5.189307
 C   3.970274   1.239844  -3.859278
 H   3.467703   2.103408  -4.346700
 H   3.287555   0.363292  -3.839950
178
Figure_S6_imid-3_modeS2_ts(CuHadd)_04 / electronic energy: -3601.991890631659 a.u. / lowest freq: -703.56 cm-1
 C   0.936801   1.323240   2.705492
 H   1.841056   0.779093   3.013545
 C  -0.315294   0.414957   2.612221
 H  -1.198312   0.874978   3.087477
 C   0.259901   1.156094   0.440175
 C   2.051809   2.706759   0.831169
 C   1.560983   3.752659   0.038119
 C   3.436945   2.619309   1.060501
 C   2.409174   4.719055  -0.489922
 H   0.487132   3.804337  -0.158911
 C   4.276920   3.617144   0.555484
 C   3.773337   4.667674  -0.207667
 H   1.991905   5.513787  -1.113990
 H   5.349827   3.522560   0.732589
 H   4.451527   5.428432  -0.600111
 C  -1.514697  -0.468319   0.546542
 C  -2.824821  -0.506996   1.044429
 C  -1.159867  -1.306202  -0.519835
 C  -3.766247  -1.378220   0.480608
 C  -2.084865  -2.211411  -1.051449
 C  -3.392009  -2.239949  -0.556594
 H  -4.113687  -2.933931  -0.972179
 S   4.222433   1.179179   1.806748
 O   5.631617   1.225064   1.320673
 O   3.499122   0.017081   1.207403
 O   4.088716   1.296665   3.269716
Cu   0.264961   1.600937  -1.417064
 C   0.726398   2.505027   3.620254
 C   1.492873   2.649942   4.789907
 C  -0.243549   3.477404   3.316961
 C   1.304670   3.755101   5.625847
 H   2.230295   1.906782   5.062011
 C  -0.427491   4.581620   4.152872
 H  -0.856791   3.374618   2.433963
 C   0.348106   4.721901   5.305883
 H   1.899820   3.860887   6.523640
 H  -1.172943   5.326984   3.907216
 H   0.204515   5.576700   5.954009
 C  -0.093612  -0.952424   3.208986
 C  -0.831713  -1.361460   4.333668
 C   0.839925  -1.844662   2.642094
 C  -0.624747  -2.632199   4.874841
 H  -1.558915  -0.702079   4.790652
 C   1.035941  -3.065452   3.168253
 H   1.406667  -1.552609   1.768062
 C   0.311483  -3.486767   4.288726
 H  -1.184779  -2.952319   5.743705
 H   1.761479  -3.731942   2.723681
 H   0.477700  -4.473283   4.701571
 N   1.108126   1.761576   1.299647
 N  -0.534426   0.348137   1.157668
 H  -0.152078  -1.286072  -0.901272
 H  -3.116574   0.141712   1.860841
 C  -1.668503  -3.175613  -2.088164
 C  -1.909211  -2.894693  -3.461946
 C  -1.057702  -4.404458  -1.707450
 C  -1.550976  -3.856025  -4.424715
 C  -0.716730  -5.331258  -2.709739
 C  -0.959657  -5.056787  -4.050371
 H  -1.731357  -3.679675  -5.476811
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H	-0.266239	-6.281433	-2.455599
H	-0.691511	-5.783841	-4.806154
C	-5.152684	-1.392531	0.978147
C	-5.499062	-2.205222	2.092903
C	-6.146962	-0.615097	0.321198
C	-6.836858	-2.222345	2.528521
C	-7.469248	-0.662728	0.798801
C	-7.806772	-1.457034	1.889510
H	-7.137558	-2.836143	3.367312
H	-8.250520	-0.086023	0.321413
H	-8.830731	-1.483817	2.239640
C	-5.825947	0.258304	-0.893202
H	-4.748919	0.207667	-1.152475
C	-6.118030	1.736252	-0.609688
H	-5.550984	2.069593	0.285840
H	-5.796840	2.355949	-1.473736
H	-7.200763	1.910482	-0.437462
C	-6.583252	-0.225975	-2.135318
H	-6.368305	-1.301090	-2.314384
H	-7.679239	-0.093402	-2.016568
H	-6.253790	0.346375	-3.028853
C	-4.469500	-3.074093	2.817238
H	-3.456097	-2.942672	2.385994
C	-4.802748	-4.562756	2.665470
H	-3.995460	-5.180846	3.113689
H	-5.760369	-4.814584	3.168010
H	-4.880466	-4.825010	1.588442
C	-4.352191	-2.681503	4.294959
H	-3.546425	-3.270864	4.780757
H	-4.096031	-1.603813	4.380982
H	-5.298682	-2.872356	4.842486
C	-0.789690	-4.764808	-0.245002
H	-1.064196	-3.931182	0.432729
C	-2.542902	-1.584117	-3.925163
H	-2.715942	-0.900351	-3.069538
C	-1.616928	-0.831146	-4.889231
H	-0.618489	-0.693961	-4.422781
H	-1.492404	-1.379669	-5.846082
H	-2.038532	0.170715	-5.117947
C	-3.915027	-1.833915	-4.560508
H	-3.823698	-2.428793	-5.493767
H	-4.567618	-2.381934	-3.847771
H	-4.403336	-0.866101	-4.803951
C	0.700517	-5.034934	0.002566
H	1.064405	-5.900443	-0.588656
H	1.298162	-4.139459	-0.265715
H	0.871667	-5.258731	1.075975
C	-1.645405	-5.960799	0.187649
H	-2.719694	-5.743243	0.004707
H	-1.363279	-6.879373	-0.368904
H	-1.512564	-6.150770	1.274358
C	-1.122950	2.308962	-2.772316
C	0.209918	2.218061	-3.323445
H	0.775354	3.151188	-3.444563
B	-1.733744	3.536696	-2.141527
O	-1.070501	4.741191	-1.896060
O	-3.075835	3.625135	-1.779261
C	-1.975524	5.590209	-1.159547
C	-3.370952	5.016796	-1.569193
C	-1.698191	5.388988	0.321436
H	-0.652641	5.638839	0.548459
H	-2.335957	6.022546	0.953188
H	-1.872203	4.339952	0.601055
C	-1.739843	7.031041	-1.557086
H	-2.482985	7.694471	-1.090786
H	-0.745866	7.361267	-1.223819
H	-1.790112	7.167951	-2.644396
C	-3.861353	5.584890	-2.893180
H	-4.177378	6.633615	-2.800968
H	-3.082100	5.527328	-3.666307
H	-4.723379	5.000481	-3.242204
C	-4.444698	5.151160	-0.509926
H	-4.204195	4.575600	0.391949
H	-4.584488	6.203807	-0.223240
H	-5.406534	4.783946	-0.892195
Na	5.291940	-0.645857	-0.193655
H	0.391151	1.534253	-4.158207
H	-1.800108	1.473676	-2.987001
H	1.439757	1.461835	-2.486849
O	3.926471	-1.998007	-1.558791
O	5.665156	-2.486137	1.210502
C	2.625979	-1.527578	-1.644495
H	2.050968	-1.894234	-0.767825
H	2.622835	-0.420614	-1.627062
C	3.936442	-3.241660	-2.175449
H	4.916226	-3.396845	-2.674931
H	3.803843	-4.033353	-1.405786
C	2.806984	-3.300984	-3.191744

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H 2.176440 -4.201793 -3.023556
C 2.025601 -2.044822 -2.932276
H 2.190643 -1.311886 -3.752162
H 0.940942 -2.250099 -2.826687
C 4.477336 -2.997933 1.725788
H 4.304881 -2.582830 2.742391
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C 6.579141 -3.526846 1.140282
H 7.221469 -3.400477 0.243007
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C 5.823911 -4.833053 1.067163
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H 5.622213 -5.096805 0.005653
C 4.543020 -4.514925 1.773108
H 3.672424 -4.980353 1.260830
H 4.586908 -4.864490 2.828288
O 5.601803 0.789135 -2.061367
C 6.038243 0.227690 -3.257761
H 7.144587 0.303504 -3.323255
H 5.760160 -0.847729 -3.271152
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H 3.804633 1.699398 -1.673445
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C 5.389666 0.939179 -4.428457
H 6.087517 1.695990 -4.850698
H 5.074328 0.228377 -5.223264
C 4.219940 1.617924 -3.796872
H 3.996474 2.597067 -4.273408
H 3.329207 0.955751 -3.849538

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Figure_S6_imid-3_modeS2_ts(CuHadd)_05 / electronic energy: -3601.992017267920 a.u. / lowest freq: -736.03 cm-1

C 1.079979 1.150351 2.722192
H 1.970807 0.572514 3.004918
C -0.194797 0.275336 2.608404
H -1.043683 0.702026 3.168147
C 0.347880 1.133846 0.468842
C 2.244997 2.543513 0.888420
C 1.812973 3.654898 0.152134
C 3.625411 2.353570 1.081728
C 2.716667 4.584313 -0.351043
H 0.741812 3.784265 -0.023515
C 4.523769 3.310798 0.600916
C 4.079450 4.427239 -0.103222
H 2.344775 5.433662 -0.930074
H 5.590818 3.131958 0.746456
H 4.800425 5.156371 -0.478994
C -1.515468 -0.394194 0.538413
C -2.801079 -0.431828 1.095527
C -1.238886 -1.159512 -0.603717
C -3.796547 -1.228467 0.516041
C -2.219935 -1.989030 -1.159334
C -3.502704 -2.015468 -0.603033
H -4.266770 -2.653252 -1.032606
S 4.310440 0.822712 1.732881
O 5.706378 0.768419 1.210616
O 3.472318 -0.238276 1.101190
O 4.227516 0.879273 3.204270
Cu 0.366304 1.650699 -1.366431
C 0.907468 2.304944 3.678588
C 1.717205 2.412857 4.822762
C -0.065025 3.291995 3.436367
C 1.567054 3.495445 5.695080
H 2.460783 1.659372 5.045697
C -0.210686 4.373640 4.308615
H -0.711267 3.217311 2.573739
C 0.606586 4.476686 5.436574
H 2.195400 3.572945 6.572934
H -0.958773 5.130436 4.110590
H 0.492685 5.314064 6.112726
C 0.027292 -1.144587 3.069276
C -0.622888 -1.625333 4.219546
C 0.873711 -2.013082 2.349953
C -0.414501 -2.942473 4.635323
H -1.282435 -0.985809 4.792567
C 1.070937 -3.278335 2.754671
H 1.367064 -1.669058 1.451758
C 0.435731 -3.771105 3.899589
H -0.908062 -3.318488 5.521972
H 1.727656 -3.924106 2.190327
H 0.602967 -4.793064 4.214091
N 1.252532 1.638674 1.334332
N -0.482428 0.342444 1.164719
H -0.247306 -1.146331 -1.025195
H -3.031477 0.158257 1.973714
C -1.892066 -2.878707 -2.291407
C -2.214270 -2.487938 -3.621332
C -1.323627 -4.160886 -2.042951

C	-1.978850	-3.393848	-4.671659
C	-1.110633	-5.030154	-3.128794
C	-1.430868	-4.646909	-4.425623
H	-2.229635	-3.136193	-5.691994
H	-0.705023	-6.020972	-2.974574
H	-1.261659	-5.331464	-5.246900
C	-5.151222	-1.251506	1.093698
C	-5.456163	-2.153408	2.150510
C	-6.152471	-0.378283	0.584666
C	-6.759505	-2.159638	2.680293
C	-7.438987	-0.419317	1.152288
C	-7.735596	-1.299826	2.187452
H	-7.027718	-2.836491	3.480756
H	-8.223998	0.231359	0.790009
H	-8.732494	-1.319008	2.608908
C	-5.876707	0.593894	-0.564033
H	-4.827995	0.514503	-0.915507
C	-6.060934	2.049166	-0.117910
H	-5.398489	2.267536	0.747027
H	-5.787117	2.735636	-0.946926
H	-7.112794	2.253784	0.172214
C	-6.753934	0.273818	-1.780383
H	-6.620375	-0.789064	-2.074606
H	-7.827567	0.454438	-1.562494
H	-6.457555	0.910982	-2.641040
C	-4.417780	-3.123437	2.717035
H	-3.435358	-2.999706	2.217278
C	-4.833381	-4.578976	2.473709
H	-4.021624	-5.265268	2.797311
H	-5.756065	-4.834373	3.036144
H	-5.014192	-4.744723	1.389980
C	-4.168431	-2.861267	4.207047
H	-3.355991	-3.521500	4.577338
H	-3.855575	-1.805947	4.358279
H	-5.078595	-3.057871	4.811350
C	-0.984257	-4.643962	-0.631619
H	-1.119950	-3.834202	0.113606
C	-2.826197	-1.125474	-3.942865
H	-2.874094	-0.487874	-3.036859
C	-1.972772	-0.354314	-4.958935
H	-0.922590	-0.295695	-4.603501
H	-1.986286	-0.841074	-5.956224
H	-2.362401	0.679312	-5.076227
C	-4.267401	-1.279924	-4.440327
H	-4.301887	-1.828613	-5.405301
H	-4.869083	-1.835711	-3.689828
H	-4.729994	-0.279975	-4.583628
C	0.484523	-5.075516	-0.518763
H	0.703150	-5.958296	-1.154152
H	1.149938	-4.241871	-0.822229
H	0.720331	-5.346717	0.531224
C	-1.923542	-5.777986	-0.207094
H	-2.980022	-5.441756	-0.281656
H	-1.784717	-6.674282	-0.848064
H	-1.725562	-6.061983	0.848734
C	-0.969210	2.511934	-2.681148
C	0.348652	2.337926	-3.249138
H	0.985005	3.227781	-3.341202
B	-1.487642	3.748364	-1.988713
O	-0.750791	4.903380	-1.715929
O	-2.812278	3.897970	-1.584202
C	-1.586082	5.773888	-0.924192
C	-3.022641	5.293668	-1.310246
C	-1.278765	5.507419	0.540750
H	-0.216105	5.696523	0.745421
H	-1.865152	6.149881	1.212190
H	-1.497598	4.459601	0.790826
C	-1.276865	7.212227	-1.279021
H	-1.963511	7.901283	-0.765664
H	-0.254604	7.468665	-0.967134
H	-1.350521	7.392591	-2.358689
C	-3.521935	5.940495	-2.594359
H	-3.773952	7.000944	-2.452248
H	-2.771639	5.868826	-3.394511
H	-4.426789	5.419830	-2.935865
C	-4.055488	5.437681	-0.212030
H	-3.816602	4.814397	0.658276
H	-4.135090	6.482995	0.120694
H	-5.044969	5.131940	-0.577790
Na	5.208408	-1.081153	-0.304645
H	0.467813	1.674717	-4.111415
H	-1.706813	1.734507	-2.911875
H	1.515098	1.453755	-2.458690
O	3.746971	-2.193108	-1.898389
O	5.184800	-3.041624	1.023592
C	2.528800	-1.531235	-1.840437
H	1.917503	-1.979704	-1.029777
H	2.695827	-0.462802	-1.602671

C 3.659194 -3.153783 -2.900722
H 4.534109 -3.048143 -3.576764
H 3.689468 -4.167345 -2.446862
C 2.372089 -2.969644 -3.687238
H 2.559828 -2.925137 -4.782221
H 1.662640 -3.796475 -3.461990
C 1.831993 -1.674067 -3.173681
H 2.124346 -0.840423 -3.848364
H 0.727671 -1.701567 -3.071794
C 4.959412 -2.970166 2.391785
H 5.823556 -2.478319 2.886462
H 4.048827 -2.363107 2.587334
C 4.508202 -4.167149 0.576255
H 3.471816 -3.884325 0.287787
H 5.024464 -4.581594 -0.315195
C 4.481710 -5.190547 1.694166
H 5.275565 -5.954193 1.539188
H 3.490364 -5.690438 1.755622
C 4.770249 -4.377352 2.926071
H 3.925296 -4.419215 3.647927
H 5.700817 -4.735310 3.419198
O 5.628194 0.425925 -2.092456
C 6.141864 -0.043759 -3.291679
H 7.144159 0.408005 -3.463743
H 6.255354 -1.147248 -3.244359
C 4.892293 1.568149 -2.386745
H 3.985741 1.595829 -1.748065
H 5.506187 2.466889 -2.159163
C 5.195063 0.343329 -4.403978
H 5.742769 0.569599 -5.344605
H 4.463244 -0.474266 -4.582393
C 4.500672 1.555366 -3.855839
H 4.861132 2.477896 -4.361860
H 3.400194 1.470855 -3.982656
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Figure_S6_imid-3_modeS2_ts(CuHadd)_06 / electronic energy: -3601.981304303318 a.u. / lowest freq: -668.67 cm-1
C 0.751728 1.281234 2.617310
H 1.574674 0.612040 2.907206
C -0.598819 0.551645 2.493874
H -1.445331 1.209895 2.761540
C 0.179815 1.058033 0.334578
C 1.976283 2.593366 0.732941
C 1.548916 3.588449 -0.158050
C 3.347112 2.494032 1.030006
C 2.443097 4.489733 -0.722974
H 0.485219 3.657384 -0.399714
C 4.235611 3.422718 0.475506
C 3.794789 4.420344 -0.389273
H 2.070402 5.248073 -1.416743
H 5.296707 3.316933 0.707472
H 4.510124 5.128211 -0.813326
C -1.645750 -0.497804 0.417831
C -2.998749 -0.352337 0.761746
C -1.270003 -1.482009 -0.508181
C -3.965655 -1.181960 0.177801
C -2.233932 -2.329533 -1.067918
C -3.581779 -2.170394 -0.733804
H -4.326845 -2.830971 -1.162624
S 4.068718 1.157863 1.997479
O 5.491686 1.099650 1.543235
O 3.344887 -0.080107 1.578224
O 3.902970 1.513994 3.416400
Cu 0.207968 1.449665 -1.538138
C 0.683237 2.446513 3.570989
C 1.272435 2.351828 4.843649
C -0.010112 3.620603 3.226958
C 1.197939 3.423319 5.738867
H 1.781317 1.445952 5.147855
C -0.081655 4.690268 4.123081
H -0.494663 3.704667 2.266205
C 0.525198 4.593241 5.377391
H 1.657815 3.344446 6.715427
H -0.611430 5.592579 3.846052
H 0.467656 5.421261 6.071968
C -0.662433 -0.709564 3.315561
C -1.545932 -0.796210 4.405357
C 0.148465 -1.820144 3.001225
C -1.602713 -1.969122 5.160812
H -2.182171 0.038413 4.672016
C 0.083228 -2.949639 3.727070
H 0.829724 -1.773295 2.161079
C -0.788955 -3.050638 4.816807
H -2.275485 -2.040834 6.005447
H 0.711081 -3.791721 3.470446
H -0.831289 -3.965256 5.393837
N 0.982208 1.706964 1.212513
N -0.650376 0.282059 1.049199
H -0.223321 -1.620470 -0.753371

H	-3.301458	0.399489	1.479630
C	-1.822931	-3.442934	-1.944860
C	-1.778390	-3.243421	-3.356431
C	-1.498357	-4.657575	-1.399568
C	-1.376458	-4.310463	-4.180261
C	-1.084628	-5.706929	-2.246583
C	-1.024155	-5.532767	-3.624269
H	-1.336214	-4.200183	-5.255865
H	-0.812054	-6.672162	-1.840778
H	-0.711162	-6.349533	-4.261968
C	-5.387061	-1.048337	0.543889
C	-5.897680	-1.753616	1.669417
C	-6.261185	-0.284671	-0.278888
C	-7.275080	-1.679895	1.947238
C	-7.631237	-0.247343	0.039068
C	-8.128175	-0.934081	1.141290
H	-7.699954	-2.214978	2.786147
H	-8.326844	0.309739	-0.574422
H	-9.186044	-0.895508	1.367677
C	-5.763022	0.473721	-1.510028
H	-4.659234	0.410287	-1.601709
C	-6.087495	1.969294	-1.414228
H	-5.670101	2.385459	-0.472685
H	-5.631077	2.511703	-2.269036
H	-7.181891	2.152319	-1.435601
C	-6.336550	-0.134148	-2.794861
H	-6.083187	-1.214669	-2.847858
H	-7.440590	-0.021064	-2.834486
H	-5.896710	0.367743	-3.683160
C	-5.005637	-2.619231	2.561071
H	-3.942154	-2.553144	2.253312
C	-5.389513	-4.098871	2.446148
H	-4.673417	-4.723844	3.021639
H	-6.412280	-4.280709	2.838572
H	-5.349366	-4.418340	1.382697
C	-5.049147	-2.149416	4.020276
H	-4.345835	-2.752089	4.632265
H	-4.743144	-1.083259	4.084252
H	-6.064323	-2.260806	4.454609
C	-1.577073	-4.928291	0.108743
H	-1.951848	-4.047051	0.668001
C	-2.170930	-1.915781	-4.004771
H	-2.442796	-1.160178	-3.240565
C	-1.001654	-1.316605	-4.794553
H	-0.122272	-1.190007	-4.127522
H	-0.714695	-1.962544	-5.650334
H	-1.286780	-0.320176	-5.193573
C	-3.409298	-2.083109	-4.893025
H	-3.196005	-2.740519	-5.762123
H	-4.241271	-2.524149	-4.303244
H	-3.741785	-1.093120	-5.272423
C	-0.190862	-5.227326	0.686936
H	0.254729	-6.135288	0.229547
H	0.479244	-4.361945	0.503572
H	-0.261164	-5.385881	1.783819
C	-2.563734	-6.060670	0.421086
H	-3.553454	-5.835872	-0.030944
H	-2.201187	-7.034405	0.030379
H	-2.699256	-6.153689	1.520041
C	-1.213743	2.152470	-2.873602
C	0.104851	2.043290	-3.448781
H	0.681756	2.967862	-3.579306
B	-1.777535	3.418303	-2.272897
O	-1.056974	4.599810	-2.078135
O	-3.106288	3.579810	-1.895950
C	-1.911557	5.510878	-1.356152
C	-3.335758	4.990281	-1.731726
C	-1.623484	5.342111	0.126916
H	-0.564757	5.553016	0.331350
H	-2.222831	6.023668	0.746227
H	-1.838161	4.310759	0.444907
C	-1.614202	6.926344	-1.800951
H	-2.317280	7.638440	-1.344499
H	-0.599857	7.217445	-1.493480
H	-1.676229	7.032216	-2.891108
C	-3.816069	5.534001	-3.069450
H	-4.083997	6.598322	-3.010067
H	-3.050287	5.415372	-3.849021
H	-4.707740	4.977436	-3.388127
C	-4.388528	5.214562	-0.666719
H	-4.169367	4.653858	0.250079
H	-4.465421	6.281617	-0.411118
H	-5.374139	4.891829	-1.027836
Na	5.207240	-0.907463	0.340347
H	0.273542	1.351065	-4.278139
H	-1.907126	1.325527	-3.071572
H	1.355787	1.261594	-2.619691
O	7.260558	-1.504137	-0.590250

O 4.591601 -3.140946 0.151293
C 7.196272 -2.153122 -1.816087
H 7.872404 -3.036668 -1.799379
H 6.160708 -2.508585 -1.997905
C 8.249734 -0.538104 -0.707821
H 8.012270 0.321040 -0.045359
H 9.224772 -0.969949 -0.389792
C 8.318967 -0.086975 -2.153870
H 7.782921 0.878265 -2.286863
H 9.374168 0.023905 -2.486507
C 7.618124 -1.185084 -2.904101
H 6.727740 -0.786545 -3.437001
H 8.298617 -1.677678 -3.632535
C 5.399871 -4.067803 0.797072
H 5.598899 -4.921802 0.112286
H 6.370060 -3.595062 1.058670
C 3.285193 -3.458378 0.491520
H 2.650978 -2.548352 0.444579
H 2.887316 -4.202749 -0.234040
C 3.288954 -4.033850 1.891066
H 2.540416 -4.848401 1.996714
H 3.085106 -3.231721 2.634195
C 4.692269 -4.546967 2.052612
H 5.164649 -4.115931 2.962769
H 4.708534 -5.657281 2.113881
O 4.275403 -0.264765 -1.636121
C 4.326900 0.993842 -2.217139
H 3.565057 1.648832 -1.744309
H 5.327953 1.442628 -2.047451
C 3.357525 -0.995590 -2.376145
H 3.616709 -2.074278 -2.331956
H 2.341677 -0.862339 -1.941303
C 4.050295 0.849679 -3.701283
H 3.377374 1.657671 -4.062614
H 5.000478 0.872403 -4.278664
C 3.399245 -0.502936 -3.809945
H 2.376321 -0.432300 -4.239001
H 4.020449 -1.182146 -4.434642
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Figure_S6_imid-3_modeS2_ts(CuHadd)_07 / electronic energy: -3601.986994980984 a.u. / lowest freq: -591.30 cm-1
C 0.540775 2.033699 2.256032
H 1.585707 1.759142 2.457440
C -0.426870 0.836806 2.391050
H -1.392948 1.130166 2.839004
C -0.241894 1.411638 0.112023
C 1.006563 3.442565 0.115318
C 0.154732 4.191826 -0.707518
C 2.383201 3.726477 0.106052
C 0.638970 5.221560 -1.505595
H -0.910179 3.945117 -0.716685
C 2.858936 4.773448 -0.689125
C 1.999107 5.524694 -1.486308
H -0.054676 5.778019 -2.141451
H 3.933430 4.965144 -0.694065
H 2.397164 6.332257 -2.104514
C -1.316446 -0.695292 0.548115
C -2.479992 -1.141333 1.190739
C -0.761235 -1.466619 -0.483625
C -3.083053 -2.343384 0.797913
C -1.347610 -2.679495 -0.859676
C -2.513444 -3.114448 -0.221608
H -2.970922 -4.053749 -0.510529
S 3.595179 2.761721 1.019592
O 4.901660 3.040352 0.348971
O 3.203127 1.335248 0.829486
O 3.529629 3.233856 2.414467
Cu -0.572384 1.628544 -1.763525
C 0.143848 3.195819 3.130134
C 0.930928 3.552004 4.239003
C -1.031723 3.921423 2.867836
C 0.561655 4.628491 5.051455
H 1.823941 2.991497 4.483257
C -1.397226 4.997757 3.680362
H -1.663036 3.649673 2.035480
C -0.599221 5.353283 4.770213
H 1.173986 4.898269 5.902149
H -2.300934 5.553743 3.466424
H -0.883611 6.185897 5.400486
C 0.163532 -0.300701 3.185205
C -0.356464 -0.619274 4.451781
C 1.225933 -1.071175 2.667516
C 0.183065 -1.684596 5.175396
H -1.171684 -0.047233 4.876870
C 1.730998 -2.103986 3.362674
H 1.636944 -0.844784 1.691643
C 1.226313 -2.432756 4.625630
H -0.210980 -1.934718 6.151829
H 2.534951 -2.690468 2.943577

H	1.643686	-3.266210	5.175538
N	0.415855	2.360425	0.814449
N	-0.654430	0.477329	0.981214
H	0.156940	-1.150201	-0.955250
H	-2.918251	-0.557761	1.990686
C	-0.716137	-3.519191	-1.896850
C	-1.235971	-3.524396	-3.221893
C	0.381329	-4.361149	-1.557707
C	-0.659532	-4.384480	-4.174250
C	0.926590	-5.196905	-2.549679
C	0.410690	-5.206121	-3.840372
H	-1.041138	-4.425199	-5.185838
H	1.751691	-5.859147	-2.323398
H	0.840653	-5.860793	-4.587587
C	-4.312187	-2.807154	1.464068
C	-4.224267	-3.646121	2.609439
C	-5.582757	-2.443980	0.937233
C	-5.413317	-4.106044	3.204603
C	-6.742146	-2.920240	1.576019
C	-6.655210	-3.741268	2.695346
H	-5.383766	-4.756738	4.068544
H	-7.724505	-2.664199	1.201504
H	-7.558768	-4.103874	3.168531
C	-5.726423	-1.571018	-0.310642
H	-4.735716	-1.270217	-0.707875
C	-6.466197	-0.266220	0.005272
H	-5.935041	0.285952	0.809941
H	-6.495010	0.379120	-0.898083
H	-7.510305	-0.459852	0.328780
C	-6.419856	-2.338266	-1.442758
H	-5.880062	-3.288384	-1.642359
H	-7.474482	-2.571367	-1.185340
H	-6.410402	-1.732443	-2.374096
C	-2.880692	-4.081278	3.197291
H	-2.033565	-3.608676	2.659207
C	-2.684789	-5.594666	3.052795
H	-1.668924	-5.881844	3.399500
H	-3.434202	-6.155970	3.649858
H	-2.780839	-5.888164	1.985338
C	-2.742390	-3.643814	4.660611
H	-1.728851	-3.898050	5.036857
H	-2.879373	-2.544212	4.741782
H	-3.487997	-4.149330	5.308967
C	0.965664	-4.413657	-0.144793
H	0.474029	-3.678257	0.523103
C	-2.405622	-2.634129	-3.641029
H	-2.705083	-1.955458	-2.816946
C	-2.023883	-1.724999	-4.816588
H	-1.091689	-1.171438	-4.579727
H	-1.866052	-2.308220	-5.747736
H	-2.831943	-0.985821	-5.003260
C	-3.640020	-3.477826	-3.977329
H	-3.457012	-4.121196	-4.863851
H	-3.903373	-4.124569	-3.113327
H	-4.506269	-2.816171	-4.192256
C	2.457044	-4.053990	-0.144401
H	3.058690	-4.805911	-0.695997
H	2.606296	-3.060516	-0.615110
H	2.836353	-4.007481	0.897597
C	0.729685	-5.786421	0.495072
H	-0.356159	-6.022762	0.493359
H	1.273449	-6.584751	-0.052726
H	1.079732	-5.779719	1.549645
C	-2.297707	1.623747	-2.898060
C	-1.117322	1.936349	-3.670366
H	-0.971499	2.983504	-3.964678
B	-3.207157	2.659546	-2.283587
O	-2.980528	4.037517	-2.314613
O	-4.418136	2.368332	-1.661091
C	-4.000753	4.664009	-1.511977
C	-5.148604	3.601230	-1.543259
C	-3.439556	4.845421	-0.111339
H	-2.525425	5.454013	-0.147367
H	-4.148119	5.350006	0.559869
H	-3.188587	3.868425	0.326081
C	-4.359978	6.002563	-2.119781
H	-5.209623	6.460029	-1.591643
H	-3.510456	6.695700	-2.043622
H	-4.621904	5.912858	-3.181298
C	-6.024615	3.731953	-2.780581
H	-6.667639	4.622386	-2.739536
H	-5.417468	3.787328	-3.695227
H	-6.672842	2.848944	-2.861926
C	-6.003690	3.563277	-0.294029
H	-5.422784	3.274008	0.590183
H	-6.462481	4.544296	-0.101913
H	-6.818275	2.836108	-0.409913
Na	5.231361	0.867111	-0.485442

H -0.803864 1.251104 -4.463689
H -2.640244 0.582080 -2.914601
H 0.415641 1.821313 -3.005526
O 6.493573 -0.632346 -1.768084
O 5.803969 -0.570099 1.319391
C 7.794185 -1.044258 -1.508760
H 8.492973 -0.453682 -2.141012
H 8.041082 -0.859869 -0.441783
C 5.904947 -1.564634 -2.617230
H 4.975498 -1.944195 -2.140963
H 5.632821 -1.075041 -3.576290
C 6.860995 -2.716586 -2.866428
H 6.359080 -3.702130 -2.750989
H 7.300819 -2.635265 -3.885201
C 7.921314 -2.515096 -1.831851
H 7.698041 -3.126032 -0.929596
H 8.932588 -2.767125 -2.218832
C 5.743259 -0.188481 2.655810
H 6.658710 0.386578 2.910715
H 4.861675 0.468774 2.815604
C 5.282192 -1.852810 1.250134
H 4.180532 -1.795018 1.106946
H 5.721522 -2.397245 0.389929
C 5.611215 -2.557716 2.543275
H 6.616035 -3.029709 2.469968
H 4.851783 -3.325790 2.802563
C 5.642070 -1.429339 3.531534
H 4.702990 -1.407289 4.127574
H 6.515768 -1.519328 4.213563
O 3.710012 0.746802 -2.263507
C 3.507253 1.155186 -3.573230
H 2.991383 2.141484 -3.576024
H 4.487263 1.269112 -4.083172
C 2.585876 0.015553 -1.910229
H 2.855104 -0.726396 -1.131100
H 1.823949 0.700339 -1.488713
C 2.660404 0.110499 -4.278015
H 1.874789 0.590211 -4.901870
H 3.296275 -0.543496 -4.914528
C 2.058390 -0.680712 -3.149383
H 0.948198 -0.657728 -3.183637
H 2.410313 -1.735727 -3.180563

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Figure_S6_imid-3_modeS2_prod(CuHadd) / electronic energy: -3602.039215307438 a.u. / lowest freq: 15.90 cm-1

C 1.044311 0.464708 3.148142
H 1.852190 -0.233865 3.405337
C -0.263654 -0.252914 2.748108
H -1.106754 0.012840 3.404126
C 0.494708 1.058131 0.927094
C 2.598369 1.919377 1.734040
C 2.479932 3.282741 1.435191
C 3.875533 1.340509 1.823481
C 3.612251 4.070412 1.250378
H 1.478709 3.715584 1.351880
C 5.005944 2.143510 1.648925
C 4.879662 3.502042 1.370219
H 3.500031 5.131697 1.019104
H 5.988636 1.670744 1.701841
H 5.773806 4.113979 1.233338
C -1.616888 -0.094460 0.576486
C -2.858771 -0.389546 1.165474
C -1.458081 -0.299635 -0.806781
C -3.904104 -0.917449 0.396730
C -2.489429 -0.864230 -1.568727
C -3.714830 -1.161801 -0.966333
H -4.509436 -1.612753 -1.549878
S 4.118583 -0.434120 2.015941
O 5.502494 -0.685131 1.521009
O 3.107930 -1.043714 1.103041
O 3.935740 -0.754980 3.444904
Cu 0.728062 2.116880 -0.669576
C 0.864465 1.451285 4.277403
C 1.640923 1.342468 5.444711
C -0.065867 2.501520 4.172670
C 1.491084 2.268122 6.481942
H 2.364106 0.544235 5.553479
C -0.211572 3.425284 5.210802
H -0.681415 2.599520 3.290213
C 0.566931 3.309304 6.364655
H 2.093149 2.178755 7.376912
H -0.929315 4.230409 5.120644
H 0.453154 4.025120 7.168418
C -0.101538 -1.755981 2.791335
C -0.224889 -2.413714 4.027990
C 0.221987 -2.515928 1.645557
C -0.052357 -3.797087 4.102898
H -0.451804 -1.855977 4.928247
C 0.374644 -3.848638 1.722354

H	0.363304	-2.038725	0.686090
C	0.240372	-4.517324	2.943493
H	-0.150900	-4.308162	5.051672
H	0.613371	-4.412688	0.833018
H	0.370252	-5.590708	2.990393
N	1.408476	1.167055	1.902982
N	-0.506665	0.284151	1.383420
H	-0.513081	-0.084430	-1.277285
H	-3.015450	-0.235181	2.224273
C	-2.255806	-1.267093	-2.971590
C	-2.574971	-0.376398	-4.034010
C	-1.828034	-2.595587	-3.260579
C	-2.500896	-0.844780	-5.358981
C	-1.763489	-3.011167	-4.603188
C	-2.095127	-2.144176	-5.636747
H	-2.770118	-0.206189	-6.189334
H	-1.474471	-4.021687	-4.858153
H	-2.047739	-2.486059	-6.662743
C	-5.179963	-1.290656	1.037889
C	-5.280834	-2.516963	1.754246
C	-6.309366	-0.431118	0.931626
C	-6.502308	-2.843153	2.371720
C	-7.513737	-0.813324	1.550438
C	-7.603747	-2.001282	2.267051
H	-6.610657	-3.762096	2.932580
H	-8.393479	-0.186996	1.483039
H	-8.537460	-2.274486	2.741777
C	-6.256842	0.891552	0.167320
H	-5.244722	1.073755	-0.243950
C	-6.557969	2.079966	1.089177
H	-5.839440	2.092683	1.936578
H	-6.451556	3.032803	0.528835
H	-7.590998	2.030109	1.492186
C	-7.207017	0.870914	-1.035510
H	-6.979979	-0.003211	-1.682693
H	-8.267131	0.812293	-0.710440
H	-7.073544	1.793168	-1.640798
C	-4.111969	-3.498192	1.861488
H	-3.232714	-3.143585	1.286008
C	-4.474709	-4.864061	1.264748
H	-3.573416	-5.512886	1.227824
H	-5.250156	-5.378106	1.870460
H	-4.853843	-4.737597	0.228470
C	-3.646364	-3.639421	3.314646
H	-2.777189	-4.327507	3.368417
H	-3.333173	-2.649153	3.709408
H	-4.452985	-4.046445	3.959788
C	-1.495955	-3.602857	-2.158076
H	-1.462972	-3.109551	-1.165189
C	-3.025674	1.060031	-3.780356
H	-2.899567	1.327421	-2.711901
C	-2.175769	2.063349	-4.573526
H	-1.098142	1.888501	-4.373972
H	-2.356144	1.980818	-5.665156
H	-2.425386	3.100087	-4.270409
C	-4.514141	1.226697	-4.100761
H	-4.712926	1.046692	-5.178621
H	-5.112571	0.509050	-3.499879
H	-4.846455	2.255172	-3.843083
C	-0.110490	-4.233925	-2.355965
H	-0.075899	-4.875277	-3.260510
H	0.660323	-3.443479	-2.448522
H	0.144202	-4.868324	-1.482196
C	-2.578548	-4.683464	-2.074343
H	-3.571900	-4.212309	-1.915747
H	-2.612955	-5.286902	-3.006225
H	-2.375019	-5.361615	-1.218197
C	0.950195	3.356820	-2.203793
C	2.268733	4.099888	-2.242492
H	2.388786	4.754911	-1.364386
B	-0.285349	4.020610	-1.632731
O	-0.293944	5.142155	-0.788459
O	-1.586198	3.513701	-1.766467
C	-1.557421	5.154239	-0.104240
C	-2.492843	4.406124	-1.110566
C	-1.379945	4.374784	1.189895
H	-0.584406	4.835670	1.793032
H	-2.294163	4.352526	1.800065
H	-1.082978	3.336385	0.970360
C	-1.957768	6.584007	0.189330
H	-2.964022	6.628638	0.631621
H	-1.258435	7.035968	0.906277
H	-1.952808	7.201309	-0.717275
C	-3.083353	5.338859	-2.158380
H	-3.821499	6.029403	-1.725964
H	-2.302541	5.934902	-2.651102
H	-3.593601	4.748373	-2.930684
C	-3.592585	3.589884	-0.462176

H -3.185848 2.785914 0.165444
H -4.244349 4.220208 0.160415
H -4.218449 3.122759 -1.234786
Na 4.812813 -1.598540 -0.559030
H 2.378192 4.757915 -3.126305
H 0.756402 2.756744 -3.106827
H 3.153320 3.439892 -2.247305
O 3.269996 -1.535218 -2.338973
O 4.462984 -3.851258 -0.139921
C 3.331589 -1.837687 -3.695015
H 4.224856 -1.342709 -4.131518
H 3.437707 -2.934736 -3.829543
C 2.140874 -0.755433 -2.116445
H 1.398336 -1.363794 -1.560459
H 2.406722 0.124939 -1.494839
C 1.566206 -0.308565 -3.444181
H 0.457008 -0.275847 -3.436748
H 1.970403 0.689800 -3.717793
C 2.080413 -1.341700 -4.389528
H 1.342870 -2.168307 -4.491144
H 2.303970 -0.910676 -5.389597
C 4.359518 -4.310796 1.166997
H 5.370720 -4.357717 1.623829
H 3.737954 -3.604477 1.760094
C 3.434531 -4.455443 -0.847273
H 2.520877 -3.825134 -0.775981
H 3.719147 -4.550014 -1.916016
C 3.184194 -5.821468 -0.245062
H 3.755438 -6.595862 -0.803164
H 2.102864 -6.077389 -0.252750
C 3.718658 -5.687997 1.153889
H 2.900409 -5.749525 1.904065
H 4.474086 -6.477501 1.361525
O 6.087960 0.092711 -1.617945
C 6.822950 -0.115525 -2.779791
H 7.907324 -0.038268 -2.547845
H 6.619026 -1.140792 -3.155453
C 5.511386 1.351334 -1.711647
H 4.531839 1.355364 -1.190197
H 6.176877 2.097265 -1.223314
C 6.431062 0.912087 -3.829629
H 7.292318 1.578553 -4.056855
H 6.077345 0.427542 -4.765954
C 5.332100 1.688449 -3.172320
H 5.425564 2.780619 -3.357276
H 4.343246 1.325587 -3.526977
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Figure_S6_imid-3_modeR1_ed(CuHadd) / electronic energy: -3601.999343742906 a.u. / lowest freq: 12.74 cm-1
C -1.685432 -1.721243 -1.211437
H -2.363758 -1.403489 -0.407043
C -0.319000 -2.210852 -0.686159
H 0.039626 -3.105868 -1.222890
C -0.014168 -0.159121 -1.829565
C -2.242380 0.334507 -2.638014
C -2.400295 0.205144 -4.020267
C -2.997518 1.300222 -1.948561
C -3.285210 1.024180 -4.717310
H -1.800534 -0.538391 -4.545749
C -3.868555 2.130770 -2.655753
C -4.015376 1.993966 -4.034736
H -3.394085 0.908502 -5.797715
H -4.430224 2.883956 -2.100263
H -4.702774 2.648947 -4.574854
C 1.896092 -0.953087 -0.574300
C 2.760723 -2.057145 -0.619165
C 2.335467 0.239411 0.025214
C 4.049439 -1.967079 -0.078238
C 3.627337 0.331132 0.565782
C 4.479593 -0.776028 0.514315
H 5.464175 -0.722849 0.963455
S -2.892544 1.506102 -0.162057
O -3.350970 0.201533 0.417201
O -3.875410 2.574713 0.167070
O -1.483900 1.818420 0.128503
Cu 0.822218 1.093016 -3.106652
C -2.380486 -2.727458 -2.093648
C -3.641138 -3.231831 -1.729072
C -1.788921 -3.166998 -3.292431
C -4.298183 -4.152885 -2.549445
H -4.117867 -2.912816 -0.811846
C -2.450859 -4.086694 -4.110820
H -0.819686 -2.791051 -3.595843
C -3.704778 -4.578659 -3.740127
H -5.268943 -4.535400 -2.262473
H -1.991868 -4.417072 -5.033588
H -4.216224 -5.290366 -4.375118
C -0.346013 -2.501291 0.794620
C -0.168744 -3.817065 1.257116

C	-0.577936	-1.474353	1.728821
C	-0.236124	-4.100811	2.623907
H	0.009326	-4.626850	0.560690
C	-0.646714	-1.764950	3.093824
H	-0.716904	-0.453154	1.400052
C	-0.474013	-3.075869	3.541510
H	-0.107113	-5.117589	2.971439
H	-0.855680	-0.978258	3.804711
H	-0.532375	-3.298617	4.598900
N	-1.308067	-0.505038	-1.967302
N	0.558408	-1.071480	-1.025405
H	1.654007	1.075230	0.120428
H	2.431203	-2.989010	-1.061255
C	4.051833	1.549126	1.289144
C	4.973606	2.459948	0.693618
C	3.575337	1.784043	2.610756
C	5.358395	3.604714	1.415562
C	3.958487	2.966167	3.270610
C	4.834859	3.865268	2.675922
H	6.071043	4.306388	1.003659
H	3.601323	3.184011	4.268411
H	5.132636	4.759331	3.208566
C	4.942968	-3.139020	-0.086381
C	4.979016	-4.008460	1.039439
C	5.806665	-3.365217	-1.193643
C	5.887094	-5.083164	1.036394
C	6.685602	-4.462991	-1.154640
C	6.724216	-5.308601	-0.051165
H	5.954730	-5.752896	1.883414
H	7.357499	-4.662821	-1.978951
H	7.414231	-6.142540	-0.035796
C	5.825254	-2.441432	-2.411878
H	5.079522	-1.627059	-2.309585
C	5.448373	-3.200686	-3.689800
H	4.463077	-3.697250	-3.558472
H	5.368615	-2.492840	-4.542439
H	6.208339	-3.969433	-3.943042
C	7.186844	-1.751589	-2.558819
H	7.444348	-1.218621	-1.618651
H	7.988375	-2.485273	-2.787199
H	7.148287	-1.004708	-3.380457
C	4.081434	-3.795674	2.260047
H	3.372709	-2.957999	2.097129
C	4.914015	-3.418611	3.490338
H	4.244851	-3.182937	4.345519
H	5.589939	-4.248273	3.787108
H	5.524810	-2.516462	3.271582
C	3.210916	-5.027286	2.539064
H	2.507943	-4.811846	3.371432
H	2.615722	-5.283257	1.636522
H	3.826117	-5.904993	2.826857
C	2.717679	0.764474	3.364109
H	2.535772	-0.143002	2.753484
C	5.598649	2.210057	-0.679375
H	5.073423	1.386018	-1.203875
C	5.493494	3.439110	-1.597769
H	4.473998	3.872527	-1.559225
H	6.218658	4.227793	-1.306559
H	5.708990	3.144947	-2.647226
C	7.061574	1.777380	-0.530554
H	7.668672	2.582313	-0.063919
H	7.130264	0.868403	0.103021
H	7.491670	1.538172	-1.526677
C	1.337862	1.338486	3.698424
H	1.414042	2.290514	4.263446
H	0.775628	1.513887	2.758568
H	0.763145	0.620081	4.317014
C	3.431753	0.269896	4.628755
H	4.440711	-0.116073	4.368284
H	3.537287	1.082469	5.377881
H	2.855073	-0.560045	5.090795
C	2.039018	2.617164	-2.462092
C	1.886706	2.592485	-3.860652
H	2.670503	2.194504	-4.512497
B	1.333912	3.609038	-1.524446
O	1.922148	4.064002	-0.367873
O	0.125770	4.209321	-1.779365
C	0.998250	4.951334	0.297483
C	-0.035763	5.298248	-0.842274
C	0.389023	4.182877	1.454276
H	1.199788	3.843480	2.112530
H	-0.281603	4.816545	2.051561
H	-0.175579	3.309764	1.105685
C	1.779505	6.139791	0.822124
H	1.110151	6.877660	1.288032
H	2.491531	5.804684	1.589265
H	2.353417	6.643473	0.034972
C	0.318247	6.571915	-1.593514

H 0.196381 7.467004 -0.967648
H 1.354408 6.547648 -1.959405
H -0.340812 6.676157 -2.466060
C -1.477642 5.326767 -0.382606
H -1.791103 4.352380 0.009916
H -1.629230 6.091102 0.394064
H -2.136849 5.574468 -1.226969
Na -5.320806 0.694272 1.429657
H 1.193301 3.284158 -4.354299
H 2.924211 2.104671 -2.068456
H 0.525843 0.364271 -4.493917
O -6.631401 -0.342599 -0.268460
O -4.513517 1.745794 3.380312
C -4.420791 3.125430 3.503216
H -4.981673 3.610273 2.676445
H -4.879437 3.437285 4.467625
C -3.322540 1.219265 3.861974
H -3.443184 0.960578 4.937121
H -3.072165 0.294793 3.303196
C -2.221370 2.244419 3.685310
H -1.602662 1.993024 2.799057
H -1.574419 2.296478 4.588062
C -2.960348 3.532386 3.461173
H -2.731052 4.273174 4.258082
H -2.704088 3.965089 2.469963
C -7.141678 -1.621132 -0.096393
H -7.957741 -1.600031 0.656380
H -6.336599 -2.292766 0.272378
C -6.159243 -0.282825 -1.572863
H -6.267035 0.752928 -1.957006
H -5.083804 -0.561150 -1.587015
C -6.955156 -1.248136 -2.430815
H -7.689762 -0.699580 -3.060626
H -6.280927 -1.847283 -3.081400
C -7.663113 -2.116904 -1.429372
H -8.763118 -1.964654 -1.494170
H -7.424328 -3.192482 -1.578205
O -5.205856 -1.353000 2.651990
C -4.204421 -2.305499 2.522765
H -3.677091 -2.172676 1.556913
H -3.470237 -2.179796 3.348359
C -6.176880 -1.920156 3.464191
H -5.958765 -1.671488 4.526810
H -7.171611 -1.501851 3.201724
C -4.836045 -3.680290 2.594547
H -4.985252 -4.092253 1.572019
H -4.207536 -4.377618 3.190562
C -6.161751 -3.423888 3.257714
H -6.239473 -3.958928 4.229360
H -6.996201 -3.735152 2.591202
178
Figure_S6_imid-3_modeR1_ts(CuHadd)_01 / electronic energy: -3601.981935926706 a.u. / lowest freq: -707.75 cm-1
C 0.957383 -2.098930 1.838215
H 1.795639 -1.966931 1.137686
C -0.379061 -2.397840 1.122489
H -0.971626 -3.173417 1.637625
C -0.482378 -0.236417 2.084400
C 1.623328 -0.072809 3.264688
C 1.426003 -0.034859 4.647421
C 2.717957 0.613460 2.708621
C 2.298920 0.667540 5.474517
H 0.563784 -0.559879 5.062717
C 3.588965 1.316084 3.542333
C 3.383601 1.343377 4.920026
H 2.127707 0.687171 6.552895
H 4.422424 1.852892 3.086018
H 4.071252 1.900854 5.559881
C -2.254070 -0.768260 0.523877
C -3.274545 -1.715418 0.346258
C -2.351671 0.476209 -0.124088
C -4.373069 -1.425362 -0.472562
C -3.441619 0.758999 -0.959944
C -4.449614 -0.194676 -1.131229
H -5.275986 0.005364 -1.802533
S 3.001710 0.668584 0.935037
O 3.339839 -0.737096 0.533592
O 4.200786 1.534111 0.738012
O 1.754750 1.174959 0.340299
Cu -1.202993 1.307368 2.928331
C 1.323681 -3.130470 2.875469
C 2.539750 -3.828588 2.776002
C 0.471837 -3.393298 3.964731
C 2.890692 -4.778480 3.739393
H 3.219763 -3.634992 1.957404
C 0.827722 -4.342869 4.926732
H -0.464363 -2.859404 4.070671
C 2.035191 -5.036286 4.813302
H 3.828121 -5.312827 3.654473

H	0.167660	-4.539950	5.761496
H	2.309334	-5.771115	5.559122
C	-0.171791	-2.813181	-0.313705
C	-0.452865	-4.131726	-0.712186
C	0.332163	-1.905014	-1.263368
C	-0.224188	-4.535341	-2.030429
H	-0.836734	-4.852295	-0.000980
C	0.557693	-2.314546	-2.580497
H	0.554076	-0.884236	-0.981625
C	0.277771	-3.627050	-2.964456
H	-0.436588	-5.553917	-2.328099
H	0.966614	-1.621290	-3.301141
H	0.457163	-3.942556	-3.983919
N	0.688668	-0.786115	2.462970
N	-1.083236	-1.104576	1.248859
H	-1.546477	1.193908	-0.036527
H	-3.210754	-2.681503	0.831275
C	-3.470651	2.003535	-1.757098
C	-4.339554	3.073310	-1.392237
C	-2.682359	2.099286	-2.940652
C	-4.377883	4.222693	-2.202776
C	-2.732448	3.286491	-3.694448
C	-3.566685	4.334199	-3.325120
H	-5.043511	5.043020	-1.971126
H	-2.143567	3.395854	-4.595443
H	-3.603679	5.231613	-3.929294
C	-5.434470	-2.427851	-0.678419
C	-5.394624	-3.278598	-1.818478
C	-6.526254	-2.501072	0.230827
C	-6.456136	-4.177450	-2.030649
C	-7.553076	-3.430616	-0.015716
C	-7.517107	-4.255022	-1.134986
H	-6.468696	-4.824404	-2.897715
H	-8.398150	-3.511888	0.655184
H	-8.322323	-4.956168	-1.313413
C	-6.630686	-1.586599	1.451838
H	-5.756321	-0.908293	1.521715
C	-6.641125	-2.398357	2.752785
H	-5.743765	-3.052073	2.798227
H	-6.615779	-1.714026	3.627681
H	-7.551109	-3.029937	2.828436
C	-7.862251	-0.677823	1.356230
H	-7.839720	-0.109038	0.402131
H	-8.802803	-1.266132	1.402045
H	-7.862459	0.051913	2.194015
C	-4.247757	-3.230391	-2.829478
H	-3.447586	-2.537918	-2.496328
C	-4.736895	-2.704596	-4.183329
H	-3.879608	-2.595006	-4.881623
H	-5.478284	-3.395372	-4.637758
H	-5.207246	-1.706287	-4.053954
C	-3.574833	-4.600333	-2.981474
H	-2.683258	-4.512246	-3.637984
H	-3.243366	-4.972151	-1.988459
H	-4.262392	-5.344878	-3.433796
C	-1.841147	0.930865	-3.463175
H	-1.914272	0.047670	-2.797276
C	-5.269200	2.991617	-0.180956
H	-4.978002	2.144918	0.474761
C	-5.196935	4.253342	0.694987
H	-4.143742	4.557343	0.856375
H	-5.738508	5.103916	0.230246
H	-5.659681	4.052411	1.684887
C	-6.712804	2.737772	-0.629567
H	-7.089807	3.580566	-1.247581
H	-6.772311	1.805552	-1.228386
H	-7.372696	2.621561	0.256719
C	-0.352739	1.293996	-3.527808
H	-0.180383	2.216820	-4.118930
H	0.043841	1.437903	-2.502121
H	0.223895	0.474877	-4.002806
C	-2.351401	0.458539	-4.830513
H	-3.437143	0.230037	-4.772024
H	-2.186413	1.230318	-5.611490
H	-1.820386	-0.468917	-5.135031
C	-2.172262	3.090333	2.587607
C	-2.011049	2.801748	3.994160
H	-2.909319	2.662943	4.604891
B	-1.163861	3.839373	1.749253
O	-1.450345	4.419240	0.519850
O	0.148162	4.099242	2.137521
C	-0.230013	4.940782	-0.028681
C	0.683912	5.088243	1.241274
C	0.298616	3.925741	-1.024089
H	-0.477864	3.738485	-1.777330
H	1.188748	4.302118	-1.547533
H	0.558829	2.974626	-0.541736
C	-0.537504	6.245464	-0.736934

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 H   0.383658   6.724403  -1.101123
 H  -1.181681   6.055235  -1.607063
 H  -1.061079   6.955994  -0.085228
 C   0.525376   6.442069   1.917957
 H   0.954488   7.257773   1.318608
 H  -0.532891   6.674045   2.105049
 H   1.040878   6.428550   2.888165
 C   2.146541   4.781513   0.993752
 H   2.287736   3.746557   0.659182
 H   2.570604   5.458528   0.236824
 H   2.723813   4.915932   1.920054
Na   5.344813  -0.315751  -0.495994
 H  -1.232052   3.348133   4.540919
 H  -3.149194   2.845935   2.157024
 H  -1.471659   1.305030   4.508570
 O   7.566037  -0.286965  -1.134526
 O   4.644674   0.487472  -2.620766
 C   5.394798   1.577851  -3.053820
 H   6.130560   1.844254  -2.266741
 H   5.952889   1.301236  -3.974381
 C   3.309871   0.785874  -2.861250
 H   3.016518   0.380414  -3.855025
 H   2.669057   0.315221  -2.089019
 C   3.146306   2.285333  -2.839693
 H   2.973918   2.629369  -1.797234
 H   2.319847   2.624837  -3.499857
 C   4.480169   2.762475  -3.319677
 H   4.441088   2.981039  -4.409839
 H   4.808207   3.669813  -2.766637
 C   7.947497  -1.022254  -2.252501
 H   7.072064  -1.136981  -2.926419
 H   8.277754  -2.034430  -1.932592
 C   8.567367   0.639293  -0.885326
 H   8.126475   1.559692  -0.447092
 H   9.291426   0.209873  -0.157731
 C   9.260788   0.955745  -2.189370
 H   8.751974   1.806965  -2.693667
 H  10.336059   1.192879  -2.036075
 C   9.070477  -0.302048  -2.981929
 H   8.793293  -0.074523  -4.034722
 H   9.998186  -0.915702  -2.964099
 O   5.322683  -2.569564  -1.315534
 C   4.130791  -2.889944  -1.958466
 H   3.439601  -2.024464  -1.919941
 H   4.348661  -3.117162  -3.024456
 C   5.605511  -3.577614  -0.400248
 H   6.659239  -3.907321  -0.521717
 H   5.480005  -3.173392   0.627355
 C   3.498399  -4.093795  -1.293455
 H   2.750451  -3.764670  -0.539299
 H   3.018575  -4.772473  -2.031539
 C   4.660524  -4.740250  -0.616064
 H   5.127175  -5.489827  -1.293115
 H   4.367980  -5.223847   0.341101
178
Figure_S6_imid-3_modeR1_ts(CuHadd)_02 / electronic energy: -3601.984095306953 a.u. / lowest freq: -688.94 cm-1
 C  -1.642819  -1.727056  -1.257804
 H  -2.314308  -1.420387  -0.442231
 C  -0.267495  -2.213585  -0.752316
 H   0.091921  -3.101111  -1.301069
 C   0.006684  -0.135007  -1.856079
 C  -2.224793   0.313879  -2.690072
 C  -2.309140   0.227080  -4.082361
 C  -3.056884   1.215745  -2.006245
 C  -3.208201   1.017107  -4.794155
 H  -1.642954  -0.464854  -4.600814
 C  -3.945603   2.016183  -2.726752
 C  -4.027584   1.914783  -4.113645
 H  -3.260474   0.935022  -5.881782
 H  -4.566666   2.724713  -2.176074
 H  -4.729928   2.545661  -4.663043
 C   1.938445  -0.937856  -0.636140
 C   2.800064  -2.045375  -0.669276
 C   2.383942   0.261679  -0.052538
 C   4.085670  -1.957932  -0.121594
 C   3.664412   0.342227   0.515060
 C   4.511862  -0.769201   0.477429
 H   5.488042  -0.722384   0.945180
 S  -2.999532   1.406014  -0.217366
 O  -3.456384   0.094548   0.346727
 O  -4.000111   2.464001   0.092038
 O  -1.602888   1.729278   0.111294
Cu   0.737827   1.313439  -2.857935
 C  -2.346201  -2.729563  -2.137669
 C  -3.603223  -3.236407  -1.763168
 C  -1.768518  -3.158942  -3.346852
 C  -4.269894  -4.150051  -2.584155
 H  -4.069536  -2.925385  -0.837532
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C	-2.439880	-4.071710	-4.165297
H	-0.802650	-2.780790	-3.658016
C	-3.689872	-4.566172	-3.784820
H	-5.237480	-4.534866	-2.289758
H	-1.991371	-4.394578	-5.095850
H	-4.208665	-5.272386	-4.419990
C	-0.285345	-2.519125	0.725650
C	-0.105887	-3.838767	1.175480
C	-0.517128	-1.501294	1.669711
C	-0.171424	-4.134956	2.539903
H	0.071244	-4.641793	0.471069
C	-0.583659	-1.803736	3.031956
H	-0.658532	-0.477931	1.349757
C	-0.409212	-3.118569	3.467337
H	-0.040880	-5.154714	2.878016
H	-0.791741	-1.022614	3.749637
H	-0.465741	-3.351009	4.522734
N	-1.281651	-0.506037	-2.009829
N	0.598546	-1.062275	-1.080679
H	1.714304	1.108347	0.021094
H	2.470703	-2.978563	-1.108615
C	4.075715	1.546444	1.266402
C	4.958210	2.497398	0.676425
C	3.643895	1.715252	2.613453
C	5.363118	3.609587	1.437724
C	4.045950	2.866708	3.315085
C	4.891217	3.801766	2.730574
H	6.054108	4.336979	1.034319
H	3.727862	3.032362	4.335869
H	5.204762	4.670805	3.294664
C	4.980150	-3.129757	-0.133423
C	5.026156	-3.997913	0.993117
C	5.829160	-3.362312	-1.251005
C	5.927220	-5.078491	0.979416
C	6.701331	-4.465791	-1.222121
C	6.748777	-5.310440	-0.118425
H	6.000502	-5.748683	1.825626
H	7.360485	-4.671519	-2.055224
H	7.433132	-6.149143	-0.111257
C	5.837844	-2.441051	-2.471350
H	5.104811	-1.616813	-2.357564
C	5.428779	-3.198795	-3.740184
H	4.438864	-3.680825	-3.590589
H	5.344730	-2.492665	-4.593831
H	6.173402	-3.979241	-4.003155
C	7.204975	-1.768217	-2.644882
H	7.486894	-1.237014	-1.710745
H	7.993132	-2.511697	-2.887539
H	7.160055	-1.022105	-3.466899
C	4.144372	-3.780860	2.224050
H	3.443730	-2.934226	2.072803
C	4.994515	-3.420712	3.447426
H	4.337307	-3.178857	4.310012
H	5.660844	-4.261228	3.735076
H	5.617011	-2.527463	3.225650
C	3.263971	-5.004647	2.505890
H	2.570406	-4.785383	3.345187
H	2.658916	-5.251410	1.607404
H	3.873025	-5.889597	2.784610
C	2.814092	0.657469	3.346309
H	2.603838	-0.215709	2.696055
C	5.526790	2.312860	-0.730901
H	4.937037	1.555520	-1.288308
C	5.460584	3.602896	-1.565984
H	4.471888	4.091351	-1.456621
H	6.244222	4.327404	-1.259738
H	5.617048	3.364940	-2.639876
C	6.969263	1.799840	-0.659659
H	7.627729	2.540128	-0.156738
H	7.011895	0.846462	-0.093685
H	7.358441	1.611247	-1.683109
C	1.448419	1.209597	3.770682
H	1.546942	2.143533	4.361661
H	0.830598	1.410263	2.871173
H	0.912372	0.465902	4.394983
C	3.580804	0.098360	4.551790
H	4.580375	-0.265044	4.230538
H	3.712920	0.869596	5.339469
H	3.027103	-0.759604	4.990077
C	1.932796	2.987483	-2.740432
C	1.409817	2.763268	-4.068242
H	2.115764	2.566824	-4.882039
B	1.287456	3.839161	-1.671501
O	1.970824	4.300424	-0.552491
O	-0.019617	4.316274	-1.695575
C	1.020517	4.925236	0.323215
C	-0.149644	5.299455	-0.651659
C	0.616598	3.894450	1.361382

H 1.522383 3.542344 1.871230
H -0.055701 4.315641 2.122345
H 0.113908 3.036083 0.898723
C 1.686444 6.108579 0.996129
H 0.971264 6.663616 1.621272
H 2.497186 5.757838 1.650213
H 2.123050 6.805426 0.269803
C 0.042611 6.665088 -1.295654
H -0.094786 7.485269 -0.576350
H 1.043975 6.761705 -1.739213
H -0.693226 6.795645 -2.101130
C -1.529093 5.185354 -0.037060
H -1.741916 4.157397 0.278049
H -1.630695 5.856251 0.829753
H -2.296485 5.473243 -0.770611
Na -5.359607 0.668155 1.452085
H 0.576049 3.394572 -4.401983
H 2.953389 2.628401 -2.566908
H 0.626177 1.333403 -4.457175
O -6.700344 -0.399463 -0.216595
O -4.425648 1.758702 3.341889
C -4.290906 3.142006 3.417850
H -4.504159 3.581708 2.421306
H -5.033495 3.546025 4.138863
C -3.219264 1.185357 3.727746
H -3.322126 0.785356 4.760074
H -2.967909 0.346403 3.047963
C -2.128937 2.229754 3.681027
H -1.630253 2.212426 2.689406
H -1.377811 2.079579 4.486340
C -2.883904 3.506686 3.852922
H -2.880404 3.810856 4.923099
H -2.456566 4.321536 3.228458
C -7.131509 -1.700519 -0.000973
H -7.914903 -1.709331 0.786010
H -6.275473 -2.320316 0.343946
C -6.281309 -0.344644 -1.539319
H -6.433285 0.681469 -1.935130
H -5.199826 -0.593022 -1.594467
C -7.081604 -1.348224 -2.346965
H -7.881943 -0.835467 -2.924691
H -6.422918 -1.913836 -3.042063
C -7.680283 -2.249130 -1.302659
H -8.790076 -2.174972 -1.316767
H -7.373975 -3.307510 -1.450801
O -5.193908 -1.345005 2.716043
C -4.192851 -2.296738 2.575571
H -3.719422 -2.205703 1.576987
H -3.415931 -2.128388 3.353006
C -6.120408 -1.883071 3.596924
H -5.852479 -1.590325 4.636645
H -7.129587 -1.480897 3.366316
C -4.807493 -3.671186 2.742915
H -4.997578 -4.134720 1.749623
H -4.146407 -4.332944 3.344300
C -6.105287 -3.393467 3.450901
H -6.139559 -3.889423 4.445528
H -6.965168 -3.734011 2.832789
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Figure_S6_imid-3_modeR1_ts(CuHadd)_03 / electronic energy: -3601.979987684155 a.u. / lowest freq: -758.54 cm-1
C -1.452449 -2.295883 -0.260875
H -2.245401 -1.710836 0.226757
C -0.087411 -2.159190 0.446448
H 0.453285 -3.119295 0.506697
C -0.026191 -0.947510 -1.593590
C -2.138458 -1.603410 -2.627726
C -2.077793 -2.602020 -3.603820
C -3.135572 -0.619984 -2.724391
C -2.995775 -2.639106 -4.648870
H -1.280112 -3.344687 -3.550308
C -4.048115 -0.652221 -3.779875
C -3.988664 -1.665208 -4.734441
H -2.926394 -3.425738 -5.403007
H -4.800366 0.136892 -3.838033
H -4.711077 -1.683828 -5.553289
C 1.977989 -0.887138 -0.238854
C 2.950375 -1.891079 -0.138157
C 2.330976 0.443492 0.022449
C 4.258111 -1.572884 0.242812
C 3.641401 0.767215 0.412290
C 4.600889 -0.246693 0.522761
H 5.605581 -0.008940 0.851898
S -3.147734 0.781423 -1.608052
O -3.156033 0.224196 -0.220294
O -4.420633 1.508446 -1.871239
O -1.918642 1.518524 -1.968496
Cu 0.330390 0.335365 -2.985813
C -1.895121 -3.729965 -0.418158

C	-3.110259	-4.157280	0.145317
C	-1.100366	-4.660835	-1.112928
C	-3.526913	-5.484078	0.005649
H	-3.736829	-3.466158	0.693395
C	-1.522739	-5.985784	-1.253128
H	-0.156892	-4.358411	-1.550205
C	-2.735718	-6.396862	-0.695529
H	-4.464989	-5.804079	0.440570
H	-0.908747	-6.694272	-1.793843
H	-3.061293	-7.423235	-0.804517
C	-0.200627	-1.577217	1.833280
C	0.150126	-2.347080	2.955511
C	-0.625754	-0.248897	2.021683
C	0.079085	-1.797804	4.238849
H	0.477891	-3.371999	2.838837
C	-0.703584	0.293018	3.305918
H	-0.885393	0.368945	1.173207
C	-0.348140	-0.479589	4.413962
H	0.353677	-2.395529	5.098222
H	-1.031907	1.315420	3.441142
H	-0.404670	-0.056747	5.408467
N	-1.191652	-1.632902	-1.561628
N	0.625885	-1.238058	-0.454615
H	1.570252	1.205815	-0.011988
H	2.683709	-2.924126	-0.325724
C	4.009890	2.154166	0.777901
C	4.782896	2.946272	-0.121727
C	3.726412	2.640462	2.088658
C	5.238698	4.207505	0.301463
C	4.229096	3.899905	2.467283
C	4.958783	4.677708	1.577478
H	5.842485	4.825648	-0.349170
H	4.078839	4.283917	3.466059
H	5.334547	5.643756	1.889510
C	5.253319	-2.646140	0.419305
C	5.312753	-3.359245	1.649581
C	6.131887	-2.984765	-0.647022
C	6.240166	-4.409047	1.780287
C	7.041578	-4.042675	-0.465942
C	7.091760	-4.744965	0.733380
H	6.307403	-4.976189	2.699335
H	7.718094	-4.332045	-1.259313
H	7.797788	-5.556794	0.852849
C	6.111084	-2.244358	-1.984461
H	5.369077	-1.420137	-1.975036
C	5.693543	-3.180669	-3.124452
H	4.707605	-3.639192	-2.895509
H	5.597643	-2.607616	-4.071451
H	6.439602	-3.988975	-3.276390
C	7.466409	-1.588618	-2.277409
H	7.769149	-0.944830	-1.424478
H	8.255822	-2.350078	-2.449460
H	7.391440	-0.951276	-3.184334
C	4.402451	-3.020952	2.831948
H	3.746590	-2.156695	2.601736
C	5.219846	-2.608254	4.062305
H	4.541260	-2.247608	4.864875
H	5.811023	-3.459772	4.459807
H	5.913096	-1.781483	3.797541
C	3.466561	-4.190415	3.158171
H	2.765281	-3.901010	3.969768
H	2.868451	-4.457493	2.260489
H	4.036855	-5.083465	3.489737
C	3.002694	1.784691	3.131376
H	2.442652	0.963233	2.641087
C	5.191824	2.443830	-1.506264
H	4.647175	1.512004	-1.760218
C	4.849606	3.454812	-2.611667
H	3.808892	3.817793	-2.498573
H	5.531464	4.330520	-2.588718
H	4.943862	2.971106	-3.607369
C	6.686141	2.103574	-1.534553
H	7.304808	3.010455	-1.364900
H	6.923897	1.359771	-0.745792
H	6.958821	1.665550	-2.518387
C	1.955682	2.578517	3.929558
H	2.428891	3.304084	4.622511
H	1.275939	3.124283	3.244257
H	1.347823	1.885531	4.546667
C	4.017150	1.130141	4.073682
H	4.741956	0.524192	3.489667
H	4.575365	1.899534	4.648825
H	3.497287	0.454492	4.786361
C	1.544774	1.996563	-3.183165
C	0.967943	1.584869	-4.444979
H	1.630978	1.205062	-5.231000
B	0.966845	3.091822	-2.320202
O	1.495641	3.493527	-1.093714

O -0.128883 3.876764 -2.664701
C 0.515126 4.315414 -0.452353
C -0.276196 4.900307 -1.671861
C -0.348401 3.417857 0.424696
H 0.295446 2.866559 1.121513
H -1.061112 4.002418 1.024477
H -0.905732 2.683887 -0.173566
C 1.222262 5.348906 0.401358
H 0.508929 6.068690 0.830321
H 1.736264 4.855289 1.237335
H 1.976502 5.907029 -0.167818
C 0.364261 6.168033 -2.218070
H 0.234490 7.023757 -1.539509
H 1.440773 6.025651 -2.389384
H -0.097479 6.425787 -3.181285
C -1.755007 5.107050 -1.415738
H -2.248072 4.137732 -1.274165
H -1.931401 5.743524 -0.535216
H -2.229739 5.594242 -2.279108
Na -5.374681 0.714677 0.411850
H 0.183019 2.227953 -4.862299
H 2.524438 1.576635 -2.927501
H 0.072489 0.219061 -4.570326
O -6.361541 -1.298631 -0.130782
O -5.011139 -0.054855 2.611591
C -4.537940 0.812284 3.586877
H -3.675895 1.386766 3.181442
H -5.338415 1.527801 3.867393
C -4.342056 -1.255510 2.802143
H -4.971183 -2.098800 2.449570
H -3.399720 -1.248259 2.215656
C -4.034233 -1.405913 4.276945
H -3.026138 -1.847160 4.433291
H -4.802180 -2.043694 4.767678
C -4.113125 0.002148 4.797804
H -4.874349 0.076244 5.605468
H -3.129811 0.349358 5.182144
C -7.379196 -1.963655 0.538278
H -8.361168 -1.578747 0.184049
H -7.300327 -1.777357 1.629873
C -5.988422 -2.084131 -1.217197
H -6.275874 -1.571772 -2.159966
H -4.886216 -2.209541 -1.204165
C -6.660148 -3.443577 -1.127467
H -7.460250 -3.526927 -1.896033
H -5.933102 -4.274445 -1.253896
C -7.260902 -3.439551 0.242587
H -8.249099 -3.947920 0.267332
H -6.564485 -3.917331 0.967104
O -5.354948 2.907962 1.181839
C -4.172887 3.586605 0.926225
H -3.348868 2.857457 0.783020
H -4.291096 4.184649 -0.003837
C -6.131218 3.757415 1.956461
H -6.763045 4.387652 1.291591
H -6.799458 3.159500 2.611535
C -3.876101 4.493318 2.103368
H -3.136080 4.015743 2.783136
H -3.489200 5.478015 1.761237
C -5.208219 4.628105 2.789204
H -5.556335 5.684122 2.795652
H -5.148318 4.247168 3.832633

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Figure_S6_imid-3_modeR1_prod(CuHadd) / electronic energy: -3602.032592781751 a.u. / lowest freq: 12.28 cm-1

C -1.562886 -1.810718 -1.429492
H -2.264271 -1.637490 -0.600388
C -0.168850 -2.262258 -0.942918
H 0.240485 -3.088612 -1.547707
C -0.020822 -0.045842 -1.769776
C -2.248885 0.394170 -2.568926
C -2.456598 0.400370 -3.950229
C -2.988618 1.273212 -1.759326
C -3.378389 1.270505 -4.527634
H -1.866345 -0.274530 -4.573609
C -3.891468 2.160331 -2.345418
C -4.092114 2.156799 -3.724468
H -3.524379 1.264762 -5.609894
H -4.434722 2.849791 -1.697279
H -4.804533 2.853846 -4.170820
C 1.986893 -0.906030 -0.724436
C 2.864101 -2.004103 -0.759394
C 2.430159 0.303946 -0.162290
C 4.160128 -1.892770 -0.239858
C 3.719816 0.405630 0.373790
C 4.586102 -0.688856 0.326641
H 5.580494 -0.611237 0.751579
S -2.812034 1.285901 0.029400
O -3.143007 -0.107455 0.469234

O	-3.858711	2.227993	0.513334
O	-1.420812	1.675680	0.310623
Cu	0.360271	1.782155	-2.272931
C	-2.182373	-2.744863	-2.436236
C	-3.414330	-3.362333	-2.157274
C	-1.550419	-3.002618	-3.666393
C	-4.005390	-4.214532	-3.094072
H	-3.919220	-3.184704	-1.216338
C	-2.145423	-3.855789	-4.600218
H	-0.602168	-2.536533	-3.903922
C	-3.372368	-4.460278	-4.314914
H	-4.955460	-4.683642	-2.873554
H	-1.655899	-4.046812	-5.546362
H	-3.832199	-5.119697	-5.039518
C	-0.181328	-2.673378	0.510224
C	-0.071563	-4.030567	0.858142
C	-0.302819	-1.713420	1.533772
C	-0.080651	-4.418567	2.201012
H	0.016223	-4.789706	0.091013
C	-0.291752	-2.105205	2.874751
H	-0.395038	-0.662319	1.295534
C	-0.182733	-3.456602	3.208387
H	0.001258	-5.465875	2.461137
H	-0.382632	-1.362723	3.655932
H	-0.182639	-3.758923	4.247445
N	-1.269329	-0.484592	-2.017936
N	0.644795	-1.042791	-1.166446
H	1.758253	1.150736	-0.095223
H	2.544080	-2.947528	-1.182223
C	4.137120	1.639370	1.060821
C	4.830708	2.653718	0.345726
C	3.822395	1.819154	2.436698
C	5.156404	3.849327	1.011831
C	4.157106	3.038567	3.053683
C	4.812792	4.040664	2.346111
H	5.679904	4.644055	0.497048
H	3.910256	3.219496	4.091394
H	5.063811	4.971364	2.838468
C	5.069646	-3.052356	-0.248574
C	5.126480	-3.914701	0.881722
C	5.937862	-3.264100	-1.355162
C	6.062106	-4.965475	0.885637
C	6.848763	-4.335155	-1.306841
C	6.908292	-5.173142	-0.198449
H	6.145965	-5.628548	1.736441
H	7.528983	-4.519991	-2.127783
H	7.621488	-5.987196	-0.176613
C	5.928133	-2.350998	-2.581653
H	5.141764	-1.573732	-2.496786
C	5.604878	-3.136651	-3.858709
H	4.647449	-3.686387	-3.733196
H	5.493428	-2.438482	-4.715767
H	6.408388	-3.862894	-4.102470
C	7.256666	-1.597479	-2.715800
H	7.463307	-1.026637	-1.784926
H	8.098757	-2.296188	-2.904852
H	7.201350	-0.875242	-3.558264
C	4.223241	-3.717508	2.100596
H	3.491622	-2.901212	1.930757
C	5.044948	-3.308203	3.327799
H	4.369658	-3.087106	4.181948
H	5.745264	-4.115605	3.629329
H	5.628860	-2.390030	3.102607
C	3.387319	-4.970722	2.388913
H	2.670973	-4.765735	3.212616
H	2.807965	-5.256043	1.484881
H	4.026032	-5.825909	2.692908
C	3.130778	0.731231	3.261210
H	3.003680	-0.200558	2.673315
C	5.244198	2.478886	-1.115942
H	4.912512	1.497473	-1.511921
C	4.589872	3.537270	-2.010446
H	3.488082	3.490040	-1.898548
H	4.936676	4.559612	-1.752223
H	4.836336	3.340991	-3.075781
C	6.770310	2.499052	-1.261981
H	7.188397	3.490943	-0.989332
H	7.223347	1.723913	-0.607216
H	7.055026	2.273091	-2.311956
C	1.722300	1.167296	3.675653
H	1.745106	2.110479	4.260952
H	1.095798	1.314606	2.770671
H	1.246636	0.379657	4.296764
C	3.971069	0.334836	4.481960
H	4.998453	0.058147	4.161949
H	4.031963	1.162821	5.218809
H	3.517451	-0.546277	4.984454
C	0.529944	3.596620	-3.047910

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C  -0.514030   3.765660  -4.141656
H  -0.473588   4.752997  -4.645224
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O   1.332905   4.763318  -0.880763
O  -0.936173   4.630285  -1.194589
C   0.736062   5.065910   0.389390
C  -0.738750   5.413271  -0.007753
C   0.828814   3.812761   1.243648
H   1.880215   3.505864   1.295062
H   0.471655   3.980568   2.270588
H   0.246437   2.990010   0.809278
C   1.506677   6.199364   1.035036
H   1.029012   6.520334   1.972835
H   2.526808   5.869174   1.277446
H   1.590228   7.071380   0.374246
C  -0.906831   6.876524  -0.395395
H  -0.835205   7.547975   0.472717
H  -0.149993   7.185051  -1.130801
H  -1.895821   7.021105  -0.852322
C  -1.770433   5.017604   1.029098
H  -1.772809   3.934894   1.198426
H  -1.587376   5.535504   1.983445
H  -2.777870   5.295409   0.686857
Na -5.091636   0.296706   1.635765
H  -1.537073   3.676603  -3.740823
H   1.560605   3.705174  -3.426643
H  -0.441121   3.015205  -4.948842
O  -6.395422  -0.714939  -0.110802
O  -4.172575   1.158099   3.667830
C  -4.092639   2.529353   3.894469
H  -4.316951   3.066024   2.948923
H  -4.852436   2.825336   4.649001
C  -2.919516   0.605634   3.911732
H  -2.952383   0.047616   4.872784
H  -2.658675  -0.105704   3.102779
C  -1.887127   1.707257   3.987279
H  -1.428302   1.870420   2.988385
H  -1.097930   1.483335   4.736874
C  -2.702605   2.895191   4.376702
H  -2.700483   3.012464   5.483135
H  -2.328177   3.825965   3.897989
C  -6.807999  -2.036389  -0.012212
H  -7.580170  -2.128732   0.780502
H  -5.940664  -2.674381   0.262324
C  -6.007157  -0.527374  -1.430194
H  -6.179377   0.529926  -1.721106
H  -4.924488  -0.756088  -1.530837
C  -6.815026  -1.457017  -2.314145
H  -7.640950  -0.902098  -2.811303
H  -6.169548  -1.934528  -3.083655
C  -7.367291  -2.471692  -1.352242
H  -8.478837  -2.431207  -1.340661
H  -7.032731  -3.500684  -1.608687
O  -4.900211  -1.854748   2.640757
C  -3.870135  -2.753948   2.401217
H  -3.455777  -2.592749   1.384914
H  -3.062228  -2.589395   3.146159
C  -5.761081  -2.478882   3.530977
H  -5.448259  -2.242305   4.572604
H  -6.793821  -2.100332   3.378012
C  -4.416174  -4.161805   2.529753
H  -4.614518  -4.596010   1.524871
H  -3.706547  -4.813716   3.084980
C  -5.702435  -3.974793   3.286979
H  -5.695612  -4.535653   4.247018
H  -6.567119  -4.301021   2.667792
178
Figure_S6_imid-3_modeR2_ed(CuHadd) / electronic energy: -3602.007795207243 a.u. / lowest freq: 16.29 cm-1
C  -1.131466  -2.058778   1.976183
H  -2.188360  -1.757381   2.019514
C  -0.161881  -0.894153   2.253578
H   0.781793  -1.237976   2.716700
C  -0.123635  -1.382750  -0.044617
C  -1.335865  -3.466723  -0.171709
C  -0.427815  -4.393128  -0.693291
C  -2.709668  -3.634600  -0.418508
C  -0.866747  -5.478178  -1.445084
H   0.638187  -4.236271  -0.514338
C  -3.142185  -4.737169  -1.160559
C  -2.230656  -5.657063  -1.671981
H  -0.137297  -6.183741  -1.849952
H  -4.211544  -4.839986  -1.354411
H  -2.587391  -6.507620  -2.256966
C   0.981729   0.641055   0.601058
C   0.437885   1.900819   0.333217
C   2.371926   0.475725   0.622076
C   1.274117   2.997761   0.101916
C   3.217210   1.581752   0.434329
```

C	2.661760	2.845138	0.185983
H	3.307147	3.703126	0.040936
S	-3.960758	-2.465500	0.132185
O	-5.107439	-2.655933	-0.803457
O	-3.356825	-1.112658	-0.044508
O	-4.264956	-2.818627	1.532767
Cu	0.395561	-1.120877	-1.927548
C	-0.910137	-3.242492	2.881634
C	-1.904878	-3.633953	3.794625
C	0.292177	-3.967840	2.831392
C	-1.701685	-4.735549	4.631596
H	-2.834658	-3.084420	3.865318
C	0.492492	-5.068767	3.668044
H	1.068803	-3.678259	2.140975
C	-0.504754	-5.453505	4.567280
H	-2.472106	-5.031475	5.331807
H	1.420992	-5.622817	3.619106
H	-0.349259	-6.305908	5.215806
C	-0.769465	0.194355	3.101284
C	-0.178386	0.552205	4.325784
C	-1.927498	0.871807	2.679623
C	-0.746907	1.554836	5.117573
H	0.719857	0.055067	4.670681
C	-2.494299	1.870444	3.474116
H	-2.387433	0.625577	1.734811
C	-1.907642	2.208106	4.695561
H	-0.287789	1.824642	6.059746
H	-3.383338	2.388185	3.138436
H	-2.345553	2.984517	5.309288
N	-0.805630	-2.371405	0.560838
N	0.124981	-0.443774	0.883179
H	2.791393	-0.500733	0.824095
H	-0.633421	2.028208	0.311721
C	4.684784	1.428329	0.548566
C	5.268948	1.128290	1.815025
C	5.519124	1.596222	-0.597258
C	6.661924	0.950080	1.895353
C	6.911471	1.455226	-0.448373
C	7.470561	1.119273	0.778475
H	7.134115	0.698221	2.835677
H	7.575153	1.590272	-1.291937
H	8.542399	0.995975	0.866126
C	0.693470	4.302953	-0.266166
C	0.450873	4.606480	-1.635816
C	0.362722	5.248476	0.743266
C	-0.131993	5.843843	-1.964195
C	-0.195152	6.482366	0.360725
C	-0.446446	6.769806	-0.976203
H	-0.342836	6.099790	-2.994133
H	-0.445635	7.229852	1.101710
H	-0.887191	7.719983	-1.249332
C	0.596465	4.968326	2.226883
H	0.974910	3.937693	2.385338
C	-0.710462	5.064886	3.023356
H	-1.482945	4.413799	2.562480
H	-0.542175	4.727320	4.067971
H	-1.092785	6.106482	3.053739
C	1.661385	5.910157	2.799424
H	2.603690	5.812878	2.218579
H	1.324102	6.967646	2.763543
H	1.876873	5.643361	3.856215
C	0.793114	3.628292	-2.759993
H	1.280926	2.715290	-2.363141
C	1.795375	4.242406	-3.744654
H	2.143542	3.469806	-4.463272
H	1.339748	5.075957	-4.319273
H	2.678814	4.628286	-3.193349
C	-0.473972	3.157178	-3.482550
H	-0.218581	2.375553	-4.229269
H	-1.180900	2.715519	-2.750470
H	-0.978095	3.996882	-4.005536
C	4.960418	1.926964	-1.983748
H	3.852709	1.928723	-1.980378
C	4.441062	1.028096	3.099248
H	3.376998	1.273693	2.914337
C	4.466947	-0.397589	3.663577
H	4.092867	-1.115920	2.904105
H	5.494745	-0.693322	3.961957
H	3.806251	-0.466137	4.554208
C	4.910288	2.045025	4.148367
H	5.930876	1.809446	4.515958
H	4.909891	3.067224	3.712631
H	4.217931	2.039901	5.017477
C	5.362476	0.874797	-3.024883
H	6.457257	0.875550	-3.207101
H	5.056310	-0.131472	-2.681263
H	4.848441	1.078666	-3.988582
C	5.403404	3.325505	-2.430254

H 5.073437 4.085011 -1.690385
H 6.507497 3.382994 -2.533883
H 4.947117 3.574884 -3.411672
C 1.531764 -2.587511 -2.824199
C 1.431232 -1.414130 -3.599730
H 0.792572 -1.361746 -4.484899
B 2.727071 -2.940341 -1.933320
O 2.922731 -4.199119 -1.392664
O 3.768285 -2.085547 -1.635195
C 4.097134 -4.131241 -0.547863
C 4.854822 -2.901085 -1.140104
C 3.623525 -3.892954 0.874551
H 2.966750 -4.718240 1.180032
H 4.460154 -3.851945 1.585327
H 3.059533 -2.952531 0.953756
C 4.846878 -5.441994 -0.642650
H 5.794608 -5.392740 -0.087011
H 4.248618 -6.253668 -0.207057
H 5.070173 -5.711304 -1.681902
C 5.720075 -3.274229 -2.334250
H 6.606329 -3.848663 -2.031547
H 5.158038 -3.871142 -3.066229
H 6.066947 -2.363677 -2.839563
C 5.660244 -2.114803 -0.131497
H 5.025322 -1.669362 0.641892
H 6.404380 -2.757182 0.360509
H 6.204587 -1.305092 -0.632117
Na -5.082319 -0.318036 -1.503679
H 2.249162 -0.683345 -3.594101
H 0.816803 -3.392700 -3.044195
H -0.289323 0.246180 -2.348210
O -6.355283 0.360926 0.401382
O -4.377928 1.961395 -1.685590
C -6.038301 0.058590 1.724351
H -6.509539 -0.906030 2.009982
H -4.937628 -0.046210 1.817599
C -7.071505 1.551153 0.397428
H -6.775282 2.169959 -0.474870
H -8.156519 1.321060 0.313898
C -6.796389 2.290575 1.685095
H -7.666250 2.903608 2.006199
H -5.895212 2.933254 1.570192
C -6.514133 1.174045 2.637168
H -5.743049 1.457114 3.386100
H -7.449814 0.869970 3.156811
C -3.472679 2.101473 -0.640089
H -2.543788 1.547563 -0.889473
H -3.914281 1.656772 0.273301
C -4.454014 3.183228 -2.336596
H -3.744062 3.188003 -3.193032
H -5.482219 3.336154 -2.727267
C -3.182113 3.572912 -0.398554
H -2.124176 3.801530 -0.640872
H -3.393690 3.866367 0.653078
C -4.094810 4.274397 -1.355330
H -5.008448 4.623710 -0.825192
H -3.592319 5.130386 -1.856645
O -3.857474 -0.815433 -3.426990
C -3.189503 0.172720 -4.138747
H -2.567109 0.769970 -3.439075
H -3.930403 0.848483 -4.616273
C -3.058782 -1.947193 -3.498479
H -2.301105 -1.920486 -2.683755
H -3.683589 -2.857397 -3.382719
C -2.314322 -0.484746 -5.193796
H -1.273516 -0.098825 -5.133489
H -2.718478 -0.308024 -6.214718
C -2.371423 -1.946010 -4.844006
H -2.990398 -2.495133 -5.587545
H -1.361838 -2.405052 -4.784227
178
Figure_S6_imid-3_modeR2_ts(CuHadd)_01 / electronic energy: -3601.993251007392 a.u. / lowest freq: -754.10 cm-1
C -1.160310 -1.969639 2.048599
H -2.222633 -1.684454 2.055714
C -0.218101 -0.779443 2.316594
H 0.720059 -1.092759 2.811349
C -0.109284 -1.334252 0.035975
C -1.264857 -3.444657 -0.069719
C -0.308279 -4.334554 -0.569117
C -2.624064 -3.666210 -0.347528
C -0.689158 -5.445165 -1.315098
H 0.748148 -4.131019 -0.382453
C -2.998694 -4.793584 -1.085394
C -2.040426 -5.682645 -1.564863
H 0.078423 -6.120989 -1.699952
H -4.058493 -4.939713 -1.303255
H -2.350776 -6.553615 -2.146366
C 0.957091 0.716033 0.653948

C	0.419385	1.970011	0.355097
C	2.346197	0.543597	0.678365
C	1.260210	3.054683	0.090212
C	3.197637	1.639242	0.460709
C	2.647879	2.898587	0.177860
H	3.296747	3.748650	0.005719
S	-3.919837	-2.524257	0.149246
O	-5.036327	-2.757220	-0.812671
O	-3.345602	-1.157796	-0.037451
O	-4.251840	-2.856791	1.548025
Cu	0.543377	-1.331529	-1.757289
C	-0.942838	-3.121781	2.995559
C	-1.961712	-3.514594	3.881190
C	0.279731	-3.815050	3.013776
C	-1.764108	-4.588675	4.754424
H	-2.906405	-2.987193	3.903240
C	0.474110	-4.888635	3.886585
H	1.079373	-3.520172	2.352461
C	-0.548265	-5.276883	4.755411
H	-2.553630	-4.886121	5.432362
H	1.418125	-5.418091	3.890015
H	-0.397138	-6.107975	5.432025
C	-0.864052	0.321394	3.119148
C	-0.303476	0.729280	4.342420
C	-2.026096	0.963082	2.654582
C	-0.904390	1.746965	5.089901
H	0.596754	0.260403	4.720134
C	-2.625511	1.976727	3.405092
H	-2.463643	0.677793	1.710303
C	-2.067648	2.365559	4.624799
H	-0.468080	2.055764	6.030941
H	-3.517622	2.466222	3.036689
H	-2.530255	3.154062	5.204012
N	-0.792271	-2.318216	0.654711
N	0.093656	-0.360117	0.942148
H	2.759342	-0.431061	0.901594
H	-0.651407	2.101436	0.327292
C	4.665082	1.476673	0.572256
C	5.252082	1.197384	1.842312
C	5.496487	1.610038	-0.580546
C	6.643469	1.006106	1.920497
C	6.887967	1.458398	-0.434248
C	7.448931	1.143140	0.797076
H	7.117303	0.769783	2.864023
H	7.549464	1.569166	-1.283037
H	8.519862	1.010997	0.882982
C	0.680459	4.343245	-0.331684
C	0.439017	4.588153	-1.713224
C	0.327100	5.320330	0.638941
C	-0.160822	5.802707	-2.092295
C	-0.251199	6.527964	0.206543
C	-0.497198	6.760345	-1.142172
H	-0.370760	6.014751	-3.132332
H	-0.523874	7.296400	0.917757
H	-0.953275	7.691201	-1.453924
C	0.548945	5.097382	2.134046
H	0.965945	4.088648	2.331504
C	-0.774298	5.166735	2.905585
H	-1.510792	4.468393	2.454956
H	-0.611453	4.871513	3.963931
H	-1.199370	6.192099	2.891787
C	1.566770	6.097822	2.693195
H	2.519996	6.023737	2.126980
H	1.187518	7.139277	2.624804
H	1.778594	5.868866	3.759564
C	0.797182	3.568879	-2.796040
H	1.301482	2.682071	-2.362101
C	1.785924	4.158439	-3.808966
H	2.152323	3.360730	-4.490170
H	1.311539	4.952926	-4.422422
H	2.659865	4.590351	-3.277024
C	-0.461670	3.042502	-3.494203
H	-0.190468	2.252458	-4.226799
H	-1.145376	2.595623	-2.743554
H	-0.997234	3.854137	-4.030066
C	4.935920	1.913781	-1.972289
H	3.828214	1.911903	-1.967071
C	4.429835	1.135257	3.132515
H	3.367467	1.387761	2.947112
C	4.444066	-0.277195	3.729681
H	4.057770	-1.008981	2.989465
H	5.470416	-0.576958	4.029031
H	3.788147	-0.317982	4.625525
C	4.915301	2.170940	4.155649
H	5.935132	1.932789	4.523706
H	4.923827	3.182775	3.696480
H	4.227400	2.193349	5.028005
C	5.340739	0.844554	-2.995188

H 6.431754 0.863735 -3.198121
H 5.064302 -0.159506 -2.621904
H 4.805194 1.014700 -3.953744
C 5.376013 3.304746 -2.444495
H 5.040556 4.078019 -1.721761
H 6.480488 3.363758 -2.543701
H 4.923796 3.532757 -3.432921
C 1.628939 -2.613988 -2.957579
C 1.445692 -1.311452 -3.557960
H 0.902325 -1.235859 -4.504062
B 2.768596 -2.986952 -2.043711
O 2.970114 -4.267671 -1.522117
O 3.784293 -2.122966 -1.636148
C 4.037611 -4.172382 -0.558635
C 4.831975 -2.931740 -1.072349
C 3.407976 -3.918033 0.801117
H 2.720971 -4.740785 1.043598
H 4.156645 -3.858269 1.603439
H 2.833735 -2.979083 0.794682
C 4.817759 -5.468668 -0.549225
H 5.695977 -5.394430 0.108818
H 4.189390 -6.288184 -0.173841
H 5.161364 -5.745114 -1.553586
C 5.798781 -3.292924 -2.190935
H 6.658274 -3.867478 -1.817749
H 5.302565 -3.885939 -2.972178
H 6.184338 -2.377024 -2.658040
C 5.549515 -2.150738 0.006592
H 4.851405 -1.721073 0.733506
H 6.261279 -2.790328 0.548528
H 6.119866 -1.326604 -0.439704
Na -5.024320 -0.426188 -1.546442
H 2.302104 -0.625284 -3.538551
H 0.908073 -3.393084 -3.239233
H 0.406766 -0.205497 -2.889765
O -6.384399 0.290315 0.251782
O -4.304361 1.853325 -1.807771
C -6.117044 0.021799 1.592764
H -6.598945 -0.935664 1.884444
H -5.020721 -0.080685 1.729286
C -7.109578 1.473374 0.191665
H -6.787150 2.071455 -0.685758
H -8.189162 1.231707 0.076455
C -6.885317 2.248345 1.468364
H -7.771306 2.860641 1.743466
H -5.986978 2.897315 1.367711
C -6.625358 1.160027 2.459010
H -5.877601 1.468638 3.221523
H -7.574076 0.865149 2.959937
C -3.476599 2.042196 -0.706653
H -2.528567 1.487711 -0.865505
H -3.980962 1.628330 0.188625
C -4.434170 3.074482 -2.452969
H -3.709922 3.120526 -3.295996
H -5.461691 3.175015 -2.862015
C -3.214166 3.523381 -0.498782
H -2.164032 3.769048 -0.759835
H -3.420290 3.836523 0.548171
C -4.149854 4.179825 -1.462908
H -5.088406 4.474840 -0.943256
H -3.688119 5.064960 -1.952568
O -3.736938 -0.945134 -3.439723
C -3.053571 0.034329 -4.147006
H -2.391184 0.593903 -3.451381
H -3.779801 0.745664 -4.594102
C -2.943998 -2.082045 -3.497924
H -2.203939 -2.059573 -2.667587
H -3.576828 -2.988205 -3.392609
C -2.230286 -0.636487 -5.231872
H -1.200559 -0.219471 -5.259031
H -2.710571 -0.506973 -6.226682
C -2.228030 -2.087139 -4.831335
H -2.798311 -2.692219 -5.570277
H -1.197942 -2.491186 -4.733338
178
Figure_S6_imid-3_modeR2_ts(CuHadd)_02 / electronic energy: -3601.990420691354 a.u. / lowest freq: -764.45 cm-1
C -1.485438 -1.721140 1.957307
H -2.477122 -1.243747 1.958728
C -0.343622 -0.737644 2.279209
H 0.517600 -1.241571 2.756312
C -0.310553 -1.210943 -0.019898
C -1.813761 -3.087333 -0.205285
C -1.021431 -4.114778 -0.727675
C -3.189170 -3.064408 -0.486836
C -1.585750 -5.128024 -1.494965
H 0.053922 -4.096080 -0.540666
C -3.750552 -4.098486 -1.242804
C -2.958711 -5.129177 -1.740534

H	-0.944778	-5.915808	-1.898109
H	-4.819174	-4.056141	-1.461130
H	-3.414163	-5.924782	-2.334509
C	1.088195	0.598003	0.681079
C	0.779587	1.930628	0.398126
C	2.426186	0.190042	0.732252
C	1.800391	2.860324	0.178342
C	3.458081	1.127876	0.563505
C	3.138409	2.468144	0.298699
H	3.927038	3.198609	0.165150
S	-4.270793	-1.714374	0.006007
O	-5.381336	-1.738875	-0.990661
O	-3.455344	-0.471656	-0.140458
O	-4.693937	-2.002060	1.389887
Cu	0.360035	-1.259696	-1.805263
C	-1.505083	-2.924803	2.864116
C	-2.597750	-3.150271	3.719656
C	-0.433909	-3.834996	2.873125
C	-2.621582	-4.270963	4.555503
H	-3.428507	-2.457229	3.747142
C	-0.461012	-4.954642	3.708487
H	0.419489	-3.674080	2.232920
C	-1.555365	-5.173757	4.548280
H	-3.466659	-4.438438	5.210649
H	0.367281	-5.651360	3.705215
H	-1.575677	-6.040721	5.195831
C	-0.781960	0.424061	3.133321
C	-0.164371	0.665230	4.373184
C	-1.805662	1.286298	2.702513
C	-0.577282	1.737137	5.170658
H	0.634421	0.024239	4.725358
C	-2.221262	2.351052	3.504793
H	-2.279877	1.130291	1.745771
C	-1.609361	2.574836	4.740119
H	-0.098348	1.916842	6.124400
H	-3.013081	3.006302	3.165102
H	-1.928236	3.403170	5.359327
N	-1.160130	-2.083250	0.557231
N	0.047489	-0.320651	0.924514
H	2.660253	-0.845298	0.940707
H	-0.252823	2.243334	0.349305
C	4.872479	0.714672	0.715329
C	5.354023	0.294580	1.991511
C	5.758661	0.740347	-0.404014
C	6.686139	-0.142491	2.105285
C	7.095199	0.339294	-0.220124
C	7.544763	-0.112762	1.014043
H	7.075178	-0.490906	3.052838
H	7.797826	0.359562	-1.042436
H	8.571642	-0.435739	1.127859
C	1.462204	4.237787	-0.225456
C	1.334189	4.556182	-1.607467
C	1.232939	5.235803	0.761132
C	0.974489	5.866491	-1.971353
C	0.891207	6.535644	0.344616
C	0.758846	6.842515	-1.005098
H	0.859526	6.139443	-3.012038
H	0.718624	7.320973	1.068579
H	0.486548	7.846292	-1.305060
C	1.343078	4.940842	2.256276
H	1.575555	3.871641	2.438321
C	0.015185	5.213014	2.972908
H	-0.803912	4.651520	2.475877
H	0.080083	4.878254	4.029900
H	-0.236405	6.294137	2.965636
C	2.486469	5.740641	2.890840
H	3.439280	5.522475	2.362363
H	2.289869	6.832487	2.842570
H	2.607384	5.450935	3.956620
C	1.564327	3.519122	-2.708073
H	1.870202	2.542434	-2.282238
C	2.703428	3.946832	-3.640909
H	2.962716	3.114821	-4.330240
H	2.417848	4.830940	-4.248794
H	3.605363	4.199527	-3.044580
C	0.276321	3.253233	-3.496286
H	0.443591	2.443913	-4.238966
H	-0.526310	2.924382	-2.804961
H	-0.064494	4.162396	-4.034715
C	5.315974	1.186864	-1.799774
H	4.227487	1.388974	-1.829866
C	4.486858	0.335698	3.252981
H	3.493820	0.780394	3.046505
C	4.229556	-1.076589	3.792851
H	3.756121	-1.705590	3.009895
H	5.174391	-1.560604	4.118293
H	3.537796	-1.031550	4.661098
C	5.109549	1.232575	4.331456

H 6.056761 0.804187 4.720668
H 5.313987 2.241861 3.914029
H 4.404470 1.347115 5.182621
C 5.555580 0.094415 -2.849364
H 6.638136 -0.091033 -3.008982
H 5.074033 -0.848027 -2.527926
H 5.106587 0.395687 -3.820062
C 6.021750 2.486815 -2.204600
H 5.803591 3.286330 -1.465585
H 7.121519 2.345127 -2.263573
H 5.660510 2.823547 -3.199288
C 1.223436 -2.681969 -3.029667
C 1.273661 -1.352754 -3.596074
H 0.755136 -1.158288 -4.539300
B 2.273443 -3.264256 -2.118408
O 2.253065 -4.576377 -1.636105
O 3.412477 -2.593297 -1.673067
C 3.303925 -4.685348 -0.656065
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H 4.732246 -6.178127 -0.008568
H 3.103117 -6.807413 -0.323998
H 4.166105 -6.395097 -1.682703
C 5.202061 -4.072479 -2.254378
H 5.956483 -4.787176 -1.896322
H 4.619721 -4.557737 -3.050227
H 5.733263 -3.220631 -2.698946
C 5.135006 -2.968346 -0.025124
H 4.519848 -2.433881 0.706819
H 5.714442 -3.736752 0.507161
H 5.850474 -2.251589 -0.447165
Na -4.973747 0.576217 -1.643577
H 2.236397 -0.827725 -3.556279
H 0.383834 -3.320157 -3.335900
H 0.448214 -0.091444 -2.896474
O -6.332007 1.226827 0.256266
O -3.902239 2.674395 -1.800014
C -7.567346 0.608025 0.404402
H -8.287389 1.028813 -0.329069
H -7.456635 -0.479801 0.206587
C -5.810207 1.452225 1.528228
H -4.844959 0.917959 1.641799
H -5.621053 2.540868 1.647696
C -6.793239 0.983051 2.583634
H -6.899937 1.720954 3.408460
H -6.472497 0.000450 2.995623
C -8.064184 0.826219 1.814566
H -8.668549 -0.032632 2.179306
H -8.660878 1.763892 1.867122
C -2.966562 2.708998 -0.773041
H -2.130360 2.021920 -1.020532
H -3.450732 2.356045 0.157421
C -3.809697 3.875788 -2.486713
H -3.119877 3.752479 -3.350754
H -4.810541 4.167349 -2.869584
C -2.464023 4.129145 -0.575135
H -1.386648 4.195914 -0.829708
H -2.619869 4.477936 0.469372
C -3.275986 4.929945 -1.544845
H -4.118265 5.429710 -1.017234
H -2.658268 5.684775 -2.078944
O -3.659296 -0.151504 -3.468578
C -2.843119 0.698645 -4.201218
H -2.049689 1.107452 -3.538558
H -3.446546 1.543505 -4.594869
C -3.117437 -1.421472 -3.603932
H -2.357170 -1.585311 -2.808460
H -3.917545 -2.183791 -3.499348
C -2.223980 -0.084271 -5.344381
H -1.137728 0.134595 -5.429791
H -2.728515 0.159193 -6.305315
C -2.469985 -1.519920 -4.969001
H -3.169088 -1.994015 -5.692809
H -1.525876 -2.104327 -4.924594
178
Figure_S6_imid-3_modeR2_ts(CuHadd)_03 / electronic energy: -3601.992698054265 a.u. / lowest freq: -733.75 cm-1
C -1.526383 -1.747391 1.761724
H -2.470765 -1.191250 1.833693
C -0.296348 -0.889074 2.112272
H 0.522708 -1.494761 2.543385
C -0.348288 -1.217619 -0.213589
C -2.019890 -2.923760 -0.499015
C -1.304742 -3.915528 -1.183223
C -3.406309 -2.810032 -0.706023

C	-1.948939	-4.784994	-2.057168
H	-0.224899	-3.982493	-1.029884
C	-4.044933	-3.701178	-1.573093
C	-3.326062	-4.682449	-2.249115
H	-1.368985	-5.546541	-2.583740
H	-5.119854	-3.589911	-1.725987
H	-3.842514	-5.362306	-2.930218
C	1.154689	0.482389	0.553953
C	0.854839	1.791928	0.168663
C	2.486122	0.102760	0.751459
C	1.876842	2.736630	0.030195
C	3.516241	1.050203	0.634558
C	3.201078	2.376004	0.301512
H	3.987132	3.116995	0.221118
S	-4.423220	-1.549606	0.075712
O	-5.630523	-1.431790	-0.791982
O	-3.614077	-0.293957	0.027791
O	-4.707507	-2.037957	1.437367
Cu	0.410690	-1.209258	-1.961223
C	-1.618469	-2.997046	2.597273
C	-2.593696	-3.103126	3.604035
C	-0.714932	-4.056087	2.409693
C	-2.674448	-4.256056	4.391057
H	-3.285704	-2.290882	3.786989
C	-0.797685	-5.207563	3.196798
H	0.047037	-3.986955	1.650122
C	-1.778748	-5.308655	4.186018
H	-3.429275	-4.331591	5.163003
H	-0.100140	-6.020263	3.040474
H	-1.842070	-6.200130	4.796444
C	-0.616333	0.259592	3.034511
C	0.035700	0.372524	4.274864
C	-1.554441	1.241120	2.664183
C	-0.257880	1.436908	5.132446
H	0.770273	-0.361951	4.580393
C	-1.854321	2.295515	3.529696
H	-2.051027	1.189684	1.705149
C	-1.206187	2.393960	4.762943
H	0.248089	1.517804	6.085755
H	-2.584304	3.040609	3.240730
H	-1.434456	3.215299	5.429675
N	-1.275653	-2.039011	0.325107
N	0.107422	-0.432766	0.777769
H	2.712888	-0.918221	1.025951
H	-0.172333	2.076344	-0.010249
C	4.921454	0.659300	0.894516
C	5.313135	0.249303	2.204425
C	5.886897	0.688313	-0.158403
C	6.636506	-0.177932	2.415668
C	7.208166	0.293249	0.122768
C	7.570158	-0.151069	1.387975
H	6.959610	-0.516566	3.391147
H	7.968623	0.315291	-0.646318
H	8.588034	-0.467357	1.576829
C	1.563411	4.098662	-0.439272
C	1.493088	4.364850	-1.835894
C	1.311305	5.137188	0.498893
C	1.178650	5.667695	-2.263449
C	1.020635	6.428034	0.020217
C	0.952093	6.685953	-1.344378
H	1.105307	5.901313	-3.317344
H	0.833928	7.243417	0.706449
H	0.715398	7.683056	-1.692837
C	1.327384	4.891499	2.006829
H	1.520660	3.823848	2.237558
C	-0.033770	5.218097	2.633512
H	-0.835545	4.655633	2.109328
H	-0.039330	4.921765	3.703786
H	-0.259382	6.303238	2.572591
C	2.451193	5.686149	2.681231
H	3.427504	5.428064	2.217620
H	2.284926	6.779873	2.585337
H	2.502275	5.430476	3.761255
C	1.723321	3.276194	-2.884739
H	2.004556	2.313966	-2.411080
C	2.885589	3.637553	-3.817206
H	3.133528	2.771478	-4.467647
H	2.630983	4.501808	-4.465864
H	3.785431	3.891410	-3.218300
C	0.440469	3.002596	-3.678430
H	0.601661	2.163133	-4.387939
H	-0.377757	2.717478	-2.983430
H	0.125210	3.896359	-4.256803
C	5.547965	1.136782	-1.583401
H	4.465448	1.338128	-1.696428
C	4.359291	0.294060	3.401656
H	3.377466	0.722739	3.121014
C	4.083880	-1.114744	3.942175

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 H   3.675459  -1.761224   3.137209
 H   5.009720  -1.580800   4.340136
 H   3.333344  -1.068449   4.759846
 C   4.894257   1.212763   4.508296
 H   5.819301   0.803527   4.965572
 H   5.111718   2.220166   4.092908
 H   4.131437   1.326264   5.308334
 C   5.861733   0.047029  -2.615085
 H   6.950390  -0.158558  -2.678994
 H   5.333392  -0.885619  -2.343924
 H   5.506249   0.361353  -3.619844
 C   6.280839   2.437927  -1.933079
 H   6.016932   3.233165  -1.204436
 H   7.381832   2.293906  -1.921734
 H   5.985009   2.782794  -2.946399
 C   1.412721  -2.595019  -3.117200
 C   1.504824  -1.256525  -3.652416
 H   1.082296  -1.045478  -4.639447
 B   2.398688  -3.208180  -2.152967
 O   2.333901  -4.530580  -1.711117
 O   3.516273  -2.562407  -1.625191
 C   3.340197  -4.690195  -0.691324
 C   4.369737  -3.582238  -1.073121
 C   2.681485  -4.422920   0.651464
 H   1.868796  -5.146321   0.799963
 H   3.383224  -4.534016   1.489779
 H   2.257222  -3.407887   0.684998
 C   3.881896  -6.102420  -0.743218
 H   4.721134  -6.228027  -0.043289
 H   3.101179  -6.821273  -0.458757
 H   4.229596  -6.368086  -1.749013
 C   5.320124  -4.044415  -2.169236
 H   6.039279  -4.788710  -1.799293
 H   4.771544  -4.487733  -3.012122
 H   5.893729  -3.191701  -2.554218
 C   5.150904  -3.021266   0.094769
 H   4.500724  -2.531382   0.828015
 H   5.707984  -3.817146   0.610171
 H   5.882436  -2.281780  -0.254451
Na  -5.144585   0.887844  -1.285588
 H   2.450809  -0.720912  -3.501651
 H   0.613308  -3.232152  -3.518919
 H   0.591018  -0.021751  -3.016763
 O  -6.392588   1.499269   0.676647
 O  -4.203040   3.103390  -1.256627
 C  -7.555826   0.823920   1.033566
 H  -8.436249   1.342135   0.597348
 H  -7.517259  -0.205984   0.620645
 C  -5.667286   1.754816   1.836649
 H  -4.608360   1.461019   1.693612
 H  -5.702723   2.845461   2.049123
 C  -6.266219   0.984268   2.991883
 H  -6.217656   1.557872   3.942963
 H  -5.746322   0.007841   3.110176
 C  -7.672910   0.765980   2.542721
 H  -8.071206  -0.211661   2.891519
 H  -8.322128   1.592838   2.907396
 C  -3.038160   3.151757  -0.504336
 H  -2.424195   2.253488  -0.730989
 H  -3.289431   3.147490   0.575974
 C  -3.938791   3.788529  -2.434906
 H  -3.579110   3.072309  -3.205660
 H  -4.872055   4.263033  -2.805541
 C  -2.281660   4.416229  -0.854296
 H  -1.198264   4.209550  -0.954748
 H  -2.441917   5.196883  -0.078198
 C  -2.881411   4.841934  -2.163693
 H  -3.347390   5.847409  -2.068526
 H  -2.118428   4.859446  -2.972566
 O  -3.939934   0.281260  -3.248374
 C  -2.556947   0.120105  -3.235962
 H  -2.194834   0.047400  -2.189521
 H  -2.091345   1.013776  -3.703000
 C  -4.491131  -0.747588  -4.003497
 H  -4.970829  -1.481751  -3.323911
 H  -5.270417  -0.337113  -4.680104
 C  -2.173289  -1.120816  -4.017078
 H  -1.943512  -1.957066  -3.322894
 H  -1.306364  -0.935104  -4.684937
 C  -3.404262  -1.425886  -4.804304
 H  -3.334479  -0.967458  -5.815725
 H  -3.577587  -2.520684  -4.893235
178
Figure_S6_imid-3_modeR2_ts(CuHadd)_04 / electronic energy: -3601.992424038614 a.u. / lowest freq: -727.14 cm-1
 C  -0.882739  -1.759374   2.499506
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 C   0.478575  -1.047597   2.451920
 H   1.318083  -1.768140   2.456311
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C	-0.419880	-1.084167	0.290174
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C	-3.546934	-2.546674	0.748817
C	-2.733104	-4.467355	-1.121760
H	-0.727981	-3.778582	-0.710117
C	-4.485852	-3.362334	0.108733
C	-4.086731	-4.318240	-0.820910
H	-2.401789	-5.204763	-1.856941
H	-5.542751	-3.206324	0.332510
H	-4.835755	-4.939939	-1.316487
C	1.407179	0.426493	0.617608
C	1.172078	1.801648	0.555655
C	2.642297	-0.087460	0.209340
C	2.173921	2.670384	0.113861
C	3.664618	0.780405	-0.207037
C	3.430635	2.163671	-0.236319
H	4.215336	2.840737	-0.551680
S	-4.174100	-1.283513	1.865541
O	-5.577552	-1.045906	1.412191
O	-3.336787	-0.071807	1.621013
O	-4.064085	-1.838363	3.225696
Cu	-0.318431	-0.923022	-1.608974
C	-0.830641	-3.072693	3.235874
C	-1.460706	-3.207297	4.485293
C	-0.128731	-4.168457	2.705828
C	-1.407008	-4.421289	5.177047
H	-1.984522	-2.371099	4.930498
C	-0.077373	-5.380908	3.398325
H	0.374251	-4.080319	1.756314
C	-0.718494	-5.508297	4.632696
H	-1.896134	-4.517913	6.137670
H	0.461358	-6.220562	2.978522
H	-0.677464	-6.447102	5.169652
C	0.671869	-0.037228	3.552819
C	1.755829	-0.161517	4.439865
C	-0.208671	1.050804	3.698617
C	1.944921	0.775344	5.459907
H	2.455411	-0.982450	4.344118
C	-0.021363	1.978797	4.725813
H	-1.037626	1.181717	3.016689
C	1.054078	1.841123	5.606327
H	2.781693	0.673457	6.138724
H	-0.706530	2.809545	4.834547
H	1.200846	2.564277	6.398023
N	-1.157132	-1.924969	1.047480
N	0.405706	-0.424706	1.124592
H	2.814533	-1.154658	0.248129
H	0.214344	2.193975	0.862367
C	4.995059	0.240792	-0.567166
C	5.811170	-0.358003	0.438420
C	5.465396	0.315290	-1.913107
C	7.045998	-0.919142	0.065894
C	6.729306	-0.222727	-2.219734
C	7.498516	-0.846634	-1.245412
H	7.678738	-1.400721	0.799612
H	7.123500	-0.172532	-3.225901
H	8.459977	-1.269403	-1.507345
C	1.888432	4.110956	-0.021598
C	1.352564	4.611871	-1.241322
C	2.135172	4.994082	1.065262
C	1.081221	5.987816	-1.349439
C	1.864438	6.365056	0.900354
C	1.339291	6.851921	-0.291460
H	0.670196	6.400340	-2.261395
H	2.054535	7.066885	1.701539
H	1.129793	7.908768	-0.395869
C	2.680174	4.501537	2.404926
H	2.787372	3.397406	2.412758
C	1.719579	4.840240	3.551625
H	0.704218	4.452945	3.321182
H	2.071732	4.367450	4.492629
H	1.655356	5.935726	3.718436
C	4.078238	5.070855	2.670073
H	4.760026	4.803399	1.834370
H	4.049923	6.176326	2.771839
H	4.492917	4.640305	3.606616
C	1.059732	3.703267	-2.435777
H	1.330337	2.650489	-2.216478
C	1.893531	4.109912	-3.656074
H	1.782562	3.352757	-4.461665
H	1.573995	5.096367	-4.053100
H	2.966702	4.167670	-3.377217
C	-0.436267	3.693821	-2.767415
H	-0.642257	2.959491	-3.574831
H	-1.015382	3.395456	-1.869317
H	-0.784156	4.693157	-3.103185
C	4.653928	0.963279	-3.038379

H	3.649817	1.269437	-2.685493
C	5.413026	-0.377207	1.917224
H	4.463646	0.167650	2.087714
C	5.187491	-1.811381	2.411458
H	4.403094	-2.306816	1.801860
H	6.120955	-2.409453	2.350689
H	4.844019	-1.800305	3.467865
C	6.451388	0.346788	2.784666
H	7.418788	-0.197413	2.800913
H	6.620828	1.373831	2.395839
H	6.081237	0.429697	3.829141
C	4.397451	-0.013600	-4.192408
H	5.338010	-0.293282	-4.710838
H	3.912325	-0.930061	-3.807596
H	3.713475	0.448698	-4.936106
C	5.349869	2.230713	-3.549371
H	5.488121	2.952243	-2.716593
H	6.342760	1.995011	-3.987154
H	4.730818	2.717182	-4.332630
C	-0.019110	-2.232536	-3.177499
C	0.092045	-0.849259	-3.579084
H	-0.611267	-0.449959	-4.314846
B	1.148185	-3.064222	-2.706188
O	1.078913	-4.425718	-2.409302
O	2.448483	-2.586918	-2.549337
C	2.344764	-4.800678	-1.827405
C	3.310527	-3.733227	-2.431013
C	2.211801	-4.663049	-0.320166
H	1.405733	-5.321720	0.031057
H	3.131941	-4.948018	0.208761
H	1.959194	-3.627343	-0.045143
C	2.660846	-6.231203	-2.206171
H	3.663397	-6.519598	-1.857227
H	1.937768	-6.916272	-1.742612
H	2.616593	-6.384327	-3.291346
C	3.780980	-4.113329	-3.828151
H	4.489880	-4.952824	-3.806629
H	2.935300	-4.394308	-4.471503
H	4.290175	-3.260865	-4.295970
C	4.495822	-3.385454	-1.557680
H	4.187452	-2.962106	-0.595628
H	5.114221	-4.273117	-1.360512
H	5.130429	-2.646559	-2.062608
Na	-5.118332	1.061956	0.424460
H	1.104251	-0.459135	-3.742566
H	-0.994235	-2.717864	-3.317715
H	-0.304670	0.386604	-2.530184
O	-3.966764	3.073380	0.474655
O	-7.199004	1.244682	-0.622592
C	-2.714174	2.992541	1.075019
H	-2.831939	2.662999	2.129209
H	-2.112368	2.233109	0.534335
C	-4.231179	4.411877	0.222711
H	-4.789032	4.511395	-0.732141
H	-4.858565	4.820154	1.045528
C	-2.921350	5.160868	0.145193
H	-3.020716	6.206332	0.509656
H	-2.542980	5.158165	-0.900702
C	-2.023893	4.345669	1.021361
H	-1.001618	4.274849	0.594877
H	-1.971003	4.790936	2.039511
C	-7.414714	2.181629	-1.622250
H	-6.606526	2.942057	-1.602153
H	-8.387845	2.690583	-1.444012
C	-7.673744	0.022470	-1.089438
H	-6.933967	-0.769494	-0.850697
H	-8.627122	-0.223388	-0.573442
C	-7.431840	1.471077	-2.954722
H	-6.405990	1.436962	-3.379560
H	-8.123129	1.962192	-3.673567
C	-7.886040	0.090531	-2.593133
H	-8.963587	-0.039198	-2.837086
H	-7.287630	-0.681035	-3.125644
O	-4.132766	0.407621	-1.618400
C	-3.424213	1.378620	-2.311127
H	-2.392487	1.433407	-1.903920
H	-3.912458	2.366235	-2.174505
C	-3.948415	-0.776357	-2.316649
H	-3.028009	-1.282208	-1.950586
H	-4.815480	-1.449212	-2.150523
C	-3.398744	1.004490	-3.781180
H	-2.383025	1.143055	-4.207618
H	-4.124262	1.620238	-4.356383
C	-3.811027	-0.442447	-3.787456
H	-4.789624	-0.563023	-4.302320
H	-3.049346	-1.087344	-4.276294

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Figure_S6_imid-3_modeR2_prod(CuHadd) / electronic energy: -3602.034857394928 a.u. / lowest freq: 17.12 cm-1

C	-1.301429	-1.887956	2.190346
H	-2.364777	-1.610176	2.233284
C	-0.356206	-0.687109	2.417476
H	0.572806	-0.981899	2.938656
C	-0.245704	-1.318483	0.158495
C	-1.498759	-3.360420	0.073233
C	-0.582498	-4.231556	-0.528585
C	-2.872616	-3.565538	-0.127394
C	-1.015701	-5.321401	-1.275613
H	0.483209	-4.025525	-0.416428
C	-3.300018	-4.680100	-0.856366
C	-2.382001	-5.562810	-1.418978
H	-0.278031	-5.978024	-1.743229
H	-4.371910	-4.810646	-1.016325
H	-2.735016	-6.421541	-1.994018
C	0.920116	0.686398	0.726295
C	0.462626	1.967336	0.414474
C	2.297091	0.428833	0.755866
C	1.369628	2.996146	0.150196
C	3.217292	1.474396	0.563122
C	2.743845	2.763318	0.272929
H	3.439810	3.578763	0.125624
S	-4.115695	-2.360291	0.355016
O	-5.228802	-2.564863	-0.617120
O	-3.464687	-1.034798	0.136530
O	-4.476166	-2.638060	1.757718
Cu	0.556427	-1.598496	-1.560242
C	-1.038231	-3.033832	3.133623
C	-2.033891	-3.456407	4.031580
C	0.201214	-3.699709	3.126862
C	-1.795783	-4.527859	4.897849
H	-2.993011	-2.956183	4.066093
C	0.435063	-4.770603	3.993290
H	0.984746	-3.387271	2.451670
C	-0.563285	-5.185484	4.877648
H	-2.567456	-4.848014	5.585923
H	1.390959	-5.278106	3.979146
H	-0.381243	-6.014830	5.548776
C	-1.002359	0.452882	3.163428
C	-0.460505	0.898029	4.382402
C	-2.144137	1.094870	2.651237
C	-1.060421	1.951468	5.079330
H	0.424374	0.430343	4.796204
C	-2.743082	2.144147	3.351756
H	-2.567462	0.784675	1.709255
C	-2.204310	2.569413	4.567878
H	-0.638396	2.288486	6.017201
H	-3.620871	2.631772	2.947784
H	-2.666268	3.385457	5.108153
N	-0.973490	-2.254527	0.791433
N	-0.011442	-0.327160	1.031342
H	2.647853	-0.567336	0.987869
H	-0.597722	2.163422	0.376756
C	4.670715	1.232787	0.741447
C	5.171852	0.859745	2.026145
C	5.576531	1.382752	-0.354541
C	6.541885	0.573675	2.165561
C	6.946281	1.139553	-0.140543
C	7.415794	0.718767	1.096673
H	6.947760	0.260559	3.118360
H	7.662932	1.262908	-0.941314
H	8.470515	0.516263	1.232085
C	0.872240	4.303550	-0.314353
C	0.686840	4.528896	-1.707929
C	0.529914	5.314420	0.624752
C	0.156256	5.761197	-2.130601
C	0.018839	6.536255	0.149817
C	-0.169583	6.751828	-1.210981
H	-0.008823	5.961002	-3.181085
H	-0.246290	7.329109	0.836698
H	-0.573481	7.694970	-1.556001
C	0.688657	5.111245	2.130545
H	1.069538	4.095058	2.360106
C	-0.661145	5.230501	2.847715
H	-1.396401	4.538530	2.384910
H	-0.546772	4.957298	3.918255
H	-1.059939	6.265037	2.792550
C	1.712483	6.091942	2.713625
H	2.683091	5.985056	2.183342
H	1.364449	7.142167	2.619263
H	1.879555	5.871712	3.789737
C	1.031295	3.470223	-2.758085
H	1.484651	2.572254	-2.291903
C	2.073105	3.993362	-3.754037
H	2.427777	3.163725	-4.402725
H	1.649551	4.789112	-4.402068
H	2.947139	4.404140	-3.206145
C	-0.228284	2.981440	-3.482051

H	0.035801	2.199856	-4.225368
H	-0.931711	2.533896	-2.749560
H	-0.739053	3.812300	-4.012386
C	5.125457	1.813225	-1.752883
H	4.020610	1.842253	-1.822471
C	4.285587	0.805430	3.274470
H	3.255027	1.144920	3.054144
C	4.171599	-0.626990	3.811198
H	3.782387	-1.303301	3.021728
H	5.157056	-1.007073	4.153665
H	3.463972	-0.656978	4.667228
C	4.792615	1.761340	4.363079
H	5.772651	1.434224	4.768929
H	4.897282	2.787065	3.948808
H	4.065111	1.800262	5.202126
C	5.580511	0.823958	-2.834894
H	6.678153	0.866109	-2.994125
H	5.305027	-0.207264	-2.549736
H	5.082345	1.062064	-3.799117
C	5.637765	3.222606	-2.076597
H	5.278363	3.949124	-1.318927
H	6.747980	3.249743	-2.093354
H	5.265419	3.544850	-3.071964
C	1.642965	-1.930876	-3.165004
C	2.069765	-0.644661	-3.852855
H	2.722821	-0.805750	-4.733020
B	2.668380	-2.638034	-2.296944
O	2.643239	-3.989397	-1.908112
O	3.775729	-2.002180	-1.725471
C	3.635220	-4.164848	-0.878464
C	4.639380	-3.009207	-1.187534
C	2.955704	-3.975107	0.469425
H	2.176672	-4.737728	0.605974
H	3.656869	-4.073058	1.309999
H	2.479841	-2.983145	0.527029
C	4.217244	-5.558501	-0.981149
H	5.045654	-5.694328	-0.270194
H	3.450220	-6.309756	-0.746030
H	4.591350	-5.770029	-1.990226
C	5.642463	-3.395479	-2.266683
H	6.378707	-4.125797	-1.901873
H	5.137583	-3.825682	-3.143184
H	6.190294	-2.503749	-2.598931
C	5.362497	-2.453823	0.021405
H	4.666983	-2.011324	0.743717
H	5.941253	-3.235707	0.534408
H	6.065804	-1.670020	-0.288524
Na	-4.803944	-0.413957	-1.716370
H	2.644712	0.000682	-3.170987
H	1.060466	-2.613251	-3.807562
H	1.231491	-0.025171	-4.210608
O	-6.472275	0.513274	-0.260683
O	-4.081105	1.893888	-1.971273
C	-6.436959	0.388853	1.126137
H	-7.070838	-0.469300	1.437344
H	-5.394829	0.186925	1.447818
C	-7.199932	1.657074	-0.556163
H	-6.802210	2.131758	-1.476764
H	-8.262633	1.378897	-0.732902
C	-7.097460	2.606204	0.613300
H	-8.008045	3.235529	0.715498
H	-6.198247	3.251385	0.502309
C	-6.923855	1.675673	1.772836
H	-6.186386	2.074164	2.503644
H	-7.899439	1.505862	2.279818
C	-3.397554	2.127802	-0.783130
H	-2.479319	1.505660	-0.765666
H	-4.042601	1.821746	0.065078
C	-4.134173	3.087591	-2.678194
H	-3.356973	3.075880	-3.472804
H	-5.128517	3.193562	-3.161054
C	-3.060224	3.601821	-0.655401
H	-1.982079	3.769796	-0.857391
H	-3.317332	3.999674	0.350658
C	-3.884834	4.236318	-1.727847
H	-4.848704	4.597315	-1.305844
H	-3.346869	5.073998	-2.223223
O	-3.009010	-1.098264	-3.124145
C	-2.143773	-0.261358	-3.814115
H	-1.226763	-0.094703	-3.205367
H	-2.632570	0.718007	-3.993764
C	-2.650951	-2.391582	-3.477536
H	-1.864415	-2.756661	-2.782348
H	-3.534987	-3.059109	-3.400933
C	-1.794761	-0.922743	-5.133118
H	-0.723026	-0.779807	-5.386381
H	-2.428270	-0.512773	-5.950429
C	-2.118832	-2.372435	-4.897165

H -2.899146 -2.718033 -5.610550
H -1.214907 -3.012891 -4.992169
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Figure_S7_imid-3_modeA_ed(AS) / electronic energy: -4442.760227951429 a.u. / lowest freq: 13.95 cm-1
C -0.723232 -0.908750 3.111383
H -1.061383 -0.014647 3.657443
C 0.756342 -0.836504 2.699020
H 1.230023 -1.833744 2.679116
C -0.584276 -0.514379 0.790347
C -2.791070 -1.111550 1.600497
C -3.196820 -2.281682 0.951265
C -3.762985 -0.203338 2.056144
C -4.549334 -2.578100 0.800790
H -2.417593 -2.954953 0.579506
C -5.116992 -0.502443 1.887465
C -5.511982 -1.691933 1.279301
H -4.851769 -3.503125 0.302730
H -5.855180 0.218954 2.243102
H -6.575089 -1.917309 1.168047
S -3.342412 1.331516 2.887141
O -4.565248 2.183488 2.801767
O -2.221444 1.945541 2.110710
O -2.983426 0.957200 4.269628
Cu -1.144253 -0.488376 -1.116134
C -1.058216 -2.144084 3.908675
C -1.531393 -2.026265 5.227583
C -0.907920 -3.427428 3.349506
C -1.851101 -3.167374 5.968985
H -1.650219 -1.053182 5.686244
C -1.227474 -4.565348 4.096056
H -0.545405 -3.545533 2.336417
C -1.699893 -4.435487 5.403784
H -2.214902 -3.068161 6.983507
H -1.107782 -5.549300 3.662810
H -1.946884 -5.317723 5.980015
N -1.395860 -0.907894 1.786042
N 0.639201 -0.346753 1.314065
C -2.339573 0.357031 -2.528139
C -3.376736 -0.577569 -2.973015
C -3.326548 -1.109616 -4.275452
C -4.464244 -0.947238 -2.157862
C -4.309807 -1.977487 -4.740128
C -5.446133 -1.816596 -2.622490
C -5.377244 -2.338282 -3.915929
H -4.245357 -2.372043 -5.757395
H -6.279011 -2.087594 -1.967037
H -6.150782 -3.019112 -4.279006
C -2.383591 1.113876 -1.337146
C -1.614761 2.375138 -1.226083
H -1.379190 2.622756 -0.181047
H -0.684464 2.345975 -1.809544
H -4.541096 -0.547440 -1.143179
H -3.227935 1.021147 -0.642748
P -3.144128 4.493704 -0.855852
O -4.356683 3.665762 -0.176518
O -2.415147 5.141313 0.271837
O -3.779806 5.444312 -1.974199
O -2.358864 3.508094 -1.818019
Na -3.269467 4.137532 2.229282
H -1.655427 0.697659 -3.316873
H -2.502170 -0.819903 -4.933038
C -5.315090 2.938768 -0.943215
H -5.741201 2.173964 -0.283419
H -6.114509 3.606836 -1.292367
H -4.846617 2.448874 -1.809287
C -4.460826 6.632436 -1.570686
H -4.790303 7.136156 -2.484015
H -5.340817 6.396066 -0.955079
H -3.792709 7.298233 -1.008835
C 1.747871 0.026521 0.521343
C 2.887455 -0.786177 0.460294
C 1.738451 1.253245 -0.154039
C 4.004792 -0.375408 -0.275338
C 2.865792 1.683642 -0.866508
C 3.999703 0.863756 -0.925999
H 4.876744 1.189842 -1.472509
H 0.881914 1.902857 -0.064053
H 2.903265 -1.740750 0.971148
C 2.880020 3.016043 -1.512064
C 2.862371 3.123458 -2.933867
C 2.947461 4.195490 -0.712943
C 2.952324 4.399286 -3.520733
C 2.998248 5.448011 -1.352482
C 3.011694 5.544801 -2.737829
H 2.967285 4.515059 -4.596269
H 3.041218 6.362841 -0.776399
H 3.066656 6.517606 -3.209543
C 5.184459 -1.252480 -0.369415

C	6.257217	-1.101825	0.552175
C	5.241584	-2.253395	-1.378887
C	7.370843	-1.954335	0.440078
C	6.369468	-3.091880	-1.438334
C	7.421295	-2.939157	-0.541043
H	8.208235	-1.862216	1.119111
H	6.441305	-3.869419	-2.187418
H	8.283896	-3.589830	-0.606903
C	4.117285	-2.445060	-2.398360
H	3.318378	-1.689688	-2.260560
C	3.446414	-3.812983	-2.226696
H	3.059481	-3.916663	-1.190188
H	2.588738	-3.908219	-2.925828
H	4.158794	-4.639852	-2.430229
C	4.625441	-2.251475	-3.832255
H	5.129964	-1.265990	-3.925233
H	5.339672	-3.051020	-4.120308
H	3.772141	-2.271160	-4.543496
C	6.237630	-0.044071	1.656731
H	5.290841	0.533603	1.644015
C	7.362029	0.978858	1.458133
H	7.275987	1.789881	2.212707
H	8.360911	0.505158	1.562253
H	7.283193	1.436298	0.448529
C	6.315903	-0.688747	3.045984
H	6.209170	0.089613	3.831191
H	5.491165	-1.422852	3.169852
H	7.285773	-1.206613	3.199009
C	2.974698	4.154181	0.816143
H	2.985671	3.113731	1.194809
C	2.735313	1.903822	-3.847205
H	2.587277	0.977898	-3.256504
C	1.508829	2.017422	-4.764733
H	0.590986	2.162737	-4.155880
H	1.606279	2.863730	-5.475775
H	1.390502	1.086726	-5.359426
C	4.013679	1.697745	-4.667743
H	4.185094	2.545963	-5.363665
H	4.889869	1.605596	-3.991456
H	3.936717	0.762653	-5.262809
C	1.719029	4.815589	1.398231
H	1.666237	5.890817	1.126949
H	0.809306	4.303759	1.017232
H	1.722715	4.737700	2.504493
C	4.250031	4.800293	1.372447
H	5.145306	4.323223	0.918863
H	4.277505	5.890582	1.165806
H	4.300143	4.652505	2.472712
H	0.456008	1.878980	3.055720
H	1.821194	3.371686	4.469569
C	1.281256	1.466490	3.622756
C	2.057997	2.318074	4.413831
C	1.574194	0.090877	3.561101
C	3.139318	1.810889	5.137442
H	3.741198	2.472952	5.746307
C	2.665800	-0.408449	4.293421
C	3.442355	0.449089	5.077632
H	2.918942	-1.460713	4.257323
H	4.279983	0.056978	5.639691
C	0.058334	-1.846594	-2.062704
H	0.953035	-1.712659	-1.432455
C	0.336447	-1.482696	-3.506376
H	0.606458	-0.424627	-3.643678
H	1.160528	-2.066993	-3.958371
H	-0.541536	-1.665074	-4.145554
B	-0.535536	-3.222043	-1.821462
O	-0.602435	-3.870399	-0.581588
O	-1.078872	-4.025348	-2.820457
C	-1.725939	-5.142035	-2.184582
C	-0.944894	-5.245884	-0.838166
C	-3.182701	-4.756324	-1.985507
H	-3.266922	-3.863750	-1.348076
H	-3.627626	-4.500352	-2.956775
H	-3.776479	-5.566171	-1.536892
C	-1.612120	-6.361767	-3.073468
H	-0.572271	-6.562659	-3.359728
H	-2.009596	-7.254776	-2.568693
H	-2.190490	-6.216044	-3.996202
C	0.359828	-6.017400	-0.980405
H	0.193070	-7.097811	-1.094416
H	0.938511	-5.666915	-1.846400
H	0.973262	-5.862891	-0.082385
C	-1.754195	-5.798631	0.315084
H	-1.133394	-5.863308	1.218154
H	-2.627710	-5.177312	0.550463
H	-2.111678	-6.813854	0.087881

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Figure_S7_imid-3_modeA_ts(AS)_01 / electronic energy: -4442.745684459335 a.u. / lowest freq: -257.30 cm-1

C	-0.680165	-0.493719	3.192983
H	-0.906247	0.489177	3.631638
C	0.781877	-0.622641	2.735351
H	1.154781	-1.658707	2.818965
C	-0.590985	-0.415554	0.840399
C	-2.812497	-0.661801	1.744098
C	-3.334774	-1.802315	1.125149
C	-3.680160	0.367925	2.150136
C	-4.707356	-1.939317	0.932210
H	-2.632496	-2.583057	0.813806
C	-5.054552	0.219389	1.948574
C	-5.570181	-0.927361	1.349347
H	-5.103124	-2.839891	0.455325
H	-5.713360	1.030638	2.263869
H	-6.648237	-1.026525	1.205780
S	-3.112401	1.882219	2.940092
O	-4.224986	2.859496	2.783934
O	-1.908696	2.323065	2.166741
O	-2.827080	1.517309	4.340168
Cu	-1.254356	-0.693785	-1.030793
C	-1.095163	-1.583651	4.147333
C	-1.425594	-1.268383	5.477057
C	-1.148855	-2.927215	3.730606
C	-1.816093	-2.273693	6.366333
H	-1.373526	-0.246720	5.830596
C	-1.540088	-3.928834	4.624069
H	-0.889768	-3.197073	2.715093
C	-1.875543	-3.602200	5.939771
H	-2.070048	-2.022614	7.388046
H	-1.581994	-4.959627	4.298985
H	-2.177566	-4.379199	6.630026
N	-1.401161	-0.590055	1.896576
N	0.659220	-0.300661	1.300345
C	-2.478012	-0.238733	-2.617927
C	-3.426460	-1.229176	-3.133638
C	-3.176381	-1.878199	-4.357522
C	-4.634826	-1.525708	-2.473496
C	-4.078073	-2.798814	-4.883674
C	-5.538182	-2.440886	-3.001712
C	-5.263993	-3.088738	-4.207508
H	-3.857066	-3.286847	-5.836026
H	-6.468903	-2.648706	-2.466621
H	-5.973998	-3.808145	-4.621939
C	-2.757166	0.630365	-1.526222
C	-1.962755	1.757546	-1.239562
H	-1.996892	2.183773	-0.233406
H	-1.018137	1.878437	-1.772871
H	-4.882380	-1.021861	-1.537231
H	-3.649367	0.467803	-0.911869
P	-3.022838	4.464753	-1.286695
O	-4.194294	4.032056	-0.210200
O	-1.989468	5.099590	-0.401584
O	-3.755476	5.498031	-2.299498
O	-2.705641	3.264279	-2.192178
Na	-2.775367	4.544483	1.733880
H	-1.718572	0.096764	-3.337889
H	-2.265607	-1.636814	-4.911512
C	-5.342693	3.314927	-0.623494
H	-5.912338	3.060185	0.277414
H	-5.974813	3.922525	-1.289684
H	-5.069163	2.388553	-1.151903
C	-4.127609	6.777977	-1.812421
H	-4.460154	7.373533	-2.669467
H	-4.956838	6.706255	-1.090964
H	-3.280030	7.285717	-1.329998
C	1.756582	-0.008717	0.459153
C	2.912481	-0.798120	0.502311
C	1.723767	1.124864	-0.364554
C	4.023300	-0.460889	-0.278335
C	2.849544	1.490297	-1.114604
C	3.998665	0.690922	-1.072894
H	4.871108	0.964551	-1.654643
H	0.849690	1.760937	-0.364936
H	2.944001	-1.680954	1.129024
C	2.845843	2.741112	-1.904578
C	2.816320	2.688871	-3.328608
C	2.895497	4.002189	-1.240928
C	2.864727	3.893465	-4.054201
C	2.907281	5.177178	-2.015064
C	2.901948	5.120102	-3.403114
H	2.863073	3.888819	-5.136122
H	2.932051	6.150694	-1.543575
H	2.925171	6.035779	-3.980051
C	5.211402	-1.331066	-0.277349
C	6.311993	-1.032206	0.572370
C	5.250002	-2.471476	-1.127274
C	7.437583	-1.875805	0.543824
C	6.389386	-3.295967	-1.102635

C	7.470542	-2.996089	-0.280271
H	8.297495	-1.671627	1.168042
H	6.448231	-4.176249	-1.729114
H	8.342293	-3.637833	-0.281690
C	4.095481	-2.824193	-2.067723
H	3.288297	-2.066821	-2.013958
C	3.452447	-4.159751	-1.675093
H	3.106042	-4.117207	-0.620095
H	2.570038	-4.362900	-2.318585
H	4.169750	-4.999933	-1.785861
C	4.552832	-2.835805	-3.531541
H	5.027144	-1.864063	-3.787393
H	5.278794	-3.653582	-3.722694
H	3.678835	-2.980130	-4.201964
C	6.308425	0.173342	1.513579
H	5.343632	0.718606	1.464821
C	7.390544	1.183295	1.115552
H	7.316402	2.090931	1.752166
H	8.406833	0.751530	1.233229
H	7.249754	1.490991	0.057148
C	6.468858	-0.260450	2.975855
H	6.361139	0.619220	3.645716
H	5.681349	-0.998153	3.240606
H	7.464790	-0.715599	3.157791
C	2.941084	4.127833	0.283484
H	2.992823	3.134690	0.770984
C	2.716746	1.371463	-4.097989
H	2.615319	0.512322	-3.405963
C	1.468682	1.340488	-4.991655
H	0.560545	1.535588	-4.381599
H	1.527592	2.097157	-5.801411
H	1.363524	0.340281	-5.463670
C	3.986137	1.116823	-4.918757
H	4.113556	1.884716	-5.710714
H	4.877176	1.132993	-4.255608
H	3.932725	0.117259	-5.400973
C	1.669326	4.804727	0.809196
H	1.574168	5.840908	0.422045
H	0.776441	4.221438	0.499284
H	1.685620	4.847498	1.917632
C	4.198793	4.872284	0.749577
H	5.105321	4.380898	0.335389
H	4.184981	5.935034	0.429425
H	4.266493	4.843196	1.858410
H	0.827060	2.132492	2.695292
H	2.396725	3.630408	3.873403
C	1.599421	1.706395	3.322688
C	2.490634	2.558621	3.981575
C	1.717099	0.310513	3.461752
C	3.504854	2.029130	4.782117
H	4.194815	2.690737	5.289562
C	2.742858	-0.211065	4.269474
C	3.628352	0.646009	4.928659
H	2.859737	-1.280876	4.389559
H	4.414908	0.236791	5.549332
C	-0.024145	-2.138194	-1.763927
H	0.840584	-1.964894	-1.105912
C	0.332133	-1.929025	-3.215574
H	0.641712	-0.898193	-3.441073
H	1.166040	-2.576119	-3.542655
H	-0.508446	-2.164385	-3.883629
B	-0.696303	-3.453065	-1.381883
O	-0.794882	-3.926588	-0.076085
O	-1.261523	-4.336861	-2.283051
C	-1.965678	-5.341788	-1.520967
C	-1.200284	-5.311162	-0.159643
C	-3.404045	-4.871521	-1.389659
H	-3.455350	-3.910134	-0.856811
H	-3.828499	-4.709966	-2.389727
H	-4.035621	-5.598961	-0.860323
C	-1.896344	-6.662148	-2.255910
H	-0.863299	-6.939124	-2.499210
H	-2.338756	-7.470285	-1.655213
H	-2.457810	-6.602126	-3.198362
C	0.067923	-6.150107	-0.187990
H	-0.151380	-7.226751	-0.180486
H	0.673509	-5.929517	-1.078056
H	0.677024	-5.922064	0.697047
C	-2.044542	-5.665508	1.044403
H	-1.429078	-5.660372	1.953164
H	-2.871939	-4.960266	1.193248
H	-2.469519	-6.674331	0.940012

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Figure_S7_imid-3_modeA_ts(AS)_02 / electronic energy: -4442.747892119929 a.u. / lowest freq: -262.85 cm-1

C	-1.124466	-0.696457	3.157928
H	-1.212212	0.249834	3.711285
C	0.322984	-1.020786	2.749278
H	0.518665	-2.107221	2.742615

C	-0.879095	-0.381691	0.833417
C	-3.162783	-0.355186	1.603953
C	-3.782431	-1.290120	0.765963
C	-3.918892	0.700050	2.143156
C	-5.143522	-1.200192	0.486537
H	-3.165081	-2.096364	0.353526
C	-5.282813	0.781148	1.850917
C	-5.897743	-0.164219	1.034232
H	-5.618047	-1.944433	-0.158341
H	-5.850629	1.615664	2.265887
H	-6.966000	-0.086093	0.822540
S	-3.223641	1.978473	3.201945
O	-4.180440	3.119475	3.112662
O	-1.908948	2.356030	2.593310
O	-3.120473	1.379437	4.543204
Cu	-1.441549	-0.254778	-1.087968
C	-1.769868	-1.808304	3.944390
C	-2.093030	-1.619007	5.299369
C	-2.041466	-3.052657	3.344991
C	-2.693620	-2.645867	6.033436
H	-1.872479	-0.681083	5.792343
C	-2.643337	-4.076069	4.083128
H	-1.789226	-3.227065	2.307019
C	-2.971291	-3.872093	5.425243
H	-2.940999	-2.491624	7.075761
H	-2.854625	-5.029034	3.616945
H	-3.436183	-4.665958	5.995370
N	-1.769181	-0.510213	1.830301
N	0.342722	-0.545864	1.351855
C	-2.390206	0.706091	-2.623869
C	-3.312605	-0.036633	-3.484643
C	-2.975275	-0.280029	-4.828974
C	-4.560720	-0.497789	-3.026827
C	-3.838973	-0.971702	-5.673193
C	-5.428286	-1.177622	-3.873351
C	-5.070390	-1.426245	-5.200194
H	-3.552412	-1.148951	-6.712562
H	-6.390848	-1.527472	-3.490645
H	-5.750750	-1.965512	-5.863254
C	-2.761530	1.314527	-1.393324
C	-1.934511	2.237007	-0.720802
H	-2.064009	2.385789	0.353582
H	-0.918097	2.380055	-1.093360
H	-4.855858	-0.324758	-1.989258
H	-3.750560	1.116753	-0.965496
P	-1.595300	5.154661	-0.803612
O	-2.048826	6.351389	-1.809655
O	-1.520760	5.596937	0.629241
O	-0.071392	4.807060	-1.271005
O	-2.525574	3.995237	-1.218176
Na	-2.587160	4.718490	2.369205
H	-1.510620	1.122209	-3.137001
H	-2.022225	0.093523	-5.213157
C	-1.445373	7.623896	-1.644320
H	-1.879388	8.296017	-2.392880
H	-1.635043	8.034058	-0.641591
H	-0.355857	7.577512	-1.800859
C	0.163480	4.419008	-2.612519
H	0.678694	5.221800	-3.159758
H	0.804661	3.528673	-2.612844
H	-0.768462	4.172702	-3.143248
C	1.524816	-0.402296	0.588448
C	2.506371	-1.401708	0.607932
C	1.755292	0.776913	-0.134730
C	3.709809	-1.219576	-0.081374
C	2.982242	0.986789	-0.781166
C	3.958926	-0.016906	-0.751416
H	4.908130	0.134424	-1.251153
H	1.012471	1.561219	-0.129185
H	2.329547	-2.326836	1.142401
C	3.271705	2.283425	-1.436315
C	3.408820	2.358596	-2.854700
C	3.439431	3.459101	-0.644698
C	3.735554	3.595418	-3.441233
C	3.715539	4.678823	-1.289535
C	3.873019	4.740728	-2.667883
H	3.868863	3.683494	-4.511141
H	3.828226	5.592608	-0.721411
H	4.103195	5.686321	-3.141813
C	4.698281	-2.310530	-0.131755
C	5.751894	-2.364106	0.821700
C	4.586715	-3.314048	-1.134357
C	6.677806	-3.421098	0.748668
C	5.525077	-4.361694	-1.151735
C	6.559431	-4.409475	-0.223023
H	7.497857	-3.487493	1.451418
H	5.462796	-5.147213	-1.893317
H	7.277071	-5.219159	-0.257661

C 3.482514 -3.286092 -2.193288
H 2.850719 -2.381365 -2.090918
C 2.538645 -4.483622 -2.037222
H 2.100541 -4.488924 -1.015999
H 1.706334 -4.410042 -2.769157
H 3.072519 -5.442349 -2.206125
C 4.068999 -3.222028 -3.608866
H 4.775755 -2.368585 -3.687278
H 4.605321 -4.158858 -3.867889
H 3.256146 -3.067364 -4.350329
C 5.910710 -1.309714 1.917505
H 5.092673 -0.561584 1.876626
C 7.215590 -0.525354 1.738800
H 7.271823 0.294785 2.486273
H 8.101412 -1.182237 1.868851
H 7.248603 -0.072056 0.724808
C 5.832939 -1.940919 3.313003
H 5.862305 -1.147180 4.089404
H 4.879772 -2.501195 3.422713
H 6.681131 -2.633821 3.493488
C 3.349790 3.444668 0.883568
H 3.220571 2.415946 1.271977
C 3.191874 1.150785 -3.767653
H 2.842210 0.272170 -3.189548
C 2.100496 1.424180 -4.813736
H 1.165472 1.756088 -4.314900
H 2.414895 2.202751 -5.539366
H 1.879700 0.495405 -5.382175
C 4.502264 0.736952 -4.447340
H 4.876376 1.538647 -5.118587
H 5.277659 0.519852 -3.682738
H 4.343969 -0.182386 -5.050589
C 2.137472 4.251154 1.366293
H 2.205239 5.312087 1.046683
H 1.203493 3.811440 0.957832
H 2.072061 4.223659 2.473552
C 4.645340 3.954860 1.528432
H 5.514401 3.383324 1.137540
H 4.802593 5.035150 1.327757
H 4.603219 3.808588 2.629232
H 0.828557 1.677657 2.975644
H 2.542829 2.777744 4.370314
C 1.475199 1.073252 3.598662
C 2.448965 1.700412 4.381607
C 1.349929 -0.328739 3.608998
C 3.303206 0.938207 5.181180
H 4.056978 1.425699 5.785705
C 2.215935 -1.085828 4.417233
C 3.183701 -0.452924 5.202168
H 2.143462 -2.166041 4.441527
H 3.845020 -1.042522 5.823745
C -0.429779 -1.761163 -2.008279
H 0.426184 -1.824641 -1.320337
C 0.021505 -1.476905 -3.420252
H 0.462387 -0.477036 -3.544475
H 0.788483 -2.192768 -3.766956
H -0.805319 -1.556776 -4.139473
B -1.325101 -2.982246 -1.802947
O -1.544661 -3.590643 -0.569602
O -1.993323 -3.643413 -2.817884
C -2.832907 -4.651559 -2.213575
C -2.133909 -4.883068 -0.834003
C -4.220669 -4.052396 -2.070104
H -4.195587 -3.154673 -1.435425
H -4.589380 -3.745332 -3.057514
H -4.939881 -4.764702 -1.642431
C -2.872330 -5.869110 -3.111122
H -1.866630 -6.227524 -3.361294
H -3.423850 -6.691396 -2.632516
H -3.384364 -5.628828 -4.052718
C -0.992100 -5.884647 -0.918438
H -1.356745 -6.913242 -1.045901
H -0.320187 -5.653178 -1.756175
H -0.401886 -5.845694 0.007008
C -3.075823 -5.250686 0.291566
H -2.509298 -5.446336 1.211130
H -3.800639 -4.454234 0.503394
H -3.635414 -6.165910 0.049330
170
Figure_S7_imid-3_modeA_ts(AS)_03 / electronic energy: -4442.746138338317 a.u. / lowest freq: -178.29 cm-1
C -1.591619 -0.687139 2.779796
H -1.979932 0.290835 3.095238
C -0.069129 -0.700368 2.584543
H 0.343270 -1.716957 2.719343
C -1.085468 -0.593668 0.483151
C -3.392300 -1.091578 0.924461
C -3.608396 -2.140189 0.018440
C -4.483086 -0.292353 1.311892

C	-4.884822	-2.441730	-0.443214
H	-2.754746	-2.738329	-0.311560
C	-5.762657	-0.608658	0.844256
C	-5.973307	-1.686039	-0.011211
H	-5.019190	-3.267575	-1.146023
H	-6.592978	0.029083	1.153213
H	-6.983153	-1.917017	-0.357272
S	-4.333874	1.168995	2.351894
O	-5.533509	1.997116	2.045344
O	-3.095680	1.868351	1.878656
O	-4.260784	0.680326	3.739248
Cu	-1.482965	-0.361814	-1.467473
C	-2.042853	-1.719323	3.786704
C	-1.861564	-1.439443	5.153654
C	-2.605994	-2.957516	3.419875
C	-2.241181	-2.366790	6.127684
H	-1.424976	-0.498583	5.465794
C	-2.983948	-3.882209	4.397707
H	-2.751583	-3.227080	2.388411
C	-2.803069	-3.587307	5.750044
H	-2.097946	-2.138966	7.176010
H	-3.414949	-4.831105	4.105348
H	-3.095726	-4.305586	6.504908
N	-2.052564	-0.903329	1.373870
N	0.034461	-0.337326	1.164993
C	-2.411325	0.826285	-2.866479
C	-3.449496	0.223678	-3.698565
C	-3.314059	0.205374	-5.098134
C	-4.609308	-0.342764	-3.139873
C	-4.291653	-0.369734	-5.905378
C	-5.582265	-0.923396	-3.944180
C	-5.427260	-0.943214	-5.332894
H	-4.166287	-0.370516	-6.990674
H	-6.468929	-1.366585	-3.482778
H	-6.191403	-1.400404	-5.965613
C	-2.648735	1.352095	-1.564660
C	-1.672438	2.104048	-0.898617
H	-1.754553	2.246678	0.178692
H	-0.671311	2.161916	-1.326825
H	-4.741579	-0.338714	-2.055943
H	-3.620665	1.222710	-1.074195
P	-1.520220	5.005325	-0.310909
O	-1.335649	6.465235	-1.009554
O	-2.312971	5.209872	0.949500
O	0.011911	4.527023	-0.006352
O	-2.011431	4.010759	-1.374635
Na	-4.145667	3.957400	1.336441
H	-1.553183	1.239199	-3.412908
H	-2.428559	0.657438	-5.553269
C	-0.578093	6.570756	-2.202834
H	-0.635886	7.611343	-2.541897
H	0.479272	6.312503	-2.033483
H	-0.977305	5.915577	-2.990747
C	0.756265	5.211272	0.982103
H	1.802720	4.905965	0.878866
H	0.701766	6.303326	0.850449
H	0.406939	4.964732	1.995305
C	1.272994	-0.159956	0.514248
C	2.139201	-1.242558	0.336245
C	1.680773	1.123002	0.133145
C	3.384480	-1.060297	-0.275560
C	2.936327	1.316058	-0.455303
C	3.783217	0.222111	-0.670145
H	4.759863	0.372815	-1.114976
H	1.041761	1.972773	0.333032
H	1.859356	-2.219550	0.698601
C	3.400043	2.676261	-0.782714
C	3.077977	3.254603	-2.042124
C	4.232970	3.376023	0.135700
C	3.603900	4.520012	-2.360227
C	4.733871	4.638246	-0.231273
C	4.416325	5.203107	-1.461749
H	3.399199	4.979841	-3.317735
H	5.386531	5.189128	0.432668
H	4.815200	6.173707	-1.727393
C	4.293000	-2.210552	-0.453130
C	4.965493	-2.761910	0.674753
C	4.495639	-2.768521	-1.748471
C	5.803649	-3.875871	0.486664
C	5.372924	-3.859506	-1.886589
C	6.007086	-4.412052	-0.779727
H	6.318474	-4.328170	1.323991
H	5.565982	-4.294743	-2.858056
H	6.667968	-5.260102	-0.905544
C	3.800835	-2.216349	-2.994771
H	3.058694	-1.438348	-2.725133
C	3.010673	-3.303677	-3.735950
H	2.338667	-3.833969	-3.032586

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H   2.386370  -2.842272  -4.530577
H   3.685254  -4.045470  -4.211980
C   4.815266  -1.548938  -3.929750
H   5.364316  -0.750209  -3.387162
H   5.548785  -2.287608  -4.316887
H   4.290547  -1.084849  -4.792169
C   4.823709  -2.171764   2.079767
H   4.184283  -1.266651   2.076038
C   6.178459  -1.708695   2.630520
H   6.034114  -1.180386   3.597352
H   6.862676  -2.566298   2.799896
H   6.654843  -1.000871   1.918518
C   4.150939  -3.169929   3.029231
H   3.989499  -2.700430   4.022960
H   3.161278  -3.471368   2.623552
H   4.775010  -4.077917   3.166625
C   4.631122   2.781096   1.488952
H   4.091334   1.831802   1.683799
C   2.228811   2.519258  -3.079923
H   1.786876   1.596615  -2.650997
C   1.043309   3.370632  -3.553828
H   0.479766   3.755387  -2.680818
H   1.378064   4.231688  -4.168923
H   0.355189   2.753130  -4.169248
C   3.092201   2.076037  -4.265217
H   3.504933   2.952552  -4.808515
H   3.934928   1.448716  -3.904497
H   2.486810   1.470076  -4.972904
C   4.261511   3.709952   2.652746
H   4.843224   4.654451   2.623265
H   3.179322   3.950774   2.618524
H   4.471462   3.205347   3.619838
C   6.125228   2.440988   1.512492
H   6.369399   1.748815   0.678281
H   6.745510   3.356961   1.413607
H   6.386515   1.935887   2.467083
H  -0.319329   2.041461   2.686760
H   0.919424   3.613341   4.125631
C   0.415188   1.656684   3.382889
C   1.120060   2.552170   4.191395
C   0.668012   0.274271   3.465434
C   2.090669   2.080696   5.078232
H   2.639709   2.776753   5.698974
C   1.651007  -0.188556   4.357472
C   2.358931   0.712279   5.157888
H   1.871752  -1.245719   4.433479
H   3.115895   0.348798   5.840698
C  -0.459192  -1.652415  -2.653531
H   0.516597  -1.140419  -2.547650
C  -0.870256  -1.754946  -4.104134
H  -0.832603  -0.793501  -4.639727
H  -0.219817  -2.446205  -4.673215
H  -1.895299  -2.142810  -4.221830
B  -0.449841  -2.982582  -1.890803
O   0.585860  -3.424095  -1.091257
O  -1.456580  -3.933130  -1.973902
C  -0.944257  -5.168862  -1.430089
C   0.204887  -4.672714  -0.482418
C  -2.073549  -5.899029  -0.734774
H  -2.563231  -5.274287   0.023393
H  -2.836715  -6.194940  -1.467385
H  -1.710414  -6.813372  -0.243528
C  -0.424060  -5.986054  -2.602455
H   0.388563  -5.464779  -3.127346
H  -0.051838  -6.969843  -2.284931
H  -1.235816  -6.147800  -3.324418
C   1.420481  -5.573748  -0.422216
H   1.162345  -6.558267  -0.005832
H   1.873320  -5.725165  -1.408976
H   2.184840  -5.125251   0.227261
C  -0.291484  -4.362166   0.918835
H   0.521953  -3.946056   1.527222
H  -1.096967  -3.617161   0.874594
H  -0.666957  -5.253716   1.438859
170
Figure_S7_imid-3_modeA_ts(AS)_04 / electronic energy: -4442.744366801986 a.u. / lowest freq: -264.99 cm-1
C   0.970692  -2.147369  -2.151946
H   1.598097  -1.586722  -2.857443
C  -0.487562  -1.656565  -2.111334
H  -1.186999  -2.479889  -1.880706
C   0.606702  -0.899617  -0.180130
C   2.680507  -2.106817  -0.160671
C   2.611992  -2.527535   1.177172
C   3.943350  -2.019513  -0.778866
C   3.755875  -2.871729   1.888040
H   1.631326  -2.601110   1.658127
C   5.084879  -2.369394  -0.050373
C   5.002549  -2.796843   1.271548
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H	3.662268	-3.210214	2.922907
H	6.052506	-2.281181	-0.547181
H	5.909606	-3.070163	1.814348
S	4.208681	-1.445634	-2.464931
O	5.665970	-1.144558	-2.557376
O	3.408313	-0.184349	-2.582921
O	3.766647	-2.533631	-3.353122
Cu	0.985879	0.027449	1.566000
C	1.055498	-3.612593	-2.521351
C	0.799571	-3.973877	-3.857507
C	1.358130	-4.631174	-1.594800
C	0.846871	-5.311916	-4.257291
H	0.564938	-3.214958	-4.593694
C	1.403241	-5.968367	-1.999603
H	1.551599	-4.416551	-0.558329
C	1.148496	-6.308874	-3.328803
H	0.648606	-5.575456	-5.288140
H	1.633545	-6.742719	-1.279192
H	1.183601	-7.345238	-3.638814
N	1.438440	-1.787329	-0.776334
N	-0.457230	-0.738528	-0.966958
C	2.181439	1.322618	2.596901
C	2.623769	0.978172	3.946751
C	2.335153	1.844458	5.015996
C	3.339473	-0.199105	4.225171
C	2.734841	1.540450	6.314174
C	3.736096	-0.505665	5.521705
C	3.432847	0.361543	6.574925
H	2.499328	2.229344	7.128910
H	4.283342	-1.431708	5.715314
H	3.741942	0.118197	7.594041
C	2.849657	0.928666	1.403549
C	2.593264	1.566917	0.174063
H	2.923890	1.091103	-0.755660
H	1.705442	2.194210	0.089221
H	3.565887	-0.891748	3.411264
H	3.667630	0.199890	1.450348
P	4.841650	3.133618	-0.892427
O	5.727003	1.760224	-0.671393
O	4.613361	3.161612	-2.375761
O	5.803384	4.324490	-0.351817
O	3.685945	3.147162	0.118344
Na	5.424651	1.151405	-3.106493
H	1.595194	2.246973	2.531683
H	1.790822	2.771705	4.818220
C	6.243055	1.445919	0.612227
H	6.368797	0.357326	0.672652
H	7.219166	1.928103	0.772800
H	5.556152	1.769307	1.409237
C	6.901438	4.731009	-1.153007
H	7.412190	5.542116	-0.622628
H	7.617535	3.907944	-1.307096
H	6.569158	5.097354	-2.134794
C	-1.547304	0.083672	-0.603769
C	-2.798711	-0.481409	-0.324418
C	-1.405236	1.478700	-0.619859
C	-3.892782	0.339485	-0.022787
C	-2.507868	2.302239	-0.356658
C	-3.746731	1.730619	-0.047814
H	-4.601832	2.367287	0.148458
H	-0.455313	1.920216	-0.890748
H	-2.925159	-1.555807	-0.347291
C	-2.401891	3.768090	-0.492613
C	-2.066934	4.568118	0.635192
C	-2.749248	4.385596	-1.727635
C	-2.114430	5.969051	0.511923
C	-2.782526	5.790393	-1.798363
C	-2.467545	6.569477	-0.691067
H	-1.890051	6.607294	1.356146
H	-3.067267	6.292392	-2.713394
H	-2.504235	7.648914	-0.763948
C	-5.209739	-0.256290	0.278121
C	-6.009614	-0.779888	-0.777501
C	-5.693246	-0.278621	1.618369
C	-7.262750	-1.338558	-0.465861
C	-6.961790	-0.831212	1.872486
C	-7.730137	-1.362112	0.843022
H	-7.894382	-1.748476	-1.242875
H	-7.365120	-0.852386	2.876224
H	-8.701694	-1.787165	1.060350
C	-4.889989	0.293216	2.788178
H	-3.886234	0.627325	2.458560
C	-4.642247	-0.762457	3.873232
H	-4.186118	-1.666408	3.423797
H	-3.941530	-0.364622	4.637624
H	-5.584543	-1.052653	4.382933
C	-5.586314	1.525741	3.375704
H	-5.756550	2.281155	2.579246

H -6.564171 1.256795 3.828194
H -4.948100 1.985270 4.160574
C -5.568310 -0.727093 -2.241672
H -4.577937 -0.241315 -2.348812
C -6.534032 0.118001 -3.081494
H -6.135988 0.237464 -4.112062
H -7.536161 -0.355620 -3.145070
H -6.640514 1.129112 -2.633319
C -5.419129 -2.137645 -2.823830
H -5.043322 -2.080833 -3.867359
H -4.689150 -2.719712 -2.221265
H -6.389601 -2.676499 -2.833332
C -3.121734 3.571063 -2.967937
H -2.965674 2.486222 -2.796947
C -1.692610 3.955436 1.983433
H -1.614760 2.852646 1.909413
C -0.318634 4.444104 2.459322
H 0.444837 4.250179 1.676154
H -0.328209 5.529654 2.689568
H -0.023942 3.902510 3.382263
C -2.771583 4.245387 3.031723
H -2.835634 5.332279 3.250860
H -3.759033 3.895748 2.663401
H -2.541112 3.704857 3.974807
C -2.235147 3.932875 -4.166633
H -2.406046 4.976963 -4.501444
H -1.164454 3.810673 -3.896512
H -2.459869 3.259083 -5.020286
C -4.605748 3.745589 -3.308103
H -5.230076 3.464094 -2.433101
H -4.831552 4.796280 -3.588249
H -4.882540 3.083914 -4.156767
H 0.547801 0.630179 -3.238944
H -0.193562 1.764075 -5.298112
C -0.275794 0.215118 -3.806411
C -0.697513 0.864707 -4.969133
C -0.920270 -0.959257 -3.375167
C -1.774846 0.360896 -5.701877
H -2.105533 0.870767 -6.597379
C -1.998929 -1.461102 -4.123252
C -2.425977 -0.799961 -5.278234
H -2.509695 -2.363696 -3.813353
H -3.260972 -1.189304 -5.846160
C -0.626633 -0.120420 2.801031
H -1.375627 0.434412 2.209173
C -0.529930 0.448955 4.197672
H -0.250670 1.514040 4.225246
H -1.494233 0.378437 4.735040
H 0.203361 -0.089441 4.818451
B -0.897574 -1.627131 2.721555
O -1.948340 -2.204053 2.034676
O -0.122209 -2.590033 3.355636
C -0.843758 -3.840741 3.299466
C -1.777039 -3.635069 2.056858
C 0.146315 -4.977357 3.161549
H 0.814805 -4.841088 2.301692
H 0.769894 -5.048917 4.063190
H -0.374171 -5.938439 3.039587
C -1.621595 -3.962729 4.600315
H -2.346230 -3.143714 4.712261
H -2.166390 -4.914678 4.665989
H -0.925857 -3.911778 5.448504
C -3.130390 -4.304015 2.158554
H -3.021398 -5.397510 2.195640
H -3.690738 -3.988680 3.045811
H -3.736667 -4.058133 1.276176
C -1.102907 -4.010913 0.750429
H -1.745642 -3.720342 -0.091460
H -0.152007 -3.469353 0.653441
H -0.907112 -5.088303 0.665660
170
Figure_S7_imid-3_modeA_ts(AS)_05 / electronic energy: -4442.741822923053 a.u. / lowest freq: -255.58 cm-1
C -1.016370 -2.898409 -2.135843
H -1.250482 -3.741222 -1.468131
C 0.438192 -2.413096 -2.007436
H 0.848525 -2.066166 -2.971897
C -0.985559 -0.819338 -1.018996
C -3.189471 -1.625118 -1.680175
C -3.766502 -0.680985 -2.537094
C -4.024500 -2.474730 -0.932921
C -5.147331 -0.604618 -2.691922
H -3.104926 -0.020108 -3.101041
C -5.410160 -2.393325 -1.097270
C -5.970923 -1.477568 -1.983916
H -5.575893 0.133717 -3.372828
H -6.040811 -3.057445 -0.503502
H -7.055403 -1.435664 -2.106173
S -3.402736 -3.708483 0.220659

O	-4.526636	-3.948954	1.173386
O	-2.247015	-3.083061	0.929069
O	-3.050711	-4.881917	-0.600796
Cu	-1.861070	0.776301	-0.217969
C	-1.401033	-3.251944	-3.550567
C	-1.798565	-4.562351	-3.869343
C	-1.378416	-2.279062	-4.567902
C	-2.168946	-4.890441	-5.176977
H	-1.819662	-5.332483	-3.109112
C	-1.750570	-2.611552	-5.873244
H	-1.076040	-1.263380	-4.349282
C	-2.146033	-3.916047	-6.177681
H	-2.473791	-5.901410	-5.414574
H	-1.732598	-1.857083	-6.649025
H	-2.433690	-4.172180	-7.189134
N	-1.767603	-1.713519	-1.646938
N	0.278644	-1.248550	-1.115393
C	-3.045679	1.529745	1.275695
C	-4.367085	2.001780	0.859508
C	-4.737656	3.341343	1.074444
C	-5.302375	1.149490	0.244709
C	-5.989759	3.810547	0.688233
C	-6.553263	1.618561	-0.141772
C	-6.905365	2.952761	0.076209
H	-6.254428	4.856226	0.868264
H	-7.259811	0.936442	-0.622359
H	-7.887244	3.320498	-0.230982
C	-2.747307	0.165124	1.541398
C	-1.511036	-0.236046	2.079911
H	-1.215101	-1.278649	1.960333
H	-0.698584	0.490492	2.132819
H	-5.038263	0.105611	0.052043
H	-3.497302	-0.615561	1.366329
P	-1.050460	-1.489391	4.683495
O	-0.908351	-1.167994	6.271492
O	-1.684200	-2.845366	4.556072
O	0.492821	-1.500212	4.149424
O	-1.678599	-0.260833	4.004487
Na	-3.202098	-3.648313	3.152202
H	-2.393534	2.290234	1.720969
H	-4.021469	4.011302	1.552340
C	-0.286275	0.040149	6.676874
H	-0.248091	0.041307	7.771860
H	0.740670	0.114720	6.286203
H	-0.854772	0.918126	6.337302
C	1.308287	-2.598896	4.513858
H	2.353717	-2.285562	4.428981
H	1.130334	-2.914545	5.553360
H	1.137490	-3.461112	3.852660
C	1.377911	-0.455859	-0.721432
C	2.173586	0.177396	-1.683278
C	1.777550	-0.427545	0.621475
C	3.345080	0.834126	-1.288805
C	2.955184	0.241142	0.993496
C	3.709845	0.860776	0.065522
H	4.631413	1.351833	0.358768
H	1.207973	-0.970298	1.364448
H	1.904562	0.129912	-2.731494
C	3.409070	0.201142	2.396690
C	2.960078	1.250389	3.359306
C	4.330303	-0.782243	2.839687
C	3.465936	1.193561	4.665468
C	4.768149	-0.748408	4.180675
C	4.351556	0.186794	5.045647
H	3.187156	1.939219	5.398181
H	5.469062	-1.490943	4.539196
H	4.722036	0.170320	6.063020
C	4.248027	1.408156	-2.303643
C	5.243595	0.589136	-2.907912
C	4.140093	2.780423	-2.659706
C	6.116547	1.165404	-3.848785
C	5.050911	3.313708	-3.590431
C	6.024082	2.513050	-4.177797
H	6.881798	0.570848	-4.330122
H	5.006284	4.357252	-3.872836
H	6.710469	2.940071	-4.897756
C	3.060362	3.689269	-2.074681
H	2.382058	3.125639	-1.401476
C	2.171659	4.267588	-3.182972
H	1.764653	3.447540	-3.812241
H	1.318400	4.814071	-2.736692
H	2.734347	4.972710	-3.829761
C	3.681584	4.803481	-1.224513
H	4.306660	4.360510	-0.419757
H	4.313058	5.476607	-1.841770
H	2.883572	5.410605	-0.747551
C	5.394957	-0.895107	-2.569184
H	4.665309	-1.209011	-1.795508

C	6.781309	-1.193018	-1.985666
H	6.824970	-2.244880	-1.630725
H	7.579706	-1.046559	-2.743007
H	6.980020	-0.524665	-1.121324
C	5.114465	-1.770477	-3.795997
H	5.155761	-2.844340	-3.514331
H	4.098675	-1.553537	-4.190687
H	5.859149	-1.590178	-4.599532
C	4.881354	-1.857763	1.903640
H	4.441521	-1.769168	0.889079
C	2.048628	2.394583	2.939992
H	1.646595	2.213196	1.921648
C	0.834845	2.519226	3.870848
H	0.362051	1.527337	4.014926
H	1.124509	2.920524	4.864633
H	0.080406	3.200611	3.425578
C	2.838193	3.706657	2.881536
H	3.238420	3.976062	3.882132
H	3.686381	3.606011	2.170678
H	2.189134	4.532948	2.527492
C	4.524589	-3.264626	2.396178
H	4.985625	-3.481029	3.382296
H	3.423259	-3.364295	2.483018
H	4.884461	-4.023431	1.669482
C	6.397016	-1.706140	1.730375
H	6.637493	-0.678357	1.384083
H	6.933143	-1.897878	2.683601
H	6.766916	-2.426117	0.969781
H	0.346398	-3.558000	0.494218
H	1.874840	-5.242580	1.439555
C	1.166444	-3.925061	-0.107979
C	2.034761	-4.876095	0.433792
C	1.363253	-3.445314	-1.416304
C	3.116273	-5.344552	-0.315781
H	3.792411	-6.075275	0.108651
C	2.456119	-3.922428	-2.160917
C	3.329433	-4.864561	-1.610018
H	2.633307	-3.566923	-3.167924
H	4.170637	-5.224386	-2.188181
C	-1.878370	2.255894	-1.576789
H	-2.964421	2.199843	-1.805749
C	-1.062572	1.947448	-2.821609
H	-1.261019	0.948810	-3.244535
H	-1.228289	2.674790	-3.637236
H	0.019214	1.975862	-2.614567
B	-1.639499	3.693081	-1.047211
O	-1.893023	4.166950	0.227084
O	-1.178843	4.710027	-1.867968
C	-1.455166	5.962104	-1.204981
C	-1.444463	5.539956	0.296340
C	-0.406829	6.984593	-1.583464
H	0.608299	6.647940	-1.343582
H	-0.447845	7.187841	-2.662038
H	-0.582614	7.934367	-1.057640
C	-2.832186	6.413857	-1.670214
H	-3.609283	5.692547	-1.376305
H	-3.102370	7.396159	-1.258606
H	-2.841238	6.491256	-2.765583
C	-2.383311	6.329868	1.182776
H	-2.102047	7.392957	1.198716
H	-3.426680	6.258672	0.851035
H	-2.333018	5.959039	2.216242
C	-0.046753	5.521720	0.889254
H	-0.086206	5.065983	1.886181
H	0.640750	4.928954	0.270187
H	0.368382	6.532829	0.998851

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Figure_S7_imid-3_modeA_ts(AS)_06 / electronic energy: -4442.737863528388 a.u. / lowest freq: -260.51 cm-1

C	-0.661713	-2.736399	-2.391476
H	-1.139213	-3.543506	-1.814370
C	0.785790	-2.453215	-1.950892
H	1.427027	-2.144531	-2.794982
C	-0.600210	-0.707111	-1.191379
C	-2.694524	-1.171462	-2.343440
C	-2.942549	-0.157338	-3.275148
C	-3.778784	-1.882125	-1.799163
C	-4.237478	0.122361	-3.701178
H	-2.091983	0.397016	-3.677350
C	-5.075905	-1.597431	-2.234667
C	-5.305598	-0.614247	-3.193795
H	-4.406929	0.913180	-4.434893
H	-5.903116	-2.159403	-1.797362
H	-6.325124	-0.412571	-3.529979
S	-3.583051	-3.197015	-0.589846
O	-4.911202	-3.313672	0.081166
O	-2.544492	-2.741275	0.381095
O	-3.203299	-4.393719	-1.366365
Cu	-1.382423	0.986755	-0.517238

C	-0.789968	-3.027850	-3.865539
C	-1.285459	-4.270152	-4.299572
C	-0.427471	-2.064921	-4.826183
C	-1.420539	-4.539882	-5.664725
H	-1.565336	-5.032552	-3.584007
C	-0.565336	-2.338651	-6.189685
H	-0.041066	-1.102354	-4.519904
C	-1.062220	-3.574800	-6.608863
H	-1.803341	-5.498323	-5.990755
H	-0.286843	-1.591601	-6.921629
H	-1.168284	-3.785441	-7.665161
N	-1.337220	-1.464316	-2.021692
N	0.592007	-1.297115	-1.055268
C	-2.731113	1.929910	0.683871
C	-3.836909	2.586360	-0.015185
C	-4.026851	3.974495	0.110426
C	-4.739537	1.869359	-0.821982
C	-5.067746	4.620186	-0.550833
C	-5.779447	2.515005	-1.483345
C	-5.949377	3.895469	-1.354808
H	-5.192890	5.700509	-0.436450
H	-6.462201	1.934424	-2.109744
H	-6.764147	4.401941	-1.877493
C	-2.709057	0.536321	0.984448
C	-1.781009	-0.022469	1.883176
H	-1.638605	-1.104182	1.863051
H	-0.915502	0.569700	2.182525
H	-4.616462	0.789572	-0.944307
H	-3.486785	-0.134837	0.599411
P	-3.371966	-1.125760	4.011411
O	-4.615309	-1.199251	2.929896
O	-2.848868	-2.533533	4.017287
O	-4.068140	-0.669187	5.402088
O	-2.477691	0.076380	3.669380
Na	-3.973359	-3.532406	2.272917
H	-2.111744	2.589072	1.303834
H	-3.337432	4.541500	0.737473
C	-5.430995	-0.062730	2.691446
H	-5.883558	-0.173003	1.697536
H	-6.231584	0.011028	3.442952
H	-4.839474	0.865145	2.710457
C	-4.849619	-1.611470	6.120158
H	-5.192386	-1.121179	7.037877
H	-5.731312	-1.929080	5.541325
H	-4.261982	-2.501770	6.385868
C	1.660039	-0.687502	-0.362890
C	2.780375	-0.216792	-1.057914
C	1.670383	-0.674138	1.037873
C	3.882672	0.269432	-0.344977
C	2.788424	-0.184182	1.731236
C	3.858262	0.281242	1.057769
H	4.726667	0.636635	1.601770
H	0.840057	-1.098337	1.585975
H	2.806321	-0.250576	-2.140197
C	2.823244	-0.243108	3.205037
C	2.461413	0.961165	4.009138
C	3.311942	-1.391221	3.878748
C	2.669939	0.905720	5.394177
C	3.459709	-1.345116	5.281355
C	3.159277	-0.252045	5.996646
H	2.449952	1.760821	6.019715
H	3.842735	-2.206388	5.813116
H	3.301962	-0.265243	7.070028
C	5.102044	0.684248	-1.063640
C	6.113386	-0.275323	-1.352036
C	5.271175	2.039946	-1.458717
C	7.275357	0.144774	-2.024907
C	6.455412	2.410767	-2.122374
C	7.442843	1.472599	-2.401054
H	8.062851	-0.558762	-2.260914
H	6.618727	3.434505	-2.432309
H	8.345344	1.777020	-2.915491
C	4.207039	3.103866	-1.193466
H	3.320805	2.669245	-0.686950
C	3.694161	3.703895	-2.508299
H	3.344008	2.895239	-3.184767
H	2.839086	4.379502	-2.308290
H	4.485342	4.287117	-3.024302
C	4.742326	4.195103	-0.258312
H	5.102280	3.738478	0.688307
H	5.577980	4.755311	-0.727812
H	3.936002	4.916119	-0.009815
C	5.977844	-1.746949	-0.957348
H	5.024203	-1.935609	-0.423619
C	7.092431	-2.165842	0.008864
H	6.905132	-3.195941	0.380580
H	8.085636	-2.147614	-0.486963
H	7.114967	-1.479389	0.881801

C	5.955225	-2.649008	-2.196846
H	5.771524	-3.702453	-1.896925
H	5.136989	-2.333517	-2.879037
H	6.918740	-2.605077	-2.746686
C	3.716757	-2.659502	3.128597
H	3.521982	-2.560497	2.040881
C	1.907129	2.223839	3.366915
H	1.686169	2.043555	2.294125
C	0.582501	2.646977	4.018367
H	-0.101356	1.776871	4.100743
H	0.746671	3.065347	5.033660
H	0.081288	3.419215	3.400097
C	2.942191	3.352061	3.429377
H	3.174986	3.622200	4.481339
H	3.879590	3.033313	2.925331
H	2.561483	4.254372	2.909287
C	2.897306	-3.868048	3.597116
H	3.084410	-4.097890	4.666623
H	1.813583	-3.668133	3.455167
H	3.169687	-4.764322	3.001068
C	5.219486	-2.924698	3.273140
H	5.793776	-2.030121	2.951578
H	5.487042	-3.163702	4.323998
H	5.518273	-3.779688	2.629628
H	0.015078	-3.638525	0.409970
H	1.084237	-5.529949	1.568765
C	0.895980	-4.093492	-0.022239
C	1.504182	-5.161225	0.642000
C	1.428115	-3.612212	-1.232898
C	2.658965	-5.746124	0.117733
H	3.133650	-6.567470	0.638621
C	2.589513	-4.209836	-1.752919
C	3.201839	-5.269854	-1.077729
H	3.022605	-3.856608	-2.680068
H	4.096709	-5.723962	-1.482978
C	-0.881528	2.423973	-1.832286
H	-1.892814	2.514831	-2.285968
C	0.124977	1.964076	-2.874408
H	-0.135590	1.004542	-3.349246
H	0.261359	2.694589	-3.692374
H	1.125304	1.819833	-2.435520
B	-0.549514	3.833391	-1.277602
O	-0.986278	4.397185	-0.094601
O	0.213185	4.735918	-2.002346
C	-0.012798	6.045575	-1.441083
C	-0.384958	5.705756	0.035910
C	1.231857	6.889476	-1.605434
H	2.114702	6.412985	-1.164035
H	1.437805	7.056128	-2.671350
H	1.103018	7.873838	-1.132327
C	-1.176873	6.657718	-2.207426
H	-2.095917	6.067173	-2.076698
H	-1.382996	7.689106	-1.889261
H	-0.939303	6.675973	-3.279500
C	-1.381591	6.652492	0.670413
H	-0.974190	7.672949	0.718733
H	-2.328146	6.689709	0.116802
H	-1.604865	6.336726	1.699200
C	0.835119	5.551134	0.925496
H	0.520654	5.180971	1.908241
H	1.548517	4.831515	0.501928
H	1.355121	6.505813	1.082314

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Figure_S7_imid-3_modeA_prod(AS) / electronic energy: -4442.756176396671 a.u. / lowest freq: 11.29 cm-1

C	-0.763660	-0.463398	3.227790
H	-1.006651	0.528649	3.635178
C	0.706409	-0.584791	2.787990
H	1.088653	-1.615173	2.891992
C	-0.646813	-0.424628	0.887647
C	-2.881673	-0.689731	1.742250
C	-3.372946	-1.829431	1.096926
C	-3.767158	0.332625	2.124039
C	-4.737267	-1.966990	0.846942
H	-2.658959	-2.610571	0.816592
C	-5.130934	0.182430	1.864560
C	-5.618909	-0.959519	1.233375
H	-5.113074	-2.869126	0.357389
H	-5.802615	0.992604	2.154819
H	-6.689454	-1.059124	1.043523
S	-3.235197	1.847096	2.941839
O	-4.328214	2.826916	2.699521
O	-1.982239	2.267013	2.239874
O	-3.040427	1.481793	4.356075
Cu	-1.310699	-0.629541	-0.968394
C	-1.174396	-1.534025	4.204310
C	-1.512392	-1.190196	5.524946
C	-1.211019	-2.887760	3.820399
C	-1.892526	-2.177823	6.438083

H	-1.473574	-0.159579	5.853064
C	-1.590711	-3.871895	4.738246
H	-0.945949	-3.179159	2.812405
C	-1.933396	-3.517117	6.044732
H	-2.151935	-1.904711	7.452746
H	-1.617266	-4.911133	4.440084
H	-2.226329	-4.280670	6.753666
N	-1.472100	-0.598662	1.926159
N	0.597720	-0.290263	1.344942
C	-2.423510	-0.325389	-2.720427
C	-3.129785	-1.370452	-3.452778
C	-2.766445	-1.667914	-4.779363
C	-4.196341	-2.085094	-2.877543
C	-3.444804	-2.645060	-5.501939
C	-4.881655	-3.049226	-3.605230
C	-4.506062	-3.338066	-4.919174
H	-3.148817	-2.860690	-6.530883
H	-5.707109	-3.592797	-3.139296
H	-5.041065	-4.102052	-5.487649
C	-2.998101	0.403042	-1.639910
C	-2.253308	1.332262	-0.936400
H	-2.614966	1.791197	-0.014788
H	-1.385282	1.808658	-1.401727
H	-4.482396	-1.891125	-1.840141
H	-3.960627	0.075267	-1.225446
P	-2.760592	4.771324	-1.362028
O	-3.967859	4.013957	-0.472379
O	-1.936361	5.378003	-0.248878
O	-3.621140	5.933202	-2.149686
O	-2.229445	3.854593	-2.420407
Na	-2.821163	4.459581	1.628092
H	-1.605183	0.170140	-3.262281
H	-1.950598	-1.110037	-5.246706
C	-4.987180	3.311697	-1.143452
H	-5.440077	2.600143	-0.438053
H	-5.774600	3.991715	-1.509375
H	-4.585878	2.755252	-2.006177
C	-4.175799	6.989738	-1.399464
H	-4.640100	7.696834	-2.098670
H	-4.954146	6.635187	-0.701696
H	-3.409336	7.522855	-0.815701
C	1.696963	0.001133	0.504781
C	2.868269	-0.762753	0.580661
C	1.644524	1.101880	-0.361983
C	3.975523	-0.431553	-0.207640
C	2.767797	1.464679	-1.117385
C	3.932780	0.691790	-1.040968
H	4.802650	0.962606	-1.627969
H	0.754385	1.714968	-0.397303
H	2.914047	-1.623238	1.236900
C	2.744634	2.690113	-1.945637
C	2.719986	2.595243	-3.367672
C	2.764642	3.970747	-1.319145
C	2.729425	3.779102	-4.128001
C	2.742263	5.122541	-2.126992
C	2.732153	5.024819	-3.512843
H	2.725433	3.742688	-5.209339
H	2.743558	6.109611	-1.683892
H	2.727251	5.923584	-4.116196
C	5.178303	-1.280425	-0.177616
C	6.272748	-0.934809	0.662012
C	5.241115	-2.441723	-0.997204
C	7.417927	-1.752035	0.651785
C	6.401693	-3.235554	-0.958577
C	7.477102	-2.889688	-0.146743
H	8.273626	-1.512400	1.269151
H	6.481365	-4.127829	-1.565511
H	8.364696	-3.509244	-0.136152
C	4.090683	-2.848570	-1.920828
H	3.257329	-2.119632	-1.870353
C	3.497510	-4.199259	-1.502103
H	3.158649	-4.152051	-0.444842
H	2.617821	-4.443003	-2.134936
H	4.241805	-5.016372	-1.606559
C	4.535573	-2.867316	-3.388175
H	4.972008	-1.883261	-3.663587
H	5.289567	-3.661066	-3.572280
H	3.661429	-3.053849	-4.048097
C	6.241959	0.293558	1.572645
H	5.265126	0.815539	1.510484
C	7.301175	1.317389	1.149210
H	7.206240	2.238839	1.762779
H	8.326929	0.911869	1.277569
H	7.153936	1.595089	0.083402
C	6.411296	-0.100069	3.045216
H	6.283096	0.793140	3.693245
H	5.640328	-0.848473	3.328097
H	7.417128	-0.528183	3.238129

C	2.818211	4.141047	0.200863
H	2.893923	3.163681	0.716631
C	2.670019	1.253479	-4.098757
H	2.605708	0.411829	-3.382082
C	1.422323	1.147310	-4.986969
H	0.509089	1.333528	-4.382565
H	1.454436	1.876040	-5.823506
H	1.349965	0.126995	-5.420739
C	3.946623	1.024471	-4.915968
H	4.043086	1.773607	-5.729935
H	4.837577	1.093641	-4.256035
H	3.930570	0.010366	-5.369654
C	1.537115	4.806066	0.717848
H	1.421676	5.831476	0.307939
H	0.653509	4.199965	0.425350
H	1.558324	4.873364	1.825199
C	4.063503	4.924564	0.634987
H	4.977070	4.438894	0.229604
H	4.026050	5.976352	0.282115
H	4.139027	4.931108	1.743671
H	0.735509	2.169379	2.681284
H	2.290933	3.704496	3.827651
C	1.503578	1.763126	3.326487
C	2.387353	2.636440	3.967358
C	1.625904	0.371806	3.503382
C	3.398279	2.132789	4.788540
H	4.082937	2.810530	5.281672
C	2.648375	-0.123581	4.331496
C	3.526187	0.754564	4.973099
H	2.769835	-1.189354	4.479583
H	4.311009	0.365354	5.608674
C	-0.147633	-2.160675	-1.608635
H	0.691385	-1.999019	-0.916196
C	0.301498	-2.025955	-3.040476
H	0.714844	-1.035797	-3.274432
H	1.098182	-2.753208	-3.274639
H	-0.506302	-2.233080	-3.754663
B	-0.825459	-3.488988	-1.220756
O	-0.943651	-3.928370	0.085644
O	-1.288470	-4.413500	-2.125606
C	-1.877564	-5.508449	-1.378846
C	-1.211942	-5.352084	0.028010
C	-3.377940	-5.277619	-1.346335
H	-3.626348	-4.325216	-0.854609
H	-3.764299	-5.230704	-2.372702
H	-3.905218	-6.086160	-0.821974
C	-1.557761	-6.808920	-2.083107
H	-0.481944	-6.926506	-2.259447
H	-1.907123	-7.669051	-1.494031
H	-2.062720	-6.845013	-3.057528
C	0.135435	-6.050669	0.126351
H	0.030096	-7.143587	0.156416
H	0.785511	-5.792106	-0.721061
H	0.643516	-5.733881	1.046981
C	-2.099055	-5.744181	1.187840
H	-1.551699	-5.643517	2.133042
H	-3.000559	-5.121868	1.249423
H	-2.412151	-6.794310	1.100040

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Figure_S7_imid-3_modeB_ed(AS) / electronic energy: -4442.756430877589 a.u. / lowest freq: 17.76 cm-1

C	0.727062	3.324353	-1.090977
H	0.540394	3.890817	-0.166269
C	-0.530732	2.619811	-1.613567
H	-0.450301	2.399429	-2.694020
C	0.833106	1.028773	-0.578092
C	2.928364	2.160798	-0.337095
C	3.826289	1.385012	-1.077763
C	3.386284	2.839783	0.806452
C	5.166236	1.301811	-0.711119
H	3.462420	0.843683	-1.953909
C	4.735906	2.756679	1.159000
C	5.626500	1.996128	0.405732
H	5.844112	0.698561	-1.318096
H	5.068265	3.284585	2.054318
H	6.677666	1.943855	0.697188
S	2.316203	3.812574	1.874280
O	3.054941	3.932016	3.166767
O	1.067355	3.010655	2.065882
O	2.109723	5.097586	1.182836
Cu	1.656814	-0.767824	-0.462763
C	1.374210	4.219525	-2.115863
C	1.356198	5.614746	-1.942493
C	1.982575	3.684400	-3.265655
C	1.949450	6.453668	-2.890626
H	0.875424	6.055884	-1.078757
C	2.575826	4.525983	-4.210608
H	1.999679	2.617872	-3.429338
C	2.561005	5.909773	-4.022526

H	1.932088	7.526544	-2.749024
H	3.045660	4.104799	-5.089985
H	3.019521	6.560641	-4.755690
N	1.567580	2.147117	-0.747962
N	-0.434524	1.334756	-0.891927
C	2.249115	-2.342430	0.717889
C	1.557485	-3.555089	0.263672
C	2.253195	-4.767161	0.134321
C	0.198533	-3.538397	-0.093561
C	1.613906	-5.919143	-0.317243
C	-0.441658	-4.685851	-0.547148
C	0.261346	-5.886503	-0.658240
H	2.179071	-6.850289	-0.409541
H	-1.499884	-4.645668	-0.811737
H	-0.241054	-6.787361	-1.018356
C	1.657018	-1.323802	1.488311
C	2.465316	-0.328945	2.234904
H	3.459766	-0.191269	1.784618
H	1.976583	0.657579	2.286675
H	-0.347770	-2.589731	-0.053261
H	0.618214	-1.444954	1.819665
P	1.729638	-0.447144	4.786367
O	2.510545	-0.928260	6.095357
O	1.238036	0.948467	4.945949
O	0.553003	-1.520937	4.534629
O	2.750123	-0.766546	3.614589
Na	1.278149	3.121225	4.528468
H	3.345066	-2.387159	0.680557
H	3.317818	-4.795296	0.380623
C	3.080252	-2.234926	6.171086
H	3.414919	-2.379399	7.202842
H	2.337977	-3.005034	5.919257
H	3.938636	-2.323638	5.492589
C	-0.641826	-1.416263	5.305105
H	-1.186399	-2.357420	5.186326
H	-0.424074	-1.271577	6.373044
H	-1.263833	-0.583664	4.950266
C	-1.501799	0.435295	-0.671681
C	-2.358954	0.085449	-1.720800
C	-1.784260	-0.006520	0.632230
C	-3.484913	-0.709499	-1.475861
C	-2.946698	-0.750174	0.894533
C	-3.781131	-1.119316	-0.168970
H	-4.683064	-1.687811	0.024900
H	-1.151173	0.308995	1.452882
H	-2.158882	0.442106	-2.723866
C	-3.367434	-1.038105	2.289728
C	-3.361077	-2.375237	2.786538
C	-3.854641	0.016923	3.118989
C	-3.858898	-2.627192	4.078638
C	-4.305295	-0.287444	4.417255
C	-4.315583	-1.593943	4.884163
H	-3.883531	-3.632478	4.477638
H	-4.668419	0.490965	5.075052
H	-4.679494	-1.807662	5.880985
C	-4.398495	-1.050510	-2.584133
C	-5.634369	-0.356319	-2.723888
C	-4.037628	-2.061176	-3.520347
C	-6.498053	-0.713945	-3.775159
C	-4.916238	-2.345986	-4.582057
C	-6.136389	-1.689728	-4.696734
H	-7.454097	-0.222304	-3.897364
H	-4.663512	-3.089623	-5.326046
H	-6.805950	-1.936111	-5.510877
C	-2.727233	-2.843696	-3.413324
H	-2.177795	-2.580592	-2.486539
C	-1.793706	-2.505572	-4.580887
H	-1.617058	-1.409468	-4.620109
H	-0.812749	-3.008757	-4.442172
H	-2.227351	-2.834566	-5.548867
C	-2.979875	-4.355647	-3.331876
H	-3.642906	-4.582979	-2.469719
H	-3.448657	-4.743174	-4.259928
H	-2.019699	-4.894512	-3.186459
C	-6.045018	0.778158	-1.782822
H	-5.235416	1.017775	-1.063979
C	-7.265494	0.380558	-0.945582
H	-7.505924	1.184727	-0.217623
H	-8.154254	0.207996	-1.588704
H	-7.048194	-0.548077	-0.375862
C	-6.306604	2.078029	-2.554595
H	-6.456397	2.917713	-1.842688
H	-5.434405	2.317763	-3.199210
H	-7.212087	1.998185	-3.191656
C	-3.922340	1.470998	2.652042
H	-3.598272	1.574548	1.599670
C	-2.819418	-3.548543	1.975846
H	-2.430037	-3.201942	1.001436

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C  -1.642956  -4.223704   2.696912
H  -0.822791  -3.490744   2.850207
H  -1.946976  -4.634894   3.681509
H  -1.248659  -5.063896   2.088979
C  -3.925948  -4.561908   1.660624
H  -4.302100  -5.048477   2.585053
H  -4.772434  -4.054661   1.150524
H  -3.536080  -5.350204   0.981556
C  -2.983637   2.349130   3.489967
H  -3.292228   2.367823   4.556139
H  -1.944726   1.960910   3.424102
H  -2.987095   3.391371   3.111653
C  -5.361245   2.003145   2.684839
H  -6.025748   1.333339   2.097863
H  -5.746046   2.074168   3.723501
H  -5.403461   3.015015   2.229022
H  -1.621283   3.341754   0.815389
H  -3.696849   4.623305   1.209356
C  -2.213288   3.669828  -0.029206
C  -3.391209   4.388213   0.199663
C  -1.804906   3.377777  -1.343350
C  -4.175489   4.811202  -0.874916
H  -5.088347   5.363825  -0.694454
C  -2.604066   3.807521  -2.417867
C  -3.781201   4.522643  -2.182446
H  -2.315778   3.593887  -3.439544
H  -4.389916   4.850973  -3.014950
C   1.812957  -1.442286  -2.389526
H   1.127501  -2.298590  -2.256698
C   1.315304  -0.487699  -3.455705
H   0.347936  -0.014935  -3.214497
H   2.029913   0.331408  -3.632100
H   1.177486  -0.969592  -4.442739
B   3.251008  -1.919579  -2.499910
O   4.289971  -1.186109  -3.089110
O   3.731876  -3.147677  -2.044476
C   5.164477  -3.131289  -2.148412
C   5.390267  -2.092567  -3.292710
C   5.724457  -2.650807  -0.816720
H   5.372152  -1.633817  -0.583047
H   5.387918  -3.318802  -0.011276
H   6.823647  -2.646457  -0.804931
C   5.652272  -4.531447  -2.455128
H   5.154542  -4.949389  -3.338801
H   6.738163  -4.544308  -2.630339
H   5.443022  -5.200539  -1.608292
C   5.219224  -2.710603  -4.674095
H   6.056697  -3.371328  -4.938505
H   4.288876  -3.292738  -4.737529
H   5.168126  -1.912608  -5.427348
C   6.700976  -1.339842  -3.221935
H   6.758481  -0.597171  -4.029651
H   6.828919  -0.811098  -2.269677
H   7.551992  -2.026761  -3.339744
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Figure_S7_imid-3_modeB_ts(AS)_01 / electronic energy: -4442.742828980603 a.u. / lowest freq: -268.37 cm-1
C   0.693791   3.551061  -0.293825
H   0.527794   3.881407   0.741837
C  -0.570367   2.972004  -0.941155
H  -0.521514   3.017285  -2.044502
C   0.833170   1.209036  -0.338108
C   2.917575   2.267758   0.156216
C   3.826414   1.717763  -0.751815
C   3.354737   2.622887   1.445719
C   5.159602   1.530450  -0.397387
H   3.479744   1.436642  -1.748681
C   4.697376   2.442011   1.784619
C   5.599107   1.899652   0.871502
H   5.847957   1.101685  -1.127871
H   5.016621   2.713511   2.792153
H   6.643936   1.761923   1.157529
S   2.255677   3.274995   2.713000
O   3.001438   3.124673   3.996713
O   1.048687   2.392249   2.702949
O   1.988690   4.675492   2.338760
Cu  1.643244  -0.579051  -0.589585
C   1.313134   4.668470  -1.091990
C   1.308570   5.980809  -0.586835
C   1.886046   4.426843  -2.353793
C   1.878928   7.024277  -1.322086
H   0.855849   6.200760   0.371529
C   2.456372   5.472290  -3.085195
H   1.893014   3.431112  -2.770139
C   2.454484   6.770015  -2.569107
H   1.871860   8.031405  -0.925766
H   2.898561   5.276097  -4.053403
H   2.895308   7.579042  -3.137041
N   1.555386   2.338897  -0.251584
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N	-0.442977	1.552137	-0.552319
C	2.218793	-2.442632	0.053504
C	1.611841	-3.562632	-0.671801
C	2.377710	-4.685511	-1.021100
C	0.260773	-3.539512	-1.055213
C	1.807683	-5.756180	-1.704258
C	-0.311039	-4.606296	-1.739119
C	0.459461	-5.724119	-2.063193
H	2.421808	-6.622463	-1.962404
H	-1.366870	-4.569571	-2.013187
H	0.011359	-6.562146	-2.601863
C	1.556654	-1.742417	1.096779
C	2.195266	-0.753334	1.874643
H	3.204366	-0.432322	1.600138
H	1.598520	0.004421	2.387568
H	-0.336397	-2.647295	-0.841127
H	0.522017	-2.002157	1.344499
P	1.798099	-1.615355	4.622967
O	2.397206	-2.494050	5.852790
O	1.240577	-0.350006	5.207138
O	0.603802	-2.551218	4.015432
O	2.859632	-1.577980	3.510710
Na	1.384930	1.839780	5.135052
H	3.315861	-2.403754	0.034480
H	3.436332	-4.710673	-0.751600
C	2.949171	-3.772682	5.585030
H	3.298795	-4.188112	6.536866
H	2.196772	-4.452477	5.155884
H	3.798494	-3.705303	4.889991
C	-0.586525	-2.681888	4.771251
H	-1.130556	-3.553356	4.390511
H	-0.377112	-2.847173	5.839477
H	-1.222473	-1.789473	4.675833
C	-1.492590	0.605025	-0.554425
C	-2.361881	0.518561	-1.647580
C	-1.747334	-0.161309	0.596566
C	-3.471067	-0.333447	-1.600679
C	-2.896151	-0.967156	0.674056
C	-3.741843	-1.066633	-0.438481
H	-4.633904	-1.679487	-0.385683
H	-1.106054	-0.055348	1.463389
H	-2.183657	1.121579	-2.529556
C	-3.298830	-1.602806	1.955018
C	-3.292213	-3.022992	2.092365
C	-3.782856	-0.795800	3.029042
C	-3.789095	-3.597486	3.277475
C	-4.226293	-1.422811	4.208588
C	-4.239110	-2.805272	4.323765
H	-3.817432	-4.671439	3.404475
H	-4.584252	-0.839115	5.046222
H	-4.600079	-3.267419	5.233654
C	-4.392149	-0.404333	-2.751211
C	-5.636962	0.285948	-2.707227
C	-4.030835	-1.153272	-3.906963
C	-6.508743	0.182545	-3.806420
C	-4.919567	-1.186551	-4.997489
C	-6.147883	-0.537724	-4.939434
H	-7.471229	0.676745	-3.797539
H	-4.667931	-1.726128	-5.900799
H	-6.824562	-0.589358	-5.782804
C	-2.708732	-1.917442	-4.004250
H	-2.146517	-1.871457	-3.049244
C	-1.798799	-1.298750	-5.071166
H	-1.639270	-0.220799	-4.854640
H	-0.808303	-1.802332	-5.065270
H	-2.242293	-1.400263	-6.084205
C	-2.940499	-3.409768	-4.276959
H	-3.578853	-3.845865	-3.478808
H	-3.427559	-3.575436	-5.260116
H	-1.970082	-3.949635	-4.283348
C	-6.049088	1.150577	-1.514040
H	-5.234892	1.215547	-0.764011
C	-7.257404	0.546083	-0.790727
H	-7.496818	1.143611	0.114877
H	-8.151404	0.527711	-1.449274
H	-7.026255	-0.491846	-0.468997
C	-6.329984	2.596812	-1.941968
H	-6.484254	3.234107	-1.045073
H	-5.464606	2.998260	-2.511012
H	-7.238692	2.664553	-2.575835
C	-3.858082	0.729088	2.949144
H	-3.546709	1.099205	1.954752
C	-2.754213	-3.950785	1.006596
H	-2.356371	-3.367929	0.155332
C	-1.587212	-4.800674	1.532688
H	-0.761313	-4.141197	1.872769
H	-1.899333	-5.449462	2.376707
H	-1.197548	-5.460362	0.730740

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C  -3.866881  -4.839481   0.438093
H  -4.251118  -5.544068   1.205425
H  -4.707399  -4.211517   0.073445
H  -3.479896  -5.430052  -0.419764
C  -2.911198   1.368280   3.973256
H  -3.209330   1.114836   5.012142
H  -1.873245   1.011553   3.801100
H  -2.918114   2.472420   3.871224
C  -5.297299   1.229682   3.131332
H  -5.967615   0.728373   2.400457
H  -5.670616   1.033394   4.157970
H  -5.345924   2.323929   2.948064
H  -1.598043   3.050471   1.616157
H  -3.672990   4.160682   2.369114
C  -2.216684   3.569166   0.895202
C  -3.394222   4.188951   1.325170
C  -1.842880   3.619479  -0.460094
C  -4.212716   4.852634   0.409499
H  -5.125359   5.328105   0.744571
C  -2.675620   4.290068  -1.373542
C  -3.852527   4.904908  -0.938149
H  -2.413941   4.341741  -2.422979
H  -4.487525   5.420069  -1.647215
C   1.789540  -0.805965  -2.606845
H   1.121408  -1.681752  -2.678225
C   1.268684   0.363214  -3.412373
H   0.285866   0.733667  -3.080790
H   1.960345   1.218611  -3.389632
H   1.151791   0.111481  -4.482725
B   3.242931  -1.219678  -2.856602
O   4.247605  -0.348891  -3.271684
O   3.730629  -2.511186  -2.728361
C   5.165157  -2.455514  -2.859460
C   5.358897  -1.162817  -3.713616
C   5.749920  -2.317248  -1.461490
H   5.401987  -1.393824  -0.972657
H   5.434457  -3.167494  -0.840777
H   6.848688  -2.307213  -1.471502
C   5.647566  -3.731105  -3.515036
H   5.123967  -3.929314  -4.458277
H   6.727129  -3.687335  -3.719981
H   5.470087  -4.588397  -2.850811
C   5.163731  -1.416267  -5.201338
H   5.996316  -1.989066  -5.632734
H   4.232008  -1.967019  -5.392919
H   5.102851  -0.456451  -5.731778
C   6.660039  -0.430623  -3.475107
H   6.689966   0.494694  -4.066317
H   6.803986  -0.162907  -2.421719
H   7.515246  -1.049983  -3.782028
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Figure_S7_imid-3_modeB_ts(AS)_02 / electronic energy: -4442.738705631423 a.u. / lowest freq: -273.52 cm-1
C   0.627776  -1.803124   2.917779
H   0.644635  -2.823216   2.508014
C  -0.743404  -1.131415   2.785837
H  -0.862564  -0.306955   3.512668
C   0.668847  -0.271708   1.141657
C   2.852198  -0.970584   1.832654
C   3.539306   0.234531   2.004039
C   3.556178  -2.113618   1.407941
C   4.910874   0.311042   1.778646
H   2.987214   1.120675   2.324363
C   4.935037  -2.027394   1.204197
C   5.614607  -0.825316   1.387749
H   5.421350   1.264002   1.929736
H   5.462428  -2.923651   0.873284
H   6.692776  -0.779358   1.219839
S   2.756878  -3.685313   1.046215
O   3.762559  -4.478529   0.283423
O   1.590937  -3.334198   0.175873
O   2.393996  -4.278118   2.345521
Cu  1.316726   1.187671  -0.026857
C   1.145605  -1.813881   4.332465
C   1.213591  -3.023243   5.046522
C   1.539762  -0.623701   4.970476
C   1.685406  -3.042994   6.362399
H   0.892015  -3.950576   4.590158
C   2.012236  -0.647605   6.285568
H   1.483959   0.320763   4.450964
C   2.087206  -1.856682   6.980561
H   1.735840  -3.978469   6.904393
H   2.318350   0.272365   6.766588
H   2.451806  -1.873689   7.999466
N   1.440625  -0.939523   2.016023
N  -0.611066  -0.519865   1.448074
C   1.866712   2.001788  -1.822902
C   1.045553   3.132829  -2.263873
C   1.636707   4.258794  -2.857142
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C	-0.348089	3.130250	-2.092321
C	0.858815	5.328667	-3.291031
C	-1.127758	4.195556	-2.527352
C	-0.527441	5.299925	-3.134018
H	1.338798	6.193688	-3.755373
H	-2.211136	4.160077	-2.401350
H	-1.138909	6.138952	-3.473680
C	1.472091	0.647952	-1.997950
C	2.322167	-0.435670	-1.692992
H	3.258061	-0.236650	-1.160770
H	1.885261	-1.420454	-1.510501
H	-0.816138	2.286752	-1.573861
H	0.492491	0.425493	-2.434698
P	3.197868	-2.395818	-3.643076
O	4.278361	-3.172612	-2.672323
O	1.948756	-3.212778	-3.474553
O	3.852593	-2.468886	-5.124577
O	3.236004	-0.892646	-3.327993
Na	2.461794	-4.641832	-1.718133
H	2.939620	2.204820	-1.712107
H	2.722819	4.288864	-2.972456
C	5.571040	-2.633206	-2.460548
H	6.066275	-3.244710	-1.697460
H	6.171458	-2.660465	-3.383210
H	5.518214	-1.591757	-2.108487
C	3.949887	-3.731702	-5.765103
H	4.368113	-3.563119	-6.763442
H	4.618355	-4.411403	-5.213586
H	2.964286	-4.208557	-5.866095
C	-1.680584	-0.131180	0.608699
C	-2.756811	0.596703	1.127602
C	-1.729004	-0.587505	-0.719638
C	-3.867207	0.884359	0.324712
C	-2.865818	-0.355374	-1.511527
C	-3.922160	0.404341	-0.991243
H	-4.806946	0.580314	-1.591325
H	-0.924108	-1.202700	-1.103539
H	-2.737704	0.926837	2.159014
C	-3.018910	-1.022509	-2.830224
C	-3.005264	-0.260702	-4.036853
C	-3.245438	-2.431092	-2.891511
C	-3.222019	-0.917800	-5.262604
C	-3.420482	-3.040731	-4.147957
C	-3.415236	-2.290733	-5.315179
H	-3.237425	-0.366206	-6.193137
H	-3.581495	-4.107538	-4.229201
H	-3.568408	-2.777685	-6.269826
C	-5.011038	1.625449	0.893437
C	-6.200596	0.928569	1.252777
C	-4.916237	3.030919	1.104972
C	-7.282421	1.658942	1.777409
C	-6.008776	3.704534	1.681963
C	-7.181043	3.027536	1.997803
H	-8.208467	1.164631	2.039658
H	-5.961783	4.766480	1.882811
H	-8.016865	3.567738	2.423756
C	-3.666133	3.830795	0.732783
H	-2.930127	3.196905	0.197410
C	-2.959475	4.352325	1.988867
H	-2.718954	3.507122	2.668386
H	-2.007242	4.852530	1.709937
H	-3.597081	5.080493	2.533494
C	-3.997575	4.981663	-0.227408
H	-4.501370	4.585292	-1.134923
H	-4.655398	5.737174	0.249701
H	-3.063901	5.495180	-0.540568
C	-6.333324	-0.589394	1.112285
H	-5.379543	-1.048154	0.781881
C	-7.380514	-0.952133	0.053726
H	-7.414595	-2.053787	-0.086040
H	-8.391145	-0.602146	0.352713
H	-7.112818	-0.487977	-0.919381
C	-6.660345	-1.249106	2.458298
H	-6.598760	-2.354334	2.363496
H	-5.928699	-0.922888	3.227506
H	-7.682665	-0.987205	2.802425
C	-3.329071	-3.310145	-1.643039
H	-3.235411	-2.710667	-0.718144
C	-2.758198	1.244824	-4.055325
H	-2.543445	1.616179	-3.037093
C	-1.534833	1.598262	-4.915581
H	-0.638726	1.058211	-4.544267
H	-1.694505	1.335777	-5.981683
H	-1.331160	2.687644	-4.866168
C	-4.001827	2.001419	-4.536263
H	-4.234024	1.761604	-5.595342
H	-4.877346	1.734013	-3.907101
H	-3.836435	3.096793	-4.450513

C	-2.184238	-4.331735	-1.623792
H	-2.249717	-5.028854	-2.485173
H	-1.207135	-3.804451	-1.661907
H	-2.216053	-4.932212	-0.692153
C	-4.694589	-4.002233	-1.537742
H	-5.506925	-3.245762	-1.587439
H	-4.840073	-4.742390	-2.352005
H	-4.778315	-4.533585	-0.566067
H	-1.357072	-3.295053	1.190296
H	-3.244682	-4.868625	1.451865
C	-2.058584	-3.155724	2.002661
C	-3.128826	-4.045066	2.142168
C	-1.898205	-2.091446	2.908537
C	-4.049782	-3.877878	3.177795
H	-4.878550	-4.566107	3.281533
C	-2.833708	-1.931427	3.946309
C	-3.901236	-2.823135	4.080050
H	-2.736068	-1.119734	4.656371
H	-4.616208	-2.694022	4.882245
C	1.085921	2.881913	1.080307
H	0.362112	3.371463	0.405904
C	0.501243	2.659166	2.457492
H	-0.395960	2.020281	2.463229
H	1.227576	2.202608	3.146634
H	0.199512	3.607882	2.938829
B	2.445284	3.584089	1.012189
O	3.414252	3.520925	2.010426
O	2.870024	4.386344	-0.036939
C	4.262025	4.692536	0.178998
C	4.381347	4.558530	1.728821
C	5.082796	3.642648	-0.555319
H	4.882953	2.633512	-0.162050
H	4.823999	3.648075	-1.623339
H	6.162344	3.832472	-0.477434
C	4.551144	6.074584	-0.365092
H	3.864750	6.824930	0.045820
H	5.580989	6.383612	-0.133950
H	4.438041	6.083367	-1.458155
C	3.918309	5.811848	2.457221
H	4.632681	6.639200	2.345051
H	2.939445	6.151168	2.089920
H	3.818361	5.595998	3.529490
C	5.745286	4.139791	2.230200
H	5.725441	4.005758	3.320329
H	6.088029	3.200316	1.780000
H	6.494804	4.911740	2.003235

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Figure_S7_imid-3_modeB_ts(AS)_03 / electronic energy: -4442.736147780118 a.u. / lowest freq: -229.89 cm-1

C	0.306971	3.481621	-1.375055
H	-0.244402	3.593592	-2.321195
C	1.336008	2.335376	-1.430194
H	2.260550	2.548118	-0.866050
C	-0.439214	1.703198	-0.025515
C	-1.890289	3.653265	-0.086027
C	-1.952812	4.575691	0.962424
C	-3.049217	3.414028	-0.852992
C	-3.145603	5.216720	1.287918
H	-1.050292	4.789722	1.535908
C	-4.240126	4.061944	-0.520621
C	-4.295965	4.948837	0.552035
H	-3.169701	5.924889	2.118611
H	-5.123987	3.864717	-1.128493
H	-5.238261	5.442101	0.799965
S	-3.058074	2.363426	-2.324035
O	-4.462913	2.423897	-2.827699
O	-2.736012	0.977439	-1.876290
O	-2.070318	2.955515	-3.243422
Cu	-1.134682	0.999146	1.690648
C	0.906477	4.804090	-0.971549
C	0.856935	5.898842	-1.852096
C	1.517667	4.965913	0.284047
C	1.409329	7.128876	-1.481734
H	0.393489	5.801697	-2.825986
C	2.067691	6.196555	0.651530
H	1.559277	4.141682	0.979506
C	2.014192	7.277695	-0.231099
H	1.368279	7.967261	-2.164984
H	2.534130	6.311851	1.621382
H	2.440535	8.230711	0.054097
N	-0.658132	2.986342	-0.369027
N	0.619178	1.251244	-0.711635
C	-2.021531	-0.184892	3.057222
C	-1.048994	-0.970668	3.818478
C	-1.084015	-0.989943	5.223194
C	-0.051834	-1.725824	3.172814
C	-0.180105	-1.760843	5.951237
C	0.841297	-2.503240	3.898755
C	0.778752	-2.530324	5.293473

H	-0.232101	-1.767153	7.042554
H	1.599528	-3.089266	3.375930
H	1.483773	-3.139723	5.863483
C	-2.472200	-0.560900	1.755088
C	-3.435403	0.195343	1.066331
H	-3.743930	1.158374	1.483378
H	-3.501135	0.122701	-0.018626
H	0.023898	-1.687087	2.082339
H	-2.102078	-1.474660	1.282449
P	-5.620467	-1.604877	0.375245
O	-7.139675	-2.084497	0.708549
O	-5.553101	-1.334782	-1.101628
O	-4.706089	-2.898646	0.777964
O	-5.230623	-0.525465	1.395937
Na	-4.972257	0.145924	-2.626881
H	-2.673795	0.473047	3.645733
H	-1.848783	-0.407551	5.744507
C	-7.477551	-2.424576	2.042892
H	-8.528212	-2.735880	2.049574
H	-6.859134	-3.256061	2.415602
H	-7.353998	-1.566806	2.719557
C	-4.822733	-4.065754	-0.014047
H	-4.228369	-4.853461	0.461931
H	-5.867186	-4.409971	-0.077752
H	-4.450138	-3.898432	-1.035353
C	1.038489	-0.109596	-0.662670
C	2.405895	-0.445282	-0.647549
C	0.087749	-1.140163	-0.804090
C	2.815661	-1.782781	-0.792434
C	0.493265	-2.472416	-0.993232
C	1.856254	-2.785247	-0.979067
H	2.173106	-3.802819	-1.174808
H	-0.963309	-0.893243	-0.879410
H	3.153688	0.332706	-0.578553
C	-0.486229	-3.510383	-1.406743
C	-0.858695	-4.562743	-0.516938
C	-1.005771	-3.498979	-2.736759
C	-1.764740	-5.543666	-0.961844
C	-1.922369	-4.494772	-3.121427
C	-2.295775	-5.501664	-2.243113
H	-2.065745	-6.355430	-0.313069
H	-2.342104	-4.506422	-4.118579
H	-2.995569	-6.263517	-2.561942
C	4.253333	-2.137345	-0.890807
C	4.947794	-1.945251	-2.121854
C	4.903625	-2.810216	0.187288
C	6.268745	-2.418171	-2.240290
C	6.221533	-3.270448	0.009494
C	6.895852	-3.066285	-1.185694
H	6.815916	-2.313279	-3.167417
H	6.732011	-3.811579	0.794498
H	7.907359	-3.433622	-1.303549
C	4.196800	-3.113877	1.506418
H	3.244021	-2.548766	1.573623
C	5.035292	-2.693772	2.723302
H	5.428721	-1.666207	2.589740
H	4.407486	-2.723724	3.638947
H	5.895407	-3.376850	2.883584
C	3.855202	-4.604474	1.593102
H	3.268257	-4.910401	0.705099
H	4.776968	-5.223283	1.632433
H	3.252798	-4.807108	2.503586
C	4.289224	-1.310587	-3.347101
H	3.273182	-0.936139	-3.114042
C	4.110156	-2.344051	-4.465311
H	3.537136	-1.898758	-5.306957
H	5.091195	-2.693699	-4.850648
H	3.539673	-3.218287	-4.084582
C	5.086264	-0.096623	-3.842039
H	4.603092	0.330249	-4.742599
H	5.118631	0.682855	-3.051022
H	6.123864	-0.368228	-4.123740
C	-0.577857	-2.466108	-3.780234
H	0.165920	-1.759437	-3.367213
C	-0.289849	-4.692412	0.893558
H	0.403590	-3.858670	1.116128
C	-1.400527	-4.639805	1.952444
H	-2.011136	-3.724183	1.825352
H	-2.070130	-5.522309	1.883568
H	-0.955922	-4.624927	2.969836
C	0.521778	-5.986616	1.035232
H	-0.134112	-6.881571	0.991680
H	1.269579	-6.060876	0.218121
H	1.056550	-5.994640	2.008592
C	-1.775696	-1.625548	-4.237587
H	-2.518400	-2.242265	-4.785540
H	-2.270513	-1.170161	-3.355780
H	-1.440236	-0.808429	-4.908747

C 0.116947 -3.133677 -4.973622
H 0.967388 -3.753889 -4.617975
H -0.584857 -3.777725 -5.543821
H 0.518732 -2.358690 -5.661021
H 0.021982 0.687803 -3.230365
H 0.565602 0.337968 -5.609398
C 0.887158 1.178636 -3.651901
C 1.178802 0.993432 -5.006600
C 1.690406 2.020397 -2.860815
C 2.245668 1.676418 -5.593397
H 2.462199 1.540975 -6.645037
C 2.760273 2.704327 -3.463200
C 3.029473 2.539430 -4.824372
H 3.370041 3.386589 -2.883657
H 3.851695 3.074511 -5.281395
C -0.230955 2.293381 2.964758
H -0.264388 3.128916 2.250608
C -1.026644 2.609110 4.211268
H -2.075640 2.879820 4.001391
H -1.047850 1.760970 4.914387
H -0.596581 3.454113 4.780766
B 1.245224 1.935185 3.169256
O 1.824773 1.781120 4.413970
O 2.187468 1.841056 2.154246
C 3.489476 1.950447 2.766266
C 3.219392 1.459750 4.230499
C 4.471509 1.101180 1.989057
H 4.076283 0.093056 1.822605
H 4.672012 1.548084 1.005743
H 5.433067 1.018643 2.515692
C 3.901873 3.413840 2.708349
H 3.193039 4.056570 3.249217
H 4.901923 3.573208 3.134875
H 3.930916 3.747602 1.662395
C 4.029002 2.172544 5.293667
H 5.107241 2.034068 5.127208
H 3.819637 3.248775 5.318706
H 3.791798 1.763668 6.285335
C 3.364148 -0.041519 4.383415
H 2.918206 -0.358746 5.335846
H 2.845441 -0.579533 3.578781
H 4.420527 -0.341035 4.388969

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Figure_S7_imid-3_modeB_ts(AS)_04 / electronic energy: -4442.733754884031 a.u. / lowest freq: -260.24 cm-1

C -0.625581 3.110783 -1.715104
H -1.244662 2.947288 -2.610244
C 0.675620 2.281249 -1.743852
H 1.539657 2.805795 -1.300674
C -0.762555 1.393737 -0.109571
C -2.699798 2.853929 -0.241475
C -2.946231 3.825986 0.732590
C -3.796002 2.236813 -0.879180
C -4.245406 4.147100 1.119384
H -2.102413 4.335031 1.199312
C -5.094343 2.569400 -0.489944
C -5.322922 3.506178 0.515480
H -4.408178 4.901127 1.892137
H -5.926685 2.082825 -0.999882
H -6.346762 3.745394 0.812021
S -3.615558 1.059436 -2.237826
O -5.012573 0.727507 -2.649141
O -2.946864 -0.145566 -1.668587
O -2.841310 1.755143 -3.280857
Cu -1.095242 0.756852 1.738064
C -0.390296 4.586005 -1.517028
C -0.788824 5.502383 -2.505889
C 0.223474 5.068344 -0.348039
C -0.575140 6.872604 -2.326627
H -1.262389 5.158206 -3.416919
C 0.434547 6.438142 -0.171399
H 0.530272 4.384046 0.427786
C 0.036026 7.340162 -1.160474
H -0.883599 7.572315 -3.092569
H 0.906257 6.799903 0.733082
H 0.200074 8.401100 -1.023198
N -1.351408 2.512595 -0.573706
N 0.334535 1.153809 -0.840129
C -1.522047 -0.442841 3.299385
C -0.334570 -0.827532 4.066085
C -0.318606 -0.712003 5.466029
C 0.817862 -1.327481 3.431221
C 0.791886 -1.113827 6.205531
C 1.919586 -1.739756 4.170010
C 1.911528 -1.640565 5.562785
H 0.777856 -1.022853 7.294220
H 2.798075 -2.135756 3.657239
H 2.780327 -1.961524 6.141943
C -1.898766 -1.099894 2.090964

C	-3.081320	-0.769095	1.399375
H	-3.619190	0.137037	1.698402
H	-3.144605	-1.008528	0.337719
H	0.847940	-1.376826	2.338367
H	-1.290546	-1.919017	1.699519
P	-5.344969	-2.399719	0.809831
O	-6.172946	-1.113868	0.192785
O	-4.729219	-3.032072	-0.404830
O	-6.478941	-3.307922	1.528004
O	-4.487869	-1.918321	1.992997
Na	-4.937143	-1.573742	-2.135773
H	-2.308431	0.077675	3.861429
H	-1.202004	-0.319002	5.977153
C	-6.875328	-0.252603	1.073714
H	-7.409347	0.486541	0.465696
H	-7.607575	-0.810381	1.677320
H	-6.189511	0.274010	1.754459
C	-7.424916	-3.985433	0.714083
H	-7.996877	-4.657493	1.362832
H	-8.121187	-3.278228	0.236782
H	-6.928773	-4.577868	-0.067645
C	1.097557	-0.040416	-0.695609
C	2.501950	-0.022106	-0.791134
C	0.438750	-1.282631	-0.618475
C	3.231041	-1.224992	-0.825145
C	1.157659	-2.486471	-0.688861
C	2.552198	-2.449860	-0.786882
H	3.105456	-3.375528	-0.892423
H	-0.642621	-1.315672	-0.614119
H	3.025319	0.919082	-0.890544
C	0.442011	-3.776697	-0.859987
C	0.402955	-4.740135	0.192990
C	-0.174590	-4.078396	-2.112037
C	-0.296692	-5.944556	-0.011136
C	-0.866813	-5.294635	-2.257170
C	-0.932982	-6.209340	-1.215803
H	-0.342155	-6.697816	0.764035
H	-1.349454	-5.549470	-3.191399
H	-1.464151	-7.142841	-1.351225
C	4.700033	-1.224526	-1.033516
C	5.229258	-1.050248	-2.346495
C	5.578802	-1.551195	0.042792
C	6.614905	-1.198652	-2.548040
C	6.954237	-1.694406	-0.217913
C	7.463520	-1.510418	-1.495293
H	7.046940	-1.101565	-3.534858
H	7.643082	-1.971582	0.568445
H	8.524018	-1.632210	-1.675525
C	5.072741	-1.821770	1.457896
H	4.011409	-1.512633	1.555837
C	5.854021	-1.024618	2.513366
H	5.943079	0.038146	2.211086
H	5.327556	-1.078971	3.489681
H	6.876263	-1.431426	2.660092
C	5.145243	-3.319966	1.768743
H	4.600333	-3.893663	0.993538
H	6.198391	-3.672861	1.788920
H	4.682107	-3.529843	2.755828
C	4.340958	-0.781584	-3.561579
H	3.284071	-0.629968	-3.266241
C	4.344596	-1.983123	-4.513712
H	3.617270	-1.818261	-5.337587
H	5.350749	-2.142503	-4.955850
H	4.041965	-2.901024	-3.965469
C	4.765679	0.499824	-4.290917
H	4.120415	0.661501	-5.176524
H	4.664789	1.373200	-3.611673
H	5.812140	0.443659	-4.653486
C	-0.079003	-3.148646	-3.323252
H	0.493280	-2.231998	-3.085407
C	1.131130	-4.543241	1.520668
H	1.602482	-3.542133	1.566320
C	0.169263	-4.633822	2.715192
H	-0.686376	-3.944053	2.578668
H	-0.226987	-5.662724	2.842464
H	0.698405	-4.353796	3.650427
C	2.261364	-5.569449	1.669801
H	1.858686	-6.598620	1.779541
H	2.920216	-5.545259	0.776521
H	2.871540	-5.335470	2.567832
C	-1.471087	-2.690343	-3.774351
H	-2.066545	-3.536189	-4.176873
H	-2.015595	-2.247577	-2.916364
H	-1.384760	-1.919457	-4.567426
C	0.681586	-3.815850	-4.475600
H	1.681311	-4.150831	-4.125236
H	0.127469	-4.691980	-4.873160
H	0.831084	-3.089091	-5.302798

H -0.282912 0.137486 -3.214204
H 0.183092 -0.382930 -5.578529
C 0.399461 0.765734 -3.768716
C 0.644838 0.477720 -5.114512
C 1.009361 1.876690 -3.157004
C 1.465651 1.315496 -5.871753
H 1.644833 1.097449 -6.916518
C 1.834352 2.712171 -3.929176
C 2.052961 2.436931 -5.281572
H 2.287080 3.592704 -3.490124
H 2.684657 3.089073 -5.870559
C -0.517171 2.403170 2.771662
H -0.831138 3.099832 1.981300
C -1.284744 2.649853 4.051129
H -2.378767 2.583559 3.921404
H -1.011217 1.933934 4.842807
H -1.084713 3.651121 4.476774
B 1.010030 2.489975 2.856637
O 1.702181 2.669882 4.038804
O 1.861791 2.517135 1.760160
C 3.125065 3.047651 2.209015
C 3.112903 2.704361 3.738781
C 4.238989 2.390649 1.423209
H 4.128269 1.300791 1.416009
H 4.225928 2.734393 0.379837
H 5.225016 2.640043 1.840651
C 3.115280 4.546662 1.947417
H 2.300603 5.048024 2.488705
H 4.062869 5.018224 2.242415
H 2.973214 4.732302 0.874379
C 3.776498 3.741058 4.621063
H 4.835326 3.866987 4.351408
H 3.284201 4.718392 4.548246
H 3.737026 3.424369 5.672241
C 3.676394 1.328391 4.035049
H 3.418036 1.039202 5.062769
H 3.258720 0.567365 3.362103
H 4.770969 1.319193 3.946807
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Figure_S7_imid-3_modeB_ts(AS)_05 / electronic energy: -4442.733814647407 a.u. / lowest freq: -253.79 cm-1
C -0.581307 3.012188 -1.327166
H -1.184238 2.629765 -2.162777
C 0.803477 2.374757 -1.228216
H 1.462630 3.005008 -0.604822
C -0.580688 1.363344 0.338616
C -2.438856 2.854098 0.517766
C -2.420656 3.113174 1.893690
C -3.666309 2.874677 -0.170131
C -3.598048 3.364951 2.591939
H -1.449654 3.141354 2.392323
C -4.838381 3.151474 0.538495
C -4.812923 3.387430 1.911034
H -3.559023 3.558316 3.666175
H -5.782524 3.148200 -0.008288
H -5.744271 3.588403 2.444283
S -3.823692 2.491152 -1.919432
O -5.280752 2.275265 -2.151779
O -3.070810 1.209292 -2.109247
O -3.264268 3.640952 -2.650033
Cu -0.995000 0.414040 2.034069
C -0.517307 4.515799 -1.423019
C -0.358542 5.105706 -2.689687
C -0.576395 5.347962 -0.289514
C -0.287213 6.495058 -2.822572
H -0.293659 4.487290 -3.576599
C -0.509628 6.737543 -0.427477
H -0.654598 4.933099 0.703416
C -0.366736 7.310876 -1.692410
H -0.169895 6.939038 -3.802609
H -0.559051 7.370201 0.449300
H -0.311312 8.386752 -1.796110
N -1.196306 2.488947 -0.072654
N 0.500804 1.168802 -0.428739
C -2.153603 -0.934407 3.083263
C -1.468828 -1.861499 3.980878
C -1.921148 -2.026990 5.301048
C -0.321284 -2.565820 3.579973
C -1.259060 -2.877848 6.181857
C 0.342239 -3.412653 4.459280
C -0.124791 -3.575828 5.765128
H -1.628715 -2.994769 7.203454
H 1.237912 -3.943596 4.129172
H 0.400262 -4.237636 6.457504
C -2.303037 -1.141181 1.686240
C -3.173802 -0.353841 0.907555
H -3.644022 0.516618 1.369654
H -3.048135 -0.286917 -0.174952
H 0.079298 -2.394731 2.576611

H	-1.793018	-1.981018	1.202183
P	-5.075984	-2.273504	-0.307678
O	-6.367898	-3.197861	0.046790
O	-5.216465	-1.856207	-1.743385
O	-3.806897	-3.286939	-0.116260
O	-4.916384	-1.238261	0.816205
Na	-5.090862	0.030709	-2.866917
H	-2.901141	-0.284599	3.560351
H	-2.804429	-1.474924	5.633846
C	-6.467037	-3.778500	1.336320
H	-7.418564	-4.320058	1.384231
H	-5.645583	-4.488325	1.521265
H	-6.451059	-3.011771	2.124290
C	-3.627063	-4.305453	-1.083473
H	-3.002100	-5.086404	-0.636532
H	-4.583548	-4.761879	-1.381494
H	-3.131303	-3.917644	-1.985822
C	1.140756	-0.090548	-0.530394
C	2.527590	-0.186770	-0.374633
C	0.403805	-1.238681	-0.881617
C	3.175650	-1.413921	-0.546493
C	1.060851	-2.459711	-1.118174
C	2.445921	-2.542269	-0.933170
H	2.961612	-3.477001	-1.119213
H	-0.663489	-1.162845	-1.049984
H	3.105026	0.688318	-0.125590
C	0.335467	-3.630731	-1.672535
C	0.149214	-4.804262	-0.882959
C	-0.075023	-3.631501	-3.039445
C	-0.416572	-5.946614	-1.480548
C	-0.686919	-4.783078	-3.568765
C	-0.842549	-5.927990	-2.800908
H	-0.544337	-6.862192	-0.918938
H	-1.024886	-4.809250	-4.596182
H	-1.294239	-6.811028	-3.234483
C	4.634693	-1.516315	-0.359852
C	5.499078	-1.452967	-1.488335
C	5.168465	-1.755188	0.937763
C	6.876736	-1.667465	-1.299646
C	6.555224	-1.949740	1.074442
C	7.395547	-1.909384	-0.032559
H	7.559537	-1.652874	-2.138673
H	6.993283	-2.148618	2.043541
H	8.458662	-2.070745	0.092218
C	4.282055	-1.839146	2.181669
H	3.223888	-1.615089	1.937127
C	4.698462	-0.805519	3.236596
H	4.712575	0.209400	2.788340
H	3.971734	-0.804112	4.076455
H	5.704054	-1.028767	3.649932
C	4.294436	-3.256058	2.765561
H	3.961266	-3.984446	1.995765
H	5.310143	-3.539233	3.113589
H	3.597720	-3.318289	3.627867
C	4.975418	-1.177522	-2.898719
H	3.892478	-0.936031	-2.883875
C	5.131691	-2.414633	-3.789405
H	4.676428	-2.226674	-4.785411
H	6.202376	-2.673211	-3.931494
H	4.609741	-3.280901	-3.329290
C	5.663697	0.042350	-3.524911
H	5.198637	0.277160	-4.505477
H	5.547243	0.925595	-2.861048
H	6.744852	-0.140697	-3.695260
C	0.157911	-2.442974	-3.970907
H	0.703083	-1.629892	-3.456948
C	0.542531	-4.873354	0.590794
H	0.906858	-3.890090	0.948255
C	-0.664178	-5.232761	1.471190
H	-1.459881	-4.467264	1.357267
H	-1.083141	-6.226471	1.211859
H	-0.363164	-5.269827	2.537182
C	1.688817	-5.868547	0.807018
H	1.370868	-6.905566	0.569170
H	2.553244	-5.601847	0.162889
H	2.024416	-5.836874	1.865753
C	-1.177616	-1.850375	-4.438256
H	-1.754470	-2.581367	-5.042632
H	-1.786628	-1.552513	-3.557982
H	-1.002935	-0.947737	-5.059563
C	1.042257	-2.835313	-5.162659
H	1.991177	-3.284190	-4.798041
H	0.531049	-3.562284	-5.827571
H	1.296185	-1.937155	-5.763372
H	-0.115494	0.805524	-3.297806
H	0.936003	0.464760	-5.505764
C	0.830295	1.283439	-3.516764
C	1.424491	1.082959	-4.766127

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C   1.451640   2.105193  -2.559975
C   2.644465   1.690442  -5.068294
H   3.102739   1.532539  -6.035909
C   2.682603   2.708370  -2.872792
C   3.272614   2.502946  -4.122428
H   3.182359   3.346725  -2.154862
H   4.218526   2.973453  -4.357359
C   0.218022   1.248911   3.456384
H  -0.582655   1.832385   3.951212
C   0.851445   0.287152   4.445277
H   0.124476  -0.232511   5.083211
H   1.454493  -0.493435   3.952980
H   1.551769   0.804791   5.126043
B   1.250763   2.244038   2.889209
O   2.613779   2.059705   3.039256
O   0.978272   3.499849   2.353713
C   2.143857   4.315291   2.623060
C   3.298705   3.257563   2.623318
C   2.285681   5.395177   1.574655
H   2.250607   4.995208   0.553642
H   1.484309   6.138030   1.677875
H   3.240078   5.927059   1.697510
C   1.930083   4.941346   3.994069
H   1.850034   4.173690   4.777493
H   2.744999   5.625979   4.266496
H   0.993333   5.514690   3.990651
C   4.411882   3.543032   3.610819
H   4.889385   4.510956   3.399776
H   4.049622   3.554946   4.645628
H   5.186688   2.767815   3.538570
C   3.883110   3.036003   1.240625
H   4.524929   2.145606   1.241550
H   3.094116   2.894199   0.492506
H   4.495563   3.889660   0.919771
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Figure_S7_imid-3_modeB_ts(AS)_06 / electronic energy: -4442.733814797944 a.u. / lowest freq: -253.80 cm-1
C  -0.581208   3.012221  -1.327143
H  -1.184157   2.629824  -2.162755
C   0.803556   2.374747  -1.228204
H   1.462729   3.004971  -0.604803
C  -0.580635   1.363360   0.338622
C  -2.438747   2.854182   0.517800
C  -2.420524   3.113262   1.893724
C  -3.666206   2.874801  -0.170085
C  -3.597901   3.365080   2.591983
H  -1.449517   3.141409   2.392349
C  -4.838262   3.151637   0.538553
C  -4.812782   3.387596   1.911091
H  -3.558859   3.558447   3.666219
H  -5.782411   3.148393  -0.008222
H  -5.744118   3.588602   2.444348
S  -3.823618   2.491285  -1.919386
O  -5.280687   2.275451  -2.151720
O  -3.070782   1.209399  -2.109211
O  -3.264161   3.641068  -2.649989
Cu -0.994971   0.414050   2.034065
C  -0.517160   4.515831  -1.422983
C  -0.358398   5.105746  -2.689648
C  -0.576199   5.347984  -0.289469
C  -0.287023   6.495096  -2.822521
H  -0.293550   4.487336  -3.576568
C  -0.509386   6.737565  -0.427419
H  -0.654398   4.933114   0.703458
C  -0.366497   7.310905  -1.692349
H  -0.169707   6.939083  -3.802556
H  -0.558771   7.370216   0.449365
H  -0.311037   8.386781  -1.796039
N  -1.196215   2.488990  -0.072631
N   0.500848   1.168791  -0.428740
C  -2.153613  -0.934370   3.083251
C  -1.468884  -1.861492   3.980872
C  -1.921235  -2.026965   5.301033
C  -0.321363  -2.565862   3.579987
C  -1.259200  -2.877852   6.181854
C   0.342108  -3.412723   4.459307
C  -0.124953  -3.575879   5.765147
H  -1.628881  -2.994758   7.203445
H   1.237762  -3.943706   4.129215
H   0.400059  -4.237710   6.457532
C  -2.303054  -1.141131   1.686229
C  -3.173796  -0.353758   0.907552
H  -3.643988   0.516712   1.369657
H  -3.048132  -0.286833  -0.174956
H   0.079244  -2.394795   2.576632
H  -1.793065  -1.980981   1.202162
P  -5.076078  -2.273348  -0.307671
O  -6.367997  -3.197682   0.046836
O  -5.216610  -1.856027  -1.743365
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O	-3.807003	-3.286814	-0.116327
O	-4.916402	-1.238130	0.816224
Na	-5.090898	0.030879	-2.866895
H	-2.901130	-0.284536	3.560338
H	-2.804499	-1.474863	5.633815
C	-6.467113	-3.778312	1.336374
H	-7.418622	-4.319902	1.384291
H	-5.645636	-4.488108	1.521325
H	-6.451159	-3.011573	2.124334
C	-3.627244	-4.305329	-1.083553
H	-3.002290	-5.086304	-0.636642
H	-4.583757	-4.761720	-1.381537
H	-3.131507	-3.917532	-1.985919
C	1.140759	-0.090577	-0.530411
C	2.527590	-0.186848	-0.374654
C	0.403768	-1.238681	-0.881647
C	3.175608	-1.414019	-0.546529
C	1.060773	-2.459730	-1.118220
C	2.445840	-2.542338	-0.933218
H	2.961499	-3.477085	-1.119272
H	-0.663523	-1.162807	-1.050012
H	3.105056	0.688218	-0.125603
C	0.335347	-3.630717	-1.672594
C	0.149045	-4.804248	-0.883028
C	-0.075141	-3.631458	-3.039504
C	-0.416788	-5.946571	-1.480627
C	-0.687085	-4.783005	-3.568834
C	-0.842763	-5.927917	-2.800987
H	-0.544593	-6.862147	-0.919024
H	-1.025054	-4.809153	-4.596252
H	-1.294490	-6.810933	-3.234570
C	4.634647	-1.516466	-0.359886
C	5.499038	-1.453123	-1.488365
C	5.168407	-1.755383	0.937726
C	6.876688	-1.667669	-1.299676
C	6.555159	-1.949981	1.074405
C	7.395487	-1.909629	-0.032592
H	7.559492	-1.653083	-2.138700
H	6.993209	-2.148892	2.043502
H	8.458597	-2.071026	0.092185
C	4.281991	-1.839337	2.181627
H	3.223832	-1.615239	1.937087
C	4.698430	-0.805744	3.236576
H	4.712601	0.209180	2.788334
H	3.971686	-0.804313	4.076421
H	5.704003	-1.029049	3.649927
C	4.294323	-3.256261	2.765490
H	3.961142	-3.984624	1.995676
H	5.310017	-3.539473	3.113526
H	3.597594	-3.318489	3.627787
C	4.975391	-1.177635	-2.898745
H	3.892458	-0.936112	-2.883901
C	5.131631	-2.414733	-3.789454
H	4.676358	-2.226749	-4.785451
H	6.202309	-2.673326	-3.931563
H	4.609672	-3.281001	-3.329348
C	5.663708	0.042228	-3.524911
H	5.198657	0.277072	-4.505473
H	5.547279	0.925463	-2.861030
H	6.744858	-0.140848	-3.695261
C	0.157841	-2.442931	-3.970954
H	0.703041	-1.629874	-3.456986
C	0.542359	-4.873369	0.590724
H	0.906723	-3.890121	0.948195
C	-0.664363	-5.232741	1.471115
H	-1.460057	-4.467238	1.357168
H	-1.083332	-6.226453	1.211804
H	-0.363359	-5.269785	2.537111
C	1.688609	-5.868606	0.806939
H	1.370628	-6.905609	0.569062
H	2.553052	-5.601920	0.162826
H	2.024196	-5.836969	1.865678
C	-1.177662	-1.850279	-4.438304
H	-1.754520	-2.581230	-5.042726
H	-1.786686	-1.552441	-3.558029
H	-1.002947	-0.947616	-5.059565
C	1.042177	-2.835292	-5.162706
H	1.991090	-3.284184	-4.798087
H	0.530956	-3.562258	-5.827613
H	1.296119	-1.937142	-5.763424
H	-0.115461	0.805563	-3.297811
H	0.936028	0.464793	-5.505774
C	0.830342	1.283454	-3.516765
C	1.424532	1.082972	-4.766130
C	1.451710	2.105181	-2.559967
C	2.644522	1.690425	-5.068291
H	3.102793	1.532520	-6.035907
C	2.682688	2.708329	-2.872779

C 3.272693 2.502903 -4.122417
H 3.182461 3.346663 -2.154841
H 4.218617 2.973388 -4.357343
C 0.218056 1.248876 3.456403
H -0.582614 1.832371 3.951217
C 0.851431 0.287088 4.445298
H 0.124435 -0.232541 5.083228
H 1.454442 -0.493528 3.953002
H 1.551779 0.804693 5.126065
B 1.250836 2.243970 2.889242
O 2.613843 2.059583 3.039290
O 0.978394 3.499796 2.353757
C 2.144011 4.315190 2.623112
C 3.298817 3.257417 2.623364
C 2.285881 5.395078 1.574715
H 2.250803 4.995116 0.553699
H 1.484534 6.137958 1.677932
H 3.240296 5.926927 1.697581
C 1.930260 4.941244 3.994125
H 1.850191 4.173587 4.777545
H 2.745196 5.625852 4.266552
H 0.993526 5.514615 3.990713
C 4.412003 3.542837 3.610869
H 4.889534 4.510751 3.399841
H 4.049745 3.554745 4.645679
H 5.186788 2.767599 3.538608
C 3.883217 3.035844 1.240670
H 4.525000 2.145423 1.241589
H 3.094218 2.894077 0.492549
H 4.495703 3.889481 0.919825

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Figure_S7_imid-3_modeB_prod(AS) / electronic energy: -4442.752883316609 a.u. / lowest freq: 17.14 cm-1

C 0.946510 1.453452 -3.161651
H 0.824460 2.524999 -2.949017
C -0.364991 0.668356 -3.040037
H -0.345694 -0.261604 -3.636690
C 0.932930 0.262046 -1.152502
C 3.098912 1.118446 -1.734780
C 3.953961 0.016530 -1.679297
C 3.586788 2.398291 -1.417665
C 5.290582 0.174864 -1.323933
H 3.566587 -0.972939 -1.929856
C 4.931435 2.544120 -1.071859
C 5.783174 1.442551 -1.025954
H 5.941276 -0.700749 -1.299203
H 5.290219 3.541880 -0.813880
H 6.831119 1.578177 -0.750857
S 2.547964 3.868600 -1.387131
O 3.328314 4.879982 -0.619649
O 1.316736 3.465901 -0.643330
O 2.320001 4.231891 -2.797510
Cu 1.604519 -0.722351 0.407606
C 1.625638 1.275965 -4.494743
C 1.704298 2.355205 -5.392900
C 2.172204 0.035686 -4.871870
C 2.332014 2.200581 -6.632466
H 1.272053 3.314869 -5.140237
C 2.800186 -0.114474 -6.111394
H 2.115738 -0.813173 -4.207597
C 2.882004 0.967658 -6.990428
H 2.389347 3.036864 -7.317154
H 3.222419 -1.071046 -6.390871
H 3.367645 0.849770 -7.950448
N 1.730226 0.862962 -2.041870
N -0.321375 0.283753 -1.612323
C 2.112776 -1.209725 2.396911
C 1.594943 -2.429228 3.015294
C 2.429524 -3.244474 3.796681
C 0.262209 -2.830260 2.820674
C 1.940951 -4.407462 4.382325
C -0.222848 -4.001441 3.391808
C 0.614109 -4.791537 4.181213
H 2.602540 -5.025899 4.993365
H -1.259907 -4.298644 3.224179
H 0.234118 -5.711887 4.630236
C 1.375454 0.005282 2.347439
C 1.796362 1.081856 1.581385
H 2.845730 1.183147 1.275199
H 1.171874 1.959199 1.427608
H -0.384969 -2.230242 2.173099
H 0.350690 0.016023 2.738599
P 1.205722 4.030926 3.649744
O 1.525308 4.468356 5.202442
O 0.346758 5.121772 3.057717
O 0.334003 2.645759 3.870081
O 2.462233 3.625575 2.914067
Na 1.785062 5.158183 1.134510
H 3.204701 -1.139280 2.297404

H	3.474736	-2.958501	3.935875
C	2.351828	3.620076	5.970558
H	2.517337	4.096605	6.944879
H	1.882499	2.636030	6.137891
H	3.327279	3.455719	5.486188
C	-0.924461	2.762708	4.494758
H	-1.379292	1.765851	4.525714
H	-0.837022	3.133905	5.529111
H	-1.588977	3.444963	3.942997
C	-1.424805	-0.206384	-0.873478
C	-2.281163	-1.160339	-1.437609
C	-1.750901	0.365368	0.369183
C	-3.443990	-1.549669	-0.766102
C	-2.959306	0.034880	1.008516
C	-3.792109	-0.938244	0.442465
H	-4.728134	-1.195954	0.922993
H	-1.120622	1.140877	0.784343
H	-2.048745	-1.597076	-2.401070
C	-3.433205	0.792903	2.194637
C	-3.581391	0.142841	3.457024
C	-3.843494	2.153677	2.052342
C	-4.156512	0.853938	4.527464
C	-4.360030	2.831487	3.172429
C	-4.526268	2.183851	4.387977
H	-4.310502	0.382596	5.488801
H	-4.658589	3.869033	3.103976
H	-4.946214	2.718068	5.230613
C	-4.322270	-2.579352	-1.349843
C	-5.500654	-2.195745	-2.049341
C	-3.997483	-3.956279	-1.194834
C	-6.345499	-3.200582	-2.555022
C	-4.860466	-4.921547	-1.745261
C	-6.023402	-4.545564	-2.408887
H	-7.259360	-2.945051	-3.074860
H	-4.639728	-5.976897	-1.654317
H	-6.680695	-5.303775	-2.814956
C	-2.746493	-4.419686	-0.444865
H	-2.175578	-3.559307	-0.040466
C	-1.787191	-5.163262	-1.381558
H	-1.543016	-4.525574	-2.258019
H	-0.840049	-5.395940	-0.849000
H	-2.232423	-6.114555	-1.741656
C	-3.112912	-5.282312	0.769048
H	-3.778473	-4.711410	1.451736
H	-3.625569	-6.217999	0.462959
H	-2.194710	-5.558778	1.328928
C	-5.874389	-0.729105	-2.271152
H	-5.082504	-0.051159	-1.892073
C	-7.153455	-0.369024	-1.507608
H	-7.365980	0.716587	-1.611787
H	-8.024927	-0.939297	-1.893137
H	-7.025529	-0.593917	-0.427091
C	-6.014369	-0.406601	-3.764299
H	-6.162817	0.685618	-3.903170
H	-5.090525	-0.704737	-4.304523
H	-6.880824	-0.933672	-4.215352
C	-3.769700	2.906560	0.723030
H	-3.441457	2.245672	-0.100410
C	-3.129777	-1.296035	3.700854
H	-2.628897	-1.710176	2.804201
C	-2.100122	-1.370537	4.839195
H	-1.205996	-0.764079	4.584459
H	-2.518843	-1.005783	5.799325
H	-1.778014	-2.419536	4.997146
C	-4.328478	-2.206888	3.992664
H	-4.820026	-1.929392	4.948973
H	-5.074018	-2.134538	3.173114
H	-3.993725	-3.264172	4.061332
C	-2.748018	4.047797	0.807092
H	-3.039053	4.793349	1.576482
H	-1.746661	3.640200	1.062514
H	-2.668254	4.568869	-0.168693
C	-5.149350	3.423322	0.291577
H	-5.879930	2.586038	0.276879
H	-5.520648	4.216041	0.973791
H	-5.093545	3.848237	-0.732854
H	-1.314256	2.956116	-1.831115
H	-3.294264	4.285277	-2.473043
C	-1.919830	2.638166	-2.670349
C	-3.044586	3.389496	-3.024437
C	-1.581177	1.482076	-3.397527
C	-3.846944	2.989582	-4.094707
H	-4.719092	3.570953	-4.364186
C	-2.396933	1.088443	-4.473020
C	-3.521825	1.841648	-4.819678
H	-2.161746	0.201149	-5.047495
H	-4.143285	1.533661	-5.650512
C	1.734831	-2.611301	-0.308258

H 1.072463 -3.089626 0.432585
C 1.217995 -2.802058 -1.714298
H 0.178426 -2.479483 -1.856478
H 1.829814 -2.280084 -2.463013
H 1.247074 -3.868314 -2.001783
B 3.191021 -3.090007 -0.089004
O 4.144744 -3.137721 -1.089073
O 3.669031 -3.604470 1.094738
C 5.086659 -3.847128 0.931854
C 5.205088 -4.010955 -0.616381
C 5.815788 -2.617394 1.448279
H 5.537898 -1.718181 0.877904
H 5.551087 -2.443147 2.500302
H 6.906968 -2.733906 1.396503
C 5.464321 -5.073477 1.732358
H 4.834970 -5.935361 1.479890
H 6.514681 -5.347910 1.559048
H 5.343468 -4.876204 2.806453
C 4.853120 -5.414788 -1.084004
H 5.631659 -6.142702 -0.817982
H 3.902215 -5.755206 -0.649611
H 4.745087 -5.419713 -2.176735
C 6.526028 -3.574457 -1.205844
H 6.500350 -3.656231 -2.300695
H 6.777895 -2.538633 -0.949639
H 7.341675 -4.215907 -0.842960
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Figure_S7_imid-3_modeC_ed(AS) / electronic energy: -4442.756964750907 a.u. / lowest freq: 15.13 cm-1
C -0.514853 -2.788972 -2.284365
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C 0.727979 -1.897086 -2.457980
H 0.711253 -1.336702 -3.409813
C -0.736623 -0.866952 -0.936585
C -2.711364 -2.232619 -1.045410
C -3.743947 -1.365317 -1.417123
C -3.001972 -3.327023 -0.207896
C -5.049290 -1.578706 -0.982710
H -3.516044 -0.511030 -2.056103
C -4.319229 -3.542775 0.204432
C -5.341512 -2.678029 -0.178392
H -5.832686 -0.883929 -1.292706
H -4.522597 -4.391574 0.859068
H -6.363378 -2.862126 0.160414
S -1.752246 -4.459770 0.422919
O -2.386173 -5.127547 1.599541
O -0.608510 -3.607070 0.869676
O -1.430559 -5.383886 -0.680274
Cu -1.765772 0.684112 -0.251866
C -1.163387 -3.161034 -3.593101
C -1.215698 -4.506233 -3.998483
C -1.728705 -2.175453 -4.424188
C -1.825765 -4.857527 -5.206467
H -0.780969 -5.284113 -3.384109
C -2.338545 -2.531491 -5.630182
H -1.699558 -1.133028 -4.137748
C -2.387841 -3.871520 -6.020874
H -1.862098 -5.895293 -5.511654
H -2.773117 -1.767747 -6.262070
H -2.860124 -4.145713 -6.955310
N -1.393246 -1.912734 -1.475474
N 0.532496 -0.918570 -1.365224
C -2.627564 1.646682 1.346863
C -2.173163 3.041791 1.332323
C -3.064907 4.090238 1.611833
C -0.848422 3.378838 1.002293
C -2.651970 5.419887 1.558290
C -0.436288 4.704057 0.941825
C -1.336717 5.735556 1.219368
H -3.367782 6.217279 1.775538
H 0.596029 4.934119 0.670964
H -1.014212 6.777829 1.166072
C -1.842728 0.550761 1.759423
C -2.446755 -0.760535 2.102231
H -3.393526 -0.927208 1.566964
H -1.774737 -1.601975 1.869492
H -0.146132 2.578825 0.741208
H -0.834312 0.736966 2.149980
P -1.765294 -1.357501 4.599103
O -2.638223 -1.518472 5.928838
O -1.000392 -2.601816 4.311969
O -0.838271 -0.056947 4.814789
O -2.819409 -0.854431 3.525610
Na -0.745061 -4.494288 3.174341
H -3.715468 1.497093 1.314780
H -4.098841 3.853521 1.880825
C -3.449057 -0.445005 6.407236
H -3.792017 -0.723307 7.408397
H -2.873834 0.489418 6.467814

H	-4.317067	-0.293517	5.752661
C	0.323903	-0.171642	5.631594
H	0.732027	0.835874	5.753742
H	0.078506	-0.574220	6.625131
H	1.073769	-0.818808	5.157593
C	1.551488	-0.112427	-0.803323
C	2.468602	0.551342	-1.630336
C	1.722266	-0.068948	0.592021
C	3.538051	1.260276	-1.069321
C	2.825858	0.592288	1.151677
C	3.721458	1.269635	0.317174
H	4.579148	1.777280	0.743225
H	1.049321	-0.623242	1.234902
H	2.352184	0.515337	-2.706712
C	3.124850	0.481439	2.598014
C	2.976540	1.612878	3.451103
C	3.654785	-0.734770	3.121687
C	3.400905	1.516739	4.789675
C	4.018780	-0.790140	4.479816
C	3.906875	0.327103	5.296632
H	3.328432	2.365058	5.457004
H	4.409904	-1.701616	4.911970
H	4.209464	0.268753	6.334294
C	4.499783	1.966304	-1.935212
C	5.702729	1.319040	-2.334484
C	4.252651	3.314732	-2.316462
C	6.639223	2.040445	-3.097693
C	5.208203	3.982180	-3.104671
C	6.387503	3.351749	-3.485153
H	7.575964	1.589234	-3.396379
H	5.051010	5.006489	-3.415806
H	7.117278	3.887452	-4.078689
C	2.998693	4.070421	-1.873818
H	2.335990	3.427214	-1.259456
C	2.161411	4.510245	-3.080671
H	1.915674	3.629688	-3.712087
H	1.208770	4.966173	-2.735609
H	2.702894	5.256902	-3.698524
C	3.365106	5.269012	-0.989465
H	3.942055	4.923363	-0.105110
H	3.971888	6.012952	-1.546885
H	2.445275	5.774422	-0.628398
C	6.021415	-0.122860	-1.935870
H	5.158711	-0.597531	-1.424427
C	7.189282	-0.166970	-0.944750
H	7.360400	-1.210571	-0.603761
H	8.123691	0.212549	-1.409883
H	6.952772	0.452902	-0.053390
C	6.308993	-0.996505	-3.163753
H	6.441413	-2.053919	-2.851939
H	5.456994	-0.943529	-3.874756
H	7.234731	-0.677394	-3.685728
C	3.854251	-1.983040	2.261202
H	3.597156	-1.790463	1.202498
C	2.363787	2.925993	2.968352
H	2.016332	2.839187	1.919576
C	1.126167	3.297441	3.798732
H	0.361966	2.495476	3.718085
H	1.378583	3.447431	4.868532
H	0.682076	4.242479	3.424888
C	3.398538	4.056626	2.990222
H	3.721459	4.285787	4.027649
H	4.288947	3.769200	2.391533
H	2.964617	4.976830	2.543456
C	2.933837	-3.114904	2.733414
H	3.181139	-3.430526	3.768731
H	1.876203	-2.775753	2.703874
H	3.032697	-3.996430	2.066898
C	5.322724	-2.427388	2.245360
H	5.970650	-1.581966	1.928705
H	5.652133	-2.781283	3.244452
H	5.460593	-3.257208	1.519838
H	1.790850	-3.183348	-0.264617
H	3.883686	-4.487537	-0.150486
C	2.404278	-3.282154	-1.149773
C	3.590045	-4.019244	-1.079666
C	2.016610	-2.673194	-2.357326
C	4.395053	-4.160847	-2.211397
H	5.311929	-4.733055	-2.155286
C	2.837719	-2.818105	-3.489259
C	4.016721	-3.564626	-3.416070
H	2.561179	-2.363720	-4.432468
H	4.641196	-3.675590	-4.293052
C	-2.010724	1.652493	-2.051238
H	-2.027265	0.793263	-2.743624
C	-0.810111	2.538318	-2.322472
H	0.155091	2.013458	-2.222599
H	-0.806898	2.972501	-3.341139

H -0.765559 3.397929 -1.635795
B -3.368504 2.333837 -1.996759
O -4.593281 1.681776 -2.178112
O -3.570994 3.695663 -1.789690
C -4.941914 3.990003 -2.107356
C -5.639976 2.615211 -1.852836
C -5.430076 5.123339 -1.229214
H -5.285539 4.908297 -0.163481
H -4.874551 6.043867 -1.457617
H -6.497639 5.324810 -1.402337
C -4.992077 4.400080 -3.572729
H -4.668910 3.578279 -4.227455
H -6.001389 4.708195 -3.880416
H -4.314004 5.248327 -3.738199
C -6.842587 2.339698 -2.730661
H -7.620043 3.104696 -2.587842
H -6.573914 2.316890 -3.794010
H -7.286120 1.366317 -2.477712
C -5.994197 2.424424 -0.386275
H -6.247671 1.372566 -0.195043
H -5.140565 2.689248 0.252347
H -6.851897 3.041867 -0.083510
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Figure_S7_imid-3_modeC_ts(AS)_01 / electronic energy: -4442.743156008483 a.u. / lowest freq: -264.88 cm-1
C -0.488640 -2.975098 -2.125358
H -0.298926 -3.850639 -1.485848
C 0.760819 -2.097891 -2.331033
H 0.771364 -1.607333 -3.320151
C -0.730841 -0.977964 -0.910249
C -2.707878 -2.341166 -0.954809
C -3.737343 -1.519663 -1.421475
C -3.001646 -3.355059 -0.023135
C -5.047843 -1.699568 -0.985816
H -3.506459 -0.727711 -2.134895
C -4.322034 -3.538244 0.392015
C -5.343386 -2.719026 -0.084472
H -5.830655 -1.041321 -1.368214
H -4.529292 -4.322221 1.121813
H -6.368076 -2.875197 0.259355
S -1.743964 -4.406816 0.719371
O -2.392771 -5.013285 1.918286
O -0.642273 -3.484275 1.132570
O -1.362543 -5.390343 -0.311282
Cu -1.732039 0.598633 -0.258154
C -1.115937 -3.419954 -3.421127
C -1.164520 -4.785859 -3.750544
C -1.664586 -2.481726 -4.316010
C -1.754149 -5.203760 -4.947417
H -0.742922 -5.528684 -3.085473
C -2.254107 -2.904487 -5.510511
H -1.638602 -1.424430 -4.087609
C -2.299470 -4.264405 -5.825911
H -1.787680 -6.257041 -5.194213
H -2.676011 -2.177085 -6.191911
H -2.755914 -4.590253 -6.751588
N -1.380959 -2.050565 -1.385808
N 0.542033 -1.041424 -1.316690
C -2.575749 1.801622 1.173599
C -2.210409 3.216644 1.079503
C -3.175444 4.220692 1.256901
C -0.895416 3.609612 0.777305
C -2.840401 5.566092 1.131809
C -0.559552 4.951587 0.647667
C -1.532119 5.938347 0.822621
H -3.608595 6.330697 1.272430
H 0.467427 5.230433 0.403077
H -1.270059 6.993365 0.715519
C -1.747005 0.811490 1.772080
C -2.178923 -0.518895 1.954560
H -3.135574 -0.825702 1.523897
H -1.446174 -1.321469 2.061438
H -0.138889 2.839139 0.596028
H -0.754521 1.087224 2.144392
P -1.813680 -1.062843 4.784973
O -2.494805 -1.046507 6.261213
O -1.014533 -2.329348 4.674770
O -0.834053 0.246430 4.786248
O -2.903267 -0.718741 3.756769
Na -0.832034 -4.174333 3.492115
H -3.650626 1.576259 1.129346
H -4.201494 3.936499 1.508254
C -3.293576 0.061476 6.642661
H -3.630899 -0.112228 7.670705
H -2.719191 1.000391 6.611607
H -4.171925 0.165482 5.989563
C 0.334502 0.199764 5.583419
H 0.759154 1.209345 5.611821
H 0.110673 -0.110340 6.616292

H	1.077716	-0.494987	5.165830
C	1.546381	-0.180618	-0.810643
C	2.464063	0.424541	-1.680892
C	1.706200	-0.024636	0.578535
C	3.524041	1.183594	-1.170553
C	2.803850	0.684303	1.092096
C	3.700358	1.299637	0.211722
H	4.553713	1.842706	0.600887
H	1.031997	-0.530360	1.258483
H	2.354830	0.305194	-2.751968
C	3.099983	0.686568	2.544499
C	2.974213	1.887304	3.302503
C	3.615673	-0.489785	3.165670
C	3.404736	1.895439	4.642593
C	3.983844	-0.438403	4.522943
C	3.893512	0.743952	5.244729
H	3.350678	2.797261	5.237527
H	4.362704	-1.316866	5.028164
H	4.200242	0.766856	6.282572
C	4.482043	1.833624	-2.083031
C	5.697444	1.175557	-2.421950
C	4.218242	3.144327	-2.570045
C	6.629646	1.849504	-3.232319
C	5.171193	3.763703	-3.399439
C	6.362649	3.123411	-3.721369
H	7.574996	1.390278	-3.488718
H	5.001982	4.758688	-3.789471
H	7.089761	3.622651	-4.348982
C	2.948247	3.911561	-2.198602
H	2.290229	3.307731	-1.541057
C	2.115944	4.241973	-3.443275
H	1.885440	3.310106	-4.002741
H	1.155462	4.713169	-3.143502
H	2.653858	4.942498	-4.115831
C	3.285614	5.181005	-1.407060
H	3.869612	4.916479	-0.499717
H	3.875240	5.895021	-2.019414
H	2.352820	5.688601	-1.083925
C	6.033291	-0.226047	-1.909888
H	5.173815	-0.671390	-1.367535
C	7.195252	-0.175902	-0.912082
H	7.378149	-1.186961	-0.489076
H	8.127498	0.178777	-1.400570
H	6.944768	0.508824	-0.073566
C	6.340425	-1.189139	-3.063846
H	6.484407	-2.217079	-2.669215
H	5.492395	-1.203834	-3.781407
H	7.265211	-0.898954	-3.604131
C	3.798879	-1.807183	2.411283
H	3.545307	-1.699722	1.340029
C	2.381443	3.167312	2.716655
H	2.019140	2.998510	1.683139
C	1.162872	3.635500	3.526505
H	0.386391	2.841936	3.538634
H	1.435746	3.885720	4.572250
H	0.725707	4.546284	3.069231
C	3.438654	4.274203	2.632286
H	3.780485	4.581017	3.643285
H	4.315193	3.920927	2.048909
H	3.016628	5.163541	2.116912
C	2.863463	-2.883709	2.974709
H	3.108433	-3.117454	4.032070
H	1.810504	-2.532938	2.919035
H	2.948268	-3.817869	2.382132
C	5.261624	-2.270372	2.434054
H	5.920550	-1.462362	2.049563
H	5.586481	-2.545175	3.459148
H	5.389266	-3.158856	1.779842
H	1.751711	-3.235718	-0.025515
H	3.841344	-4.522828	0.241641
C	2.394491	-3.389364	-0.881664
C	3.578957	-4.115137	-0.724678
C	2.045702	-2.862256	-2.138524
C	4.423266	-4.323519	-1.816801
H	5.339560	-4.885949	-1.693050
C	2.905467	-3.074966	-3.230425
C	4.084187	-3.807991	-3.069366
H	2.660080	-2.683223	-4.209662
H	4.738501	-3.971590	-3.915825
C	-1.989065	1.489476	-2.081285
H	-1.970058	0.591956	-2.721666
C	-0.813606	2.389842	-2.387534
H	0.164362	1.900384	-2.255745
H	-0.827741	2.750640	-3.432869
H	-0.807763	3.295209	-1.763901
B	-3.372733	2.144957	-2.095884
O	-4.565636	1.454043	-2.273511
O	-3.594239	3.506906	-1.981862

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C  -4.961603   3.756633  -2.374129
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C  -5.506690   4.932267  -1.592719
H  -5.415064   4.787752  -0.509754
H  -4.956658   5.847094  -1.853425
H  -6.567287   5.101129  -1.830372
C  -4.949978   4.071508  -3.862795
H  -4.581019   3.218218  -4.449360
H  -5.949634   4.336425  -4.234583
H  -4.282610   4.923096  -4.051734
C  -6.798187   2.027807  -2.974585
H  -7.596598   2.781685  -2.916494
H  -6.478419   1.944890  -4.020420
H  -7.232505   1.062458  -2.679923
C  -6.064951   2.278186  -0.602745
H  -6.314012   1.236183  -0.360268
H  -5.247918   2.594400   0.060498
H  -6.943628   2.898901  -0.378769
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Figure_S7_imid-3_modeC_ts(AS)_02 / electronic energy: -4442.739381669286 a.u. / lowest freq: -279.72 cm-1
C   0.605150  -1.461999   3.195530
H   0.592251  -2.551272   3.044501
C  -0.768265  -0.804762   2.953169
H  -0.938630   0.067739   3.607551
C   0.674772  -0.235624   1.190244
C   2.810581  -1.093155   1.890041
C   3.668204   0.008699   1.933416
C   3.332011  -2.359989   1.563903
C   5.026747  -0.128988   1.659925
H   3.265298   0.988289   2.190133
C   4.699280  -2.490231   1.312042
C   5.546714  -1.384671   1.357513
H   5.668240   0.753768   1.700905
H   5.082781  -3.479524   1.056765
H   6.612302  -1.509223   1.152178
S   2.312321  -3.834225   1.399624
O   3.164227  -4.825091   0.682659
O   1.157100  -3.416047   0.548265
O   1.948129  -4.248359   2.768002
Cu  1.474568   1.020965  -0.115231
C   1.179385  -1.147826   4.553154
C   1.400898  -2.178802   5.483216
C   1.507792   0.174069   4.908797
C   1.944522  -1.893337   6.739260
H   1.150111  -3.203416   5.240660
C   2.052160   0.454355   6.165078
H   1.344795   0.986370   4.213429
C   2.271123  -0.578474   7.079481
H   2.112229  -2.692531   7.449629
H   2.304335   1.473095   6.429606
H   2.692425  -0.359874   8.052160
N   1.422099  -0.858991   2.112723
N  -0.606948  -0.297298   1.571962
C   2.208352   1.600516  -1.936747
C   1.663625   2.854268  -2.462107
C   2.508374   3.811184  -3.047185
C   0.290747   3.144607  -2.384123
C   2.002200   5.015517  -3.528898
C  -0.215694   4.347190  -2.861704
C   0.638576   5.291539  -3.435141
H   2.680040   5.746433  -3.977061
H  -1.285286   4.551489  -2.784207
H   0.240633   6.238919  -3.805632
C   1.536362   0.350536  -2.042792
C   2.141381  -0.878597  -1.702573
H   3.104705  -0.866261  -1.182431
H   1.503587  -1.734669  -1.473867
H  -0.380322   2.427492  -1.900720
H   0.529894   0.319302  -2.474370
P   2.628118  -3.117972  -3.456902
O   3.650266  -3.918045  -2.442276
O   1.295162  -3.736023  -3.146281
O   3.187765  -3.442938  -4.942147
O   2.873394  -1.605127  -3.320333
Na  1.726374  -4.994847  -1.230346
H   3.300498   1.561838  -1.818674
H   3.577959   3.597596  -3.132205
C   5.012376  -3.537897  -2.350503
H   5.454071  -4.078329  -1.505160
H   5.562081  -3.799313  -3.268092
H   5.112321  -2.455568  -2.177815
C   3.058765  -4.762142  -5.449543
H   3.399035  -4.748479  -6.490629
H   3.682611  -5.472512  -4.884606
H   2.014305  -5.104092  -5.419572
C  -1.673690   0.045728   0.705443
C  -2.754597   0.804299   1.175930
C  -1.713665  -0.474855  -0.599803
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C	-3.859323	1.044840	0.349168
C	-2.839984	-0.276506	-1.412574
C	-3.906682	0.493233	-0.935693
H	-4.786136	0.639238	-1.551452
H	-0.908848	-1.107679	-0.950434
H	-2.738399	1.203902	2.182609
C	-2.963279	-0.972446	-2.715658
C	-2.929164	-0.233859	-3.935492
C	-3.188497	-2.381280	-2.748683
C	-3.139942	-0.914774	-5.149361
C	-3.343465	-3.017484	-3.994082
C	-3.329264	-2.289858	-5.176131
H	-3.152846	-0.381597	-6.090387
H	-3.499497	-4.086421	-4.054695
H	-3.473000	-2.795871	-6.122280
C	-4.993407	1.849477	0.838697
C	-6.139052	1.203934	1.382875
C	-4.962536	3.266585	0.714147
C	-7.236225	1.990899	1.778696
C	-6.073213	4.009911	1.154183
C	-7.196491	3.376819	1.674406
H	-8.133389	1.532356	2.172625
H	-6.081073	5.089368	1.080297
H	-8.047305	3.965455	1.992927
C	-3.775128	4.004692	0.093827
H	-2.980575	3.297964	-0.220919
C	-3.123028	4.953417	1.106450
H	-2.823880	4.388844	2.015504
H	-2.210647	5.409793	0.666293
H	-3.815903	5.769530	1.400390
C	-4.196446	4.755667	-1.175379
H	-4.640215	4.045019	-1.905215
H	-4.937839	5.550262	-0.949030
H	-3.312463	5.232103	-1.647970
C	-6.223286	-0.316288	1.528947
H	-5.256413	-0.797575	1.274523
C	-7.263420	-0.898024	0.565653
H	-7.260314	-2.007499	0.626246
H	-8.283323	-0.531706	0.808825
H	-7.016231	-0.608711	-0.478284
C	-6.523591	-0.727299	2.976195
H	-6.469459	-1.832204	3.073891
H	-5.774304	-0.276849	3.661604
H	-7.538252	-0.406104	3.290466
C	-3.291502	-3.229864	-1.480087
H	-3.217684	-2.606994	-0.568699
C	-2.675637	1.272609	-3.976597
H	-2.420717	1.657888	-2.969303
C	-1.481488	1.616691	-4.880286
H	-0.575128	1.073071	-4.540857
H	-1.679060	1.356170	-5.940299
H	-1.274359	2.705473	-4.839988
C	-3.931832	2.025587	-4.429464
H	-4.200529	1.763637	-5.474751
H	-4.787240	1.776168	-3.766854
H	-3.759197	3.121732	-4.371963
C	-2.142130	-4.242745	-1.411503
H	-2.195037	-4.970623	-2.248064
H	-1.168696	-3.710124	-1.459523
H	-2.180587	-4.806488	-0.456693
C	-4.654612	-3.927212	-1.380860
H	-5.470327	-3.176354	-1.456905
H	-4.784149	-4.684304	-2.182154
H	-4.748712	-4.439540	-0.399690
H	-1.364056	-3.012758	1.416899
H	-3.228584	-4.602304	1.720071
C	-2.061351	-2.865061	2.230185
C	-3.117710	-3.765601	2.395825
C	-1.911468	-1.775940	3.108264
C	-4.029337	-3.592055	3.438707
H	-4.846119	-4.290662	3.565477
C	-2.838264	-1.608600	4.152179
C	-3.886917	-2.517205	4.318590
H	-2.745803	-0.780670	4.843919
H	-4.593997	-2.384009	5.127087
C	1.493678	2.651518	1.123241
H	1.546298	2.138539	2.097512
C	0.185266	3.397468	0.984424
H	-0.702626	2.746905	1.041638
H	0.052065	4.153776	1.780153
H	0.117363	3.951697	0.037433
B	2.773582	3.448816	0.857668
O	4.029737	3.089977	1.334377
O	2.827024	4.644312	0.161106
C	4.118329	5.236655	0.416184
C	4.994978	3.985197	0.741028
C	4.558419	6.023375	-0.799223
H	4.562616	5.408745	-1.707184

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 H   3.872687   6.864323  -0.971293
 H   5.567143   6.437419  -0.655060
 C   3.956024   6.160062   1.614936
 H   3.658560   5.600343   2.513060
 H   4.881692   6.707145   1.841855
 H   3.170426   6.897758   1.403546
 C   6.114513   4.233883   1.727938
 H   6.810731   4.995784   1.348230
 H   5.735175   4.568493   2.701087
 H   6.691100   3.313053   1.892990
 C   5.526262   3.314651  -0.515574
 H   5.934933   2.325012  -0.269128
 H   4.722732   3.175308  -1.252339
 H   6.325283   3.901303  -0.990004
170
Figure_S7_imid-3_modeC_ts(AS)_03 / electronic energy: -4442.737028981568 a.u. / lowest freq: -266.30 cm-1
 C  -1.350344   2.401846  -1.730509
 H  -2.120856   1.944161  -2.360754
 C   0.044144   1.793348  -1.955383
 H   0.841379   2.520030  -1.719853
 C  -0.780609   1.003232   0.075230
 C  -2.781051   2.258985   0.462872
 C  -2.561794   2.648087   1.792502
 C  -4.107660   2.087908   0.017125
 C  -3.621130   2.835350   2.675671
 H  -1.535273   2.829761   2.119747
 C  -5.161696   2.303587   0.909625
 C  -4.930062   2.663118   2.233488
 H  -3.417336   3.139936   3.704528
 H  -6.178165   2.160846   0.539485
 H  -5.771101   2.816688   2.912734
 S  -4.558218   1.567950  -1.644808
 O  -5.996730   1.185044  -1.581321
 O  -3.710750   0.362435  -1.912349
 O  -4.284984   2.720625  -2.521979
Cu  -0.821269   0.220913   1.900121
 C  -1.367829   3.893009  -1.975037
 C  -1.326932   4.354221  -3.303485
 C  -1.402656   4.839755  -0.931382
 C  -1.322064   5.723619  -3.582185
 H  -1.300114   3.650370  -4.126191
 C  -1.394989   6.208314  -1.215242
 H  -1.411216   4.537112   0.103778
 C  -1.355816   6.650220  -2.538767
 H  -1.290355   6.066195  -4.608360
 H  -1.413721   6.927400  -0.406426
 H  -1.348975   7.710547  -2.755625
 N  -1.614284   1.992482  -0.320485
 N   0.062843   0.741826  -0.927897
 C  -1.533650  -1.255927   3.135790
 C  -0.622814  -1.857099   4.113085
 C  -1.064688  -2.087484   5.426565
 C   0.698049  -2.208806   3.786363
 C  -0.228041  -2.676116   6.371638
 C   1.533503  -2.794295   4.730255
 C   1.074408  -3.035523   6.025990
 H  -0.595612  -2.852634   7.385187
 H   2.558272  -3.053818   4.462057
 H   1.735703  -3.491587   6.766010
 C  -1.636353  -1.668992   1.784227
 C  -2.711658  -1.299047   0.953757
 H  -3.403375  -0.519699   1.287115
 H  -2.616522  -1.398168  -0.128389
 H   1.081980  -1.976467   2.789336
 H  -0.902057  -2.372278   1.381671
 P  -5.004852  -2.928942   0.038238
 O  -6.085296  -1.682549   0.050543
 O  -4.587950  -2.998317  -1.402726
 O  -5.865527  -4.210508   0.540772
 O  -3.999472  -2.731653   1.180630
Na  -5.571346  -1.083663  -2.299926
 H  -2.425822  -0.774202   3.564166
 H  -2.085586  -1.806660   5.700653
 C  -6.649924  -1.234239   1.269697
 H  -7.323594  -0.401365   1.037292
 H  -7.225464  -2.033731   1.761138
 H  -5.874770  -0.881187   1.966986
 C  -6.881132  -4.726213  -0.304633
 H  -7.263177  -5.642408   0.159176
 H  -7.713909  -4.013322  -0.412935
 H  -6.489369  -4.967673  -1.303244
 C   1.122144  -0.182312  -0.786183
 C   2.400435   0.263294  -0.441368
 C   0.921978  -1.536805  -1.096769
 C   3.473201  -0.630265  -0.382920
 C   2.004250  -2.432453  -1.074116
 C   3.275895  -1.977916  -0.701876
 H   4.115873  -2.663036  -0.694300
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H	-0.058368	-1.879525	-1.404879
H	2.569924	1.307943	-0.247594
C	1.843811	-3.827661	-1.538472
C	1.545940	-4.864431	-0.609239
C	2.109977	-4.150333	-2.900266
C	1.517986	-6.196794	-1.060436
C	2.085444	-5.500536	-3.296661
C	1.784615	-6.507615	-2.387959
H	1.308047	-7.008761	-0.376882
H	2.313501	-5.784042	-4.315273
H	1.771184	-7.540183	-2.712764
C	4.821174	-0.129071	-0.055313
C	5.584951	0.546628	-1.048685
C	5.343610	-0.294041	1.258004
C	6.844678	1.065785	-0.698855
C	6.616145	0.229270	1.551972
C	7.351011	0.907807	0.586282
H	7.447477	1.592225	-1.427029
H	7.047135	0.114765	2.537770
H	8.325524	1.308579	0.834215
C	4.576117	-1.033413	2.354344
H	3.570863	-1.342209	2.003056
C	4.336081	-0.135774	3.575767
H	3.856635	0.814666	3.262607
H	3.658105	-0.643843	4.293859
H	5.285884	0.098923	4.100044
C	5.309774	-2.320629	2.749705
H	5.457533	-2.961670	1.854275
H	6.300411	-2.097407	3.198932
H	4.712487	-2.893675	3.488026
C	5.088236	0.712469	-2.486271
H	4.101814	0.227191	-2.630749
C	6.034123	0.030827	-3.482729
H	5.594394	0.058221	-4.502792
H	7.022336	0.535845	-3.513590
H	6.182127	-1.032837	-3.198301
C	4.893225	2.192421	-2.834687
H	4.460966	2.289444	-3.853396
H	4.191302	2.661262	-2.113314
H	5.856591	2.743641	-2.808608
C	2.470993	-3.082801	-3.934163
H	2.338100	-2.062643	-3.519049
C	1.301695	-4.583757	0.870222
H	1.284734	-3.494625	1.059612
C	-0.061179	-5.120546	1.329840
H	-0.864485	-4.749785	0.657855
H	-0.080809	-6.230319	1.332743
H	-0.279042	-4.768061	2.360761
C	2.436528	-5.156321	1.726852
H	2.494664	-6.261019	1.630292
H	3.406781	-4.715484	1.412518
H	2.272117	-4.907080	2.795571
C	1.556119	-3.153816	-5.163887
H	1.711686	-4.090375	-5.738076
H	0.492449	-3.096105	-4.849416
H	1.770576	-2.302347	-5.842598
C	3.944098	-3.199415	-4.339528
H	4.591058	-3.128158	-3.439110
H	4.143128	-4.165992	-4.849176
H	4.216976	-2.371064	-5.027890
H	-1.335096	-0.227608	-3.220302
H	-1.028301	-1.043546	-5.526175
C	-0.566320	0.213482	-3.841214
C	-0.392897	-0.254144	-5.146345
C	0.246098	1.248889	-3.344554
C	0.603619	0.291191	-5.959573
H	0.738895	-0.075342	-6.968844
C	1.253090	1.782618	-4.167421
C	1.431840	1.302099	-5.467259
H	1.892515	2.578960	-3.808426
H	2.207929	1.719435	-6.095647
C	0.303534	1.182732	3.304160
H	1.038285	0.367971	3.443409
C	-0.457725	1.467395	4.585741
H	-0.894863	0.571296	5.052322
H	0.180923	1.936078	5.357976
H	-1.284534	2.178605	4.426301
B	0.998846	2.426038	2.731162
O	2.149139	2.442734	1.964609
O	0.579739	3.714749	3.030876
C	1.681806	4.602502	2.750053
C	2.471459	3.814410	1.648564
C	1.135038	5.944670	2.314889
H	0.419474	5.847179	1.489681
H	0.612289	6.427978	3.151143
H	1.943759	6.617354	1.994473
C	2.475999	4.744250	4.039871
H	2.886381	3.778006	4.366768

H 3.308765 5.452805 3.932285
H 1.816869 5.114373 4.836666
C 3.976633 3.973126 1.694528
H 4.271528 5.018841 1.524130
H 4.395038 3.647116 2.654227
H 4.439865 3.361476 0.907906
C 1.951122 4.121473 0.254899
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H 0.886644 3.864113 0.183609
H 2.069792 5.182063 -0.002622
170
Figure_S7_imid-3_modeC_ts(AS)_04 / electronic energy: -4442.743915610607 a.u. / lowest freq: -272.34 cm-1
C 2.575193 -1.458084 -1.665408
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C 1.329611 -0.669854 0.167012
C 3.619984 -1.102747 0.708201
C 3.487211 -1.779731 1.928383
C 4.775732 -0.329989 0.480354
C 4.467144 -1.689431 2.913061
H 2.606264 -2.406743 2.085005
C 5.758570 -0.262588 1.472385
C 5.610804 -0.929118 2.684385
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H 6.641178 0.347537 1.276251
H 6.390834 -0.855035 3.444724
S 5.079754 0.624762 -1.014191
O 6.185985 1.565378 -0.670828
O 3.815678 1.384604 -1.266300
O 5.428214 -0.353253 -2.060724
Cu 0.895798 -0.162138 2.035963
C 3.221827 -2.766622 -2.056208
C 3.516734 -2.988265 -3.413693
C 3.525149 -3.779377 -1.124177
C 4.100295 -4.188277 -3.828984
H 3.295073 -2.228166 -4.152745
C 4.106246 -4.978929 -1.544743
H 3.300462 -3.665669 -0.075807
C 4.394866 -5.183143 -2.895162
H 4.322886 -4.347013 -4.876195
H 4.328742 -5.753350 -0.821962
H 4.844506 -6.113117 -3.218174
N 2.517997 -1.197665 -0.198948
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C 0.847263 1.376873 3.409463
C -0.286916 1.430516 4.335313
C -0.069751 1.717563 5.693235
C -1.604165 1.185094 3.911319
C -1.134683 1.792793 6.587782
C -2.666848 1.258515 4.804019
C -2.438280 1.568680 6.146080
H -0.944312 2.025175 7.638221
H -3.681618 1.054773 4.459115
H -3.274337 1.620655 6.846991
C 0.831885 1.902800 2.095684
C 1.993854 2.017635 1.300889
H 2.934958 1.599826 1.668114
H 1.898356 2.055422 0.217678
H -1.780150 0.889077 2.873119
H -0.110967 2.260261 1.668550
P 2.358455 4.796272 0.307480
O 2.070601 6.264500 0.944131
O 3.357872 4.985137 -0.796974
O 0.901575 4.320419 -0.263831
O 2.647561 3.820776 1.463877
Na 5.007860 3.552346 -1.213012
H 1.835838 1.271695 3.881854
H 0.951237 1.893782 6.043531
C 1.081627 6.402817 1.950492
H 1.331076 7.283935 2.552935
H 0.086521 6.552412 1.504592
H 1.048092 5.522854 2.610434
C 0.405473 4.952738 -1.430561
H -0.655837 4.701626 -1.521655
H 0.496362 6.048284 -1.370399
H 0.931187 4.606655 -2.332393
C -0.803722 -0.205430 -0.831045
C -1.808186 -1.166435 -0.698188
C -1.155055 1.146500 -0.974708
C -3.154357 -0.793153 -0.694652
C -2.508603 1.524607 -0.998444
C -3.505172 0.552056 -0.848232
H -4.550521 0.836983 -0.881450
H -0.382076 1.891087 -1.117721
H -1.547682 -2.207520 -0.626987
C -2.902971 2.923371 -1.273691
C -3.225976 3.802624 -0.200854

C	-3.072026	3.356476	-2.620213
C	-3.705083	5.091963	-0.496460
C	-3.570750	4.650545	-2.860953
C	-3.873755	5.507770	-1.810782
H	-3.969506	5.779949	0.295525
H	-3.740531	5.001382	-3.869868
H	-4.255208	6.499532	-2.017448
C	-4.196498	-1.832498	-0.604321
C	-4.524004	-2.605045	-1.754405
C	-4.850566	-2.081745	0.634698
C	-5.485237	-3.624999	-1.634460
C	-5.814477	-3.104610	0.698095
C	-6.119964	-3.869972	-0.421870
H	-5.754026	-4.234519	-2.487109
H	-6.336874	-3.315738	1.621771
H	-6.861085	-4.655783	-0.351206
C	-4.553138	-1.265398	1.892996
H	-3.740273	-0.532963	1.713689
C	-4.066830	-2.159158	3.041575
H	-3.212463	-2.781199	2.705042
H	-3.723518	-1.532475	3.891912
H	-4.874286	-2.828506	3.405056
C	-5.783369	-0.451396	2.311144
H	-6.116793	0.190351	1.467812
H	-6.622211	-1.114967	2.609593
H	-5.535084	0.207216	3.169012
C	-3.878190	-2.351171	-3.118535
H	-3.161068	-1.506567	-3.075650
C	-4.927163	-1.948961	-4.162424
H	-4.426800	-1.660245	-5.111645
H	-5.627634	-2.783737	-4.374787
H	-5.507727	-1.074295	-3.798473
C	-3.073752	-3.570228	-3.584657
H	-2.555926	-3.341095	-4.540362
H	-2.304480	-3.828353	-2.826193
H	-3.730668	-4.450637	-3.745205
C	-2.773098	2.447674	-3.812652
H	-2.290075	1.503830	-3.487316
C	-3.102614	3.382757	1.260517
H	-2.654156	2.374939	1.337816
C	-2.176856	4.326607	2.039894
H	-1.203001	4.416544	1.517116
H	-2.620491	5.338423	2.145125
H	-1.989299	3.924700	3.057667
C	-4.483177	3.297038	1.920590
H	-4.976904	4.291232	1.949967
H	-5.129100	2.591732	1.355673
H	-4.387063	2.922341	2.960761
C	-1.789003	3.106387	-4.788435
H	-2.221754	4.011759	-5.261332
H	-0.857092	3.388934	-4.253631
H	-1.530037	2.395958	-5.600187
C	-4.068632	2.045916	-4.525642
H	-4.760036	1.556851	-3.806229
H	-4.574257	2.931347	-4.965981
H	-3.847539	1.321361	-5.338529
H	1.643869	1.130759	-2.908467
H	1.260142	2.058948	-5.158223
C	1.177061	0.512623	-3.663951
C	0.957593	1.043623	-4.937192
C	0.802930	-0.811982	-3.373466
C	0.339518	0.269569	-5.922486
H	0.164408	0.685384	-6.906200
C	0.172830	-1.578898	-4.368915
C	-0.060915	-1.037216	-5.635573
H	-0.126721	-2.599964	-4.169809
H	-0.544860	-1.634206	-6.397631
C	0.192280	-1.642877	3.239399
H	-0.816178	-1.209096	3.372572
C	0.931860	-1.734002	4.560625
H	0.923168	-0.794825	5.136393
H	0.512494	-2.509823	5.228900
H	1.990149	-2.010449	4.423691
B	0.084342	-2.975915	2.488582
O	-0.891690	-3.315797	1.567663
O	0.930517	-4.048038	2.735058
C	0.281676	-5.234846	2.231434
C	-0.642331	-4.659418	1.103323
C	1.337466	-6.212401	1.763416
H	2.033067	-5.753981	1.049964
H	1.926180	-6.569074	2.619191
H	0.879875	-7.090465	1.284938
C	-0.515128	-5.824959	3.385852
H	-1.282906	-5.123764	3.743133
H	-1.012107	-6.763746	3.104117
H	0.159379	-6.037493	4.226163
C	-1.972975	-5.364244	0.940639
H	-1.831962	-6.414729	0.646914

H -2.567629 -5.338944 1.861353
H -2.560616 -4.871593 0.153634
C 0.077631 -4.585984 -0.233052
H -0.581412 -4.190579 -1.015484
H 0.956151 -3.933428 -0.154446
H 0.410569 -5.575282 -0.573466
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Figure_S7_imid-3_modeC_ts(AS)_05 / electronic energy: -4442.742404258524 a.u. / lowest freq: -266.68 cm-1
C -0.551418 -2.898495 -2.224144
H -0.389119 -3.795760 -1.607682
C 0.721524 -2.047866 -2.395886
H 0.748771 -1.525723 -3.368475
C -0.748857 -0.934234 -0.948999
C -2.764470 -2.231718 -1.053636
C -3.763397 -1.371982 -1.516725
C -3.097020 -3.249116 -0.139363
C -5.082325 -1.515477 -1.093310
H -3.501314 -0.576377 -2.214892
C -4.425150 -3.394054 0.265939
C -5.416150 -2.535221 -0.205888
H -5.839458 -0.826315 -1.472874
H -4.663045 -4.181757 0.982338
H -6.447483 -2.662042 0.130218
S -1.882255 -4.368419 0.573454
O -2.556954 -4.981870 1.754423
O -0.739655 -3.510114 1.011535
O -1.545641 -5.335156 -0.488645
Cu -1.706802 0.645738 -0.240888
C -1.179142 -3.290266 -3.536410
C -1.255319 -4.644325 -3.906807
C -1.699653 -2.313543 -4.406612
C -1.844676 -5.013025 -5.119873
H -0.855083 -5.415627 -3.261232
C -2.289080 -2.687254 -5.617407
H -1.651993 -1.264213 -4.146144
C -2.362132 -4.035864 -5.973704
H -1.899506 -6.057449 -5.398446
H -2.689386 -1.930619 -6.279734
H -2.818379 -4.323666 -6.912002
N -1.425093 -1.971140 -1.465471
N 0.524413 -1.021338 -1.348127
C -2.511434 1.816825 1.236575
C -2.116013 3.225647 1.201569
C -3.070554 4.237874 1.389640
C -0.786153 3.608591 0.955188
C -2.710765 5.581598 1.337693
C -0.425687 4.949599 0.898519
C -1.386788 5.944479 1.090214
H -3.471470 6.351990 1.487286
H 0.612871 5.221532 0.698907
H -1.103829 6.998376 1.042293
C -1.710016 0.781448 1.794923
C -2.180407 -0.542870 1.920329
H -3.146829 -0.798867 1.478399
H -1.473151 -1.372637 1.983283
H -0.034938 2.835603 0.763213
H -0.709912 1.014215 2.176241
P -1.834018 -1.217418 4.728568
O -2.520829 -1.223265 6.202384
O -1.074452 -2.504641 4.584918
O -0.815022 0.060650 4.771719
O -2.908813 -0.809369 3.707743
Na -0.953523 -4.319951 3.356959
H -3.591499 1.620713 1.183870
H -4.108600 3.959495 1.594179
C -3.289195 -0.104258 6.612994
H -3.625790 -0.292712 7.638705
H -2.691342 0.820308 6.600005
H -4.167867 0.036968 5.967427
C 0.346448 -0.044143 5.573745
H 0.808227 0.948205 5.622563
H 0.104939 -0.364226 6.599558
H 1.065398 -0.758760 5.147465
C 1.546533 -0.199844 -0.814852
C 2.466214 0.427548 -1.666276
C 1.718728 -0.105701 0.577903
C 3.542154 1.146037 -1.133053
C 2.830196 0.565114 1.112412
C 3.730983 1.201709 0.251120
H 4.595253 1.715581 0.655546
H 1.040898 -0.629021 1.240776
H 2.345631 0.356512 -2.740466
C 3.131547 0.505505 2.562252
C 3.057291 1.673380 3.371439
C 3.597086 -0.704225 3.151564
C 3.484137 1.588213 4.713173
C 3.955874 -0.691767 4.515307
C 3.904812 0.431913 5.242072

H	3.465303	2.462509	5.350499
H	4.296226	-1.597590	4.999843
H	4.205671	0.403882	6.282215
C	4.496219	1.822689	-2.024914
C	5.690633	1.190051	-2.441304
C	4.258490	3.235048	-2.441777
C	6.596976	1.928447	-3.230955
C	5.236341	3.847498	-3.243378
C	6.352030	3.195774	-3.605988
H	7.527026	1.476694	-3.550558
H	5.106895	4.870440	-3.572877
H	7.083736	3.711540	-4.215904
C	3.025577	4.012247	-1.999157
H	2.368359	3.374500	-1.372825
C	2.185600	4.450324	-3.203938
H	1.917299	3.565824	-3.820545
H	1.245111	4.929214	-2.856668
H	2.737134	5.176951	-3.836922
C	3.417877	5.213866	-1.131960
H	4.005860	4.870636	-0.254033
H	4.023505	5.945329	-1.707302
H	2.508068	5.730072	-0.760665
C	6.030956	-0.243711	-2.039153
H	5.188743	-0.712224	-1.488318
C	7.236317	-0.271293	-1.093386
H	7.422788	-1.309491	-0.744178
H	8.151365	0.102755	-1.599619
H	7.032933	0.361251	-0.202679
C	6.274431	-1.128787	-3.267804
H	6.436119	-2.180304	-2.949426
H	5.389491	-1.097738	-3.938861
H	7.169888	-0.801586	-3.835811
C	3.734246	-2.006818	2.365039
H	3.511569	-1.854607	1.292031
C	2.520450	3.002997	2.848520
H	2.158857	2.899761	1.805858
C	1.316666	3.476835	3.676342
H	0.508863	2.715575	3.642790
H	1.592923	3.659834	4.735123
H	0.919775	4.427444	3.265683
C	3.621407	4.069311	2.826362
H	3.969696	4.308306	3.853345
H	4.486279	3.712347	2.227985
H	3.237932	5.000885	2.357663
C	2.734496	-3.049543	2.878358
H	2.936742	-3.312864	3.937921
H	1.700107	-2.650236	2.798259
H	2.795307	-3.975370	2.269689
C	5.171663	-2.542566	2.406696
H	5.878888	-1.756868	2.064005
H	5.457254	-2.865904	3.429276
H	5.271804	-3.415444	1.727332
H	1.658663	-3.303521	-0.130605
H	3.722534	-4.636200	0.109528
C	2.310181	-3.432897	-0.984164
C	3.480808	-4.183688	-0.842193
C	1.987265	-2.847729	-2.222027
C	4.338177	-4.357685	-1.930295
H	5.244109	-4.939009	-1.818102
C	2.858960	-3.027821	-3.310378
C	4.024589	-3.784619	-3.164362
H	2.634066	-2.590291	-4.275037
H	4.687935	-3.922944	-4.008287
C	-1.938567	1.615490	-2.024956
H	-1.913487	0.748804	-2.706333
C	-0.752673	2.522161	-2.268268
H	0.220465	2.023155	-2.134846
H	-0.741879	2.926115	-3.297743
H	-0.755923	3.400608	-1.607025
B	-3.318103	2.280176	-2.023788
O	-4.515541	1.607077	-2.238145
O	-3.531929	3.637109	-1.850861
C	-4.896892	3.914016	-2.230715
C	-5.591509	2.535728	-1.981518
C	-5.432290	5.056032	-1.394472
H	-5.351772	4.855623	-0.319546
H	-4.865929	5.974405	-1.602775
H	-6.488267	5.252431	-1.631221
C	-4.884109	4.298270	-3.702870
H	-4.519858	3.471218	-4.328654
H	-5.882855	4.584939	-4.060666
H	-4.212211	5.154239	-3.851755
C	-6.743001	2.225715	-2.913297
H	-7.541444	2.975409	-2.815131
H	-6.423548	2.198330	-3.962170
H	-7.178163	1.246197	-2.670643
C	-6.013556	2.359792	-0.531705
H	-6.272236	1.309337	-0.340071

H -5.196443 2.635687 0.149401
H -6.887851 2.976188 -0.280026
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Figure_S7_imid-3_modeC_ts(AS)_06 / electronic energy: -4442.738698912161 a.u. / lowest freq: -278.31 cm-1
C 0.637612 -1.434755 3.210247
H 0.643953 -2.524507 3.062346
C -0.746274 -0.800907 2.962572
H -0.931474 0.070439 3.614503
C 0.691723 -0.211940 1.202412
C 2.840239 -1.027905 1.907742
C 3.674396 0.092604 1.934119
C 3.387779 -2.286987 1.595089
C 5.034591 -0.019149 1.656937
H 3.250482 1.066384 2.179014
C 4.757095 -2.391609 1.342839
C 5.580878 -1.267657 1.371190
H 5.656057 0.878456 1.680474
H 5.161290 -3.375490 1.098734
H 6.648308 -1.372138 1.164255
S 2.396611 -3.781220 1.437532
O 3.267848 -4.759185 0.726067
O 1.236404 -3.386855 0.581283
O 2.036307 -4.196463 2.806507
Cu 1.455164 1.053651 -0.113016
C 1.202882 -1.106116 4.568050
C 1.436347 -2.129353 5.503609
C 1.511103 0.222140 4.918237
C 1.971595 -1.830038 6.760041
H 1.201255 -3.158571 5.264966
C 2.047102 0.516268 6.174951
H 1.339121 1.028648 4.218052
C 2.277885 -0.508933 7.095039
H 2.148555 -2.623318 7.474777
H 2.283705 1.539793 6.435371
H 2.692701 -0.279608 8.068036
N 1.447406 -0.819983 2.127959
N -0.589446 -0.293491 1.581111
C 2.145839 1.646681 -1.943948
C 1.528242 2.866022 -2.470365
C 2.309881 3.859020 -3.081792
C 0.143817 3.085475 -2.366036
C 1.731008 5.028923 -3.566636
C -0.435483 4.252333 -2.849283
C 0.356085 5.232360 -3.451389
H 2.360043 5.789380 -4.036357
H -1.513023 4.398879 -2.754236
H -0.098510 6.151936 -3.826766
C 1.533603 0.365073 -2.034706
C 2.192842 -0.831207 -1.677752
H 3.153473 -0.770131 -1.156118
H 1.590543 -1.709447 -1.436927
H -0.477516 2.342955 -1.854587
H 0.529721 0.282173 -2.465384
P 2.732081 -3.066265 -3.419596
O 3.758675 -3.858678 -2.403579
O 1.404240 -3.697495 -3.113336
O 3.298912 -3.383945 -4.903645
O 2.961361 -1.551005 -3.280287
Na 1.842794 -4.952721 -1.194821
H 3.239422 1.663551 -1.836737
H 3.387551 3.701185 -3.184815
C 5.116584 -3.466115 -2.302865
H 5.560040 -4.011624 -1.461703
H 5.672085 -3.712438 -3.221175
H 5.206173 -2.384962 -2.117550
C 3.186663 -4.704700 -5.411110
H 3.530683 -4.687494 -6.450886
H 3.816148 -5.407867 -4.843473
H 2.145928 -5.058121 -5.384962
C -1.658980 0.020587 0.707382
C -2.756752 0.760394 1.167638
C -1.684925 -0.514938 -0.592083
C -3.865102 0.966203 0.337500
C -2.812440 -0.347441 -1.409889
C -3.896406 0.404502 -0.943436
H -4.777599 0.524640 -1.562427
H -0.867029 -1.136195 -0.933021
H -2.752471 1.167799 2.171389
C -2.918098 -1.062086 -2.703575
C -2.901098 -0.351387 -3.936683
C -3.109608 -2.472909 -2.730910
C -3.088405 -1.077860 -5.131267
C -3.246119 -3.107118 -3.982767
C -3.240760 -2.408577 -5.125385
H -3.107611 -0.568033 -6.085452
H -3.378277 -4.179769 -4.040791
H -3.368076 -2.931005 -6.065722
C -5.020824 1.735605 0.824340

C	-6.174363	1.089933	1.328184
C	-5.023755	3.224541	0.733631
C	-7.273560	1.887563	1.709230
C	-6.176578	3.897930	1.171781
C	-7.245436	3.229052	1.631283
H	-8.176461	1.420467	2.080543
H	-6.223405	4.978635	1.132259
H	-8.117127	3.789700	1.946298
C	-3.843917	4.003289	0.166453
H	-3.037414	3.310754	-0.151047
C	-3.233727	4.926801	1.226327
H	-2.936602	4.334805	2.118507
H	-2.325318	5.421919	0.821356
H	-3.953832	5.712544	1.537867
C	-4.253010	4.790386	-1.084197
H	-4.651269	4.095855	-1.854924
H	-5.026850	5.550653	-0.848335
H	-3.372133	5.314716	-1.509860
C	-6.261197	-0.429689	1.458813
H	-5.289433	-0.905340	1.210704
C	-7.289839	-1.002528	0.478268
H	-7.287966	-2.112445	0.529748
H	-8.312374	-0.637581	0.712288
H	-7.030058	-0.704596	-0.560156
C	-6.578589	-0.851741	2.898917
H	-6.516595	-1.956864	2.991342
H	-5.842559	-0.399779	3.597539
H	-7.599791	-0.538214	3.199987
C	-3.200200	-3.319400	-1.461476
H	-3.141909	-2.690374	-0.552851
C	-2.690092	1.158827	-4.013833
H	-2.455231	1.574178	-3.013727
C	-1.499144	1.512787	-4.917623
H	-0.580509	1.004641	-4.556606
H	-1.681042	1.217460	-5.971351
H	-1.322712	2.607786	-4.905197
C	-3.963813	1.863717	-4.493498
H	-4.216552	1.568959	-5.534056
H	-4.816500	1.604946	-3.830738
H	-3.823627	2.965514	-4.460666
C	-2.031270	-4.308725	-1.385794
H	-2.064511	-5.037300	-2.222804
H	-1.068744	-3.756573	-1.427673
H	-2.064219	-4.872908	-0.430926
C	-4.549312	-4.043697	-1.367160
H	-5.379592	-3.309273	-1.446211
H	-4.660459	-4.802850	-2.169320
H	-4.636844	-4.558014	-0.386481
H	-1.286320	-3.038819	1.448895
H	-3.137893	-4.645050	1.738586
C	-1.999064	-2.889094	2.248197
C	-3.048971	-3.798613	2.405420
C	-1.876848	-1.787542	3.115028
C	-3.983477	-3.620263	3.427025
H	-4.795938	-4.325170	3.546491
C	-2.825865	-1.616282	4.138316
C	-3.869565	-2.532411	4.294937
H	-2.756429	-0.777729	4.819869
H	-4.594517	-2.395387	5.086791
C	1.445178	2.696132	1.109944
H	1.520584	2.192994	2.088048
C	0.121723	3.417345	0.984167
H	-0.753013	2.752393	1.071283
H	-0.008672	4.185482	1.768902
H	0.024202	3.952613	0.028750
B	2.707932	3.511569	0.817842
O	3.977912	3.170114	1.269351
O	2.731931	4.705740	0.117169
C	4.019946	5.316564	0.345139
C	4.919659	4.078224	0.659133
C	4.427626	6.103417	-0.881590
H	4.423319	5.485679	-1.787324
H	3.729495	6.935984	-1.044048
H	5.433835	6.529884	-0.757739
C	3.866946	6.243790	1.542180
H	3.591978	5.684984	2.447985
H	4.789237	6.803893	1.750279
H	3.068401	6.970330	1.340941
C	6.050642	4.345752	1.628032
H	6.727955	5.119210	1.237574
H	5.681372	4.673781	2.607278
H	6.645263	3.434813	1.783610
C	5.442686	3.413670	-0.604295
H	5.863801	2.427791	-0.363326
H	4.633359	3.267355	-1.333282
H	6.230414	4.008833	-1.086906

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Figure_S7_imid-3_modeC_prod(AS) / electronic energy: -4442.751813336476 a.u. / lowest freq: 17.37 cm-1

C	-0.651741	-1.916313	-3.113639
H	-0.510903	-2.983232	-2.882466
C	0.643109	-1.090914	-2.980879
H	0.690353	-0.259560	-3.705045
C	-0.789420	-0.564885	-1.207221
C	-2.838602	-1.709968	-1.747854
C	-3.832387	-0.740986	-1.887392
C	-3.174412	-2.987079	-1.264927
C	-5.153624	-1.021661	-1.547431
H	-3.567935	0.245651	-2.266847
C	-4.504139	-3.264058	-0.944917
C	-5.491724	-2.289540	-1.082896
H	-5.908252	-0.240392	-1.658368
H	-4.745461	-4.255500	-0.557544
H	-6.524524	-2.524694	-0.817753
S	-1.949596	-4.274524	-0.985845
O	-2.621223	-5.267712	-0.100232
O	-0.832144	-3.592921	-0.267929
O	-1.594496	-4.803334	-2.316229
Cu	-1.675231	0.592920	0.112605
C	-1.309430	-1.771843	-4.461590
C	-1.458057	-2.891241	-5.299087
C	-1.792756	-0.523572	-4.898047
C	-2.079603	-2.764409	-6.545028
H	-1.090791	-3.861985	-4.991651
C	-2.414627	-0.402140	-6.143679
H	-1.691305	0.353925	-4.273153
C	-2.558333	-1.521575	-6.966546
H	-2.190102	-3.630743	-7.184319
H	-2.785661	0.560536	-6.470800
H	-3.039876	-1.425900	-7.931095
N	-1.494913	-1.329917	-2.042922
N	0.474937	-0.495794	-1.633644
C	-2.459917	1.449266	1.858524
C	-2.096010	2.808950	2.252088
C	-3.074795	3.717723	2.685085
C	-0.760804	3.246301	2.195104
C	-2.731498	5.016082	3.049277
C	-0.418923	4.547107	2.544924
C	-1.404132	5.438061	2.974299
H	-3.507383	5.706137	3.389396
H	0.621474	4.871343	2.476446
H	-1.136473	6.461038	3.247654
C	-1.650184	0.318594	2.169877
C	-1.906273	-0.935607	1.643134
H	-2.897858	-1.193243	1.250894
H	-1.212559	-1.765781	1.790764
H	0.010655	2.561966	1.828565
H	-0.684773	0.484276	2.661517
P	-1.750746	-2.872895	4.281486
O	-1.789594	-3.723109	5.698088
O	-0.706525	-3.580217	3.442080
O	-1.135922	-1.423185	4.790161
O	-3.136150	-2.593859	3.775029
Na	-1.190430	-4.905271	1.756324
H	-3.527698	1.253717	1.681097
H	-4.115206	3.389254	2.755176
C	-2.671896	-3.280283	6.704342
H	-2.715593	-4.048213	7.487407
H	-2.327514	-2.337063	7.161677
H	-3.688011	-3.117554	6.311088
C	0.218098	-1.402079	5.176716
H	0.425770	-0.437631	5.658285
H	0.456277	-2.202765	5.896616
H	0.886202	-1.521885	4.309052
C	1.521263	0.085172	-0.873213
C	2.462544	0.922259	-1.490198
C	1.696197	-0.268628	0.476827
C	3.564003	1.397919	-0.768953
C	2.835528	0.153368	1.182122
C	3.761351	0.994249	0.554759
H	4.647266	1.317591	1.087948
H	0.999116	-0.947690	0.949425
H	2.337533	1.206835	-2.527649
C	3.134667	-0.380554	2.533134
C	3.123557	0.481072	3.670856
C	3.516868	-1.747584	2.686621
C	3.503872	-0.039648	4.922445
C	3.835566	-2.226114	3.970917
C	3.838838	-1.378698	5.070144
H	3.534057	0.590956	5.800657
H	4.108958	-3.261582	4.124436
H	4.108728	-1.762383	6.045695
C	4.529937	2.313885	-1.401913
C	5.709603	1.796783	-2.006268
C	4.309517	3.718824	-1.349296
C	6.649866	2.698907	-2.537445
C	5.268105	4.577092	-1.918189

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C   6.424423   4.070603  -2.501119
H   7.569544   2.342642  -2.981967
H   5.131136   5.650230  -1.897739
H   7.157081   4.748052  -2.920758
C   3.080790   4.325952  -0.669692
H   2.416264   3.538363  -0.260481
C   2.231024   5.121739  -1.667437
H   1.945132   4.472842  -2.522848
H   1.300368   5.476610  -1.175055
H   2.781248   6.005339  -2.053369
C   3.487059   5.195177   0.526303
H   4.103313   4.600142   1.233423
H   4.068782   6.083292   0.201584
H   2.582691   5.547622   1.065697
C   6.000128   0.296629  -2.068494
H   5.136620  -0.294306  -1.699176
C   7.187458  -0.064227  -1.169363
H   7.338220  -1.165044  -1.160806
H   8.121466   0.419406  -1.526083
H   6.986671   0.264793  -0.127168
C   6.239171  -0.171822  -3.509619
H   6.352783  -1.276229  -3.533340
H   5.372896   0.105996  -4.147348
H   7.160315   0.274922  -3.937736
C   3.627847  -2.711779   1.503772
H   3.429423  -2.199996   0.543402
C   2.720601   1.953235   3.585099
H   2.358422   2.207658   2.568601
C   1.562378   2.275291   4.540907
H   0.685727   1.637948   4.305492
H   1.846058   2.117691   5.601593
H   1.262208   3.337247   4.430867
C   3.921036   2.864730   3.866993
H   4.283663   2.739195   4.909119
H   4.752196   2.631255   3.168904
H   3.634007   3.927843   3.719553
C   2.593635  -3.837824   1.621315
H   2.772217  -4.456985   2.525302
H   1.571465  -3.406748   1.676792
H   2.640986  -4.498655   0.731014
C   5.049352  -3.274494   1.370469
H   5.782653  -2.441428   1.313595
H   5.310893  -3.928796   2.228057
H   5.135609  -3.872862   0.438629
H   1.557406  -3.061023  -1.287737
H   3.581833  -4.448859  -1.542057
C   2.198033  -2.912856  -2.145736
C   3.346011  -3.698293  -2.283969
C   1.884513  -1.936285  -3.108479
C   4.187652  -3.521211  -3.383756
H   5.075607  -4.130775  -3.489578
C   2.741023  -1.764244  -4.209951
C   3.882001  -2.559156  -4.348628
H   2.522589  -1.021742  -4.967274
H   4.533574  -2.424454  -5.202260
C  -1.899656   2.139572  -1.198768
H  -1.891804   1.553680  -2.131330
C  -0.722818   3.080003  -1.156379
H   0.246497   2.582957  -1.302407
H  -0.797998   3.835420  -1.958841
H  -0.669829   3.653297  -0.220721
B  -3.287122   2.792147  -0.994778
O  -4.474972   2.226591  -1.411521
O  -3.472300   4.046129  -0.458859
C  -4.821602   4.459860  -0.795441
C  -5.553073   3.088095  -0.968879
C  -5.370119   5.336586   0.307473
H  -5.332721   4.844615   1.286069
H  -4.785967   6.264210   0.378056
H  -6.413941   5.613102   0.100335
C  -4.728594   5.240186  -2.097207
H  -4.346856   4.614634  -2.916595
H  -5.703317   5.645488  -2.401402
H  -4.037246   6.083456  -1.968492
C  -6.645926   3.082160  -2.015100
H  -7.432161   3.808523  -1.763969
H  -6.259354   3.325235  -3.012145
H  -7.117159   2.091214  -2.070727
C  -6.066706   2.526503   0.345622
H  -6.362278   1.476866   0.214031
H  -5.290918   2.562409   1.122662
H  -6.940401   3.081352   0.713640
170
Figure_S7_imid-3_modeD_ed(AS) / electronic energy: -4442.757427819045 a.u. / lowest freq: 12.40 cm-1
C   0.410647   0.018323   3.272467
H   0.684755  -0.964074   3.678020
C  -1.053287   0.072252   2.782674
H  -1.587192   0.965074   3.148267
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C	0.391114	0.324174	0.923065
C	2.582071	0.288392	1.898302
C	3.128978	1.425395	1.290936
C	3.438246	-0.770016	2.257418
C	4.493306	1.527254	1.042597
H	2.458229	2.232489	0.986125
C	4.808681	-0.656980	2.005814
C	5.339751	0.481588	1.405806
H	4.880689	2.422514	0.551279
H	5.449215	-1.501507	2.266769
H	6.413682	0.544356	1.214326
S	2.878422	-2.289783	3.036131
O	3.970039	-3.282975	2.822377
O	1.645045	-2.713434	2.303508
O	2.649723	-1.949878	4.453068
Cu	1.169089	0.790239	-0.864214
C	0.720730	1.087332	4.290221
C	1.063585	0.734226	5.607390
C	0.654032	2.449974	3.944030
C	1.349714	1.723026	6.553099
H	1.099803	-0.304374	5.908636
C	0.938472	3.435035	4.894692
H	0.378019	2.746652	2.939881
C	1.289291	3.071936	6.196680
H	1.613816	1.443025	7.564679
H	0.883652	4.481094	4.625363
H	1.508648	3.836099	6.931075
N	1.169106	0.237878	2.018861
N	-0.886377	0.195783	1.316222
C	2.317004	0.182187	-2.452669
C	3.264120	1.199569	-2.912139
C	2.919175	2.026046	-3.998514
C	4.536393	1.371036	-2.338024
C	3.795142	2.997086	-4.472369
C	5.411757	2.343884	-2.809426
C	5.046502	3.167244	-3.876454
H	3.501603	3.625791	-5.317197
H	6.394910	2.456387	-2.343177
H	5.736255	3.929176	-4.248124
C	2.483618	-0.713276	-1.377093
C	1.880880	-2.066359	-1.404917
H	1.680180	-2.462106	-0.396741
H	0.954292	-2.090324	-1.991559
H	4.846388	0.726315	-1.512245
H	3.357959	-0.606247	-0.720480
P	3.684463	-4.011115	-1.302938
O	4.856467	-3.138475	-0.626382
O	3.049319	-4.870172	-0.265925
O	4.335985	-4.775769	-2.552665
O	2.751340	-3.018971	-2.120810
Na	2.498872	-4.927057	1.891384
H	1.554373	-0.092486	-3.195065
H	1.944424	1.891687	-4.477169
C	5.667310	-2.284314	-1.431176
H	6.142000	-1.560241	-0.759145
H	6.446591	-2.860125	-1.950145
H	5.064383	-1.742629	-2.175746
C	5.147562	-5.924423	-2.314922
H	5.541764	-6.242841	-3.284616
H	5.989296	-5.689707	-1.647042
H	4.557356	-6.740786	-1.877552
C	-1.958469	0.050366	0.396768
C	-3.231681	0.566223	0.689674
C	-1.780504	-0.695105	-0.778093
C	-4.306508	0.330659	-0.178965
C	-2.855273	-0.947552	-1.637065
C	-4.120949	-0.437917	-1.333232
H	-4.956198	-0.631655	-1.996507
H	-0.815570	-1.119076	-1.001045
H	-3.390061	1.151485	1.586462
C	-2.654874	-1.791394	-2.832365
C	-2.560491	-1.194854	-4.122444
C	-2.505172	-3.200425	-2.685293
C	-2.286559	-2.016444	-5.231099
C	-2.234420	-3.976647	-3.826921
C	-2.123198	-3.388819	-5.081683
H	-2.192186	-1.593764	-6.222687
H	-2.108095	-5.048493	-3.749850
H	-1.911817	-4.003354	-5.947407
C	-5.634213	0.902241	0.108332
C	-6.581782	0.155761	0.862025
C	-5.982918	2.177022	-0.418887
C	-7.864133	0.698437	1.065172
C	-7.272781	2.682136	-0.175123
C	-8.200372	1.948692	0.556829
H	-8.616079	0.150174	1.617009
H	-7.570801	3.647329	-0.563072
H	-9.191396	2.349999	0.726032

C -5.007033 3.004259 -1.256561
H -4.032761 2.488824 -1.358965
C -4.700991 4.349952 -0.588684
H -4.324490 4.183001 0.443305
H -3.914323 4.887228 -1.160551
H -5.604160 4.994028 -0.543944
C -5.530730 3.198548 -2.684226
H -5.746333 2.210856 -3.145494
H -6.456687 3.811165 -2.694303
H -4.762883 3.708733 -3.304484
C -6.259473 -1.226282 1.431989
H -5.198870 -1.497483 1.252084
C -7.100903 -2.308499 0.746493
H -6.797103 -3.313844 1.109232
H -8.182581 -2.168554 0.955562
H -6.938496 -2.274326 -0.352302
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C -2.643368 -3.900361 -1.331093
H -2.890930 -3.178501 -0.526981
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H -2.975087 0.826231 -3.398092
C -1.415585 0.938385 -4.837870
H -0.594355 0.709422 -4.126836
H -1.138981 0.555328 -5.842642
H -1.522164 2.042737 -4.896581
C -3.882315 0.613951 -5.299180
H -3.671731 0.241989 -6.323657
H -4.815327 0.139218 -4.926738
H -4.050802 1.710895 -5.353584
C -1.326697 -4.569856 -0.918442
H -1.035958 -5.366903 -1.634371
H -0.516083 -3.813696 -0.872793
H -1.428225 -5.025112 0.088952
C -3.796459 -4.911473 -1.343391
H -4.737023 -4.409624 -1.656913
H -3.588867 -5.754654 -2.035112
H -3.949291 -5.324786 -0.323291
H -0.926056 -2.471508 1.710040
H -2.227889 -4.453661 2.377910
C -1.638031 -2.387687 2.520361
C -2.377062 -3.513947 2.892506
C -1.835226 -1.157966 3.177416
C -3.307884 -3.429313 3.929920
H -3.878710 -4.302663 4.217416
C -2.775868 -1.084681 4.219292
C -3.502581 -2.217431 4.596325
H -2.943706 -0.152515 4.744222
H -4.224275 -2.153182 5.400309
C 0.424264 2.580291 -1.526312
H 0.721972 2.497235 -2.586530
C -1.077756 2.745000 -1.392407
H -1.393306 2.798764 -0.337599
H -1.463017 3.671790 -1.859067
H -1.649637 1.924133 -1.849879
B 1.223747 3.713793 -0.885599
O 0.635223 4.770763 -0.197054
O 2.607163 3.869741 -0.921425
C 2.901323 5.231757 -0.565673
C 1.675672 5.615497 0.329981
C 4.238946 5.287115 0.141538
H 4.265658 4.637305 1.025516
H 5.039548 4.964440 -0.539792
H 4.471140 6.311917 0.467165
C 2.955828 6.033683 -1.859014
H 1.992160 6.001082 -2.388001
H 3.215235 7.087201 -1.683124
H 3.715212 5.601288 -2.525007
C 1.240735 7.061982 0.213456
H 2.050032 7.743445 0.514338
H 0.939859 7.315387 -0.810371
H 0.382164 7.254656 0.871321
C 1.870270 5.248034 1.791464
H 0.910837 5.350185 2.315783
H 2.209490 4.209229 1.908275
H 2.600118 5.901350 2.290009
170
Figure_S7_imid-3_modeD_ts(AS)_01 / electronic energy: -4442.744184694649 a.u. / lowest freq: -259.20 cm-1
C 0.482095 0.089062 3.254720
H 0.803924 -0.864808 3.693004
C -0.994496 0.081675 2.800761
H -1.552535 0.956036 3.172974
C 0.394288 0.339357 0.903029
C 2.612064 0.432962 1.847002
C 3.073161 1.595996 1.218904
C 3.546233 -0.535434 2.262140

C	4.429526	1.810716	0.998570
H	2.342250	2.338329	0.890108
C	4.908527	-0.295271	2.062447
C	5.354633	0.865745	1.436139
H	4.750914	2.715834	0.479619
H	5.615963	-1.059802	2.388366
H	6.424411	1.023377	1.281850
S	3.089738	-2.119605	2.987521
O	4.310758	-2.969035	2.883980
O	1.999028	-2.650703	2.113714
O	2.678129	-1.843085	4.376199
Cu	1.186063	0.766402	-0.896059
C	0.785775	1.208491	4.220089
C	1.188848	0.920402	5.536054
C	0.660428	2.553626	3.823589
C	1.474442	1.955500	6.431073
H	1.274395	-0.103562	5.875243
C	0.944919	3.584900	4.723710
H	0.341290	2.801566	2.818886
C	1.354516	3.286254	6.024871
H	1.785331	1.725390	7.441932
H	0.845530	4.616844	4.415376
H	1.574246	4.086198	6.720003
N	1.205393	0.282213	1.973989
N	-0.868641	0.196543	1.330017
C	2.402216	0.298632	-2.478137
C	3.328839	1.322477	-2.952426
C	2.965584	2.133084	-4.044579
C	4.595615	1.521428	-2.374408
C	3.818813	3.123915	-4.517317
C	5.446345	2.515136	-2.844413
C	5.060693	3.327348	-3.912977
H	3.515395	3.742095	-5.366010
H	6.426286	2.651964	-2.378894
H	5.732041	4.106308	-4.282956
C	2.653655	-0.622987	-1.425810
C	1.901173	-1.802244	-1.275372
H	1.893682	-2.306874	-0.305396
H	1.009114	-1.925474	-1.887961
H	4.925160	0.879077	-1.554176
H	3.513404	-0.477581	-0.761851
P	3.358865	-4.306707	-1.432803
O	4.434290	-3.626728	-0.384324
O	2.523021	-5.178925	-0.541059
O	4.276435	-5.124783	-2.490392
O	2.747707	-3.195379	-2.300034
Na	3.239936	-4.679699	1.571484
H	1.633677	-0.000320	-3.204294
H	1.999136	1.968482	-4.530224
C	5.461909	-2.777856	-0.866697
H	5.796490	-2.148478	-0.032418
H	6.316101	-3.363386	-1.239642
H	5.097514	-2.131623	-1.680789
C	4.861822	-6.351310	-2.081011
H	5.412507	-6.754055	-2.938068
H	5.567673	-6.203985	-1.248251
H	4.097243	-7.078061	-1.771642
C	-1.964250	0.010618	0.447575
C	-3.223832	0.554781	0.744314
C	-1.820591	-0.791201	-0.693102
C	-4.319993	0.294905	-0.089689
C	-2.915177	-1.066898	-1.519658
C	-4.168988	-0.528674	-1.211292
H	-5.019343	-0.735469	-1.850926
H	-0.866609	-1.237183	-0.914359
H	-3.353046	1.186560	1.613877
C	-2.742469	-1.944484	-2.696657
C	-2.711877	-1.386154	-4.007690
C	-2.550253	-3.344900	-2.514899
C	-2.480276	-2.238055	-5.103150
C	-2.320592	-4.151153	-3.644810
C	-2.287200	-3.602107	-4.920918
H	-2.437542	-1.844927	-6.110317
H	-2.162819	-5.216593	-3.541631
H	-2.106744	-4.239642	-5.776965
C	-5.628052	0.913429	0.191801
C	-6.578207	0.232886	1.002415
C	-5.948614	2.176922	-0.379142
C	-7.833908	0.829646	1.220072
C	-7.212012	2.737898	-0.119347
C	-8.141822	2.069150	0.669406
H	-8.586217	0.333291	1.818637
H	-7.486999	3.697676	-0.536648
H	-9.112115	2.513235	0.851421
C	-4.969110	2.936134	-1.275125
H	-4.022539	2.375240	-1.397312
C	-4.582404	4.285067	-0.657703
H	-4.169199	4.129438	0.361953

H -3.800513 4.775833 -1.275975
H -5.457358 4.965420 -0.592824
C -5.534820 3.113977 -2.688911
H -5.818870 2.125570 -3.109545
H -6.427129 3.774634 -2.686736
H -4.764925 3.563433 -3.352158
C -6.285982 -1.132844 1.624794
H -5.246477 -1.456970 1.412437
C -7.199935 -2.210615 1.030886
H -6.917295 -3.209688 1.426496
H -8.264295 -2.018993 1.283162
H -7.089671 -2.232841 -0.074629
C -6.407406 -1.088267 3.153043
H -6.117184 -2.069748 3.583816
H -5.728575 -0.310931 3.564600
H -7.446583 -0.866086 3.473198
C -2.584288 -4.004135 -1.134367
H -2.821186 -3.267593 -0.340760
C -2.884080 0.111196 -4.265800
H -3.093183 0.657847 -3.328249
C -1.598546 0.722174 -4.836817
H -0.744245 0.508326 -4.159519
H -1.370310 0.312918 -5.843422
H -1.705250 1.825049 -4.919192
C -4.083786 0.388364 -5.180232
H -3.920417 -0.018933 -6.199808
H -5.000795 -0.069039 -4.750778
H -4.250689 1.483541 -5.265071
C -1.216236 -4.600141 -0.778878
H -0.928834 -5.403823 -1.488793
H -0.439201 -3.807299 -0.800408
H -1.239863 -5.030619 0.243744
C -3.688459 -5.065370 -1.048783
H -4.666096 -4.618732 -1.330664
H -3.477820 -5.925767 -1.717862
H -3.769385 -5.444528 -0.007378
H -0.646418 -2.488251 1.864950
H -1.848346 -4.524244 2.565747
C -1.406645 -2.417539 2.631438
C -2.089780 -3.573159 3.020602
C -1.718759 -1.175811 3.216601
C -3.083234 -3.503503 3.999477
H -3.610318 -4.399542 4.300395
C -2.722368 -1.117411 4.199260
C -3.395056 -2.277900 4.591818
H -2.981676 -0.175641 4.666612
H -4.162954 -2.225635 5.352707
C 0.419391 2.501959 -1.640329
H 0.702515 2.389792 -2.700358
C -1.082596 2.594161 -1.485043
H -1.385979 2.690273 -0.430968
H -1.503452 3.480160 -1.994847
H -1.618431 1.730076 -1.901861
B 1.177902 3.698611 -1.041355
O 0.525868 4.741759 -0.405008
O 2.544337 3.919648 -1.091614
C 2.764466 5.315817 -0.793552
C 1.517053 5.670686 0.083474
C 4.093955 5.478731 -0.089513
H 4.152163 4.882371 0.829444
H 4.914218 5.165738 -0.751352
H 4.266929 6.531064 0.179158
C 2.777987 6.057000 -2.122718
H 1.818121 5.952254 -2.648923
H 2.984263 7.128809 -1.995544
H 3.558664 5.630813 -2.767063
C 0.998512 7.081369 -0.101632
H 1.765363 7.821995 0.168187
H 0.686902 7.269990 -1.136002
H 0.128376 7.252993 0.546426
C 1.724475 5.380422 1.559961
H 0.758462 5.448629 2.077528
H 2.126215 4.371003 1.725962
H 2.411150 6.098620 2.028962

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Figure_S7_imid-3_modeD_ts(AS)_02 / electronic energy: -4442.745381055473 a.u. / lowest freq: -275.78 cm-1

C -0.771787 -0.843775 3.217681
H -0.743354 0.036026 3.876603
C 0.616582 -1.226987 2.664164
H 0.787167 -2.316490 2.672129
C -0.723082 -0.432668 0.888139
C -2.868168 -0.092966 1.918518
C -3.702131 -0.851722 1.089958
C -3.388846 1.042502 2.564676
C -5.036280 -0.507017 0.900516
H -3.277463 -1.716889 0.576116
C -4.734214 1.372694 2.379512
C -5.557437 0.606388 1.556973

H	-5.654048	-1.105500	0.227311
H	-5.117616	2.267007	2.873881
H	-6.602983	0.890800	1.420763
S	-2.411539	2.130454	3.617738
O	-3.152498	3.423439	3.636932
O	-1.092948	2.302876	2.930049
O	-2.325508	1.453965	4.923766
Cu	-1.616477	-0.101299	-0.885998
C	-1.452759	-1.987585	3.925213
C	-1.761226	-1.893390	5.293369
C	-1.789147	-3.163398	3.228262
C	-2.402626	-2.949658	5.947361
H	-1.501482	-1.006813	5.857140
C	-2.430683	-4.216458	3.886243
H	-1.553248	-3.261884	2.176168
C	-2.738840	-4.109055	5.244249
H	-2.637714	-2.869731	7.000816
H	-2.687985	-5.116922	3.344182
H	-3.235173	-4.925516	5.752603
N	-1.501960	-0.474794	1.983256
N	0.516883	-0.789013	1.252374
C	-2.593938	1.153712	-2.197344
C	-3.710457	0.620922	-2.973875
C	-3.479641	0.128694	-4.272059
C	-5.026505	0.583401	-2.478098
C	-4.514586	-0.407823	-5.031517
C	-6.060736	0.049523	-3.237855
C	-5.810535	-0.456374	-4.515418
H	-4.310328	-0.786808	-6.035950
H	-7.075759	0.031869	-2.831985
H	-6.624681	-0.876853	-5.110731
C	-2.682629	1.704483	-0.896287
C	-1.652913	2.471177	-0.311376
H	-1.579527	2.514584	0.777166
H	-0.700902	2.544109	-0.841481
H	-5.243218	0.982223	-1.484466
H	-3.612924	1.600950	-0.326882
P	-0.959458	5.287324	-0.411650
O	-1.519930	6.594933	-1.198122
O	-0.389584	5.611686	0.938375
O	0.264680	4.756342	-1.350354
O	-2.135885	4.290447	-0.524876
Na	-1.273022	4.739520	2.803657
H	-1.712514	1.434784	-2.790591
H	-2.468388	0.176782	-4.686956
C	-0.728922	7.772661	-1.185811
H	-1.269153	8.538674	-1.752970
H	-0.562398	8.135548	-0.161029
H	0.250633	7.606319	-1.661567
C	-0.008057	4.432326	-2.703915
H	0.523790	3.505452	-2.955466
H	-1.082294	4.272240	-2.881940
H	0.344997	5.232265	-3.370970
C	1.634111	-0.707146	0.382171
C	2.626151	-1.701622	0.396040
C	1.809357	0.420902	-0.433551
C	3.773564	-1.566214	-0.397067
C	2.963982	0.566053	-1.211759
C	3.946197	-0.428244	-1.191088
H	4.841691	-0.317181	-1.791926
H	1.074036	1.210102	-0.424462
H	2.508259	-2.580418	1.017163
C	3.167747	1.790879	-2.010195
C	2.963212	1.767995	-3.419120
C	3.544614	3.001903	-1.363019
C	3.121959	2.961473	-4.147135
C	3.683099	4.169314	-2.135907
C	3.475445	4.145908	-3.510404
H	2.957909	2.983006	-5.216355
H	3.954820	5.109307	-1.674191
H	3.584617	5.055451	-4.086994
C	4.803430	-2.620796	-0.405282
C	5.901801	-2.547832	0.495704
C	4.728189	-3.674817	-1.358230
C	6.907298	-3.529296	0.418669
C	5.749751	-4.641337	-1.382937
C	6.825800	-4.565690	-0.505274
H	7.767392	-3.493299	1.073962
H	5.723354	-5.455441	-2.095299
H	7.607953	-5.312903	-0.546737
C	3.584679	-3.777029	-2.367948
H	2.856819	-2.954908	-2.229576
C	2.792526	-5.076633	-2.182592
H	2.424466	-5.149147	-1.136701
H	1.911993	-5.084927	-2.860034
H	3.416742	-5.966483	-2.408476
C	4.101083	-3.640842	-3.805048
H	4.671369	-2.693308	-3.913770

H 4.759281 -4.491805 -4.079643
H 3.246552 -3.612266 -4.514691
C 6.038171 -1.421286 1.521077
H 5.142976 -0.765873 1.519073
C 7.230975 -0.519881 1.184025
H 7.269292 0.339950 1.886751
H 8.188359 -1.078302 1.254502
H 7.122448 -0.118674 0.153415
C 6.148973 -1.971250 2.948687
H 6.159969 -1.132632 3.676551
H 5.275156 -2.619331 3.174141
H 7.079953 -2.558687 3.089093
C 3.811693 3.073785 0.142121
H 3.721629 2.075923 0.616666
C 2.544624 0.499022 -4.162088
H 2.507336 -0.370054 -3.479023
C 1.133598 0.644442 -4.742982
H 0.417903 0.896393 -3.932183
H 1.096289 1.440152 -5.516545
H 0.809530 -0.313637 -5.202880
C 3.558383 0.123745 -5.250006
H 3.576834 0.876875 -6.065257
H 4.574935 0.042900 -4.808790
H 3.293871 -0.861456 -5.690564
C 2.785579 3.974726 0.838252
H 2.844108 5.017801 0.463275
H 1.761207 3.582358 0.664597
H 2.967131 3.988423 1.932852
C 5.244351 3.537153 0.434140
H 5.969596 2.883177 -0.096091
H 5.404098 4.588220 0.114633
H 5.450210 3.467960 1.523932
H 1.373482 1.426674 2.600299
H 3.217950 2.496272 3.838940
C 1.984085 0.827897 3.262561
C 3.032235 1.437605 3.957853
C 1.740878 -0.550805 3.409073
C 3.839982 0.682741 4.810776
H 4.650623 1.156781 5.348730
C 2.561588 -1.300893 4.269300
C 3.601068 -0.683826 4.970520
H 2.393992 -2.362344 4.403359
H 4.227033 -1.267740 5.632790
C -1.364776 -1.698178 -2.122053
H -1.604027 -1.225331 -3.088610
C 0.043697 -2.249832 -2.125641
H 0.302685 -2.735555 -1.171679
H 0.191524 -3.024842 -2.900030
H 0.809931 -1.485133 -2.320618
B -2.451167 -2.733973 -1.791020
O -2.163214 -4.056843 -1.495810
O -3.819805 -2.509722 -1.784073
C -4.470141 -3.797475 -1.828351
C -3.395874 -4.739759 -1.184284
C -5.778507 -3.722511 -1.071754
H -5.638332 -3.408311 -0.029740
H -6.452594 -3.001240 -1.555474
H -6.284328 -4.699023 -1.064916
C -4.726706 -4.116568 -3.294208
H -3.787301 -4.168377 -3.863514
H -5.258008 -5.069880 -3.421796
H -5.340850 -3.321460 -3.738566
C -3.346023 -6.132838 -1.776454
H -4.304278 -6.654499 -1.638004
H -3.116291 -6.114325 -2.848428
H -2.568577 -6.728016 -1.278412
C -3.504500 -4.824067 0.328843
H -2.610505 -5.320443 0.729666
H -3.572706 -3.829680 0.790555
H -4.383188 -5.402578 0.646116
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Figure_S7_imid-3_modeD_ts(AS)_03 / electronic energy: -4442.751658658786 a.u. / lowest freq: -273.13 cm-1
C -1.391245 -1.122972 2.714846
H -1.818509 -0.248604 3.219640
C 0.121540 -0.985814 2.447757
H 0.643802 -1.954811 2.535210
C -1.023635 -0.745796 0.410341
C -3.296190 -1.277656 0.924821
C -3.534221 -2.149743 -0.149674
C -4.376840 -0.562262 1.473826
C -4.810860 -2.318313 -0.673904
H -2.696282 -2.720462 -0.561889
C -5.658330 -0.753685 0.945528
C -5.882243 -1.621406 -0.119198
H -4.960531 -3.003987 -1.511055
H -6.481192 -0.183602 1.379385
H -6.892556 -1.747032 -0.514467
S -4.223083 0.632094 2.811670

O	-5.480531	1.431981	2.778140
O	-3.055949	1.499234	2.448329
O	-4.032230	-0.152579	4.043717
Cu	-1.595072	-0.520475	-1.494011
C	-1.711044	-2.337403	3.557530
C	-1.382002	-2.303185	4.925139
C	-2.307568	-3.503051	3.035991
C	-1.641978	-3.401572	5.748956
H	-0.923724	-1.421062	5.355111
C	-2.563616	-4.600010	3.863495
H	-2.567149	-3.587243	1.994267
C	-2.232393	-4.549568	5.218491
H	-1.384474	-3.362272	6.799461
H	-3.017274	-5.492313	3.451633
H	-2.431878	-5.400467	5.856881
N	-1.936267	-1.143742	1.328319
N	0.141875	-0.574111	1.035091
C	-2.613218	0.604805	-2.879418
C	-3.376327	-0.079818	-3.919079
C	-2.786342	-0.266241	-5.183948
C	-4.676881	-0.576338	-3.717520
C	-3.461711	-0.930642	-6.202556
C	-5.349886	-1.244348	-4.736043
C	-4.746843	-1.427862	-5.982545
H	-2.981676	-1.062299	-7.175237
H	-6.360248	-1.620994	-4.557630
H	-5.279462	-1.951539	-6.779505
C	-3.076212	0.959367	-1.589550
C	-2.332374	1.809371	-0.740325
H	-2.512674	1.764455	0.337114
H	-1.317426	2.073922	-1.039617
H	-5.171546	-0.434323	-2.753772
H	-4.050494	0.602232	-1.234815
P	-2.425730	4.653336	-0.032091
O	-2.476870	6.082687	-0.806254
O	-3.030038	4.863891	1.325427
O	-0.832098	4.308222	0.052813
O	-2.982311	3.576713	-0.984782
Na	-4.386489	3.550838	2.490811
H	-1.737531	1.156409	-3.246139
H	-1.778182	0.120721	-5.359975
C	-1.896442	6.191020	-2.095712
H	-2.189646	7.161248	-2.511829
H	-0.797319	6.145553	-2.045191
H	-2.252060	5.393222	-2.764007
C	-0.021448	5.074130	0.923829
H	1.022853	4.886237	0.655670
H	-0.215815	6.152801	0.818488
H	-0.178009	4.791319	1.974954
C	1.319816	-0.164271	0.368330
C	2.392756	-1.052742	0.217012
C	1.479262	1.177985	-0.006836
C	3.604983	-0.616363	-0.332466
C	2.694987	1.623010	-0.545576
C	3.750487	0.719759	-0.721305
H	4.697095	1.065241	-1.120482
H	0.681618	1.885523	0.173855
H	2.302559	-2.072609	0.554942
C	2.906049	3.055974	-0.842058
C	2.458330	3.605696	-2.076931
C	3.644403	3.863884	0.070504
C	2.780679	4.940519	-2.383267
C	3.942181	5.192051	-0.285762
C	3.511305	5.721601	-1.496106
H	2.482570	5.380784	-3.325250
H	4.519858	5.826204	0.373293
H	3.754111	6.744674	-1.753287
C	4.756766	-1.539281	-0.414635
C	5.497847	-1.852572	0.761246
C	5.135395	-2.105812	-1.665546
C	6.578743	-2.748171	0.664682
C	6.237065	-2.979938	-1.710133
C	6.941848	-3.302213	-0.556768
H	7.157524	-3.013566	1.539514
H	6.556409	-3.420976	-2.645103
H	7.782637	-3.981869	-0.611354
C	4.389930	-1.795442	-2.962603
H	3.527844	-1.129180	-2.774197
C	3.812243	-3.068928	-3.593917
H	3.155858	-3.587254	-2.864935
H	3.203759	-2.810524	-4.486147
H	4.615032	-3.765348	-3.913767
C	5.293500	-1.050487	-3.951729
H	5.697046	-0.130421	-3.477075
H	6.141161	-1.687548	-4.281356
H	4.709094	-0.748950	-4.847350
C	5.177329	-1.229676	2.121331
H	4.338883	-0.508092	2.048348

C	6.368240	-0.425534	2.657962
H	6.067033	0.136576	3.567996
H	7.218985	-1.088361	2.921504
H	6.706728	0.306492	1.894296
C	4.739099	-2.301181	3.126376
H	4.490595	-1.830204	4.100754
H	3.834537	-2.824952	2.749078
H	5.542454	-3.047734	3.298349
C	4.138812	3.330957	1.416684
H	3.745757	2.312045	1.612166
C	1.694438	2.775478	-3.105851
H	1.418911	1.791773	-2.684436
C	0.371442	3.439430	-3.510580
H	-0.244450	3.637174	-2.609550
H	0.538961	4.394561	-4.049585
H	-0.200333	2.765464	-4.182485
C	2.568281	2.494335	-4.332621
H	2.829368	3.435731	-4.861004
H	3.504831	1.983450	-4.020819
H	2.030386	1.826784	-5.039388
C	3.644697	4.195896	2.583857
H	4.103165	5.206377	2.566887
H	2.541409	4.301879	2.538834
H	3.909393	3.714632	3.549140
C	5.667319	3.221724	1.429076
H	6.007886	2.565588	0.599987
H	6.141111	4.219630	1.314672
H	6.009372	2.776138	2.387468
H	-0.346824	1.723709	2.594489
H	0.741891	3.363772	4.076788
C	0.415831	1.389187	3.285744
C	1.035264	2.323097	4.119692
C	0.784170	0.031781	3.341271
C	2.036479	1.916275	5.004711
H	2.519362	2.642322	5.645732
C	1.788068	-0.367154	4.239423
C	2.415006	0.572957	5.061882
H	2.079359	-1.406907	4.309394
H	3.190378	0.258434	5.748313
C	-0.627510	-1.711694	-2.829805
H	-1.381623	-1.868231	-3.618329
C	0.556374	-0.920185	-3.334940
H	1.248721	-0.645979	-2.524889
H	1.164922	-1.477552	-4.070216
H	0.268645	0.017591	-3.838325
B	-0.375251	-3.006150	-2.060492
O	0.795965	-3.367057	-1.415920
O	-1.341288	-4.001869	-1.937060
C	-0.682283	-5.190735	-1.456158
C	0.559068	-4.600531	-0.702542
C	-1.647357	-5.970278	-0.588682
H	-2.073955	-5.350216	0.209051
H	-2.479653	-6.350003	-1.196770
H	-1.152115	-6.835382	-0.124132
C	-0.286149	-6.006368	-2.677409
H	0.423999	-5.457075	-3.311638
H	0.170812	-6.966713	-2.401030
H	-1.179460	-6.217764	-3.280140
C	1.808340	-5.452334	-0.768239
H	1.655640	-6.415186	-0.258947
H	2.115776	-5.654995	-1.800919
H	2.639100	-4.936658	-0.267478
C	0.231125	-4.252119	0.739893
H	1.108011	-3.836648	1.251084
H	-0.573635	-3.504805	0.772268
H	-0.084010	-5.132612	1.315142

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Figure_S7_imid-3_modeD_ts(AS)_04 / electronic energy: -4442.747191445505 a.u. / lowest freq: -270.71 cm-1

C	-0.785304	-1.481038	2.676611
H	-1.367413	-0.740379	3.239343
C	0.658039	-1.024696	2.388013
H	1.359734	-1.877034	2.369122
C	-0.585641	-0.873376	0.404114
C	-2.663419	-1.938679	0.899697
C	-2.728805	-2.770095	-0.230013
C	-3.861902	-1.511635	1.500483
C	-3.949372	-3.168838	-0.763703
H	-1.796174	-3.125993	-0.678284
C	-5.082372	-1.933509	0.962376
C	-5.134937	-2.751806	-0.162378
H	-3.964302	-3.811675	-1.646815
H	-5.998338	-1.582738	1.441030
H	-6.101864	-3.060780	-0.566153
S	-3.936624	-0.415394	2.922935
O	-5.352674	0.043893	2.998678
O	-3.033870	0.733397	2.587992
O	-3.500175	-1.212259	4.083060
Cu	-1.259308	-0.660029	-1.464928

C	-0.823603	-2.780258	3.449791
C	-0.470227	-2.754833	4.811589
C	-1.178354	-4.014155	2.867724
C	-0.471945	-3.927899	5.570939
H	-0.193893	-1.821973	5.287355
C	-1.176546	-5.185090	3.630973
H	-1.442955	-4.092975	1.826714
C	-0.824816	-5.142521	4.981029
H	-0.198356	-3.894670	6.617579
H	-1.445242	-6.128231	3.172775
H	-0.824025	-6.050911	5.569420
N	-1.355236	-1.536666	1.299721
N	0.535047	-0.496199	1.020563
C	-2.530873	0.251811	-2.778652
C	-3.234638	-0.551741	-3.775151
C	-2.673442	-0.695569	-5.058766
C	-4.464972	-1.184471	-3.518307
C	-3.304399	-1.453682	-6.038947
C	-5.095072	-1.943565	-4.499816
C	-4.517813	-2.086430	-5.763202
H	-2.848015	-1.550346	-7.026933
H	-6.051853	-2.423792	-4.278780
H	-5.016305	-2.681484	-6.531678
C	-2.980742	0.513714	-1.458037
C	-2.426896	1.544613	-0.672333
H	-2.570297	1.516601	0.411659
H	-1.511746	2.023743	-1.019142
H	-4.942570	-1.073305	-2.541866
H	-3.825839	-0.047521	-1.042903
P	-4.444645	3.521531	0.032573
O	-5.401892	2.206521	0.297042
O	-4.060036	3.963053	1.414770
O	-5.403345	4.574051	-0.746779
O	-3.394185	3.162781	-1.031442
Na	-4.815230	2.357749	2.862312
H	-1.812966	0.970839	-3.196716
H	-1.725494	-0.195903	-5.279714
C	-6.114551	1.616045	-0.776981
H	-6.290221	0.560892	-0.529146
H	-7.086066	2.111354	-0.925817
H	-5.546231	1.670655	-1.718681
C	-6.370170	5.296282	0.000064
H	-6.898125	5.955331	-0.697435
H	-7.104623	4.623326	0.470282
H	-5.899317	5.905999	0.784082
C	1.564235	0.221910	0.368381
C	2.817874	-0.368703	0.157100
C	1.378697	1.576468	0.054596
C	3.871723	0.377908	-0.385450
C	2.433559	2.330065	-0.479063
C	3.675417	1.725441	-0.706730
H	4.497398	2.311096	-1.102247
H	0.435930	2.056331	0.279616
H	2.987154	-1.396326	0.439048
C	2.276884	3.779310	-0.725054
C	1.781384	4.241921	-1.976639
C	2.739946	4.712420	0.245460
C	1.804042	5.621884	-2.249191
C	2.736358	6.082855	-0.073691
C	2.275352	6.528565	-1.306968
H	1.467918	6.003743	-3.203870
H	3.105579	6.816505	0.630450
H	2.288553	7.586323	-1.536775
C	5.208214	-0.231758	-0.549774
C	6.053947	-0.402528	0.583996
C	5.661745	-0.626958	-1.841171
C	7.322963	-0.983142	0.403459
C	6.944501	-1.190873	-1.967961
C	7.759586	-1.371402	-0.857255
H	7.989600	-1.128933	1.243127
H	7.322445	-1.495056	-2.935090
H	8.742194	-1.809919	-0.975700
C	4.806513	-0.455851	-3.095910
H	3.816626	-0.031095	-2.845897
C	4.530365	-1.804796	-3.772279
H	4.042403	-2.494553	-3.053155
H	3.847736	-1.665889	-4.637015
H	5.465552	-2.273576	-4.143002
C	5.455731	0.529169	-4.074883
H	5.648110	1.497929	-3.565860
H	6.415043	0.132465	-4.468939
H	4.773772	0.718573	-4.931449
C	5.642916	0.046027	1.987656
H	4.635579	0.508769	1.986403
C	6.592944	1.123425	2.525130
H	6.204725	1.526922	3.484971
H	7.609891	0.714630	2.702174
H	6.663876	1.962254	1.800472

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C   5.566748  -1.148561   2.946021
H   5.231954  -0.811238   3.949371
H   4.835445  -1.893069   2.564287
H   6.555115  -1.640700   3.060204
C   3.266281   4.270769   1.611620
H   3.121992   3.180935   1.762191
C   1.273559   3.282739  -3.049573
H   1.189700   2.259650  -2.641009
C  -0.136124   3.653689  -3.531493
H  -0.823225   3.752260  -2.664830
H  -0.135361   4.606681  -4.100047
H  -0.528898   2.857948  -4.199283
C   2.256813   3.209526  -4.221937
H   2.341116   4.191965  -4.733201
H   3.261015   2.907088  -3.854729
H   1.915906   2.451228  -4.958972
C   2.503423   4.953060   2.754635
H   2.695487   6.045827   2.779076
H   1.412140   4.782043   2.637129
H   2.822602   4.527552   3.729492
C   4.772125   4.531125   1.724698
H   5.308065   4.019352   0.897001
H   4.995300   5.618087   1.678740
H   5.156599   4.130193   2.686926
H  -0.333162   1.505501   2.824985
H   0.485018   3.188911   4.428534
C   0.517477   1.271591   3.452114
C   0.982611   2.230909   4.354801
C   1.150759   0.018573   3.357677
C   2.092454   1.957657   5.157726
H   2.456008   2.705203   5.850722
C   2.260552  -0.249309   4.176647
C   2.731842   0.719251   5.067383
H   2.757633  -1.209569   4.130123
H   3.590035   0.507374   5.691796
C  -0.103572  -1.572428  -2.872257
H  -0.826157  -1.858558  -3.653503
C   0.864636  -0.518612  -3.356716
H   1.494912  -0.133289  -2.541511
H   1.567243  -0.900723  -4.119472
H   0.367546   0.349531  -3.818598
B   0.470784  -2.814966  -2.192669
O   1.712324  -2.918324  -1.590194
O  -0.220008  -4.020845  -2.131798
C   0.719290  -5.040065  -1.730273
C   1.792689  -4.211030  -0.948140
C  -0.012736  -6.081182  -0.909886
H  -0.568137  -5.632037  -0.077144
H  -0.735802  -6.616307  -1.540474
H   0.684173  -6.825563  -0.497858
C   1.279676  -5.661363  -3.000293
H   1.821631  -4.919506  -3.603843
H   1.965065  -6.491418  -2.780029
H   0.456063  -6.054317  -3.611136
C   3.209822  -4.729273  -1.062741
H   3.299069  -5.733132  -0.622462
H   3.549133  -4.780052  -2.103804
H   3.896456  -4.064374  -0.521210
C   1.413323  -4.024146   0.510476
H   2.166532  -3.418485   1.028526
H   0.446192  -3.507556   0.582050
H   1.346778  -4.978104   1.049879
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Figure_S7_imid-3_modeD_ts(AS)_05 / electronic energy: -4442.743469571735 a.u. / lowest freq: -217.01 cm-1
C  -0.169281   3.864799  -0.631695
H  -0.311886   4.119665  -1.692643
C   1.178207   3.166783  -0.362014
H   1.722941   3.600983   0.491556
C  -0.582094   1.629994   0.044430
C  -2.540589   2.978115  -0.540465
C  -3.324174   3.577937   0.447724
C  -3.131335   2.639648  -1.773702
C  -4.675068   3.839722   0.231733
H  -2.860241   3.836518   1.400677
C  -4.486081   2.902517  -1.982049
C  -5.256106   3.503466  -0.987450
H  -5.269568   4.304037   1.021722
H  -4.921583   2.644580  -2.948761
H  -6.313425   3.708911  -1.169958
S  -2.168584   1.975194  -3.143931
O  -3.156737   1.741325  -4.240117
O  -1.605317   0.676408  -2.676868
O  -1.169441   3.014908  -3.448172
Cu -1.893111   0.353726   0.889248
C  -0.385713   5.088124   0.225435
C  -0.657825   6.330155  -0.374445
C  -0.335677   5.004330   1.629995
C  -0.877489   7.463146   0.414841
```

H	-0.704104	6.423011	-1.452325
C	-0.557033	6.139358	2.414570
H	-0.131630	4.059621	2.116396
C	-0.827874	7.367862	1.807708
H	-1.088009	8.415649	-0.054030
H	-0.520102	6.065810	3.493744
H	-0.999636	8.245949	2.416678
N	-1.143195	2.799643	-0.308526
N	0.753525	1.790334	0.011344
C	-3.367151	-1.046835	1.090110
C	-4.680311	-0.575318	1.521032
C	-5.289203	-1.141282	2.655165
C	-5.364860	0.444523	0.836520
C	-6.539473	-0.708167	3.084548
C	-6.612302	0.881577	1.270383
C	-7.206920	0.306921	2.395566
H	-6.997195	-1.161979	3.967120
H	-7.121589	1.683966	0.729918
H	-8.186014	0.651608	2.736595
C	-2.938672	-1.025861	-0.268352
C	-1.805677	-1.723976	-0.701743
H	-1.422005	-1.497583	-1.693493
H	-1.096315	-2.109259	0.032363
H	-4.895976	0.920025	-0.031311
H	-3.552631	-0.532747	-1.030966
P	-2.839443	-3.781987	-2.569055
O	-4.203835	-4.666959	-2.401736
O	-3.049432	-2.580279	-3.446454
O	-1.928544	-4.846978	-3.381540
O	-2.269855	-3.572664	-1.153653
Na	-2.823617	-0.610178	-4.368412
H	-2.911691	-1.797870	1.746421
H	-4.754785	-1.917606	3.209235
C	-5.190747	-4.192631	-1.504985
H	-6.044875	-4.877935	-1.553957
H	-4.815519	-4.162930	-0.469900
H	-5.539271	-3.182570	-1.777557
C	-1.484619	-6.021544	-2.724050
H	-0.784057	-6.532196	-3.394427
H	-0.970730	-5.782107	-1.781424
H	-2.323813	-6.699010	-2.505837
C	1.680476	0.718650	0.132698
C	2.928461	0.915762	0.752213
C	1.442349	-0.490133	-0.537273
C	3.916814	-0.079245	0.691063
C	2.421048	-1.490755	-0.593942
C	3.654328	-1.284556	0.030855
H	4.429251	-2.038788	-0.041890
H	0.540317	-0.604839	-1.108573
H	3.152095	1.856831	1.238183
C	2.193925	-2.724775	-1.378503
C	2.057666	-4.032097	-0.676436
C	2.193458	-2.713258	-2.799847
C	2.010154	-5.242404	-1.517738
C	2.069227	-3.931482	-3.506883
C	1.996318	-5.124040	-2.901200
H	1.961516	-6.226935	-1.072136
H	2.054295	-3.923340	-4.588985
H	1.927211	-6.021328	-3.503437
C	5.276294	0.179696	1.209049
C	6.289599	0.666778	0.334513
C	5.607040	-0.132366	2.554904
C	7.600029	0.823462	0.832645
C	6.928914	0.082784	2.986535
C	7.900231	0.553896	2.107284
H	8.396370	1.163458	0.184039
H	7.222642	-0.138103	4.004208
H	8.915143	0.690380	2.459351
C	4.597119	-0.732920	3.528420
H	3.604256	-0.849934	3.048184
C	4.385871	0.184784	4.739419
H	4.057551	1.190179	4.399092
H	3.598828	-0.230091	5.402791
H	5.317028	0.291913	5.334128
C	5.036723	-2.137610	3.965577
H	5.168282	-2.786583	3.073482
H	5.992387	-2.104895	4.529508
H	4.269159	-2.601191	4.618589
C	6.012756	0.982732	-1.135941
H	4.927559	0.925963	-1.360073
C	6.699338	-0.040217	-2.047151
H	6.431188	0.153604	-3.107880
H	7.804083	0.011131	-1.944650
H	6.360870	-1.066195	-1.787547
C	6.438512	2.411544	-1.497994
H	6.156396	2.633053	-2.548085
H	5.927957	3.139914	-0.832512
H	7.535688	2.549536	-1.410213

C 2.345980 -1.420608 -3.600594
H 2.478461 -0.548364 -2.933459
C 1.935663 -4.146886 0.832161
H 1.872351 -3.137290 1.286553
C 0.653833 -4.891069 1.227945
H -0.233812 -4.366844 0.816569
H 0.657774 -5.936110 0.854480
H 0.559988 -4.927053 2.332631
C 3.170263 -4.833638 1.423336
H 3.249850 -5.883477 1.069235
H 4.090003 -4.285284 1.128560
H 3.109849 -4.834669 2.532835
C 1.087035 -1.147371 -4.432643
H 0.946364 -1.918476 -5.218736
H 0.194484 -1.143380 -3.772703
H 1.157850 -0.156175 -4.926014
C 3.600467 -1.451812 -4.482845
H 4.494035 -1.677213 -3.862202
H 3.515863 -2.215565 -5.283861
H 3.753322 -0.460572 -4.960604
H 1.062401 1.638066 -2.666323
H 2.486372 1.834074 -4.669820
C 1.856111 2.372639 -2.681766
C 2.657275 2.482535 -3.822029
C 2.075426 3.214149 -1.575423
C 3.670177 3.441412 -3.877321
H 4.285750 3.528047 -4.763197
C 3.099703 4.174658 -1.642037
C 3.886746 4.291113 -2.790689
H 3.276992 4.847659 -0.812333
H 4.669934 5.036724 -2.835710
C -1.932455 1.132894 2.788193
H -1.176836 1.924281 2.670179
C -3.263454 1.673728 3.266686
H -3.879415 2.157026 2.490021
H -3.892387 0.885172 3.701461
H -3.123643 2.433208 4.057468
B -1.419572 -0.086815 3.554223
O -2.268266 -0.951530 4.233683
O -0.093178 -0.478707 3.687250
C -0.052891 -1.446113 4.763016
C -1.483604 -2.065473 4.702054
C 1.066255 -2.428488 4.517173
H 1.021405 -2.851649 3.509503
H 2.032136 -1.926409 4.626667
H 1.034878 -3.253055 5.243312
C 0.189987 -0.673563 6.050614
H -0.636641 0.017772 6.266592
H 0.311912 -1.343373 6.913225
H 1.106815 -0.077538 5.951746
C -2.030750 -2.530850 6.033844
H -1.391084 -3.310799 6.471845
H -2.110997 -1.706040 6.752019
H -3.034344 -2.958706 5.902538
C -1.583822 -3.176685 3.669495
H -2.638333 -3.431813 3.494678
H -1.142608 -2.870551 2.710042
H -1.072831 -4.090232 4.002976
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Figure_S7_imid-3_modeD_ts(AS)_06 / electronic energy: -4442.739372191179 a.u. / lowest freq: -246.64 cm-1
C -0.258536 3.783467 -0.223958
H -0.513920 4.106599 -1.244521
C 1.129088 3.115197 -0.136074
H 1.737597 3.500305 0.697850
C -0.538880 1.493953 0.318911
C -2.586186 2.811387 0.052496
C -3.269490 3.282375 1.175531
C -3.306933 2.564867 -1.132517
C -4.644224 3.505474 1.139649
H -2.707211 3.474834 2.090238
C -4.685310 2.782900 -1.159930
C -5.353645 3.255029 -0.031158
H -5.156607 3.869677 2.033028
H -5.220917 2.592768 -2.091649
H -6.431687 3.426600 -0.070940
S -2.493013 2.085848 -2.666287
O -3.592113 1.932729 -3.666716
O -1.841515 0.767091 -2.420569
O -1.562926 3.190244 -2.963472
Cu -1.680844 0.090529 1.192935
C -0.422209 4.935877 0.736708
C -0.776243 6.208917 0.256573
C -0.237255 4.754821 2.120597
C -0.943599 7.277090 1.143029
H -0.925722 6.376191 -0.802810
C -0.407009 5.825292 3.002752
H 0.031336 3.783937 2.515853
C -0.759833 7.085513 2.514577

H	-1.217217	8.254090	0.766148
H	-0.266239	5.677108	4.065573
H	-0.891093	7.913588	3.199000
N	-1.166959	2.664285	0.112655
N	0.780474	1.700044	0.160820
C	-3.114839	-1.354497	1.322398
C	-4.351117	-0.981078	2.002342
C	-4.758330	-1.707091	3.136630
C	-5.165336	0.079226	1.565755
C	-5.932438	-1.386453	3.808485
C	-6.338392	0.402268	2.241178
C	-6.728532	-0.327879	3.366057
H	-6.229606	-1.964580	4.686908
H	-6.951919	1.236105	1.888755
H	-7.649139	-0.071992	3.895907
C	-2.830527	-1.077695	-0.047278
C	-1.899028	-1.829913	-0.782368
H	-1.545651	-1.424394	-1.729149
H	-1.205592	-2.486784	-0.253962
H	-4.863345	0.668660	0.694441
H	-3.445796	-0.364551	-0.609391
P	-3.323443	-2.981009	-2.969231
O	-4.422093	-1.755912	-2.815329
O	-2.420241	-2.481795	-4.060119
O	-4.210406	-4.274687	-3.375546
O	-2.790129	-3.350377	-1.575362
Na	-3.014155	-0.280433	-4.304211
H	-2.604022	-2.222083	1.758571
H	-4.125535	-2.521651	3.496901
C	-5.489964	-1.871464	-1.887944
H	-5.846359	-0.860313	-1.652413
H	-6.321482	-2.452180	-2.315355
H	-5.159462	-2.357859	-0.957303
C	-4.749255	-4.349351	-4.686912
H	-5.252605	-5.317768	-4.779903
H	-5.487091	-3.551195	-4.865282
H	-3.960794	-4.278953	-5.449455
C	1.736566	0.648558	0.102083
C	3.045711	0.840749	0.581763
C	1.441713	-0.526268	-0.606840
C	4.039837	-0.120031	0.338389
C	2.433536	-1.481838	-0.863312
C	3.728728	-1.280259	-0.378280
H	4.507387	-2.000124	-0.602109
H	0.470930	-0.644300	-1.053389
H	3.305821	1.753113	1.103018
C	2.151085	-2.642270	-1.735409
C	2.129170	-4.026285	-1.172027
C	1.998320	-2.493601	-3.137523
C	1.987018	-5.095127	-2.073047
C	1.822387	-3.653838	-3.920407
C	1.830259	-4.885892	-3.387585
H	1.991948	-6.115924	-1.713731
H	1.696088	-3.568244	-4.991961
H	1.709241	-5.740236	-4.042503
C	5.441791	0.132404	0.731013
C	6.349402	0.712386	-0.200919
C	5.917671	-0.278499	2.005071
C	7.701376	0.865340	0.171806
C	7.272548	-0.060241	2.315860
C	8.137549	0.505888	1.383391
H	8.419663	1.275592	-0.525417
H	7.675170	-0.353387	3.276430
H	9.180776	0.642154	1.639788
C	5.029105	-0.990433	3.021408
H	3.993433	-1.097407	2.638853
C	4.926879	-0.186184	4.323752
H	4.550261	0.836557	4.107888
H	4.216808	-0.675473	5.022444
H	5.911564	-0.108182	4.830249
C	5.544035	-2.412970	3.284669
H	5.587635	-2.980851	2.330645
H	6.556137	-2.398852	3.740496
H	4.865571	-2.953067	3.975883
C	5.916381	1.129760	-1.606812
H	4.814659	1.064390	-1.722303
C	6.520974	0.193005	-2.658054
H	6.143382	0.459484	-3.668480
H	7.629579	0.260848	-2.663620
H	6.225746	-0.856725	-2.444756
C	6.280854	2.590670	-1.901353
H	5.883976	2.883908	-2.895255
H	5.835691	3.255734	-1.130969
H	7.379080	2.745720	-1.921164
C	2.053994	-1.133738	-3.830342
H	2.233885	-0.320900	-3.101443
C	2.245179	-4.295085	0.320665
H	2.238866	-3.337881	0.880068

C 1.051284 -5.109705 0.836599
H 0.101387 -4.585454 0.599675
H 1.023135 -6.123297 0.385916
H 1.123242 -5.233247 1.936582
C 3.567636 -4.996229 0.647726
H 3.609583 -6.004878 0.184472
H 4.422018 -4.393661 0.272911
H 3.678189 -5.104582 1.748048
C 0.720456 -0.818172 -4.518197
H 0.512120 -1.531394 -5.342708
H -0.106383 -0.872784 -3.780028
H 0.737489 0.207148 -4.941409
C 3.220799 -1.062352 -4.823106
H 4.171542 -1.318941 -4.308722
H 3.072312 -1.759457 -5.674237
H 3.313944 -0.031590 -5.226793
H 0.815294 1.796496 -2.546449
H 2.034563 2.205315 -4.651515
C 1.592821 2.547538 -2.571113
C 2.277942 2.777993 -3.767662
C 1.906462 3.290651 -1.418164
C 3.267536 3.760369 -3.830645
H 3.793041 3.940531 -4.759417
C 2.907737 4.274530 -1.492669
C 3.577805 4.512107 -2.695600
H 3.156178 4.873134 -0.625047
H 4.343357 5.275481 -2.746028
C -1.528008 0.703314 3.145091
H -0.798971 1.519870 3.031255
C -2.816130 1.161720 3.796208
H -3.512556 1.702579 3.133946
H -3.387151 0.318427 4.208041
H -2.613509 1.844123 4.641996
B -0.927511 -0.567563 3.741237
O -1.696334 -1.524571 4.392326
O 0.415589 -0.925117 3.731427
C 0.564711 -2.005683 4.681325
C -0.850606 -2.659059 4.657471
C 1.683904 -2.914906 4.235588
H 1.573748 -3.207012 3.187204
H 2.643306 -2.399236 4.339902
H 1.725844 -3.825047 4.850558
C 0.891882 -1.379149 6.028343
H 0.068257 -0.745591 6.386951
H 1.098143 -2.139812 6.794156
H 1.783660 -0.745976 5.930219
C -1.274890 -3.302879 5.959567
H -0.580343 -4.105536 6.247545
H -1.321190 -2.575248 6.778784
H -2.273301 -3.749762 5.854243
C -1.008828 -3.636102 3.504043
H -2.067337 -3.905186 3.383151
H -0.657536 -3.194623 2.559807
H -0.450332 -4.565722 3.678153

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Figure_S7_imid-3_modeD_prod(AS) / electronic energy: -4442.755071742211 a.u. / lowest freq: 10.93 cm-1

C 0.469581 0.109625 3.311199
H 0.736396 -0.865138 3.741968
C -0.997872 0.176207 2.828871
H -1.506860 1.094890 3.161791
C 0.431928 0.328959 0.965027
C 2.638762 0.351641 1.923585
C 3.158973 1.493096 1.306081
C 3.513661 -0.679235 2.309652
C 4.520659 1.622321 1.050807
H 2.463906 2.287906 1.029353
C 4.882051 -0.532050 2.069541
C 5.388166 0.604315 1.441160
H 4.885432 2.515139 0.538305
H 5.543990 -1.348875 2.363062
H 6.460668 0.687899 1.253622
S 2.963161 -2.208758 3.085274
O 4.074983 -3.175880 2.878680
O 1.749850 -2.624261 2.316018
O 2.699461 -1.868655 4.494112
Cu 1.336612 0.593344 -0.791004
C 0.810539 1.206415 4.288275
C 1.158632 0.891095 5.613351
C 0.779990 2.557762 3.892776
C 1.480982 1.905055 6.520078
H 1.173889 -0.137536 5.949494
C 1.101574 3.567690 4.804238
H 0.509006 2.827818 2.879489
C 1.454116 3.241670 6.115669
H 1.748935 1.654203 7.538270
H 1.075563 4.604265 4.495960
H 1.702745 4.025131 6.819769
N 1.223435 0.276858 2.045973

N	-0.840770	0.236742	1.356333
C	2.614156	0.158040	-2.434318
C	3.475005	1.135670	-3.078833
C	3.012361	1.791468	-4.235948
C	4.759115	1.454305	-2.597827
C	3.796363	2.741319	-4.881054
C	5.544252	2.396108	-3.249316
C	5.065931	3.047625	-4.389350
H	3.419700	3.239133	-5.777349
H	6.541851	2.625972	-2.867495
H	5.686797	3.789062	-4.897683
C	2.955176	-0.645893	-1.315763
C	2.015868	-1.499452	-0.763026
H	2.172318	-2.006676	0.191546
H	1.205779	-1.881645	-1.389705
H	5.149852	0.956800	-1.706627
H	3.874164	-0.430256	-0.756266
P	2.569671	-4.852153	-1.439084
O	3.783072	-4.106324	-0.542237
O	1.761238	-5.494715	-0.334688
O	3.433369	-5.988609	-2.261495
O	2.025396	-3.916185	-2.472749
Na	2.698627	-4.736529	1.577964
H	1.767931	-0.197065	-3.039384
H	2.025757	1.536691	-4.633742
C	4.808993	-3.421982	-1.221855
H	5.290828	-2.727397	-0.518884
H	5.575958	-4.115231	-1.606222
H	4.409761	-2.847648	-2.074184
C	3.990783	-7.066441	-1.545142
H	4.493424	-7.728035	-2.262341
H	4.739525	-6.728920	-0.807635
H	3.221375	-7.645952	-1.011333
C	-1.927934	0.118329	0.452579
C	-3.147752	0.760298	0.716747
C	-1.816142	-0.692043	-0.687011
C	-4.235688	0.595102	-0.149924
C	-2.904633	-0.866933	-1.549493
C	-4.118359	-0.228471	-1.274861
H	-4.962461	-0.358759	-1.942341
H	-0.893772	-1.212465	-0.888582
H	-3.250869	1.399474	1.584312
C	-2.770751	-1.743316	-2.730909
C	-2.617579	-1.176115	-4.028917
C	-2.738724	-3.157187	-2.562522
C	-2.417523	-2.034939	-5.125120
C	-2.531106	-3.970765	-3.691385
C	-2.373342	-3.413832	-4.955122
H	-2.283878	-1.636838	-6.122343
H	-2.489109	-5.047802	-3.596962
H	-2.213769	-4.057082	-5.811015
C	-5.495919	1.315646	0.101987
C	-6.510937	0.717210	0.898376
C	-5.700015	2.601715	-0.471541
C	-7.714528	1.417706	1.099894
C	-6.916813	3.265403	-0.232007
C	-7.910522	2.677391	0.543424
H	-8.512299	0.987910	1.691137
H	-7.104071	4.244913	-0.652027
H	-8.842517	3.201507	0.712217
C	-4.642251	3.279845	-1.343876
H	-3.742175	2.643332	-1.449758
C	-4.157858	4.589851	-0.711636
H	-3.781197	4.397007	0.315819
H	-3.324433	5.015522	-1.310597
H	-4.974272	5.340625	-0.661973
C	-5.161936	3.509099	-2.767859
H	-5.513954	2.548379	-3.201125
H	-5.999038	4.238345	-2.779775
H	-4.345036	3.899695	-3.411853
C	-6.340640	-0.666133	1.527615
H	-5.334936	-1.083458	1.315447
C	-7.347265	-1.662718	0.941515
H	-7.150980	-2.680907	1.340649
H	-8.390083	-1.378924	1.196630
H	-7.243496	-1.699013	-0.164248
C	-6.454406	-0.601076	3.055543
H	-6.247027	-1.600547	3.493199
H	-5.710675	0.118284	3.460365
H	-7.470219	-0.287648	3.374760
C	-2.921915	-3.820885	-1.196162
H	-3.132497	-3.070178	-0.407891
C	-2.629794	0.334026	-4.269519
H	-2.830961	0.886762	-3.333408
C	-1.264478	0.822836	-4.767687
H	-0.470670	0.516913	-4.053773
H	-1.027527	0.405759	-5.769037
H	-1.258214	1.931837	-4.835467

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C  -3.750235   0.738882  -5.235320
H  -3.576468   0.331023  -6.252977
H  -4.727311   0.367272  -4.858766
H  -3.806291   1.846177  -5.308018
C  -1.643767  -4.550800  -0.767378
H  -1.396163  -5.375760  -1.467918
H  -0.792836  -3.837633  -0.736382
H  -1.771068  -4.979675   0.248630
C  -4.128362  -4.768197  -1.191424
H  -5.038089  -4.225024  -1.526188
H  -3.962645  -5.640572  -1.857606
H  -4.310181  -5.144859  -0.161959
H  -0.836540  -2.425283   1.925941
H  -2.188609  -4.356264   2.642784
C  -1.588277  -2.289223   2.691837
C  -2.357954  -3.385719   3.089674
C  -1.807110  -1.021101   3.263075
C  -3.346731  -3.230784   4.063602
H  -3.942028  -4.080914   4.370455
C  -2.806413  -0.876764   4.241083
C  -3.567349  -1.978682   4.641747
H  -2.996165   0.087316   4.696217
H  -4.333681  -1.859922   5.396731
C   0.753189   2.392064  -1.525685
H   1.025388   2.247993  -2.583668
C  -0.733497   2.609097  -1.373843
H  -1.035128   2.747640  -0.325064
H  -1.054800   3.525918  -1.899024
H  -1.340620   1.799217  -1.798637
B   1.609646   3.545419  -0.948040
O   1.032027   4.590733  -0.261575
O   2.966994   3.725411  -1.114587
C   3.238781   5.126268  -0.857401
C   2.075207   5.523123   0.114458
C   4.626074   5.275873  -0.274302
H   4.750277   4.718478   0.661951
H   5.377361   4.913201  -0.989621
H   4.846579   6.332905  -0.066812
C   3.153363   5.838710  -2.199510
H   2.155065   5.735172  -2.648860
H   3.379002   6.910102  -2.111488
H   3.878271   5.394124  -2.894208
C   1.556430   6.932881  -0.073532
H   2.352739   7.669531   0.104932
H   1.159932   7.092315  -1.083128
H   0.747684   7.137243   0.640756
C   2.400486   5.279552   1.577666
H   1.481856   5.377637   2.170257
H   2.810069   4.275466   1.752864
H   3.126970   6.009506   1.959745
66
Figure_S8_imid-2-Cu-H / electronic energy: -2884.087226671726 a.u. / lowest freq: 26.36 cm-1
C   0.618428   1.397213   0.194580
H   0.960404   1.185433   1.221721
C  -0.914970   1.396045   0.050953
H  -1.246677   2.084311  -0.744739
C  -0.055055  -0.627110  -0.810741
C   2.330388  -0.194817  -0.850743
C   2.927746   0.151511  -2.066065
C   3.072470  -0.924728   0.094205
C   4.246800  -0.198018  -2.341790
H   2.332734   0.692753  -2.804177
C   4.395320  -1.271469  -0.188574
C   4.985102  -0.904912  -1.395930
H   4.693520   0.080648  -3.298331
H   4.953010  -1.843662   0.554725
H   6.021654  -1.182042  -1.599210
C  -2.452011  -0.453687  -0.759021
C  -3.044345  -0.008396  -1.969843
C  -3.190249  -1.304746   0.099903
C  -4.373569  -0.350154  -2.258769
C  -4.515227  -1.634245  -0.217771
C  -5.114007  -1.153225  -1.385012
S   2.389069  -1.449653   1.677396
O   3.305869  -2.524235   2.148747
O   1.047313  -2.036702   1.354652
O   2.335152  -0.247816   2.525823
Cu  0.349636  -2.497505  -1.046443
C   1.274219   2.661119  -0.302441
C   2.046935   3.443406   0.574230
C   1.139283   3.070376  -1.642497
C   2.669562   4.609734   0.119488
H   2.169431   3.152051   1.609994
C   1.764358   4.236583  -2.092643
H   0.559020   2.482900  -2.341138
C   2.528595   5.005966  -1.212516
H   3.262889   5.206193   0.800400
H   1.657937   4.542543  -3.125342
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 H   3.012543   5.908429  -1.562882
 C  -1.646596   1.743481   1.324673
 C  -2.593660   2.784303   1.328104
 C  -1.412892   1.034397   2.518651
 C  -3.290163   3.105226   2.497015
 H  -2.798588   3.346946   0.425789
 C  -2.112409   1.358509   3.684318
 H  -0.691235   0.229994   2.551691
 C  -3.050414   2.392691   3.673783
 H  -4.017760   3.906480   2.489708
 H  -1.927119   0.806389   4.596577
 H  -3.591322   2.642094   4.577445
 N   0.982972   0.215740  -0.622759
 N  -1.163192  -0.000599  -0.375165
Na   1.720123  -4.281511   1.164070
 H   0.717182  -4.022093  -1.171190
 C  -2.297567   0.812829  -2.988439
 H  -2.413391   0.355465  -3.993900
 H  -2.712476   1.842199  -3.012436
 H  -1.211815   0.866751  -2.784249
 C  -2.607027  -1.886604   1.358092
 H  -2.724606  -2.990798   1.346977
 H  -1.528537  -1.672415   1.462079
 H  -3.141008  -1.476413   2.240868
 C  -6.536782  -1.517043  -1.694119
 H  -6.631426  -2.620689  -1.771323
 H  -7.199577  -1.152245  -0.881333
 H  -6.875615  -1.067327  -2.651656
 H  -5.084742  -2.272506   0.448627
 H  -4.829033   0.005972  -3.175770
92
Figure_S8_imid-2_modeS1_ed(CuHadd) / electronic energy: -3372.985295587232 a.u. / lowest freq: 19.76 cm-1
 C   2.501782   0.080516   0.237398
 H   2.454064  -0.282579   1.275852
 C   2.031235   1.534268   0.065652
 H   2.539214   2.012930  -0.790012
 C   0.359264   0.104889  -0.760875
 C   1.478119  -2.031429  -0.792425
 C   1.608824  -2.439362  -2.123796
 C   1.335149  -2.996753   0.216188
 C   1.610635  -3.791165  -2.456150
 H   1.692894  -1.670236  -2.894558
 C   1.350765  -4.351629  -0.124252
 C   1.491567  -4.750059  -1.451267
 H   1.706823  -4.092941  -3.501268
 H   1.220390  -5.088952   0.670046
 H   1.496662  -5.813364  -1.700206
 C  -0.202618   2.443779  -0.699755
 C  -0.089915   2.989236  -2.008181
 C  -1.085978   3.052370   0.227267
 C  -0.848294   4.116439  -2.356491
 C  -1.823126   4.183751  -0.149117
 C  -1.712332   4.715285  -1.436869
 S   1.046246  -2.570190   1.939650
 O   0.292447  -3.736383   2.490243
 O   0.168738  -1.360515   1.914761
 O   2.370573  -2.349237   2.545767
Cu  -0.935814  -0.802233  -1.968580
 C   3.883802  -0.170705  -0.313064
 C   4.923651  -0.562091   0.548895
 C   4.155038  -0.026271  -1.686985
 C   6.205802  -0.803947   0.046635
 H   4.745027  -0.677411   1.610503
 C   5.438093  -0.270278  -2.184501
 H   3.373371   0.267834  -2.373968
 C   6.462818  -0.658597  -1.318615
 H   7.000882  -1.104128   0.716838
 H   5.637516  -0.159237  -3.242482
 H   7.455930  -0.846909  -1.705489
 C   2.233927   2.397273   1.288583
 C   2.885013   3.639032   1.164861
 C   1.789941   1.989573   2.561785
 C   3.082504   4.452162   2.284632
 H   3.237338   3.983698   0.200584
 C   1.991534   2.805575   3.678570
 H   1.275791   1.048720   2.695672
 C   2.636567   4.035839   3.540367
 H   3.581782   5.406536   2.178080
 H   1.642442   2.485124   4.651621
 H   2.789688   4.667131   4.406046
 N   1.461257  -0.633953  -0.529057
 N   0.601924   1.346582  -0.290937
 C  -2.048852  -2.344464  -1.151498
 C  -2.046607  -2.357955  -2.560995
 H  -2.914883  -1.982925  -3.111860
 B  -3.176717  -1.631317  -0.408662
 O  -4.197251  -0.977575  -1.060798
 O  -3.318026  -1.551617   0.973790
```

C	-4.882661	-0.163610	-0.082759
C	-4.624201	-0.957607	1.238189
C	-4.192632	1.189207	-0.096471
H	-4.262802	1.628137	-1.100438
H	-4.633878	1.897897	0.617142
H	-3.126379	1.065958	0.135309
C	-6.339436	-0.039063	-0.465471
H	-6.902140	0.502452	0.308304
H	-6.435764	0.524295	-1.402729
H	-6.808883	-1.018604	-0.613136
C	-5.605103	-2.100159	1.433445
H	-6.606245	-1.730550	1.693391
H	-5.691190	-2.715786	0.527732
H	-5.267512	-2.748906	2.252982
C	-4.532270	-0.102658	2.481325
H	-3.701389	0.609577	2.426174
H	-5.461428	0.464949	2.631648
H	-4.384810	-0.727072	3.373990
Na	-1.787949	-2.399255	2.523082
H	-1.405523	-3.043515	-3.125344
H	-1.334013	-2.981112	-0.613085
H	-0.613808	-0.266384	-3.422937
C	-1.264997	2.535112	1.628599
H	-0.725347	3.196158	2.337227
H	-2.339469	2.545493	1.904509
H	-0.907051	1.492313	1.736967
C	0.827911	2.426224	-3.062708
H	0.245489	2.204275	-3.981515
H	1.609618	3.175111	-3.309071
H	1.330475	1.492372	-2.756890
C	-2.509565	5.920464	-1.841945
H	-3.149838	6.286137	-1.011094
H	-1.821855	6.739063	-2.141725
H	-3.163577	5.662944	-2.701550
H	-0.762241	4.534630	-3.353324
H	-2.491905	4.648112	0.566552

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Figure_S8_imid-2_modeS1_ts(CuHadd) / electronic energy: -3372.973372247575 a.u. / lowest freq: -703.95 cm-1

C	2.545261	0.064208	0.204399
H	2.503680	-0.272128	1.252647
C	2.082408	1.516666	-0.000413
H	2.556119	1.953247	-0.897703
C	0.381083	0.081935	-0.734469
C	1.476935	-2.058210	-0.776359
C	1.580253	-2.485828	-2.104050
C	1.317894	-3.005955	0.246335
C	1.547012	-3.840857	-2.419606
H	1.682459	-1.729740	-2.885325
C	1.300871	-4.365485	-0.077698
C	1.417581	-4.783678	-1.400538
H	1.626372	-4.158526	-3.461374
H	1.165312	-5.090150	0.727270
H	1.396829	-5.850043	-1.635287
C	-0.181570	2.417005	-0.689631
C	-0.161288	2.893844	-2.029349
C	-1.012174	3.062523	0.260743
C	-0.952030	3.996838	-2.382968
C	-1.777638	4.173006	-0.120914
C	-1.755406	4.639741	-1.438234
S	1.069013	-2.553616	1.972336
O	0.284184	-3.694833	2.533196
O	0.231601	-1.317040	1.954788
O	2.408417	-2.374226	2.557276
Cu	-1.002899	-0.846674	-1.685896
C	3.918747	-0.210460	-0.354759
C	4.964871	-0.589744	0.504864
C	4.175312	-0.101322	-1.734872
C	6.238967	-0.855374	-0.005830
H	4.797223	-0.677392	1.571008
C	5.450328	-0.369287	-2.240692
H	3.388100	0.184152	-2.419918
C	6.481415	-0.745967	-1.377135
H	7.039058	-1.146321	0.662479
H	5.638580	-0.285920	-3.303251
H	7.468232	-0.953002	-1.770499
C	2.350564	2.426739	1.174658
C	2.993342	3.661498	0.965205
C	1.975589	2.072408	2.485562
C	3.249920	4.519807	2.038158
H	3.293078	3.965801	-0.029946
C	2.236030	2.933829	3.555164
H	1.469913	1.138602	2.686344
C	2.871927	4.156393	3.331956
H	3.742068	5.468237	1.865628
H	1.939674	2.654605	4.557932
H	3.070589	4.822785	4.161305
N	1.493065	-0.656536	-0.535084
N	0.638642	1.330769	-0.285208

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 C  -2.308510  -2.392581  -1.279437
 C  -2.158073  -2.155178  -2.697858
 H  -3.004616  -1.701610  -3.224363
 B  -3.351928  -1.651559  -0.486192
 O  -4.311508  -0.825970  -1.054774
 O  -3.483013  -1.669646   0.912655
 C  -4.865018  -0.015366  -0.002316
 C  -4.682733  -0.929935   1.253284
 C  -4.014679   1.241517   0.066584
 H  -4.037830   1.753845  -0.904851
 H  -4.362716   1.948635   0.831730
 H  -2.969060   0.974133   0.276855
 C  -6.303126   0.320873  -0.327791
 H  -6.773470   0.873224   0.498497
 H  -6.349217   0.957127  -1.221730
 H  -6.899670  -0.578023  -0.525642
 C  -5.810057  -1.936067   1.410782
 H  -6.745806  -1.452155   1.722522
 H  -5.997699  -2.476046   0.472453
 H  -5.544176  -2.675214   2.178659
 C  -4.440695  -0.183597   2.547385
 H  -3.529125   0.425357   2.503710
 H  -5.284883   0.480087   2.782654
 H  -4.337565  -0.888448   3.385521
Na  -1.799812  -2.441411   2.287660
 H  -1.648362  -2.907159  -3.309724
 H  -1.682920  -3.171236  -0.823482
 H  -1.093219  -0.961112  -3.271785
 C  -1.120073   2.593869   1.686792
 H  -0.567303   3.292360   2.348087
 H  -2.182485   2.584547   2.007241
 H  -0.733019   1.564428   1.817439
 C   0.677984   2.273794  -3.117908
 H   0.018060   1.935558  -3.944526
 H   1.387698   3.030621  -3.513344
 H   1.267153   1.401786  -2.785207
 C  -2.588482   5.817959  -1.850277
 H  -3.173688   6.223913  -0.997838
 H  -1.929700   6.622818  -2.239033
 H  -3.297314   5.512179  -2.648454
 H  -0.939348   4.361211  -3.404279
 H  -2.405397   4.666408   0.612221
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Figure_S8_imid-2_modeS1_prod(CuHadd) / electronic energy: -3373.016852320262 a.u. / lowest freq: 16.52 cm-1
 C   2.788008  -0.219253   0.126599
 H   2.844972  -0.473727   1.196583
 C   2.437087   1.258816  -0.129534
 H   2.854338   1.610804  -1.088408
 C   0.522069  -0.052370  -0.525007
 C   1.378522  -2.304078  -0.439617
 C   1.740858  -3.005844  -1.592135
 C   0.792633  -3.002506   0.632456
 C   1.547454  -4.382109  -1.682255
 H   2.152867  -2.454122  -2.438666
 C   0.609253  -4.382037   0.538110
 C   0.985521  -5.072988  -0.612179
 H   1.829617  -4.910494  -2.595226
 H   0.158191  -4.905580   1.382476
 H   0.833208  -6.152703  -0.671111
 C   0.188066   2.323953  -0.614209
 C   0.173752   2.803852  -1.950442
 C  -0.535220   3.026113   0.381419
 C  -0.513838   3.987899  -2.253283
 C  -1.204288   4.212491   0.050273
 C  -1.196407   4.696900  -1.261298
 S   0.247656  -2.176913   2.141430
 O  -0.416339  -3.240030   2.946849
 O  -0.781892  -1.173436   1.706677
 O   1.453536  -1.584622   2.741451
Cu  -1.164566  -0.988528  -0.803533
 C   4.045827  -0.672185  -0.571576
 C   5.117194  -1.189538   0.178273
 C   4.169718  -0.592759  -1.971784
 C   6.285319  -1.618346  -0.459256
 H   5.050726  -1.261915   1.256713
 C   5.338980  -1.023772  -2.604569
 H   3.358200  -0.208487  -2.575355
 C   6.396148  -1.535793  -1.849167
 H   7.105163  -2.015594   0.125118
 H   5.424320  -0.962746  -3.681793
 H   7.300778  -1.869440  -2.340830
 C   2.889338   2.199105   0.962100
 C   3.659385   3.331095   0.634886
 C   2.551448   1.976428   2.310668
 C   4.076619   4.217957   1.631681
 H   3.934809   3.533150  -0.392754
 C   2.970828   2.866131   3.303624
 H   1.958433   1.120376   2.598571
```

C 3.732375 3.986074 2.964764
H 4.666574 5.086711 1.369594
H 2.702692 2.687720 4.336895
H 4.055408 4.674374 3.735003
N 1.574238 -0.889252 -0.401566
N 0.962059 1.189774 -0.257234
C -2.570419 -2.333541 -1.315112
C -2.479229 -2.676358 -2.787359
H -2.687035 -1.800336 -3.422167
B -3.577175 -1.358929 -0.782111
O -4.259804 -0.370002 -1.501793
O -3.916414 -1.246274 0.599244
C -4.656472 0.634786 -0.556870
C -4.910863 -0.209582 0.730209
C -3.478151 1.582428 -0.385811
H -3.186984 1.985904 -1.365896
H -3.707284 2.428135 0.277992
H -2.609364 1.038081 0.023374
C -5.869014 1.372225 -1.080053
H -6.260787 2.072846 -0.328070
H -5.602056 1.956687 -1.971117
H -6.674209 0.683269 -1.363444
C -6.279857 -0.871589 0.725765
H -7.087108 -0.142402 0.882641
H -6.465800 -1.391680 -0.224135
H -6.338369 -1.613199 1.534377
C -4.678370 0.535160 2.028313
H -3.641534 0.882697 2.116874
H -5.341117 1.409261 2.107855
H -4.891060 -0.113483 2.891026
Na -2.700680 -2.337055 2.224066
H -3.200125 -3.455722 -3.103180
H -2.364673 -3.199663 -0.658919
H -1.484097 -3.046889 -3.089786
C -0.646259 2.531612 1.798061
H -0.095944 3.217053 2.475688
H -1.712772 2.511089 2.104878
H -0.253838 1.504375 1.918563
C 0.863150 2.091544 -3.085418
H 0.135216 1.907151 -3.903618
H 1.687178 2.725638 -3.474508
H 1.282774 1.110855 -2.796293
C -1.926137 5.958414 -1.618528
H -2.422461 6.409077 -0.732799
H -1.210149 6.698347 -2.034161
H -2.702485 5.736621 -2.380821
H -0.520573 4.359570 -3.271903
H -1.749306 4.749822 0.817886

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Figure_S8_imid-2_modeS2_ed(CuHadd) / electronic energy: -3372.986290612261 a.u. / lowest freq: 19.66 cm-1

C -1.964089 -0.024305 1.047876
H -2.974197 0.079767 0.627743
C -1.237065 1.326378 1.259380
H -0.687894 1.322202 2.211323
C -0.183920 0.155005 -0.498988
C -1.234271 -2.002045 -0.444511
C -0.083322 -2.799993 -0.420252
C -2.423955 -2.530762 -0.971974
C -0.110341 -4.114727 -0.870681
H 0.843329 -2.363156 -0.041498
C -2.445869 -3.862163 -1.397461
C -1.305898 -4.658818 -1.338460
H 0.803854 -4.712860 -0.848449
H -3.374721 -4.248302 -1.821122
H -1.346907 -5.694917 -1.681041
C 0.664662 2.364517 -0.110308
C 1.740496 2.588724 0.788202
C 0.571249 3.151665 -1.287109
C 2.668253 3.606813 0.520893
C 1.510627 4.165100 -1.523187
C 2.556057 4.397831 -0.624749
S -3.882666 -1.526544 -1.334555
O -4.575005 -2.264209 -2.415711
O -3.303236 -0.230485 -1.816128
O -4.654003 -1.391328 -0.085218
Cu 0.875720 -0.363520 -2.095357
C -2.030424 -0.851567 2.308152
C -3.268315 -1.117931 2.918658
C -0.856999 -1.360981 2.895096
C -3.330883 -1.890429 4.082490
H -4.184875 -0.722182 2.501149
C -0.923833 -2.133648 4.057296
H 0.107408 -1.160867 2.450202
C -2.160267 -2.399945 4.649876
H -4.287846 -2.092251 4.546085
H -0.016383 -2.525111 4.498675
H -2.211098 -2.997877 5.550581
C -2.149701 2.527967 1.242040

C -2.151611 3.424682 2.326826
C -2.991563 2.788154 0.145195
C -2.976033 4.553688 2.311688
H -1.511863 3.255496 3.184038
C -3.813330 3.918510 0.133805
H -3.017617 2.117105 -0.699512
C -3.805554 4.800971 1.215867
H -2.969895 5.238576 3.149752
H -4.457058 4.109860 -0.714964
H -4.442435 5.675995 1.205425
N -1.104712 -0.670770 0.023669
N -0.281323 1.333918 0.132503
C 2.875814 0.098915 -1.914189
C 2.582003 -0.510849 -3.142725
H 2.778111 -1.578530 -3.294563
B 3.473981 -0.650358 -0.710823
O 3.544073 -2.022693 -0.607163
O 4.072027 -0.010877 0.348842
C 4.114189 -2.336163 0.689739
C 4.842631 -1.001925 1.069314
C 2.965416 -2.654976 1.630034
H 2.386377 -3.503173 1.241005
H 3.322658 -2.929387 2.631823
H 2.289335 -1.795161 1.732707
C 5.025224 -3.535534 0.544612
H 5.549282 -3.745574 1.488103
H 4.437444 -4.426436 0.285372
H 5.775374 -3.391619 -0.241777
C 6.261897 -0.930288 0.526987
H 6.936410 -1.620012 1.052516
H 6.296615 -1.167078 -0.545682
H 6.651260 0.088209 0.657007
C 4.826540 -0.669064 2.544939
H 3.807909 -0.589771 2.942505
H 5.361879 -1.435207 3.123867
H 5.329830 0.291456 2.718788
Na -2.252639 -0.360418 -3.796482
H 2.490331 0.073630 -4.063511
H 2.932706 1.195825 -1.899125
H -0.110067 -0.895367 -3.239915
C -0.504173 2.947535 -2.321483
H -0.035518 2.759194 -3.310511
H -1.163784 2.089851 -2.099981
H -1.132287 3.860677 -2.388373
C 3.564872 5.478492 -0.882694
H 3.549824 6.209615 -0.047128
H 4.578933 5.032004 -0.955794
H 3.351050 6.021204 -1.828034
C 1.944460 1.744906 2.017502
H 3.000702 1.783284 2.357445
H 1.313300 2.128310 2.844519
H 1.702861 0.682672 1.809450
H 1.429061 4.769861 -2.419170
H 3.488064 3.785461 1.207400
92
Figure_S8_imid-2_modeS2_ts(CuHadd) / electronic energy: -3372.965950138900 a.u. / lowest freq: -777.97 cm-1
C -1.874727 -0.496039 1.027594
H -2.839667 -0.762274 0.570883
C -1.664456 1.027889 1.159816
H -1.090829 1.270673 2.070311
C -0.264782 0.216162 -0.548532
C -0.444119 -2.166552 -0.315829
C 0.905653 -2.520854 -0.203021
C -1.351695 -3.090720 -0.855453
C 1.345270 -3.790797 -0.559166
H 1.612822 -1.773834 0.164286
C -0.906541 -4.375399 -1.183081
C 0.428226 -4.735067 -1.021163
H 2.405924 -4.037987 -0.469512
H -1.623824 -5.076652 -1.613566
H 0.755889 -5.742683 -1.286075
C -0.288053 2.598829 -0.291359
C 0.729094 3.141338 0.536051
C -0.790756 3.369911 -1.367517
C 1.156543 4.461131 0.332487
C -0.340253 4.684801 -1.550947
C 0.622339 5.237627 -0.699532
S -3.023409 -2.640669 -1.358625
O -3.291446 -3.538970 -2.519298
O -2.897446 -1.225093 -1.827248
O -3.917917 -2.824330 -0.205089
Cu 1.089440 -0.047220 -1.861127
C -1.717221 -1.228658 2.336395
C -2.820152 -1.873982 2.922172
C -0.469527 -1.284044 2.986264
C -2.675705 -2.564804 4.129202
H -3.793225 -1.839803 2.448931
C -0.329379 -1.977192 4.191385

H	0.395354	-0.798478	2.555833
C	-1.431512	-2.617561	4.762521
H	-3.529436	-3.059467	4.574028
H	0.634724	-2.018750	4.681611
H	-1.321754	-3.153985	5.696108
C	-2.945741	1.824529	1.173472
C	-3.218382	2.698381	2.242319
C	-3.876436	1.726444	0.122485
C	-4.393624	3.455421	2.256717
H	-2.520907	2.799124	3.064573
C	-5.049443	2.485985	0.140557
H	-3.697356	1.064203	-0.711620
C	-5.308052	3.349953	1.206567
H	-4.594459	4.125830	3.082357
H	-5.758205	2.404677	-0.673345
H	-6.216838	3.937611	1.218923
N	-0.802430	-0.853127	0.073339
N	-0.834262	1.317294	-0.027719
C	3.061629	0.467350	-2.119114
C	2.592460	-0.443005	-3.143581
H	2.916587	-1.489538	-3.072195
B	3.775504	0.070173	-0.847037
O	4.021525	-1.236791	-0.423606
O	4.338140	0.991404	0.029981
C	4.644194	-1.171510	0.877285
C	5.241427	0.277233	0.890486
C	3.562428	-1.357292	1.930233
H	3.068998	-2.329707	1.796396
H	3.973671	-1.336030	2.948973
H	2.796825	-0.571892	1.856066
C	5.672980	-2.277697	0.984563
H	6.236218	-2.202386	1.926253
H	5.179443	-3.259367	0.970946
H	6.387407	-2.252200	0.153063
C	6.621485	0.342103	0.251088
H	7.389581	-0.136559	0.874401
H	6.627035	-0.143304	-0.735052
H	6.907701	1.392935	0.107929
C	5.262477	0.940766	2.251271
H	4.258074	1.025708	2.682368
H	5.893530	0.378734	2.955184
H	5.677141	1.954719	2.169306
Na	-2.297371	-1.724337	-4.008546
H	2.588591	-0.096340	-4.182504
H	3.067907	1.532450	-2.385066
H	1.033491	-0.823576	-3.273165
C	-1.800442	2.829376	-2.344662
H	-1.423906	2.964415	-3.380627
H	-1.994237	1.748640	-2.205772
H	-2.756971	3.382245	-2.235011
C	1.101742	6.646376	-0.893336
H	0.896557	7.239105	0.022917
H	2.195094	6.645053	-1.087134
H	0.593463	7.137532	-1.750277
C	1.402092	2.347539	1.623704
H	2.502167	2.479371	1.557273
H	1.057948	2.707686	2.615524
H	1.203389	1.263157	1.539631
H	-0.740533	5.277194	-2.365751
H	1.920717	4.883932	0.975169

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Figure_S8_imid-2_modeS2_prod(CuHadd) / electronic energy: -3373.009403035306 a.u. / lowest freq: 14.98 cm-1

C	-2.148344	0.464675	0.911052
H	-3.062182	0.512323	0.304467
C	-1.321974	1.778343	0.888673
H	-1.017589	2.068662	1.905472
C	-0.081886	0.072265	-0.179025
C	-1.381298	-1.905436	0.173455
C	-0.329533	-2.703729	0.651392
C	-2.491785	-2.531598	-0.417365
C	-0.379368	-4.090128	0.565462
H	0.533322	-2.207646	1.102950
C	-2.538759	-3.928090	-0.484349
C	-1.496221	-4.707965	0.005284
H	0.457101	-4.682986	0.942207
H	-3.405524	-4.389130	-0.960709
H	-1.552704	-5.796321	-0.061115
C	0.968069	2.230137	-0.161679
C	1.800218	2.681944	0.895303
C	1.252675	2.640313	-1.490277
C	2.847708	3.573392	0.622370
C	2.317096	3.520281	-1.732732
C	3.111250	3.992933	-0.683470
S	-3.844253	-1.630820	-1.182693
O	-4.473919	-2.602240	-2.127105
O	-3.201016	-0.521814	-1.953238
O	-4.729456	-1.182880	-0.094342
Cu	1.235456	-0.978895	-1.119900

C	-2.508049	0.038557	2.313764
C	-3.839995	0.118854	2.756424
C	-1.518607	-0.415897	3.206858
C	-4.177032	-0.263321	4.058363
H	-4.617300	0.486607	2.098847
C	-1.860543	-0.797622	4.506976
H	-0.484561	-0.481333	2.895770
C	-3.188835	-0.722928	4.932161
H	-5.204889	-0.199207	4.391262
H	-1.094706	-1.150552	5.185475
H	-3.451836	-1.017535	5.939848
C	-2.044372	2.945840	0.260832
C	-2.192199	4.149697	0.974638
C	-2.555561	2.865381	-1.047367
C	-2.837547	5.244424	0.391654
H	-1.803688	4.246032	1.980861
C	-3.199297	3.962219	-1.626611
H	-2.458433	1.955419	-1.619536
C	-3.340234	5.151071	-0.907935
H	-2.945539	6.166888	0.947394
H	-3.588479	3.890124	-2.633964
H	-3.838389	5.999942	-1.358112
N	-1.214285	-0.499449	0.273861
N	-0.136800	1.379564	0.103149
C	2.493695	-2.117080	-2.152087
C	1.965175	-3.519585	-2.378203
H	1.823174	-4.054063	-1.425173
B	3.462014	-1.838224	-1.024878
O	3.632031	-2.644970	0.112767
O	4.241284	-0.674793	-0.907559
C	4.247273	-1.827319	1.121217
C	5.059373	-0.803158	0.264294
C	3.125257	-1.156249	1.903536
H	2.473953	-1.924529	2.344369
H	3.495133	-0.523042	2.722241
H	2.508084	-0.536820	1.231183
C	5.083369	-2.697894	2.034677
H	5.633644	-2.089796	2.767813
H	4.438705	-3.389691	2.594378
H	5.808807	-3.300063	1.473447
C	6.409953	-1.355539	-0.167465
H	7.121110	-1.410620	0.669051
H	6.308735	-2.360609	-0.600542
H	6.843251	-0.700759	-0.935822
C	5.223568	0.561861	0.899533
H	4.252444	1.034852	1.083599
H	5.763600	0.497714	1.855698
H	5.795109	1.225689	0.236274
Na	-3.917163	-1.304567	-4.071213
H	2.645438	-4.153104	-2.980016
H	2.719766	-1.571474	-3.083558
H	0.987808	-3.555551	-2.892661
C	0.453598	2.174566	-2.679749
H	1.132516	1.696002	-3.416821
H	-0.326654	1.436118	-2.421978
H	-0.039614	3.046470	-3.158753
C	4.253392	4.930169	-0.945776
H	4.095661	5.876073	-0.386094
H	5.203039	4.463165	-0.609188
H	4.344678	5.172188	-2.026071
C	1.631444	2.208345	2.314380
H	2.622010	2.080726	2.800609
H	1.047959	2.956720	2.889707
H	1.126898	1.223898	2.360335
H	2.526974	3.836477	-2.748204
H	3.477866	3.927573	1.430474

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Figure_S8_imid-2_modeR1_ed(CuHadd) / electronic energy: -3372.981777696869 a.u. / lowest freq: 19.37 cm-1

C	2.598340	-0.248897	0.514345
H	2.283950	-0.578886	1.517191
C	2.319122	1.236877	0.254280
H	2.992752	1.645313	-0.518754
C	0.643140	-0.055057	-0.782574
C	1.611808	-2.303867	-0.618873
C	2.446410	-2.868998	-1.587022
C	0.803808	-3.150545	0.157017
C	2.507268	-4.247449	-1.767416
H	3.034434	-2.211222	-2.228523
C	0.869628	-4.532728	-0.024891
C	1.725815	-5.084962	-0.974590
H	3.164486	-4.663942	-2.533498
H	0.234562	-5.166835	0.596431
H	1.773466	-6.168804	-1.100302
C	0.350785	2.322360	-0.894828
C	0.701281	2.742948	-2.208199
C	-0.578330	3.091244	-0.150828
C	0.136104	3.913501	-2.735332
C	-1.111698	4.265649	-0.699408

C -0.763060 4.678497 -1.986714
S -0.444564 -2.502202 1.275366
O -1.033053 -3.674676 1.957670
O -1.427602 -1.866380 0.326929
O 0.215588 -1.526176 2.160646
Cu -0.927424 -0.656247 -1.886332
C 4.034107 -0.649914 0.274611
C 4.771496 -1.256436 1.307592
C 4.659068 -0.428986 -0.967904
C 6.101107 -1.635635 1.100748
H 4.319053 -1.437717 2.274617
C 5.988259 -0.810914 -1.170044
H 4.116038 0.024500 -1.786000
C 6.708935 -1.413341 -0.136760
H 6.660526 -2.102638 1.901009
H 6.458935 -0.641885 -2.129884
H 7.738025 -1.708733 -0.295230
C 2.421045 2.108274 1.484114
C 3.233267 3.257817 1.458320
C 1.725853 1.797711 2.669198
C 3.343326 4.075406 2.586843
H 3.781194 3.526561 0.563762
C 1.840370 2.617752 3.795305
H 1.080512 0.933458 2.723762
C 2.647952 3.755601 3.754383
H 3.968760 4.958194 2.555600
H 1.297319 2.373109 4.698989
H 2.733589 4.390398 4.626781
N 1.642550 -0.887651 -0.429692
N 0.949542 1.173473 -0.310514
C -2.617048 0.563616 -1.834282
C -2.596298 -0.318954 -2.932163
H -2.274035 0.010804 -3.925769
B -3.437202 0.226644 -0.583268
O -3.724908 1.086280 0.442115
O -4.046005 -1.012682 -0.406372
C -4.335841 0.334855 1.515104
C -4.889855 -0.934877 0.774621
C -3.246024 0.011306 2.524197
H -2.827394 0.945218 2.921356
H -3.642396 -0.560468 3.374517
H -2.428334 -0.558771 2.065719
C -5.403281 1.194675 2.159447
H -5.943208 0.633584 2.935772
H -4.937341 2.064029 2.642452
H -6.134234 1.569066 1.432583
C -6.315638 -0.764056 0.280670
H -7.034359 -0.732413 1.110775
H -6.427510 0.157400 -0.306739
H -6.587813 -1.608711 -0.366578
C -4.736966 -2.222387 1.558719
H -3.682857 -2.439192 1.779811
H -5.282354 -2.170320 2.511756
H -5.161566 -3.068283 0.996551
Na -2.881956 -3.010393 -0.932119
H -3.268299 -1.184877 -2.961404
H -2.263223 1.589126 -1.989402
H -0.428056 -1.869767 -2.796705
C 1.667975 1.992346 -3.089001
H 1.158589 1.702225 -4.032100
H 2.529421 2.648405 -3.334702
H 2.066788 1.071370 -2.629937
C -1.028230 2.693811 1.226002
H -2.115824 2.879542 1.340301
H -0.853021 1.617334 1.420967
H -0.497649 3.310157 1.979902
C -1.361049 5.933690 -2.551491
H -2.466714 5.837101 -2.585776
H -1.092213 6.797318 -1.907421
H -0.994085 6.135245 -3.580389
H 0.404990 4.231753 -3.736204
H -1.813534 4.858487 -0.123505
92
Figure_S8_imid-2_modeR1_ts(CuHadd) / electronic energy: -3372.965984629026 a.u. / lowest freq: -740.12 cm-1
C 2.680006 -0.301509 0.546554
H 2.321038 -0.629060 1.535486
C 2.463551 1.200759 0.298097
H 3.202087 1.607035 -0.413823
C 0.784378 -0.019912 -0.827144
C 1.671944 -2.297667 -0.691782
C 2.491158 -2.841598 -1.685675
C 0.837342 -3.158864 0.040622
C 2.518839 -4.212744 -1.924520
H 3.100831 -2.171176 -2.293160
C 0.870393 -4.532938 -0.198159
C 1.718758 -5.064306 -1.166815
H 3.167405 -4.612249 -2.706793
H 0.215226 -5.178005 0.389643

H 1.742165 -6.142726 -1.337181
C 0.569841 2.362568 -0.916285
C 1.068868 2.886648 -2.138993
C -0.462738 3.053412 -0.239021
C 0.572974 4.105632 -2.624148
C -0.934413 4.272780 -0.744894
C -0.420154 4.804070 -1.930029
S -0.402058 -2.517814 1.167810
O -1.107584 -3.705471 1.718239
O -1.331139 -1.766739 0.250429
O 0.278205 -1.662655 2.151064
Cu -0.866024 -0.564807 -1.696285
C 4.107780 -0.751908 0.352475
C 4.784705 -1.401267 1.400722
C 4.783469 -0.538167 -0.864267
C 6.105188 -1.828961 1.233787
H 4.291964 -1.578959 2.348523
C 6.103275 -0.968580 -1.026616
H 4.287170 -0.050778 -1.692502
C 6.763833 -1.613160 0.021360
H 6.617944 -2.328791 2.045404
H 6.613342 -0.804207 -1.966934
H 7.785700 -1.946168 -0.106272
C 2.498791 2.037271 1.554277
C 3.375996 3.134462 1.640957
C 1.664661 1.747863 2.651067
C 3.414580 3.922374 2.795142
H 4.029929 3.384939 0.814916
C 1.706791 2.538636 3.802702
H 0.972510 0.918697 2.615517
C 2.580712 3.625010 3.874928
H 4.091411 4.765082 2.851722
H 1.058147 2.310453 4.638525
H 2.611083 4.236956 4.767108
N 1.740278 -0.894243 -0.440519
N 1.130901 1.191268 -0.344171
C -2.764855 0.290479 -1.947550
C -2.478401 -0.770270 -2.893244
H -2.348307 -0.506031 -3.948953
B -3.627403 0.102707 -0.728759
O -4.070596 1.129045 0.096232
O -4.195042 -1.126314 -0.305886
C -4.742138 0.545810 1.224396
C -5.250944 -0.802807 0.630619
C -3.718192 0.336668 2.332084
H -3.286702 1.302910 2.622517
H -4.172471 -0.099381 3.232748
H -2.894644 -0.313292 2.000972
C -5.841070 1.479694 1.683523
H -6.439669 1.020974 2.484003
H -5.406845 2.406565 2.082124
H -6.514278 1.752995 0.861898
C -6.535426 -0.644642 -0.167746
H -7.401151 -0.452066 0.480902
H -6.455660 0.179647 -0.889916
H -6.736073 -1.566110 -0.731482
C -5.392772 -1.920431 1.642276
H -4.447760 -2.140762 2.158188
H -6.127404 -1.653454 2.415472
H -5.760050 -2.841065 1.163468
Na -3.089928 -3.152122 -0.010650
H -3.057258 -1.698918 -2.799178
H -2.534254 1.315418 -2.264164
H -1.019820 -1.574362 -2.926795
C 2.117634 2.187148 -2.965095
H 1.752172 2.070954 -4.007345
H 3.046448 2.795170 -2.976539
H 2.364277 1.175865 -2.594172
C -1.084024 2.526434 1.023023
H -2.182373 2.665713 0.980792
H -0.890229 1.443675 1.165835
H -0.698112 3.096489 1.892828
C -0.947503 6.109678 -2.448972
H -2.038180 6.022556 -2.638184
H -0.772454 6.907650 -1.696945
H -0.448969 6.404958 -3.396711
H 0.963197 4.509264 -3.551527
H -1.713544 4.809752 -0.215474
92
Figure_S8_imid-2_modeR1_prod(CuHadd) / electronic energy: -3373.017513844781 a.u. / lowest freq: 20.32 cm-1
C 2.766629 -0.155573 0.144805
H 2.759980 -0.450376 1.205790
C 2.397868 1.320823 -0.077800
H 2.852273 1.713099 -1.003760
C 0.538726 -0.015193 -0.631547
C 1.476619 -2.254180 -0.559041
C 1.970389 -2.916516 -1.686717
C 0.887941 -3.009452 0.472186

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C   1.923795  -4.304875  -1.780689
H   2.382505  -2.325244  -2.505989
C   0.847593  -4.400337   0.372338
C   1.373455  -5.050267  -0.741448
H   2.317713  -4.800270  -2.670518
H   0.386138  -4.964462   1.184137
H   1.338051  -6.139979  -0.801454
C   0.153792   2.357206  -0.628268
C   0.184613   2.887955  -1.944995
C  -0.614412   3.013054   0.365242
C  -0.512164   4.071123  -2.231114
C  -1.289566   4.200522   0.052107
C  -1.243517   4.732166  -1.238786
S   0.189244  -2.252666   1.949733
O  -0.475695  -3.365840   2.685986
O  -0.857875  -1.289022   1.471895
O   1.318294  -1.619358   2.650585
Cu  -1.128671  -0.916926  -1.067370
C   4.078224  -0.552765  -0.485381
C   5.109374  -1.078291   0.313564
C   4.292508  -0.413275  -1.869914
C   6.326722  -1.456486  -0.260608
H   4.973334  -1.196415   1.381390
C   5.510868  -0.793809  -2.439344
H   3.513299  -0.022345  -2.510973
C   6.527350  -1.314595  -1.635565
H   7.115028  -1.860563   0.361290
H   5.665859  -0.687133  -3.505166
H   7.470041  -1.609200  -2.078214
C   2.777998   2.233288   1.064298
C   3.527128   3.397294   0.808063
C   2.395855   1.952382   2.390159
C   3.880650   4.258077   1.851271
H   3.835573   3.644492  -0.200134
C   2.751916   2.816097   3.429723
H   1.814668   1.072332   2.624649
C   3.493270   3.968022   3.160859
H   4.454849   5.151696   1.643432
H   2.449474   2.593056   4.444700
H   3.766894   4.636222   3.967098
N   1.604035  -0.833085  -0.483683
N   0.933614   1.223743  -0.282548
C  -2.569912  -2.202053  -1.610153
C  -2.230583  -3.580147  -1.077109
H  -3.050759  -4.319112  -1.174878
B  -3.590966  -1.316965  -0.955668
O  -4.294268  -0.288383  -1.592216
O  -3.932272  -1.334103   0.424379
C  -4.715749   0.627181  -0.572901
C  -4.941620  -0.322567   0.645572
C  -3.562232   1.589911  -0.338240
H  -3.309372   2.093171  -1.282052
H  -3.797083   2.361977   0.407763
H  -2.667585   1.033484  -0.009007
C  -5.951782   1.368190  -1.032738
H  -6.357725   1.997526  -0.227135
H  -5.705948   2.026440  -1.877021
H  -6.739639   0.681108  -1.365087
C  -6.299744  -1.004145   0.604641
H  -7.115123  -0.303058   0.831753
H  -6.491756  -1.447917  -0.381993
H  -6.335871  -1.810461   1.350294
C  -4.704947   0.326618   1.994245
H  -3.659898   0.640773   2.114784
H  -5.345333   1.211277   2.123068
H  -4.949470  -0.366443   2.813530
Na  -2.752145  -2.405688   2.135025
H  -1.955227  -3.574044  -0.006815
H  -2.625957  -2.172377  -2.710261
H  -1.356769  -4.029317  -1.577960
C   0.937170   2.234829  -3.075830
H   0.245727   2.056662  -3.926360
H   1.754425   2.906467  -3.412927
H   1.378892   1.258859  -2.803895
C  -0.763190   2.468609   1.760298
H  -1.836082   2.441499   2.042514
H  -0.377751   1.435125   1.851698
H  -0.229447   3.128186   2.475522
C  -1.990657   5.996231  -1.547643
H  -3.073138   5.846679  -1.350213
H  -1.614465   6.818547  -0.903284
H  -1.865464   6.296768  -2.609666
H  -0.483350   4.477407  -3.235731
H  -1.870809   4.705475   0.815519
92
Figure_S8_imid-2_modeR2_ed(CuHadd) / electronic energy: -3372.981529315850 a.u. / lowest freq: 17.41 cm-1
C  -2.379724   0.610235   0.707918
H  -3.099310   0.714161  -0.118463
```

C	-1.351460	1.756697	0.767448
H	-1.103791	1.990695	1.813097
C	-0.271806	-0.193333	-0.014863
C	-1.936584	-1.895927	0.356158
C	-1.318713	-2.794973	1.234386
C	-2.916673	-2.367607	-0.533047
C	-1.661804	-4.142549	1.241764
H	-0.562035	-2.404061	1.918299
C	-3.264089	-3.722047	-0.508257
C	-2.647418	-4.606666	0.370688
H	-1.165752	-4.826376	1.934023
H	-4.012380	-4.075539	-1.220210
H	-2.931428	-5.661105	0.369303
C	1.032189	1.837810	-0.155961
C	1.809988	2.360469	0.910082
C	1.455095	2.059071	-1.492510
C	2.946005	3.133947	0.627920
C	2.605368	2.821312	-1.741378
C	3.345336	3.368876	-0.689407
S	-3.730667	-1.343231	-1.775776
O	-4.020490	-2.291781	-2.885661
O	-2.708243	-0.338558	-2.196383
O	-4.914172	-0.757826	-1.123546
Cu	0.746626	-1.624479	-0.947193
C	-3.120668	0.414940	2.007238
C	-4.510893	0.614760	2.065219
C	-2.436889	0.026174	3.175306
C	-5.202713	0.425370	3.265349
H	-5.060435	0.920746	1.184198
C	-3.133081	-0.162521	4.372332
H	-1.366127	-0.134654	3.157084
C	-4.514923	0.036312	4.417401
H	-6.273146	0.581019	3.302218
H	-2.600826	-0.463673	5.265309
H	-5.052648	-0.110130	5.345199
C	-1.801810	3.026384	0.087184
C	-1.865892	4.228905	0.815562
C	-2.140845	3.041243	-1.277904
C	-2.261045	5.415654	0.191051
H	-1.607171	4.251817	1.866856
C	-2.534254	4.229921	-1.898668
H	-2.101607	2.136645	-1.863667
C	-2.594493	5.416418	-1.165014
H	-2.306858	6.335886	0.758960
H	-2.792070	4.230762	-2.949835
H	-2.899194	6.336220	-1.647205
N	-1.504174	-0.544070	0.405829
N	-0.178272	1.141833	0.105158
C	2.063307	-2.826732	0.135147
C	1.799011	-3.317493	-1.152327
H	1.085569	-4.132944	-1.319057
B	3.351019	-2.030355	0.403039
O	4.036571	-2.034074	1.593916
O	3.998389	-1.309631	-0.577349
C	5.155118	-1.121200	1.458901
C	5.338204	-1.042979	-0.095855
C	4.713749	0.199307	2.060243
H	4.407407	0.048620	3.103590
H	5.510881	0.954556	2.042857
H	3.852172	0.592068	1.508845
C	6.342808	-1.682348	2.208136
H	7.232334	-1.054324	2.055551
H	6.134290	-1.705696	3.286146
H	6.583789	-2.704396	1.892411
C	6.231405	-2.146687	-0.638625
H	7.283321	-1.995490	-0.360142
H	5.918408	-3.135040	-0.273351
H	6.170923	-2.160079	-1.735009
C	5.785282	0.306668	-0.610384
H	5.071141	1.095097	-0.350155
H	6.766577	0.580135	-0.197199
H	5.876671	0.285549	-1.704335
Na	-1.581948	-1.494396	-3.805259
H	2.519202	-3.163630	-1.962681
H	1.513150	-3.267292	0.974708
H	0.242591	-1.686744	-2.466054
C	1.486322	2.075859	2.353089
H	2.405765	2.091287	2.976186
H	0.798911	2.854542	2.742548
H	1.034427	1.068399	2.468582
C	0.708431	1.524011	-2.685657
H	1.388702	0.891920	-3.294280
H	-0.166474	0.908056	-2.412314
H	0.351389	2.370580	-3.309225
C	4.573717	4.188025	-0.958128
H	4.441361	5.206920	-0.537264
H	5.453889	3.709632	-0.479049
H	4.773968	4.280520	-2.046780

```
 H   2.920393   2.993231  -2.764299
 H   3.536204   3.542596   1.440340
92
Figure_S8_imid-2_modeR2_ts(CuHadd) / electronic energy: -3372.965179483431 a.u. / lowest freq: -710.22 cm-1
 C  -2.121997   0.474637   0.943029
 H  -3.009185   0.609050   0.308689
 C  -1.202632   1.720816   0.982211
 H  -0.868935   1.922899   2.010772
 C  -0.097489  -0.015381  -0.190091
 C  -1.532933  -1.915385   0.169619
 C  -0.625993  -2.814528   0.749616
 C  -2.649781  -2.422693  -0.515385
 C  -0.830325  -4.187215   0.677996
 H   0.252092  -2.408742   1.257739
 C  -2.852962  -3.805309  -0.572569
 C  -1.955817  -4.686087   0.023081
 H  -0.109370  -4.865843   1.138964
 H  -3.721929  -4.177238  -1.117975
 H  -2.131482  -5.762469  -0.033179
 C   1.070174   2.097194  -0.127784
 C   1.928795   2.520491   0.921505
 C   1.345453   2.517923  -1.456142
 C   3.001809   3.378255   0.639356
 C   2.439941   3.357707  -1.707569
 C   3.266003   3.792236  -0.667355
 S  -3.834291  -1.381607  -1.375991
 O  -4.434503  -2.265345  -2.421034
 O  -3.026307  -0.306632  -2.028434
 O  -4.789010  -0.900734  -0.363247
Cu   0.941272  -1.053891  -1.418483
 C  -2.555716   0.031024   2.319090
 C  -3.907517   0.112849   2.696556
 C  -1.616504  -0.459838   3.246374
 C  -4.312228  -0.299256   3.969778
 H  -4.648763   0.501870   2.010318
 C  -2.026097  -0.871271   4.517551
 H  -0.568962  -0.528890   2.982917
 C  -3.373029  -0.792396   4.878718
 H  -5.354888  -0.233970   4.252675
 H  -1.298529  -1.251306   5.222963
 H  -3.688676  -1.110833   5.863781
 C  -1.850031   2.975713   0.446242
 C  -1.911012   4.133065   1.245005
 C  -2.377180   3.022871  -0.857274
 C  -2.485932   5.307039   0.749115
 H  -1.509475   4.131624   2.250712
 C  -2.950106   4.198692  -1.349388
 H  -2.347937   2.151786  -1.493159
 C  -3.004402   5.340179  -0.547121
 H  -2.527212   6.192630   1.369980
 H  -3.351968   4.224473  -2.354014
 H  -3.447988   6.250223  -0.929807
 N  -1.244001  -0.532005   0.302491
 N  -0.063373   1.286579   0.148710
 C   2.169241  -2.716872  -1.565490
 C   1.883095  -2.124487  -2.847033
 H   1.331441  -2.713228  -3.586666
 B   3.224726  -2.208046  -0.617502
 O   3.594121  -2.841013   0.567099
 O   3.971801  -1.043793  -0.819520
 C   4.398752  -1.905432   1.309553
 C   5.016561  -1.028702   0.171284
 C   3.447541  -1.114504   2.192488
 H   2.892660  -1.803606   2.843799
 H   3.967564  -0.388272   2.832297
 H   2.715509  -0.579182   1.570688
 C   5.408394  -2.662063   2.144011
 H   6.092786  -1.970207   2.656635
 H   4.896969  -3.255408   2.914377
 H   6.007544  -3.350376   1.535079
 C   6.248381  -1.670045  -0.449248
 H   7.115755  -1.635077   0.224825
 H   6.060258  -2.720202  -0.713340
 H   6.514782  -1.133788  -1.370183
 C   5.304169   0.403025   0.567085
 H   4.397048   0.914605   0.906541
 H   6.046376   0.447805   1.377274
 H   5.706008   0.964530  -0.287501
Na  -3.331753  -1.070699  -4.210404
 H   2.664257  -1.513944  -3.316218
 H   1.574548  -3.593148  -1.279442
 H   0.729179  -0.900037  -2.995941
 C   1.756175   2.061976   2.345123
 H   2.745625   1.921694   2.829986
 H   1.189970   2.827059   2.915854
 H   1.232666   1.087470   2.402155
 C   0.496411   2.122505  -2.635473
 H   1.131714   1.626642  -3.399288
```

H -0.318299 1.425283 -2.374136
H 0.040824 3.030477 -3.083801
C 4.438631 4.688153 -0.939314
H 4.322669 5.636432 -0.373427
H 5.374283 4.184704 -0.616284
H 4.525983 4.931918 -2.019515
H 2.644332 3.678144 -2.722869
H 3.651942 3.709692 1.441320
92
Figure_S8_imid-2_modeR2_prod(CuHadd) / electronic energy: -3373.009128484981 a.u. / lowest freq: 15.59 cm-1
C -2.292701 0.540112 0.777097
H -3.096353 0.594495 0.029109
C -1.382718 1.794845 0.797330
H -1.164912 2.103000 1.830762
C -0.139792 -0.042489 -0.015951
C -1.600469 -1.914104 0.327915
C -0.706037 -2.746352 1.017123
C -2.664851 -2.497231 -0.380619
C -0.878623 -4.125513 1.037169
H 0.128054 -2.280784 1.548329
C -2.842502 -3.883388 -0.335005
C -1.964778 -4.696453 0.374959
H -0.167614 -4.751028 1.580647
H -3.668890 -4.316633 -0.900929
H -2.118961 -5.777241 0.394572
C 1.020126 2.058859 -0.046791
C 1.768147 2.540400 1.058750
C 1.465065 2.349426 -1.362729
C 2.893685 3.347127 0.837549
C 2.604546 3.144343 -1.551271
C 3.317156 3.648171 -0.458888
S -3.747367 -1.561808 -1.470250
O -4.268036 -2.567806 -2.443097
O -2.843058 -0.597770 -2.171887
O -4.782918 -0.933370 -0.634081
Cu 1.191877 -1.169032 -0.840224
C -2.888515 0.239933 2.130724
C -4.270239 0.386195 2.344647
C -2.071828 -0.171419 3.201699
C -4.824838 0.110224 3.598091
H -4.918665 0.722658 1.545983
C -2.630991 -0.446899 4.452468
H -1.003860 -0.283902 3.066740
C -4.006638 -0.308128 4.650226
H -5.889734 0.223952 3.754575
H -1.997017 -0.767531 5.268983
H -4.438109 -0.521073 5.619708
C -1.958145 2.978789 0.059421
C -2.113814 4.211937 0.719411
C -2.325944 2.882183 -1.295187
C -2.625666 5.320305 0.038171
H -1.835566 4.319917 1.760394
C -2.836378 3.992952 -1.972491
H -2.221601 1.948731 -1.827576
C -2.986056 5.211246 -1.306665
H -2.741067 6.265191 0.553291
H -3.116172 3.908611 -3.014597
H -3.381354 6.070618 -1.832596
N -1.340685 -0.520259 0.358172
N -0.153353 1.286489 0.156800
C 2.460198 -2.296733 -1.871682
C 2.702589 -1.819315 -3.289712
H 3.419088 -2.451266 -3.849955
B 3.455323 -1.974879 -0.779901
O 3.552644 -2.659589 0.444907
O 4.340021 -0.887004 -0.793233
C 4.235886 -1.785699 1.358344
C 5.140069 -0.948837 0.396286
C 3.177804 -0.926428 2.037144
H 2.452684 -1.571236 2.553450
H 3.604331 -0.235217 2.777814
H 2.625596 -0.339493 1.285326
C 4.989549 -2.610399 2.378617
H 5.595705 -1.969020 3.035295
H 4.286646 -3.167342 3.013535
H 5.654914 -3.338492 1.899109
C 6.437223 -1.665967 0.050185
H 7.138085 -1.684067 0.896966
H 6.248239 -2.702605 -0.262313
H 6.929824 -1.147834 -0.784057
C 5.427566 0.460667 0.870527
H 4.505151 1.040549 0.986271
H 5.956906 0.458243 1.834916
H 6.060762 0.986804 0.142764
Na -2.922157 -1.686520 -4.252732
H 3.124099 -0.801848 -3.307673
H 2.052074 -3.320247 -1.812530
H 1.789836 -1.781083 -3.909389

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C   1.425461   2.178564   2.479384
H   2.344733   2.118419   3.100313
H   0.760112   2.954203   2.911713
H   0.936368   1.185036   2.536101
C   0.760613   1.843320  -2.594588
H   1.477892   1.278191  -3.226134
H  -0.084080   1.168029  -2.369188
H   0.370423   2.704065  -3.177418
C   4.542538   4.489830  -0.662474
H   4.395355   5.483502  -0.189372
H   5.418043   3.991197  -0.195384
H   4.759680   4.642784  -1.741048
H   2.937910   3.368407  -2.558155
H   3.460876   3.724580   1.680925
123
Figure_S9_imid-2_modeA_ed(AS) / electronic energy: -4442.824230082218 a.u. / lowest freq: -7.03 cm-1
C   0.884598   2.216842   1.640257
H  -0.027365   2.753898   1.935143
C   1.603139   2.833048   0.422792
H   2.696280   2.835519   0.562730
C   0.686658   0.742986  -0.210985
C  -0.086393  -0.129702   1.932670
C   0.657323  -1.303341   2.109834
C  -1.309437   0.014761   2.615979
C   0.232265  -2.290265   2.996076
H   1.592425  -1.411236   1.549052
C  -1.732925  -0.991837   3.487953
C  -0.959258  -2.129451   3.698497
H   0.835091  -3.191180   3.135629
H  -2.689327  -0.861924   3.997170
H  -1.298631  -2.896875   4.397762
S  -2.389704   1.442610   2.441272
O  -3.717200   0.997510   2.963528
O  -2.476516   1.736184   0.980742
O  -1.782042   2.521007   3.246256
Cu  0.191548  -0.957666  -1.158002
C   1.781673   2.086040   2.848830
C   1.531560   2.855235   3.999285
C   2.877441   1.201956   2.846325
C   2.354110   2.735617   5.123471
H   0.704192   3.552678   4.026818
C   3.695658   1.084212   3.972933
H   3.091091   0.594217   1.979387
C   3.434233   1.850139   5.110905
H   2.154427   3.331230   6.004831
H   4.532402   0.397922   3.964115
H   4.069236   1.758466   5.982534
N   0.473012   0.888172   1.110585
N   1.251573   1.881044  -0.653319
C  -1.314694  -2.268088  -1.563750
C  -1.161824  -3.555240  -0.876703
C  -0.845667  -4.716661  -1.606542
C  -1.390330  -3.696677   0.504745
C  -0.753131  -5.958524  -0.984168
C  -1.294838  -4.936895   1.128033
C  -0.976200  -6.077398   0.388448
H  -0.511042  -6.843258  -1.578377
H  -1.477483  -5.014007   2.203887
H  -0.905215  -7.051738   0.877850
C  -1.840029  -1.099417  -0.971107
C  -2.522952  -0.090978  -1.812804
H  -2.603383   0.883581  -1.313158
H  -2.036114   0.035189  -2.788514
H  -1.658805  -2.820510   1.099544
H  -2.125746  -1.095664   0.087114
P  -5.115503  -0.071587  -1.286107
O  -4.944713  -0.700629   0.195363
O  -5.350361   1.386763  -1.084820
O  -6.260478  -0.906943  -2.029457
O  -3.888569  -0.541391  -2.170530
Na -4.972020   1.856834   1.151787
H  -1.336116  -2.331165  -2.660194
H  -0.691329  -4.639292  -2.686141
C  -4.765291  -2.100542   0.407092
H  -4.264048  -2.221208   1.374832
H  -5.737451  -2.612236   0.433751
H  -4.139191  -2.547531  -0.379083
C  -7.628035  -0.651428  -1.711357
H  -8.229604  -1.321796  -2.332032
H  -7.836832  -0.862371  -0.652243
H  -7.897143   0.389544  -1.934015
C   1.790043   1.999563  -1.962600
C   3.172082   1.774514  -2.201426
C   0.968725   2.438264  -3.031533
C   3.707363   2.020680  -3.473508
C   1.530981   2.666136  -4.295424
C   2.896027   2.464549  -4.520155
H  -0.958081   3.796836   0.023125
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H	-1.633993	6.090220	-0.548810
C	-0.197148	4.556292	-0.083674
C	-0.586122	5.858670	-0.408268
C	1.162526	4.241015	0.099395
C	0.375017	6.860973	-0.553316
H	0.072151	7.868892	-0.805814
C	2.121122	5.260726	-0.048538
C	1.727181	6.562311	-0.372934
H	3.175520	5.049876	0.079685
H	2.471685	7.339573	-0.487060
C	1.794135	-1.680882	-2.200822
H	2.255985	-0.709635	-2.432701
C	1.434068	-2.423001	-3.471057
H	0.719805	-1.876809	-4.112166
H	2.309263	-2.642145	-4.113522
H	0.973687	-3.400265	-3.257837
B	2.620306	-2.419127	-1.162636
O	3.214483	-1.826487	-0.041636
O	2.892426	-3.784244	-1.189683
C	3.498418	-4.140199	0.067144
C	4.130328	-2.783288	0.518350
C	2.377614	-4.595945	0.986115
H	1.635704	-3.795082	1.125004
H	1.850970	-5.443624	0.526809
H	2.743093	-4.914762	1.973335
C	4.495366	-5.256621	-0.156620
H	5.229295	-4.997795	-0.929845
H	5.039508	-5.491112	0.770265
H	3.977364	-6.170336	-0.478977
C	5.491475	-2.537134	-0.115627
H	6.266894	-3.194612	0.301655
H	5.456677	-2.691574	-1.203278
H	5.795221	-1.497097	0.065258
C	4.209531	-2.590115	2.018014
H	4.636987	-1.605171	2.251301
H	3.224668	-2.649522	2.498587
H	4.857163	-3.350779	2.478383
C	4.100044	1.226151	-1.151445
H	4.682309	0.378286	-1.570590
H	4.803645	2.019246	-0.823104
H	3.554860	0.835467	-0.274514
C	-0.502511	2.700295	-2.868151
H	-0.704919	3.782306	-3.012492
H	-1.070204	2.126867	-3.630299
H	-0.877015	2.402649	-1.873280
C	3.496957	2.710843	-5.873007
H	3.949157	1.772025	-6.256580
H	2.734463	3.057051	-6.602877
H	4.286117	3.487999	-5.794522
H	4.762956	1.851279	-3.654593
H	0.898762	3.008519	-5.106775

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Figure_S9_imid-2_modeA_ts(AS)_01 / electronic energy: -4442.810823094441 a.u. / lowest freq: -256.81 cm-1

C	-1.004553	-2.433521	-1.210225
H	-1.993032	-2.225345	-1.641565
C	-1.060903	-2.937022	0.247757
H	-0.370367	-3.780233	0.405208
C	-0.057929	-0.794510	0.223075
C	0.174986	-0.348525	-2.146642
C	1.547607	-0.065665	-2.191602
C	-0.662244	0.154752	-3.159612
C	2.088284	0.681971	-3.233275
H	2.186285	-0.469133	-1.397600
C	-0.104772	0.912465	-4.193963
C	1.260840	1.172884	-4.240931
H	3.163585	0.876924	-3.261904
H	-0.774833	1.306678	-4.959628
H	1.675431	1.759953	-5.062861
S	-2.439800	-0.117712	-3.239157
O	-2.962054	0.983921	-4.099384
O	-2.955172	0.030469	-1.842851
O	-2.614802	-1.462936	-3.812930
Cu	0.902874	0.940681	0.665059
C	-0.258020	-3.381949	-2.117501
C	-0.954762	-4.127629	-3.084297
C	1.133858	-3.557384	-1.994464
C	-0.271234	-5.012200	-3.923853
H	-2.028406	-4.033462	-3.183077
C	1.813104	-4.441661	-2.836801
H	1.694256	-3.005375	-1.252946
C	1.111629	-5.166986	-3.802268
H	-0.815063	-5.581095	-4.666834
H	2.883764	-4.565993	-2.740232
H	1.638817	-5.852529	-4.453016
N	-0.286453	-1.138008	-1.059192
N	-0.568830	-1.761979	0.998931
C	1.038587	2.980798	0.512573
C	2.290763	3.621907	0.104050

C	2.998859	4.423756	1.018385
C	2.798138	3.516879	-1.204188
C	4.171456	5.075540	0.647916
C	3.964093	4.174937	-1.577250
C	4.662584	4.953499	-0.652215
H	4.700122	5.693551	1.377509
H	4.336178	4.073396	-2.600378
H	5.580025	5.469094	-0.945417
C	0.047265	2.522630	-0.397550
C	-1.250914	2.180187	0.028600
H	-1.864784	1.527754	-0.598156
H	-1.436228	2.124549	1.102626
H	2.270218	2.908196	-1.941296
H	0.258868	2.501446	-1.472372
P	-3.827090	3.604439	0.254464
O	-4.371327	5.098253	0.595228
O	-4.847705	2.955055	-0.634508
O	-3.739302	2.866613	1.709238
O	-2.355722	3.730989	-0.183946
Na	-4.509757	1.824623	-2.510917
H	0.696101	3.242548	1.523701
H	2.604923	4.548956	2.030249
C	-3.595469	5.945656	1.425677
H	-4.162802	6.871050	1.576098
H	-3.406191	5.483512	2.407086
H	-2.629723	6.188756	0.959365
C	-4.933789	2.423441	2.328244
H	-4.667037	2.014292	3.309474
H	-5.645270	3.251049	2.476199
H	-5.426843	1.638697	1.736460
C	-0.389043	-1.790719	2.406942
C	0.614209	-2.609254	2.990069
C	-1.259653	-1.057768	3.252296
C	0.696555	-2.720321	4.385054
C	-1.143622	-1.178466	4.644278
C	-0.176071	-2.011657	5.214130
H	-3.422847	-1.504007	0.188380
H	-5.639328	-2.212396	0.980267
C	-3.538260	-2.492678	0.605318
C	-4.800090	-2.891912	1.053747
C	-2.437481	-3.364084	0.698724
C	-4.979086	-4.165202	1.597970
H	-5.956766	-4.472765	1.945711
C	-2.631511	-4.645479	1.247668
C	-3.895949	-5.041445	1.693796
H	-1.804105	-5.338228	1.338497
H	-4.035181	-6.027835	2.117007
C	2.310515	0.575212	2.088300
H	1.793318	-0.274855	2.551882
C	2.579084	1.653498	3.109982
H	1.664114	2.076347	3.558810
H	3.187516	1.280542	3.954572
H	3.147617	2.492375	2.684679
B	3.491223	0.083310	1.252375
O	3.457366	-1.037915	0.427946
O	4.733006	0.693440	1.216627
C	5.508873	0.060546	0.176238
C	4.816514	-1.337216	0.047200
C	5.342322	0.908334	-1.071944
H	4.283118	0.959100	-1.364465
H	5.672978	1.934971	-0.864437
H	5.924789	0.523201	-1.921010
C	6.960274	0.009017	0.600189
H	7.082463	-0.464869	1.581678
H	7.563969	-0.549227	-0.130090
H	7.372467	1.025022	0.665914
C	5.352065	-2.350804	1.046799
H	6.375831	-2.666307	0.802519
H	5.351485	-1.945289	2.068387
H	4.713423	-3.244111	1.039695
C	4.829258	-1.921347	-1.349168
H	4.328049	-2.898518	-1.354918
H	4.315958	-1.278907	-2.075616
H	5.860225	-2.075563	-1.699366
C	1.655117	-3.325040	2.171787
H	2.662527	-3.131899	2.597372
H	1.459688	-4.417410	2.191221
H	1.680451	-2.975181	1.123314
C	-2.332411	-0.147311	2.721554
H	-3.329556	-0.530818	3.023785
H	-2.195592	0.869187	3.146268
H	-2.313474	-0.057359	1.620789
C	-0.054749	-2.141716	6.704187
H	0.956438	-1.814496	7.025846
H	-0.809324	-1.520642	7.232214
H	-0.203909	-3.201723	6.999216
H	1.459807	-3.348827	4.830224
H	-1.816410	-0.620938	5.285952

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Figure_S9_imid-2_modeA_ts(AS)_02 / electronic energy: -4442.811963393518 a.u. / lowest freq: -238.21 cm-1

C	0.269581	2.423842	1.581451
H	-0.744823	2.776167	1.810738
C	0.921862	3.140285	0.379864
H	1.970248	3.404702	0.590289
C	0.525871	0.881714	-0.202302
C	-0.221506	-0.070960	1.907008
C	0.708347	-1.106108	2.071910
C	-1.457150	-0.144317	2.577732
C	0.440543	-2.175306	2.922754
H	1.664232	-1.035506	1.540532
C	-1.714062	-1.227558	3.422333
C	-0.769136	-2.232280	3.610411
H	1.182975	-2.967052	3.051677
H	-2.682972	-1.270470	3.922756
H	-0.984955	-3.063530	4.285253
S	-2.774819	1.066899	2.387116
O	-4.009503	0.379871	2.864726
O	-2.861336	1.342130	0.920671
O	-2.397221	2.234072	3.206030
Cu	0.452831	-0.945899	-1.062002
C	1.107565	2.507922	2.835635
C	0.666509	3.275577	3.928186
C	2.340974	1.835047	2.930220
C	1.435394	3.356529	5.092995
H	-0.267904	3.819513	3.878074
C	3.105271	1.917610	4.097196
H	2.705752	1.236972	2.107608
C	2.652528	2.676763	5.178262
H	1.088078	3.949067	5.929479
H	4.049095	1.392402	4.163849
H	3.245956	2.740405	6.081126
N	0.162227	1.024135	1.084911
N	0.886287	2.089654	-0.660356
C	-0.578007	-2.661215	-1.486732
C	-0.150178	-3.933271	-0.898461
C	0.476703	-4.907833	-1.698866
C	-0.397402	-4.258086	0.449586
C	0.864179	-6.135199	-1.170785
C	-0.012396	-5.485426	0.977105
C	0.626214	-6.430721	0.172458
H	1.346498	-6.872470	-1.816948
H	-0.217369	-5.706605	2.028358
H	0.928551	-7.395192	0.587069
C	-1.451062	-1.743962	-0.831398
C	-2.104467	-0.717510	-1.532630
H	-2.555802	0.101509	-0.966485
H	-1.770659	-0.479642	-2.543444
H	-0.910386	-3.544247	1.095877
H	-1.719761	-1.885800	0.220690
P	-4.996455	-1.119785	-1.467031
O	-4.757588	-1.585093	0.097674
O	-5.507633	0.285825	-1.331238
O	-6.097853	-2.167999	-2.035467
O	-3.744511	-1.456965	-2.287575
Na	-5.261894	0.807180	0.877328
H	-0.568193	-2.633327	-2.584530
H	0.638147	-4.702139	-2.759710
C	-4.398736	-2.923431	0.397951
H	-3.923095	-2.933189	1.387610
H	-5.285672	-3.574797	0.423831
H	-3.689589	-3.326382	-0.342185
C	-7.454243	-2.013769	-1.647996
H	-8.030736	-2.795980	-2.153822
H	-7.580943	-2.132498	-0.560140
H	-7.847252	-1.030368	-1.942861
C	1.463896	2.280949	-1.943287
C	2.871980	2.388616	-2.092421
C	0.634176	2.448805	-3.080457
C	3.416219	2.702935	-3.345366
C	1.208692	2.752095	-4.322934
C	2.593822	2.886457	-4.459414
H	-1.749136	3.452650	-0.258425
H	-2.891432	5.496058	-1.010684
C	-1.180725	4.366240	-0.354301
C	-1.834093	5.525341	-0.781428
C	0.194471	4.389886	-0.055491
C	-1.124516	6.720474	-0.914512
H	-1.631742	7.617072	-1.246496
C	0.897823	5.601047	-0.192360
C	0.239926	6.758325	-0.619485
H	1.957723	5.651165	0.023858
H	0.789527	7.684823	-0.724315
C	2.196581	-1.278946	-2.054084
H	2.408091	-0.220911	-2.257212
C	2.081407	-2.056167	-3.342828
H	1.285729	-1.684998	-4.010355

H 3.015235 -2.017206 -3.933923
H 1.884388 -3.124055 -3.170557
B 3.128377 -1.807103 -0.966025
O 3.492009 -1.088416 0.169599
O 3.723294 -3.055672 -0.980746
C 4.332119 -3.264633 0.312846
C 4.579825 -1.799428 0.797291
C 3.306909 -3.989730 1.167314
H 2.392162 -3.386072 1.264526
H 3.020877 -4.933827 0.683227
H 3.685544 -4.221126 2.173235
C 5.584080 -4.096317 0.145585
H 6.268792 -3.660414 -0.592132
H 6.122383 -4.194174 1.099695
H 5.324810 -5.107871 -0.195230
C 5.874009 -1.213426 0.253882
H 6.758490 -1.664617 0.724835
H 5.952662 -1.355063 -0.833165
H 5.898037 -0.133918 0.454177
C 4.505904 -1.606712 2.296801
H 4.679677 -0.552670 2.552267
H 3.529755 -1.893768 2.707830
H 5.277010 -2.203284 2.805564
C 3.831283 2.118557 -0.964464
H 4.621280 1.415890 -1.304828
H 4.307195 3.068301 -0.642936
H 3.337464 1.645571 -0.096793
C -0.864272 2.334709 -3.016466
H -1.321264 3.320577 -3.244004
H -1.213177 1.597613 -3.769733
H -1.225517 2.000438 -2.027349
C 3.207175 3.212856 -5.789526
H 3.899531 2.398618 -6.090661
H 2.434773 3.327209 -6.579617
H 3.776047 4.163474 -5.714475
H 4.491223 2.788844 -3.458253
H 0.569028 2.887970 -5.187535
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Figure_S9_imid-2_modeA_ts(AS)_03 / electronic energy: -4442.811278359693 a.u. / lowest freq: -239.08 cm-1
C 2.758738 -1.600401 0.625757
H 3.425640 -1.044968 -0.046175
C 2.041636 -2.787943 -0.050328
H 2.065529 -3.681133 0.591803
C 0.437898 -1.126533 0.473669
C 1.735702 0.449645 1.787897
C 0.957571 0.493478 2.953290
C 2.605941 1.519443 1.509939
C 1.075025 1.543843 3.857004
H 0.279175 -0.338402 3.157728
C 2.727108 2.562850 2.432749
C 1.984493 2.569726 3.609564
H 0.459596 1.551763 4.759062
H 3.407014 3.383413 2.195687
H 2.098512 3.390927 4.320471
S 3.562253 1.649366 -0.006506
O 3.868935 3.102091 -0.156321
O 2.652978 1.190922 -1.100775
O 4.758934 0.808454 0.182819
Cu -1.105652 0.145867 0.764610
C 3.538883 -2.014947 1.850667
C 4.944760 -2.009279 1.825587
C 2.880234 -2.433179 3.022643
C 5.674453 -2.395408 2.953841
H 5.478311 -1.714966 0.931000
C 3.613793 -2.816996 4.148481
H 1.800477 -2.452019 3.069968
C 5.009815 -2.796601 4.114959
H 6.756402 -2.386386 2.926642
H 3.099171 -3.130285 5.047598
H 5.576573 -3.094807 4.987453
N 1.618221 -0.708245 0.969650
N 0.651029 -2.290857 -0.159202
C -1.871544 2.031733 0.576211
C -2.035697 2.812592 1.804250
C -3.279945 2.821862 2.466340
C -0.996582 3.593661 2.341343
C -3.468265 3.573262 3.621670
C -1.189243 4.347561 3.495064
C -2.424375 4.339909 4.144202
H -4.441442 3.564710 4.118978
H -0.366053 4.949557 3.889136
H -2.574891 4.933820 5.048757
C -0.666940 1.969104 -0.181421
C -0.651085 1.570979 -1.526956
H 0.307847 1.326146 -1.985762
H -1.526392 1.074598 -1.947822
H -0.023226 3.617243 1.846594
H 0.270721 2.365089 0.225862

P	0.270851	3.827538	-3.100364
O	1.096369	4.374237	-1.779851
O	1.338035	3.114684	-3.881249
O	-0.288920	5.171570	-3.815300
O	-1.013958	3.122080	-2.641433
Na	3.145412	3.152646	-2.453829
H	-2.807817	1.819545	0.041793
H	-4.093798	2.219187	2.056035
C	0.451547	5.149094	-0.784103
H	1.083057	5.128296	0.113585
H	0.330779	6.193782	-1.109405
H	-0.540686	4.740528	-0.536427
C	0.626336	6.011756	-4.501672
H	0.044820	6.798527	-4.994107
H	1.338727	6.484132	-3.806864
H	1.191233	5.453381	-5.261609
C	-0.407910	-3.104552	-0.645948
C	-0.844070	-4.241381	0.087168
C	-0.963195	-2.858147	-1.927283
C	-1.814179	-5.092553	-0.460597
C	-1.927967	-3.731341	-2.449525
C	-2.361834	-4.841207	-1.719801
H	2.498678	-1.174529	-2.249180
H	3.395261	-1.831075	-4.441944
C	2.770841	-2.206136	-2.416321
C	3.281086	-2.574760	-3.663943
C	2.614472	-3.163458	-1.396536
C	3.642499	-3.901016	-3.908554
H	4.036792	-4.185113	-4.875608
C	2.984549	-4.496451	-1.655421
C	3.495121	-4.860664	-2.904878
H	2.872767	-5.258098	-0.893742
H	3.774736	-5.888733	-3.095512
C	-2.485304	-0.555667	2.091751
H	-2.571305	0.271726	2.814947
C	-2.062521	-1.854056	2.735112
H	-1.022297	-1.878126	3.103993
H	-2.691768	-2.103003	3.609201
H	-2.180168	-2.690543	2.034469
B	-3.677987	-0.652664	1.135052
O	-4.656345	0.317213	0.959581
O	-3.908533	-1.745279	0.309251
C	-4.966870	-1.385929	-0.606786
C	-5.724550	-0.273624	0.186779
C	-4.321490	-0.838875	-1.868330
H	-3.703320	0.043892	-1.648810
H	-3.678144	-1.602591	-2.318221
H	-5.068347	-0.552280	-2.620769
C	-5.788673	-2.616846	-0.918556
H	-6.141952	-3.113020	-0.006414
H	-6.662769	-2.362385	-1.535300
H	-5.185370	-3.341042	-1.481749
C	-6.731853	-0.845410	1.171759
H	-7.614556	-1.256072	0.662381
H	-6.285551	-1.642270	1.783144
H	-7.072729	-0.051595	1.849746
C	-6.363655	0.797467	-0.669734
H	-6.890244	1.525623	-0.038066
H	-5.620242	1.346051	-1.260828
H	-7.101014	0.362030	-1.359521
C	-0.299723	-4.593197	1.446403
H	-1.122791	-4.922057	2.115987
H	0.430941	-5.423299	1.350651
H	0.185098	-3.728272	1.935402
C	-0.526516	-1.708847	-2.792796
H	-0.025719	-2.100197	-3.703061
H	-1.409108	-1.112390	-3.101874
H	0.172689	-1.031552	-2.274165
C	-3.401349	-5.769261	-2.276531
H	-4.274828	-5.804855	-1.591891
H	-3.753047	-5.437226	-3.276500
H	-2.975826	-6.790183	-2.373799
H	-2.146248	-5.960381	0.098251
H	-2.341109	-3.542827	-3.433878

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Figure_S9_imid-2_modeA_ts(AS)_04 / electronic energy: -4442.810573649339 a.u. / lowest freq: -253.19 cm-1

C	2.926049	0.643990	-1.056116
H	3.473042	0.324991	-0.157961
C	2.322680	2.060157	-0.955656
H	2.456748	2.611069	-1.899442
C	0.560063	0.486699	-0.945633
C	1.695319	-1.583862	-1.468538
C	0.886228	-1.991680	-2.539885
C	2.449445	-2.551071	-0.780183
C	0.847111	-3.319740	-2.949533
H	0.306922	-1.232544	-3.070931
C	2.423035	-3.878747	-1.219316
C	1.640793	-4.264480	-2.303091

H	0.203507	-3.609079	-3.783238
H	3.011630	-4.612905	-0.666792
H	1.633091	-5.308031	-2.624684
S	3.413618	-2.207627	0.699852
O	3.542704	-3.527694	1.385165
O	2.582535	-1.277143	1.523814
O	4.696353	-1.643156	0.245566
Cu	-1.104653	-0.665771	-0.821352
C	3.830237	0.488548	-2.255519
C	5.225506	0.468014	-2.082651
C	3.304532	0.406231	-3.559147
C	6.074196	0.340877	-3.186244
H	5.658612	0.560451	-1.094682
C	4.156746	0.278160	-4.659356
H	2.237072	0.432933	-3.725999
C	5.540376	0.242941	-4.473163
H	7.146937	0.322970	-3.043676
H	3.743742	0.207865	-5.657310
H	6.199007	0.145171	-5.326413
N	1.702251	-0.196943	-1.156728
N	0.883311	1.776682	-0.754210
C	-2.027658	-2.236963	0.157899
C	-2.316919	-3.443176	-0.621363
C	-3.566209	-3.579020	-1.258946
C	-1.392218	-4.496099	-0.749484
C	-3.867406	-4.713206	-2.006412
C	-1.698086	-5.630608	-1.495012
C	-2.934736	-5.744576	-2.132250
H	-4.841837	-4.795350	-2.494597
H	-0.962769	-6.435388	-1.576699
H	-3.172804	-6.635936	-2.717479
C	-0.787833	-1.981760	0.794241
C	-0.592842	-0.923327	1.698715
H	0.432347	-0.601296	1.880739
H	-1.369366	-0.164326	1.805006
H	-0.420863	-4.435729	-0.253195
H	0.064712	-2.646004	0.618677
P	0.032242	-1.074701	4.583536
O	-0.791220	-1.052164	5.986508
O	1.337578	-1.764854	4.854328
O	0.245627	0.504080	4.222288
O	-0.920990	-1.577103	3.483882
Na	2.721671	-2.827293	3.495373
H	-2.910883	-1.693598	0.521023
H	-4.292176	-2.768227	-1.162707
C	-2.069349	-0.440650	6.023190
H	-2.467502	-0.564507	7.036758
H	-2.006927	0.635286	5.796209
H	-2.759543	-0.910130	5.307024
C	1.206809	1.247346	4.947632
H	1.139306	2.290092	4.616890
H	1.014374	1.212170	6.031716
H	2.226653	0.879261	4.761936
C	-0.093221	2.809344	-0.781769
C	-0.402371	3.482609	-1.994584
C	-0.698700	3.248740	0.422524
C	-1.311573	4.550157	-1.985492
C	-1.601414	4.321249	0.399321
C	-1.918662	4.966407	-0.799016
H	2.588548	1.419945	1.726954
H	3.520965	2.818406	3.521731
C	2.953184	2.408644	1.485676
C	3.479532	3.200119	2.510270
C	2.898515	2.893603	0.164530
C	3.952988	4.483455	2.231523
H	4.358552	5.095319	3.026824
C	3.381246	4.188369	-0.102750
C	3.903696	4.977046	0.926379
H	3.348548	4.593328	-1.106598
H	4.270155	5.972503	0.711396
C	-2.469103	-0.440144	-2.315001
H	-2.652330	-1.480774	-2.631638
C	-1.973686	0.430867	-3.445563
H	-0.949908	0.209592	-3.793981
H	-2.614277	0.346040	-4.342518
H	-1.999984	1.491078	-3.161541
B	-3.623215	0.143814	-1.496257
O	-4.669216	-0.584299	-0.937735
O	-3.755998	1.495948	-1.203861
C	-4.821696	1.634615	-0.237813
C	-5.675386	0.356728	-0.506165
C	-4.196782	1.618997	1.146838
H	-3.664808	0.675143	1.336261
H	-3.478560	2.441168	1.234784
H	-4.947025	1.751408	1.937917
C	-5.539592	2.943871	-0.480122
H	-5.872664	3.040285	-1.520458
H	-6.417217	3.038283	0.175566

H	-4.871006	3.787348	-0.262640
C	-6.648863	0.540687	-1.659964
H	-7.488056	1.195642	-1.387160
H	-6.150545	0.970517	-2.540347
H	-7.063245	-0.434173	-1.950125
C	-6.386639	-0.203791	0.706335
H	-6.974678	-1.088204	0.425705
H	-5.682167	-0.508450	1.490185
H	-7.081444	0.534158	1.132881
C	0.229618	3.116468	-3.311770
H	-0.519225	3.175373	-4.129991
H	1.052970	3.825524	-3.537858
H	0.623097	2.083325	-3.307936
C	-0.379699	2.638402	1.758391
H	0.129381	3.390514	2.396756
H	-1.313237	2.316508	2.263377
H	0.274835	1.756228	1.670523
C	-2.893928	6.106544	-0.823655
H	-3.740868	5.857968	-1.497400
H	-3.301371	6.318498	0.187776
H	-2.388831	7.021386	-1.198808
H	-1.547942	5.064087	-2.910482
H	-2.057472	4.654858	1.324470

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Figure_S9_imid-2_modeA_ts(AS)_05 / electronic energy: -4442.807971544134 a.u. / lowest freq: -254.61 cm-1

C	-1.129093	-2.202920	-1.358266
H	-2.098593	-1.896483	-1.771229
C	-1.226809	-2.823060	0.052773
H	-0.633253	-3.747971	0.126191
C	-0.054703	-0.772257	0.203790
C	0.177160	-0.124796	-2.124021
C	1.562977	0.093673	-2.138186
C	-0.618377	0.473326	-3.119592
C	2.155216	0.863868	-3.134774
H	2.172575	-0.386656	-1.363984
C	-0.007316	1.247827	-4.110537
C	1.369773	1.439173	-4.130563
H	3.238395	1.010183	-3.138472
H	-0.645330	1.711139	-4.864463
H	1.825850	2.040129	-4.919904
S	-2.409312	0.323848	-3.227361
O	-2.840459	1.484919	-4.060962
O	-2.930173	0.465114	-1.834197
O	-2.673577	-0.984786	-3.850738
Cu	0.988827	0.867212	0.789506
C	-0.449856	-3.123711	-2.348547
C	-1.226007	-3.794183	-3.315591
C	0.886784	-3.339839	-2.301455
C	-0.621337	-4.657413	-4.234145
H	-2.299215	-3.656952	-3.352681
C	1.513458	-4.199428	-3.212450
H	1.498722	-2.843838	-1.562085
C	0.758232	-4.859385	-4.184012
H	-1.219937	-5.168913	-4.976703
H	2.583659	-4.353109	-3.162878
H	1.238284	-5.525409	-4.889166
N	-0.335486	-0.967267	-1.100042
N	-0.607421	-1.778805	0.896100
C	1.197286	2.911021	0.781934
C	2.441199	3.529643	0.315220
C	3.292393	4.180840	1.228218
C	2.801185	3.555191	-1.045545
C	4.458560	4.811031	0.802901
C	3.962140	4.189305	-1.471323
C	4.802279	4.817313	-0.549592
H	5.098976	5.311442	1.533142
H	4.215396	4.191355	-2.534959
H	5.714902	5.315813	-0.884413
C	0.120555	2.558793	-0.078173
C	-1.148038	2.200157	0.416301
H	-1.826458	1.626094	-0.218757
H	-1.257748	2.050438	1.491432
H	2.158169	3.074200	-1.784936
H	0.245452	2.619619	-1.164561
P	-3.768886	3.561882	0.576694
O	-4.381909	4.763902	1.486258
O	-4.637336	3.460868	-0.643554
O	-3.902596	2.234566	1.520733
O	-2.249227	3.781268	0.462997
Na	-4.362616	2.403699	-2.557803
H	0.951300	3.105866	1.835023
H	3.015380	4.211394	2.284905
C	-3.765774	5.072956	2.724343
H	-4.279014	5.946505	3.142380
H	-3.852890	4.236919	3.436069
H	-2.700357	5.312131	2.593027
C	-5.172595	1.628265	1.670521
H	-5.085664	0.857896	2.445046

H -5.937481 2.355021 1.986770
H -5.506661 1.153326 0.736220
C -0.356145 -1.986720 2.278538
C 0.637832 -2.909307 2.700380
C -1.144706 -1.328927 3.255806
C 0.793677 -3.188499 4.065254
C -0.957136 -1.619561 4.614464
C 0.002540 -2.550454 5.023154
H -3.416660 -1.137775 0.122416
H -5.695068 -1.653165 0.886380
C -3.639519 -2.136087 0.468219
C -4.936206 -2.424765 0.901268
C -2.640996 -3.128181 0.487596
C -5.253302 -3.706551 1.354835
H -6.257901 -3.928677 1.690701
C -2.974373 -4.416643 0.944437
C -4.273693 -4.701769 1.375023
H -2.228556 -5.201091 0.975630
H -4.520298 -5.694903 1.727587
C 2.401189 0.320579 2.151037
H 1.860075 -0.550523 2.542956
C 2.699957 1.302948 3.257900
H 1.796517 1.701938 3.749392
H 3.307854 0.849565 4.062841
H 3.280795 2.165045 2.900021
B 3.560680 -0.128140 1.264488
O 3.480905 -1.153440 0.326805
O 4.822110 0.441154 1.276602
C 5.547160 -0.071852 0.137522
C 4.821253 -1.432899 -0.129105
C 5.343063 0.927388 -0.987083
H 4.274145 1.017939 -1.230307
H 5.682547 1.920271 -0.661334
H 5.892502 0.656754 -1.899935
C 7.011864 -0.196641 0.492878
H 7.161020 -0.792554 1.401417
H 7.575813 -0.667976 -0.325235
H 7.446145 0.796985 0.667922
C 5.364696 -2.565132 0.728604
H 6.372427 -2.870170 0.414593
H 5.406472 -2.280955 1.789417
H 4.705852 -3.439160 0.639657
C 4.773933 -1.854400 -1.582466
H 4.225667 -2.801025 -1.683169
H 4.274305 -1.111866 -2.217091
H 5.787428 -2.013312 -1.978641
C 1.590151 -3.571984 1.742437
H 2.630880 -3.453773 2.110866
H 1.354663 -4.654146 1.669756
H 1.554515 -3.122391 0.734203
C -2.206629 -0.326788 2.901400
H -3.199982 -0.717562 3.205991
H -2.014803 0.625539 3.439106
H -2.235170 -0.102880 1.821029
C 0.200406 -2.862607 6.477557
H 1.241862 -2.615966 6.773439
H -0.494345 -2.280270 7.119539
H 0.019301 -3.943681 6.654755
H 1.550019 -3.896054 4.386329
H -1.568223 -1.118472 5.356563
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Figure_S9_imid-2_modeA_ts(AS)_06 / electronic energy: -4442.809206671704 a.u. / lowest freq: -237.84 cm-1
C 0.287500 2.421980 1.580482
H -0.724946 2.779907 1.810125
C 0.940055 3.135141 0.376334
H 1.989748 3.396365 0.584057
C 0.530489 0.878069 -0.204099
C -0.221202 -0.069481 1.906303
C 0.704649 -1.107717 2.073528
C -1.457318 -0.136714 2.576660
C 0.432526 -2.174333 2.926230
H 1.660921 -1.041291 1.542382
C -1.718841 -1.217660 3.422831
C -0.777765 -2.225581 3.613190
H 1.171853 -2.968679 3.057014
H -2.688200 -1.255961 3.922748
H -0.997148 -3.054893 4.289270
S -2.769524 1.079936 2.383337
O -4.007129 0.399577 2.862957
O -2.855071 1.351870 0.916306
O -2.386403 2.247423 3.199256
Cu 0.448434 -0.949714 -1.062666
C 1.127808 2.502571 2.836221
C 0.678519 3.274989 3.926580
C 2.312393 1.851150 2.924979
C 1.440513 3.359177 5.095693
H -0.255431 3.819034 3.870068
C 3.091307 1.921056 4.086967

H	2.673971	1.254481	2.099422
C	2.654280	2.676146	5.177178
H	1.092551	3.952593	5.931239
H	4.032377	1.389479	4.140792
H	3.253327	2.733273	6.076715
N	0.167789	1.022932	1.082983
N	0.898498	2.083547	-0.662692
C	-0.589814	-2.660598	-1.486343
C	-0.167824	-3.933141	-0.895011
C	0.453571	-4.913025	-1.693189
C	-0.414869	-4.252644	0.454313
C	0.836345	-6.140410	-1.161665
C	-0.034612	-5.479969	0.985248
C	0.598891	-6.430592	0.182810
H	1.314542	-6.881850	-1.806116
H	-0.239108	-5.696824	2.037500
H	0.897577	-7.395028	0.600137
C	-1.459428	-1.738380	-0.833356
C	-2.107237	-0.709906	-1.536582
H	-2.555232	0.111991	-0.972002
H	-1.772009	-0.475349	-2.547693
H	-0.923616	-3.534357	1.099036
H	-1.730265	-1.877585	0.218501
P	-5.000596	-1.100580	-1.469168
O	-4.761898	-1.565592	0.095708
O	-5.505983	0.307194	-1.333972
O	-6.107183	-2.144643	-2.035366
O	-3.751059	-1.443525	-2.290869
Na	-5.258667	0.829247	0.874391
H	-0.579140	-2.634944	-2.584178
H	0.614462	-4.711471	-2.754916
C	-4.409257	-2.905338	0.396975
H	-3.932688	-2.916348	1.386201
H	-5.299335	-3.552346	0.424407
H	-3.702783	-3.312570	-0.343401
C	-7.462708	-1.982965	-1.647973
H	-8.043222	-2.763041	-2.152508
H	-7.589863	-2.099409	-0.559914
H	-7.850815	-0.998049	-1.944296
C	1.477175	2.270476	-1.945791
C	2.885868	2.370126	-2.094966
C	0.648485	2.441619	-3.083240
C	3.431929	2.679982	-3.348225
C	1.224787	2.740358	-4.326004
C	2.610657	2.866814	-4.462536
H	-1.730511	3.456066	-0.259448
H	-2.866958	5.502927	-1.011142
C	-1.159280	4.367760	-0.356101
C	-1.809315	5.528857	-0.782896
C	0.216266	4.386993	-0.058687
C	-1.096015	6.721660	-0.916967
H	-1.600653	7.619805	-1.248710
C	0.923368	5.595898	-0.196427
C	0.268808	6.755188	-0.623210
H	1.983613	5.642705	0.018840
H	0.821295	7.679888	-0.728762
C	2.191631	-1.293088	-2.052573
H	2.406922	-0.236473	-2.259087
C	2.074676	-2.074237	-3.338784
H	1.281543	-1.701803	-4.008609
H	3.009425	-2.041474	-3.928810
H	1.872695	-3.140650	-3.163071
B	3.120916	-1.821254	-0.962294
O	3.485374	-1.100943	0.172013
O	3.712282	-3.071538	-0.973396
C	4.319108	-3.279410	0.321314
C	4.569924	-1.813789	0.803223
C	3.291163	-4.000551	1.175788
H	2.377613	-3.394720	1.270556
H	3.003695	-4.944935	0.693106
H	3.667886	-4.230902	2.182670
C	5.569261	-4.114426	0.157061
H	6.255967	-3.681461	-0.580525
H	6.106137	-4.211912	1.112011
H	5.307950	-5.125940	-0.182299
C	5.866915	-1.232702	0.261289
H	6.749031	-1.686340	0.734297
H	5.946931	-1.375903	-0.825449
H	5.894316	-0.153054	0.460366
C	4.493385	-1.617341	2.302133
H	4.666785	-0.562592	2.554947
H	3.516445	-1.903017	2.712224
H	5.263418	-2.212721	2.813903
C	3.843664	2.095901	-0.966713
H	4.629648	1.388439	-1.306410
H	4.324998	3.043280	-0.646297
H	3.347348	1.626673	-0.098408
C	-0.850585	2.335800	-3.019323

H -1.302115 3.324087 -3.247269
H -1.203500 1.600351 -3.772332
H -1.213755 2.003821 -2.030144
C 3.225951 3.188142 -5.792988
H 3.913725 2.369643 -6.093075
H 2.454275 3.305897 -6.583287
H 3.800187 4.135615 -5.719033
H 4.507408 2.759720 -3.461142
H 0.585968 2.878789 -5.190824
123
Figure_S9_imid-2_modeA_prod(AS) / electronic energy: -4442.821144031133 a.u. / lowest freq: 10.64 cm-1
C 0.160199 2.607079 -1.362756
H 1.218031 2.783848 -1.601771
C -0.292280 3.259650 -0.038271
H -1.297959 3.696998 -0.133216
C -0.280022 0.919884 0.229788
C 0.156551 0.113947 -2.015779
C -0.950216 -0.717344 -2.234228
C 1.350726 -0.123597 -2.722322
C -0.884690 -1.762463 -3.152923
H -1.871833 -0.510853 -1.679093
C 1.402583 -1.184499 -3.629989
C 0.295741 -1.999125 -3.853218
H -1.762634 -2.388986 -3.328730
H 2.343111 -1.366516 -4.153203
H 0.358501 -2.816196 -4.574469
S 2.851794 0.864379 -2.546992
O 3.952660 -0.017869 -3.019685
O 2.987549 1.134619 -1.082186
O 2.630411 2.067428 -3.366080
Cu -0.481755 -0.986729 0.841296
C -0.694783 3.020931 -2.534995
C -0.149209 3.807504 -3.564746
C -2.049014 2.642230 -2.610280
C -0.936730 4.192918 -4.653568
H 0.882554 4.131637 -3.522998
C -2.832135 3.030364 -3.701068
H -2.496085 2.043891 -1.827516
C -2.276083 3.803024 -4.722823
H -0.508823 4.797484 -5.442756
H -3.871287 2.734244 -3.754744
H -2.884220 4.103210 -5.566298
N 0.001878 1.158867 -1.059935
N -0.360668 2.091922 0.869069
C 0.021748 -3.020089 1.061668
C -0.836336 -4.151020 0.727556
C -1.215393 -5.056225 1.736413
C -1.267947 -4.400765 -0.587711
C -1.996655 -6.168789 1.440758
C -2.042214 -5.516099 -0.882725
C -2.413420 -6.403336 0.130161
H -2.276071 -6.861662 2.237419
H -2.368834 -5.690606 -1.910839
H -3.025138 -7.277472 -0.103737
C 0.902818 -2.392235 0.135095
C 1.653118 -1.302878 0.530791
H 2.223128 -0.687079 -0.166076
H 1.853054 -1.149835 1.596224
H -0.998170 -3.704905 -1.386694
H 0.832013 -2.636843 -0.932926
P 4.776003 -2.311823 1.271023
O 4.360906 -2.407338 -0.358634
O 5.364787 -0.919343 1.322071
O 5.958041 -3.453779 1.364526
O 3.654508 -2.795111 2.135803
Na 5.027138 -0.124270 -0.774153
H 0.302103 -2.934003 2.121280
H -0.872038 -4.886287 2.760179
C 3.802275 -3.601754 -0.854057
H 3.258843 -3.374986 -1.782827
H 4.580148 -4.350369 -1.078274
H 3.100472 -4.044809 -0.128320
C 7.185478 -3.212025 0.714776
H 7.838024 -4.076934 0.888276
H 7.058465 -3.091255 -0.374886
H 7.684432 -2.310952 1.104123
C -0.740744 2.201333 2.232343
C -2.059957 2.589946 2.584407
C 0.215282 1.989608 3.257924
C -2.381061 2.817804 3.929683
C -0.140077 2.211352 4.595930
C -1.429263 2.633801 4.935637
H 2.412940 3.083267 0.496975
H 3.896714 4.837137 1.370795
C 2.004017 4.060335 0.701235
C 2.850906 5.055192 1.197184
C 0.642166 4.329225 0.473120
C 2.349731 6.329561 1.469733

H	3.006727	7.098897	1.854254
C	0.149574	5.618186	0.750809
C	1.000385	6.610878	1.245964
H	-0.894480	5.856689	0.590223
H	0.612239	7.598657	1.458323
C	-2.244069	-1.072237	1.827329
H	-2.207901	-0.028051	2.161323
C	-2.299424	-1.996115	3.016598
H	-1.443478	-1.885782	3.701252
H	-3.201975	-1.795298	3.620902
H	-2.364005	-3.054321	2.729630
B	-3.342510	-1.214172	0.757125
O	-3.583613	-0.271680	-0.227619
O	-4.238886	-2.255597	0.704972
C	-5.052097	-2.082420	-0.482403
C	-4.896496	-0.552733	-0.772879
C	-4.442917	-2.948691	-1.569798
H	-3.410885	-2.638237	-1.790181
H	-4.408662	-3.992046	-1.229846
H	-5.024881	-2.910857	-2.500774
C	-6.465187	-2.527150	-0.175494
H	-6.873919	-2.014164	0.703324
H	-7.131958	-2.335190	-1.028328
H	-6.485188	-3.606409	0.026188
C	-5.888398	0.297530	0.003938
H	-6.911730	0.178700	-0.377113
H	-5.887421	0.042092	1.072808
H	-5.614032	1.356648	-0.088925
C	-4.919316	-0.181447	-2.238838
H	-4.819177	0.905439	-2.352964
H	-4.108386	-0.656243	-2.804973
H	-5.873367	-0.474527	-2.699652
C	-3.168886	2.703721	1.571895
H	-4.071962	2.174549	1.943727
H	-3.419092	3.772732	1.409978
H	-2.905512	2.235734	0.604284
C	1.625050	1.542181	2.977445
H	2.336341	2.329938	3.303323
H	1.837589	0.610658	3.543031
H	1.806640	1.331781	1.908053
C	-1.806333	2.875689	6.367847
H	-2.641320	2.201365	6.652605
H	-0.952944	2.686921	7.053432
H	-2.131881	3.929669	6.494601
H	-3.386712	3.121383	4.198383
H	0.596724	2.057146	5.375990

123

Figure_S9_imid-2_modeB_ed(AS) / electronic energy: -4442.818766626988 a.u. / lowest freq: 15.87 cm-1

C	-2.806732	-1.062423	1.252922
H	-3.033964	-1.950462	0.647844
C	-3.483191	0.230019	0.745422
H	-3.854965	0.833885	1.588009
C	-1.143815	0.426691	0.443566
C	-0.306380	-1.583511	1.508230
C	0.613377	-1.053534	2.419964
C	-0.136405	-2.909122	1.059989
C	1.660540	-1.823701	2.913446
H	0.481344	-0.022239	2.753718
C	0.918642	-3.673451	1.564610
C	1.811342	-3.142564	2.491932
H	2.343286	-1.376027	3.635673
H	1.033019	-4.695198	1.199079
H	2.624970	-3.760396	2.880105
S	-1.161368	-3.679841	-0.203736
O	-0.363602	-4.834639	-0.711269
O	-1.310548	-2.645196	-1.274836
O	-2.426177	-4.076125	0.442568
Cu	0.674210	1.236406	0.207394
C	-3.129654	-1.357072	2.697888
C	-3.879878	-2.496369	3.038327
C	-2.688908	-0.498936	3.723716
C	-4.172515	-2.776571	4.376466
H	-4.245226	-3.165198	2.269867
C	-2.982917	-0.783806	5.059810
H	-2.113266	0.386624	3.489106
C	-3.722992	-1.922418	5.386298
H	-4.749893	-3.656093	4.630463
H	-2.636415	-0.121305	5.842385
H	-3.950282	-2.141614	6.421519
N	-1.365762	-0.737717	1.083966
N	-2.346694	0.932579	0.114373
C	2.148618	1.554165	-1.216891
C	2.021765	2.944489	-1.663134
C	2.880579	3.919564	-1.117944
C	1.062756	3.367364	-2.601618
C	2.765619	5.258711	-1.476859
C	0.944414	4.708292	-2.955100
C	1.790957	5.664283	-2.390973

H 3.441020 5.996454 -1.035889
H 0.186291 5.009801 -3.682480
H 1.695388 6.717018 -2.667080
C 1.342786 0.486781 -1.624041
C 1.747159 -0.903595 -1.308965
H 2.228723 -0.974720 -0.319777
H 0.886264 -1.590572 -1.322458
H 0.405937 2.633894 -3.071159
H 0.615890 0.602870 -2.432331
P 2.376722 -2.546836 -3.259434
O 2.245041 -3.907319 -2.390707
O 1.108378 -2.438050 -4.033320
O 3.749563 -2.626970 -4.074084
O 2.774316 -1.385661 -2.253984
Na -0.354677 -4.055973 -2.990512
H 3.061079 1.333219 -0.653802
H 3.628632 3.600650 -0.386917
C 3.226450 -4.283126 -1.427242
H 2.834827 -5.154879 -0.893319
H 4.173914 -4.549786 -1.916736
H 3.408294 -3.471104 -0.707807
C 3.845562 -3.493762 -5.204642
H 4.837622 -3.340722 -5.639168
H 3.743694 -4.546571 -4.904369
H 3.079798 -3.252413 -5.953546
C -2.461945 2.190556 -0.531462
C -2.698884 3.371505 0.217042
C -2.366121 2.272362 -1.943928
C -2.805892 4.603274 -0.445484
C -2.487492 3.516332 -2.578530
C -2.689219 4.683320 -1.835544
H -3.554552 -1.315314 -1.553387
H -5.440890 -1.640739 -3.092198
C -4.490529 -0.821109 -1.343145
C -5.561356 -1.009691 -2.221178
C -4.631935 -0.001265 -0.208160
C -6.785480 -0.384289 -1.977478
H -7.613466 -0.530736 -2.658928
C -5.872338 0.621688 0.026724
C -6.940852 0.430233 -0.854152
H -6.013881 1.262510 0.888192
H -7.889822 0.915587 -0.666147
C 1.441868 2.411402 1.718225
H 1.623449 3.311544 1.104609
C 0.533134 2.735539 2.892833
H -0.231942 3.479707 2.630576
H -0.013306 1.862553 3.291623
H 1.071836 3.158262 3.762734
B 2.785047 1.785635 2.077135
O 3.045432 1.043216 3.233534
O 3.957079 1.907517 1.320288
C 4.933537 1.005380 1.870123
C 4.478778 0.923804 3.358513
C 4.784809 -0.329184 1.150362
H 3.799125 -0.776962 1.354675
H 4.871977 -0.181227 0.063742
H 5.556102 -1.052206 1.452205
C 6.317108 1.578311 1.656174
H 6.397614 2.602449 2.041713
H 7.080322 0.960915 2.152147
H 6.555937 1.604613 0.584048
C 4.959143 2.114602 4.176217
H 6.038008 2.068636 4.380269
H 4.746066 3.062477 3.661891
H 4.433267 2.129997 5.140482
C 4.842469 -0.367550 4.059302
H 4.434171 -0.377762 5.079737
H 4.466061 -1.254044 3.534933
H 5.935045 -0.465905 4.138731
C -2.882544 3.352135 1.710205
H -2.501043 4.291212 2.164417
H -3.963076 3.261785 1.946620
H -2.334680 2.511237 2.177853
C -2.188506 1.056028 -2.813930
H -1.850332 0.171180 -2.241961
H -3.150010 0.820388 -3.315278
H -1.430992 1.251303 -3.600254
C -2.788149 6.017909 -2.514163
H -2.679806 5.925894 -3.615853
H -3.775287 6.476409 -2.294637
H -1.984868 6.686281 -2.138418
H -2.985332 5.508206 0.123991
H -2.415831 3.574025 -3.658577
123
Figure_S9_imid-2_modeB_ts(AS)_01 / electronic energy: -4442.804622855016 a.u. / lowest freq: -220.83 cm-1
C 2.993033 0.207844 1.306336
H 3.389600 1.136430 0.873487
C 3.399561 -1.068640 0.530876

H	3.698490	-1.862273	1.229230
C	1.065745	-0.750314	0.318627
C	0.631530	1.128390	1.768917
C	-0.383795	0.585367	2.564312
C	0.703297	2.525704	1.607205
C	-1.305030	1.404527	3.206709
H	-0.432605	-0.498808	2.689445
C	-0.228699	3.337061	2.258181
C	-1.226568	2.786979	3.058638
H	-2.071552	0.941720	3.828364
H	-0.166762	4.415616	2.104759
H	-1.943277	3.440309	3.561255
S	1.886121	3.350023	0.527638
O	1.317603	4.705845	0.285364
O	1.886266	2.552614	-0.738254
O	3.176637	3.359124	1.240332
Cu	-0.893756	-1.013910	-0.099504
C	3.370931	0.141227	2.766412
C	4.339072	1.016190	3.289591
C	2.768743	-0.800788	3.622801
C	4.686584	0.958964	4.642625
H	4.831984	1.737932	2.651446
C	3.118683	-0.853401	4.974658
H	2.025656	-1.490715	3.244307
C	4.075673	0.026774	5.484762
H	5.432110	1.636698	5.037986
H	2.647790	-1.577458	5.626873
H	4.346249	-0.015565	6.531843
N	1.515934	0.212077	1.139843
N	2.128323	-1.441590	-0.125717
C	-2.503378	-0.692148	-1.342666
C	-2.819939	-1.866031	-2.156856
C	-3.930689	-2.663375	-1.817764
C	-2.041080	-2.257888	-3.262211
C	-4.239206	-3.807407	-2.547502
C	-2.346471	-3.405616	-3.985645
C	-3.446424	-4.189356	-3.631141
H	-5.105781	-4.410752	-2.265880
H	-1.721365	-3.689901	-4.835585
H	-3.685132	-5.091385	-4.199349
C	-1.507605	0.263551	-1.672386
C	-1.291817	1.407100	-0.885413
H	-1.780367	1.482496	0.090633
H	-0.345852	1.943527	-0.986727
H	-1.185640	-1.654265	-3.566603
H	-0.931120	0.173920	-2.596325
P	-1.697051	3.792334	-2.540610
O	-1.174756	5.137243	-1.744660
O	-0.474919	3.340925	-3.289849
O	-2.894819	4.339863	-3.491165
O	-2.422963	2.865413	-1.555730
Na	1.253656	4.448579	-2.130237
H	-3.274481	-0.402267	-0.620950
H	-4.537307	-2.372783	-0.956816
C	-1.959942	5.704122	-0.710685
H	-1.354898	6.471116	-0.213425
H	-2.872264	6.171146	-1.114392
H	-2.250636	4.942754	0.027710
C	-2.584444	5.296296	-4.491070
H	-3.478785	5.432529	-5.109005
H	-2.310858	6.266417	-4.047257
H	-1.758025	4.955091	-5.131899
C	1.962680	-2.550001	-0.998350
C	2.031347	-3.879493	-0.506850
C	1.650639	-2.332481	-2.364997
C	1.713122	-4.949804	-1.357449
C	1.352118	-3.423442	-3.193453
C	1.357069	-4.727263	-2.690169
H	3.595624	0.791921	-1.500881
H	5.441194	1.098327	-3.096327
C	4.458049	0.146936	-1.434213
C	5.504229	0.322792	-2.344009
C	4.524369	-0.859257	-0.453956
C	6.628873	-0.502487	-2.285672
H	7.437898	-0.365861	-2.991506
C	5.664166	-1.683776	-0.404808
C	6.708714	-1.504815	-1.316701
H	5.745628	-2.469433	0.335957
H	7.580395	-2.144862	-1.272404
C	-1.828260	-2.459829	1.005806
H	-2.241710	-3.070174	0.185175
C	-0.888653	-3.274610	1.869359
H	-0.258367	-3.945637	1.270461
H	-0.214290	-2.659065	2.488526
H	-1.425823	-3.926463	2.583877
B	-2.985879	-1.773522	1.747041
O	-2.969278	-1.402351	3.087280
O	-4.229326	-1.512190	1.182867

C -5.003060 -0.754405 2.137784
C -4.346711 -1.188713 3.484436
C -4.787247 0.719316 1.829744
H -3.732551 1.004857 1.963668
H -5.061262 0.922817 0.785135
H -5.401322 1.369083 2.468913
C -6.463063 -1.124864 1.998194
H -6.615195 -2.209427 2.057640
H -7.065450 -0.647414 2.784580
H -6.851975 -0.783683 1.029007
C -4.874274 -2.525675 3.983758
H -5.902886 -2.446760 4.361331
H -4.857198 -3.285404 3.189484
H -4.239687 -2.884721 4.805202
C -4.422691 -0.155932 4.586839
H -3.858898 -0.494196 5.466965
H -4.027493 0.820694 4.282936
H -5.466603 -0.006188 4.898321
C 2.463571 -4.190860 0.901997
H 2.143910 -5.209875 1.207619
H 3.570353 -4.147842 0.965439
H 2.022692 -3.474534 1.623181
C 1.718893 -0.964593 -2.991904
H 1.470878 -0.161847 -2.271560
H 2.740491 -0.798686 -3.389215
H 1.011431 -0.880052 -3.842176
C 1.004782 -5.890561 -3.570248
H 0.746142 -5.561862 -4.599388
H 1.866189 -6.588653 -3.629469
H 0.130557 -6.427068 -3.144908
H 1.748573 -5.966911 -0.984175
H 1.115587 -3.254557 -4.237658
123
Figure_S9_imid-2_modeB_ts(AS)_02 / electronic energy: -4442.807730103428 a.u. / lowest freq: -251.09 cm-1
C 1.684569 2.748898 -0.547531
H 2.633190 2.691893 0.002076
C 0.502325 3.245922 0.311195
H -0.071910 4.027078 -0.210037
C 0.093332 1.001876 -0.320140
C 1.957417 0.505059 -1.780293
C 1.229223 -0.003754 -2.863343
C 3.297595 0.102850 -1.607362
C 1.792049 -0.920226 -3.746886
H 0.202688 0.343212 -3.000004
C 3.855540 -0.804403 -2.511739
C 3.113762 -1.322398 -3.570563
H 1.199794 -1.304773 -4.580222
H 4.888035 -1.118737 -2.350585
H 3.571624 -2.037315 -4.257130
S 4.335642 0.620652 -0.227121
O 5.482535 -0.329149 -0.211404
O 3.480517 0.432440 0.985091
O 4.722581 2.017600 -0.493287
Cu -0.791982 -0.762275 -0.688675
C 1.881997 3.584901 -1.789525
C 3.017140 4.404448 -1.919129
C 0.925583 3.576644 -2.823244
C 3.200356 5.183096 -3.065850
H 3.756224 4.451190 -1.129988
C 1.113630 4.355966 -3.967843
H 0.037847 2.963077 -2.746120
C 2.251062 5.157051 -4.090230
H 4.077539 5.810307 -3.158505
H 0.376275 4.339309 -4.759967
H 2.394769 5.760918 -4.976852
N 1.259610 1.366199 -0.892974
N -0.328436 2.027181 0.428202
C -0.920248 -2.794211 -0.609261
C -2.158263 -3.478534 -0.236820
C -2.766716 -4.354726 -1.153593
C -2.729588 -3.362636 1.043682
C -3.886697 -5.101443 -0.801441
C -3.848662 -4.110024 1.396113
C -4.430546 -4.987352 0.478301
H -4.333675 -5.783722 -1.528489
H -4.274488 -4.004465 2.397383
H -5.307121 -5.575824 0.759466
C 0.057117 -2.352304 0.329335
C 1.386592 -2.119028 -0.062798
H 1.613102 -2.114914 -1.130720
H 2.042751 -1.507137 0.561056
H -2.292801 -2.676994 1.775455
H -0.170911 -2.339840 1.400001
P 3.400122 -3.775505 1.273369
O 4.866052 -3.402046 0.622661
O 3.296074 -2.841892 2.446352
O 3.534986 -5.341237 1.677653
O 2.339920 -3.786829 0.162423

Na	4.922696	-1.255816	1.974773
H	-0.542600	-3.047849	-1.610811
H	-2.330253	-4.466378	-2.150173
C	5.269618	-3.977569	-0.608013
H	6.125811	-3.403797	-0.981327
H	5.572226	-5.027829	-0.474166
H	4.458879	-3.937605	-1.350272
C	4.466387	-5.705158	2.684213
H	4.368673	-6.783680	2.849563
H	5.500483	-5.488354	2.373448
H	4.263583	-5.178827	3.628373
C	-1.543054	2.007402	1.162392
C	-2.630127	2.822621	0.758242
C	-1.618876	1.318520	2.400790
C	-3.707781	3.027142	1.630035
C	-2.723053	1.521911	3.240756
C	-3.754414	2.392019	2.873225
H	1.905761	1.974215	2.311725
H	2.535732	2.861533	4.519100
C	1.630011	2.984957	2.570196
C	1.988034	3.485481	3.824785
C	0.915414	3.783726	1.659916
C	1.638063	4.788655	4.184282
H	1.915368	5.175013	5.156492
C	0.568687	5.095403	2.033206
C	0.929430	5.592957	3.288991
H	0.015321	5.733918	1.355912
H	0.657518	6.602547	3.568699
C	-2.251442	-0.366358	-2.048252
H	-2.002276	0.689278	-2.254493
C	-2.114700	-1.232834	-3.284873
H	-2.769242	-0.893680	-4.109717
H	-1.095241	-1.271233	-3.703390
H	-2.409233	-2.273768	-3.080967
B	-3.630306	-0.461427	-1.376457
O	-4.531419	-1.473583	-1.663872
O	-4.177549	0.469427	-0.510669
C	-5.480655	-0.006892	-0.102353
C	-5.831671	-1.027809	-1.235217
C	-5.327292	-0.673121	1.253358
H	-4.656660	-1.540120	1.196027
H	-4.900659	0.036554	1.971303
H	-6.293301	-1.010140	1.654534
C	-6.437965	1.162748	-0.013936
H	-6.422194	1.774971	-0.923483
H	-7.467223	0.809867	0.146237
H	-6.181194	1.812622	0.831241
C	-6.486071	-0.361123	-2.437447
H	-7.514304	-0.038269	-2.223706
H	-5.911914	0.516030	-2.768596
H	-6.521879	-1.073161	-3.272882
C	-6.647320	-2.218662	-0.781865
H	-6.839849	-2.890744	-1.629891
H	-6.124945	-2.799011	-0.011792
H	-7.620355	-1.900451	-0.379624
C	-2.695376	3.463236	-0.602355
H	-3.681778	3.253975	-1.068020
H	-2.570585	4.561883	-0.504675
H	-1.924695	3.064612	-1.290512
C	-0.541135	0.386452	2.889018
H	0.272852	0.234464	2.157322
H	-0.097589	0.789720	3.823570
H	-0.985167	-0.607624	3.106176
C	-4.922479	2.627088	3.785683
H	-4.822064	2.056960	4.733649
H	-4.991376	3.707584	4.031678
H	-5.860195	2.308878	3.284140
H	-4.524089	3.675322	1.331960
H	-2.769636	1.008286	4.194222

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Figure_S9_imid-2_modeB_ts(AS)_03 / electronic energy: -4442.809989169532 a.u. / lowest freq: -267.59 cm-1

C	-2.590260	-2.028577	-0.469909
H	-3.487016	-1.576242	-0.027067
C	-1.671974	-2.721256	0.558643
H	-1.381694	-3.730040	0.225987
C	-0.509834	-0.885565	-0.382951
C	-2.074414	-0.068512	-2.049828
C	-1.192197	-0.009074	-3.136639
C	-3.224319	0.747467	-2.059818
C	-1.418090	0.851871	-4.206437
H	-0.321282	-0.667756	-3.128891
C	-3.450615	1.589120	-3.151673
C	-2.557732	1.651934	-4.217541
H	-0.711230	0.879640	-5.038697
H	-4.337696	2.223380	-3.132882
H	-2.754302	2.326792	-5.052885
S	-4.411004	0.861604	-0.704167
O	-5.212985	2.087202	-0.991992

O	-3.596002	1.048411	0.532578
O	-5.208986	-0.377546	-0.734229
Cu	0.909805	0.425002	-0.939455
C	-3.012010	-2.959012	-1.582425
C	-4.346018	-3.394448	-1.672293
C	-2.078478	-3.423496	-2.528921
C	-4.740307	-4.260393	-2.696696
H	-5.080536	-3.073997	-0.944781
C	-2.477588	-4.288155	-3.551631
H	-1.044466	-3.110345	-2.481181
C	-3.807760	-4.705017	-3.636747
H	-5.769348	-4.589887	-2.759441
H	-1.754651	-4.635416	-4.278404
H	-4.115128	-5.375480	-4.428836
N	-1.719889	-0.935292	-0.981284
N	-0.479394	-1.845871	0.547786
C	1.590802	2.361172	-1.078181
C	2.986651	2.726083	-0.840180
C	3.752892	3.257359	-1.893435
C	3.585228	2.638407	0.430658
C	5.057627	3.694051	-1.685957
C	4.887241	3.078913	0.638968
C	5.630653	3.612149	-0.416678
H	5.628816	4.110152	-2.519269
H	5.330845	3.000290	1.635233
H	6.653876	3.957030	-0.249925
C	0.600537	2.268167	-0.063686
C	-0.773684	2.280009	-0.364161
H	-1.061202	2.323924	-1.416719
H	-1.507137	1.819843	0.297507
H	3.021751	2.219738	1.269241
H	0.890219	2.262700	0.991478
P	-1.831419	4.433517	1.405239
O	-1.063901	5.817086	1.794296
O	-3.270107	4.595404	1.804774
O	-1.076045	3.308093	2.324385
O	-1.463439	4.063205	-0.040914
Na	-4.855802	3.272970	0.966824
H	1.228006	2.584208	-2.092775
H	3.300685	3.347390	-2.885189
C	0.326702	5.907684	1.533540
H	0.625146	6.953440	1.669657
H	0.907379	5.279993	2.229006
H	0.563391	5.597839	0.503741
C	-1.331258	3.299046	3.716686
H	-0.627135	2.599324	4.181179
H	-1.180932	4.294694	4.163434
H	-2.357013	2.968252	3.937153
C	0.658951	-2.119886	1.350082
C	1.430407	-3.285068	1.112781
C	0.920445	-1.342098	2.507349
C	2.363603	-3.708200	2.068632
C	1.875172	-1.779163	3.436312
C	2.580879	-2.969515	3.234311
H	-2.669733	-0.715288	2.164178
H	-3.620851	-0.916970	4.424211
C	-2.735974	-1.690856	2.621073
C	-3.275629	-1.801751	3.905152
C	-2.279606	-2.831725	1.936569
C	-3.367563	-3.052111	4.519901
H	-3.785190	-3.136739	5.514779
C	-2.378018	-4.086197	2.566165
C	-2.919648	-4.193268	3.850697
H	-2.031391	-4.982665	2.067366
H	-2.990109	-5.161919	4.328374
C	2.197403	-0.569532	-2.150236
H	1.648560	-1.522835	-2.244686
C	2.379638	0.119377	-3.487911
H	2.953682	-0.497262	-4.205132
H	1.436212	0.377272	-3.996896
H	2.945764	1.057728	-3.383388
B	3.502307	-0.786727	-1.372222
O	4.683206	-0.129345	-1.678358
O	3.690445	-1.713098	-0.358701
C	5.046845	-1.580780	0.121276
C	5.758075	-0.883741	-1.084229
C	5.018389	-0.703669	1.361323
H	4.645322	0.302438	1.127215
H	4.354634	-1.143266	2.114556
H	6.014910	-0.604089	1.814005
C	5.597649	-2.951631	0.452010
H	5.457658	-3.658245	-0.374678
H	6.672138	-2.895286	0.679551
H	5.099217	-3.368984	1.335151
C	6.230822	-1.878213	-2.135811
H	7.092595	-2.467490	-1.792663
H	5.427661	-2.574766	-2.415588
H	6.532252	-1.334015	-3.041082

C	6.881263	0.053298	-0.700366
H	7.308764	0.519426	-1.599070
H	6.532052	0.858619	-0.043734
H	7.688854	-0.489652	-0.187912
C	1.303871	-4.091323	-0.151599
H	2.310933	-4.269441	-0.584500
H	0.831946	-5.070128	0.075099
H	0.708698	-3.567494	-0.923962
C	0.189009	-0.063503	2.816041
H	-0.500975	0.246897	2.011096
H	-0.396396	-0.186211	3.751305
H	0.924270	0.755225	2.962663
C	3.584303	-3.447421	4.242779
H	3.646642	-2.761522	5.114238
H	3.293463	-4.454360	4.609162
H	4.588363	-3.508287	3.773722
H	2.932353	-4.615480	1.899049
H	2.058652	-1.192067	4.328920

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Figure_S9_imid-2_modeB_ts(AS)_04 / electronic energy: -4442.805082698800 a.u. / lowest freq: -234.02 cm-1

C	-0.052561	-2.741591	0.279920
H	-1.069708	-2.935019	0.637952
C	0.971310	-2.498741	1.409343
H	1.918796	-3.017745	1.197011
C	0.615104	-0.466451	0.262560
C	-0.796414	-1.069861	-1.585130
C	-0.118538	-0.241874	-2.494968
C	-2.125833	-1.441576	-1.877761
C	-0.728829	0.237108	-3.647305
H	0.922577	0.017430	-2.295359
C	-2.719412	-0.970289	-3.053645
C	-2.041328	-0.131624	-3.933641
H	-0.160517	0.882802	-4.321423
H	-3.752016	-1.260417	-3.253676
H	-2.538045	0.225691	-4.838008
S	-3.176962	-2.426848	-0.794106
O	-4.563865	-2.251337	-1.307419
O	-3.038072	-1.785134	0.552972
O	-2.681265	-3.811264	-0.866760
Cu	0.551828	1.484573	-0.235646
C	0.356238	-3.906130	-0.592405
C	0.152843	-5.211355	-0.108792
C	0.974705	-3.737574	-1.845623
C	0.537869	-6.319506	-0.868573
H	-0.306424	-5.369262	0.859509
C	1.358870	-4.848045	-2.602353
H	1.172316	-2.756880	-2.241703
C	1.138577	-6.138066	-2.115831
H	0.372529	-7.319327	-0.488576
H	1.832563	-4.707194	-3.565408
H	1.437833	-6.996647	-2.702911
N	-0.071289	-1.418987	-0.411726
N	1.178944	-1.041381	1.329904
C	-0.483991	3.251794	-0.396650
C	0.130419	4.426975	0.212543
C	0.802097	5.356800	-0.604073
C	0.101412	4.670868	1.598900
C	1.442110	6.464225	-0.057956
C	0.737873	5.780898	2.144294
C	1.419904	6.678664	1.321135
H	1.959366	7.168941	-0.713407
H	0.701238	5.946857	3.223552
H	1.922529	7.547473	1.752298
C	-1.316050	2.319234	0.281125
C	-2.184386	1.462961	-0.414201
H	-2.072259	1.371639	-1.495659
H	-2.610520	0.596227	0.097711
H	-0.434070	3.988207	2.261466
H	-1.424122	2.370185	1.368448
P	-5.067033	1.839119	0.082638
O	-5.847667	0.768767	-0.901256
O	-4.914494	1.072881	1.365408
O	-6.085900	3.100076	0.178197
O	-3.857871	2.423819	-0.659728
Na	-5.375490	-1.117195	0.675214
H	-0.603087	3.304867	-1.487825
H	0.815068	5.199768	-1.686336
C	-6.048169	1.076083	-2.269583
H	-6.399301	0.165936	-2.769717
H	-6.805330	1.866231	-2.393095
H	-5.112801	1.409194	-2.743385
C	-7.331301	2.918474	0.832183
H	-7.815031	3.899075	0.901281
H	-7.988647	2.240831	0.264977
H	-7.197306	2.514322	1.846247
C	2.107778	-0.350507	2.150932
C	3.500294	-0.587101	2.017909
C	1.648949	0.529250	3.163481

C 4.396623 0.017580 2.910960
C 2.570370 1.131712 4.031711
C 3.940250 0.877196 3.913112
H -1.337401 -1.751091 2.726299
H -2.083936 -2.435796 4.968444
C -0.724636 -2.432805 3.299268
C -1.153183 -2.820079 4.571751
C 0.484776 -2.924063 2.773228
C -0.382031 -3.701594 5.332188
H -0.715118 -4.000305 6.317678
C 1.252220 -3.812405 3.548529
C 0.819032 -4.197823 4.820603
H 2.188899 -4.204901 3.172633
H 1.416376 -4.880569 5.410926
C 2.325468 2.344217 -0.803242
H 1.952753 3.192220 -1.400062
C 3.019384 2.826062 0.453263
H 3.820140 3.557765 0.235998
H 2.350596 3.327044 1.173954
H 3.515085 2.005153 0.990325
B 3.158902 1.440831 -1.721835
O 4.356498 0.848239 -1.360892
O 2.858896 1.194892 -3.054992
C 3.833767 0.253835 -3.563027
C 5.030127 0.458665 -2.578131
C 3.233626 -1.135636 -3.449802
H 3.040530 -1.386608 -2.396975
H 2.281654 -1.177266 -3.996391
H 3.895475 -1.905629 -3.869038
C 4.134477 0.590221 -5.007042
H 4.430634 1.639101 -5.129270
H 4.942914 -0.044599 -5.397710
H 3.246170 0.417681 -5.630323
C 5.924833 1.620669 -2.982395
H 6.528109 1.385387 -3.870036
H 5.336280 2.523959 -3.196699
H 6.612898 1.855620 -2.159364
C 5.860123 -0.780792 -2.325398
H 6.661791 -0.560376 -1.607648
H 5.262535 -1.604775 -1.917828
H 6.332315 -1.129356 -3.255360
C 4.070004 -1.450751 0.925488
H 5.016120 -1.011091 0.546894
H 4.289614 -2.461760 1.327084
H 3.379361 -1.532966 0.061928
C 0.190958 0.832189 3.376918
H -0.456312 0.422082 2.580039
H -0.135668 0.409671 4.350154
H 0.040644 1.930434 3.399715
C 4.925243 1.522564 4.843053
H 4.420047 2.178468 5.583637
H 5.487050 0.738813 5.393533
H 5.640498 2.138914 4.258635
H 5.460350 -0.169374 2.815745
H 2.214217 1.799142 4.808108

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Figure_S9_imid-2_modeB_ts(AS)_05 / electronic energy: -4442.808593485546 a.u. / lowest freq: -188.35 cm-1

C -0.708499 -2.612285 0.661535
H -1.802386 -2.673346 0.637141
C -0.139689 -2.103872 2.005712
H 0.663328 -2.758986 2.378708
C 0.348873 -0.513851 0.324418
C -0.488629 -1.523418 -1.694197
C 0.592751 -1.055258 -2.458038
C -1.676609 -1.883607 -2.364341
C 0.511388 -0.915231 -3.837799
H 1.528713 -0.809538 -1.953869
C -1.734948 -1.760549 -3.756600
C -0.661123 -1.275660 -4.496964
H 1.380371 -0.540234 -4.383993
H -2.669226 -2.030914 -4.250227
H -0.744721 -1.183655 -5.581486
S -3.196122 -2.422222 -1.556038
O -4.253544 -2.330247 -2.605009
O -3.447550 -1.421112 -0.472865
O -2.954832 -3.794640 -1.079342
Cu 0.788169 1.221856 -0.603604
C -0.156791 -3.971770 0.302545
C -0.791258 -5.121112 0.805945
C 1.014157 -4.123278 -0.462829
C -0.286444 -6.393019 0.519986
H -1.678279 -5.030716 1.420921
C 1.516709 -5.395935 -0.746366
H 1.545081 -3.262591 -0.834363
C 0.864888 -6.530571 -0.258621
H -0.785829 -7.272113 0.906236
H 2.415749 -5.501448 -1.339901
H 1.256032 -7.515682 -0.477544

N	-0.296607	-1.534206	-0.285036
N	0.428108	-0.795088	1.629875
C	0.033281	2.972543	-1.416525
C	0.581970	4.221616	-0.895421
C	1.596276	4.897203	-1.600389
C	0.138427	4.784126	0.316987
C	2.164187	6.064714	-1.099114
C	0.702219	5.953562	0.814800
C	1.726134	6.595133	0.115500
H	2.953188	6.568044	-1.662894
H	0.337986	6.369917	1.757009
H	2.172018	7.511237	0.509505
C	-1.018759	2.250225	-0.797237
C	-1.738604	1.234085	-1.438027
H	-1.466992	0.960633	-2.460633
H	-2.261009	0.471650	-0.858314
H	-0.672571	4.309700	0.872868
H	-1.353391	2.530521	0.204629
P	-4.557510	2.182090	-0.968830
O	-5.041484	3.739734	-0.968798
O	-5.799521	1.337202	-0.993893
O	-3.759412	2.039437	0.456130
O	-3.474071	2.001052	-2.040815
Na	-5.709939	-0.802367	-1.593444
H	0.214090	2.781308	-2.483454
H	1.938260	4.493220	-2.557495
C	-4.050167	4.745723	-0.860058
H	-4.484556	5.689578	-1.209782
H	-3.723779	4.873775	0.184643
H	-3.167402	4.511680	-1.476458
C	-4.508218	1.962894	1.653004
H	-3.798131	1.944584	2.488406
H	-5.171328	2.834075	1.776815
H	-5.121484	1.050178	1.688544
C	1.291607	-0.072722	2.492009
C	2.605328	-0.542801	2.747532
C	0.825758	1.083391	3.165168
C	3.406610	0.114696	3.691570
C	1.654157	1.728269	4.094455
C	2.939871	1.247475	4.363751
H	-2.515711	-0.702188	1.929039
H	-4.188961	-0.468705	3.719658
C	-2.347060	-1.196826	2.875736
C	-3.298903	-1.060091	3.889644
C	-1.184313	-1.962154	3.086291
C	-3.102654	-1.684726	5.122928
H	-3.840283	-1.576969	5.907559
C	-0.999495	-2.588688	4.332322
C	-1.954523	-2.448702	5.343700
H	-0.114456	-3.181948	4.525686
H	-1.803299	-2.932098	6.300206
C	2.736846	1.818273	-0.742624
H	2.649519	2.528104	-1.582187
C	3.095221	2.539587	0.539715
H	4.022498	3.135173	0.443498
H	2.322837	3.248221	0.885806
H	3.283707	1.840004	1.366620
B	3.690612	0.698563	-1.181794
O	4.728124	0.196642	-0.415210
O	3.686294	0.134518	-2.451269
C	4.690943	-0.906795	-2.479220
C	5.639382	-0.474150	-1.314537
C	3.999871	-2.226521	-2.186629
H	3.572945	-2.219737	-1.174478
H	3.186754	-2.395714	-2.905283
H	4.692750	-3.076162	-2.257175
C	5.334045	-0.931075	-3.848368
H	5.714400	0.055813	-4.138808
H	6.169571	-1.645537	-3.877517
H	4.602335	-1.244877	-4.605710
C	6.666070	0.558756	-1.754791
H	7.439717	0.120657	-2.400326
H	6.192129	1.387098	-2.300439
H	7.162677	0.980765	-0.870816
C	6.320054	-1.614462	-0.589679
H	6.940043	-1.224491	0.228777
H	5.604036	-2.323612	-0.158375
H	6.980504	-2.169432	-1.271589
C	3.196735	-1.725469	2.027700
H	4.214944	-1.472349	1.669317
H	3.269951	-2.586032	2.724795
H	2.603580	-2.025304	1.142519
C	-0.547089	1.652895	2.938631
H	-1.075941	1.163804	2.101129
H	-1.154892	1.534669	3.860027
H	-0.466638	2.733108	2.700005
C	3.827062	1.939992	5.356046
H	3.325671	2.822432	5.807500

H 4.097562 1.234970 6.170077
H 4.754123 2.283543 4.850509
H 4.407867 -0.249051 3.893500
H 1.291517 2.609538 4.611070
123
Figure_S9_imid-2_modeB_prod(AS) / electronic energy: -4442.815393661368 a.u. / lowest freq: 16.03 cm-1
C -3.016431 -1.141563 0.783650
H -3.162187 -2.001878 0.119318
C -3.726522 0.143352 0.303870
H -4.324420 0.594548 1.109366
C -1.388333 0.485963 0.235193
C -0.506375 -1.545302 1.214579
C 0.379128 -0.906650 2.093461
C -0.299949 -2.904134 0.905019
C 1.441670 -1.590407 2.670367
H 0.203961 0.139207 2.356387
C 0.767479 -3.579524 1.504114
C 1.633138 -2.938280 2.383928
H 2.095298 -1.054186 3.358255
H 0.917030 -4.628166 1.243503
H 2.458173 -3.492078 2.837556
S -1.278835 -3.842608 -0.288352
O -0.422337 -5.014859 -0.634552
O -1.435362 -2.929298 -1.455608
O -2.537889 -4.211425 0.382414
Cu 0.472476 1.122661 -0.224173
C -3.432486 -1.537750 2.180995
C -4.366571 -2.572892 2.363382
C -2.941384 -0.857652 3.312097
C -4.776608 -2.939226 3.648633
H -4.784682 -3.092200 1.510314
C -3.353311 -1.228045 4.595154
H -2.233945 -0.047655 3.206037
C -4.268025 -2.269700 4.763780
H -5.492764 -3.740089 3.779601
H -2.963952 -0.705565 5.459353
H -4.586835 -2.554467 5.758091
N -1.579287 -0.756518 0.711052
N -2.587063 1.026275 -0.029850
C 2.216149 1.250888 -1.422709
C 2.807984 2.524496 -1.820434
C 4.183942 2.746446 -1.639859
C 2.039492 3.540816 -2.419512
C 4.774463 3.932854 -2.063716
C 2.628451 4.729360 -2.835435
C 4.000495 4.928129 -2.662126
H 5.847648 4.083592 -1.924648
H 2.014468 5.509453 -3.291217
H 4.463816 5.862174 -2.988290
C 1.172955 0.637003 -2.172139
C 0.561273 -0.507842 -1.707265
H 1.064571 -1.097643 -0.932411
H -0.307476 -0.963147 -2.182492
H 0.959935 3.405164 -2.535835
H 0.755177 1.168382 -3.034293
P 3.074807 -2.733829 -1.965473
O 2.857174 -4.278515 -1.376402
O 1.948906 -2.635858 -2.976130
O 4.525458 -2.862118 -2.731154
O 3.280478 -1.757477 -0.845068
Na 0.537302 -4.351886 -2.618505
H 2.834057 0.570834 -0.817902
H 4.784124 1.968453 -1.165029
C 3.720526 -4.746380 -0.363836
H 3.237754 -5.592763 0.142515
H 4.681891 -5.090560 -0.780508
H 3.926733 -3.958878 0.377753
C 4.623507 -3.693289 -3.865884
H 5.652987 -3.635058 -4.241295
H 4.404483 -4.747046 -3.622965
H 3.938710 -3.375694 -4.667618
C -2.768543 2.395888 -0.365062
C -3.246583 3.316875 0.606086
C -2.589166 2.837925 -1.701332
C -3.540239 4.635388 0.231300
C -2.880965 4.166478 -2.042226
C -3.356261 5.065913 -1.083920
H -3.115395 -1.003651 -2.130026
H -4.596285 -1.306552 -4.071827
C -4.141865 -0.671858 -2.065737
C -4.979526 -0.845763 -3.170641
C -4.626769 -0.071242 -0.889074
C -6.309500 -0.424089 -3.114075
H -6.956900 -0.558586 -3.970900
C -5.969237 0.348001 -0.844022
C -6.803897 0.171549 -1.951636
H -6.371306 0.817241 0.045206
H -7.834651 0.498937 -1.909023

C 1.134883 2.561222 1.037148
H 1.429844 3.325623 0.298704
C 0.055683 3.081411 1.956733
H -0.721397 3.637972 1.418153
H -0.436744 2.292946 2.547372
H 0.469188 3.788265 2.699212
B 2.401832 2.037341 1.754742
O 2.413964 1.539745 3.047233
O 3.671062 2.126302 1.230270
C 4.578792 1.480623 2.154458
C 3.793633 1.598644 3.499609
C 4.744219 0.044027 1.692431
H 3.791171 -0.503179 1.723489
H 5.088615 0.022897 0.649916
H 5.479716 -0.499471 2.302155
C 5.901719 2.214712 2.132483
H 5.774317 3.291817 2.295960
H 6.579034 1.824884 2.906081
H 6.397348 2.079672 1.161193
C 3.975894 2.954599 4.164209
H 4.982880 3.070395 4.587472
H 3.806677 3.775344 3.452515
H 3.250913 3.063060 4.982084
C 4.064302 0.489247 4.490081
H 3.412972 0.594047 5.368393
H 3.904498 -0.507364 4.062124
H 5.105684 0.534747 4.839812
C -3.426404 2.952362 2.056278
H -2.977476 3.736450 2.702415
H -4.508708 2.874056 2.289749
H -2.925239 2.001894 2.314345
C -2.139315 1.925781 -2.807601
H -1.815078 0.938292 -2.438555
H -2.972077 1.778276 -3.526821
H -1.284709 2.385947 -3.345125
C -3.671571 6.486307 -1.451567
H -3.477331 6.683704 -2.527299
H -4.741867 6.696493 -1.243583
H -3.042974 7.175519 -0.849193
H -3.905582 5.336696 0.973274
H -2.746543 4.496640 -3.066050
123
Figure_S9_imid-2_modeC_ed(AS) / electronic energy: -4442.825163621003 a.u. / lowest freq: 15.84 cm-1
C 3.205488 -0.863902 -0.708812
H 3.538004 -1.382355 0.201595
C 3.460976 0.655765 -0.683453
H 3.741867 1.025940 -1.683323
C 1.135151 0.275973 -0.522131
C 0.975498 -2.107865 -0.911247
C 0.126417 -2.195246 -2.019257
C 1.055434 -3.190970 -0.017261
C -0.592723 -3.357930 -2.274502
H 0.046734 -1.336214 -2.689080
C 0.332037 -4.355475 -0.285231
C -0.475791 -4.449294 -1.415978
H -1.238563 -3.398408 -3.153239
H 0.394559 -5.179625 0.427687
H -1.028537 -5.370642 -1.613214
S 1.982638 -3.130759 1.523431
O 1.303678 -4.113099 2.420296
O 1.798872 -1.743630 2.051197
O 3.378435 -3.478855 1.199273
Cu -0.845114 0.520651 -0.624829
C 3.810783 -1.539346 -1.914951
C 4.848350 -2.474617 -1.755374
C 3.348055 -1.248065 -3.212643
C 5.405728 -3.109304 -2.869469
H 5.231246 -2.710252 -0.770796
C 3.907606 -1.886063 -4.322965
H 2.549447 -0.533444 -3.363703
C 4.935200 -2.816396 -4.151728
H 6.204067 -3.828271 -2.738404
H 3.543494 -1.659515 -5.316690
H 5.367742 -3.309462 -5.012650
N 1.721851 -0.912791 -0.749162
N 2.119793 1.175046 -0.340951
C -2.596906 0.652345 0.433588
C -2.949018 2.070598 0.535688
C -4.206064 2.523942 0.097250
C -2.052075 3.023505 1.049932
C -4.546551 3.871691 0.172408
C -2.386087 4.371631 1.116903
C -3.638727 4.805032 0.677363
H -5.529853 4.200300 -0.174136
H -1.662751 5.090976 1.509408
H -3.904184 5.863662 0.725813
C -1.598948 0.017311 1.200461
C -1.605802 -1.458985 1.359072

H -1.948771 -1.972916 0.449437
H -0.612379 -1.847514 1.621701
H -1.068029 2.692193 1.382876
H -1.071539 0.579633 1.981658
P -2.369892 -1.395823 3.887198
O -3.287496 -2.400856 4.722771
O -0.982343 -1.330944 4.429040
O -3.142931 0.015168 3.886349
O -2.547339 -1.922844 2.394414
Na 0.930918 -2.480294 4.202086
H -3.354710 0.028901 -0.055161
H -4.907698 1.801843 -0.325988
C -4.645062 -2.643655 4.356645
H -5.089138 -3.248006 5.153429
H -5.203815 -1.702348 4.263077
H -4.697618 -3.194920 3.408564
C -2.685598 1.115199 4.666817
H -3.343281 1.960280 4.438612
H -2.738984 0.897178 5.742410
H -1.652218 1.382906 4.406037
C 1.845614 2.559744 -0.215335
C 1.853634 3.406503 -1.353037
C 1.637135 3.122235 1.068645
C 1.677360 4.787884 -1.189223
C 1.460007 4.506292 1.200567
C 1.475785 5.340814 0.078400
H 3.657529 0.109841 2.025040
H 5.390169 0.867406 3.592628
C 4.464071 0.723979 1.654596
C 5.447460 1.152918 2.550226
C 4.524219 1.090544 0.297199
C 6.502199 1.950846 2.103056
H 7.262358 2.282952 2.798214
C 5.593780 1.894171 -0.140662
C 6.575463 2.320599 0.758650
H 5.667442 2.198058 -1.177465
H 7.392725 2.940200 0.412758
C -1.338515 1.185999 -2.504997
H -0.448686 0.906622 -3.092758
C -1.563703 2.686839 -2.465672
H -0.850826 3.242095 -1.830638
H -1.504233 3.160482 -3.464171
H -2.560240 2.932565 -2.068032
B -2.554844 0.322506 -2.796174
O -2.535567 -0.982851 -3.299939
O -3.872896 0.727427 -2.568011
C -4.747133 -0.229459 -3.185607
C -3.867387 -1.521708 -3.203738
C -6.019839 -0.340594 -2.371153
H -5.815668 -0.561334 -1.315378
H -6.578689 0.604873 -2.411610
H -6.676187 -1.130368 -2.765843
C -5.062581 0.276911 -4.586418
H -4.153715 0.345528 -5.200949
H -5.782228 -0.369432 -5.108493
H -5.497717 1.283397 -4.520313
C -4.118461 -2.436318 -4.385371
H -5.163748 -2.778413 -4.403423
H -3.903325 -1.938728 -5.338965
H -3.481391 -3.329767 -4.323471
C -3.971719 -2.308665 -1.905057
H -3.211251 -3.100367 -1.880964
H -3.806041 -1.663568 -1.030490
H -4.955813 -2.784749 -1.791538
C 2.019670 2.881572 -2.755019
H 1.268527 3.349082 -3.426172
H 3.035083 3.131980 -3.126700
H 1.867050 1.787450 -2.818178
C 1.604050 2.286639 2.322168
H 0.713538 2.547510 2.931472
H 1.547117 1.202133 2.108418
H 2.511836 2.491600 2.926784
C 1.268095 6.820115 0.218866
H 2.154964 7.360399 -0.174093
H 0.370594 7.126320 -0.358880
H 1.118942 7.113581 1.279785
H 1.683262 5.437161 -2.057530
H 1.301848 4.932542 2.184544
123
Figure_S9_imid-2_modeC_ts(AS)_01 / electronic energy: -4442.810779672690 a.u. / lowest freq: -218.49 cm-1
C 3.250845 0.124217 0.997015
H 3.660729 1.011622 0.495888
C 3.388414 -1.174999 0.173325
H 3.657143 -2.028278 0.816220
C 1.104832 -0.589401 0.302842
C 1.110417 1.268767 1.850581
C 0.223383 0.819808 2.833830
C 1.295209 2.652578 1.668777

C	-0.442897	1.719981	3.658272
H	0.073143	-0.254505	2.959465
C	0.619261	3.546079	2.502084
C	-0.235930	3.088054	3.501304
H	-1.115232	1.335698	4.426732
H	0.762626	4.615029	2.336371
H	-0.748833	3.804003	4.147176
S	2.323130	3.358240	0.371034
O	1.835485	4.758352	0.207490
O	2.027536	2.557661	-0.857132
O	3.717439	3.262787	0.840117
Cu	-0.893036	-0.707123	0.221814
C	3.860692	0.007359	2.372364
C	4.991069	0.771159	2.712395
C	3.315348	-0.868311	3.330891
C	5.556066	0.669152	3.987206
H	5.441657	1.440074	1.990528
C	3.882905	-0.965756	4.604186
H	2.447079	-1.469447	3.095031
C	5.001661	-0.196887	4.932708
H	6.425964	1.260791	4.241495
H	3.454674	-1.637725	5.336637
H	5.440473	-0.273911	5.919069
N	1.773672	0.281590	1.073608
N	2.007176	-1.362473	-0.319012
C	-2.686008	-0.269674	-0.673094
C	-3.257837	-1.392514	-1.413102
C	-4.563085	-1.832325	-1.128972
C	-2.528990	-2.083607	-2.399383
C	-5.112941	-2.919394	-1.800149
C	-3.075836	-3.173441	-3.066962
C	-4.372077	-3.599037	-2.769288
H	-6.129597	-3.242954	-1.563608
H	-2.483233	-3.700207	-3.819077
H	-4.802736	-4.457158	-3.290429
C	-1.662653	0.571417	-1.198902
C	-1.224130	1.726043	-0.529635
H	-1.557261	1.904086	0.497092
H	-0.260146	2.166524	-0.793993
H	-1.506872	-1.773134	-2.625308
H	-1.260317	0.372038	-2.196198
P	-2.009842	3.671109	-2.592111
O	-2.987686	4.916436	-2.968737
O	-0.629018	4.029399	-3.064326
O	-2.619148	2.419870	-3.448328
O	-2.270621	3.291219	-1.126382
Na	1.288199	4.555022	-2.114563
H	-3.325445	0.141045	0.117162
H	-5.138524	-1.314983	-0.358965
C	-4.367256	4.833424	-2.653685
H	-4.846226	5.748905	-3.019069
H	-4.840611	3.967291	-3.142205
H	-4.527691	4.754544	-1.568646
C	-2.434251	2.387651	-4.851012
H	-2.834621	1.434864	-5.217380
H	-2.973075	3.209458	-5.349481
H	-1.369699	2.454923	-5.120238
C	1.618004	-2.450901	-1.139626
C	1.588156	-3.771331	-0.623289
C	1.319649	-2.233028	-2.508342
C	1.295273	-4.843352	-1.478381
C	1.022317	-3.324036	-3.336708
C	1.007083	-4.626778	-2.828536
H	3.571290	0.691418	-1.860436
H	5.207558	0.770035	-3.692303
C	4.335500	-0.069048	-1.911984
C	5.264339	-0.020279	-2.955028
C	4.396013	-1.092398	-0.948108
C	6.264296	-0.990187	-3.048248
H	6.982398	-0.951460	-3.857078
C	5.409816	-2.063191	-1.052766
C	6.337216	-2.010311	-2.097546
H	5.481454	-2.866805	-0.330357
H	7.111938	-2.762554	-2.171005
C	-1.428881	-2.245642	1.452336
H	-0.495913	-2.349754	2.028684
C	-1.761322	-3.486860	0.652623
H	-1.123039	-3.646544	-0.232905
H	-1.670267	-4.407288	1.257448
H	-2.794974	-3.461669	0.279669
B	-2.577166	-1.629062	2.254937
O	-2.442457	-0.778940	3.346432
O	-3.914842	-1.854422	1.963139
C	-4.698641	-1.343077	3.059410
C	-3.752207	-0.253348	3.662409
C	-6.012877	-0.813902	2.525080
H	-5.866491	-0.075905	1.726111
H	-6.612803	-1.637241	2.112880

H -6.602492 -0.341253 3.324142
C -4.943689 -2.500646 4.016028
H -4.000594 -2.891169 4.423608
H -5.587228 -2.210045 4.858062
H -5.440040 -3.319563 3.478308
C -3.868284 -0.079208 5.161703
H -4.893208 0.201037 5.444859
H -3.598871 -0.994042 5.702812
H -3.202381 0.722615 5.509670
C -3.898558 1.089393 2.963185
H -3.090105 1.766054 3.269020
H -3.846910 0.985621 1.870307
H -4.853489 1.574583 3.208431
C 1.819026 -4.079019 0.832587
H 1.035812 -4.775559 1.199796
H 2.812268 -4.558284 0.957959
H 1.765500 -3.176092 1.469629
C 1.323637 -0.861196 -3.131201
H 0.391667 -0.706953 -3.713797
H 1.380458 -0.049445 -2.380930
H 2.186466 -0.773210 -3.823762
C 0.672770 -5.791891 -3.712855
H 1.524365 -6.504192 -3.729335
H -0.227293 -6.310596 -3.320548
H 0.464571 -5.468391 -4.754939
H 1.272430 -5.853595 -1.085377
H 0.797238 -3.153549 -4.383248
123
Figure_S9_imid-2_modeC_ts(AS)_02 / electronic energy: -4442.811522350486 a.u. / lowest freq: -249.65 cm-1
C -2.981507 -0.783340 1.259697
H -3.307638 -1.708497 0.765262
C -3.521835 0.506384 0.599421
H -3.899024 1.216772 1.351882
C -1.168489 0.436064 0.342980
C -0.561079 -1.567100 1.572815
C 0.353602 -1.078661 2.508867
C -0.502841 -2.923697 1.193140
C 1.300788 -1.916565 3.089832
H 0.310176 -0.023563 2.786021
C 0.440794 -3.756627 1.794749
C 1.334394 -3.264578 2.744900
H 1.998717 -1.500786 3.818681
H 0.471828 -4.802748 1.486960
H 2.064025 -3.936682 3.202606
S -1.502970 -3.630172 -0.130890
O -0.896686 -4.961858 -0.418035
O -1.303547 -2.700614 -1.283862
O -2.891222 -3.713290 0.360739
Cu 0.708587 1.066273 0.049347
C -3.312234 -0.874969 2.730033
C -4.147992 -1.901979 3.203689
C -2.786164 0.053887 3.647938
C -4.449667 -1.996793 4.565617
H -4.569543 -2.628579 2.520680
C -3.089521 -0.045766 5.008405
H -2.132604 0.847382 3.312736
C -3.920915 -1.069954 5.467103
H -5.094106 -2.789829 4.922304
H -2.677804 0.670471 5.707629
H -4.154922 -1.145843 6.521085
N -1.513994 -0.650407 1.050731
N -2.298323 1.063723 -0.016223
C 2.402836 1.282502 -1.077012
C 2.508319 2.596915 -1.708509
C 3.645105 3.395337 -1.486888
C 1.483049 3.119566 -2.518029
C 3.746249 4.664812 -2.046747
C 1.580331 4.391278 -3.072278
C 2.713034 5.172665 -2.836765
H 4.638177 5.268102 -1.860932
H 0.764738 4.777042 -3.688814
H 2.790173 6.173219 -3.268467
C 1.614691 0.216564 -1.601847
C 1.607262 -1.055230 -0.998591
H 2.023521 -1.167902 0.008375
H 0.801468 -1.751053 -1.249470
H 0.590615 2.519778 -2.702858
H 1.067276 0.342760 -2.541078
P 2.597271 -3.240963 -2.608520
O 2.130837 -4.484069 -1.631554
O 1.435245 -3.095927 -3.548989
O 3.960566 -3.769857 -3.311507
O 3.087220 -2.074237 -1.737870
Na -0.201466 -4.457280 -2.654504
H 3.232614 1.024608 -0.409691
H 4.443594 3.010426 -0.850071
C 2.954473 -4.874810 -0.547064
H 2.427921 -5.661636 0.005234

H 3.918005 -5.273281 -0.901808
H 3.152016 -4.029900 0.130800
C 3.877157 -4.832498 -4.248174
H 4.882033 -4.993753 -4.653377
H 3.536758 -5.764570 -3.769864
H 3.193498 -4.587669 -5.073796
C -2.287400 2.269192 -0.763121
C -2.489215 3.516585 -0.120057
C -2.154614 2.229588 -2.174816
C -2.573428 4.687419 -0.886873
C -2.239756 3.417613 -2.914189
C -2.443719 4.645594 -2.277435
H -3.537197 -1.229233 -1.554689
H -5.325431 -1.566736 -3.206845
C -4.449448 -0.658690 -1.462749
C -5.463880 -0.854527 -2.403741
C -4.615349 0.265642 -0.414511
C -6.654760 -0.131733 -2.310325
H -7.439024 -0.283826 -3.040513
C -5.821300 0.986485 -0.330721
C -6.833395 0.787461 -1.274412
H -5.978349 1.709241 0.460319
H -7.756366 1.348281 -1.203330
C 1.057615 2.474949 1.491968
H 0.224489 2.241020 2.173622
C 0.970443 3.878779 0.932412
H 0.197169 4.015681 0.157315
H 0.745635 4.624762 1.715786
H 1.916975 4.192708 0.470563
B 2.425316 2.017751 2.007094
O 2.651293 0.971785 2.895076
O 3.625101 2.592831 1.608473
C 4.669873 2.076907 2.456291
C 4.072226 0.708966 2.925700
C 5.950937 1.965177 1.657160
H 5.818998 1.372440 0.743274
H 6.300333 2.963835 1.360457
H 6.747747 1.498723 2.254765
C 4.845623 3.060810 3.603784
H 3.928852 3.143586 4.204135
H 5.668951 2.771968 4.271530
H 5.071794 4.056659 3.199418
C 4.472051 0.301286 4.328469
H 5.565346 0.221815 4.415423
H 4.117917 1.016829 5.080024
H 4.052319 -0.682896 4.578721
C 4.365464 -0.424135 1.952366
H 3.762524 -1.305784 2.210020
H 4.127217 -0.155077 0.913558
H 5.423310 -0.719695 1.982034
C -2.586633 3.648865 1.376264
H -1.967916 4.503460 1.723020
H -3.642779 3.830778 1.665144
H -2.211921 2.750435 1.900864
C -1.939148 0.947493 -2.936283
H -1.089921 1.063227 -3.641124
H -1.703371 0.090788 -2.277842
H -2.850155 0.710245 -3.524207
C -2.514017 5.918376 -3.068869
H -3.497412 6.406737 -2.903712
H -1.706657 6.606091 -2.739779
H -2.392560 5.730976 -4.157026
H -2.726186 5.641926 -0.395840
H -2.139165 3.382984 -3.992937
123
Figure_S9_imid-2_modeC_ts(AS)_03 / electronic energy: -4442.811687210238 a.u. / lowest freq: -237.15 cm-1
C 2.879620 1.190014 1.215339
H 3.103196 2.132153 0.697668
C 3.588560 -0.043206 0.608978
H 4.050013 -0.668752 1.389243
C 1.248431 -0.280514 0.323628
C 0.375200 1.680895 1.458901
C -0.485195 1.111098 2.400706
C 0.153079 3.007153 1.034755
C -1.533811 1.842974 2.949002
H -0.317007 0.077758 2.710336
C -0.897319 3.732451 1.598728
C -1.731867 3.163746 2.558943
H -2.180698 1.368346 3.688453
H -1.061424 4.752582 1.247792
H -2.545930 3.753234 2.987499
S 1.074796 3.795734 -0.300073
O 0.332663 5.055039 -0.596673
O 0.967944 2.842403 -1.445888
O 2.446995 4.030747 0.186287
Cu -0.532324 -1.151207 0.043781
C 3.162141 1.368946 2.687820
C 3.859863 2.503408 3.139431

C	2.728697	0.415846	3.628763
C	4.117839	2.679104	4.502250
H	4.207771	3.251563	2.438338
C	2.987700	0.596502	4.990080
H	2.179399	-0.459258	3.311068
C	3.682211	1.726833	5.426696
H	4.656107	3.554577	4.841745
H	2.647372	-0.139355	5.707081
H	3.882039	1.865344	6.481337
N	1.443746	0.874625	0.979558
N	2.453745	-0.779130	0.011075
C	-2.174759	-1.625191	-1.084781
C	-2.091009	-2.961132	-1.671821
C	-3.112575	-3.903014	-1.454070
C	-0.980957	-3.357586	-2.439691
C	-3.021175	-5.187304	-1.981942
C	-0.884548	-4.642561	-2.960827
C	-1.906128	-5.566274	-2.732936
H	-3.825984	-5.904267	-1.802517
H	-0.005856	-4.926690	-3.544905
H	-1.833588	-6.578053	-3.138403
C	-1.527164	-0.482935	-1.642040
C	-1.712303	0.797858	-1.093156
H	-2.147223	0.886479	-0.092366
H	-1.026177	1.600727	-1.377838
H	-0.175486	-2.643505	-2.614432
H	-0.954825	-0.569095	-2.570729
P	-3.134090	2.873351	-2.571194
O	-2.916740	4.039244	-1.430534
O	-2.003948	3.086170	-3.537584
O	-4.597027	3.196021	-3.198313
O	-3.349931	1.523460	-1.871385
Na	-0.399936	4.453219	-2.747338
H	-3.044504	-1.454231	-0.440751
H	-3.973436	-3.617303	-0.846428
C	-3.816685	4.096669	-0.337691
H	-3.523013	4.940601	0.297374
H	-4.851765	4.255266	-0.679285
H	-3.784229	3.170989	0.258562
C	-4.758450	4.359689	-3.993163
H	-5.790914	4.367326	-4.359744
H	-4.587213	5.275792	-3.405948
H	-4.073794	4.357866	-4.853701
C	2.606865	-2.008608	-0.679269
C	2.946652	-3.191919	0.024083
C	2.499539	-2.048640	-2.093167
C	3.186125	-4.377196	-0.685601
C	2.741238	-3.249768	-2.774587
C	3.078525	-4.414225	-2.078083
H	3.392988	1.609163	-1.600848
H	5.130490	2.112307	-3.265865
C	4.370011	1.161082	-1.490883
C	5.354728	1.450657	-2.439232
C	4.647327	0.300112	-0.412385
C	6.626414	0.886106	-2.323018
H	7.387523	1.110260	-3.059123
C	5.933780	-0.260374	-0.305548
C	6.915725	0.031987	-1.256790
H	6.177559	-0.931078	0.509008
H	7.901379	-0.406282	-1.168163
C	-0.724490	-2.547614	1.526521
H	0.064844	-2.191508	2.208017
C	-0.461565	-3.947480	1.016441
H	0.340022	-4.015478	0.261777
H	-0.169937	-4.637540	1.828529
H	-1.354695	-4.382373	0.546298
B	-2.143789	-2.245314	2.015989
O	-2.504221	-1.200637	2.859620
O	-3.258495	-2.979397	1.635387
C	-4.372188	-2.556608	2.447021
C	-3.946760	-1.112088	2.874053
C	-5.639187	-2.623303	1.620603
H	-5.555990	-2.050281	0.688118
H	-5.861962	-3.665829	1.354697
H	-6.499046	-2.233960	2.184975
C	-4.459977	-3.514850	3.625573
H	-3.552786	-3.476682	4.244827
H	-5.324012	-3.297102	4.268231
H	-4.566611	-4.542158	3.252259
C	-4.403269	-0.709600	4.261144
H	-5.499629	-0.743580	4.338728
H	-3.982939	-1.361343	5.036348
H	-4.092718	0.320521	4.484939
C	-4.366930	-0.054844	1.862644
H	-3.898581	0.908304	2.107822
H	-4.067491	-0.315727	0.837252
H	-5.455565	0.094345	1.861383
C	3.032060	-3.244503	1.525876

H	2.504795	-4.145585	1.904553
H	4.096593	-3.295210	1.835888
H	2.552804	-2.370294	2.003129
C	2.147777	-0.837628	-2.917596
H	1.333829	-1.085958	-3.629785
H	1.796586	0.012397	-2.303906
H	3.036071	-0.518489	-3.501482
C	3.315312	-5.703835	-2.807547
H	4.346748	-6.062425	-2.606588
H	2.589924	-6.468037	-2.456935
H	3.192581	-5.581944	-3.904822
H	3.443352	-5.283028	-0.148142
H	2.658311	-3.276196	-3.855064

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Figure_S9_imid-2_modeC_ts(AS)_04 / electronic energy: -4442.802341399660 a.u. / lowest freq: -226.82 cm-1

C	1.481747	2.781798	-0.534930
H	2.427511	2.779579	0.020997
C	0.266290	3.197869	0.318931
H	-0.326512	3.973740	-0.187675
C	-0.031112	0.953133	-0.383944
C	1.928106	0.564283	-1.758705
C	1.259314	-0.045250	-2.828317
C	3.299609	0.288715	-1.570753
C	1.903745	-0.934825	-3.681463
H	0.209693	0.206184	-2.982641
C	3.941180	-0.585120	-2.452318
C	3.257100	-1.204165	-3.495843
H	1.347009	-1.402018	-4.496915
H	4.996711	-0.800190	-2.278808
H	3.783942	-1.893652	-4.158648
S	4.286224	0.892126	-0.185594
O	5.504611	0.038038	-0.157412
O	3.433748	0.630517	1.015568
O	4.566424	2.315847	-0.442438
Cu	-0.778233	-0.869793	-0.829791
C	1.634088	3.642318	-1.767035
C	2.710181	4.540558	-1.877091
C	0.689288	3.580228	-2.809450
C	2.850300	5.340898	-3.014974
H	3.434985	4.632847	-1.079035
C	0.833841	4.381463	-3.945103
H	-0.156634	2.909730	-2.744509
C	1.915030	5.259264	-4.049292
H	3.682544	6.028467	-3.092725
H	0.105933	4.322759	-4.743951
H	2.025096	5.880215	-4.928901
N	1.142495	1.381470	-0.902655
N	-0.519547	1.943031	0.374903
C	-0.647311	-2.919826	-0.801104
C	-1.850240	-3.711849	-0.571285
C	-2.458437	-4.361936	-1.660065
C	-2.420874	-3.879210	0.703065
C	-3.591087	-5.148790	-1.485888
C	-3.548801	-4.671154	0.877695
C	-4.141201	-5.309053	-0.214203
H	-4.044762	-5.647094	-2.346140
H	-3.974338	-4.792571	1.877528
H	-5.028222	-5.931295	-0.072068
C	0.212087	-2.406913	0.206883
C	1.544483	-2.068170	-0.074638
H	1.865071	-2.038356	-1.117511
H	2.105032	-1.426031	0.609381
H	-1.978870	-3.380001	1.569579
H	-0.097417	-2.423713	1.255839
P	3.666048	-3.555563	1.312941
O	5.046999	-2.959079	0.640527
O	3.472111	-2.674859	2.514975
O	4.027643	-5.097035	1.668339
O	2.592477	-3.691107	0.225661
Na	4.958566	-0.919036	2.045945
H	-0.186283	-3.070859	-1.787731
H	-2.020192	-4.248897	-2.656199
C	5.485134	-3.418960	-0.625289
H	6.308765	-2.771685	-0.947555
H	5.845462	-4.458236	-0.567643
H	4.675401	-3.368250	-1.368885
C	5.017168	-5.358103	2.650428
H	5.035723	-6.440094	2.820989
H	6.014991	-5.037950	2.311153
H	4.786221	-4.850930	3.598520
C	-1.707414	1.832932	1.147393
C	-2.829492	2.645483	0.841494
C	-1.717271	1.069454	2.346677
C	-3.878764	2.760083	1.762649
C	-2.798815	1.180684	3.232443
C	-3.868888	2.035700	2.956302
H	1.699556	1.936254	2.306749
H	2.244992	2.781996	4.551753

C 1.368198 2.922126 2.590812
C 1.677421 3.399090 3.867340
C 0.628752 3.711233 1.692621
C 1.252549 4.669410 4.261656
H 1.491938 5.037549 5.250860
C 0.205320 4.989586 2.101830
C 0.517187 5.463952 3.379455
H -0.371195 5.619562 1.435850
H 0.186343 6.447743 3.686278
C -2.342341 -0.780413 -2.143526
H -2.274951 -1.767148 -2.632187
C -2.240549 0.339776 -3.161887
H -1.462008 0.176227 -3.923560
H -3.180007 0.472797 -3.730458
H -2.038261 1.319117 -2.703209
B -3.635372 -0.744458 -1.311206
O -4.277520 -1.860894 -0.806895
O -4.382895 0.406013 -1.089187
C -5.721739 -0.039478 -0.772053
C -5.440628 -1.409439 -0.083957
C -6.424690 0.977826 0.094395
H -5.912821 1.133404 1.047507
H -6.486627 1.944501 -0.423176
H -7.450391 0.650289 0.316941
C -6.457846 -0.195429 -2.096352
H -5.986709 -0.962206 -2.728283
H -7.512394 -0.469405 -1.953722
H -6.427366 0.756332 -2.644177
C -6.547699 -2.430052 -0.229853
H -7.487151 -2.053049 0.200712
H -6.727623 -2.689143 -1.280978
H -6.282593 -3.355644 0.299666
C -5.040272 -1.254723 1.374595
H -4.650316 -2.209648 1.750303
H -4.245958 -0.503790 1.482134
H -5.885888 -0.959802 2.011287
C -2.955598 3.399677 -0.454662
H -3.945496 3.192265 -0.913157
H -2.871883 4.489594 -0.261084
H -2.187736 3.101145 -1.192869
C -0.590538 0.158874 2.758367
H -0.988177 -0.864136 2.924278
H 0.217931 0.088339 2.010486
H -0.148055 0.524046 3.709004
C -5.011808 2.171568 3.919569
H -5.099434 3.229058 4.246358
H -5.957809 1.865614 3.426042
H -4.865950 1.537081 4.819534
H -4.721099 3.405464 1.539612
H -2.796238 0.607239 4.152442

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Figure_S9_imid-2_modeC_ts(AS)_05 / electronic energy: -4442.803159881789 a.u. / lowest freq: -206.12 cm-1

C -2.281253 -2.412453 -0.343749
H -3.167149 -2.097143 0.222970
C -1.173020 -3.023453 0.538800
H -0.784055 -3.954112 0.098620
C -0.369991 -0.999878 -0.396638
C -2.194976 -0.326929 -1.843166
C -1.430042 -0.040178 -2.980490
C -3.445576 0.303744 -1.688482
C -1.869411 0.860998 -3.944347
H -0.475575 -0.554575 -3.094353
C -3.888854 1.185473 -2.677858
C -3.112918 1.471982 -3.797452
H -1.243177 1.070331 -4.814544
H -4.849972 1.679774 -2.528796
H -3.479098 2.175629 -4.547430
S -4.497395 0.153471 -0.233227
O -5.380032 1.354980 -0.265772
O -3.570285 0.230670 0.937797
O -5.217033 -1.125262 -0.360691
Cu 0.769823 0.561172 -0.997054
C -2.705112 -3.342723 -1.454413
C -3.980891 -3.932805 -1.435992
C -1.824544 -3.653804 -2.508511
C -4.374519 -4.798506 -2.460835
H -4.667872 -3.734616 -0.623671
C -2.222882 -4.518941 -3.531095
H -0.831808 -3.224261 -2.540161
C -3.497740 -5.089049 -3.508795
H -5.358956 -5.247836 -2.440096
H -1.541904 -4.748669 -4.340346
H -3.804418 -5.759989 -4.300737
N -1.612683 -1.200206 -0.887253
N -0.121841 -1.982415 0.479672
C 1.108794 2.592202 -1.087403
C 2.453063 3.101750 -0.840706
C 3.228562 3.546010 -1.926741

C	3.003058	3.197050	0.450132
C	4.506587	4.058295	-1.734520
C	4.278861	3.713161	0.641695
C	5.038874	4.143278	-0.448213
H	5.091328	4.396929	-2.593291
H	4.687974	3.782024	1.653215
H	6.042176	4.547879	-0.293016
C	0.134368	2.343697	-0.086500
C	-1.227757	2.236483	-0.401157
H	-1.513697	2.214011	-1.452657
H	-1.921967	1.757277	0.292341
H	2.426163	2.862971	1.316815
H	0.421133	2.356794	0.967960
P	-2.244600	4.457037	1.208178
O	-2.983256	5.908865	1.215290
O	-2.952392	3.588464	2.210135
O	-0.716788	4.790830	1.683296
O	-2.102572	4.002941	-0.252689
Na	-4.655436	2.202272	1.859818
H	0.723798	2.785800	-2.098490
H	2.808411	3.488805	-2.935332
C	-2.494289	6.940782	0.374952
H	-3.137438	7.816603	0.517218
H	-1.459909	7.214928	0.634891
H	-2.522201	6.645053	-0.683843
C	-0.482030	5.142791	3.034340
H	0.597605	5.289536	3.156761
H	-0.995933	6.079675	3.303644
H	-0.816803	4.352217	3.722417
C	1.087180	-2.088265	1.217756
C	1.987141	-3.153219	0.957684
C	1.311399	-1.257060	2.347809
C	3.016878	-3.431787	1.865969
C	2.370436	-1.542474	3.221364
C	3.211259	-2.636180	2.997309
H	-2.218674	-1.300216	2.420680
H	-2.884794	-1.805806	4.733460
C	-2.119242	-2.309723	2.785711
C	-2.496612	-2.593568	4.100873
C	-1.609510	-3.321987	1.953750
C	-2.370731	-3.891284	4.600457
H	-2.662575	-4.109765	5.619512
C	-1.487224	-4.626120	2.468837
C	-1.866826	-4.906733	3.784860
H	-1.093438	-5.427144	1.855672
H	-1.767911	-5.912151	4.173159
C	2.269489	0.031039	-2.275297
H	2.428502	0.972306	-2.828428
C	1.899369	-1.097224	-3.221991
H	1.215302	-0.783070	-4.025679
H	2.782959	-1.519500	-3.735765
H	1.423592	-1.951302	-2.714696
B	3.535653	-0.245057	-1.446439
O	4.424673	0.723760	-1.015638
O	4.011391	-1.520851	-1.169488
C	5.425013	-1.376781	-0.909770
C	5.490547	0.059691	-0.306214
C	5.907360	-2.476708	0.005709
H	5.387216	-2.473860	0.966956
H	5.753238	-3.458786	-0.461267
H	6.982701	-2.365743	0.206517
C	6.131387	-1.474834	-2.256135
H	5.822654	-0.663564	-2.931184
H	7.224654	-1.437066	-2.152975
H	5.869815	-2.428011	-2.735874
C	6.790164	0.790857	-0.560779
H	7.642278	0.232550	-0.145690
H	6.966172	0.946006	-1.632653
H	6.770252	1.779153	-0.081378
C	5.140050	0.083056	1.172295
H	5.006572	1.122021	1.501057
H	4.197833	-0.450712	1.354730
H	5.923370	-0.373021	1.793647
C	1.892439	-4.010648	-0.275541
H	2.887431	-4.076286	-0.764193
H	1.563352	-5.032828	0.005835
H	1.191610	-3.594863	-1.024208
C	0.434215	-0.083511	2.694446
H	1.058883	0.830587	2.775288
H	-0.353585	0.111632	1.945667
H	-0.056153	-0.263832	3.674104
C	4.328495	-2.953093	3.948018
H	4.190248	-3.975921	4.357218
H	5.300855	-2.904607	3.414932
H	4.359113	-2.236857	4.796464
H	3.684276	-4.266237	1.681617
H	2.529369	-0.914254	4.090428

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Figure_S9_imid-2_modeC_ts(AS)_06 / electronic energy: -4442.802591917493 a.u. / lowest freq: -226.51 cm-1

C	-0.972277	-2.620871	0.515988
H	-2.044746	-2.634502	0.287829
C	-0.648793	-2.210804	1.971820
H	0.059426	-2.910718	2.442812
C	0.200591	-0.558380	0.509004
C	-0.260736	-1.435004	-1.683874
C	0.981681	-1.029415	-2.192967
C	-1.319456	-1.650113	-2.589728
C	1.181500	-0.795655	-3.547878
H	1.806692	-0.910432	-1.488322
C	-1.095036	-1.448141	-3.955446
C	0.135375	-1.013449	-4.440278
H	2.160186	-0.454568	-3.893476
H	-1.930790	-1.608318	-4.637661
H	0.270642	-0.847068	-5.510606
S	-3.004729	-2.083748	-2.118278
O	-3.828411	-1.832364	-3.337092
O	-3.374804	-1.122826	-1.033798
O	-2.975053	-3.496771	-1.704730
Cu	1.018745	1.153756	-0.202906
C	-0.393581	-3.970942	0.169007
C	-1.200808	-5.117165	0.274897
C	0.957944	-4.121270	-0.194685
C	-0.678289	-6.381233	-0.012771
H	-2.235030	-5.032152	0.584551
C	1.476391	-5.387587	-0.481372
H	1.610797	-3.262572	-0.256801
C	0.658316	-6.516003	-0.394144
H	-1.309012	-7.257320	0.065145
H	2.514279	-5.496297	-0.766918
H	1.062056	-7.495612	-0.614926
N	-0.354579	-1.514200	-0.268909
N	0.008737	-0.902134	1.785698
C	0.646610	2.964629	-1.136332
C	1.177157	4.204969	-0.576040
C	2.103667	4.961354	-1.314826
C	0.788008	4.690874	0.686473
C	2.618118	6.155448	-0.817475
C	1.302697	5.882456	1.184779
C	2.221186	6.621978	0.435738
H	3.335047	6.726044	-1.412660
H	0.987902	6.237199	2.169183
H	2.625541	7.557360	0.829287
C	-0.573495	2.369457	-0.719246
C	-1.264737	1.417590	-1.482841
H	-0.840903	1.108190	-2.441008
H	-1.942495	0.709735	-1.006677
H	0.082128	4.121282	1.294802
H	-1.059305	2.714186	0.198497
P	-4.041542	2.549801	-1.507109
O	-4.334611	4.152867	-1.432638
O	-5.334637	1.878859	-1.872504
O	-3.583708	2.186826	0.024619
O	-2.783493	2.315516	-2.357505
Na	-5.330501	-0.272286	-2.472222
H	0.981482	2.735928	-2.158575
H	2.421236	4.597194	-2.296108
C	-3.266584	5.005597	-1.058243
H	-3.553802	6.034317	-1.304478
H	-3.064057	4.944688	0.023717
H	-2.340974	4.753875	-1.600318
C	-4.577320	2.141471	1.030400
H	-4.070726	2.045242	1.997574
H	-5.185077	3.060174	1.044516
H	-5.249043	1.280209	0.897916
C	0.654942	-0.217074	2.846848
C	1.875520	-0.706161	3.379774
C	0.053671	0.926467	3.428941
C	2.445280	-0.080260	4.497174
C	0.648882	1.534107	4.543369
C	1.838858	1.034367	5.082258
H	-2.944203	-0.740251	1.546076
H	-4.910134	-0.548827	3.012622
C	-2.961106	-1.288795	2.477026
C	-4.079300	-1.176760	3.307217
C	-1.871451	-2.098062	2.850371
C	-4.124753	-1.872172	4.517146
H	-4.991145	-1.783983	5.159753
C	-1.930463	-2.795672	4.070551
C	-3.051889	-2.681490	4.897847
H	-1.107574	-3.424456	4.386857
H	-3.088098	-3.219778	5.836118
C	2.986661	1.187841	0.310112
H	2.902341	0.775173	1.328838
C	3.669068	2.541465	0.362068
H	3.143826	3.281624	0.987121
H	4.692311	2.467837	0.778478

H 3.780428 2.991999 -0.635866
B 3.758606 0.192946 -0.575148
O 4.209639 -1.044653 -0.159796
O 4.198012 0.481001 -1.860120
C 5.309783 -0.397048 -2.139259
C 5.020287 -1.626919 -1.206558
C 5.340777 -0.724058 -3.616274
H 4.404227 -1.178425 -3.961684
H 5.510942 0.188395 -4.203811
H 6.158461 -1.423289 -3.843355
C 6.569085 0.360457 -1.742160
H 6.563577 0.617481 -0.673167
H 7.482427 -0.212227 -1.953544
H 6.620571 1.300117 -2.308574
C 6.255225 -2.233518 -0.570128
H 6.946892 -2.612333 -1.336440
H 6.794899 -1.512123 0.054869
H 5.970806 -3.080560 0.068865
C 4.210817 -2.719001 -1.882290
H 3.908511 -3.459643 -1.131384
H 3.303473 -2.331304 -2.362850
H 4.800365 -3.243155 -2.647083
C 2.621655 -1.863145 2.769401
H 3.685522 -1.583448 2.617004
H 2.575041 -2.737674 3.451287
H 2.220137 -2.153447 1.780708
C -1.229682 1.516632 2.913084
H -1.111450 2.610781 2.773721
H -1.530623 1.090391 1.938747
H -2.040774 1.339041 3.649832
C 2.476045 1.686310 6.274213
H 2.551439 0.952775 7.104379
H 3.494910 2.037535 6.006754
H 1.885732 2.558116 6.628370
H 3.375343 -0.456880 4.908045
H 0.179217 2.401798 4.992430
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Figure_S9_imid-2_modeC_prod(AS) / electronic energy: -4442.820902045555 a.u. / lowest freq: -8.85 cm-1
C 3.402455 -0.485734 0.332176
H 3.739729 0.507364 0.663059
C 3.291274 -0.628636 -1.201593
H 3.609784 -1.629799 -1.531092
C 1.129063 -0.605560 -0.268033
C 1.560851 -0.685840 2.114176
C 0.929008 -1.853963 2.547783
C 1.736272 0.386529 3.007618
C 0.488220 -1.974136 3.862267
H 0.789107 -2.672883 1.838853
C 1.287554 0.252926 4.322375
C 0.674559 -0.921310 4.754678
H 0.006949 -2.899488 4.185266
H 1.409242 1.101451 4.997938
H 0.334571 -1.006258 5.788836
S 2.475246 1.964384 2.540015
O 1.959517 2.943095 3.536226
O 1.931568 2.268059 1.181032
O 3.933724 1.757700 2.577053
Cu -0.868637 -0.638715 -0.128516
C 4.274902 -1.544275 0.958442
C 5.467238 -1.183578 1.610157
C 3.910107 -2.903182 0.904699
C 6.274262 -2.161340 2.199631
H 5.776623 -0.147364 1.659213
C 4.719631 -3.876664 1.496313
H 2.996551 -3.207495 0.410311
C 5.900547 -3.506237 2.143719
H 7.190799 -1.875934 2.699561
H 4.430655 -4.918794 1.453286
H 6.526602 -4.261352 2.601159
N 1.984626 -0.638491 0.756478
N 1.831336 -0.499864 -1.404024
C -2.865418 0.065355 -0.082938
C -3.696841 0.012607 -1.278190
C -4.949944 -0.625152 -1.238672
C -3.272776 0.577330 -2.496078
C -5.750701 -0.685656 -2.374175
C -4.070696 0.511039 -3.631518
C -5.314103 -0.122123 -3.575149
H -6.724358 -1.178498 -2.324514
H -3.717066 0.947297 -4.568399
H -5.942376 -0.176594 -4.466926
C -1.950115 1.129413 0.174349
C -1.050196 1.071670 1.216457
H -1.194185 0.378475 2.056707
H -0.248113 1.804928 1.305247
H -2.293879 1.057011 -2.556200
H -1.802018 1.920104 -0.570509
P -2.091930 4.475598 1.144516

O	-2.665257	5.995673	0.876581
O	-1.065694	4.213181	0.065258
O	-3.454237	3.573833	0.924899
O	-1.670460	4.293358	2.583245
Na	0.632512	4.203104	1.891444
H	-3.240984	-0.492067	0.784096
H	-5.286827	-1.076840	-0.303704
C	-3.594376	6.519742	1.801329
H	-3.803412	7.560311	1.523407
H	-4.543696	5.958265	1.789863
H	-3.199612	6.499354	2.829013
C	-4.099867	3.644116	-0.329149
H	-4.776392	2.782850	-0.417763
H	-4.693574	4.567547	-0.428894
H	-3.379405	3.613747	-1.164239
C	1.213558	-0.523947	-2.680416
C	1.206456	-1.709835	-3.459625
C	0.658634	0.664468	-3.220214
C	0.680100	-1.682012	-4.759181
C	0.127093	0.656889	-4.517170
C	0.134593	-0.509406	-5.288350
H	3.234021	2.131675	-1.002395
H	4.508871	3.765855	-2.319946
C	3.918683	1.774319	-1.754688
C	4.642462	2.707363	-2.502082
C	4.079815	0.395451	-1.982195
C	5.536156	2.276320	-3.484173
H	6.095391	3.000169	-4.062691
C	4.985060	-0.025737	-2.974645
C	5.707658	0.910821	-3.719740
H	5.129353	-1.079356	-3.179091
H	6.399675	0.577106	-4.482104
C	-1.332225	-2.462434	-0.894822
H	-0.315984	-2.879268	-0.878233
C	-1.944783	-2.461842	-2.271421
H	-1.585178	-1.658544	-2.936264
H	-1.726789	-3.406500	-2.798422
H	-3.037459	-2.363549	-2.237406
B	-2.202668	-3.003072	0.259903
O	-1.714408	-3.391288	1.491274
O	-3.570891	-3.141709	0.176650
C	-3.997821	-3.916606	1.323825
C	-2.855197	-3.636315	2.355947
C	-5.369472	-3.447443	1.756125
H	-5.394676	-2.370425	1.961831
H	-6.105732	-3.656374	0.968147
H	-5.694210	-3.975940	2.663720
C	-4.045498	-5.370796	0.883331
H	-3.055037	-5.730440	0.571027
H	-4.411826	-6.027936	1.683677
H	-4.724431	-5.471605	0.026258
C	-2.541024	-4.798581	3.271473
H	-3.425645	-5.080045	3.860344
H	-2.204973	-5.680055	2.712711
H	-1.747497	-4.526840	3.980277
C	-3.091203	-2.370339	3.161827
H	-2.174103	-2.093294	3.698054
H	-3.367382	-1.522785	2.518992
H	-3.891191	-2.500860	3.903000
C	1.711249	-3.030080	-2.939811
H	0.969272	-3.827513	-3.157303
H	2.668817	-3.284593	-3.440189
H	1.861833	-3.027788	-1.843702
C	0.648171	1.969814	-2.468501
H	-0.360160	2.428529	-2.515723
H	0.905246	1.851576	-1.399401
H	1.369791	2.670626	-2.937361
C	-0.445100	-0.518384	-6.672226
H	0.339653	-0.804993	-7.403573
H	-1.275328	-1.254031	-6.723119
H	-0.842849	0.479244	-6.955969
H	0.675632	-2.586722	-5.356721
H	-0.292915	1.568301	-4.926985

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Figure_S9_imid-2_modeD_ed(AS) / electronic energy: -4442.828215219654 a.u. / lowest freq: -8.44 cm-1

C	2.971778	1.141990	-0.472217
H	3.449087	0.537108	0.311195
C	2.332548	2.441744	0.053252
H	2.454098	3.265587	-0.670072
C	0.611993	0.934843	-0.521837
C	1.805220	-0.775236	-1.741279
C	1.138687	-0.723265	-2.973856
C	2.482946	-1.952667	-1.382576
C	1.194093	-1.790314	-3.863835
H	0.598387	0.192033	-3.230009
C	2.537553	-3.018479	-2.286131
C	1.917038	-2.934572	-3.529105
H	0.675530	-1.722738	-4.822838

H	3.067379	-3.923734	-1.983457
H	1.979060	-3.773247	-4.226050
S	3.303558	-2.176953	0.198805
O	3.347747	-3.654142	0.411475
O	2.431389	-1.532492	1.228861
O	4.634492	-1.557441	0.058686
Cu	-1.086315	-0.055861	-0.877214
C	3.970386	1.391135	-1.576717
C	5.345315	1.231615	-1.328588
C	3.554114	1.817331	-2.852151
C	6.280025	1.469182	-2.340593
H	5.696717	0.932984	-0.349139
C	4.491920	2.052327	-3.861358
H	2.505646	1.961177	-3.069543
C	5.853695	1.876126	-3.606779
H	7.336179	1.341397	-2.141482
H	4.162325	2.372760	-4.841201
H	6.578820	2.059784	-4.388986
N	1.774358	0.396120	-0.939357
N	0.899889	2.073437	0.133006
C	-2.104351	-1.773652	-0.451624
C	-2.341010	-2.606203	-1.631486
C	-3.648894	-2.737950	-2.135485
C	-1.311241	-3.306664	-2.283797
C	-3.914156	-3.531083	-3.247410
C	-1.575231	-4.091692	-3.402298
C	-2.877800	-4.210576	-3.891650
H	-4.938121	-3.615349	-3.620449
H	-0.753324	-4.617510	-3.896641
H	-3.084239	-4.829866	-4.767727
C	-0.904481	-1.714589	0.291939
C	-0.939185	-1.375802	1.732223
H	0.051519	-1.092745	2.113239
H	-1.656902	-0.575934	1.957361
H	-0.285768	-3.230487	-1.912029
H	-0.027838	-2.290156	-0.030798
P	-0.392009	-3.539784	3.151607
O	0.330417	-4.317698	1.926078
O	0.715946	-3.030820	4.009225
O	-1.432511	-4.558704	3.813380
O	-1.434902	-2.514852	2.541665
Na	2.644713	-3.471224	2.709145
H	-3.020231	-1.438508	0.049234
H	-4.455177	-2.179944	-1.650342
C	-0.411818	-4.987048	0.906464
H	0.253800	-5.093028	0.042207
H	-0.727278	-5.981455	1.251508
H	-1.295881	-4.404472	0.609106
C	-0.948413	-5.590696	4.672740
H	-1.823913	-6.127330	5.049600
H	-0.306158	-6.294868	4.124045
H	-0.387559	-5.169320	5.517296
C	-0.095958	3.051938	0.397636
C	-0.410191	4.046648	-0.567324
C	-0.688630	3.127151	1.681937
C	-1.262714	5.105125	-0.222361
C	-1.524935	4.205003	2.001825
C	-1.812610	5.195081	1.059596
H	2.502997	1.014041	2.414825
H	3.366867	1.787253	4.583441
C	2.881545	2.023511	2.499588
C	3.370710	2.458326	3.734299
C	2.877318	2.888117	1.388244
C	3.862028	3.757756	3.874651
H	4.239610	4.093168	4.831892
C	3.376827	4.194419	1.542510
C	3.865673	4.624532	2.779674
H	3.383897	4.884575	0.708069
H	4.245926	5.631867	2.889762
C	-2.224619	1.006074	-2.203903
H	-1.598505	1.898245	-2.343110
C	-2.530233	0.321619	-3.517678
H	-3.205597	-0.537382	-3.392901
H	-3.027589	0.992439	-4.244604
H	-1.636001	-0.067493	-4.038993
B	-3.353448	1.240465	-1.217158
O	-4.593292	0.599993	-1.247253
O	-3.285230	2.115237	-0.124151
C	-4.629605	2.312334	0.347121
C	-5.328522	0.977850	-0.070108
C	-4.635452	2.559608	1.841169
H	-4.022873	1.826586	2.380203
H	-4.250013	3.558775	2.075907
H	-5.660341	2.509323	2.237122
C	-5.192111	3.519291	-0.390122
H	-5.244460	3.338670	-1.473115
H	-6.197473	3.789614	-0.037424
H	-4.532077	4.381934	-0.228800

C -6.793177 1.120887 -0.428559
H -7.371384 1.512538 0.421347
H -6.938821 1.793179 -1.282993
H -7.217316 0.143017 -0.696221
C -5.150718 -0.112384 0.976512
H -5.436104 -1.085950 0.553569
H -4.107448 -0.178139 1.314550
H -5.776143 0.065063 1.862583
C 0.148801 4.033990 -1.965535
H 0.629855 3.072643 -2.221187
H -0.669492 4.193374 -2.699320
H 0.891194 4.851767 -2.076342
C -0.445658 2.093985 2.745469
H 0.083065 2.559419 3.603600
H -1.417070 1.688457 3.098576
H 0.157915 1.246495 2.376397
C -2.704811 6.342605 1.433930
H -3.701358 5.961048 1.738850
H -2.256586 6.900977 2.282491
H -2.844511 7.045724 0.585486
H -1.490942 5.868169 -0.957677
H -1.957928 4.272405 2.993604
123
Figure_S9_imid-2_modeD_ts(AS)_01 / electronic energy: -4442.816117249291 a.u. / lowest freq: -255.52 cm-1
C 3.177446 0.452157 -0.478116
H 3.482463 -0.268670 0.294640
C 2.857053 1.857116 0.068613
H 3.157163 2.641563 -0.646313
C 0.842113 0.802781 -0.529621
C 1.593242 -1.100163 -1.808297
C 0.982072 -0.849286 -3.044519
C 1.939008 -2.419111 -1.471288
C 0.771278 -1.874973 -3.960446
H 0.701397 0.180524 -3.281134
C 1.730840 -3.441952 -2.401584
C 1.170476 -3.173145 -3.647111
H 0.301514 -1.655425 -4.921763
H 2.003877 -4.460071 -2.117852
H 1.024312 -3.983916 -4.363980
S 2.645376 -2.868489 0.117227
O 2.335467 -4.317162 0.289139
O 1.922106 -2.052965 1.139914
O 4.085742 -2.571536 0.014447
Cu -1.022472 0.172432 -0.876329
C 4.219765 0.474469 -1.569460
C 5.504502 -0.042279 -1.324731
C 3.939575 1.032022 -2.831368
C 6.479056 -0.021464 -2.326831
H 5.756999 -0.454015 -0.355863
C 4.916480 1.049582 -3.830632
H 2.965036 1.446281 -3.045948
C 6.184631 0.521364 -3.579544
H 7.464565 -0.423547 -2.130538
H 4.690078 1.474079 -4.800147
H 6.940431 0.536646 -4.354091
N 1.842486 0.023546 -0.973235
N 1.377523 1.825349 0.155254
C -2.463729 -1.240897 -0.565842
C -2.912628 -2.010055 -1.722524
C -4.232529 -1.860241 -2.189129
C -2.068524 -2.907387 -2.400360
C -4.687699 -2.578510 -3.290546
C -2.521735 -3.617695 -3.506760
C -3.834042 -3.458822 -3.957840
H -5.716223 -2.446957 -3.635348
H -1.844620 -4.304391 -4.021812
H -4.189043 -4.020055 -4.825205
C -1.309949 -1.555318 0.211214
C -1.108030 -1.008410 1.490875
H -0.119425 -1.111905 1.941865
H -1.687635 -0.134707 1.794516
H -1.037972 -3.042470 -2.062351
H -0.609474 -2.334528 -0.110165
P -1.239587 -3.273968 3.290550
O -0.816250 -4.224961 2.008976
O 0.062943 -3.098303 4.016482
O -2.337701 -4.149456 4.102758
O -2.061657 -2.078024 2.786545
Na 1.593093 -4.038912 2.590066
H -3.256237 -0.677323 -0.060982
H -4.891982 -1.149149 -1.683817
C -1.800952 -4.703776 1.106810
H -1.297834 -4.966059 0.167173
H -2.299755 -5.599471 1.507273
H -2.563570 -3.937311 0.901119
C -1.892372 -5.255465 4.872979
H -2.766104 -5.671302 5.386367
H -1.452606 -6.039926 4.236885

H -1.147840 -4.949246 5.621394
C 0.628230 2.997860 0.442924
C 0.522690 4.044612 -0.512558
C 0.078531 3.186293 1.734764
C -0.084068 5.256123 -0.151930
C -0.507838 4.413943 2.070251
C -0.590166 5.449587 1.136659
H 2.731658 0.384921 2.407353
H 3.762338 0.914743 4.576027
C 3.321978 1.286252 2.501901
C 3.905002 1.583093 3.736793
C 3.496774 2.149876 1.403490
C 4.669098 2.741652 3.890225
H 5.118998 2.970479 4.847617
C 4.270650 3.313030 1.570931
C 4.852215 3.605244 2.808172
H 4.420385 3.999381 0.746808
H 5.443825 4.503575 2.928387
C -1.897865 1.437746 -2.207592
H -1.071343 2.149544 -2.338064
C -2.337271 0.835794 -3.517633
H -3.162722 0.120932 -3.395341
H -2.703906 1.604736 -4.222869
H -1.532201 0.300494 -4.050329
B -2.956731 1.929388 -1.220662
O -4.300533 1.590499 -1.280772
O -2.693575 2.752474 -0.128197
C -3.966822 3.245027 0.345726
C -4.950126 2.112718 -0.102641
C -3.919762 3.454962 1.843514
H -3.511234 2.583029 2.368858
H -3.300753 4.322998 2.097857
H -4.927311 3.651786 2.237477
C -4.227801 4.562231 -0.368693
H -4.301850 4.422426 -1.456357
H -5.152482 5.041997 -0.019396
H -3.395645 5.252297 -0.178137
C -6.335286 2.593274 -0.480513
H -6.820198 3.102206 0.365135
H -6.310572 3.284597 -1.331350
H -6.968446 1.740573 -0.761815
C -5.048890 0.995474 0.924380
H -5.544950 0.122033 0.478845
H -4.060115 0.681238 1.285502
H -5.637423 1.299584 1.800807
C 1.052147 3.927238 -1.917480
H 1.336014 2.892905 -2.181664
H 0.271302 4.245454 -2.640380
H 1.937952 4.585537 -2.036626
C 0.103242 2.114843 2.788258
H 0.726440 2.448353 3.644382
H -0.929665 1.923533 3.148055
H 0.507451 1.160295 2.408073
C -1.219662 6.755143 1.526702
H -2.270806 6.587111 1.840878
H -0.656493 7.201722 2.372944
H -1.218300 7.477991 0.683338
H -0.154130 6.055810 -0.880390
H -0.908699 4.562822 3.066657

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Figure_S9_imid-2_modeD_ts(AS)_02 / electronic energy: -4442.816120685304 a.u. / lowest freq: -265.70 cm-1

C 3.061736 0.475909 -0.821852
H 3.480885 0.298755 0.178481
C 2.431650 1.870919 -0.998435
H 2.610939 2.263945 -2.013414
C 0.707446 0.271730 -0.911672
C 1.903946 -1.814665 -1.115402
C 1.289688 -2.345273 -2.258981
C 2.526785 -2.686027 -0.206307
C 1.332414 -3.709581 -2.527154
H 0.799661 -1.654603 -2.950670
C 2.573898 -4.053719 -0.491686
C 1.997533 -4.565145 -1.650612
H 0.852095 -4.100603 -3.426785
H 3.057001 -4.714436 0.230124
H 2.048966 -5.636527 -1.855979
S 3.248218 -2.137001 1.346407
O 3.248158 -3.349823 2.216967
O 2.307882 -1.109421 1.889363
O 4.591194 -1.627718 1.022805
Cu -0.968166 -0.824533 -0.829428
C 4.123909 0.181567 -1.853155
C 5.479165 0.166995 -1.478237
C 3.788382 -0.048979 -3.200718
C 6.473448 -0.096535 -2.424919
H 5.769148 0.368538 -0.454840
C 4.785561 -0.313368 -4.143603
H 2.757295 -0.033214 -3.522122

C	6.126915	-0.339527	-3.755847
H	7.513838	-0.108524	-2.126793
H	4.517818	-0.497119	-5.176054
H	6.898029	-0.543366	-4.487435
N	1.869722	-0.402073	-0.959818
N	0.985773	1.584125	-0.844341
C	-2.140284	-2.150097	0.207961
C	-2.403092	-3.452795	-0.397089
C	-3.711204	-3.775123	-0.804446
C	-1.392565	-4.410499	-0.596160
C	-3.996970	-5.005220	-1.388003
C	-1.677270	-5.636261	-1.188435
C	-2.980800	-5.941956	-1.586368
H	-5.020018	-5.234146	-1.696151
H	-0.873668	-6.361943	-1.340072
H	-3.202355	-6.906172	-2.049710
C	-0.988559	-1.833623	0.980570
C	-0.886272	-0.623306	1.694067
H	0.105678	-0.307917	2.019854
H	-1.593461	0.180176	1.476702
H	-0.365937	-4.186582	-0.295349
H	-0.171315	-2.556787	1.086711
P	-0.733747	-0.346244	4.585247
O	-1.664352	-0.136378	5.900076
O	0.474951	-1.127981	5.012025
O	-0.333599	1.168831	4.125735
O	-1.642311	-0.847641	3.445946
Na	1.912656	-2.420941	3.934780
H	-3.036033	-1.543015	0.378014
H	-4.501062	-3.030230	-0.674817
C	-2.883092	0.577522	5.771590
H	-3.311953	0.683187	6.774409
H	-2.718973	1.580858	5.348690
H	-3.596575	0.039358	5.130829
C	0.708241	1.845983	4.803456
H	0.743665	2.870740	4.415845
H	0.528873	1.888657	5.889312
H	1.682281	1.365470	4.627563
C	0.008536	2.572746	-1.142331
C	-0.246686	2.958385	-2.486628
C	-0.622610	3.283814	-0.091746
C	-1.091224	4.046512	-2.749825
C	-1.446277	4.378154	-0.386098
C	-1.684625	4.763101	-1.706815
H	2.483262	1.687743	1.764322
H	3.249440	3.383346	3.370159
C	2.864468	2.628597	1.391233
C	3.296768	3.589751	2.308839
C	2.916823	2.886855	0.007351
C	3.787016	4.817048	1.858681
H	4.119994	5.560897	2.570834
C	3.415836	4.126597	-0.432725
C	3.847275	5.084706	0.489408
H	3.465278	4.357653	-1.489516
H	4.226655	6.036834	0.141603
C	-2.034704	-0.528189	-2.533781
H	-1.359763	0.174973	-3.039752
C	-2.315463	-1.745331	-3.379205
H	-3.014012	-2.442370	-2.895098
H	-2.777998	-1.477863	-4.347571
H	-1.411640	-2.327101	-3.631613
B	-3.195742	0.167475	-1.824600
O	-4.444730	-0.403132	-1.623150
O	-3.133035	1.443180	-1.265973
C	-4.493474	1.856032	-1.007808
C	-5.223181	0.489827	-0.799688
C	-4.546643	2.764951	0.200782
H	-3.988627	2.352280	1.050126
H	-4.130190	3.752144	-0.031646
H	-5.587898	2.922541	0.517513
C	-4.976256	2.592274	-2.248769
H	-4.984678	1.934384	-3.129139
H	-5.986638	3.003556	-2.116845
H	-4.296611	3.426268	-2.465274
C	-6.660955	0.464388	-1.274551
H	-7.261249	1.223339	-0.752106
H	-6.739174	0.644822	-2.353451
H	-7.112111	-0.515895	-1.067768
C	-5.144418	0.006909	0.641245
H	-5.448061	-1.047460	0.699485
H	-4.128893	0.093942	1.052363
H	-5.812646	0.581884	1.296957
C	0.371997	2.261973	-3.669799
H	0.864564	1.312466	-3.395800
H	-0.413956	2.019048	-4.416001
H	1.119767	2.930809	-4.144797
C	-0.438502	2.923718	1.354569
H	0.061281	3.759889	1.887028

H -1.429146 2.740283 1.821242
H 0.167581 2.011349 1.485123
C -2.572475 5.939651 -1.989579
H -3.581988 5.758769 -1.564682
H -2.142346 6.850970 -1.523550
H -2.678732 6.119075 -3.080591
H -1.277523 4.341873 -3.776043
H -1.910459 4.933078 0.421570
123
Figure_S9_imid-2_modeD_ts(AS)_03 / electronic energy: -4442.807707406971 a.u. / lowest freq: -260.34 cm-1
C -1.148180 1.888501 1.639143
H -2.122668 1.500986 1.962270
C -1.208167 2.745741 0.356959
H -0.604436 3.661734 0.459922
C -0.020165 0.757510 -0.122950
C 0.187340 -0.286455 2.044282
C 1.557921 -0.565425 1.932674
C -0.585050 -1.043142 2.947253
C 2.162193 -1.561677 2.687895
H 2.158025 0.020507 1.232672
C 0.040922 -2.027553 3.719627
C 1.402008 -2.290124 3.599946
H 3.225472 -1.765021 2.547683
H -0.577107 -2.607311 4.406458
H 1.861559 -3.071145 4.209485
S -2.365840 -0.868463 3.161869
O -2.800018 -2.123704 3.843062
O -2.941872 -0.804622 1.782033
O -2.571183 0.347723 3.965773
Cu 0.993657 -0.811070 -0.919448
C -0.520122 2.635358 2.791684
C -1.334991 3.189119 3.794778
C 0.870268 2.842292 2.854574
C -0.767430 3.902632 4.854794
H -2.411091 3.076620 3.752937
C 1.434368 3.554977 3.915718
H 1.517848 2.450013 2.086351
C 0.616437 4.082093 4.917431
H -1.401781 4.321208 5.625372
H 2.506003 3.701176 3.958911
H 1.054040 4.635551 5.738135
N -0.321876 0.731360 1.194980
N -0.575487 1.860359 -0.643790
C 1.015908 -2.874283 -1.225722
C 2.255064 -3.569132 -0.883977
C 3.194117 -3.861933 -1.892084
C 2.569009 -3.945282 0.434716
C 4.416540 -4.452281 -1.586619
C 3.791077 -4.531973 0.740925
C 4.728360 -4.776823 -0.265550
H 5.132101 -4.660792 -2.385649
H 4.013536 -4.805655 1.775927
H 5.690607 -5.234411 -0.023592
C -0.024570 -2.570830 -0.317177
C -1.266586 -2.056286 -0.739690
H -1.882687 -1.509501 -0.022699
H -1.371246 -1.767250 -1.786779
H 1.845555 -3.774963 1.233550
H 0.108473 -2.773810 0.750574
P -3.979666 -3.220211 -1.062491
O -4.597590 -4.211827 -2.195983
O -4.895979 -3.295583 0.124092
O -4.014385 -1.745894 -1.763756
O -2.476330 -3.528753 -0.924282
Na -4.335777 -2.826685 2.214771
H 0.762502 -2.860620 -2.294320
H 2.953890 -3.617544 -2.930491
C -3.923397 -4.338982 -3.435584
H -4.519128 -5.004618 -4.070471
H -3.822766 -3.365591 -3.941328
H -2.920725 -4.772365 -3.305294
C -5.253253 -1.066538 -1.850439
H -5.092773 -0.154755 -2.436539
H -6.017575 -1.676513 -2.357222
H -5.629595 -0.789792 -0.854710
C -0.268513 2.320462 -1.950937
C 0.742490 3.296116 -2.150442
C -1.043722 1.892752 -3.056998
C 0.926082 3.857861 -3.422250
C -0.821912 2.454956 -4.321693
C 0.150729 3.440296 -4.508512
H -3.417285 1.128040 -0.031474
H -5.682900 1.810338 -0.709781
C -3.621286 2.175260 -0.206331
C -4.909025 2.557126 -0.592836
C -2.608492 3.140203 -0.046461
C -5.200174 3.902209 -0.827583
H -6.197661 4.195596 -1.128104

C -2.915617 4.492556 -0.284260
C -4.204434 4.868870 -0.673429
H -2.157811 5.258205 -0.174111
H -4.430986 5.911344 -0.856079
C 2.645051 -0.466114 -2.076790
H 2.867843 -1.498844 -2.376589
C 2.368210 0.395721 -3.289959
H 2.459739 1.466244 -3.064502
H 3.096839 0.209392 -4.099809
H 1.376700 0.237340 -3.748426
B 3.728984 0.015666 -1.110557
O 4.349401 1.252499 -1.182474
O 4.247687 -0.743640 -0.066347
C 5.475068 -0.113774 0.353708
C 5.239940 1.380233 -0.053843
C 5.673336 -0.338489 1.837228
H 4.820122 0.018440 2.427955
H 5.803145 -1.410558 2.042067
H 6.574787 0.179539 2.195684
C 6.600827 -0.768822 -0.433170
H 6.476670 -0.614800 -1.514660
H 7.588363 -0.384977 -0.141622
H 6.588420 -1.851570 -0.247582
C 6.486105 2.118841 -0.493024
H 7.230218 2.150315 0.315986
H 6.950999 1.653435 -1.370573
H 6.238424 3.155941 -0.757532
C 4.509590 2.169128 1.019511
H 4.197092 3.141788 0.617928
H 3.610090 1.636122 1.354864
H 5.142419 2.354116 1.898268
C 1.681329 3.725030 -1.055182
H 1.629830 3.059771 -0.173784
H 2.728027 3.688635 -1.424365
H 1.445427 4.764494 -0.745844
C -2.124515 0.855849 -2.935311
H -3.102776 1.307251 -3.202934
H -1.913751 0.014173 -3.628166
H -2.200901 0.442734 -1.914716
C 0.359873 4.027992 -5.873196
H 0.643069 3.224593 -6.585471
H -0.579774 4.506602 -6.220938
H 1.164076 4.794254 -5.870110
H 1.694959 4.607751 -3.568763
H -1.418117 2.128726 -5.166582

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Figure_S9_imid-2_modeD_ts(AS)_04 / electronic energy: -4442.807721719831 a.u. / lowest freq: -259.92 cm-1

C -1.152471 1.887257 1.637361
H -2.126977 1.498982 1.959382
C -1.212445 2.744354 0.354929
H -0.616632 3.665196 0.460677
C -0.016381 0.759864 -0.121923
C 0.180339 -0.288888 2.044311
C 1.550500 -0.571391 1.934627
C -0.595070 -1.044380 2.945901
C 2.150895 -1.570931 2.688579
H 2.153414 0.014236 1.236770
C 0.027117 -2.032387 3.716793
C 1.387342 -2.299441 3.597763
H 3.213828 -1.776967 2.549553
H -0.593560 -2.611078 4.402150
H 1.843720 -3.083331 4.205985
S -2.374746 -0.862172 3.164232
O -2.814468 -2.117704 3.841149
O -2.952566 -0.790497 1.785691
O -2.571927 0.352485 3.972413
Cu 0.996210 -0.809035 -0.919458
C -0.527053 2.635103 2.790758
C -1.345513 3.197897 3.785873
C 0.864075 2.834306 2.862320
C -0.781142 3.912679 4.846719
H -2.421919 3.090839 3.737298
C 1.424964 3.548354 3.924264
H 1.514914 2.434872 2.100601
C 0.603262 4.084488 4.918070
H -1.418322 4.338044 5.611222
H 2.497111 3.688517 3.974257
H 1.038436 4.638881 5.739435
N -0.325004 0.730501 1.194494
N -0.568997 1.863722 -0.643261
C 1.011261 -2.872743 -1.226528
C 2.249414 -3.571258 -0.888618
C 3.185803 -3.864571 -1.899040
C 2.565038 -3.950298 0.428852
C 4.407509 -4.458121 -1.596855
C 3.786335 -4.540275 0.731733
C 4.721176 -4.785513 -0.276919
H 5.121070 -4.666899 -2.397601

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 H   4.010161  -4.816192   1.765835
 H   5.682856  -5.245656  -0.037592
 C  -0.024671  -2.565454  -0.314151
 C  -1.266573  -2.046050  -0.730817
 H  -1.874589  -1.489703  -0.014602
 H  -1.378526  -1.767026  -1.779973
 H   1.843563  -3.779476   1.229369
 H   0.113071  -2.766883   0.753256
 P  -3.987573  -3.204929  -1.056896
 O  -4.582154  -4.204478  -2.196360
 O  -4.927856  -3.271578   0.111345
 O  -4.005488  -1.736520  -1.771480
 O  -2.488228  -3.512469  -0.879990
Na  -4.352282  -2.807310   2.203165
 H   0.754716  -2.857446  -2.294388
 H   2.944218  -3.617706  -2.936554
 C  -3.885749  -4.334799  -3.423222
 H  -4.461567  -5.015146  -4.060927
 H  -3.790122  -3.365249  -3.937480
 H  -2.879394  -4.752734  -3.272281
 C  -5.251342  -1.090959  -1.958492
 H  -5.064436  -0.154861  -2.496245
 H  -5.940646  -1.706411  -2.557925
 H  -5.733897  -0.860512  -0.997370
 C  -0.252942   2.328724  -1.946598
 C   0.757580   3.307138  -2.134812
 C  -1.018444   1.903336  -3.060380
 C   0.949569   3.874315  -3.402939
 C  -0.788489   2.471285  -4.321078
 C   0.183186   3.459632  -4.496596
 H  -3.402601   1.106974  -0.051504
 H  -5.671204   1.768219  -0.739175
 C  -3.616435   2.152650  -0.223386
 C  -4.905871   2.522745  -0.615281
 C  -2.614216   3.127030  -0.054752
 C  -5.209404   3.865749  -0.846393
 H  -6.208226   4.150195  -1.151038
 C  -2.933681   4.477141  -0.288828
 C  -4.224286   4.841880  -0.683240
 H  -2.184206   5.249903  -0.171613
 H  -4.460476   5.882720  -0.862975
 C   2.650028  -0.465146  -2.072876
 H   2.871389  -1.497609  -2.374745
 C   2.379275   0.400976  -3.284274
 H   2.466887   1.470834  -3.054013
 H   3.113743   0.219680  -4.090015
 H   1.391231   0.242110  -3.749884
 B   3.732084   0.011708  -1.102162
 O   4.353378   1.248470  -1.167626
 O   4.248019  -0.752312  -0.060133
 C   5.475075  -0.125205   0.364874
 C   5.242166   1.370735  -0.036987
 C   5.670249  -0.356073   1.847834
 H   4.816044  -0.001015   2.438256
 H   5.798977  -1.429026   2.048649
 H   6.571284   0.160015   2.210095
 C   6.601688  -0.778198  -0.422504
 H   6.479813  -0.619686  -1.503607
 H   7.589078  -0.396666  -0.127444
 H   6.587634  -1.861694  -0.241435
 C   6.489811   2.109773  -0.471221
 H   7.232299   2.138203   0.339398
 H   6.956133   1.646749  -1.349262
 H   6.243404   3.147871  -0.732973
 C   4.510885   2.156262   1.038261
 H   4.200770   3.131117   0.640206
 H   3.609814   1.623468   1.369690
 H   5.142210   2.336680   1.919047
 C   1.687447   3.733626  -1.031087
 H   1.627547   3.067849  -0.150698
 H   2.737055   3.696009  -1.391743
 H   1.450326   4.773092  -0.722675
 C  -2.096654   0.862409  -2.951655
 H  -3.074346   1.311968  -3.224360
 H  -1.878050   0.024522  -3.646701
 H  -2.178870   0.444312  -1.933776
 C   0.401133   4.053484  -5.857232
 H   0.691462   3.253716  -6.570715
 H  -0.536990   4.531438  -6.209955
 H   1.203529   4.821551  -5.844964
 H   1.717969   4.626365  -3.540663
 H  -1.377401   2.146985  -5.171805
123
Figure_S9_imid-2_modeD_ts(AS)_05 / electronic energy: -4442.807644380910 a.u. / lowest freq: -260.13 cm-1
 C  -0.331492   2.365787   1.502201
 H  -1.413485   2.520163   1.594568
 C   0.318919   3.182676   0.367192
 H   1.253222   3.660428   0.702365
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C	0.442136	0.886295	-0.191963
C	-0.379324	-0.202183	1.802470
C	0.654944	-1.145919	1.898440
C	-1.608707	-0.482861	2.430865
C	0.494300	-2.333991	2.600058
H	1.608133	-0.937660	1.406201
C	-1.751238	-1.674826	3.149135
C	-0.713620	-2.597284	3.242011
H	1.319838	-3.047993	2.632301
H	-2.715976	-1.874177	3.618898
H	-0.855354	-3.522497	3.804955
S	-3.056847	0.582847	2.346773
O	-4.212589	-0.276402	2.730923
O	-3.163146	0.996313	0.911720
O	-2.808728	1.693664	3.281409
Cu	0.685328	-0.939531	-1.038074
C	0.315291	2.638542	2.839217
C	-0.322406	3.476256	3.771164
C	1.582390	2.114616	3.152506
C	0.277959	3.750548	5.003793
H	-1.280358	3.925302	3.541279
C	2.179566	2.389580	4.385305
H	2.105727	1.492887	2.444077
C	1.525899	3.203991	5.312581
H	-0.222483	4.391793	5.717773
H	3.151122	1.973802	4.619509
H	1.989633	3.417997	6.266793
N	-0.108540	0.965170	1.040401
N	0.636446	2.138284	-0.629057
C	-0.181719	-2.715610	-1.636725
C	0.449980	-3.950695	-1.177300
C	1.323887	-4.644835	-2.036835
C	0.229705	-4.485506	0.105484
C	1.994608	-5.787172	-1.612530
C	0.901918	-5.626108	0.530680
C	1.799441	-6.275371	-0.319588
H	2.673643	-6.302108	-2.296309
H	0.719535	-6.016084	1.535767
H	2.330185	-7.168878	0.017399
C	-1.154228	-1.974371	-0.916597
C	-1.962363	-1.007187	-1.542409
H	-2.506075	-0.293677	-0.916273
H	-1.672791	-0.653663	-2.532425
H	-0.479404	-4.003291	0.780691
H	-1.377206	-2.231501	0.124774
P	-4.807786	-1.684521	-1.598971
O	-4.630292	-2.091803	-0.012687
O	-5.472511	-0.340369	-1.531217
O	-5.745880	-2.853169	-2.221436
O	-3.470280	-1.905200	-2.322666
Na	-5.437697	0.175190	0.710957
H	-0.159539	-2.560684	-2.723861
H	1.472583	-4.275197	-3.055106
C	-4.095773	-3.352948	0.352895
H	-3.612996	-3.244631	1.333223
H	-4.890847	-4.110259	0.426928
H	-3.347562	-3.697315	-0.377608
C	-7.132466	-2.845999	-1.920365
H	-7.588329	-3.689014	-2.451011
H	-7.312070	-2.972668	-0.840795
H	-7.610911	-1.913135	-2.251182
C	1.384939	2.432000	-1.798420
C	2.750433	2.805724	-1.701253
C	0.745796	2.470884	-3.062391
C	3.430379	3.259759	-2.840447
C	1.456843	2.909530	-4.188096
C	2.790419	3.312981	-4.082672
H	-2.228614	2.917255	-0.662881
H	-3.657481	4.672330	-1.627403
C	-1.861066	3.932708	-0.700257
C	-2.675936	4.926575	-1.248872
C	-0.581634	4.249590	-0.207021
C	-2.224943	6.246651	-1.310647
H	-2.856946	7.015227	-1.736356
C	-0.139021	5.583556	-0.274306
C	-0.957990	6.574774	-0.823224
H	0.842058	5.858635	0.092418
H	-0.608806	7.598052	-0.872471
C	2.505544	-1.421330	-1.843000
H	2.282949	-2.421508	-2.236156
C	2.925315	-0.488254	-2.956469
H	3.458750	0.392935	-2.577488
H	3.632408	-0.977271	-3.650743
H	2.096690	-0.130677	-3.591464
B	3.441318	-1.553397	-0.639651
O	4.549480	-0.752463	-0.418824
O	3.317544	-2.521892	0.349861
C	4.584453	-2.587912	1.037692

C 5.148108 -1.140339 0.836994
C 4.346940 -2.985392 2.478625
H 3.650019 -2.306448 2.986127
H 3.921819 -3.998252 2.523195
H 5.288421 -2.993708 3.046824
C 5.420677 -3.643908 0.328943
H 5.606413 -3.370439 -0.719704
H 6.391217 -3.801307 0.819834
H 4.878621 -4.599282 0.332113
C 6.653849 -1.060983 0.705361
H 7.148915 -1.440485 1.611030
H 7.019825 -1.635823 -0.153945
H 6.966630 -0.016878 0.567450
C 4.658879 -0.174745 1.901595
H 4.902700 0.855595 1.612429
H 3.570732 -0.247285 2.025535
H 5.123724 -0.369158 2.877856
C 3.534229 2.679641 -0.422674
H 2.999784 2.081062 0.338341
H 4.496065 2.161586 -0.621925
H 3.748523 3.688995 -0.013902
C -0.689103 2.066507 -3.257818
H -1.278037 2.941153 -3.605498
H -0.747174 1.265216 -4.024263
H -1.151808 1.680663 -2.332216
C 3.522911 3.783568 -5.304766
H 3.540508 2.973320 -6.063807
H 3.006249 4.669139 -5.731063
H 4.570794 4.067728 -5.069924
H 4.471402 3.550984 -2.760189
H 0.965469 2.943566 -5.154046
123
Figure_S9_imid-2_modeD_ts(AS)_06 / electronic energy: -4442.807603325020 a.u. / lowest freq: -264.33 cm-1
C -0.292954 2.382648 1.496744
H -1.371892 2.552912 1.596308
C 0.361119 3.185071 0.353710
H 1.306221 3.647992 0.679388
C 0.445824 0.884936 -0.196832
C -0.378298 -0.182773 1.808353
C 0.641378 -1.142518 1.902870
C -1.608284 -0.441120 2.445288
C 0.465828 -2.325154 2.610176
H 1.595319 -0.951370 1.405121
C -1.766536 -1.628689 3.167423
C -0.743123 -2.567200 3.258499
H 1.280630 -3.051519 2.641138
H -2.731844 -1.811455 3.642568
H -0.896944 -3.488180 3.825219
S -3.041108 0.645748 2.363677
O -4.207098 -0.194277 2.760190
O -3.150996 1.049956 0.926589
O -2.772676 1.758729 3.290148
Cu 0.662389 -0.948103 -1.033510
C 0.367276 2.652126 2.827804
C -0.251397 3.503154 3.760459
C 1.629430 2.112396 3.133748
C 0.362355 3.775060 4.987027
H -1.204658 3.964468 3.535638
C 2.240088 2.384963 4.360447
H 2.138588 1.480760 2.423932
C 1.605032 3.212778 5.288785
H -0.123490 4.426733 5.701645
H 3.207750 1.957101 4.588952
H 2.079241 3.425056 6.238223
N -0.093251 0.977094 1.039700
N 0.653024 2.132347 -0.641854
C -0.224411 -2.716057 -1.626036
C 0.389621 -3.957172 -1.159269
C 1.255261 -4.668320 -2.013389
C 0.160768 -4.481255 0.126357
C 1.909704 -5.817205 -1.581309
C 0.816853 -5.628217 0.559312
C 1.706528 -6.294891 -0.285742
H 2.582406 -6.345478 -2.261168
H 0.628274 -6.009241 1.566684
H 2.224531 -7.193497 0.057459
C -1.191051 -1.958987 -0.914138
C -1.975074 -0.978850 -1.550172
H -2.512892 -0.253888 -0.932534
H -1.669016 -0.633343 -2.537960
H -0.542221 -3.985328 0.797862
H -1.428404 -2.209576 0.125854
P -4.810726 -1.653520 -1.579299
O -4.586093 -2.127440 -0.018830
O -5.471617 -0.311681 -1.449931
O -5.769066 -2.796108 -2.220212
O -3.494819 -1.843953 -2.350423
Na -5.435764 0.248132 0.750774

H -0.195091 -2.565681 -2.713580
H 1.410300 -4.307070 -3.033725
C -4.089280 -3.426501 0.258339
H -3.623459 -3.408302 1.251880
H -4.902546 -4.168148 0.259800
H -3.335490 -3.733267 -0.483376
C -7.148717 -2.790910 -1.888356
H -7.619076 -3.621854 -2.425339
H -7.305621 -2.937955 -0.807852
H -7.631139 -1.850190 -2.189739
C 1.397313 2.410157 -1.817814
C 2.769851 2.760250 -1.732442
C 0.748610 2.458240 -3.076593
C 3.448623 3.199055 -2.878324
C 1.458275 2.881198 -4.209115
C 2.799774 3.260461 -4.115556
H -2.199378 2.959682 -0.653942
H -3.607620 4.736196 -1.609270
C -1.815379 3.968811 -0.696727
C -2.618666 4.974944 -1.240037
C -0.526521 4.265444 -0.215568
C -2.146634 6.287305 -1.308389
H -2.769713 7.065393 -1.729956
C -0.062808 5.591914 -0.289126
C -0.870220 6.595454 -0.832764
H 0.925765 5.851569 0.068623
H -0.504791 7.612789 -0.886991
C 2.474934 -1.458804 -1.839014
H 2.238116 -2.457604 -2.227098
C 2.904357 -0.536487 -2.957889
H 3.458228 0.334562 -2.584896
H 3.596001 -1.041238 -3.656368
H 2.078329 -0.163651 -3.587544
B 3.411649 -1.597760 -0.637349
O 4.529279 -0.808618 -0.422347
O 3.279893 -2.561849 0.355557
C 4.548950 -2.640554 1.038318
C 5.127231 -1.199466 0.832830
C 4.312936 -3.033297 2.480724
H 3.625314 -2.346200 2.989987
H 3.876890 -4.041356 2.528423
H 5.256548 -3.051077 3.045189
C 5.371636 -3.705864 0.327655
H 5.555894 -3.435445 -0.722056
H 6.342555 -3.872310 0.814820
H 4.820615 -4.656016 0.334105
C 6.633341 -1.135049 0.697142
H 7.127149 -1.518809 1.601708
H 6.991696 -1.713528 -0.162940
H 6.955945 -0.094102 0.557856
C 4.650456 -0.226746 1.896494
H 4.900599 0.800795 1.602691
H 3.562454 -0.291052 2.025724
H 5.118296 -0.421624 2.871253
C 3.561166 2.625191 -0.459356
H 3.023158 2.036817 0.307061
H 4.513517 2.091931 -0.664035
H 3.793930 3.632154 -0.054804
C -0.695459 2.081549 -3.259056
H -1.270661 2.967573 -3.600871
H -0.776023 1.282218 -4.025496
H -1.156771 1.703893 -2.329368
C 3.530629 3.714693 -5.344799
H 3.527290 2.902403 -6.101857
H 3.026594 4.608426 -5.769189
H 4.585375 3.980367 -5.119259
H 4.495221 3.472077 -2.807164
H 0.959626 2.922216 -5.171064

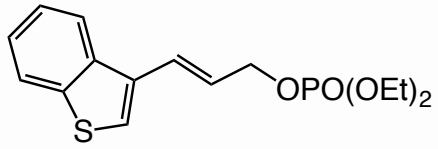
123

Figure_S9_imid-2_modeD_prod(AS) / electronic energy: -4442.827233578473 a.u. / lowest freq: 20.31 cm-1

C 3.302350 -0.047818 -0.637081
H 3.659354 -0.506622 0.295743
C 3.044615 1.469759 -0.520349
H 3.356133 1.999654 -1.434124
C 0.977980 0.366663 -0.724953
C 1.613214 -1.899579 -1.248936
C 0.943582 -2.082941 -2.466891
C 1.902860 -3.011698 -0.441114
C 0.579662 -3.354063 -2.897469
H 0.737579 -1.203448 -3.082753
C 1.536613 -4.284953 -0.888541
C 0.886929 -4.461630 -2.107402
H 0.061906 -3.476397 -3.851448
H 1.753676 -5.138739 -0.244054
H 0.611997 -5.466602 -2.434814
S 2.722977 -2.914893 1.165104
O 2.227671 -4.103430 1.912462
O 2.227656 -1.658325 1.806809

O	4.163387	-2.912179	0.866653
Cu	-0.900834	-0.284390	-0.983665
C	4.243606	-0.397917	-1.762418
C	5.503702	-0.954416	-1.481539
C	3.881972	-0.170139	-3.103866
C	6.377909	-1.286364	-2.520852
H	5.814132	-1.126376	-0.458924
C	4.758804	-0.504441	-4.139489
H	2.919678	0.259515	-3.348005
C	6.005334	-1.063291	-3.848521
H	7.345880	-1.715404	-2.296374
H	4.471290	-0.330339	-5.168276
H	6.683454	-1.321395	-4.651592
N	1.932750	-0.562225	-0.891923
N	1.565667	1.525479	-0.420881
C	-2.618789	-1.611386	-0.721247
C	-3.321592	-2.353706	-1.756566
C	-4.570343	-1.888079	-2.215576
C	-2.809644	-3.540696	-2.316836
C	-5.268688	-2.572759	-3.203676
C	-3.508444	-4.220972	-3.306954
C	-4.739256	-3.739106	-3.758722
H	-6.233035	-2.191871	-3.547370
H	-3.091826	-5.138798	-3.728685
H	-5.285671	-4.274850	-4.538135
C	-1.472173	-2.071942	-0.027838
C	-0.823960	-1.260425	0.891774
H	0.151607	-1.529298	1.301769
H	-1.365271	-0.449588	1.402338
H	-1.854823	-3.942509	-1.972645
H	-0.969743	-2.983585	-0.376487
P	-1.620413	-1.063898	4.163224
O	-1.667487	-2.579654	3.440861
O	-0.154446	-0.954710	4.516580
O	-2.529077	-1.317309	5.511192
O	-2.374028	-0.065747	3.336987
Na	0.990723	-2.674066	3.603048
H	-3.193812	-0.807007	-0.247965
H	-4.968680	-0.958389	-1.804169
C	-2.894818	-3.032897	2.915880
H	-2.700750	-3.901711	2.272115
H	-3.588849	-3.340973	3.715967
H	-3.388428	-2.249993	2.316464
C	-2.040785	-2.191812	6.502858
H	-2.774217	-2.224100	7.318533
H	-1.910172	-3.217304	6.116658
H	-1.075849	-1.852226	6.910656
C	0.858552	2.750485	-0.311198
C	0.834099	3.667726	-1.393748
C	0.304300	3.134986	0.934092
C	0.314199	4.955449	-1.201089
C	-0.186624	4.436190	1.103332
C	-0.183395	5.348399	0.045203
H	2.873112	0.807249	2.157722
H	3.966594	1.915339	4.059563
C	3.516380	1.653292	1.970921
C	4.135554	2.281118	3.055056
C	3.724016	2.120484	0.660190
C	4.969738	3.380704	2.844436
H	5.447940	3.866387	3.685155
C	4.567954	3.229181	0.461322
C	5.186147	3.853826	1.548590
H	4.745213	3.616402	-0.534320
H	5.831987	4.707006	1.386057
C	-1.583799	0.813016	-2.535232
H	-0.695935	1.427551	-2.728136
C	-2.015125	0.064789	-3.767494
H	-2.944748	-0.501573	-3.624796
H	-2.208749	0.762329	-4.601735
H	-1.257745	-0.644425	-4.141667
B	-2.639225	1.550763	-1.684498
O	-3.990762	1.274255	-1.723016
O	-2.341000	2.532003	-0.757094
C	-3.597782	3.152525	-0.375899
C	-4.624268	2.007122	-0.644262
C	-3.557292	3.595466	1.069492
H	-3.165987	2.815283	1.732663
H	-2.940464	4.492715	1.191418
H	-4.569357	3.856653	1.410045
C	-3.792300	4.345612	-1.297156
H	-3.872333	4.037593	-2.349130
H	-4.693247	4.917986	-1.037081
H	-2.929687	5.018954	-1.211549
C	-5.986087	2.473430	-1.109096
H	-6.454203	3.125215	-0.357519
H	-5.929224	3.023339	-2.056005
H	-6.650377	1.611544	-1.260297
C	-4.762930	1.071021	0.547173

H	**-5.307272**	**0.162601**	**0.252595**
H	**-3.789934**	**0.775931**	**0.965458**
H	**-5.330041**	**1.540887**	**1.361903**
C	**1.344864**	**3.319887**	**-2.767009**
H	**1.566011**	**2.241429**	**-2.879185**
H	**0.575441**	**3.574321**	**-3.526569**
H	**2.265760**	**3.902049**	**-2.979927**
C	**0.225242**	**2.199612**	**2.109485**
H	**0.851899**	**2.588949**	**2.938838**
H	**-0.825732**	**2.133137**	**2.457977**
H	**0.557827**	**1.173552**	**1.865412**
C	**-0.722337**	**6.733115**	**0.255590**
H	**-1.786460**	**6.678226**	**0.566926**
H	**-0.138477**	**7.243082**	**1.050435**
H	**-0.659890**	**7.341526**	**-0.671607**
H	**0.303931**	**5.656274**	**-2.027936**
H	**-0.583219**	**4.738850**	**2.065974**



^{1}H NMR of 1-5

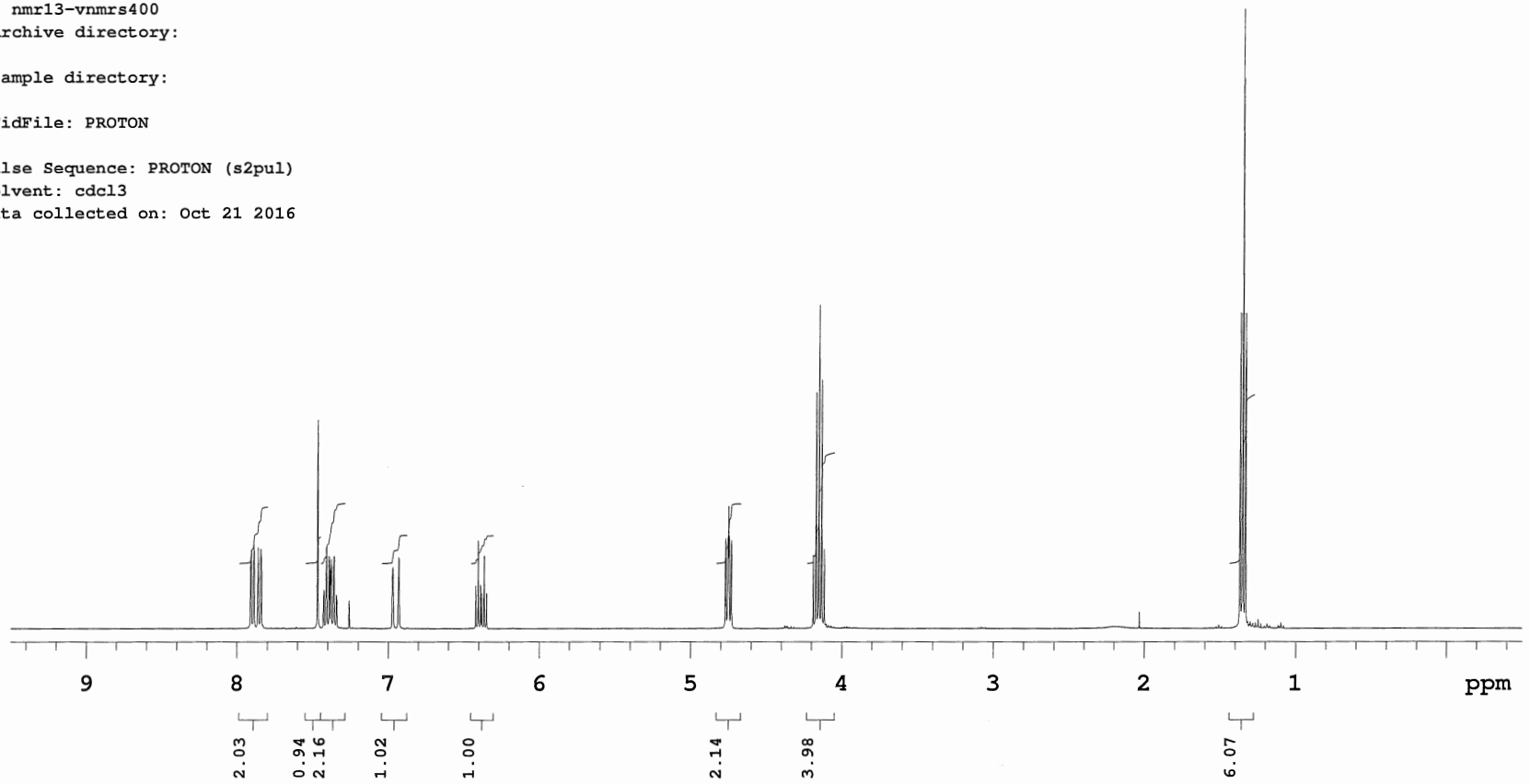
JL-V-33-PD

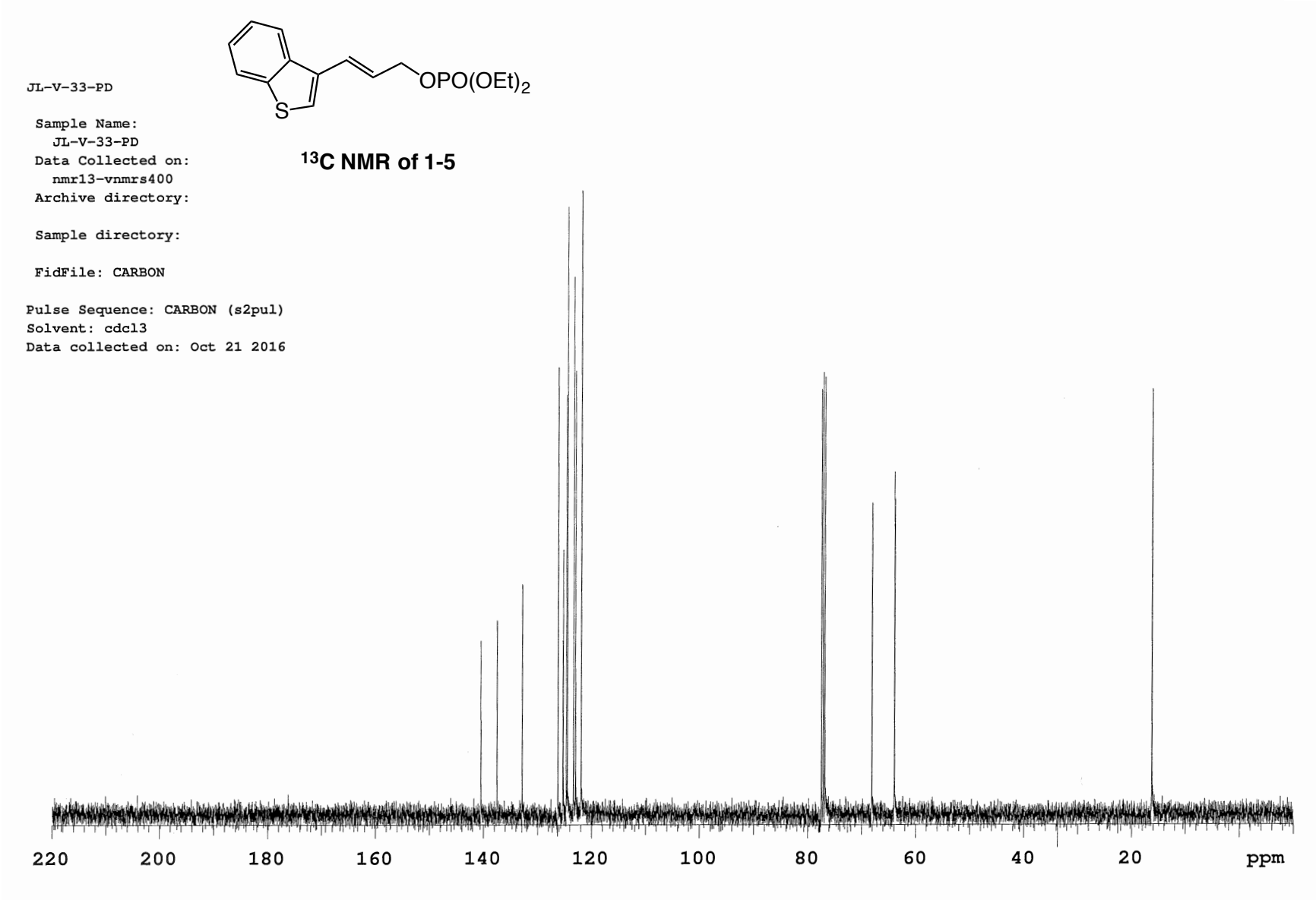
Sample Name:
JL-V-33-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

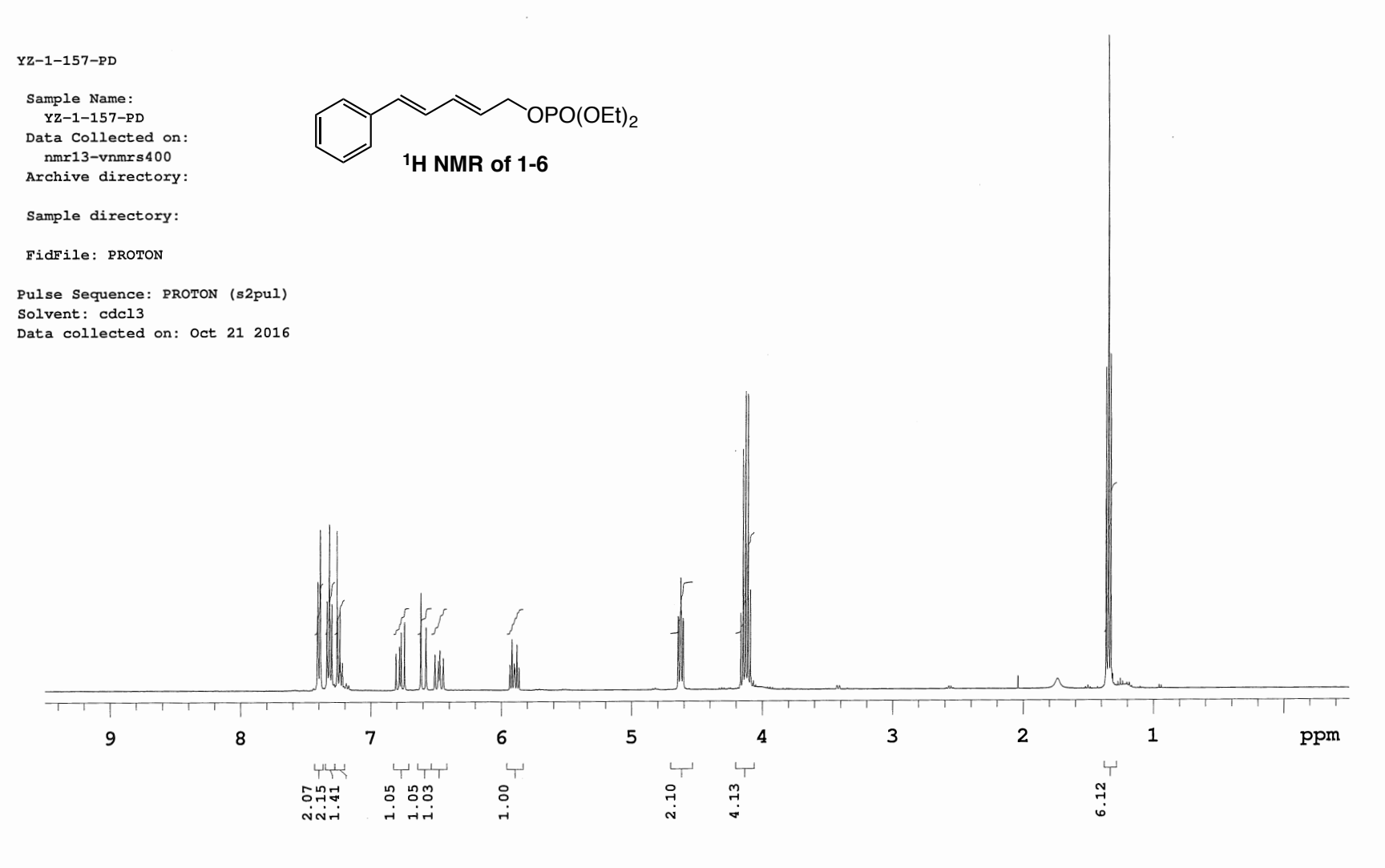
Sample directory:

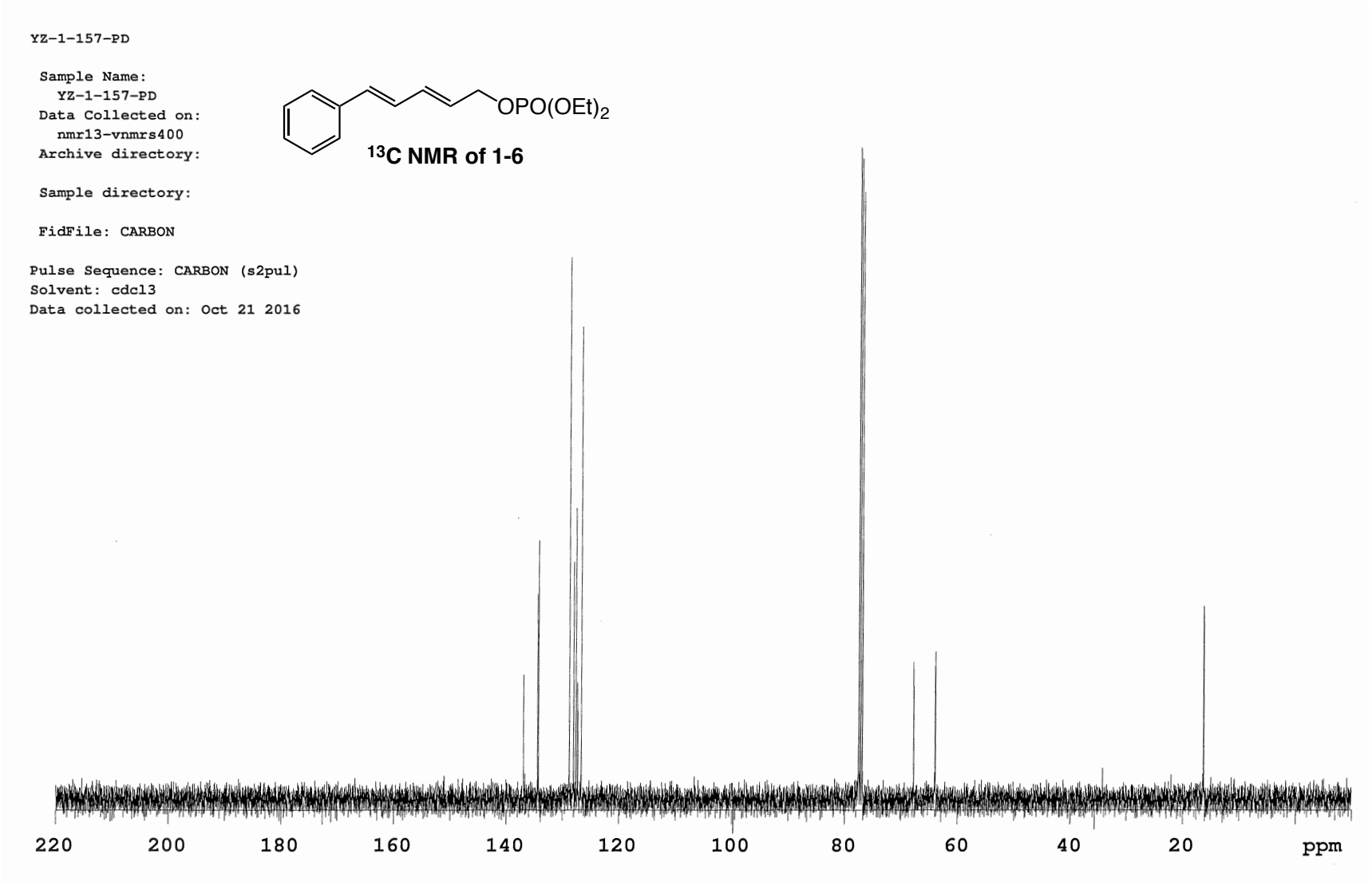
FidFile: PROTON

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




JL-V-33-PD
Sample Name:
JL-V-33-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 21 2016
OPO(OEt)2
S
13C NMR of 1-5
220
200
180
160
140
120
100
80
60
40
20
ppm


YZ-1-157-PD
Sample Name:
YZ-1-157-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 21 2016
OPO(OEt)2
1H NMR of 1-6
9
8
7
6
5
4
3
2
1
ppm
2.07
2.15
1.41
1.05
1.05
1.03
1.00
2.10
4.13
6.12


YZ-1-157-PD
Sample Name:
YZ-1-157-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 21 2016
OPO(OEt)2
13C NMR of 1-6
220
200
180
160
140
120
100
80
60
40
20
ppm

Sample Name:
SR-IV-166-phos
Data Collected on:
vnmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: SR-IV-166-phos

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

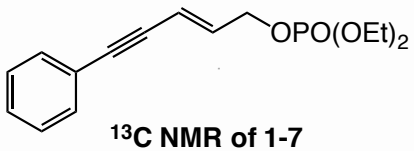
^{1}H NMR of 1-7

Sample Name:
SR-IV-166-phos-carbon
Data Collected on:
vnmr13-vnmrs400
Archive directory:

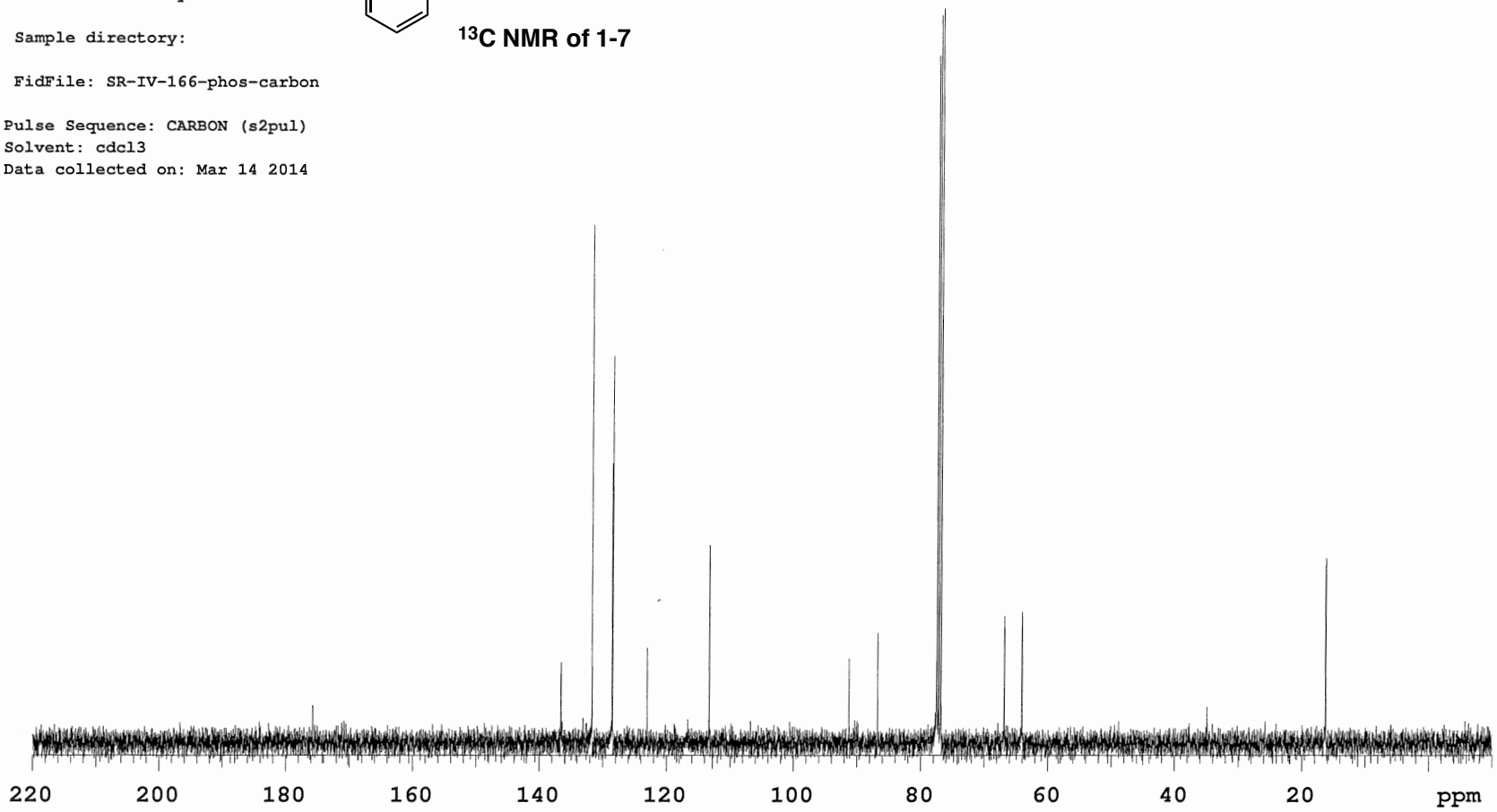
Sample directory:

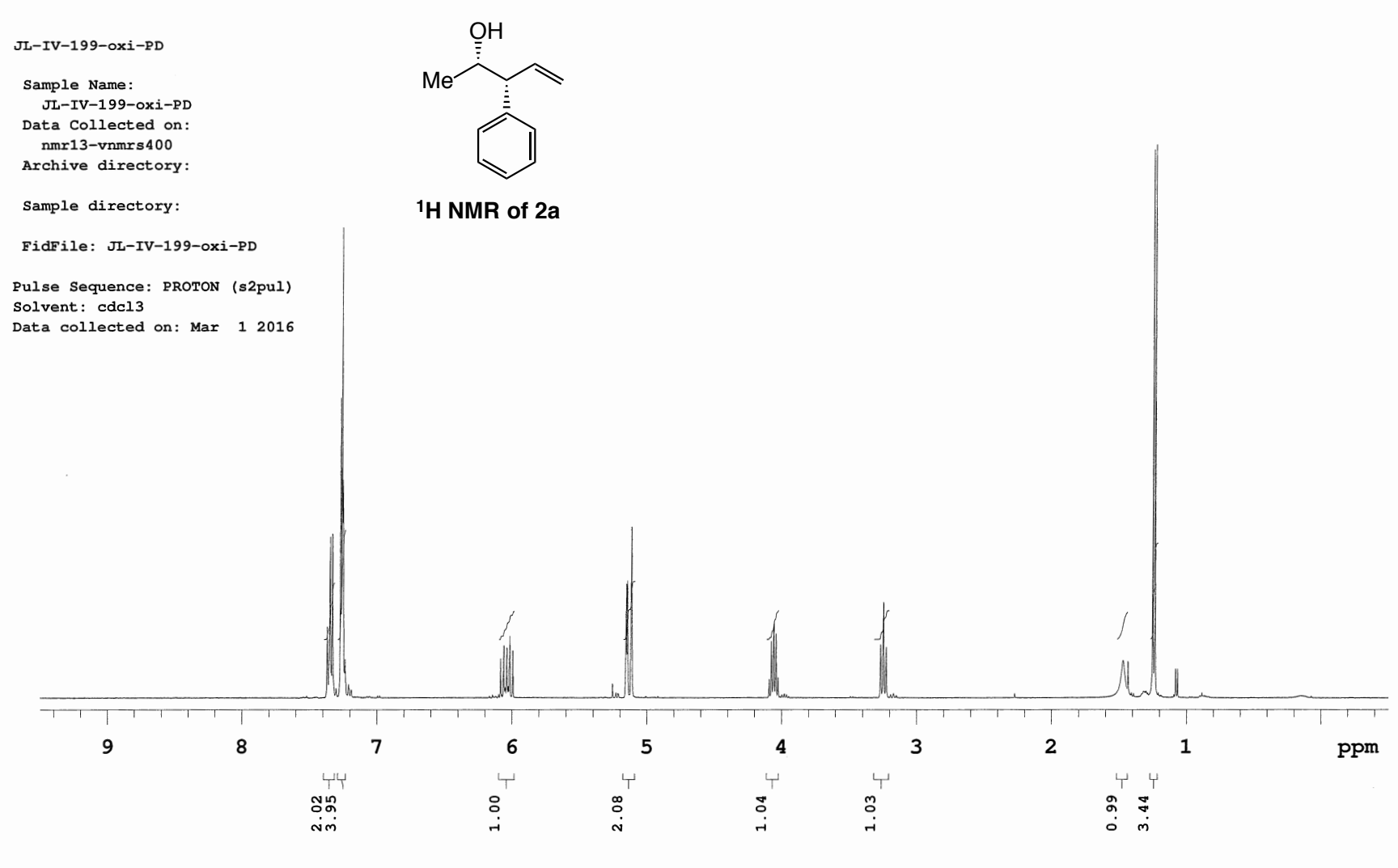
FidFile: SR-IV-166-phos-carbon

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



^{13}C NMR of 1-7




JL-IV-199-oxi-PD
Sample Name:
JL-IV-199-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: JL-IV-199-oxi-PD
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 1 2016
OH
Me
1H NMR of 2a
9
8
7
6
5
4
3
2
1
ppm
2.02
3.95
1.00
2.08
1.04
1.03
0.99
3.44

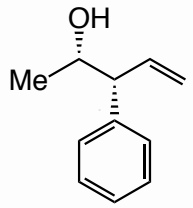
JL-IV-199-PD-C

Sample Name:
JL-IV-199-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 8 2016



^{13}C NMR of 2a

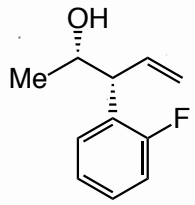
JL-IV-225-2-oxi-PD

Sample Name:
JL-IV-225-2-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

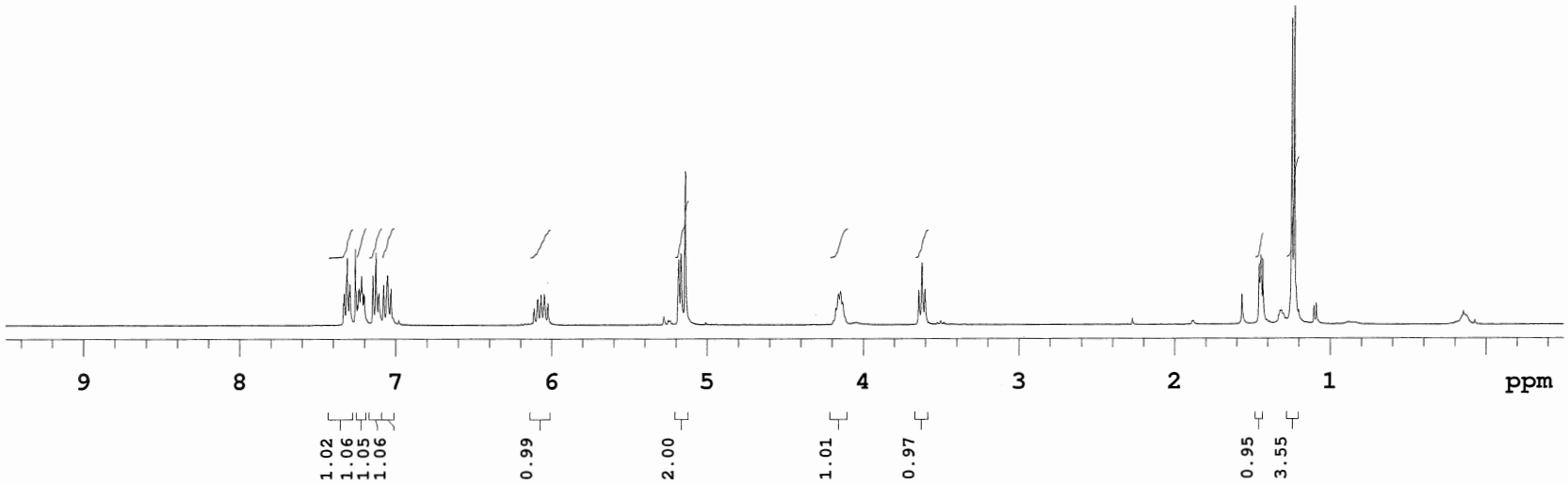
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 26 2016



^{1}H NMR of 2b



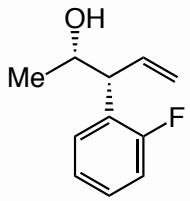
JL-IV-225-2-oxi-PD-C

Sample Name:
JL-IV-225-2-oxi-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: JL-IV-225-2-oxi-PD-C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 26 2016



^{13}C NMR of 2b

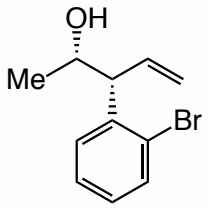
JL-IV-217-2-oxi-PD

Sample Name:
JL-IV-217-2-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

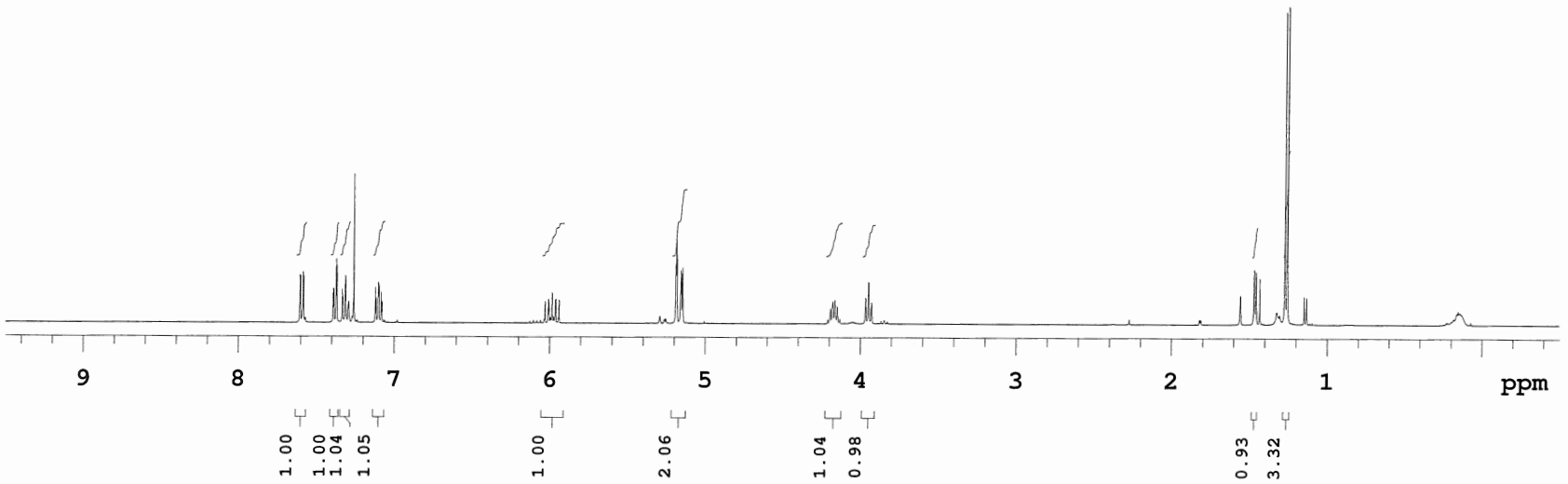
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 18 2016



^{1}H NMR of 2c



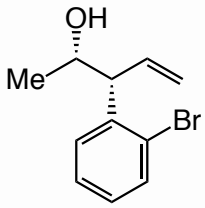
JL-IV-217-2-oxi-PD-C

Sample Name:
JL-IV-217-2-oxi-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 20 2016



^{13}C NMR of 2c

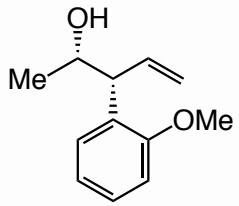
JL-IV-209-1-oxi-PD-prep

Sample Name:
JL-IV-209-1-oxi-PD-prep
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: JL-IV-209-oxi-PD-prep

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 11 2016



^{1}H NMR of 2d

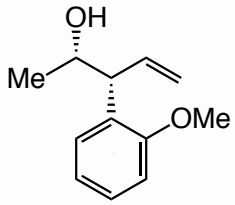
JL-IV-209-oxi-PD-C

Sample Name:
JL-IV-209-oxi-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 13 2016



^{13}C NMR of 2d

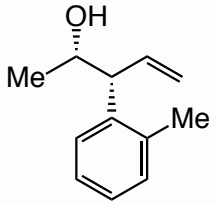
JL-IV-261-1-oxi-PD

Sample Name:
JL-IV-261-1-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: JL-IV-261-1-oxi-PD

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 23 2016



^{1}H NMR of 2e

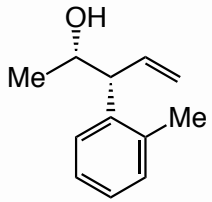
JL-IV-261PD-C

Sample Name:
JL-IV-261PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 15 2016



^{13}C NMR of 2e

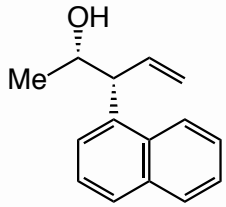
JL-IV-207-1-oxi-PD

Sample Name:
JL-IV-207-1-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 12 2016



^{1}H NMR of 2f

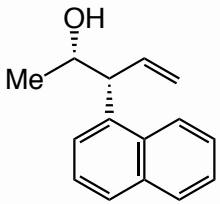
JL-IV-207-1-oxi-PD-C

Sample Name:
JL-IV-207-1-oxi-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

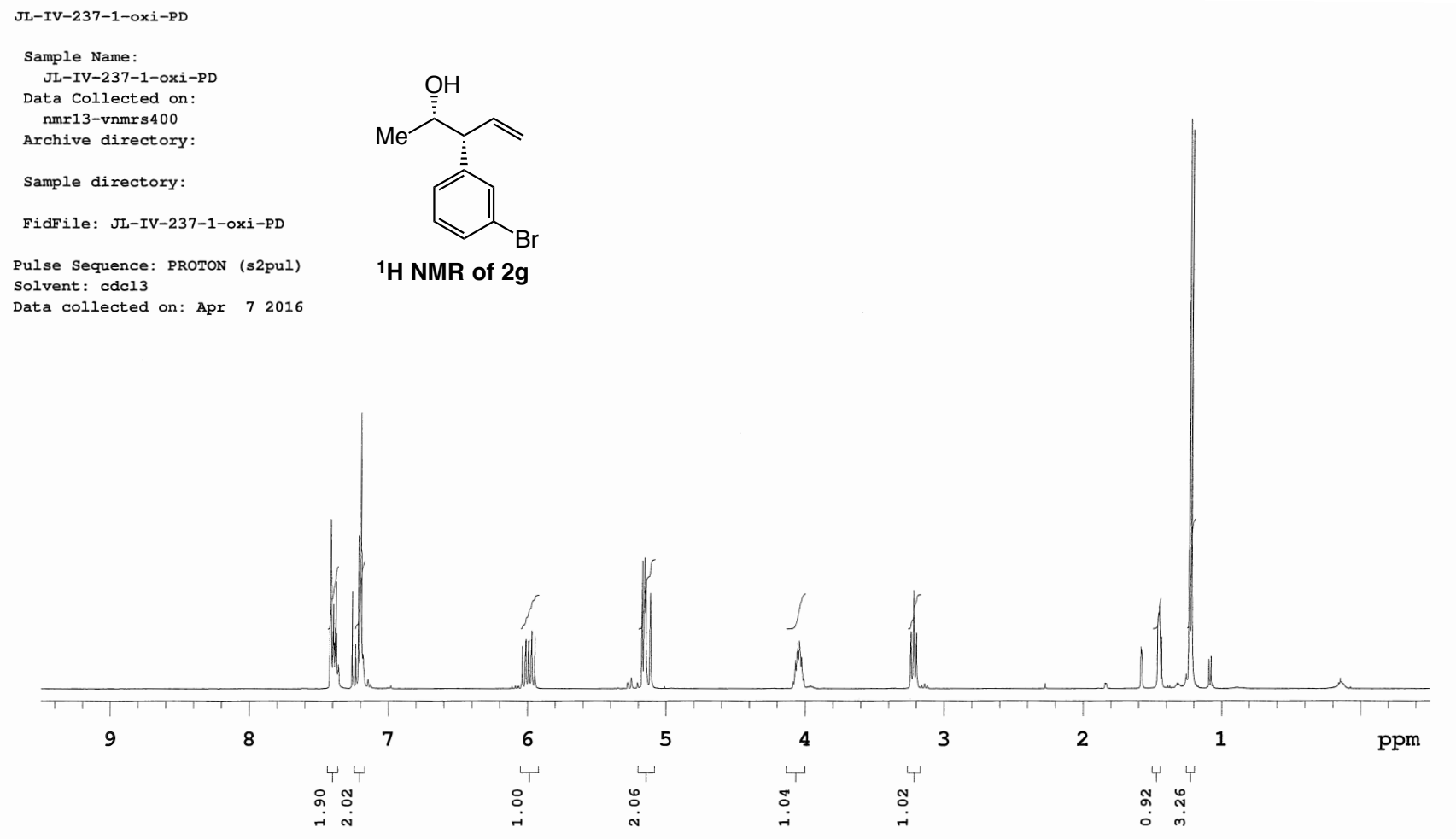
Sample directory:

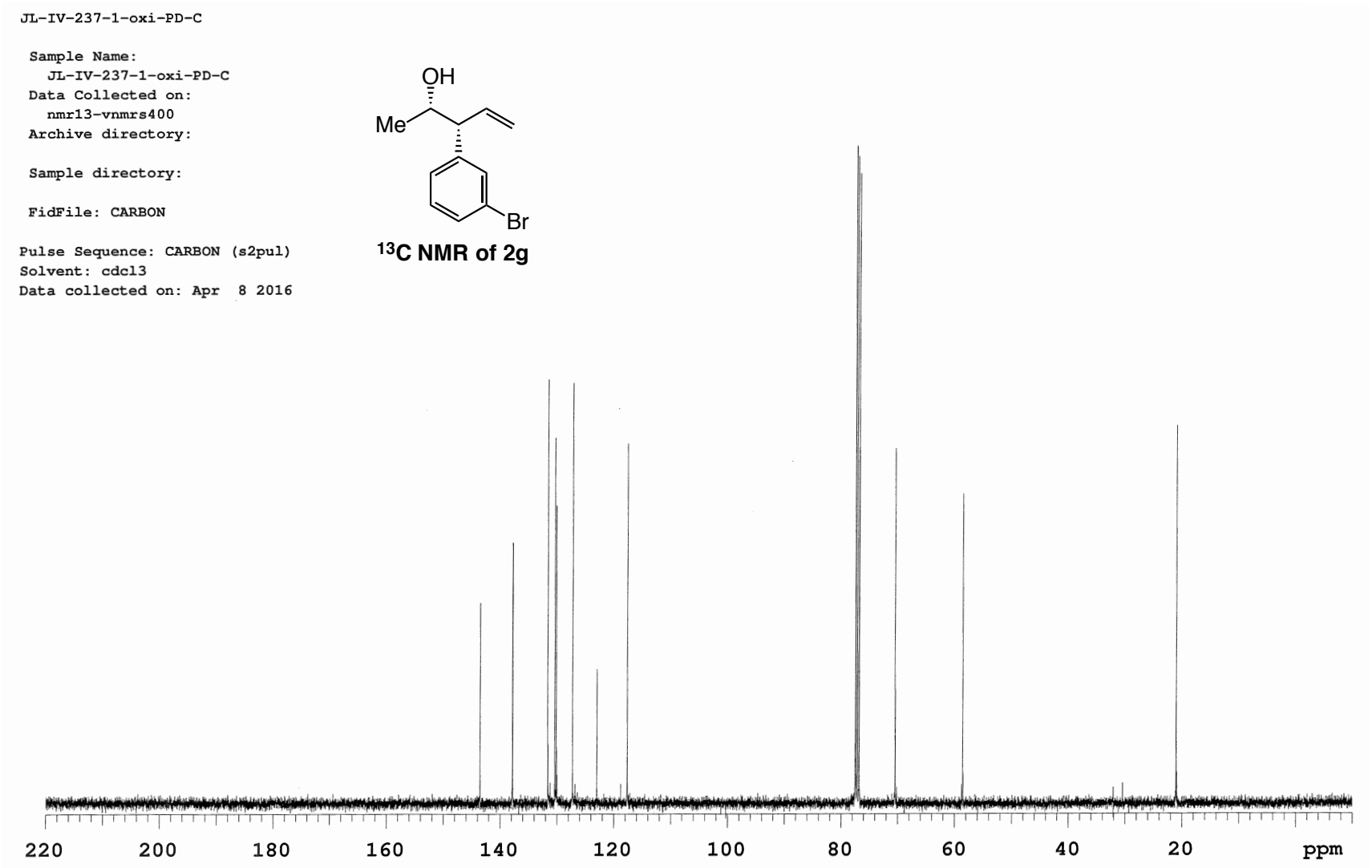
FidFile: CARBON

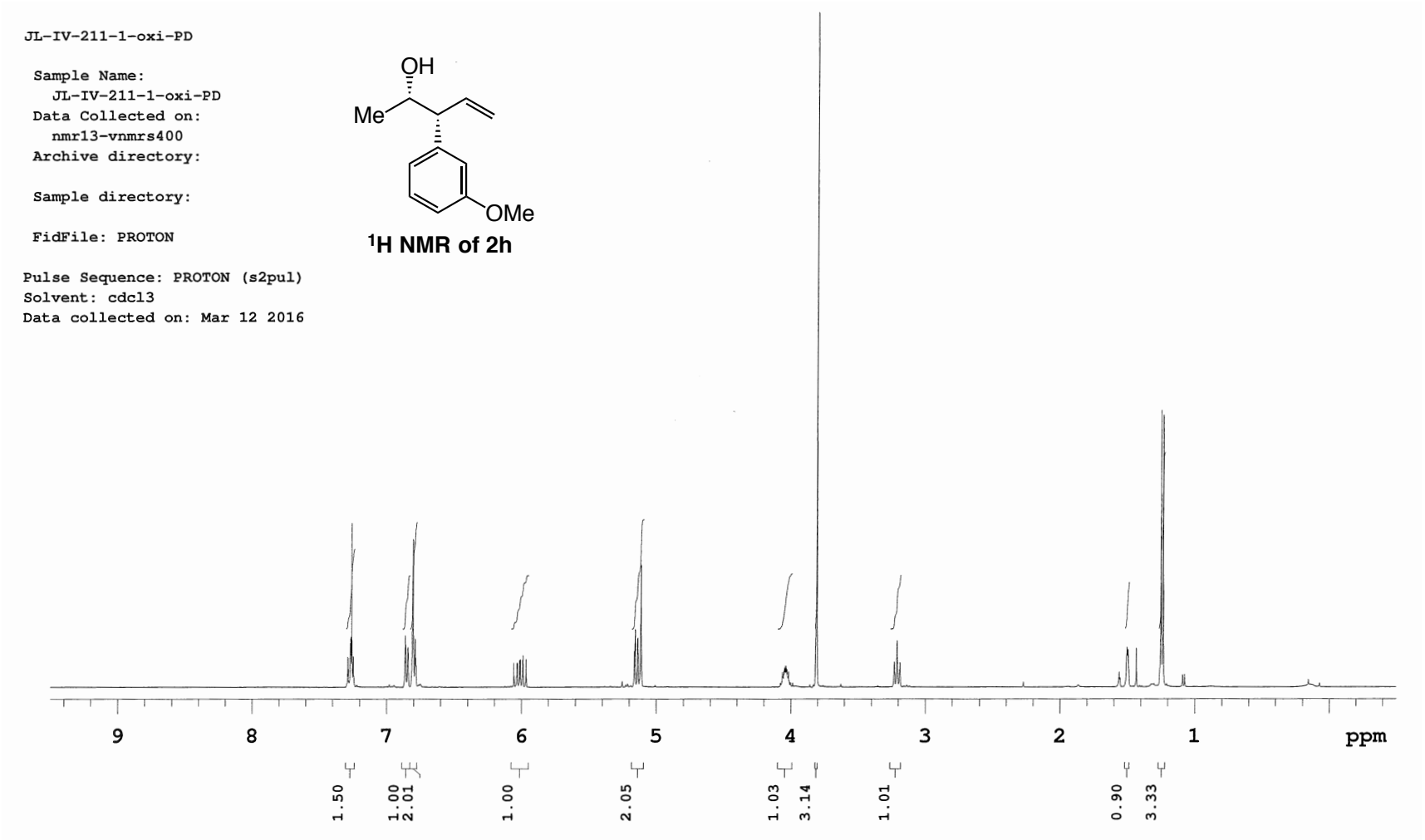
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 14 2016



^{13}C NMR of 2f


JL-IV-237-1-oxi-PD
Sample Name:
JL-IV-237-1-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: JL-IV-237-1-oxi-PD
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 7 2016
OH
Me
Br
1H NMR of 2g
9
8
7
6
5
4
3
2
1
ppm
1.90
2.02
1.00
2.06
1.04
1.02
0.92
3.26


JL-IV-237-1-oxi-PD-C
Sample Name:
JL-IV-237-1-oxi-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 8 2016
OH
Me
Br
13C NMR of 2g
220
200
180
160
140
120
100
80
60
40
20
ppm


JL-IV-211-1-oxi-PD
Sample Name:
JL-IV-211-1-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 12 2016
OH
Me
OMe
9
8
7
6
5
4
3
2
1
ppm
1.50
1.00
2.01
1.00
2.05
1.03
3.14
1.01
0.90
3.33

^{1}H NMR of 2h

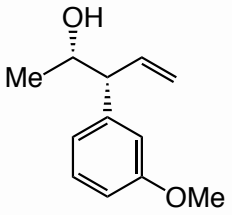
JL-IV-211-1-oxi-PD-C

Sample Name:
JL-IV-211-1-oxi-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 15 2016



^{13}C NMR of 2h

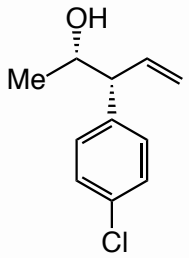
JL-IV-233-2-oxi-PD

Sample Name:
JL-IV-233-2-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

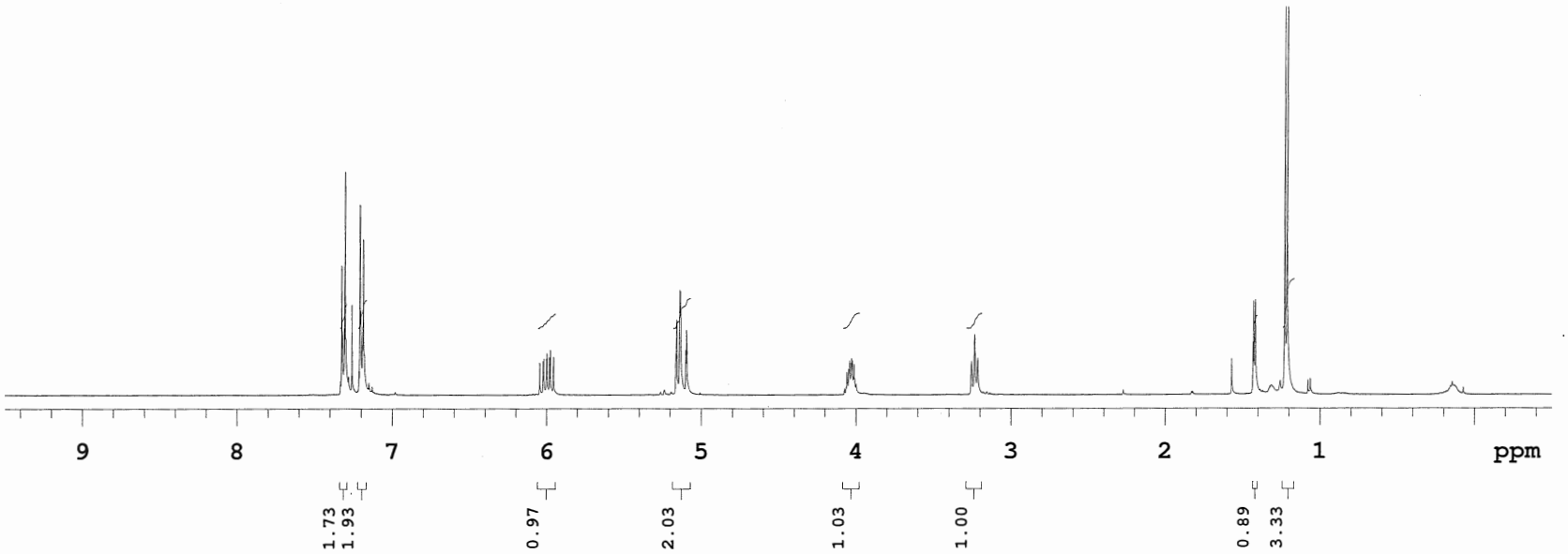
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 4 2016



^{1}H NMR of 2i



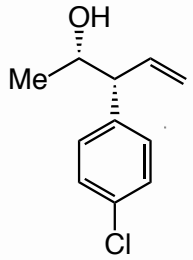
JL-IV-233-2-oxi-PD-C

Sample Name:
JL-IV-233-2-oxi-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

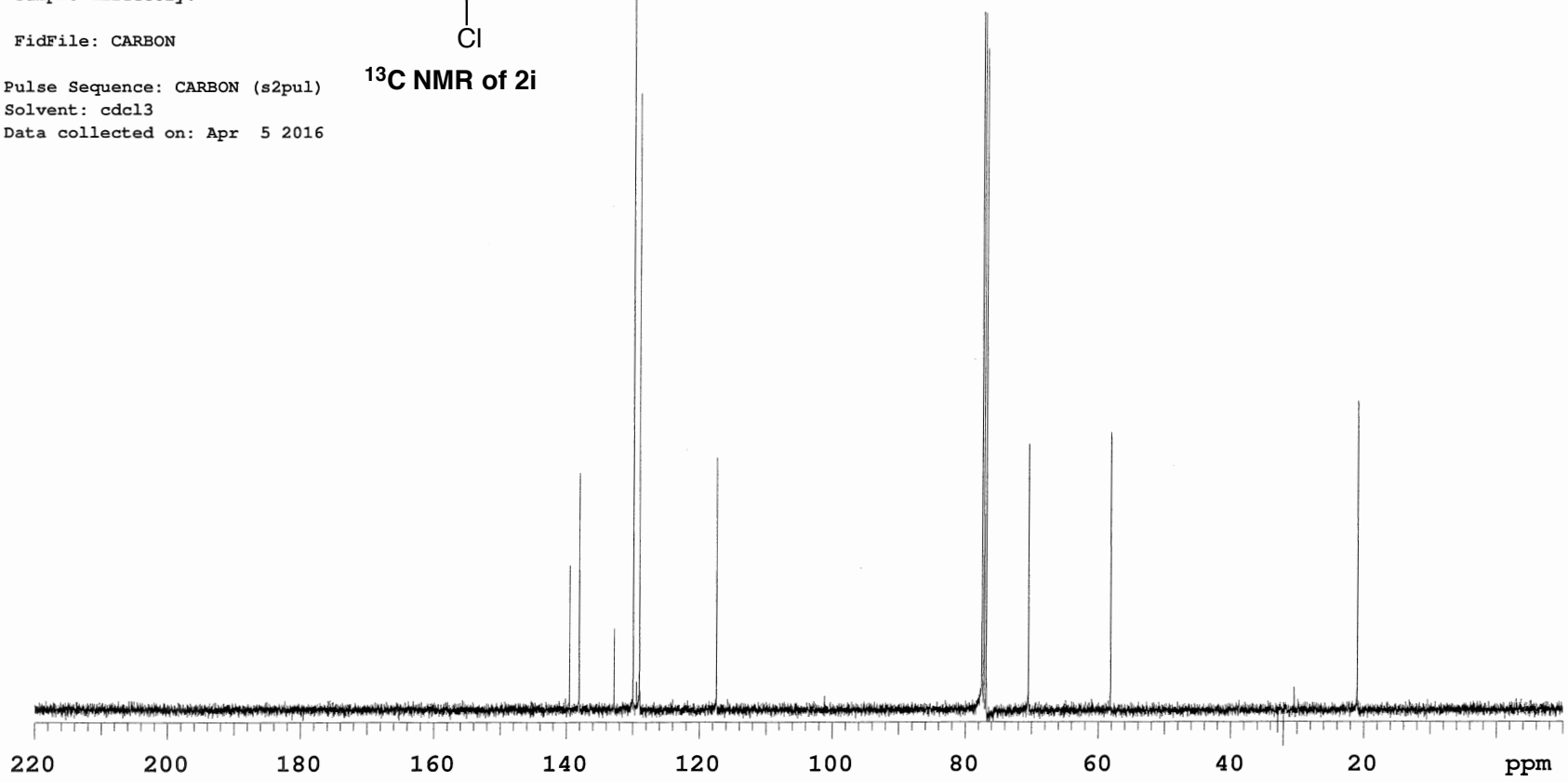
Sample directory:

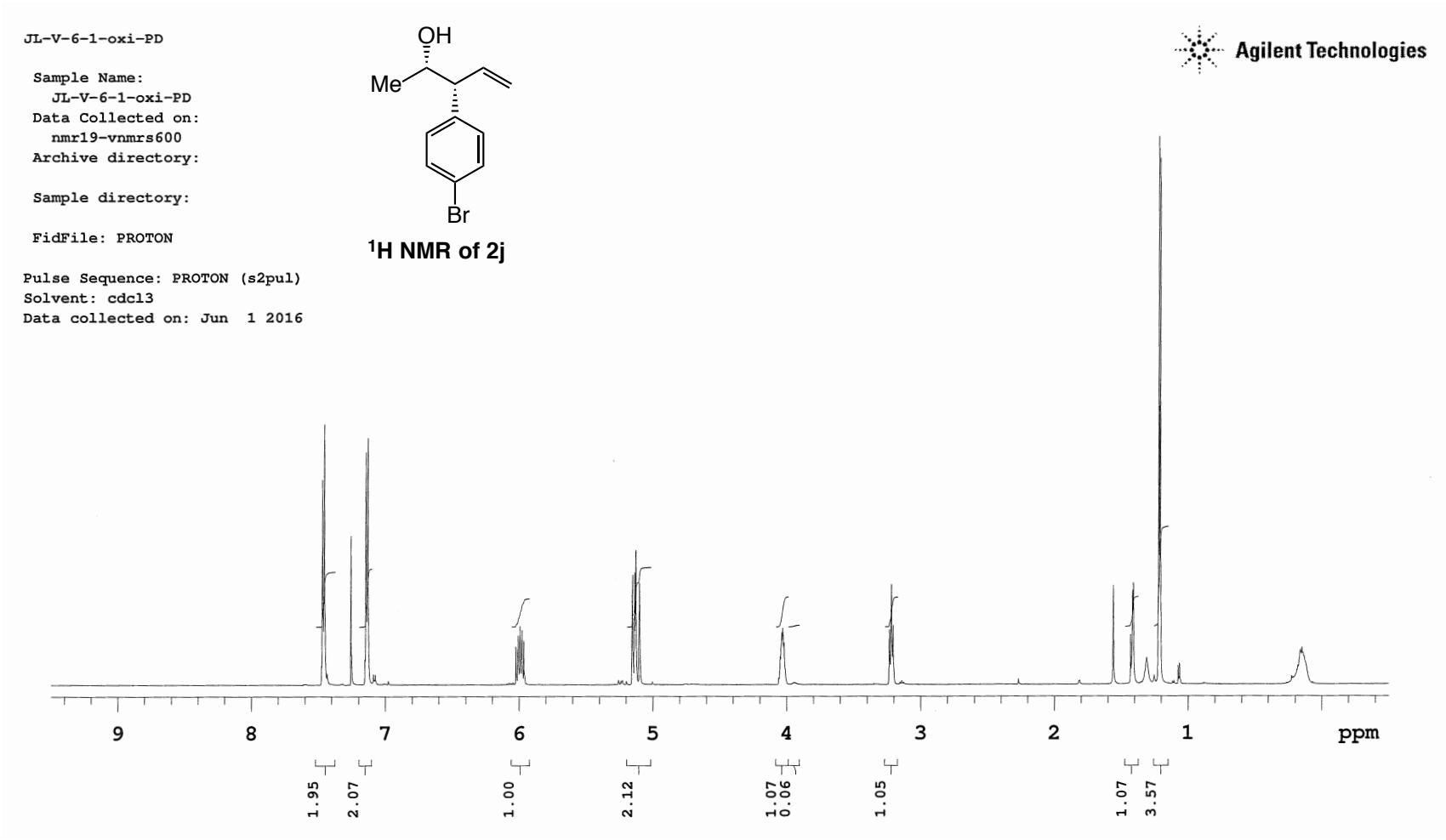
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 5 2016



^{13}C NMR of 2i




JL-V-6-1-oxi-PD
Sample Name:
JL-V-6-1-oxi-PD
Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 1 2016
OH
Me
Br
Agilent Technologies
9
8
7
6
5
4
3
2
1
ppm
1.95
2.07
1.00
2.12
1.07
0.06
1.05
1.07
3.57

^{1}H NMR of 2j

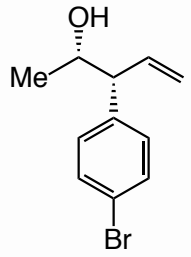
JL-V-6-PD-C

Sample Name:
JL-V-6-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: JL-V-6-PD-C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 2 2016



^{13}C NMR of 2j

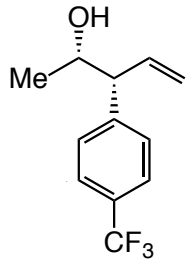
Jl-IV-215-2-oxi-PD

Sample Name:
Jl-IV-215-2-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

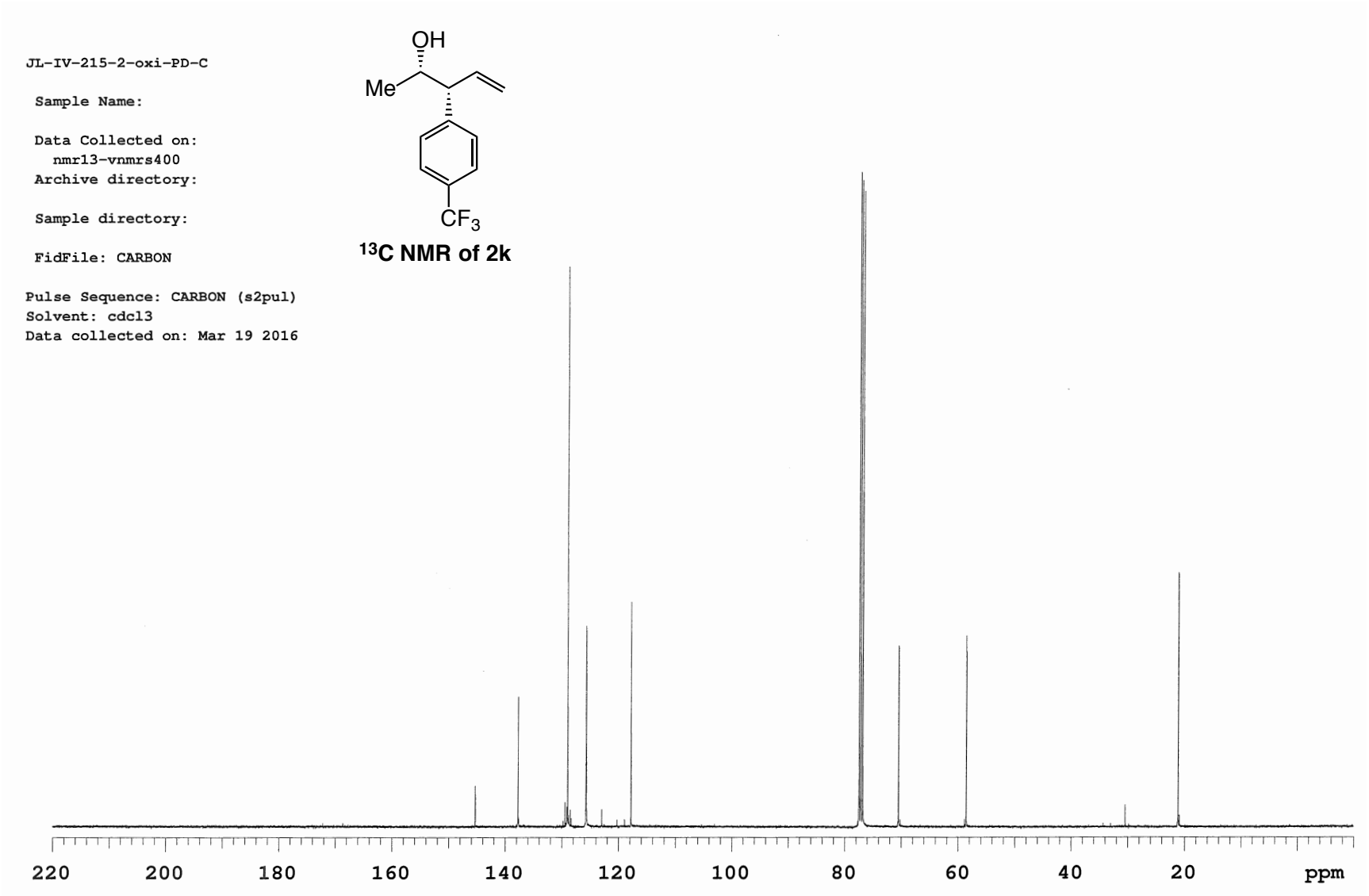
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 18 2016



^{1}H NMR of 2k


JL-IV-215-2-oxi-PD-C
Sample Name:
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 19 2016
OH
Me
CF3
13C NMR of 2k
220
200
180
160
140
120
100
80
60
40
20
ppm

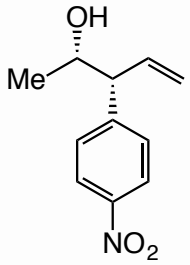
JL-IV-231-2-oxi-PD

Sample Name:
JL-IV-231-2-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

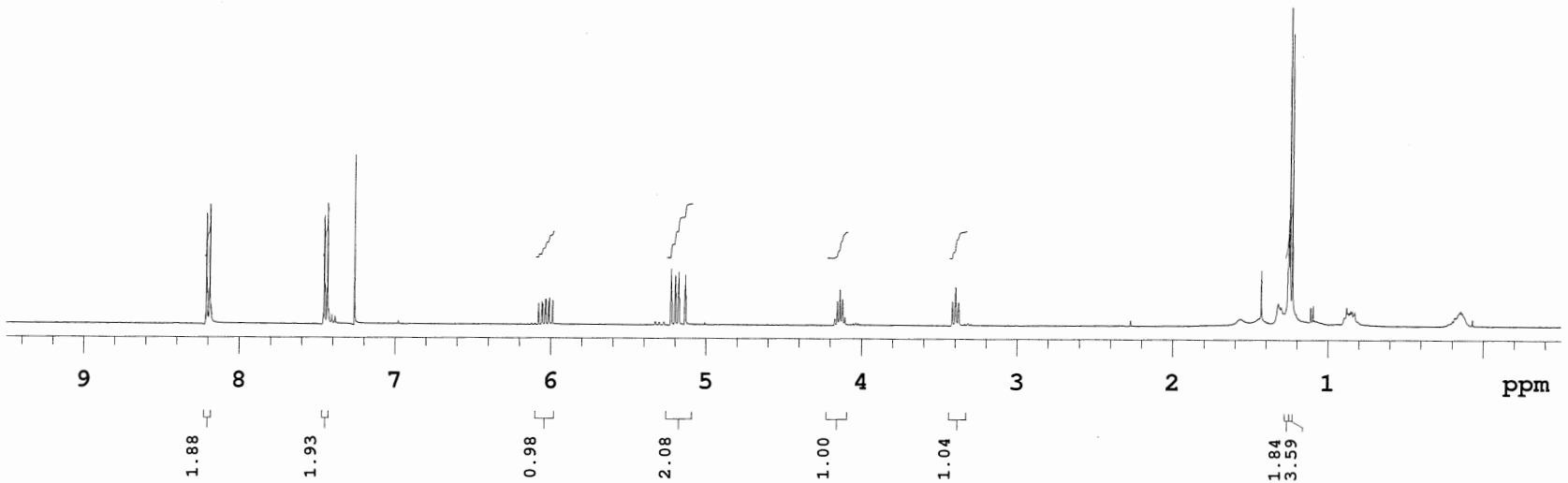
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 2 2016



^{1}H NMR of 2l



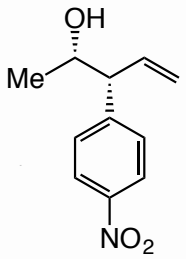
JL-IV-232-2-oxi-PD-C

Sample Name:
JL-IV-232-2-oxi-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

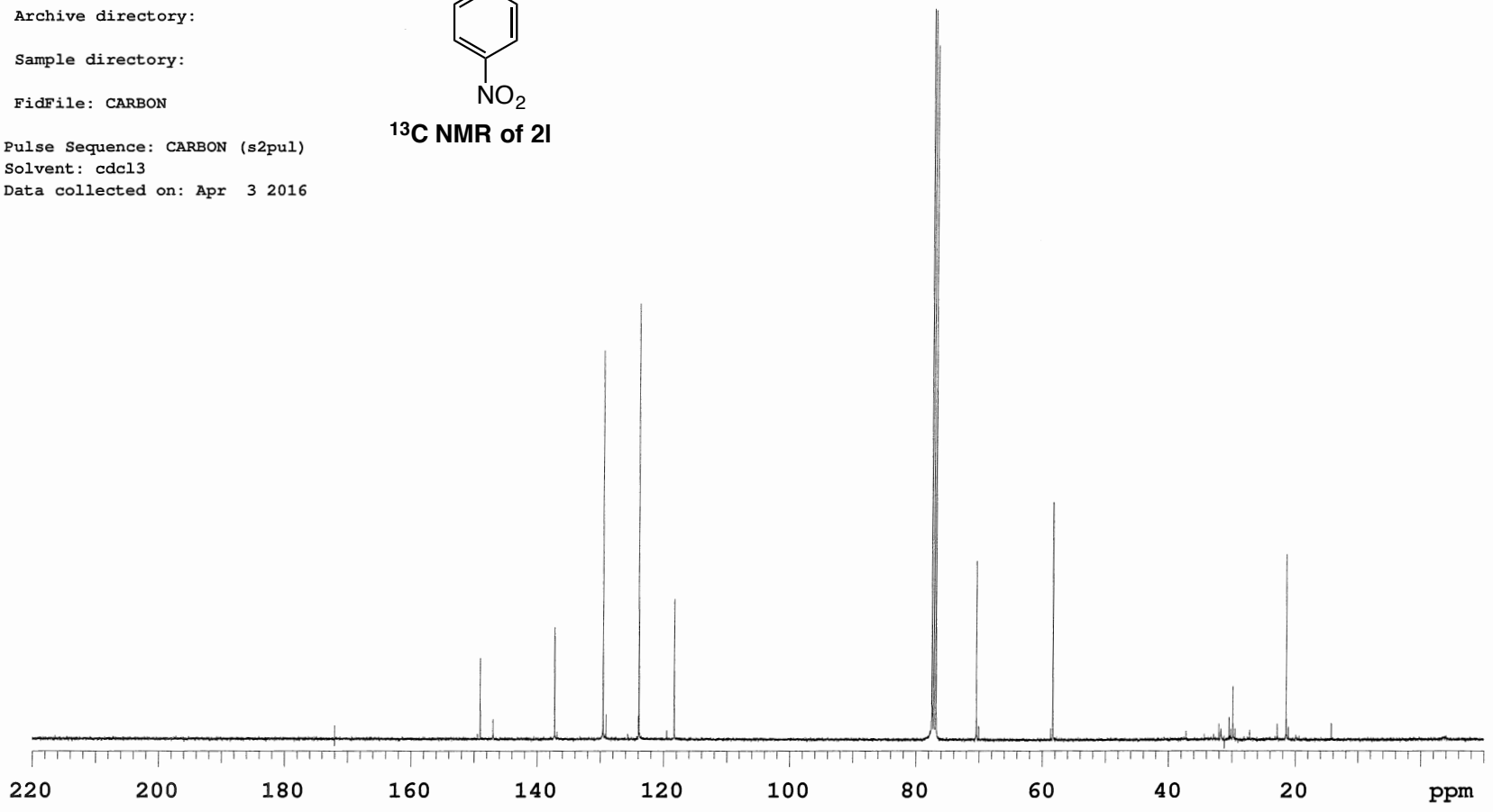
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 3 2016



^{13}C NMR of 2l



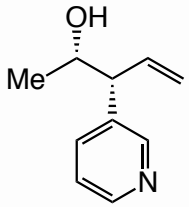
JL-V-86-2-oxi-PD

Sample Name:
JL-V-86-2-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

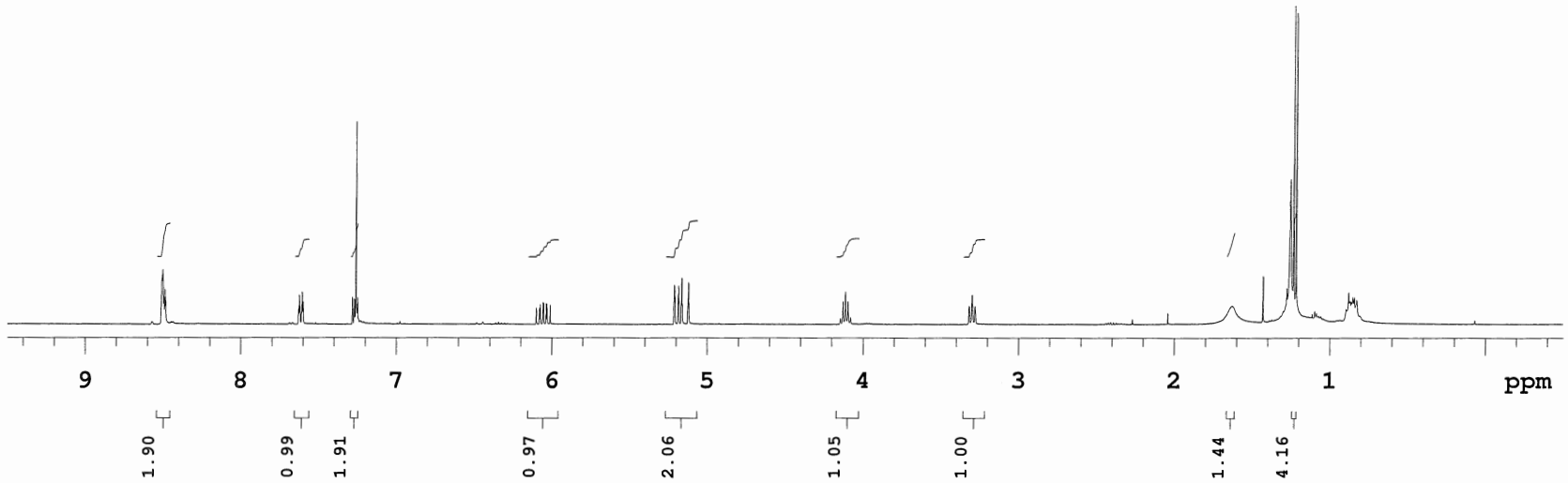
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 19 2016



^{1}H NMR of 4



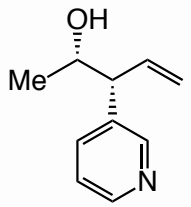
JL-V-86-2-oxi-PD-C

Sample Name:
JL-V-86-2-oxi-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 20 2016



^{13}C NMR of 4

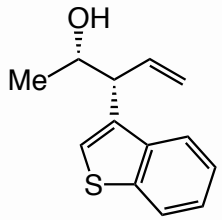
JL-V-38-2-oxi-PD

Sample Name:
JL-V-38-2-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 5 2016



^{1}H NMR of 5

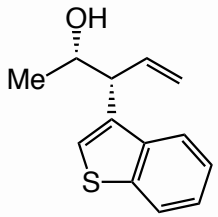
JL-V-38-2-oxi-PD-C

Sample Name:
JL-V-38-2-oxi-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

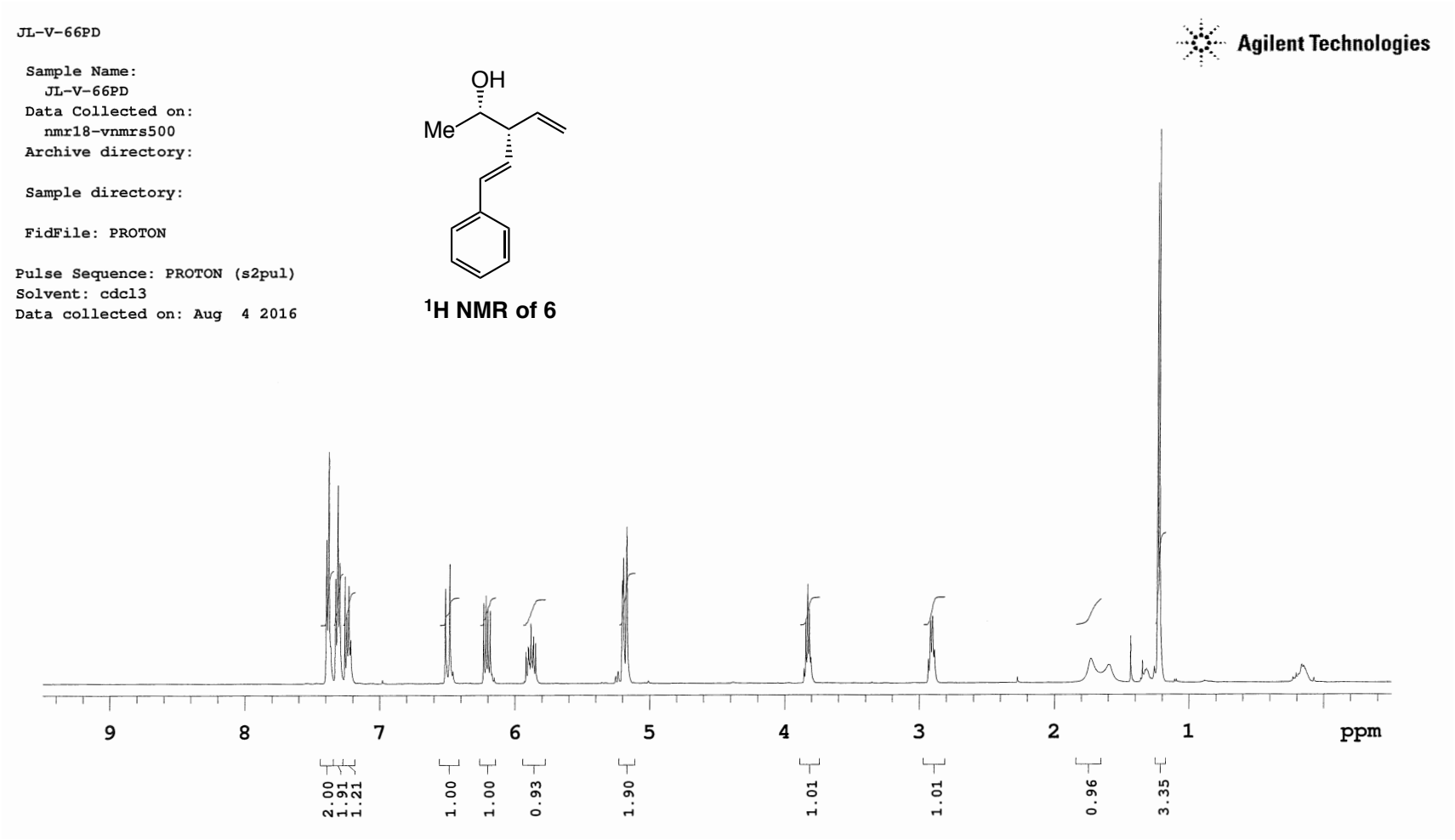
Sample directory:

FidFile: CARBON

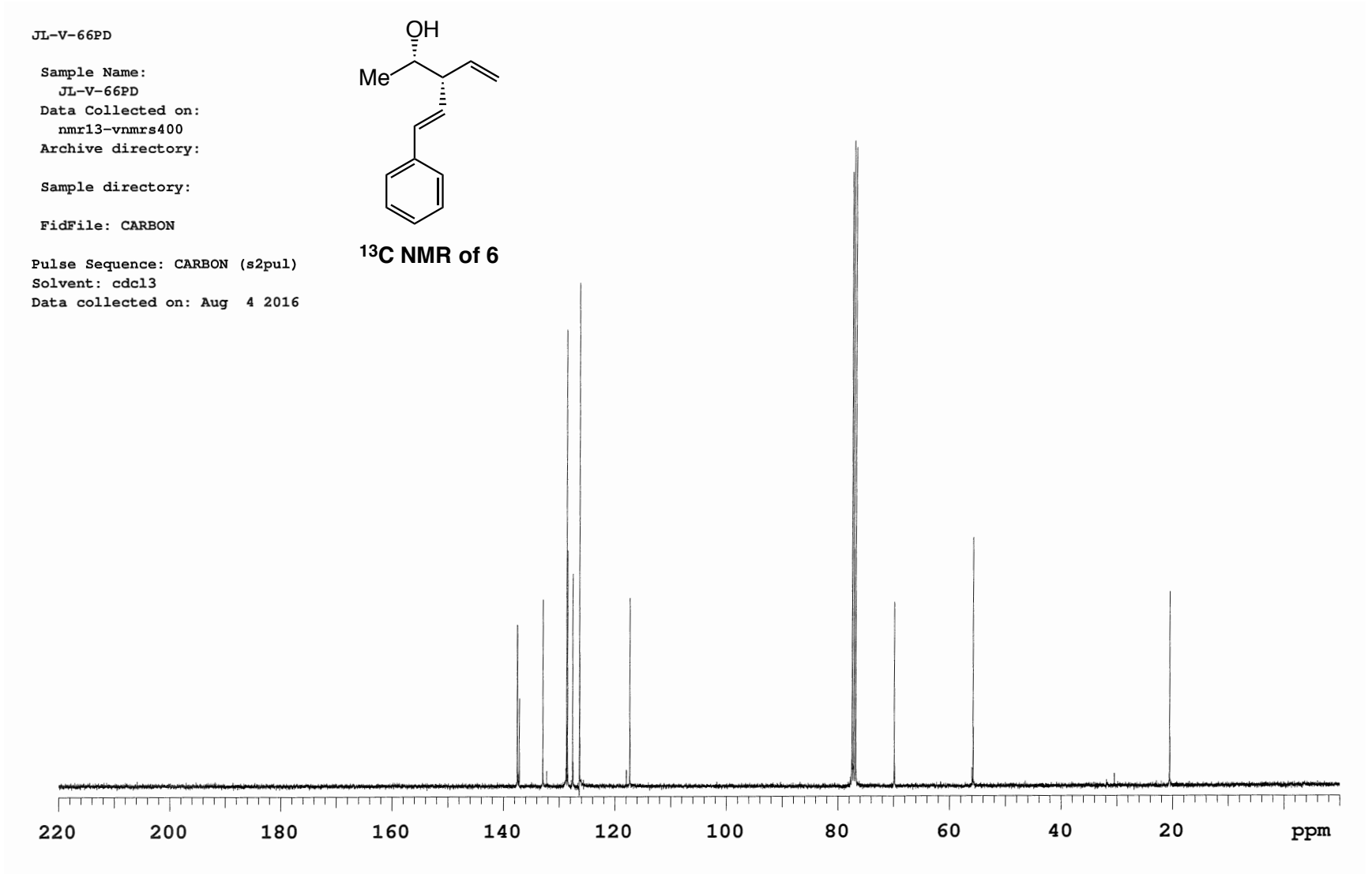
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 6 2016



^{13}C NMR of 5


JL-V-66PD
Sample Name:
JL-V-66PD
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 4 2016
Agilent Technologies
OH
Me
9
8
7
6
5
4
3
2
1
ppm
2.00
1.91
1.21
1.00
1.00
0.93
1.90
1.01
1.01
0.96
3.35

^{1}H NMR of 6


JL-V-66PD
Sample Name:
JL-V-66PD
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 4 2016
OH
Me
13C NMR of 6
220
200
180
160
140
120
100
80
60
40
20
ppm

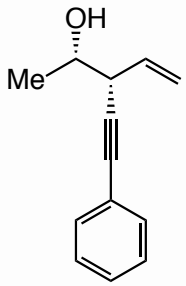
JL-IV-247-2-oxi-PD

Sample Name:
JL-IV-247-2-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2016



^{1}H NMR of 7

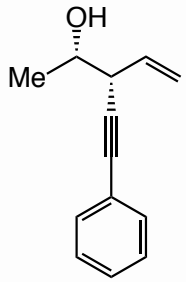
JL-IV-247-2-oxi-PD-C

Sample Name:
JL-IV-247-2-oxi-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 19 2016



^{13}C NMR of 7

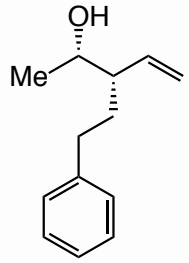
JL-IV-219-2-oxi-PD

Sample Name:
JL-IV-219-2-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 18 2016



^{1}H NMR of 8

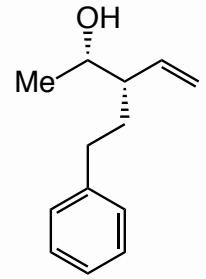
JL-IV-219-2-oxi-PD-C

Sample Name:
JL-IV-219-2-oxi-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:

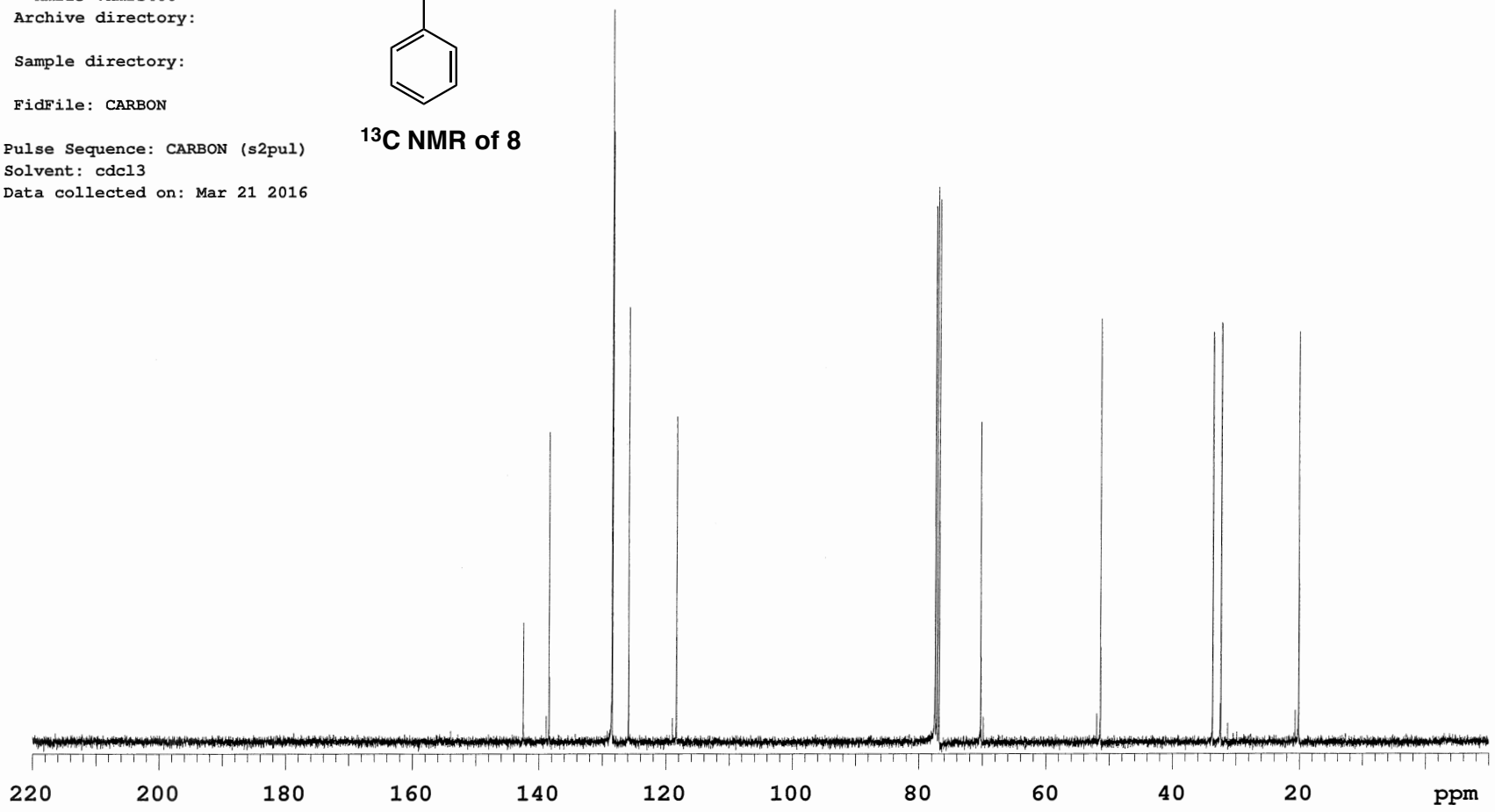
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 21 2016



^{13}C NMR of 8



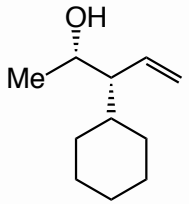
JL-IV-259-2-oxi-PD

Sample Name:
JL-IV-259-2-oxi-PD
Data Collected on:
nmr13-vnmrs400
Archive directory:

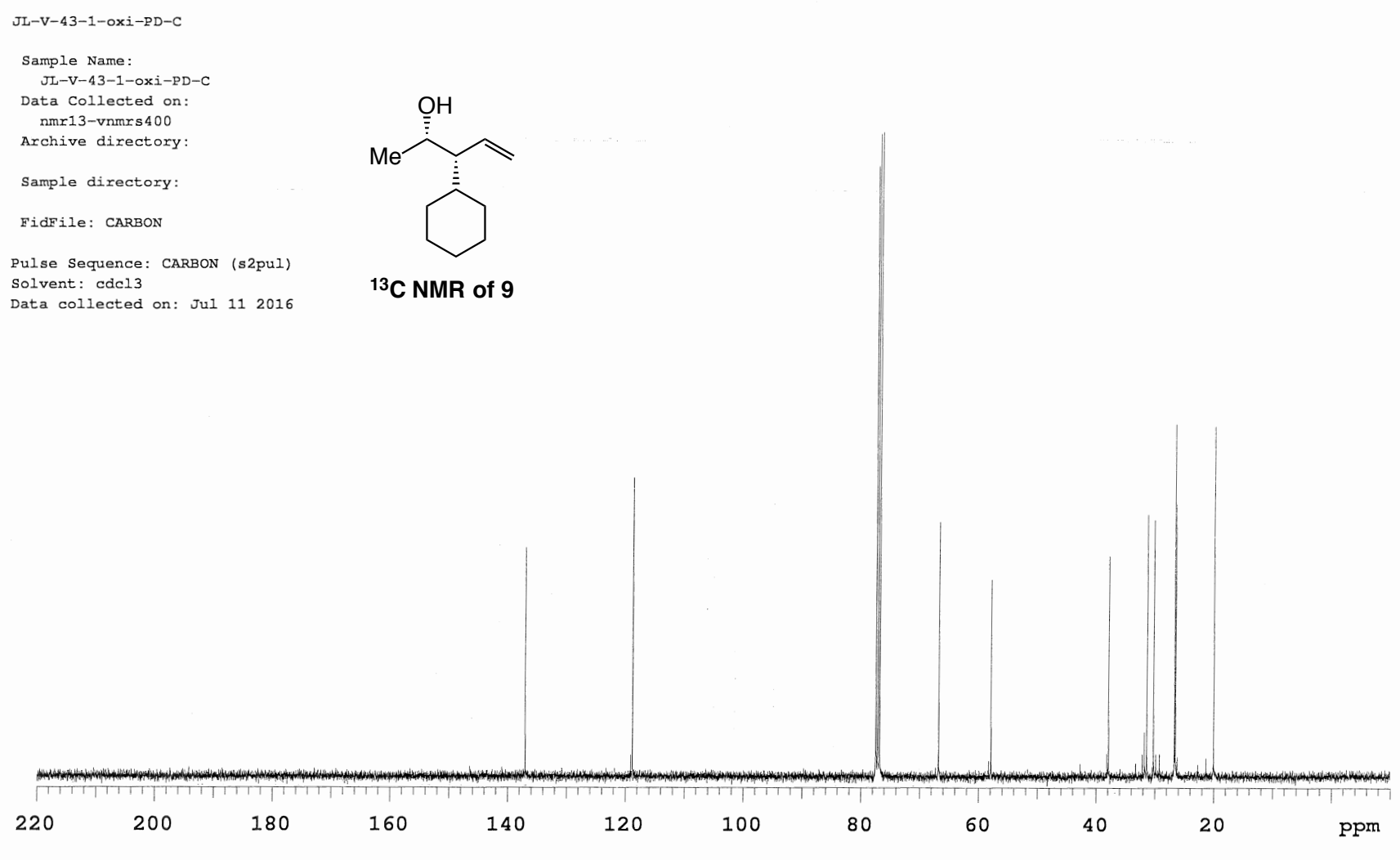
Sample directory:

FidFile: JL-IV-259-2-oxi-PD

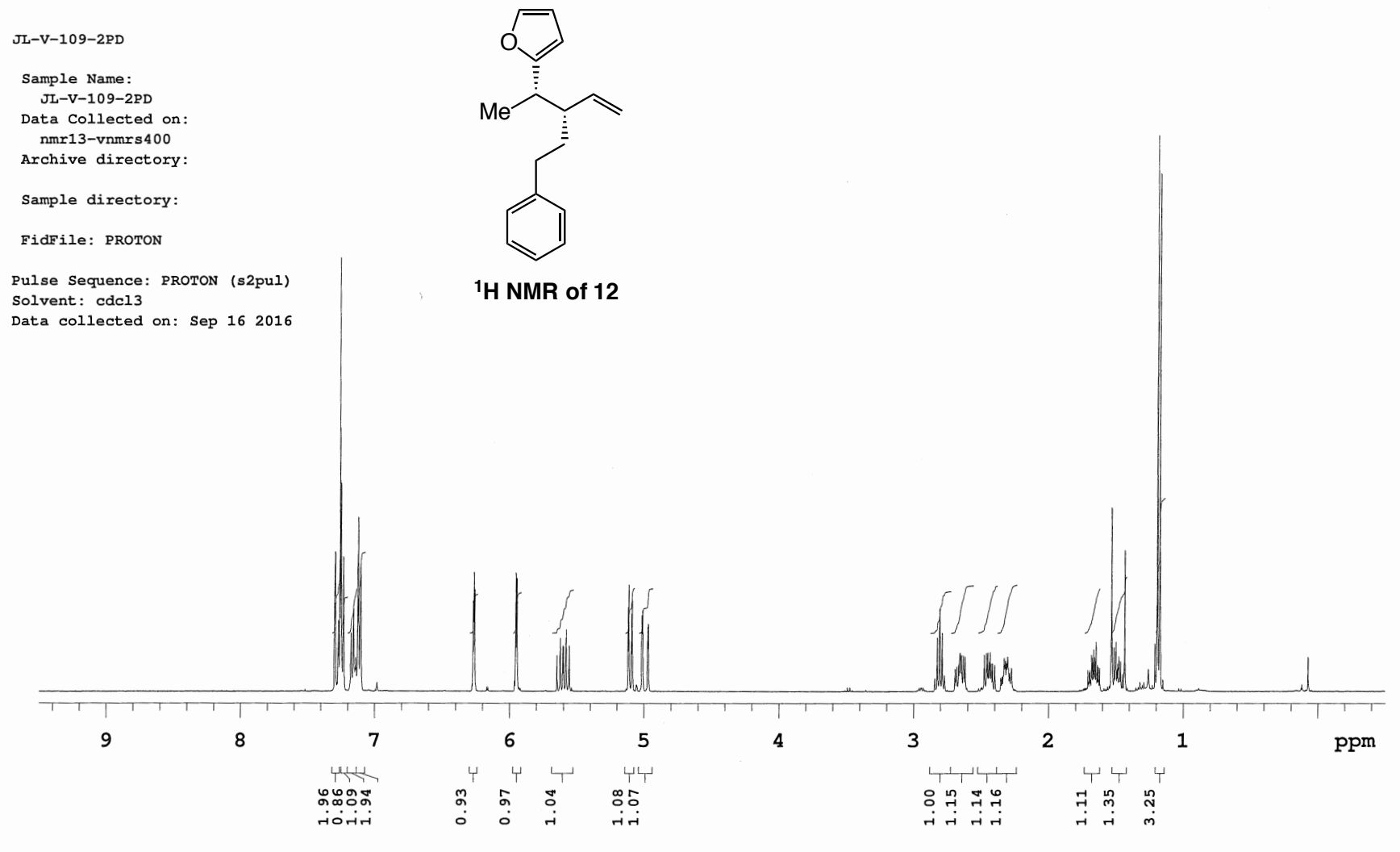
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 23 2016



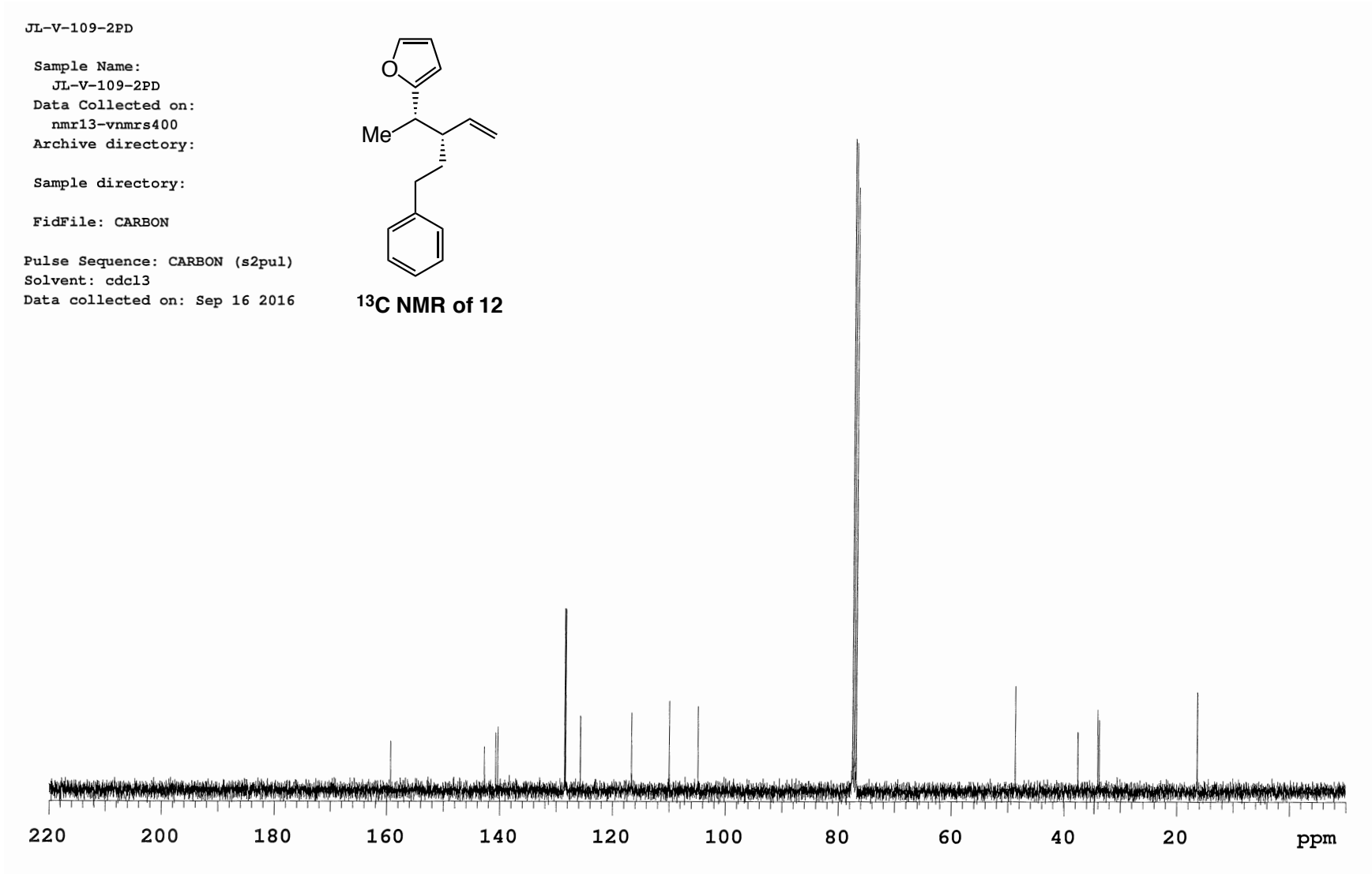
^{1}H NMR of 9


JL-V-43-1-oxi-PD-C
Sample Name:
JL-V-43-1-oxi-PD-C
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 11 2016
OH
Me
220
200
180
160
140
120
100
80
60
40
20
ppm

^{13}C NMR of 9


JL-V-109-2PD
Sample Name:
JL-V-109-2PD
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 16 2016
O
Me
9
8
7
6
5
4
3
2
1
ppm
1.96
0.86
1.09
1.94
0.93
0.97
1.04
1.08
1.07
1.00
1.15
1.14
1.16
1.11
1.35
3.25

^{1}H NMR of 12


JL-V-109-2PD
Sample Name:
JL-V-109-2PD
Data Collected on:
nmr13-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 16 2016
O
Me
220
200
180
160
140
120
100
80
60
40
20
ppm

^{13}C NMR of 12