SUPPORTING INFORMATION

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1 General

Infrared (IR) spectra were recorded on a Bruker FT-IR Alpha (ATR mode) spectrophotometer, λ_{max} in cm^{-1}. Bands are characterized as broad (br), strong (s), medium (m), and weak (w). ^1H NMR spectra were recorded on a Varian Unity INOVA 400 (400 MHz), Varian Unity INOVA 500 (500 MHz) or Varian Unity INOVA 600 (600 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 7.26 ppm). Data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, sep = septet, bs = broad singlet, m = multiplet), and coupling constants (Hz). ^{13}C NMR spectra were recorded on a Varian Unity INOVA 400 (100 MHz), Varian Unity INOVA 500 (125 MHz) or or Varian Unity INOVA 600 (150 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 77.16 ppm). High-resolution mass spectrometry was performed on a JEOL AccuTOF DART (positive mode), or ESI (positive mode) at the Mass Spectrometry Facility at Boston College. Enantiomer ratios were determined by GC (Alltech Associated Chiraldex B-DM (30 m x 0.25 mm), Chiraldex G-TA (30 m x 0.25 mm), β-dex 120 (30 m x 0.25 mm), Chiraldex M-DM (30 m x 0.25 mm)) or HPLC analysis (Chiral Technologies Chiralpak AZ–H (4.6 x 250 mm), Chiralcel OD–H (4.6 x 250 mm), Chiralpak AD–H (4.6 x 250 mm), Chiralcel OJ–H (4.6 x 250 mm), Chiralcel OZ–H (4.6 x 250 mm) and Chiralcel OZ–3 (4.6 x 150 mm)) in comparison with authentic racemic materials. Specific rotations were measured on an ATAGO® AP-300 Automatic Polarimeter or a Rudolph Research Analytical Autopol IV Polarimeter. Unless otherwise noted, all reactions were carried out with distilled and degassed solvents under an atmosphere of dry N_2 in oven- (135 °C) or flame-dried glassware with standard dry box or vacuum-line techniques. Solvents were purified under a positive pressure of dry argon by a modified Innovative Technologies purification system: toluene, benzene and hexanes were purified through a copper oxide and alumina column; CH_2Cl_2 and Et_2O were purged with Ar and purified by passage through two alumina columns. Tetrahydrofuran (Fisher Scientific, Inc.) was purified by distillation from sodium benzophenone ketyl immediately prior to use unless otherwise specified. All work-up and purification procedures were carried out in air.

2 Reagents

Acetic acid was purchased from Fisher and used as received.

Allylic phosphates were prepared according to previously reported methods.[1]

Ammonium tetrafluoroborate was purchased from Strem Inc. and used as received.

Racemic-2,2'-bis(diphenylphosphino)-1,1'-binapthyl (*rac*-binap) was purchased from Aldrich and used as received.

Bis[(pinacolato)boryl]methane was prepared according to previously reported methods.[2]

Diisobutyl(oct-1-en-2-yl)aluminum was prepared according to previously reported methods.[3]

(Dimethylphenylsilyl)boronic acid pinacol ester [$PhMe_2Si$–B(pin)] was purchased from Aldrich and distilled prior to use.

(−)-(*S,S*)-Diphenylethylenediamine was purchased from Astatech Inc. and used as received.

1,4-Dioxane (99%, anhydrous) was purchased from Aldrich and used as received.

Formaldehyde (37% aqueous solution) was purchased from Aldrich and used as received.

***N*-Methyl-*N*-methylidneiminium iodide (Eschenmoser's salt)** was purchased from Aldrich and used as received.

Palladium (II) acetate was purchased from Aldrich and used as received.

Triethyl orthoformate was purchased from Aldrich and distilled from Na prior to used.

Trifluoroacetic acid was purchased from Oakwood Inc. and used as received.

Tris(dibenzylideneacetone)dipalladium(0) was purchased from Strem Inc. and used as received.

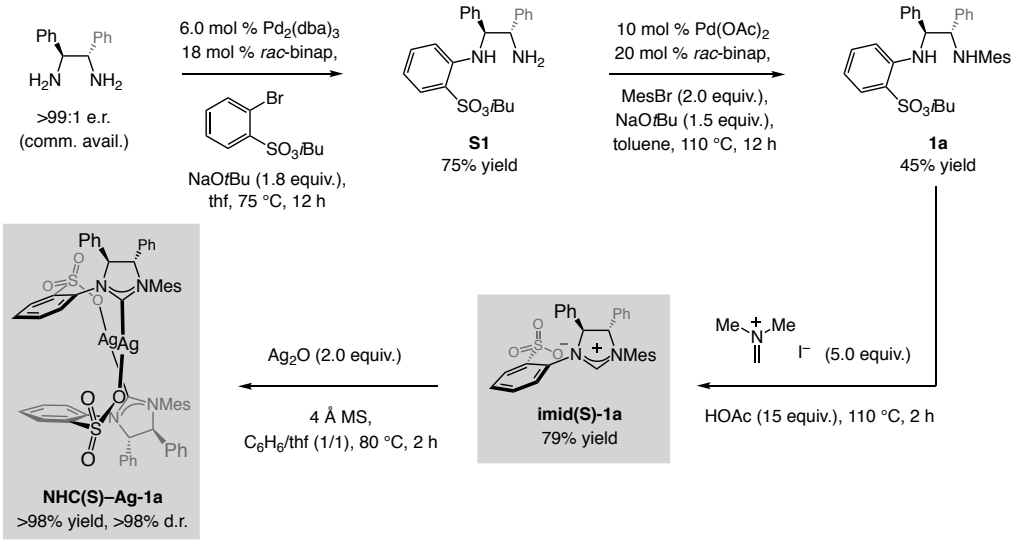
Silver (I) oxide was prepared by previously reported methods.[4]

Sodium methoxide was purchased from Strem Inc. and used as received.

Sodium perborate tetrahydrate was purchased from Aldrich and used as received.

NOTE: It is imperative that Cu and imidazolinium salts are rigorously dried in order to achieve optimal efficiency and enantioselectivity.

3 Sulfonate N-Heterocyclic Carbenes[5]



3.1 *iso*-Butyl-2-((1*S*,2*S*)-2-amino-1,2-diphenylethylamino)benzenesulfonate (S1)

In a glove box, an oven-dried 250 mL round bottom flask was charged with (–)-(*S*,*S*)-diphenylethylenediamine (1.00 g, 4.71 mmol), $Pd_2(dba)_3$ (258 mg, 0.283 mmol), *rac*-binap (528 mg, 0.848 mmol) and NaO*t*-Bu (815 mg, 8.48 mmol). The flask was removed from the glove box and fitted with a reflux condenser. A solution of *iso*-butyl-2-bromobenzenesulfonate[5a] (1.38 g, 4.71 mmol) in thf (47 mL) was added through syringe and the mixture was allowed to stir at 75 °C (the solution turned dark-red upon heating and remained as such for the duration). After 15 h, the mixture was allowed to cool to 22 °C and the volatiles were removed in vacuo, affording deep red oil. This was dissolved in toluene and purified by silica gel chromatography (100% hexanes (to elute toluene) to 50% Et_2O/hexanes) to afford 1.50 g (3.53

mmol, 75% yield) of **S1** as yellow solid. **Mp:** 157–159 °C; **IR (neat):** 3364 (br), 2966 (w), 2874 (w), 1601 (m), 1504 (m), 1461 (m), 1167 (m), 978 (m) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 7.67 (1H, dd, *J* = 8.1, 1.7 Hz), 7.49 (2H, d, *J* = 8.1 Hz), 7.44 (1H, d, *J* = 7.0 Hz) 7.35–7.22 (8H, m), 7.13 (1H, dd, *J* = 8.1, 7.2 Hz), 6.57 (1H, dd, *J* = 8.1, 7.2 Hz), 6.31 (1H, d, *J* = 8.1 Hz), 4.59 (1H, dd, *J* = 7.0, 3.5 Hz), 4.40 (1H, d, *J* = 3.5 Hz), 3.74 (1H, dd, *J* = 9.3, 6.8 Hz), 3.70 (1H, dd, *J* = 9.3, 6.6 Hz), 1.95 (1H, ddqq, *J* = 6.8, 6.8, 6.8, 6.6 Hz), 1.51 (2H, br), 0.92 (3H, d, *J* = 6.8 Hz), 0.85 (3H, d, *J* = 6.8 Hz); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 145.8, 142.6, 140.7, 135.1, 130.8, 128.8, 128.4, 127.6, 127.6, 127.1, 126.8, 116.5, 115.1, 113.6, 76.3, 63.0, 61.2, 28.1, 18.8, 18.7; **HRMS (EI+):** Calcd for $C_{24}H_{29}N_2O_3S$: 425.1899 (M^++H); found: 425.1895. Specific rotation: $[\alpha]_D^{25}$ –98.9 (*c* 1.00, $CHCl_3$).

3.2 *iso*-Butyl-2-((1*S*,2*S*)-2-(mesitylamino)-1,2-diphenylethylamino)benzenesulfonate (1a)

In a glove box, an oven-dried 50 mL round bottom flask was charged with **S1** (0.800 g, 1.88 mmol), $Pd(OAc)_2$ (42.0 mg, 0.188 mmol), *rac*-binap (234 mg, 0.376 mmol) and NaO*t*-Bu (272 mg, 2.83 mmol). The flask was removed from the glove box and attached to a reflux condenser. A solution of 2-bromomesitylene (577 μL, 3.77 mmol) dissolved in toluene (19 mL) was added by syringe and the mixture was allowed to stir at 110 °C (the mixture turned dark-red upon heating and remained so afterwards). After 18 h, the mixture was allowed to cool to 22 °C, loaded on silica gel and purified by silica gel chromatography (100% petroleum ether (for eluting toluene) to 20% Et_2O/petroleum ether) to afford pale yellow solid, which was rinsed with petroleum ether to give 441 mg (0.811 mmol, 43% yield) of diamine **1a** as white solid. **Mp:** 164–166 °C; **IR (neat):** 3352 (m), 2962 (m), 2917 (w), 2861 (w), 1596 (s), 1350 (s) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 7.82 (1H, dd, *J* = 8.1, 1.7 Hz), 7.42 (1H, d, *J* = 4.5 Hz), 7.30–7.12 (9H, m), 7.07–7.04 (2H, m), 6.75–6.72 (3H, m), 6.57 (1H, d, *J* = 8.4 Hz), 4.97 (1H, dd, *J* = 7.0, 4.5 Hz), 4.57 (1H, d, *J* = 7.0 Hz), 3.88 (1H, dd, *J* = 9.3, 6.6 Hz), 3.78 (1H, dd, *J* = 9.3, 6.4 Hz), 3.65 (1H, br s), 2.20 (3H, s), 2.15 (6H, s), 2.01 (1H, ddqq, *J* = 6.6, 6.4, 4.2, 4.0 Hz), 0.99 (3H, d, *J* = 4.0 Hz,), 0.97 (3H, d, *J* = 4.2 Hz); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 145.7, 140.9, 140.2, 140.1, 135.1, 131.1, 130.9, 129.8, 129.2, 128.4, 128.2, 128.1, 127.8, 127.6, 117.6, 115.8, 113.9, 76.2, 66.7, 62.0, 28.2, 20.5, 19.2, 18.8; **HRMS (EI+):** Calcd for $C_{33}H_{39}N_2O_3S$: 543.2681 (M^++1); found: 543.2680. Specific rotation: $[\alpha]_D^{25}$ –94.4 (*c* 0.100, $CHCl_3$).

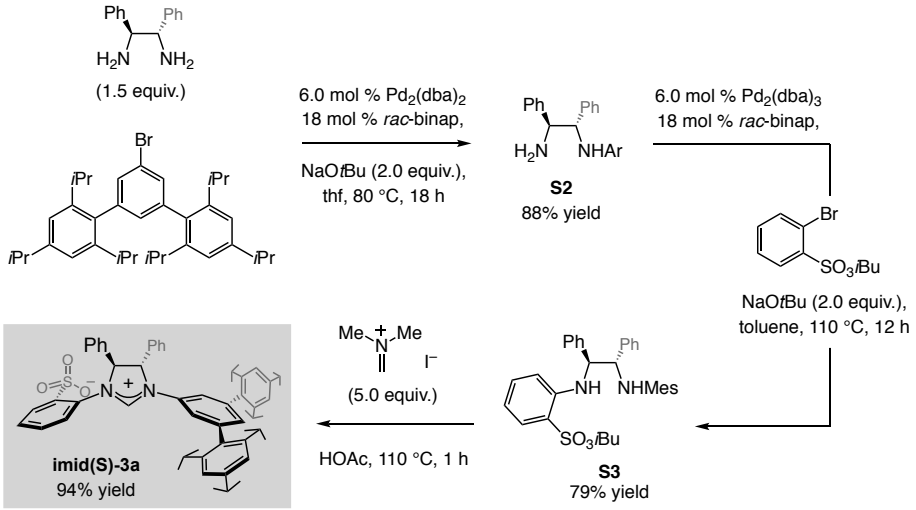
3.3 Imid(S)-1a

An oven-dried 2-dram vial was charged with diamine **1a** (1.56 g, 2.87 mmol) and Eschenmoser's salt (2.60 g, 14.3 mmol). The vial was sealed (septum) and purged with N_2, after which acetic acid (2.48 mL, 43.0 mmol) was added by syringe. The vial was sealed (screw cap) and the solution was allowed to stir at 110 °C (the heterogeneous mixture turned yellow and then black/homogeneous upon heating). After 2 h, the mixture was allowed to cool to 22 °C and transferred into an Erlenmeyer flask, and was diluted with Et_2O (5 mL) and water (5 mL). The solution was neutralized by *slow* addition of an aqueous solution of saturated K_2CO_3 until gas evolution ceased. Dichloromethane (10 mL) was added and the aqueous layer was separated. The aqueous layer was washed with CH_2Cl_2 (2 × 10 mL) and the combined organic layers were dried over Na_2SO_4, filtered and concentrated in vacuo to afford yellow solid, which was purified by silica gel chromatography (100% CH_2Cl_2 to 0.5% MeOH/CH_2Cl_2 to 1.0% MeOH/CH_2Cl_2) to afford 1.12 g (2.26 mmol, 79% yield) of **imid(S)-1a** as white solid. (Note: Separation of a yellow impurity by silica gel chromatography can often be tedious. Note: After silica gel chromatography, precipitation of **imid(S)-1a**

from a CH_2Cl_2 solution with hexenes leads to removal of trace quantities of the impurity; crystalline material was then secured by recrystallization from CH_2Cl_2:Et_2O. **Mp:** 223–225 °C; **IR (neat):** 3058 (m), 2914 (m), 2861 (w), 1623 (s), 1579 (m), 1230 (s) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 8.72 (1H, s), 8.23 (1H, dd, *J* = 7.9, 1.5 Hz), 7.67–7.64 (2H, m, Ar**H**), 7.50–7.47 (2H, m), 7.43–7.41 (3H, m), 7.36–7.30 (4H, m), 7.10 (1H, td, *J* = 7.9, 1.5 Hz), 6.93 (1H, s), 6.73 (1H, s), 6.72 (1H, dd, *J* = 7.9, 1.5 Hz), 6.56 (1H, d, *J* = 11.8 Hz), 5.53 (1H, d, *J* = 11.8 Hz), 2.60 (3H, s), 2.23 (3H, s), 2.00 (3H, s); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 158.7, 144.0, 140.4, 138.6, 135.0, 134.3, 131.5, 130.7, 130.5, 130.5, 130.3, 130.0, 129.9, 129.7, 129.6, 129.1, 129.1, 127.5, 76.2, 74.5, 21.0, 18.8, 18.5; **HRMS (EI+):** Calcd for $C_{30}H_{29}N_2O_3S$: 497.1899 (M^++H), Found 497.1886; **Elemental Analysis:** Anal Calcd for $C_{30}H_{28}N_2O_3S$: C 72.55; H 5.68; N 5.64; found C 72.27; H 5.41; N 5.45. Specific Rotation: $[\alpha]_D^{25}$ –14.9 (*c* 0.50, $CHCl_3$).

3.4 Complex NHC(S)-Ag-1a

An oven-dried 10 mL round bottom flask was charged with **imid(S)-1a** (100 mg, 0.201 mmol), Ag_2O (93.0 mg, 0.400 mmol), and oven-dried powdered <5 micron 4Å MS (~ 50 mg). The flask was purged with N_2, fitted with a reflux condenser, and covered with aluminum foil. Tetrahydrofuran (1.0 mL) and benzene (1.0 mL) were added by syringe, resulting in a heterogeneous black mixture, which was allowed to stir at 80 °C for 1 h. The mixture was allowed to cool to 22 °C and passed through a short plug of celite (4 x 1 cm) eluted with thf (ca. 20 mL). The volatiles were removed in vacuo, affording 119 mg (0.197 mmol, 98% yield) of **NHC(S)-Ag-1a** as white solid (stored in the dark). Further purification was carried out by recrystallization (CH_2Cl_2:Et_2O). **Mp:** 247–249 °C (decomp.); **IR (neat):** 3062 (w), 3026 (w), 2908 (w), 1608 (w), 1480 (s), 1455 (s), 1226 (s), 1201 (s), 1027 (m), 754 (s) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 8.27 (1H, br d, *J* = 7.3 Hz), 7.50–7.44 (2H, m), 7.32–6.95 (9H, m), 6.80 (2H, br s), 6.55 (1H, br d, *J* = 10.4 Hz), 6.33 (2H, br s), 5.18 (1H, br d, *J* = 10.4 Hz), 2.46 (3H, s), 2.29 (3H, s), 1.42 (3H, s); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 205.6 ($J_{C^{109}Ag}$ = 186.8 Hz, $J_{C^{107}Ag}$ = 182.5 Hz), 143.4, 138.6, 138.5, 136.5, 135.7, 135.2, 134.1, 131.1, 130.6, 130.0, 129.9, 129.6, 128.9, 128.8, 128.6, 128.5, 128.4, 128.2, 76.5, 74.0, 68.6, 21.1, 19.0, 17.9. Specific rotation: $[\alpha]_D^{25}$ –104 (*c* 0.50, $CHCl_3$).



3.5 3,5-Bis(2,4,6-tri-*iso*-propylbenzene)-((*1S,2S*)-2-amino-1,2-diphenylethylamino) benzene (S2)

In a glove box, a flame-dried 100 mL round-bottom flask was charged with 5'-bromo-2,2",4,4",6,6"-hexaisopropyl-1,1':3',1"-terphenyl[6] (4.24 g, 7.55 mmol), (–)-(*S,S*)-diphenylethylenediamine (2.41 g, 11.3 mmol), $Pd_2(dba)_3$ (415 mg, 0.453 mmol), *rac*-binap (846 mg, 1.36 mmol) and NaO*t*-Bu (1.31 g, 13.6 mmol). Tetrahydrofuran (20 mL) was added, and, after being fitted with a reflux condenser, the flask was removed from the glove box. The mixture was allowed to stir for 18 h at 80 °C, after which it was allowed to cool to 22 °C. The volatiles were removed in vacuo, and the resulting red oil was purified by silica gel chromatography (1:5 EtOAc:hexanes, R_f = 0.2) to afford 4.61 g (6.64 mmol, 88% yield) of **S2** as pale yellow solid. **Mp:** 86–88 °C. **IR (neat)**: 2960 (s), 2929 (m), 2868 (m), 1590 (s), 1493 (m), 1459 (s), 1433 (m), 1382 (m), 1361 (m), 1315 (w), 1265 (w), 1216 (s), 1110 (s), 1071 (w), 1028 (w), 993 (w), 908 (s), 877 (w), 853 (w), 753 (s), 731 (s), 698 (s), 666 (m), 649 (m) cm−1; **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ 7.34–7.26 (4H, m), 7.24–7.18 (6H, m), 6.95 (2H, d, *J* = 1.2 Hz), 6.92 (2H, s), 6.27 (2H, s), 6.19 (1H, s), 4.97 (1H, d, *J* = 7.6 Hz), 4.59 (1H, dd, *J* = 7.6, 4.0 Hz), 4.34 (1H, d, *J* = 3.2 Hz), 2.86 (2H, q, *J* = 6.8 Hz), 2.71 (2H, q, *J* = 6.8 Hz), 2.55 (2H, q, *J* = 6.8 Hz), 1.38 (2H, d, *J* = 2.8 Hz), 1.24 (12H, d, J = 6.8 Hz), 1.10 (6H, d, J = 6.8 Hz), 0.99 (6H, d, J = 6.8 Hz), 0.89 (12H, dd, *J* = 11.2, 6.8 Hz); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ 147.4, 147.1, 146.6, 146.5, 142.9, 141.3, 141.0, 137.6, 128.4, 128.3, 127.5, 127.4, 127.2, 127.1, 121.3, 120.4, 120.3, 114.2, 77.4, 63.8, 60.9, 34.4, 30.3, 30.2, 24.6, 24.5, 24.3, 24.2, 24.1; **MS (TOF MS ES+)**: Calcd for $C_{50}H_{74}N_2O_5$ $[M+5H_2O]^+$: 782.5; found: 782.3. Specific rotation: $[\alpha]_D^{23.8}$ –52.4 (*c* 0.93, $CHCl_3$).

3.6 3,5-Bis(2,4,6-tri-*iso*-propylbenzene)-((*1S,2S*)-2-((2-*iso*-butylsulfonyl)benzene)-amino-1,2-diphenylethylamino)benzene (S3)

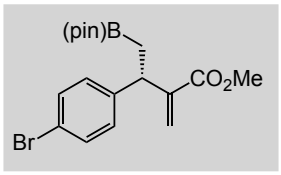
In a glove box, a flame-dried 100 mL round-bottom flask was charged with diamine **S2** (5.14 g, 7.42 mmol), isobutyl-2-bromobenzenesulfonate (3.96 g, 13.5 mmol), $Pd_2(dba)_3$ (407 mg, 0.445 mmol), *rac*-binap (739 mg, 1.19 mmol), and NaO*t*-Bu (1.43 g, 14.8 mmol), and toluene (40 mL) was added. The flask was fitted with a reflux condenser and removed from the glove box, after which the mixture was allowed to stir for 12 h at reflux (110 °C). The solution was allowed to cool to 22 °C and loaded onto a silica gel column. Chromatographic purification of the resulting red oil (1:9 Et_2O:hexanes, R_f = 0.18) afforded 5.31 g (5.86 mmol, 79% yield) of **S3** as pale yellow solid. **Mp:** 98–100 °C. **IR (neat):** 3388 (br), 2960 (s), 2929 (m), 2868 (m), 17 02 (s), 1590 (s), 1513 (s), 1467 (m), 1430 (m), 1351 (w), 1315 (w), 1266 (s), 1241 (s), 1216 (s), 1173 (w), 1162 (w), 1104 (w), 1071 (w), 1029 (m), 976 (m), 943 (m), 908 (m), 877 (m), 846 (m), 815 (m), 752 (s), 731 (s), 700 (s), 667 (m), 649 (m), 592 (s), 526 (m) cm−1; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 7.69 (1H, dd, *J* = 8.0, 1.6 Hz), 7.27–7.20 (5H, m), 7.17 (1H, t, *J* = 7.8 Hz), 7.06 (2H, dd, *J* = 7.8, 1.2 Hz), 7.00–6.95 (7H, m), 6.63 (1H, t, *J* = 8.0 Hz), 6.58 (1H, d, *J* = 6.0 Hz), 6.43 (2H, d, *J* = 1.2 Hz), 6.37 (1H, s), 4.94 (2H, dt, *J* = 5.6, 5.2 Hz), 4.25 (1H, d, *J* = 8.4 Hz), 3.69 (2H, d, *J* = 6.0 Hz), 2.89 (2H, q, *J* = 7.2 Hz), 2.76 (2H, q, *J* = 7.2 Hz), 2.66 (2H, q, *J* = 7.2 Hz), 1.85-1.81 (1H, m), 1.27 (12H, d, *J* = 7.2 Hz), 1.10 (6H, d, *J* = 7.2 Hz), 1.01 (12H, dd, *J* = 6.8, 2.8 Hz), 0.98 (6H, d, *J* = 7.2 Hz), 0.81 (6H, dd, *J* = 6.8, 6.4 Hz); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ 147.4, 146.5, 146.4, 145.7, 145.4, 141.6, 138.1, 137.6, 137.3, 135.2, 130.8, 128.4, 128.3, 128.2, 128.1, 127.9, 122.5, 120.45, 120.40, 117.5, 116.1, 114.8, 113.8, 77.4, 76.3, 62.4, 60.7, 34.4, 30.4, 30.3, 28.1, 24.5, 24.4, 24.23, 24.20, 24.1, 18.75, 18.73; **HRMS (MALDI-TOF):** Calcd for $C_{60}H_{77}N_2O_3S$ $[M+H]^+$: 905.5655; found: 905.5617. Specific rotation: $[\alpha]_D^{23.5}$ –113.2 (*c* 1.00, $CHCl_3$).

imid(S)-3a:[7] Diamine **S3** (1.52 g, 1.68 mmol) and Eschenmoser's salt (1.55 g, 8.39 mmol) were weighed out into a screw cap vial, which was sealed with a septum and purged with N_2. Acetic acid (10.0 mL) was added to the mixture, which was allowed to stir vigorously for 30 min at 22 °C (preliminary stirring at 22 °C is needed for high yield and reproducibility) before it was allowed to heat to 110 °C (the mixture becomes an orange homogeneous solution). After 1 h, the mixture was allowed to cool to 22 °C and diluted with Et_2O (10 mL) and water (10 mL). The solution was neutralized by the *slow* addition of a saturated solution of aqueous K_2CO_3 until gas evolution ceased. The aqueous layer was washed with CH_2Cl_2 (4 x 100 mL) and the combined organic layers were dried over $MgSO_4$, filtered, and concentrated in vacuo to afford red oil, which was purified by silica gel chromatography (10% EtOAc in hexanes to 20% acetone in CH_2Cl_2) to furnish 1.36 g (1.58 mmol, 94% yield) of **imid(S)-3a** as white solid. **Mp:** >300 °C. **IR (neat)**: 3004 (w), 2958 (s), 2928 (m), 2867 (w), 2356 (w), 2340 (w), 2214 (w), 2197 (w), 2190 (w), 2167 (w), 2006 (w), 1978 (w), 1966 (w), 1614 (s), 1583 (s), 1542 (w), 1496 (m), 1475 (s), 1458 (m), 1434 (w), 1382 (m), 1361 (m), 1314 (m), 1279 (s), 1235 (s), 1223 (s), 1201 (s), 1141 (s), 1095 (m), 1075 (m), 1051 (m), 1021 (s), 939 (w), 892 (m), 876 (m), 866 (w), 817 (w), 791 (m), 755 (s), 734 (s), 709 (s), 665 (w), 646 (m), 629 (w), 608 (s), 576 (s), 558 (w), 537 (m), 512 (w), 494 (s), 475 (s), 460 (m), 442 (m), 428 (w), 415 (w) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ 9.19 (1H, s), 8.27 (1H, dd, *J* = 7.8, 1.2 Hz), 7.60–7.57 (2H, m), 7.46–7.43 (5H, m), 7.35 (1H, t, *J* = 7.6 Hz), 7.32 (2H, t , *J* = 3.2 Hz), 7.29 (2H, t, J = 1.2 Hz), 7.26 (1H, s), 7.07 (1H, t, *J* = 8.0 Hz), 7.01 (2H, d, *J* = 1.2 Hz), 6.95 (2H, s), 6.94 (1H, s), 6.54 (1H, dd, *J* = 8.2, 1.2 Hz), 6.11 (1H, d, *J* = 10.4 Hz), 5.86 (1H, d, *J* = 10.4 Hz), 2.89 (2H, q, *J* = 6.8 Hz), 2.47 (2H, q, *J* = 6.8 Hz), 2.26 (2H, q, *J* = 6.8 Hz), 1.27 (12H, d, J = 6.8 Hz), 1.20 (6H, d, *J* = 6.8 Hz), 0.99 (6H, d, *J* = 6.8 Hz), 0.94 (6H, d, *J* = 6.8 Hz), 0.88 (6H, d, *J* = 6.8 Hz); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ 157.6, 148.6, 146.1, 145.8, 143.9, 143.0, 135.1, 134.6, 134.1, 133.3, 132.1, 130.9, 130.4, 130.2, 129.9, 129.7, 129.6, 129.3, 128.9, 128.7, 127.4, 121.6, 120.7, 120.5, 74.9, 34.3, 30.4, 30.3, 29.6, 24.2, 24.17, 24.13, 24.0, 23.8; **HRMS (MALDI-TOF)**: Calcd for $C_{57}H_{66}N_2NaO_3S$ $[M+Na]^+$: 881.4692; found: 881.4714. Specific rotation: $[\alpha]_D^{22.6}$ –160.4 (*c* 0.46, $CHCl_3$)

4 EAS of Bis[(pinacolato)boryl]methane to Trisubstituted Allylic Phosphates (Scheme 22a)

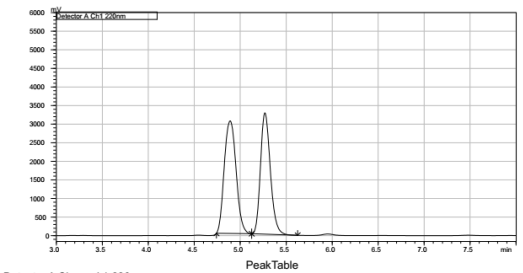
4.1 Representative Procedure

An oven-dried 1-dram vial in a N_2-filled glove box was charged with **NHC(S)–Ag-5a** (7.4 mg, 0.011 mmol), CuCl(1.0 mg, 0.01 mmol), and NaOMe (8.4 mg, 0.15 mmol). The vial was sealed (phenolic open top cap with red PFTE/white silicon septum and electrical tape). After addition of thf by syringe (0.5 mL), the resulting blue solution was allowed to stir five min at 22 °C. A solution of bis[(pinacolato)boryl]methane (40.2 mg, 0.15 mmol) in thf (0.5 mL) was added, causing the mixture to turn brown. The mixture was allowed to stir for five min at 22 °C, after which it was charged with a solution of allylic phosphate (0.1 mmol) in thf (0.5 mL). The mixture was allowed to stir at 22 °C for 12 h, after which it was passed through a short plug of silica gel and eluted with Et_2O (3 mL). The resulting solution was concentrated in vacuo, affording yellow oil residue, which was purified by silica gel chromatography to afford the desired product as colorless oil.



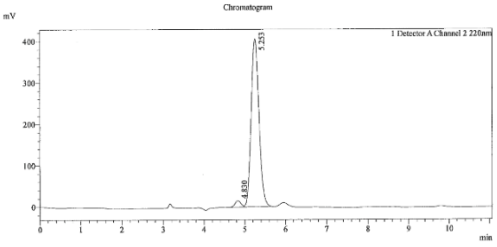
4.2 Methyl-(*R*)-3-(4-bromophenyl)-2-methylene-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) butanoate

IR (neat): 2977 (w), 2931, (w), 1721 (w), 1627 (w), 1485 (w), 1467 (w), 1438 (w), 1367 (m), 1317 (s), 1269 (m), 1214 (w), 1141 (s), 1098 (w), 1072 (w), 1036 (w), 1010 (s), 967 (m), 890 (w), 845 (m), 817 (w) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 7.37–7.33 (2H, m), 7.12–7.09 (2H, m), 6.26 (1H, s), 5.68 (1H, s), 4.11 (1H, t, *J* = 8 Hz), 3.62 (3H, s), 1.35–1.23 (2H, m), 1.11 (12H, s); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 167.2, 145.0, 143.7, 131.3, 129.7, 123.9, 120.0, 83.4, 51.9, 41.6, 24.9; **HMRS (ESI$^+$):** Calcd for $C_{18}H_{25}BBrO_4$ [M+H$^+$]: 395.1029; found: 395.1023. Specific rotation $[\alpha]^{20}$ –37.0 (*c* 0.81, $CHCl_3$) for a sample of 98:2 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material; Chiracel OJ-H, 99% hexanes, 1% *i*PrOH, 1.0 mL/min, 220 nm.



Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Area %
1	4.886	27126918	3026732	52.640
2	5.265	24406309	3265872	47.360
Total		51533227	6294604	100.000

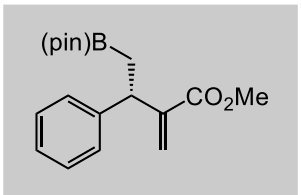


Peak Table

Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Conc.
1	4.830	153111	15342	2.774
2	5.253	5365817	405171	97.226
Total		5518928	420513	

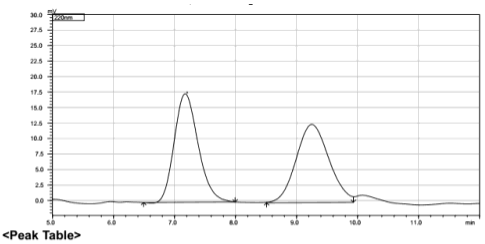
Retention Time	Area	Area %	Retention Time	Area	Area %
4.886	27126918	52.640	4.830	153111	2.774
5.265	24406309	47.360	5.253	5365817	97.226



4.3 Methyl-(*R*)-2-methylene-3-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) butanoate

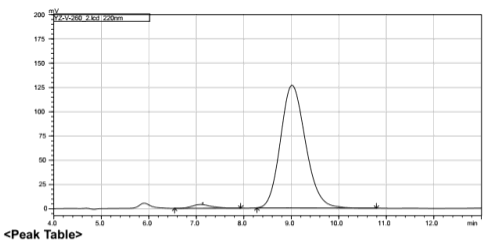
IR (neat): 2978 (w), 2931 (w), 1722 (m), 1626 (w), 1493 (w), 1437 (w), 1389 (w), 1359 (m), 1320 (m), 1272 (w), 1212 (w), 1143 (s), 1111 (w), 1082 (w), 1059 (w), 1006 (w), 986 (w) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 7.23 (4H, d, *J* = 4.3 Hz,), 7.18 – 7.10 (1H, m), 6.25 (1H, s), 5.68 (1H, t, *J* = 1.2 Hz), 4.17 (1H, t, *J* = 8.2 Hz), 3.65 (3H, s), 1.34 (2H, dd, *J* = 8.3, 4.7 Hz), 1.11 (6H, s), 1.10 (6H, s); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 167.5, 145.5, 144.6, 128.3, 127.9, 126.3, 123.6, 83.3, 51.9, 42.1, 24.8, 24.8; **HMRS (ESI$^+$):** Calcd for $C_{18}H_{26}BO_4$ [M+H$^+$]: 317.1919; found: 317.1923. Specific rotation $[\alpha]^{20}$ –79.1 (*c* 0.3, $CHCl_3$) for

a sample of 98:2 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material; Chiracel OJ-H, 99% hexanes, 1% *i*PrOH, 1.0 mL/min, 220 nm.



<Peak Table>
220nm

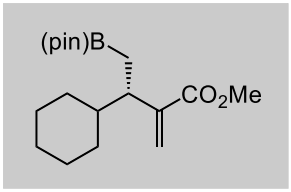
Peak#	Ret. Time	Area	Area%
1	7.174	476410	50.171
2	9.251	473163	49.829
Total		949573	100.000



<Peak Table>
220nm

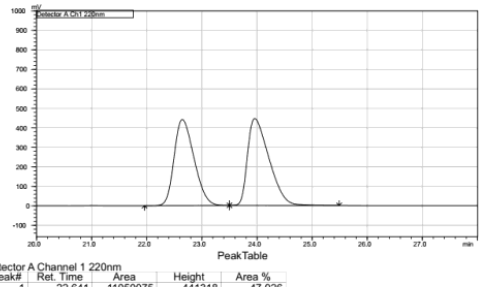
Peak#	Ret. Time	Area	Area%
1	7.088	109648	2.312
2	9.015	4632424	97.688
Total		4742072	100.000

Retention Time	Area	Area %	Retention Time	Area	Area %
7.174	476410	50.171	7.088	109648	2.312
9.251	473163	59.829	9.015	4632424	97.688



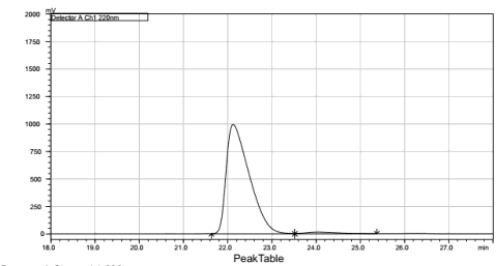
4.4 Methyl-(*R*)-3-cyclohexyl-2-methylene-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) butanoate

IR (neat): 2978 (w), 2924 (w), 2851 (w), 1719 (m), 1623 (w), 1437 (w), 1364 (m), 1320 (m), 1268 (w), 1227 (w), 1200 (w), 1143 (s), 1001 (w), 967 (w) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 6.18 (1H, s), 5.48 (1H, s), 3.73 (3H, s), 2.71 (1H, dt, J = 6.0, 10.8 Hz), 1.72–1.59 (5H, m), 1.39–1.30 (1H, m), 1.26–1.05 (5H, m), 1.18 (6H, s), 1.16 (6H, s), 0.98–0.78 (2H, m); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ 168.2, 145.2, 124.4, 83.1, 51.8, 43.0, 41.8, 31.3, 29.7, 26.71, 26.69, 26.68, 25.0, 24.7; **HRMS (ESI$^+$):** Calcd for $C_{18}H_{32}BO_4$ [M+H$^+$]: 323.2394; found: 323.2302. Specific rotation $[\alpha]^{20}$ –1.31 (*c* 1.91, $CHCl_3$) for a sample of 98:2 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material; Chiracel OZ-H, 99.5% hexanes, 0.5% *i*PrOH, 1.0 mL/min, 220 nm.



Detector A Channel 1 220nm

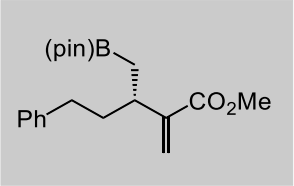
Peak#	Ret. Time	Area	Height	Area %
1	22.641	11050075	441318	47.926
2	23.955	12006674	445674	52.074
Total		23056749	886992	100.000



Detector A Channel 1 220nm

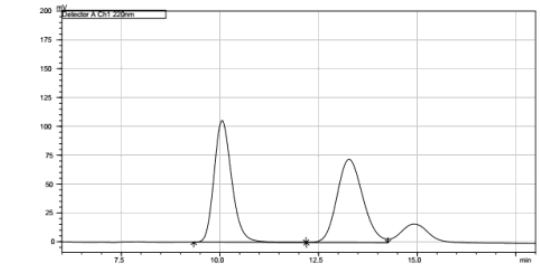
Peak#	Ret. Time	Area	Height	Area %
1	22.119	36006160	994059	97.789
2	24.043	813956	15548	2.211
Total		36820117	1009607	100.000

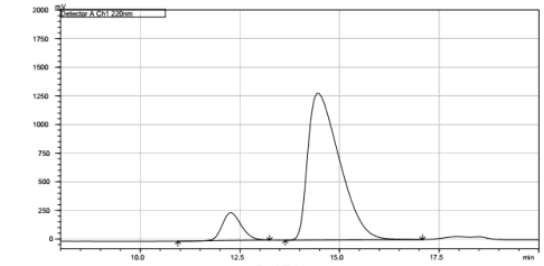
Retention Time	Area	Area %	Retention Time	Area	Area %
22.641	11050075	47.926	22.119	36006160	97.789
23.955	12006674	52.073	24.043	813958	2.211



4.5 Methyl-(*R*)-2-methylene-5-phenyl-3-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl) pentanoate

IR (neat): 3025 (w), 2977 (w), 2926 (w), 2855 (w), 1719 (m), 1625 (w), 1496 (w), 1454 (w), 1437 (w), 1369 (m), 1321 (m), 1269 (m), 1197 (m), 1143 (s), 1107 (w), 1030 (w), 1004 (w), 968 (w) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz)**: δ 7.27–7.23 (2H, m), 7.17–7.14 (3H, m), 6.20 (1H, s), 5.58 (1H, s), 3.75 (3H, s), 2.96 (1H, m), 2.55 (2H, m), 1.92–1.83 (1H, m), 1.80–1.71 (1H, m), 1.21 (6H, s), 1.20 (6H, s), 1.08 (2H, dq, J = 6.8, 15.6 Hz); **^{13}C NMR ($CDCl_3$, 100 MHz)**: δ 167.9, 145.7, 142.8, 128.5, 128.4, 125.7, 124.0, 83.2, 51.8, 38.7, 36.6, 33.7, 24.9; **HRMS (ESI$^+$):** Calcd for $C_{20}H_{30}BO_4$ [M+H$^+$]: 345.2247; found: 345.2247. Specific rotation $[\alpha]^{20}$ –25.7 (*c* 1.36, $CHCl_3$) for a sample of 90:10 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material; Chiracel OJ-H, 99% hexanes, 1% *i*PrOH, 1.0 mL/min, 220 nm.





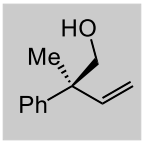
Retention Time	Area	Area %	Retention Time	Area	Area %
10.050	3282514	49.878	12.265	8172576	10.319
13.269	3298602	50.122	14.455	71023094	89.681

5 EAS of Bis[(pinacolato)boryl]methane to *Z*-Trisubstituted Allylic Phosphates (Scheme 22b)

5.1 Representative Procedure

An oven-dried 1-dram vial in a N_2-filled glove box and equipped with a stir bar was charged with **NHC(S)-Ag-5b** (4.0 mg, 2.75 μmol) and CuCl (0.5 mg, 5 μmol). Tetrahydrofuran (0.8 mL) was added and the mixture was allowed to stir for two h at 22 °C, after which NaOMe (6.5 mg, 120 μmol) was added and the vial was sealed (capped with phenolic open-top cap with a red PFTE/white silicon septum and electrical

tape) and removed from the glove box. A solution of allylic phosphate (0.10 mmol) and bis[(pinacolato)boryl]methane (40.2 mg, 0.15 mmol) in thf (0.3 mL) was added by syringe and the mixture was allowed to stir for 24 h at 22 °C, after which it was passed through a short plug of silica gel and eluted with Et_2O. The volatiles were removed in vacuo, and $NaBO_3 \cdot 4H_2O$ (46.2 mg, 0.30 mmol), thf (1 mL) and H_2O (1 mL) was added to the yellow oil. The mixture was allowed to stir for three h at 22 °C, after which H_2O and Et_2O were added, the organic layer separated, and the aqueous layer was washed with Et_2O (3 x 2 mL). The combined organic layers were dried with Na_2SO_4 and the volatiles were in vacuo. The resulting yellow oil was purified by silica gel chromatography to afford the desired product as colorless oil.

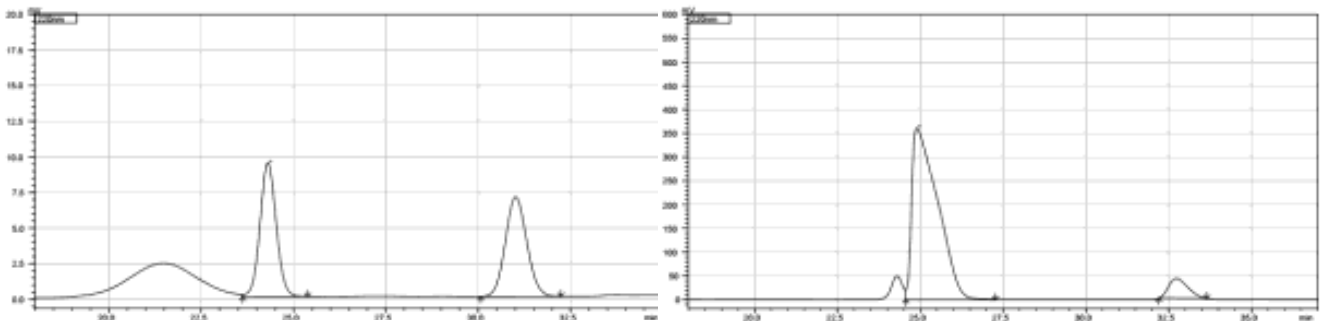


5.2 (*S*)-2-Methyl-2-phenylbut-3-en-1-ol[8]

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.36–7.24 (5H, m), 6.08 (1H, dd, J = 17.6, 10.8 Hz), 5.28 (1H, dd, J = 10.8, 1.2 Hz), 5.16 (1H, dd, J = 17.6, 1.2 Hz), 3.80 (2H, d, J = 6.4 Hz), 1.44 (3H, s), 1.35 (1H, br, s). Specific rotation: $[\alpha]_D^{20}$ 16.3 (*c* 1.0, EtOH) for an enantiomerically enriched sample of 92:8 e.r.

5.2.1 Determination of stereochemical identity

Previously reported specific rotation: $[\alpha]_D^{20}$ −18.1 (*c* 1.9, EtOH) for an enantiomerically enriched sample of 90.5:9.5 e.r. (*R* major).[9] Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material; Chiralpak AZ-H column, 99.5% hexanes, 0.5% *i*PrOH, 1.0 mL/min, 220 nm.



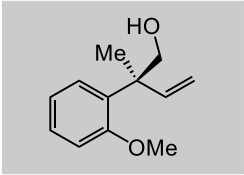
220nm

Peak#	Ret. Time	Area	Area%
1	24.306	288015	50.454
2	31.013	282834	49.546
Total		570849	100.000

220nm

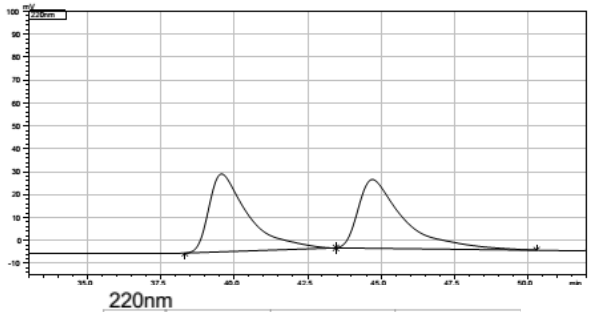
Peak#	Ret. Time	Area	Area%
1	24.895	19490025	92.084
2	32.731	1675487	7.916
Total		21165511	100.000

Retention Time	Area	Area %	Retention Time	Area	Area %
24.306	288015	50.454	24.895	19490025	92.084
31.013	282834	49.546	32.731	1675487	7.916



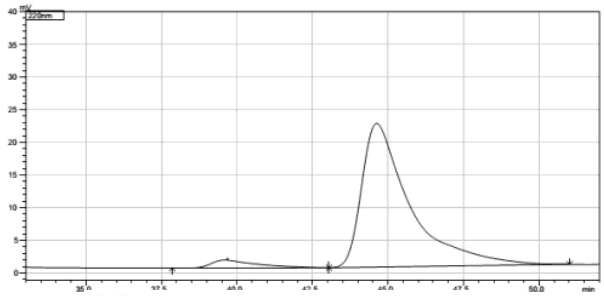
5.3 (*S*)-2-(2-Methoxyphenyl)-2-methylbut-3-en-1-ol

IR (neat): 3421 (br), 2936 (w), 2881 (w), 1598 (w), 1498 (s), 1462 (m), 1434 (m), 1240 (s), 1027 (s), 914 (m), 753 (s), 700 (w) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 7.29 (1H, dd, *J* = 8.0, 1.6 Hz), 7.24–7.20 (1H, m), 6.94–6.88 (2H, m), 6.20 (1H, dd, *J* = 18.0, 10.4 Hz), 5.16 (1H, dd, *J* = 10.8, 1.2 Hz), 5.03 (1H, dd, *J* = 18.0, 1.2 Hz), 3.98–3.93 (1H, m), 3.89–3.84 (1H, m), 3.80 (3H, s), 1.44 (3H, s); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 157.9, 144.0, 132.3, 129.1, 128.0, 120.7, 113.2, 111.9, 68.5, 55.2, 47.0, 21.7; **HRMS (ESI$^+$):** Calcd for $C_{12}H_{16}O_2$ $[M+H]^+$: 193.1229; found: 193.123. Specific rotation: $[\alpha]_D^{20}$ 14.4 (*c* 0.5, $CHCl_3$) for an enantiomerically enriched sample of 95:5 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material; Chiralcel OD-H column, 99% hexanes, 1% *i*PrOH, 0.5 mL/min, 220 nm.



220nm

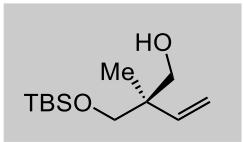
Peak#	Ret. Time	Area	Area%
1	39.564	3181337	49.712
2	44.708	3218168	50.288
Total		6399505	100.000



220nm

Peak#	Ret. Time	Area	Area%
1	39.588	123905	4.814
2	44.621	2449898	95.186
Total		2573804	100.000

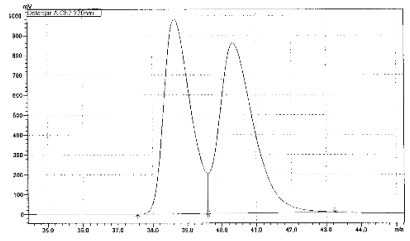
Retention Time	Area	Area %	Retention Time	Area	Area %
39.564	3181337	49.712	39.588	123905	4.814
44.708	3218168	50.288	44.621	2449898	95.186

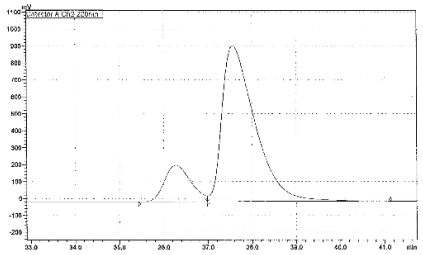


5.4 (*R*)-2-(((*tert*-Butyldimethylsilyl)oxy)methyl)-2-methylbut-3-en-1-ol

IR (neat): 2927 (m), 1723 (s), 1470 (m), 1268 (s), 1096 (s), 1027 (m), 837 (s), 776 (m), 709 (s) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 5.81 (1H, dd, *J* = 17.6, 10.8 Hz), 5.13 (1H, dd, *J* = 6.8, 1.2 Hz), 5.09 (1H, dd, *J* = 12.8, 1.2 Hz), 3.63–3.45 (4H, m), 2.52 (1H, br), 1.00 (3H, s), 0.89 (9H, s), 0.04 (6H, s); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 141.5, 114.6, 70.6, 70.0, 43.2, 26.0, 18.6, 18.3, –5.50, –5.48; **HRMS (ESI$^+$):** Calcd for $C_{12}H_{25}OSi$ $[M+H–H_2O]^+$: 213.1675; found: 213.168. Specific rotation: $[\alpha]_D^{20}$ 0.2 (*c* 1.0, $CHCl_3$) for an

enantiomerically enriched sample of 84:16 e.r. Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material of benzoate derivatives; Chiralcel OD-H column, 100% hexanes, 0.2 mL/min, 220 nm.





<Peak Table>
Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark
1	38.643	52778054	979513	47.222		M
2	40.337	58987079	856206	52.778		V M
Total		111765133	1835820			

<Peak Table>
Detector A Channel 2 220nm

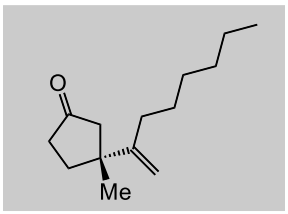
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark
1	36.267	8858598	214675	15.701		M
2	37.567	47563137	922089	84.299		V M
Total		56421734	1136664			

Retention Time	Area	Area %	Retention Time	Area	Area %
38.643	52778054	47.222	36.267	8858598	15.701
40.337	58987079	52.778	37.567	47563137	84.299

6 ECA of Alkenyl–Al Compounds to Cyclic Enones (Schemes 49-50)

6.1 Representative Procedure

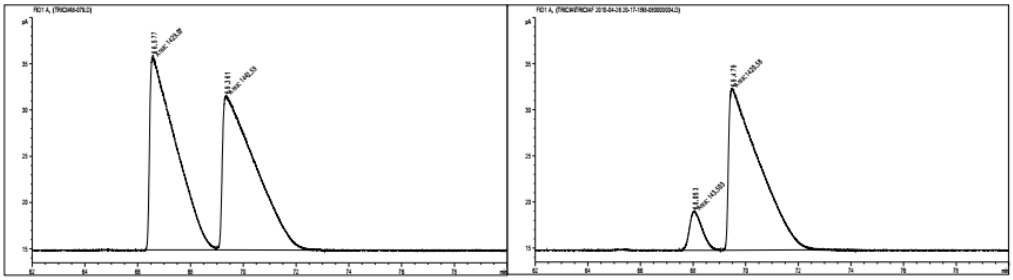
In a glove box, an oven-dried 4-dram vial was charged with **NHC(S)–Ag-2d** (2.70 mg, 2.50 μmol) and $CuCl_2$•$2H_2O$ (0.850 mg, 5.00 μmol). The vial was sealed (septum), and thf (1.0 mL) was added by syringe and the resulting blue solution was allowed to stir for five min. To this mixture was added (syringe, at –78 °C, sequentially), diisobutyl(oct-1-en-2-yl)aluminum (160 μL, 0.20 mmol, 1.25 M) (CAUTION: Flammable!) and 3-methylcyclopentenone (9.9 μL, 0.10 mmol), which resulted in a brown solution. The mixture was allowed to stir for 12 h at –50 °C, after which the reaction was quenched by the addition of a saturated solution aqueous of sodium potassium tartrate (2 mL). The mixture was washed with Et_2O (2 x 1 mL), passed through a short plug of silica gel (2 cm x 1 cm), and eluted with Et_2O. The organic layer was dried over $MgSO_4$, filtered, and the volatiles were removed in vacuo to furnish yellow oil, which was purified by silica gel chromatography to afford 17.7 mg of (*R*)-3-methyl-3-(oct-1-en-2-yl)cyclopentan-1-one as colorless oil (0.085 mmol, 85% yield).



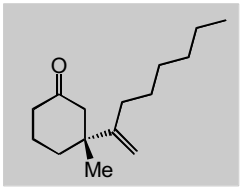
6.2 (*R*)-3-Methyl-3-(oct-1-en-2-yl)cyclopentanone

IR (neat): 2956 (m), 2926 (s), 2856 (m), 1745 (s), 1637 (w), 1588 (w), 1465 (m), 1406 (w), 1377 (w), 1249 (w), 1160 (w), 895 (w), 725 (w) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 4.81 (1H, s), 4.81 (1H, s), 2.41 (1H,

d, J = 17.6 Hz), 2.31–2.27 (2H, m), 2.13 (1H, d, J = 17.6 Hz), 2.07–2.01 (3H, m), 1.91–1.85 (1H, m), 1.49–1.43 (2H, m), 1.36–1.25 (6H, m), 1.17 (3H, s), 0.89 (3H, t, J = 6.0 Hz); **^{13}C NMR ($CDCl_3$, 100 MHz):** 219.2, 155.0, 107.7, 51.5, 45.5, 36.7, 34.0, 32.0, 31.7, 29.5, 28.9, 26.2, 22.8, 14.2; **HRMS (EI+):** Calcd for $C_{14}H_{25}O$ $[M+H]^+$: 209.1905; found: 209.1903. Specific rotation: $[\alpha]_D^{24}$ –10.0 (*c* 1.04, $CHCl_3$) for an enantiomerically enriched sample of 91:9 e.r. Enantiomeric purity was determined by GC analysis in comparison with authentic racemic material; CDMDM column, 15 psi, 120 °C.

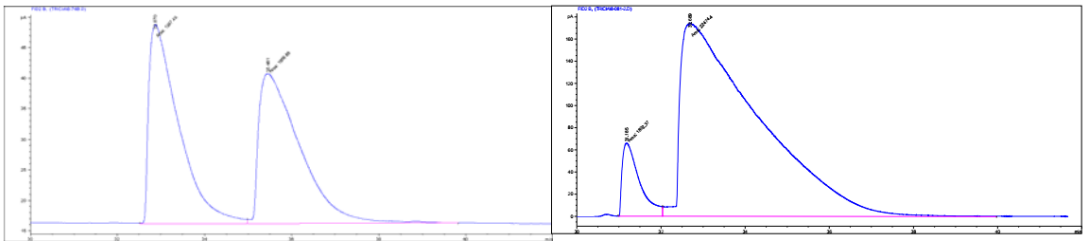


Retention Time	Area	Area %	Retention Time	Area	Area %
66.577	1429.1	49.765	68.053	143.5	9.175
69.361	1442.6	50.235	69.479	1420.6	90.825

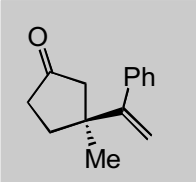


6.3 (*R*)-3-Methyl-3-(oct-1-en-2-yl)cyclohexanone

IR (neat): 2955 (m), 2929 (s), 2858 (m), 1714 (s), 1634 (w), 1457 (m), 1423 (w), 1377 (w), 1350 (w), 1289 (m), 1226 (w), 1080 (w), 903 (m) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 4.85 (2H, s), 2.60 (1H, dd, J = 14.0, 1.2 Hz), 2.33–2.17 (3H, m), 2.00–1.90 (3H, m), 1.86–1.68 (2H, m), 1.62–1.60 (1H, m), 1.47–1.41 (2H, m), 1.36–1.26 (6H, m), 1.08 (3H, s), 0.89 (3H, t, J = 5.6 Hz); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 211.9, 154.3, 109.7, 52.9, 44.4, 40.1, 35.0, 32.0, 30.8, 29.6, 29.1, 26.9, 22.8, 22.0, 14.2; **HRMS (EI+):** Calcd for $C_{15}H_{27}O$ $[M+H]^+$: 223.2062; found: 223.2064. Specific rotation: $[\alpha]_D^{24}$ +25.2 (*c* 1.42, $CHCl_3$) for an enantiomerically enriched sample of 92:8 e.r. Enantiomeric purity was determined by GC analysis in comparison with authentic racemic material; CDGTA column, 15 psi, 140 °C.

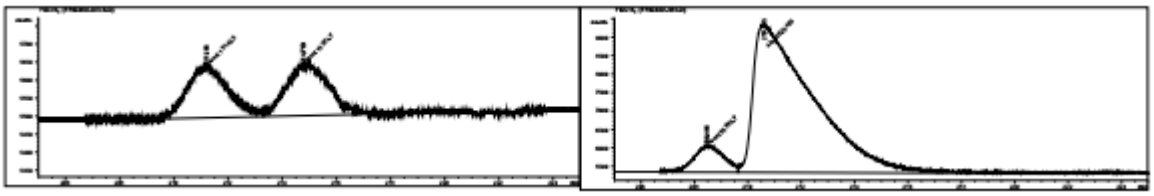


Retention Time	Area	Area %	Retention Time	Area	Area %
32.870	1557.5	49.219	31.185	1892.4	7.766
35.461	1606.9	50.781	32.689	22474.4	92.234

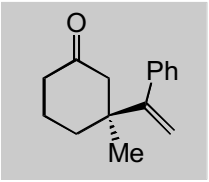


6.4 (*S*)-3-Methyl-3-(1-phenylvinyl)cyclopentanone

IR (neat): 2959 (w), 2873 (w), 1741 (s), 1627 (w), 1598 (w), 1573 (w), 1492 (w), 1441 (w), 1405 (w), 1375 (w), 1280 (w), 1249 (w), 1231 (w), 1208 (w), 1165 (m), 1120 (w), 1074 (w), 1028 (w), 980 (w), 906 (m), 877 (w), 812 (w), 774 (w), 812 (w), 774 (w), 752 (m), 702 (w) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** 7.30–7.22 (3H, m), 7.14–7.12 (2H, m), 5.16 (1H, d, J = 0.8 Hz), 4.94 (1H, d, J = 0.8 Hz), 2.48 (1H, d, J = 17.2 Hz), 2.30–2.26 (2H, m), 2.19–2.11 (2H, m), 1.87–1.81 (1H, m), 1.23 (3H, s); **^{13}C NMR ($CDCl_3$, 100 MHz):** 218.6, 156.4, 142.3, 128.7, 128.0, 127.1, 113.7, 51.9, 45.1, 36.6, 34.5, 26.6; **HRMS (EI+):** Calcd for $C_{14}H_{17}O$ $[M+H]^+$: 201.1279; found: 201.1285. Specific Rotation: $[\alpha]_D^{24}$ –11.3 (*c* 0.73, $CHCl_3$) for an enantiomerically enriched sample of 92:8 e.r. Enantiomeric purity was determined by GC analysis in comparison with authentic racemic material; β-dex column, 15 psi, 120 °C.



Retention Time	Area	Area %	Retention Time	Area	Area %
211.195	15142.8	49.620	208.466	55789.7	8.189
214.783	15374.7	50.380	210.635	625469.2	91.81



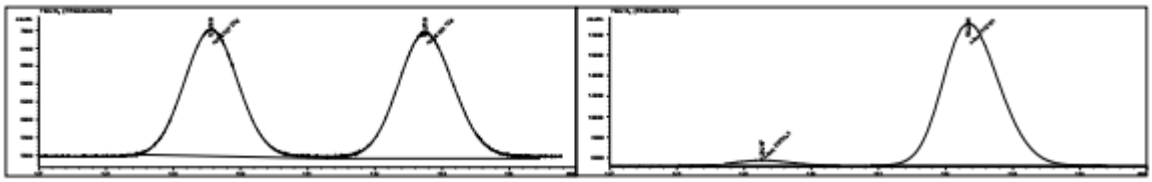
6.5 (*S*)-3-Methyl-3-(1-phenylvinyl)cyclohexanone

IR (neat): 2956 (m), 2872 (w), 1707 (s), 1625 (w), 1491 (w), 1441 (w), 1421 (w), 1399 (w), 1375 (w), 1349 (w), 1289 (w), 1226 (m), 1135 (w), 1074 (w), 1028 (w), 951 (w), 909 (m), 773 (m), 703 (s), 676 (w), 636 (w), 614 (w), 571 (w), 538 (m), 503 (m), 440 (w), 420 (w) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 7.30–7.23 (3H, m), 7.11–7.08 (2H, m), 5.18 (1H, d, J = 0.8 Hz), 4.91 (1H, d, J = 1.2 Hz), 2.66 (1H, d, J = 14.0 Hz), 2.32–2.22 (3H, m), 1.96–1.79 (3H, m), 1.63–1.57 (1H, m), 1.13 (3H, s); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 211.6, 156.4, 142.2, 129.2, 127.7, 126.9, 115.1, 52.8, 44.2, 40.9, 35.0, 26.7, 22.2; **HRMS (EI+):** Calcd

for $C_{15}H_{19}O$ $[M+H]^+$: 215.1436; found: 215.1438. Specific rotation: $[\alpha]_D^{24}$ +32.2 (*c* 0.980, $CHCl_3$) for an enantiomerically enriched sample of 96:4 e.r.

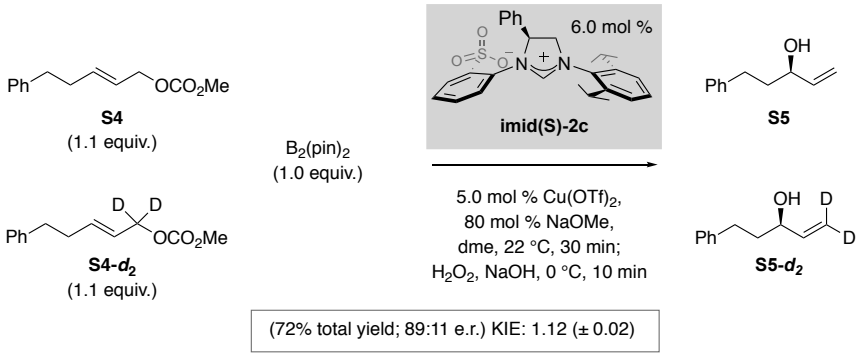
6.5.1 Determination of Stereochemical Identity

Formerly reported specific rotation: $[\alpha]_D^{20}$ –33.4 (*c* 1.00, $CHCl_3$) for an enantiomerically enriched sample of 94:6 e.r. of the *R* enantiomer.[10] Enantiomeric purity was determined by GC analysis in comparison with authentic racemic material; β-dex column, 15 psi, 140 °C.



Retention Time	Area	Area %	Retention Time	Area	Area %
129.56	82723.2	48.794	129.267	29758.8	3.413
132.75	86812.9	51.206	132.336	842161.3	96.587

7 Kinetic Isotope Effect Experiments



7.1 (*E*)-Methyl (5-phenylpent-2-en-1-yl-1,1-*d*$_2$) carbonate

This compound was prepared according to a previously reported procedure.[11] **IR (neat):** 3025 (w), 2952 (w), 2851 (w), 1741 (s), 1494 (w), 1439 (m), 1275 (s), 1179 (m), 1050 (m), 969 (m), 924 (m), 790 (m), 747 (m), 698 (m) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 7.33–7.25 (2H, m), 7.22–7.15 (3H, m), 5.87 (1H, dt, *J* = 15.4, 6.7 Hz), 5.62 (1H, d, *J* = 15.4 Hz), 3.79 (3H, s), 2.74–2.66 (2H, m), 2.47–2.24 (2H, m); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 155.8, 141.6, 136.5, 128.5, 128.5, 126.1, 123.9, 68.0 (m), 54.8, 35.4, 34.1; **HRMS (DART):** Calcd for $C_{13}H_{18}D_2O_3N$ $[M+NH_4^+]$: 240.1569. Found: 240.157.

7.2 Competition experiment between S4 and S4-*d*$_2$ and determination of the secondary kinetic isotope effect (SKIE) for C–O bond cleavage at Cα

In a N_2-filled glove box, an oven-dried 1-dram vial ("Vial 1") equipped with a stir bar was charged with the corresponding imidazolinium salt (2.8 mg, 6.0 μmol), NaOMe (4.3 mg, 80 μmol), $Cu(OTf)_2$ (1.8 mg, 5.0

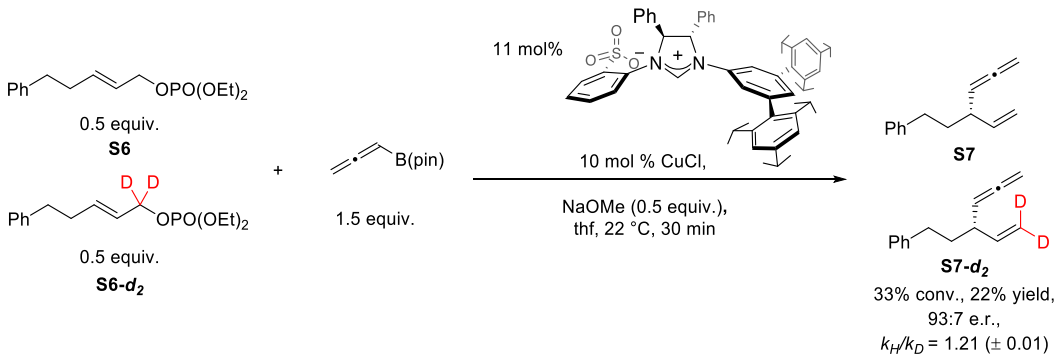
μmol) and dme (0.4 mL), and the mixture was allowed to stir for 1 h at 22 °C. At this point, $B_2(pin)_2$ (25.4 mg, 0.10 mmol) was added and the mixture was allowed to stir for an additional 30 min.

In an N_2-filled glove box, a second oven-dried 1-dram vial ("Vial 2") was charged with **S4** (24.2 mg, 0.11 mmol), **S4-*d*$_2$** (24.4 mg, 0.11 mmol) and dme (0.1 mL). The solution in Vial 2 was transferred to Vial 1 and the resulting mixture was allowed to stir for 30 min at 22 °C. The solution was passed through a short plug of silica gel (4 cm x 1 cm) and eluted with Et_2O. The filtrate was concentrated in vacuo and the resulting yellow oil was dissolved in Et_2O, after which, at 0 °C, H_2O_2 (30 wt% in H_2O, 125 μL) and NaOH (2.0 M in H_2O, 0.5 mL) were added, and the mixture was allowed to stir for 1 h at 0 °C. The solution was passed through a short plug of silica gel (4 cm x 1 cm) and eluted with Et_2O. The filtrate was concentrated in vacuo and the resulting yellow oil was purified by silica gel chromatography to afford a mixture of **S5** and **S5-*d*$_2$** as colorless oil (11.7 mg, 0.072 mmol, 72% yield). The ratio of **S5**:**S5-*d*$_2$** was determined by analysis of the ^{1}H NMR spectrum of the purified product.

The relative rates corresponding to the reactions with **S5** and **S5-*d*$_2$**, respectively, were determined by the use of the following formula:

$$k_H/k_D = n_{S2}/n_{S2\text{-}d2}$$

Accordingly, we measured SKIE (k_H/k_D = 1.12 +/– 0.02) as the average of three independent experiments (1.10, 1.12, 1.14).



7.3 (*E*)-Diethyl (5-phenylpent-2-en-1-yl-1,1-*d*$_2$) phosphate

This material was prepared according to a previously reported procedure.[11] **IR (neat):** 3472 (br), 3024 (w), 2980 (w), 2928 (w), 1667 (w), 1495 (w), 1453 (w), 1392 (w), 1263 (m), 1015 (s), 968 (s), 799 (m), 746 (m), 698 (m) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 7.32–7.24 (2H, m), 7.23–7.14 (3H, m), 5.84 (1H, dt, *J* = 15.4, 6.6 Hz), 5.64 (1H ,d, J = 15.4 Hz), 4.17–3.99 (4H, m), 2.90–2.57 (2H, m), 2.51–2.26 (2H, m), 1.55–1.09 (6H, m); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 141.5, 135.5, 128.5 (d, *J* = 3.1 Hz), 126.0, 125.1, 125.1, 68.4–66.7 (m), 63.8 (d, *J* = 5.7 Hz), 35.3, 34.0, 16.2 (d, *J* = 6.7 Hz); **HRMS (DART):** Calcd for $C_{15}H_{22}D_2O_4P$ [M+H$^+$]: 301.1538. Found: 301.1533.

7.4 Competition experiment between S6 and S6-*d*$_2$ and determination of the secondary kinetic isotope effect (SKIE) for C–O bond cleavage at Cα

In a N_2-filled glove box an oven-dried 1-dram vial ("Vial 1") equipped with a stir bar was charged with the corresponding imidazolinium salt (9.3 mg, 11.0 μmol), NaOMe (2.7 mg, 50 μmol), CuCl (1.0 mg, 10.0

μmol), and thf (0.7 mL). The mixture was allowed to stir for 1 h at 22 °C. The allenyl–B(pin) compound (24.9 mg, 0.15 mmol) was added and the mixture was allowed to stir for another 30 min at 22 °C.

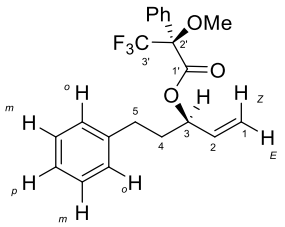
In a N_2-filled glove box, a second oven-dried 1-dram vial ("Vial 2") was charged with **S6** (14.9 mg, 0.05 mmol), **S6-*d*$_2$** (15.0 mg, 0.05 mmol), and thf (0.3 mL). The solution in Vial 2 was transferred to Vial 1 and the mixture was allowed to stir for 30 min at 22 °C. The mixture was passed through a short plug of silica gel (4 cm x 1 cm) and eluted with Et_2O. The filtrate was concentrated in vacuo and the resulting yellow oil was purified by silica gel chromatography to afford a mixture of **S7** and **S7-*d*$_2$** as colorless oil (4.1 mg, 0.022 mmol, 22% yield). The ratio of **S7**:**S7-*d*$_2$** was determined by analysis of the ^{1}H NMR spectrum of the purified product.

The relative rates corresponding to the reactions with **S7** and **S7-*d*$_2$**, respectively, were determined through the use of the following formula:

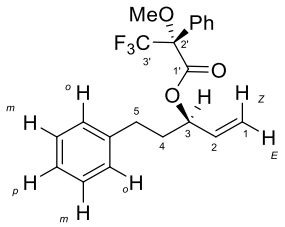
$$k_H/k_D = n_{S4}/n_{S4\text{-}d2}$$

According, we measured SKIE (k_H/k_D = 1.21 +/– 0.01) as the average of three independent experiments (1.20, 1.21, 1.22).

8 Absolute Stereochemistry of Enantioselective Boryl Substitution Products



***(S)*-S8**



***(R)*-S8**

8.1 (*R*)-5-Phenylpent-1-en-3-yl (*S*)-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate (*S*-S8)

This compound was prepared according to a previously reported procedure.[12] The secondary alcohol substrate was accessed by oxidation of the enantiomerically enriched allylic boronate, synthesized by enantioselective boryl substitution with an *E* allylic carbonate.[11b] **IR (neat):** 3025 (w), 2952 (w), 1745 (s), 1496 (w), 1452 (w), 1257 (s), 1168 (s), 1121 (m), 1015 (m), 719 (m), 698 (m) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 7.59–7.50 (2H, m), 7.43–7.38 (3H, m), 7.33–7.25 (2H, m), 7.23–7.18 (1H, m), 7.16–7.12 (2H, m), 5.77 (1H, ddd, *J* = 17.3, 10.5, 6.9 Hz), 5.48 (1H, q, *J* = 6.9 Hz), 5.30 (1H, dt, *J* = 17.2, 1.2 Hz), 5.25 (1H, dt, *J* = 10.5, 1.1 Hz), 3.57 (3H, d, *J* = 1.3 Hz), 2.71–2.60 (2H, m), 2.15–1.91 (2H, m); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 165.9, 141.0, 134.9, 132.4, 129.7, 128.7, 128.5, 128.5, 127.6, 126.3, 123.5 (q, *J* = 288.5 Hz), 118.9, 84.8 (q, *J* = 27.7 Hz), 77.2, 55.6, 35.9, 31.4; **HRMS (DART):** Calcd for $C_{21}H_{25}NO_3F_3$ [M+NH_4^+]: 396.1781; found: 396.1782. Specific rotation: $[\alpha]_D^{20}$ –23.1 (*c* 0.26, $CHCl_3$).

8.2 (*R*)-5-Phenylpent-1-en-3-yl (*R*)-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate (*R*-S8)

This compound was prepared according to a formerly reported procedure.[12] **IR (neat):** 3064 (w), 2948 (w), 2924 (w), 1745 (s), 1496 (w), 1452 (w), 1257 (m), 1268 (s), 1121 (m), 1015 (m), 990 (m), 698 (m) cm^{-1};

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.60–7.52 (2H, m), 7.45–7.37 (3H, m), 7.31–7.22 (2H, m), 7.18 (1H, t, *J* = 7.4 Hz), 7.11–7.04 (1H, m), 5.86 (1H, ddd, *J* = 17.4, 10.4, 7.1 Hz), 5.49 (1H, q, *J* = 7.0 Hz), 5.38 (1H, dt, *J* = 17.2, 1.1 Hz), 5.30 (1H, dt, *J* = 10.5, 1.0 Hz), 3.57 (3H, d, *J* = 1.3 Hz), 2.54 (2H, dt, *J* = 9.2, 5.8 Hz), 2.08–1.87 (2H, m); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 166.0, 141.0, 135.1, 132.6, 129.8, 128.6, 128.6, 128.4, 127.5, 126.2, 123.6 (q, J = 288.7 Hz), 119.3, 84.6 (q, J = 28.0 Hz), 55.6, 35.9, 31.1; **HRMS (DART):** Calcd for $C_{21}H_{25}NO_3F_3$ [M+NH_4^+]: 396.1781; found: 396.1774. Specific rotation: $[\alpha]_D^{20}$ –33.6 (*c* 0.27, $CHCl_3$).

Table S1. Comparison of the chemical shift between **(*S*)-S8** and **(*R*)-S8.**

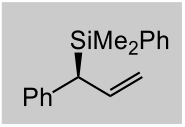
	δ ***S*-S8**	δ ***R*-S8**	$\Delta\delta^{SR}$ ($= \delta_{(S)\text{-}S8} - \delta_{(R)\text{-}S8}$)	
			ppm	Hz
1*E*	5.25	5.30	–0.05	–20
1*Z*	5.30	5.38	–0.08	–32
2	5.77	5.86	–0.09	–36
3	5.48	5.49	–0.01	–4
4	2.03	1.98	0.05	20
5	2.65	2.54	0.11	44
Ph-*o*-H	7.14	7.08	0.06	24
Ph-*m*-H	7.29	7.26	0.03	12
Ph-*p*-H	7.20	7.18	0.02	8

On the basis of the previously reported data,[12] because the hydrogen atoms on C1 and C2 have smaller chemical shift on **(*S*)-S8** (vs. H atoms on C4 and C5), the absolute configuration is determined as *R*.

9 Catalytic Enantioselective Silyl Substitution

9.1 Representative Procedure

In a N_2-filled glove box, an oven-dried 1-dram vial equipped with a stir bar was charged with **imid(S)-1a** (0.6 mg, 1.25 μmol), CuCl (0.1 mg, 1.00 μmol), and NaOMe (4.3 mg, 80 μmol). The vial was capped (phenolic open top cap with a red PFTE/white silicon septum, sealed with electrical tape), and removed from the glove box. Tetrahydrofuran (0.5 mL) was added and the mixture was allowed to stir for 1 h at 22 °C, after which the solution was allowed to cool to –78 °C. Allylic phosphate (0.10 mmol) and (dimethylphenylsilyl)boronic acid pinacol ester (39.3 mg, 0.15 mmol in 0.5 mL thf) were added by syringe, and the mixture was allowed to stir for 12 h at –50 °C, after which it was passed through a short plug of silica gel and eluted with Et_2O (3 mL). The volatiles were removed in vacuo to afford yellow oil residue, which was purified by silica gel chromatography to furnish the desired product as colorless oil.

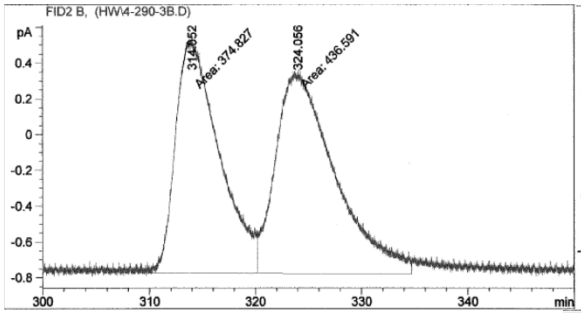


9.2 (*S*)-Dimethyl(phenyl)(1-phenylallyl)silane[13]

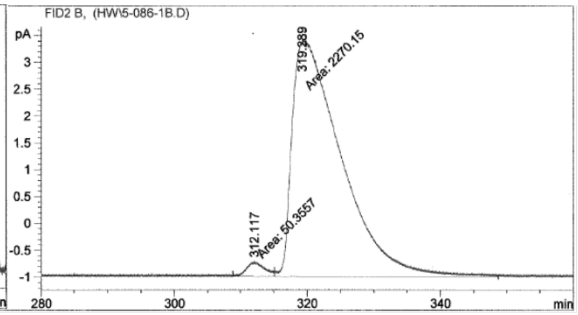
^{1}H NMR (CDCl$_3$, 400 MHz): δ 7.36–7.24 (5H, m), 7.19–7.15 (2H, m), 7.09–7.05 (2H, m), 6.92–6.89 (1H, m), 6.10 (1H, ddd, *J* = 16.8, 10.0, 10.0 Hz), 4.95–4.87 (2H, m), 3.13 (1H, d, *J* = 10.0 Hz), 0.26 (3H, s), 0.23 (3H, s). Specific rotation: $[\alpha]_D^{20}$ +11.5 (*c* 0.87, $CHCl_3$) for a sample with 98:2 e.r.

9.2.1 Determination of stereochemical identity

Previous reported specific rotation: $[\alpha]_D^{20}$ –7.3 (c 0.77, $CHCl_3$) for an enantiomerically enriched sample of 98:2 e.r. of the *R* enantiomer. Enantiomeric purity was determined by GC analysis in comparison with authentic racemic material; Chiraldex GTA column, 90 °C, 20 psi.

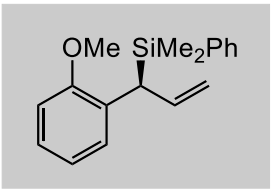


Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	314.052	MF	4.7378	374.82727	1.31858	46.19407
2	324.056	FM	6.4235	436.59125	1.13280	53.80593



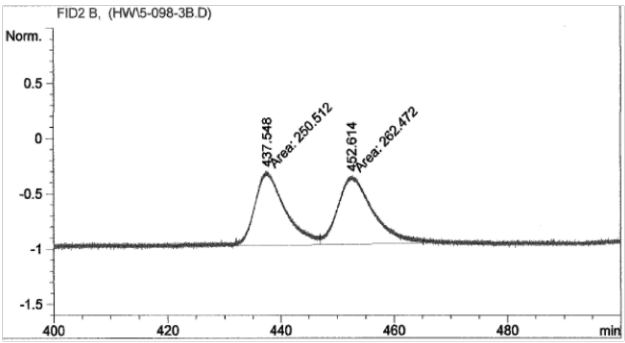
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	312.117	MF	2.9409	50.35573	2.85377e-1	2.17003
2	319.289	FM	8.5346	2270.15088	4.43321	97.82997

Retention Time	Area	Area %	Retention Time	Area	Area %
314.052	374.82727	46.19407	312.117	50.35573	2.17003
324.056	436.59125	53.80593	319.289	2270.15088	97.82997

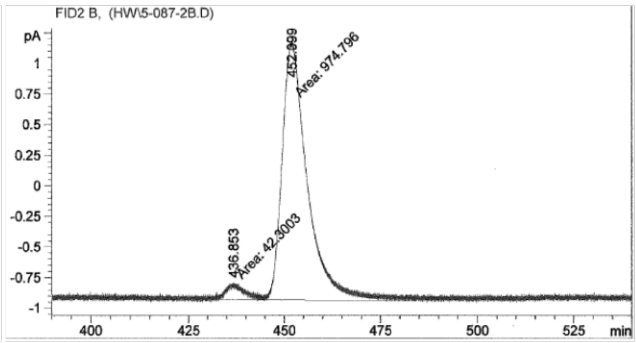


9.3 (*S*)-(1-(2-Methoxyphenyl)allyl)dimethyl(phenyl)silane[14]

^{1}H NMR (CDCl$_3$, 400 MHz): δ 7.39–7.27(5H, m), 7.10–7.05 (1H, m), 6.99–6.96 (1H, m), 6.87–6.83 (1H, m), 6.76–6.74 (1H, m), 6.14 (1H, ddd, *J* = 16.8, 10.6, 9.6 Hz), 4.95–4.90 (2H, m), 3.74 (1H, d, *J* = 9.6 Hz), 3.62 (3H, s), 0.27 (3H, s), 0.23 (3H, s). Specific rotation: $[\alpha]_D^{20}$ +18.2 (*c* 1.10, $CHCl_3$) for a sample with 96:4 e.r. Enantiomeric purity was determined by GC analysis in comparison with authentic racemic material; Chiraldex GTA column, 100 °C, 20 psi.

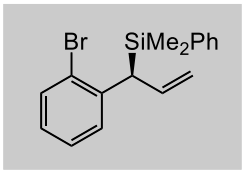


Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	437.548	MF	6.1890	250.51210	6.74616e-1	48.83429
2	452.614	FM	7.0300	262.47195	6.22267e-1	51.16571



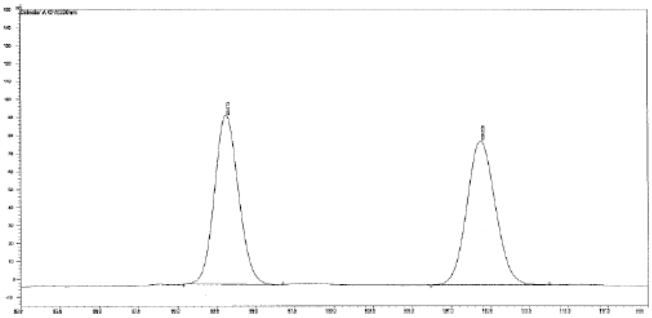
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	436.853	MF	4.8178	42.30031	1.46335e-1	4.15893
2	452.099	FM	7.6677	974.79626	2.11884	95.84107

Retention Time	Area	Area %	Retention Time	Area	Area %
437.548	250.51210	48.83429	436.853	42.30031	4.15893
452.614	262.47195	51.16571	452.099	974.79626	95.84107

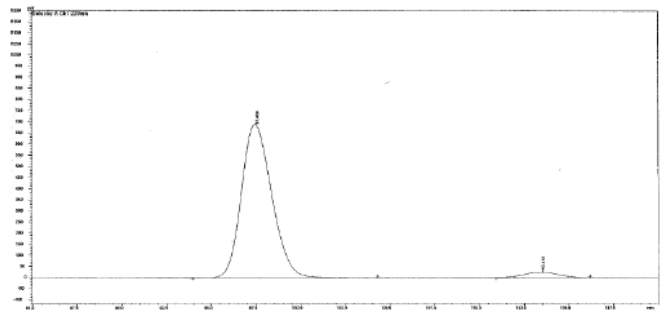


9.4 (*S*)-(1-(2-Bromophenyl)allyl)dimethyl(phenyl)silane[14]

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.53–7.50 (1H, m), 7.44–7.30 (5H, m), 7.18–7.14 (1H, m), 6.98–6.93 (2H, m), 6.00 (1H, ddd, *J* = 16.8, 10.0, 9.2 Hz), 4.98–4.88 (2H, m), 3.88 (1H, d, *J* = 9.2 Hz), 0.31 (3H, s), 0.29 (3H, s); optical rotation: $[\alpha]_D^{20}$ +33.3 (*c* 0.60, $CHCl_3$) for a sample with 96:4 e.r. Enantiomeric purity was determined by HPLC analysis of the boron–hydride addition (9-BBN)/oxidation product in comparison with authentic racemic material; Chiralcel OD-H column, 98% hexanes, 2% *i*PrOH, 0.3 mL/min, 220 nm.

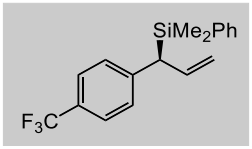


Peak#	Ret. Time	Area	Height	Area %	Height %
1	93.073	10168769	94153	50.143	53.988
2	109.359	10110945	80242	49.857	46.012
Total		20279714	174396	100.000	100.000



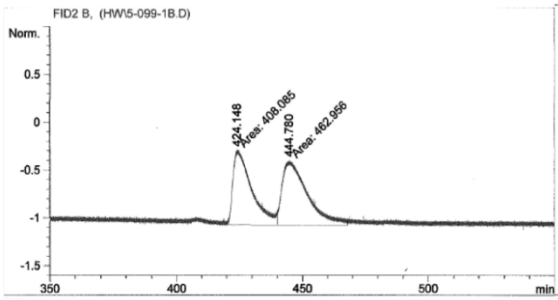
Peak#	Ret. Time	Area	Height	Area %	Height %
1	97.450	80743856	690283	96.101	96.436
2	113.418	3275903	25515	3.899	3.564
Total		84019759	715798	100.000	100.000

Retention Time	Area	Area %	Retention Time	Area	Area %
93.073	10168769	50.143	97.450	80743856	96.436
109.359	10110945	49.857	113.418	3275903	3.564

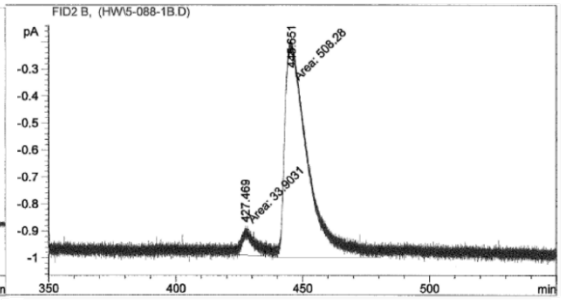


9.5 (*S*)-Dimethyl(phenyl)(1-(4-(trifluoromethyl)phenyl)allyl)silane[13]

^{1}H NMR (CDCl$_3$, 400 MHz): δ 7.42 (2H, d, *J* = 8.0 Hz), 7.40–7.30 (5H, m), 6.99 (2H, d, *J* = 8.0 Hz), 6.09 (1H, ddd, *J* = 17.0, 10.0, 10.0 Hz), 5.02–4.93 (2H, m), 3.22 (1H, d, *J* = 10.0 Hz), 0.28 (3H, s), 0.27 (3H, s). Specific rotation: $[\alpha]_D^{20}$ +14.8 (*c* 1.35, $CHCl_3$) for a sample with 94:6 e.r. Enantiomeric purity was determined by GC analysis in comparison with authentic racemic material; Chiraldex GTA column, 90 °C, 15 psi.

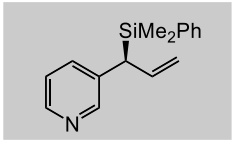


Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	424.148	MF	8.6812	408.08533	7.83464e-1	46.85027
2	444.780	FM	11.4220	462.95630	6.75533e-1	53.14973



Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	427.469	MM	5.1951	33.90314	1.08766e-1	6.25308
2	445.651	MM	10.3398	508.27985	8.19296e-1	93.74692

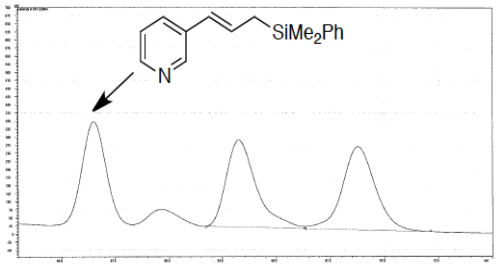
Retention Time	Area	Area %	Retention Time	Area	Area %
424.148	408.08533	46.85027	427.469	33.90314	6.25308
444.780	462.95630	53.14973	445.651	508.27985	93.74692



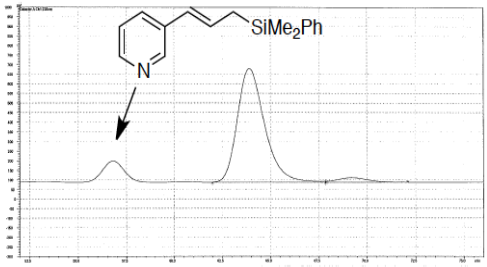
9.6 (*S*)-3-(1-(Dimethyl(phenyl)silyl)allyl)pyridine (mixture with S_N2 product)

IR (neat): 3070 (m), 3049 (m), 2957 (s), 2925 (s), 2853 (m), 1626 (m), 1588 (m), 1571 (m), 1477 (s), 1426 (s), 1410 (m), 1249 (s), 1182 (m), 1114 (s), 1078 (m), 1024 (m), 900 (s), 825 (s), 776 (s), 736 (s), 714 (s), 699 (s), 655 (m), 573 (m), 470 (m) cm^{-1}; **^{1}H NMR (CDCl$_3$, 400 MHz):** δ 8.36-8.24 (2H, ap d), 7.40–7.29 (5H, m), 7.17–7.11 (2H, m), 6.06 (1H, ddd, *J* = 16.8, 10.0, 10.0 Hz), 5.03–4.93 (2H, m), 3.14 (1H, d, *J* = 10.0 Hz), 0.29 (6H, s); **^{13}C NMR (CDCl$_3$, 100 MHz):** δ 149.1, 147.7, 147.5, 146.4, 138.2, 137.6, 136.6, 135.9, 134.6, 134.4, 133.7, 133.2, 132.1, 130.1, 129.7, 129.6, 129.4, 128.0, 127.8, 125.7, 125.4, 123.2, 114.2, 41.6, –4.5, –4.7; **HRMS (ESI$^+$)** Calcd for $C_{16}H_{20}N_1Si_1$ [M+H]: 254.13650; found: 254.13549. Specific rotation: $[\alpha]_D^{20}$ +7.68 (*c* 1.30, $CHCl_3$) for a sample with 96:4 e.r. Enantiomeric purity was

determined by HPLC analysis of product in comparison with authentic racemic material; Chiralcel OD-H column, 95% hexanes, 5% *i*PrOH, 0.1 mL/min, 220 nm.

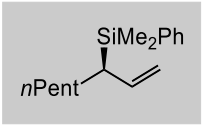


Peak#	Ret. Time	Area	Height	Area %	Height %
1	63.259	26168918	268910	48.874	51.063
2	68.776	27374405	257710	51.126	48.937
Total		53543323	526620	100.000	100.000



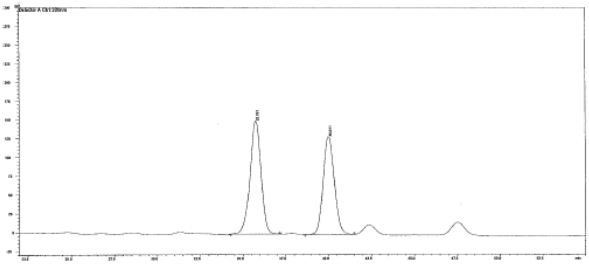
Peak#	Ret. Time	Area	Height	Area %	Height %
1	63.903	58469676	593971	95.667	96.025
2	69.221	2648418	24589	4.333	3.975
Total		61118094	618560	100.000	100.000

Retention Time	Area	Area %	Retention Time	Area	Area %
63.259	26168918	48.874	63.903	58469676	95.667
68.776	27374405	51.126	69.221	2648418	4.333

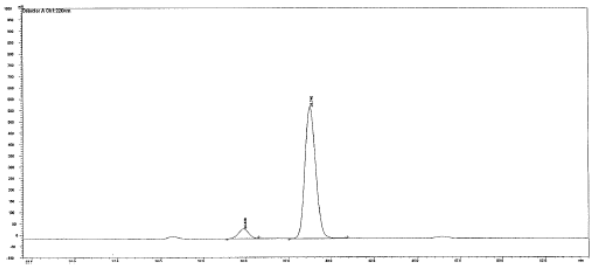


9.7 (*R*)-Dimethyl(oct-1-en-3-yl)(phenyl)silane[15]

^{1}H NMR (CDCl$_3$, 400 MHz): 7.51–7.49 (2H, m), 7.36–7.34 (3H, m), 5.59 (1H, ddd, J = 17.0, 10.0, 10.0 Hz), 4.90–4.79 (2H, m), 1.76–1.72 (1H, m), 1.44–1.13 (8H, m), 0.85 (3H, t, J = 7.0 Hz), 0.27 (3H, s), 0.26 (3H, s). Specific rotation: $[\alpha]_D^{20}$ –74.9 (*c* 0.80, $CHCl_3$) for a sample with 94:6 er. Enantiomeric purity was determined by HPLC analysis of the hydroboration (9-BBN)/oxidation product in comparison with authentic racemic material; Chiralcel OD-H column, 98% hexanes, 2% *i*PrOH, 0.3 mL/min, 220 nm.



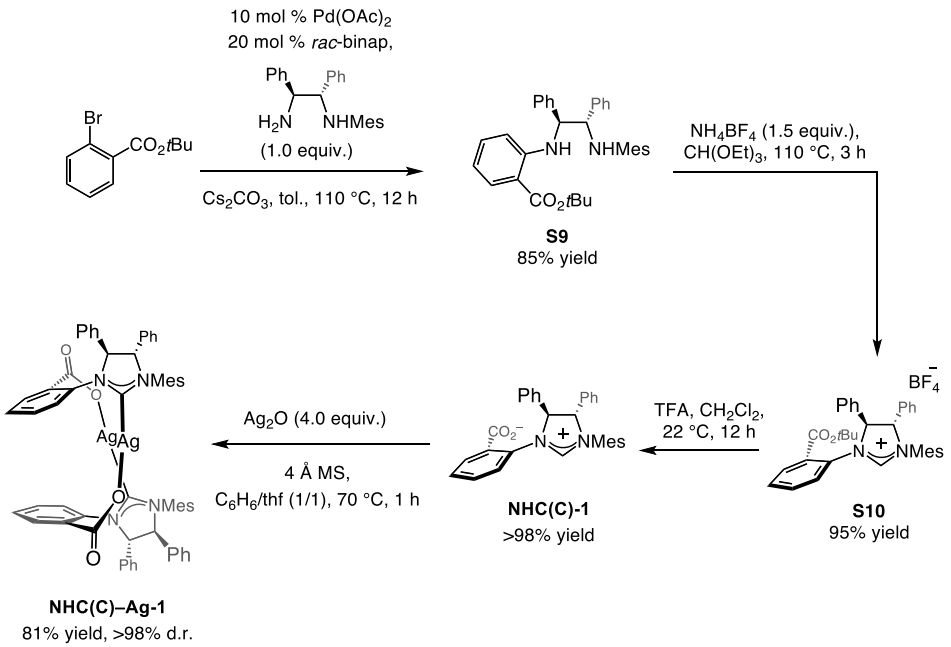
Peak#	Ret. Time	Area	Height	Area %	Height %
1	35.761	6731132	150566	53.184	53.540
2	40.011	5925289	130657	46.816	46.460
Total		12656421	281223	100.000	100.000



Peak#	Ret. Time	Area	Height	Area %	Height %
1	34.838	1742379	42401	6.385	6.792
2	38.746	25544831	581895	93.615	93.208
Total		27287210	624296	100.000	100.000

Retention Time	Area	Area %	Retention Time	Area	Area %
35.761	6731132	53.184	34.838	1742379	6.385
40.011	5925289	46.816	38.746	25544831	93.615

10 Carboxylate NHC–Metal Complex



1.1 Imidazolinium salt S10

In a glove box, an oven-dried 100 mL round bottom flask was charged with (1*S*,2*S*)-N^1-mesityl-1,2-diphenylethane-1,2-diamine (990 mg, 3.00 mmol), $Pd(OAc)_2$ (67 mg, 0.3 mmol), *rac*-binap (373 mg, 0.6 mmol), and Cs_2CO_3 (1.95 g, 6.00 mmol). The flask was removed from the glove box and fitted with a reflux condenser, after which it was charged with a solution of *tert*-butyl 2-bromobenzoate (771 mg, 3.00 mmol in 25 mL tol.), and the resulting mixture was allowed to stir at for 15 h 110 °C. After the mixture was allowed to cool to 22 °C, the volatiles were removed in vacuo, affording dark-red oil, which was dissolved in toluene and purified by silica gel chromatography (100% hexanes to elute toluene, to 5% EtOAc/hexanes), giving to afford 1.29 g (2.55 mmol, 85% yield) of **S9** as yellow solid. An oven-dried 10-dram vial was charged **S9** (396 mg, 0.78 mmol), after which NH_4BF_4 (123 mg, 1.17 mmol) and triethyl orthoformate (5 mL) were added. The mixture was allowed to stir for 3 h at 110 °C, after which it was allowed to cool to 22 °C. The volatiles were removed in vacuo and the resulting yellow oil was purified by silica gel chromatography (5% MeOH in CH_2Cl_2) and recrystallization (CH_2Cl_2/Et_2O/hexanes) to afford 447 mg (0.74 mmol, 95% yield) of **S10** as white solid. **IR (neat):** 3066 (w), 2979 (w), 2930 (w), 1700 (m), 1619 (s), 1597 (m), 1578 (m), 1484 (w), 1456 (w), 1394 (m), 1369 (m), 1303 (m), 1142 (m), 1052 (s), 1032 (s), 756 (s),730 (s), 698 (s) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ 8.22 (1H, s), 7.87 (1H, dd, *J* = 8.0,1.6 Hz), 7.67 (1H, d, *J* = 8.0 Hz), 7.49–7.41 (3H, m), 7.38-7.36 (2H, m), 7.31–7.22 (7H, m), 6.83 (1H, s), 6.61 (1H, s), 6.12 (1H, d, *J* = 11.2 Hz), 5.58 (1H, d, *J* = 11.2 Hz), 2.58 (3H, s), 2.10 (3H, s), 1.97 (3H, s), 1.59 (9H, s); **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 164.8, 158.3, 140.2, 136.3, 135.3, 134.5, 134.3, 134.3, 132.0, 131.9, 130.9, 130.5, 130.4, 130.2, 130.0, 129.7, 129.7, 129.2, 128.9, 128.6, 127.3, 83.3, 76.0, 74.7, 28.3, 21.0, 18.7, 18.1; **HRMS (ES+):** Calcd for $C_{35}H_{37}N_2O_2$: 517.2855; found: 517.2849. Specific rotation: $[\alpha]_D^{20}$ –238.9 (*c* 1.00, $CHCl_3$).

10.1 Carboxylate imidazolinium salt NHC(C)-1

A 2-dram vial was charged with **S10** (413 mg, 0.68 mmol), and trifluoroacetic acid (1 mL) and CH_2Cl_2 (3 mL) were added by syringe. The resulting mixture was allowed to stir at 22 °C. After 12 hours, the mixture was neutralized through the addition of saturated aqueous solution of $NaHCO_3$, and acidified with 4M HCl solution. The organic layer was separated and the aqueous solution was washed with CH_2Cl_2 (5 mL) for three times. The combined organic layers were dried over Na_2SO_4 and concentrated in vacuo. The resulting yellow solid was purified by recrystallization with CH_2Cl_2 and hexanes to afford 313 mg (0.68 mmol, >98% yield) **NHC(C)-1** as white solid. **IR (neat):** 3035 (w), 1703 (m), 1685 (m), 1618 (s), 1596 (s), 1485 (w), 1455 (w), 1263 (m), 1220 (m), 1180 (s), 1128 (s), 1093 (m), 731(s), 716 (s), 698 (s) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 8.91 (1H, s), 7.91 (1H, d, *J* = 7.8 Hz), 7.57–7.50 (2H, m), 7.47–7.40 (6H, m), 7.41–7.34 (5H, m), 6.92 (1H, s), 6.75 (1H, s), 6.22 (1H, d, *J* = 11.1 Hz), 5.61 (1H, d, *J* = 10.9 Hz), 2.58 (3H, s), 2.22 (3H, s), 2.04 (3H, s); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 167.9, 158.6, 140.2, 137.0, 134.8, 134.8, 133.5, 132.2, 131.9, 131.8, 130.6, 130.2, 130.2, 130.1, 129.8, 129.8, 129.6, 129.3, 129.3, 129.1, 128.6, 128.1, 76.2, 74.8, 21.0, 18.9, 18.3; **HRMS (ES+):** Calcd for $C_{31}H_{29}N_2O_2$ [M+H]: 461.2229; found: 461.2220. Specific rotation: $[\alpha]_D^{20}$ –210.5 (*c* 1.00, $CHCl_3$).

10.2 Complex NHC(C)-Ag-1

In a glove box, an oven-dried 6-dram vial was charged with Ag_2O (100 mg, 0.43 mmol), **NHC(C)-1** (50 mg, 0.11 mmol) and 4 Å molecular sieve (~50 mg). The vial was wrapped in aluminum foil and thf (5 mL) and benzene (5 mL) were added to the solution, resulting in the formation of a black heterogeneous mixture, which was allowed to stir at for one h at 70 °C. The mixture was allowed to cool to 22 °C and filtered through a short plug of celite (4 x 1 cm) and eluted with CH_2Cl_2. The volatiles were removed in vacuo to afford 50 mg (0.089 mmol, 81% yield) of **NHC(C)-Ag-1** as white solid. **Mp:** This compound decomposed upon heating. **IR (neat):** 1602 (m), 1477 (s), 1455 (s), 1227 (s), 1193 (s), 904 (s) cm^{-1}; **^{1}H NMR ($CDCl_3$, 400 MHz,):** δ 8.26–8.22 (1H, m), 7.47-6.96 (11H, m), 6.82 (1H, t, *J* = 7.2 Hz), 6.62-6.50 (2H, m), 6.39-6.34 (1H, m), 6.07 (1H, bs), 5.14 (1H, d, *J* = 6.8 Hz), 3.76 (3H, s), 2.45 (3H, s), 1.42 (3H, s). **^{13}C NMR ($CDCl_3$, 100 MHz):** δ 206.0 (C_{NHC}, $J_{^{109}Ag}$ =186.5, $J_{^{107}Ag}$ = 172.8 Hz), 157.9, 143.5, 140.4, 138.6, 135.9, 135.8, 135.2, 131.2, 130.6, 130.1, 129.8, 129.6, 129.2, 129.1, 129.0, 128.8, 128.7, 128.5, 128.3, 114.1, 113.2, 74.0, 55.3, 19.4. 205.6

11 Density Functional Theory (DFT) Calculations

11.1 Computational Details

DFT computations[16] were performed with the Gaussian 09/Gaussian 16 suite of programs.[17] Geometries were optimized with the M06–L[18] functional and the def2-SVP basis set[19] in conjunction with the corresponding Coulomb fitting basis set to speed up calculations.[20] The effect of a polar reaction medium (dichloromethane) was approximated by means of the SMD solvation model.[21] Several conformers have been investigated through manual screening, and only the most stable transition state structure is reported. Stationary points were probed through vibrational analysis and Gibbs free energy corrections were performed under standard conditions (298.15 K, 1.0 atm). Transition states have been verified through Intrinsic Reaction Coordinate calculations (IRC) by the use of the L(ocal) Q(uadratic) A(approximation) method,[22,23] followed by subsequent optimization of the end points with the abovementioned optimization protocol. We also probed the performance of various density functionals through single point energy calculations at the geometries optimized with the level described above by means of the SMD solvation model with DCM as solvent and the larger def2-TZVPP[19] basis set. Several state-of-the-art DFT approaches and benchmark studies have been developed by Truhlar,[24,25] Grimme,[26,27] Head-Gordon,[28,29] et al.[30,31] with emphasis on treatment of dispersion interactions[32] and employed, for example, in modeling the olefin metathesis reaction.[33,34,35,36] A notable impact of dispersion is related to the correct description of ligand association/dissociation steps during a catalytic cycle.[36] Nonetheless, there have been raised concerns regarding the accurate modeling of dispersion interactions in solution.[37,38] In particular, although structural information regarding catalyst precursors is available through x-ray christallography,[34] there is minimal information regarding their structure and that of related reactive intermediates in solution. Here, we are solely concerned with evaluation with M06–L/def2-TZVPP//M06–L/def2-SVP $_{CH2Cl2(SMD)}$, while additional free energy values corresponding to MN15/def2-TZVPP//M06–L/def2-SVP$_{CH2Cl2(SMD)}$ and ω–B97XD/def2-TZVPP//M06–L/def2-SVP$_{CH2Cl2(SMD)}$ are provided in Schemes S1–S13. A file for convenient viewing of computed geometries with the program Mercury 3.3 is appended as separate "coordinates.xyz" file in Section 13.[39] The "coordinates.xyz" file can be generated by copying all the coordinates in Section 13 into a text file without blank lines and changing the extension to (.xyz).

11.2 General Features

The principal features considered here are consistent within the recently reviewed framework of reactions promoted by nucleophilic Cu(I) complexes.[40] Examples that involve enantioselective allylic substitution (EAS) of allylic phosphates, which are promoted by NHC–Cu complexes bearing sulfonate containing NHC ligands have previously been investigated with respect to the function to the sulfonate group.[41,42,43] The latter likely binds an alkali metal cation and assists the displacement of the phosphate anion by establishing a cationic bridge. Enantioselective 1,4- and 1,6-conjugate additions promoted by NHC–Cu complexes that contain an alcohol group are mechanistically related.[44,45,46]

11.3 Stereochemical Models

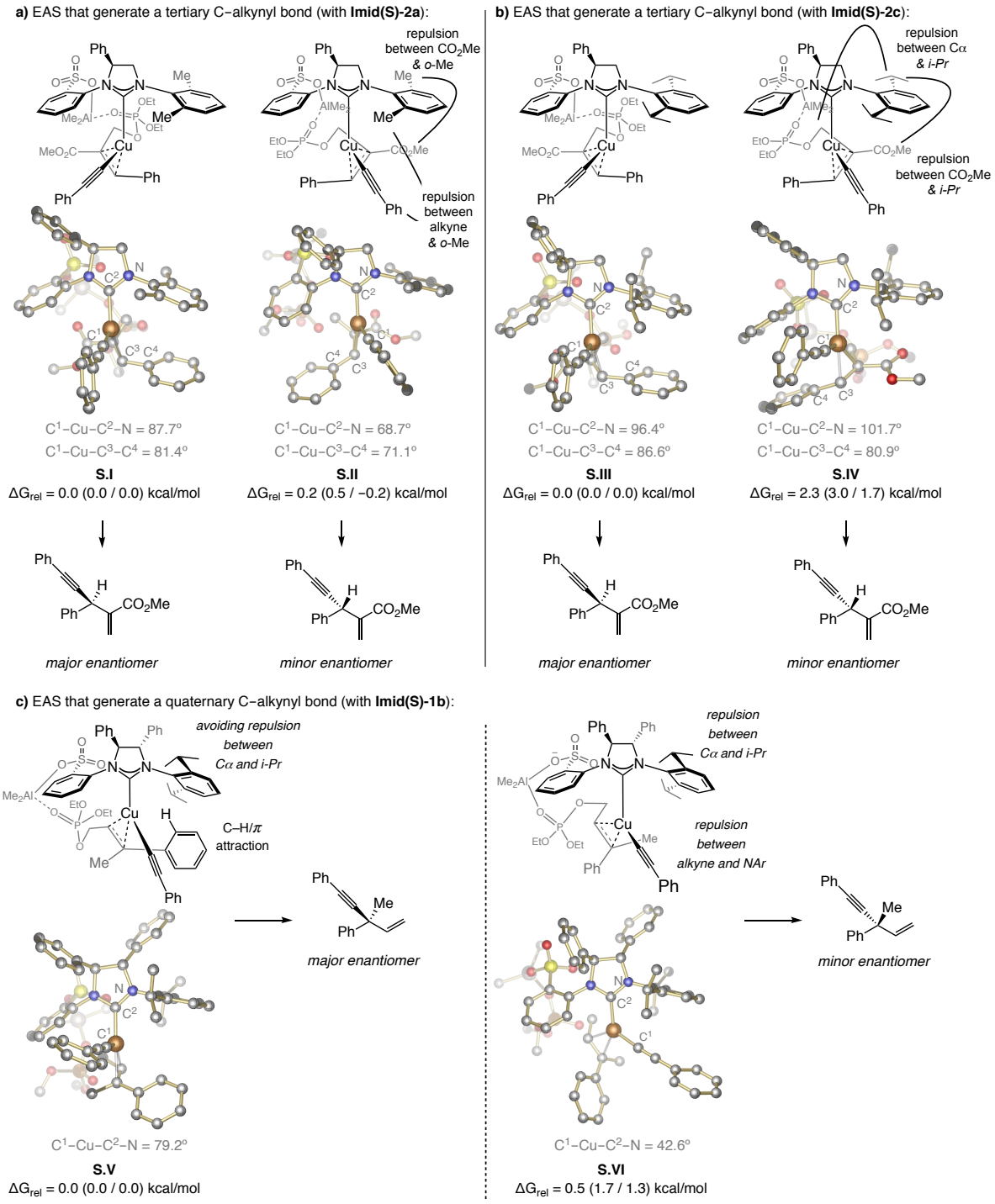
In addition to the previously investigated transformations (see Section 12.2), we provide DFT analyses for a selected range of transformations. These include previously undisclosed investigations regarding EAS involving organoaluminum compounds (see Section 12.3.1), insight into ECA promoted by organozinc and organoaluminum compounds (see Section 12.3.2), proto-boryl additions to aryl alkenes (see Section 12.3.3), and comparison of migratory insertion versus π-allyl formation pathways in boryl substitutions (see Section 12.3.4). In all cases, several conformers have been investigated through manual screening and only the most stable transition state structure is reported. It is worth noting that the dynamic structure present in solution is probably not adequately described by a single geometry. Furthermore, we make assumptions regarding the coordination of cationic Lewis acidic fragments (i.e., $AlMe_2^+$, $ZnMe^+$ or Na^+) to the sulfonate or phenolate functionality of the ligand on the one hand, and to the Lewis basic functionality of the substrate on the other. Discrete solvent molecules have not been included.

11.3.1 Stereochemical models for EAS

The stereochemical models for EAS between bis[(pinacolato)boryl]methane and di- and trisubstituted allyl phosphates (cf. Scheme 34), a rationale for EAS of alkenyl moieties derived from Al/Cu exchange (cf. Scheme 36), and stereochemical models for EAS with silyl-substituted alkenyl–Al compounds (cf. Scheme 37) are shown in Schemes S4, S5 and S6. This includes additional single point energies obtained with MN15/def2-TZVPP//M06–L/def2-$SVP_{CH2Cl2(SMD)}$ and ω–B97XD/def2-TZVPP//M06–L/def2-SVP_{CH2Cl2} (SMD).

Other notable investigations merit mention:

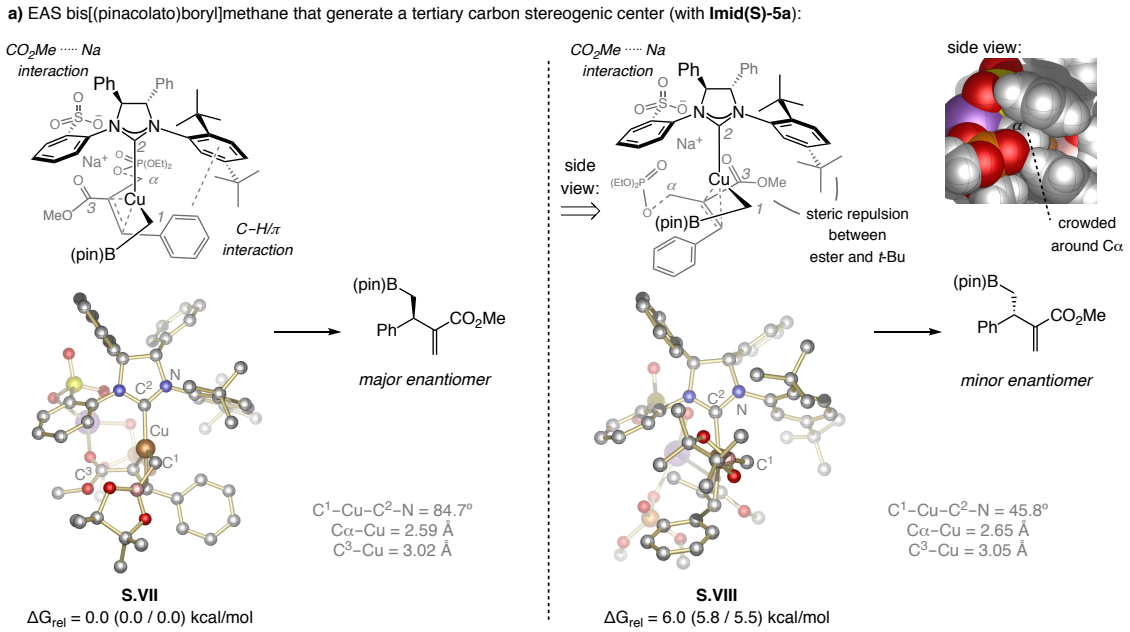
(i) In EAS involving alkynyl–Al reagents and trisubstituted allyl phosphates containing an ester moiety the Ph ring on the substrate occupies the empty space underneath the NAr unit (**S.I**; Scheme S1a). In the less favorable transition state there is likely repulsion between the rear *ortho*-Me group on the NAr unit and the ester, along with repulsion between the *ortho*-Me group that is oriented to the front and the alkyne moiety. The latter interaction causes the nucleophile to move closer to the substrate's Ph group, as indicated by the contracted C^1–Cu–C^3–C^4 dihedral angle (71.7º in **S.II** vs. 81.4º in **S.I**). The smaller energy difference between **S.I** and **S.II** (0.2 kcal/mol with M06L) suggests that entropic factors probably play a significant role in achieving high enantioselectivity and that they are not adequately captured by a single transition state geometry. With the sterically more demanding **imid(S)-2c**, the computed energy difference is larger (2.3 kcal/mol with M06L; Scheme S1b). This is probably owing to the stronger repulsion between the ester and the *i*-Pr group on the NAr, which leads to rotation of the substrate, causing a short H·····H contact between Cα and the rear *i*Pr group (1.99 Å). In EAS reactions that generate a quaternary C–alkynyl bond, **S.V** is favored because of the stabilizing C–H/π interaction and because repulsion between Cα and the rear *ortho i*-Pr group is avoided (**S.V**; Scheme S1c). Increased repulsion between Cα and the rear *ortho i*Pr group in **S.VI** leads to rotation of the substrate and forces the nucleophile underneath the NAr ring, as indicated by the contracted C^1–Cu–C^2–N dihedral angle (42.6º).



Scheme S1. Stereochemical models for EAS involving alkynyl–Al reagents and trisubstituted allyl phosphates (promoted by **imid(S)-2a**, **imid(S)-2c** and **imid(S)-1b**, respectively; see Schemes 8a–b in the manuscript for methodology). Free energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ωB97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.

(ii) In EAS reactions with bis[(pinacolato)boryl]methane, which generate a tertiary carbon stereogenic center, the Na^+ binds simultaneously the sulfonate, the phosphate, and the ester moiety (Scheme S2). Here, **S.VII** is likely favored owing to stabilizing C–H/π interaction, while the B(pin) group can be oriented towards the available space (front). In **S.VIII**, Na^+ is coordinated to the ester also, albeit at the expense of steric pressure caused by the proximity of Cα and the NAr^{SO3} ring. This is highlighted by the

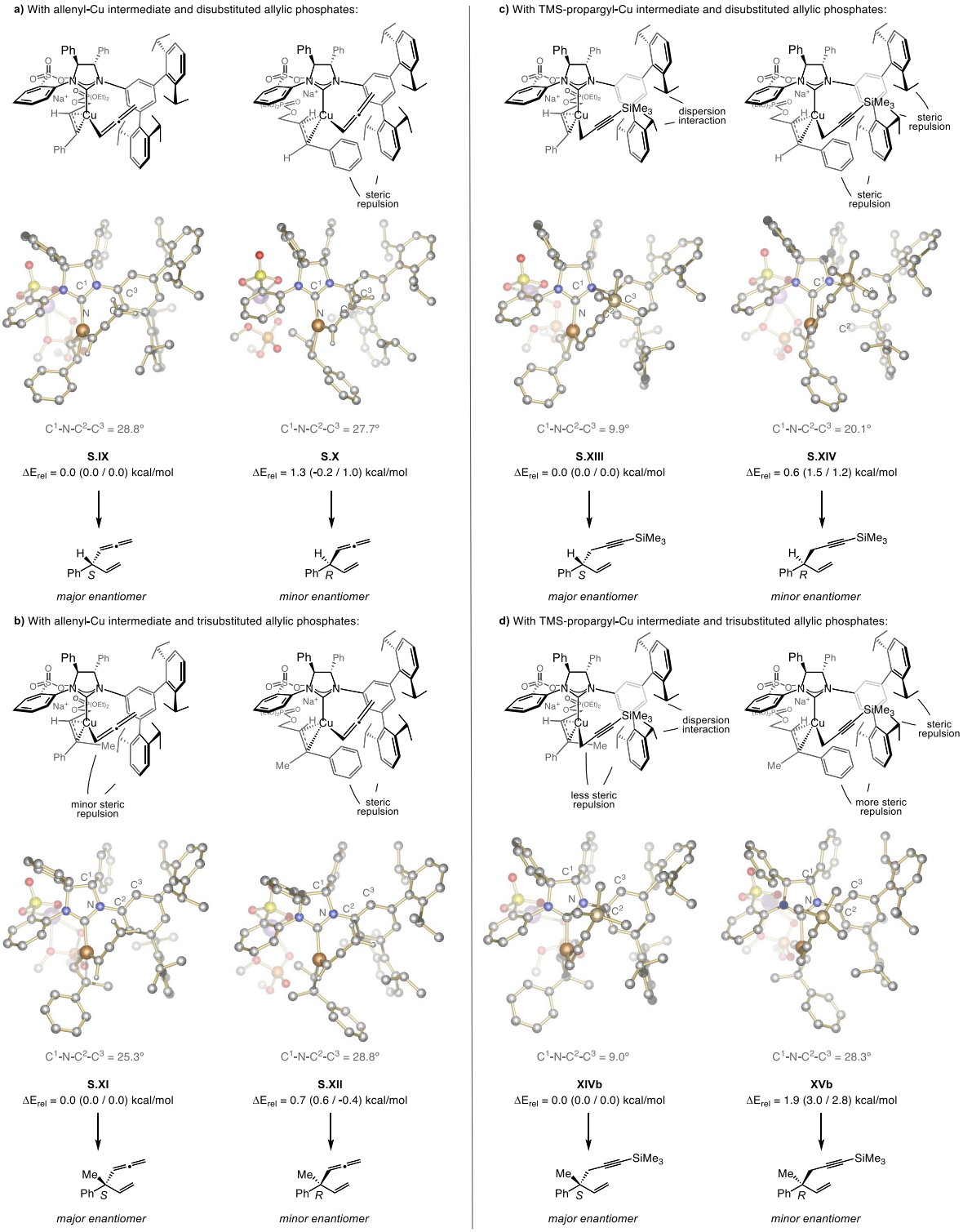
side view (space filling model) and is a consequence of the fact that Cα must interact with the transition metal more closely during π-allyl formation, as reflected in the distances to Cu (Cα–Cu = 2.65 Å vs C^3–Cu = 3.05 Å). Furthermore, there is likely steric repulsion between the ester and *t*-Bu group.



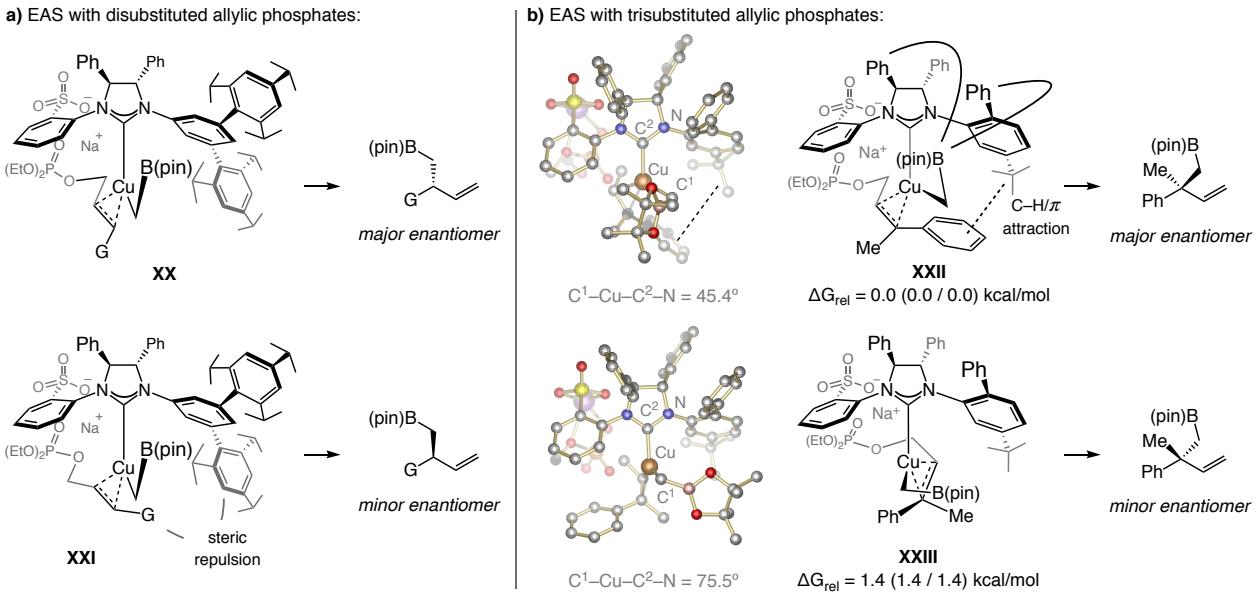
Scheme S2. EAS with bis[(pinacolato)boryl]methane that generate a tertiary carbon stereogenic center (promoted by **imid(S)-5a**) (see Scheme 22a in the manuscript for methodology). Free energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ω–B97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.

(iii) In EAS reactions with allenyl–B(pin) or trimethylsilylpropargyl–B(pin) and di- or trisubstituted allylic phosphates, respectively, the substrate probably approaches the Cu-based complex such that steric repulsion between the phenyl substituent and the NAr moiety acan be circumvented (Scheme S3). In the energetically most favorable transition states (based on electronic energies) the nucleophile is oriented up and to the right, as drwan, while the sizeable NAr ring is nearly coplanar with the heterocyclic ring (C^1–N–C^2–C^3 dihedral angle = 28.8º in **S.IX**; Scheme S3a). In **S.X**, which leads to the minor enantiomer, there is steric pressure caused by the propinquity of the substrate's phenyl moiety and the *meta* substituent of the NAr. Although we only show the energetically most preferred transition state, there is probably a considerable degree of conformational mobility around the N–Ar bond, which can result in non-negligible repulsion between it and the substrate's Me group in **S.XI**, leading to diminished enantioselectivity for trisubstituted alkene substrates (see Schemes S3b and 30 in the manuscript). For the trimethylsilylpropargyl system, e.r. is high regardless of whether a di- or trisubstituted allylic phosphate is involved (see Scheme 30 in the manuscript). This might arise from the more restricted rotation around the N–Ar bond, partly as the result of favorable dispersion interaction between the $SiMe_3$ group and the NHC's *i*-Pr substituents, which leads to contraction of the C^1–N–C^2–C^3 dihedral angle (9.9º in **S.XIII**; Scheme S3c). In the case of trisubstituted alkenes, the substrate's Me group likely associates with the π-cloud of the *m*-aryl substituent in **XIVb**, thus circumventing interaction with the NHC's *i*Pr groups (see Schemes S3d and 30d in the manuscript). In the alternative transition state **XVb**, which leads to the minor enantiomer, steric repulsion between the substrate's Ph group and the NAr ring causes the C^1–N–C^2–C^3 dihedral angle (28.3º) to expand,

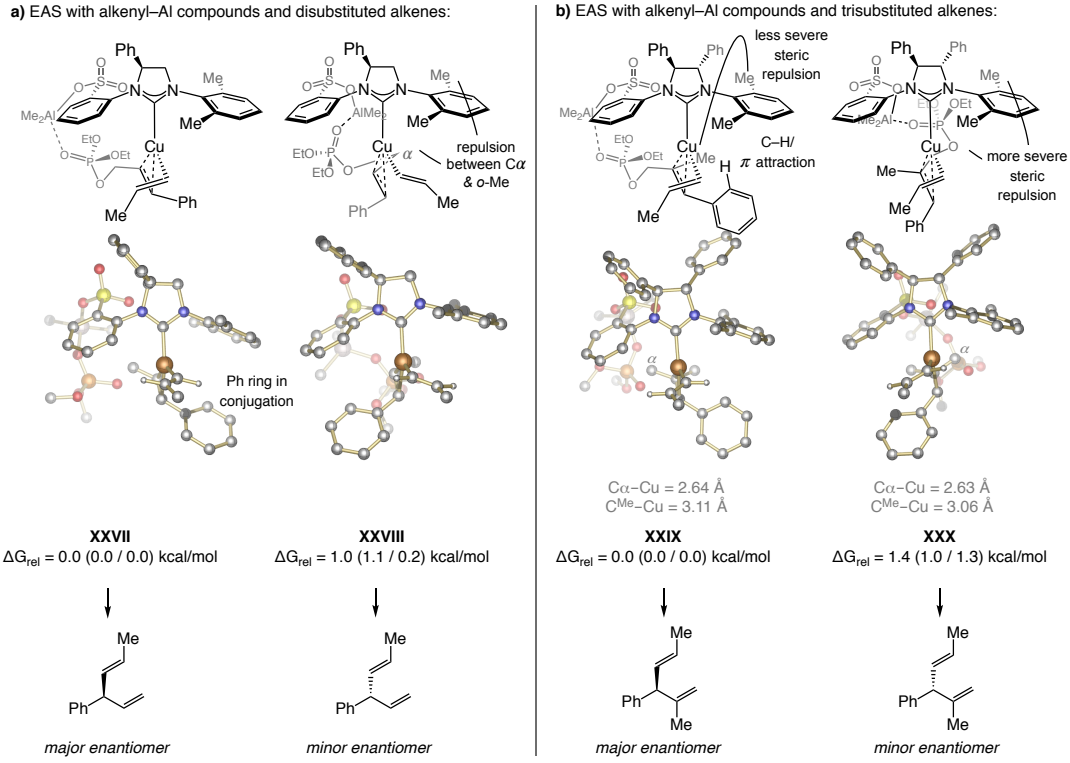
thus converting an attractive dispersive association between the $SiMe_3$ group and the NHC's *i*-Pr substituents (see **XIVb**) into a repulsive interaction involving one of the *i*-Pr units (**XVb**).



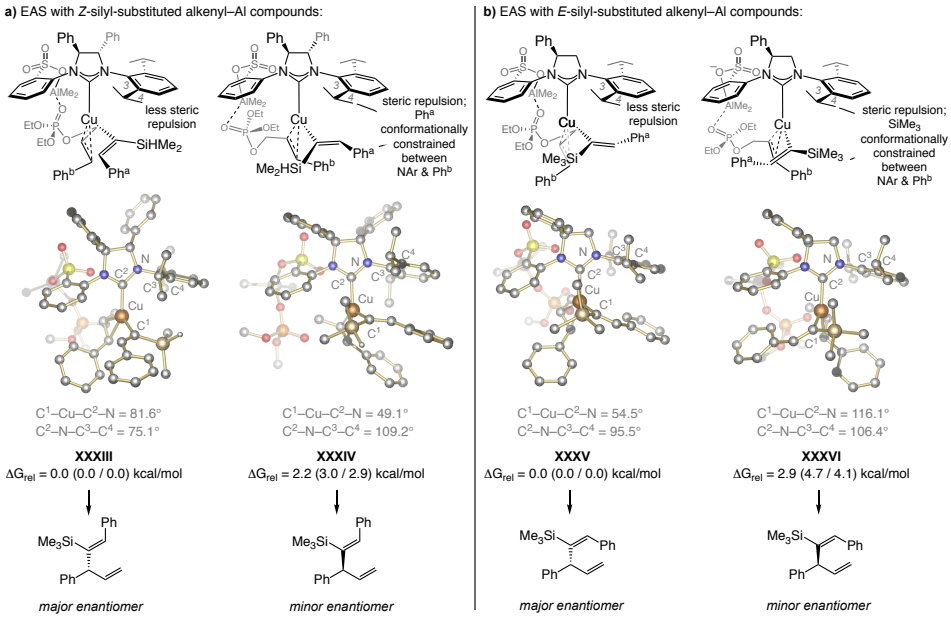
Scheme S3. Stereochemical models for EAS involving allenyl–B(pin) or trimethylsilylpropargyl–B(pin) compounds and di- or trisubstituted allyl phosphates (with catalyst derived from **imid(S)-3a**; see Schemes 13, 19 and 32 in the manuscript for methodology). Electronic energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ωB97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.



Scheme S4. High enantioselectivity in certain transformations due to a combination of sulfonate bridging and dispersive attraction (see Schemes 34 and 21–22 in the manuscript for methodology). Free energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ω–B97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.



Scheme S5. Rationale for EAS of alkenyl moieties derived from Cu/Al exchange (with catalysts derived from **imid(S)-2a** and **imid(S)-1a**, respectively; see Schemes 5 and 36a–b in the manuscript for methodology). Free energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ω–B97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.



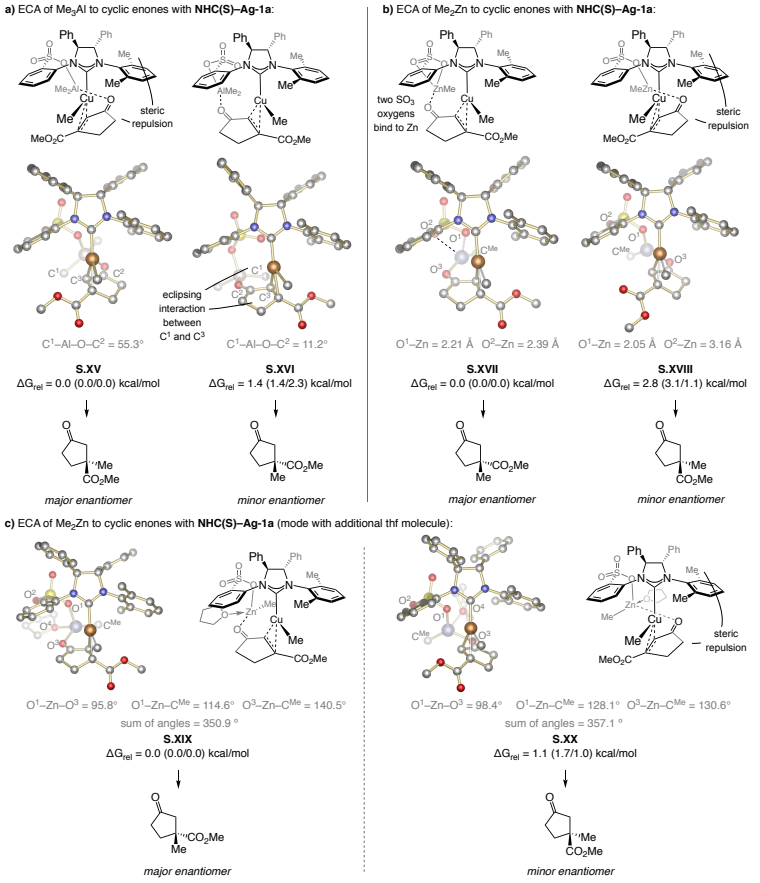
Scheme S6. Rationale for EAS with silyl-substituted alkenyl–Al compounds (promoted by **imid(S)-1b** and **imid(S)-2c**, respectively; see Schemes 6 and 37 in the manuscript for methodology). Free energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ω–B97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.

11.3.2 Stereochemical models for ECA

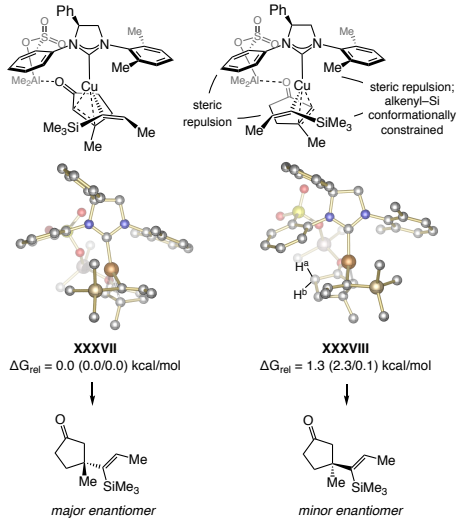
The stereochemical models for ECA of silyl-substituted alkenyl–Al reagents to cyclic enones (see Scheme 59), models illustrating the effect of **imid(O)-2a** and **imid(S)-2a** in ECA of aryl–Al reagents to cyclic enones (see Scheme 60), as well as stereochemical models for addition of β–alkenyl–Al reagents to acyclic enones (see Scheme 61) are shown in Schemes S8, S9 and S10 including additional single point energies obtained with MN15/def2-TZVPP//M06–L/def2-SVP$_{CH2Cl2(SMD)}$ and ω–B97XD/def2-TZVPP//M06–L/def2-SVP$_{CH2Cl2(SMD)}$. Other notable trends merit note:

(i) ECA of (alkyl)$_3$–Al compounds to β–ester-substituted cyclic enone promoted by **NHC(S)–Ag-1a** occur with opposite sense of enantioselectivity compared to when (alkyl)$_2$–Zn compounds are used (Scheme S7). We attribute this trend to different coordination geometries of the Lewis acidic fragment involving the sulfonate and the Lewis basic site within a substrate. In case of Al-based species, severe steric repulsion is likely avoided in **S.XV**, as indicated by the C^1–Al–O–C^2 dihedral angle (55.3º; Scheme S7a). In contrast, severe eclipsing interaction might contribute to the destabilization of **S.XVI** (C^1–Al–O–C^2 dihedral angle of 11.2º). Such coordination geometries might overrule the steric interaction between the rear *ortho*-Me group on the NAr unit and the substrate in the transition state that leads to the major enantiomer (**S.XV**). In the case of a Lewis acidic MeZn$^+$ fragment (Scheme S7b) the sulfonate group might serve as bidentate ligand to Zn, favoring mode of addition **S.XVII** (O^1–Zn = 2.21 Å and O^2–Zn = 2.39 Å). This latter coordination mode is unlikely in **S.XVIII**, which is additionally disfavored due to steric interaction between the rear *o*-Me group on the NAr unit and the substrate. Furthermore, the geometry surrounding the Zn ion in **S.XVII** is nearly planar (sum of angles [O^1–Zn–C^{Me}, O^1–Zn–O^3, O^3–Zn–C^{Me}] = 359.0º), suggesting severe eclipsing interaction between Zn–Me and the substrate (as present with Al–Me in **S.XVI**) are absent in **S.XVII**. A stereochemical model involving thf to Zn coordination offers a plausible rationale for the

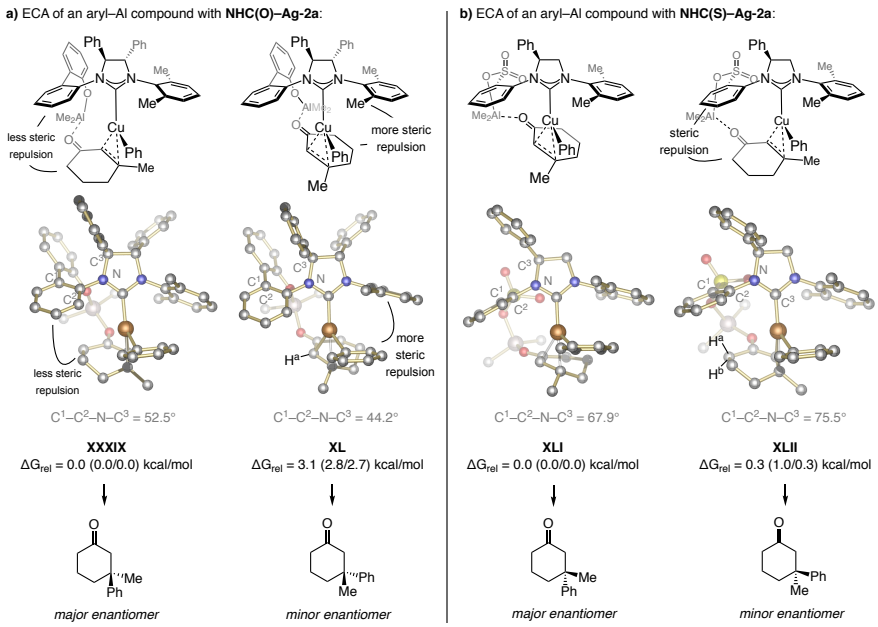
aforementioned findings (Scheme S7c). Calculations suggest that, while the additional thf molecule causes distortion from planarity, the effect is minor (350.9° and 357.1° in **S.XIX** and **S.XX**, respectively).



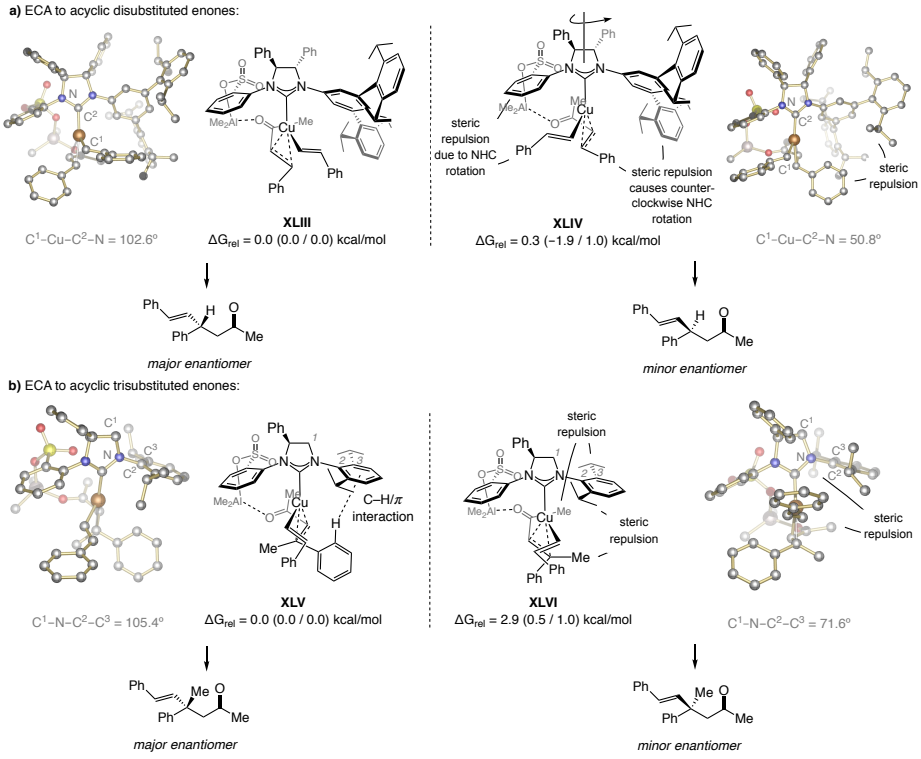
Scheme S7. Rationale for ECA of Me_3Al and Me_2Zn reagents to β-ester-substituted cyclic enones (with catalyst derived from **imid(S)-1a**; see Schemes 39 and 40 in manuscript for methodology). Free energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ω–B97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.



Scheme S8. Rationale for high enantioselectivity in ECA with silyl-substituted alkenyl–Al compounds (promoted by **imid(S)-2a**; see Schemes 51 and 59 in the manuscript for methodology). Free energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ω–B97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.



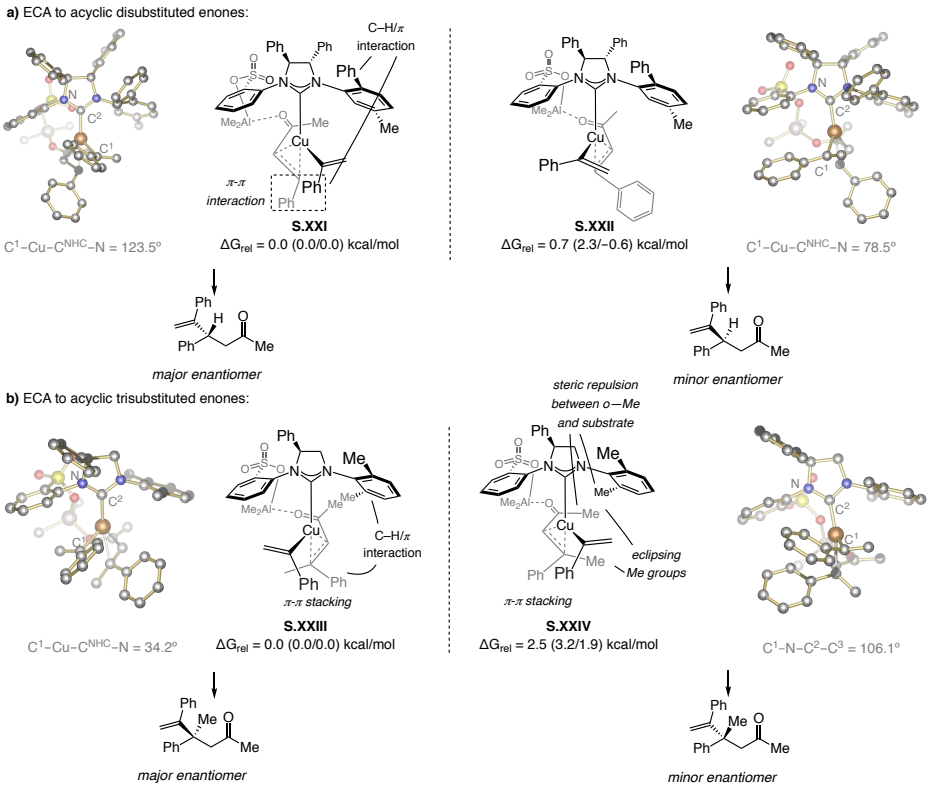
Scheme S9. Rationale for high enantioselectivity in ECA with aryl–Al compounds (with catalysts derived from **imid(O)-2a** and **imid(S)-2a**, respectively; see Scheme 55 and 60 in the manuscript for methodology). Free energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ωB97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.



Scheme S10. Rationale for high e.r. in ECA of β-alkenyl–Al compounds (promoted by **imid(S)-3a** and **imid(S)-2c**, respectively; see Schemes 47, 53, and 61 in the manuscript for methodology). Free energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ωB97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.

(ii) It is probable that dispersive interactions impact ECA of α–alkenyl–Al reagents to acyclic disubstituted enones (Scheme S11a). The expanded C^1–Cu–C^2–N dihedral angle in **S.XXI** (123.5°) is a

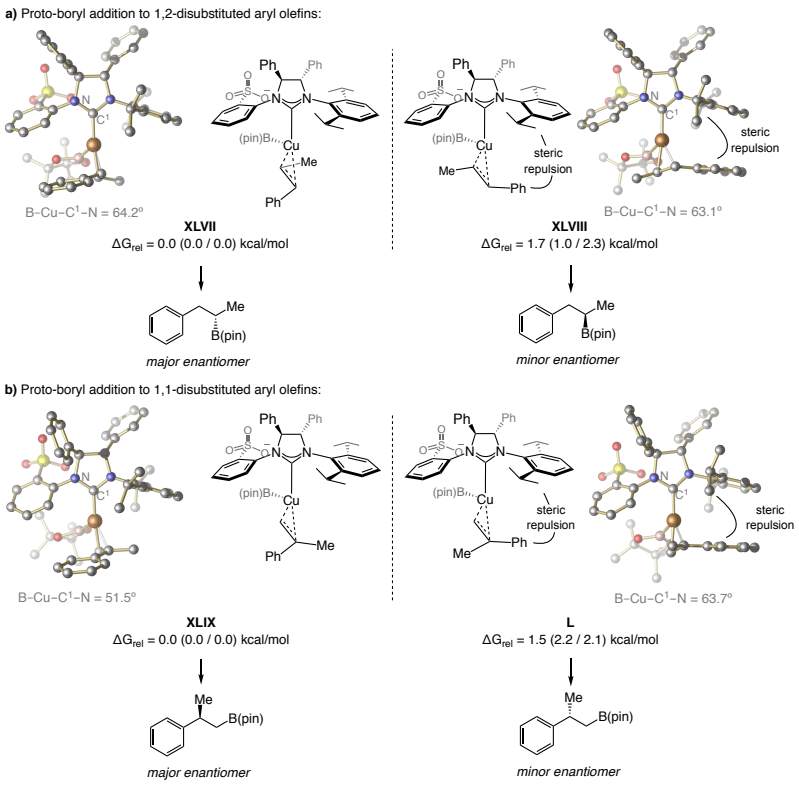
result of the nucleophile occupying the open quadrant below the *ortho*-phenyl ring that is at the front. As such, the phenyl substituent of the alkenyl group can point to the front, thus avoiding steric repulsion with the NAr^{SO3} unit. There is also stabilizing π–π stacking interaction between the nucleophile and the substrate's phenyl ring, and C–H/π interaction between the nucleophile and the NHC's *ortho* phenyl moiety. In **S.XXII**, steric factors are likely to dominate, forcing the alkenyl phenyl moiety to be oriented to the left (as drawn), and, as such, it is not conformationally constrained between the ligand and the substrate. For ECA to trisubstituted acyclic enones, a contracted C^1–Cu–C^2–N dihedral angle can be adopted in **S.XXIII** (34.2º) so that the alkenyl phenyl moiety can be oriented to the front (Scheme S11b). Similar to **S.XXI**, π–π stacking and C–H/π interactions are stabilizing factors (**S.XXIII**). The minor transition state **S.XXIV** is destabilized owing to steric interaction between the rear *ortho*-Me group on the NAr unit and the substrate, as well as the eclipsing Me groups.



Scheme S11. Rationale for high e.r. in ECA of α-alkenyl–Al compounds (with catalysts derived from **imid(S)-6b** and **NHC(S)-Ag-2a**, respectively; see Schemes 47 and 53 in the manuscript for methodology). Free energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ω–B97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.

11.3.3 Stereochemical models for proto-boryl addition

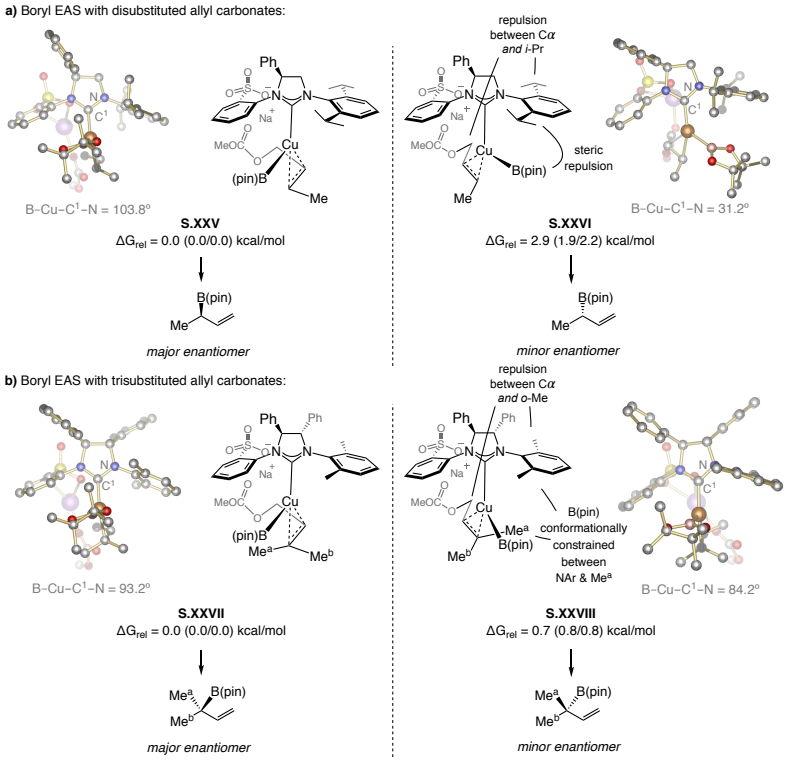
The stereochemical models for proto-boryl addition (see Scheme 64) are provided in Scheme S12. This includes additional single point energies obtained with MN15/def2-TZVPP//M06–L/def2-$SVP_{CH2Cl2(SMD)}$ and ω–B97XD/def2-TZVPP//M06–L/def2-$SVP_{CH2Cl2(SMD)}$.



Scheme S12. Stereochemical models accounting for the high enantioselectivity in proto-boryl additions to aryl alkenes (with catalyst derived from **imid(S)-1b**; see Schemes 64, 66 and 68 for the methodology). Free energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ω–B97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.

11.3.4 Stereochemical models for boryl substitution

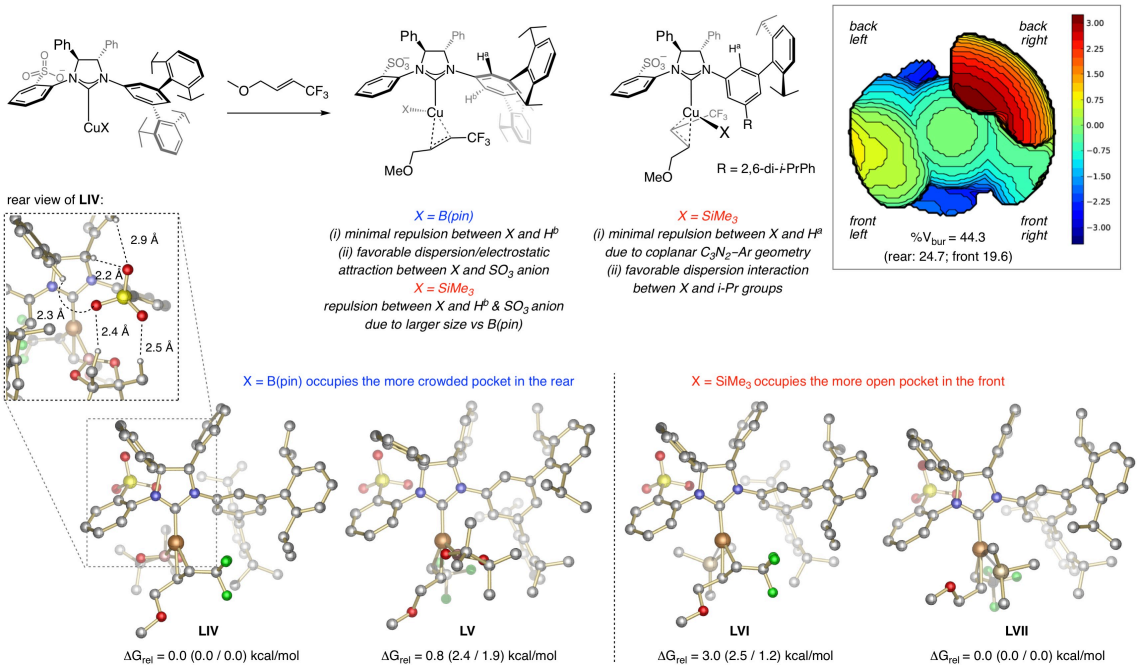
Based on the experimentally obtained KIE (Scheme 72c) we propose a π-allyl mechanism for EAS boryl substitution. The corresponding stereochemical model for reaction of disubstituted allyl carbonates (see Scheme 72a for the methodology) suggests that there is steric repulsion between Cα and the rear *ortho* *i*Pr group in the transition state leading to the minor enantiomer (**S.XXVI**, Scheme S13a), causing repulsion between the B(pin) nucleophile and the NAr unit, as indicated by the contracted B–Cu–C^1–N dihedral angle (31.2º). Similarly, repulsion between Cα and the rear *o*-Me group in **S.XXVIII** (leading to rotation of the substrate) is the reason why reactions of trisubstituted allyl carbonates are enantioselective (Scheme S13b). This results in the B(pin) group being conformationally constrained between NAr and Me[a]. The small energy difference (0.7 kcal/mol) is likely the result of a small model substrate being applied and due to the difficulty of accurately capturing the conformational flexibility with a single structure.



Scheme S13. Stereochemical models accounting for the high enantioselectivity in boryl substitution with di- and trisubstituted allyl carbonates as electrophiles (with catalysts derived from **imid(S)-2c** and **imid(S)-1a**, respectively; see Scheme 75 for the methodology). Free energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ωB97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.

11.3.5 Stereochemical models for silyl substitution

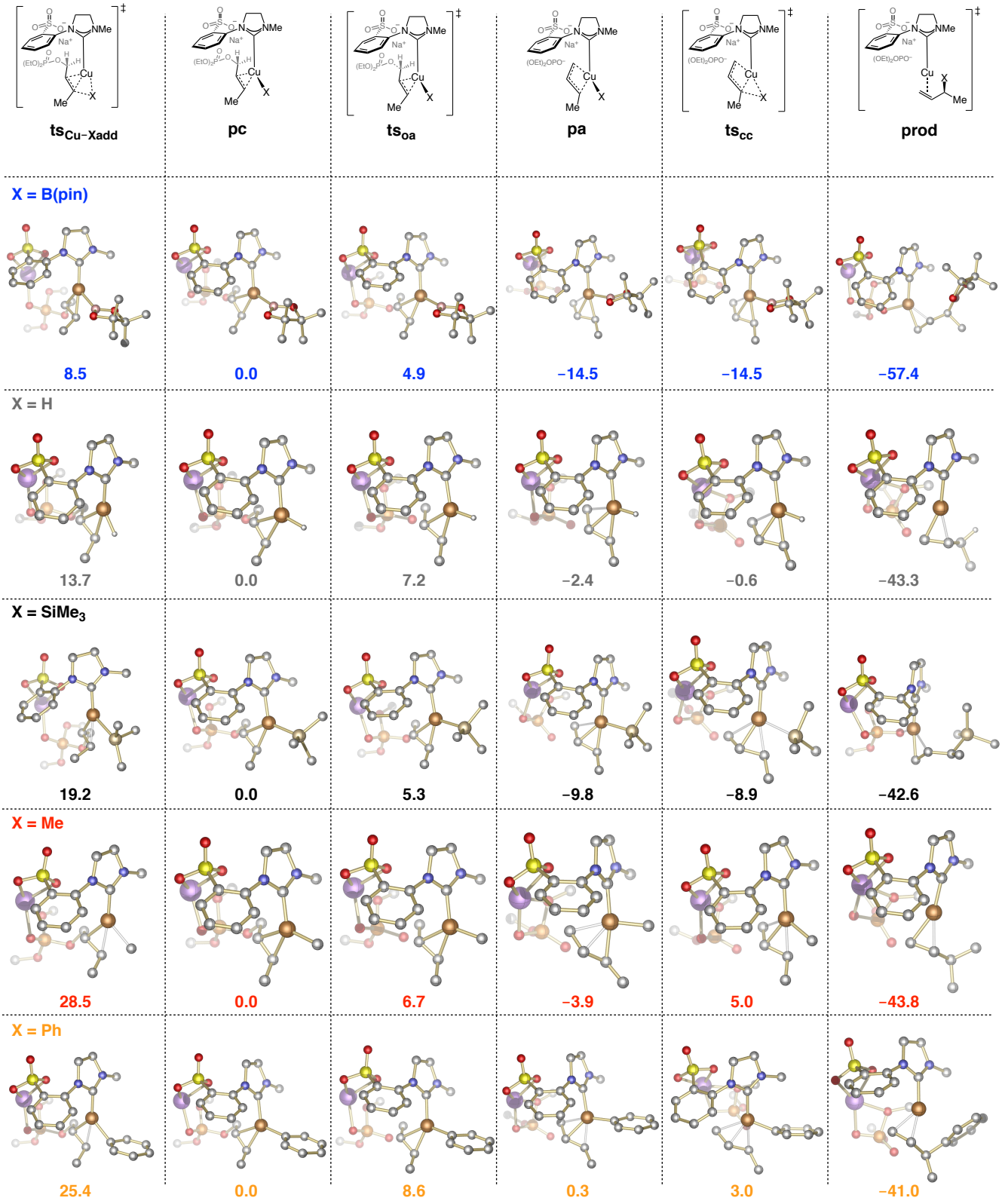
The stereochemical model for enantioselective boryl and silyl substitution reactions, involving F_3C-alkenes as substrates (cf. Scheme 79b) are provided (Scheme S14). This includes additional single point energies obtained with MN15/def2-TZVPP//M06–L/def2-SVP$_{CH2Cl2(SMD)}$ and ω–B97XD/def2-TZVPP//M06–L/ def2-SVP$_{CH2Cl2(SMD)}$.



Scheme S14. Stereochemical models for enantioselective boryl and silyl substitutions involving F_3C-alkenes (with catalyst derived from **imid(S)-3a**; see Schemes 76 and 79 for the methodology). Free energy values correspond to the **M06L**/Def2-TZVPP//M06L/Def2-SVP (**MN15**/Def2-TZVPP//M06L/Def2-SVP and **ω–B97XD**/Def2-TZVPP//M06L/Def2-SVP) levels of theory.

11.3.6 Comparison of migratory insertion versus π-allyl formation

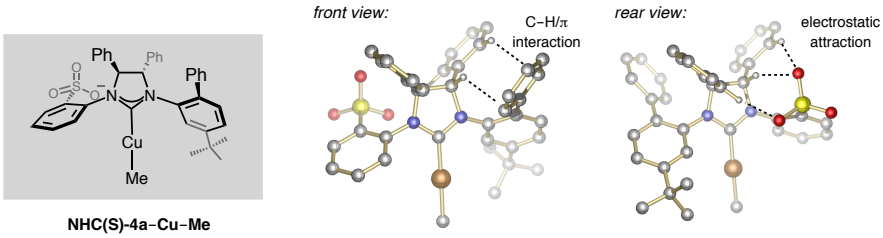
The DFT optimized geometries for the energy diagram shown in Scheme 29 (including free energies obtained with M06/def2-TZVPP//M06–L/def2-SVP$_{DCM(SMD)}$) are shown in Scheme S15.



Scheme S15. Evaluation of two boryl substitution pathways (promoted by a model NHC–sulfonate ligand; see Scheme 29 in the manuscript). Free energy values correspond to the **M06**/Def2-TZVPP//M06L/Def2-SVP level of theory.

11.4 Steric Maps

To gain a greater understanding of the selectivity profiles exhibited by sulfonate NHC ligands, we investigated the steric properties in more detail (Scheme S16).[47,48] We optimized the most commonly applied ligands (in their anionic form) while bound to a neutral Cu–Me fragment. To derive the steric maps and buried volume values (%V_{bur}), we applied a sphere with a 3.5 Å radius and placed the carbene carbon at a 2.0 Å distance from the Cu center. Ligand **NHC(S)-1b** (with two *ortho* isopropyl groups) covers the largest space of the sphere (%V_{bur} = 47.2; Scheme S16a). On the other hand, ligands with either a *tert*-butyl (**NHC(S)-3b** or **NHC(S)-4a**) or 2,4,6-triisopropylphenyl substituent at the *meta* position (**NHC(S)-3a** or **NHC(S)-4b**) cover the largest space on the opposite side of the sphere, close to the Cu–Me fragment (parts highlighted in red in the back-right quadrant; Schemes S16b–c). Notably, buried volume values increase by ~2.5–3.0% when a *tert*-butyl group is changed to a 2,4,6-triisopropylphenyl substituent (Scheme S16b–c). In all cases the front-left quadrant is partly blocked by the C–H bonds of the NAr ring that contains the sulfonate. This is because there is probably some electrostatic attraction between the sulfonate, which resides in the rear-left quadrant (as drawn), and the C–H bonds of the phenyl rings on the NHC backbone; the result is that the sulfonate moves away from the metal center (e.g. **NHC(S)-4a–Cu–Me**; rear view below). Likewise, edge-to-face aromatic interactions might exist between the *ortho* phenyl substituent and phenyl rings on the NHC backbone (see front view).

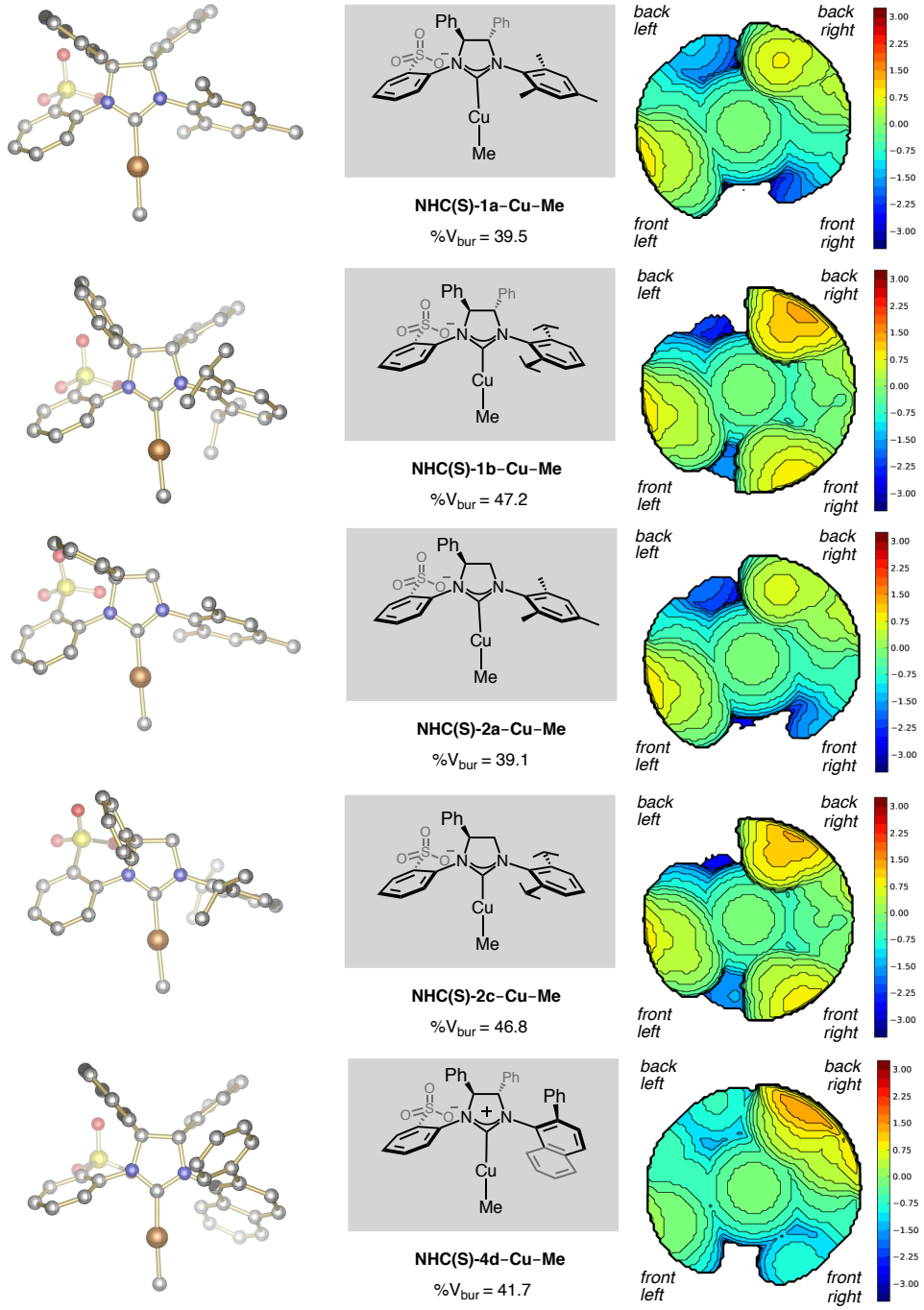


NHC(S)-4a–Cu–Me

The abovementioned electrostatic interaction creates an open pocket beneath the sulfonate group (at least when the ligand is in its anionic form; e.g., relevant to Cu–B(pin) additions to alkenes). Comparison with IPr (%V_{bur} = 53.4 for **IPr–Cu–Me**; Scheme S16d) shows, that the sulfonate ligands are noticeably smaller (%V_{bur} = 46.8 for **NHC(S)-2c–Cu–Me**; Scheme S16a).

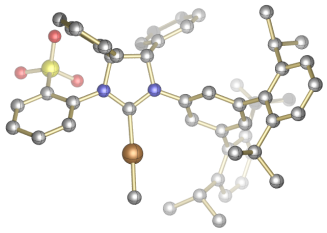
It should be noted that these steric maps represent just a snapshot obtained from a single geometry, whereas the situation in solution may be more complex. Notably, the highlighted parts in red are conformationally mobile in ligands bearing a 3,5-disubstituted NAr unit, owing to more facile rotation around the N–Ar bond (Scheme S16b). In contrast, the areas highlighted in red will be more rigid in case of 2,5-disubstitution (Scheme S16c).

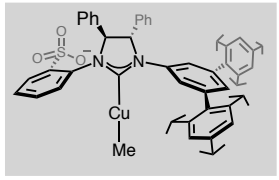
a) NHC ligands bearing a 2,6-disubstituted NAr unit



Scheme S16a. Steric maps and buried volumes (%V_{bur}) of commonly applied NHC-sulfonate ligands in their corresponding anionic Cu–Me complexes. Structures have been optimized with M06L/Def2-SVP in dichloromethane as solvent (SMD solvation model).

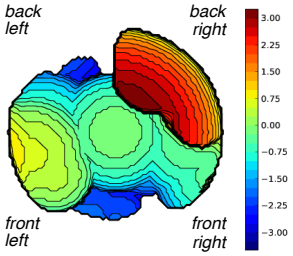
b) NHC ligands bearing a 3,5-disubstituted NAr unit

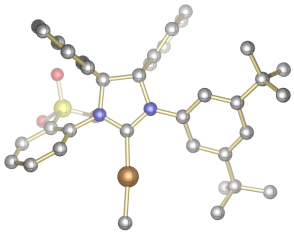


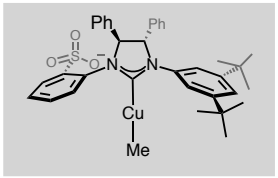


NHC(S)-3a–Cu–Me

$\%V_{bur}$ = 44.3

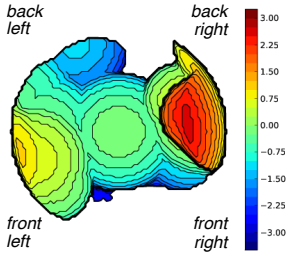




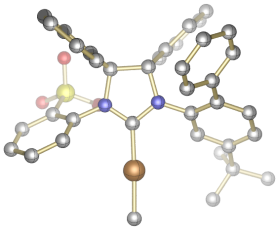


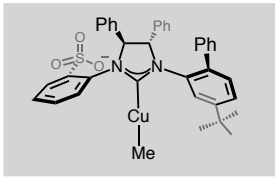
NHC(S)-3b–Cu–Me

$\%V_{bur}$ = 41.5



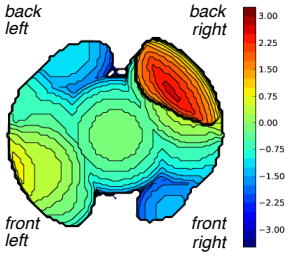
c) NHC ligands bearing a 2,5-disubstituted NAr unit

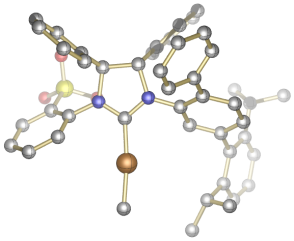


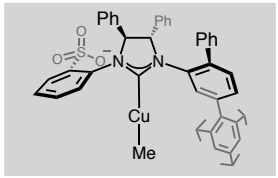


NHC(S)-4a–Cu–Me

$\%V_{bur}$ = 41.4

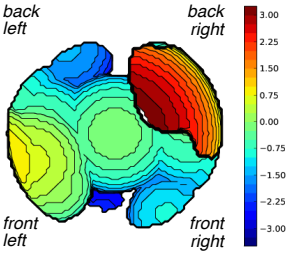




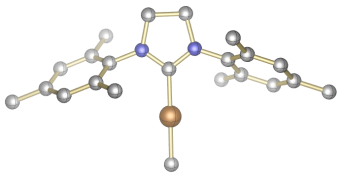


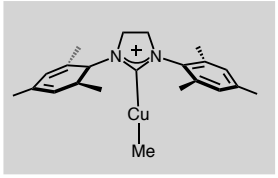
NHC(S)-4b–Cu–Me

$\%V_{bur}$ = 43.0



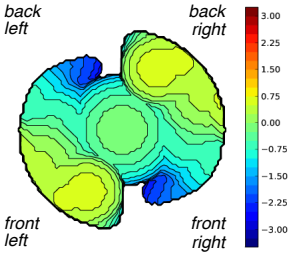
d) representative achiral monodentated NHC ligands

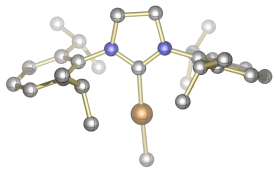


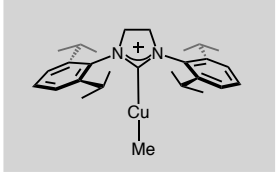


SIMes–Cu–Me

$\%V_{bur}$ = 41.4

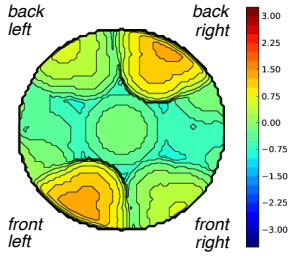






IPr–Cu–Me

$\%V_{bur}$ = 53.4



Scheme S16b–d. Steric maps and buried volumes ($\%V_{bur}$) of commonly applied NHC-sulfonate ligands in their corresponding anionic Cu–Me complexes. Structures have been optimized with M06L/Def2-SVP in dichloromethane as solvent (SMD solvation model).

12 Coordinates After Optimization with M06L/Def2SVP$_{CH2Cl2(SMD)}$

110
Scheme_S1_S.I / electronic energy: -5188.84834855 a.u. / lowest freq: -254.54 cm-1

C	-0.319833	3.030643	1.750614
H	0.723630	3.341324	1.905610
C	-0.797097	2.133914	2.901901
H	-1.695624	2.528000	3.402170
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C	0.043054	2.428189	-0.704342
C	-0.913422	2.469433	-1.724749
C	1.382107	2.721389	-1.003549
C	-0.549666	2.820037	-3.021327
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C	1.736275	3.099923	-2.299972
C	0.774462	3.156952	-3.303734
H	-1.307401	2.846768	-3.807442
H	2.782156	3.314753	-2.525956
H	1.066108	3.448343	-4.315071
C	-1.559833	-0.306400	2.930164
C	-0.632090	-1.092008	3.641568
C	-2.927783	-0.641348	2.856005
C	-1.101082	-2.265746	4.247913
C	-3.343319	-1.830328	3.466254
C	-2.437898	-2.637946	4.151256
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S	2.685197	2.592212	0.221944
O	3.880350	2.160301	-0.641027
O	2.336677	1.548315	1.199049
O	2.899170	3.940338	0.758647
Cu	-1.188677	-0.656128	-0.316971
C	-1.153793	4.250509	1.453701
C	-0.530514	5.478229	1.209841
C	-2.547975	4.159632	1.345950
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C	1.212530	-0.928524	-1.985554
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C	-4.122069	-0.697663	-1.500955
C	6.362747	1.413974	0.993889
C	5.844765	0.575166	-2.310830
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H	6.504620	-0.305649	-2.397738
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H	0.777344	-3.790836	1.053665
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H	-2.924073	-3.626398	-1.166886
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H	-0.195140	-5.501452	2.541172
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H	-7.632238	-2.475620	-3.925833
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H	-9.178992	-0.654901	-3.213396
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H	-4.131412	1.139403	2.838949
H	-4.871686	-0.244861	2.022942
H	1.142006	-0.006730	2.991499
H	1.462188	-1.589758	3.729464
H	1.004028	-0.223501	4.739164
C	1.450589	-0.816009	-4.310130
H	1.012102	-1.300221	-5.187221
H	2.536363	-0.981824	-4.297198
H	1.254823	0.263550	-4.340176
O	4.372272	-0.654185	0.088274
H	6.791558	-2.006033	0.398896
C	6.354697	-2.979662	0.131395
P	3.894357	-2.096051	0.017815
H	6.933061	-3.771701	0.618647
H	6.412608	-3.117490	-0.958799
O	3.767807	-2.441007	-1.556799
O	5.012002	-3.092095	0.600967
O	2.622098	-2.450978	0.786277
C	3.310407	-3.732555	-1.951454
H	3.962152	-4.527922	-1.559435
H	3.334203	-3.765318	-3.046471
H	2.280318	-3.918180	-1.609616
H	0.586679	-1.695662	1.332220
H	1.643801	-0.381578	0.550236

110

Scheme_S1_S.II / electronic energy: -5188.84776449 a.u. / lowest freq: -248.07 cm-1

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H	2.436705	-3.483162	1.776474
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C	-0.213068	-1.488947	-1.254409
C	0.471419	-0.789517	-2.254796
C	-1.591025	-1.733787	-1.405764
C	-0.199720	-0.332064	-3.386233
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C	-1.562896	-0.583987	-3.535179
H	0.348673	0.219157	-4.153506
H	-3.327617	-1.462523	-2.645615
H	-2.095382	-0.229670	-4.420932
C	2.098579	-0.867586	2.925301
C	1.192901	-0.380443	3.888012
C	3.491393	-0.726383	3.059938
C	1.720096	0.289089	4.998713
C	3.970622	-0.044086	4.185685
C	3.095127	0.461441	5.143005
H	3.489074	0.990163	6.014640
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O	-3.966917	-2.169426	-0.434034
O	-2.081934	-1.988813	1.170980
O	-2.336620	-4.008044	-0.294019
Cu	1.109049	1.009013	0.295355
C	1.584243	-3.971010	-0.678845
C	1.067502	-5.099408	-1.322321
C	2.857672	-3.505418	-1.035468
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H	0.067008	-5.453904	-1.058152
C	3.604105	-4.166222	-2.007847
H	3.263773	-2.610973	-0.550015
C	3.085118	-5.300533	-2.637569
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H	4.596072	-3.795997	-2.278639
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N	0.487454	-1.846962	-0.076623
N	1.569112	-1.544546	1.783928
C	-0.475368	2.295849	0.736993
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H	5.049416	0.088743	4.303448
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C	4.428620	-1.296678	2.046568

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C	-1.375009	1.325942	0.225555
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H	-7.227806	-2.500761	-0.453578
H	-6.780873	-1.054293	-1.360939
H	-4.878995	-3.210729	2.472484
H	-6.054101	-2.032830	3.062340
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C	1.604769	3.850781	-3.543444
H	2.556812	3.615943	-1.623743
C	-0.778943	3.483120	-3.594571
H	-1.709814	2.992013	-1.714538
C	0.404922	3.800607	-4.259164
H	2.535604	4.112374	-4.052147
H	-1.725804	3.472358	-4.140830
H	0.393300	4.023987	-5.328610
C	2.949042	1.210522	-0.247101
C	5.513890	1.275855	-0.955419
C	6.135358	0.145108	-1.527265
C	6.292238	2.436519	-0.760163
C	7.478989	0.178142	-1.888061
H	5.545863	-0.761668	-1.687329
C	7.635997	2.460465	-1.121058
H	5.826070	3.320536	-0.318067
C	8.236306	1.333708	-1.686235
H	7.940816	-0.708064	-2.330648
H	8.221208	3.369294	-0.959336
H	9.291546	1.356083	-1.968624
H	4.066798	-1.135477	1.022122
H	4.552334	-2.384355	2.175095
H	5.426992	-0.847838	2.126768
H	-0.661756	-0.223792	2.776450
H	-0.843130	-0.110267	4.537124
H	-0.531404	-1.671093	3.751246
C	0.364698	3.630708	4.060203
H	1.364445	3.963046	4.354701
H	0.044931	2.792680	4.691326
H	-0.350569	4.455987	4.178255
O	-4.571409	0.345295	0.765747
H	-5.049215	2.643333	-2.751982
C	-4.469615	1.709487	-2.811195
P	-4.374492	1.528473	-0.188298
H	-3.408175	1.957252	-2.960773
H	-4.824144	1.128988	-3.670486
O	-5.494532	2.653089	0.047928
O	-4.653865	0.904912	-1.651754
O	-3.053317	2.283676	-0.116147
C	-6.875950	2.297929	0.054519
H	-7.444362	3.227870	0.162940
H	-7.112016	1.637496	0.901299
H	-7.172640	1.809230	-0.885600
H	-1.837352	0.623191	0.922755
H	-1.275661	0.997066	-0.810457

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Scheme_S1_S.III / electronic energy: -5345.97000961 a.u. / lowest freq: -295.85 cm-1

C	-0.786111	2.823941	1.596312
H	0.059476	3.526384	1.562943
C	-0.604971	1.819972	2.744073
H	-1.349576	1.946436	3.542786
C	-0.782874	0.624313	0.749394
C	-0.476420	2.356827	-0.901152
C	-1.486164	2.257149	-1.862738
C	0.789939	2.837997	-1.276395
C	-1.248789	2.647651	-3.177739
H	-2.459716	1.868342	-1.556215
C	1.014793	3.251868	-2.591194
C	-0.001979	3.159309	-3.537350
H	-2.045344	2.560989	-3.919952
H	2.002934	3.617751	-2.875359
H	0.187892	3.476415	-4.565037
C	-0.774989	-0.750280	2.763331
C	0.424108	-1.246999	3.323543
C	-1.984119	-1.483464	2.825034
C	0.388451	-2.501294	3.946043

C	-1.953530	-2.741465	3.438616
C	-0.782859	-3.247269	3.995516
H	-0.785585	-4.232483	4.469164
S	2.138956	2.972319	-0.103025
O	3.359946	2.695594	-0.999231
O	2.000581	1.914093	0.911491
O	2.148429	4.353680	0.387416
Cu	-1.039742	-0.810192	-0.598414
C	-2.076882	3.607384	1.621974
C	-2.063301	4.974032	1.917799
C	-3.304089	2.977577	1.373559
C	-3.254430	5.698513	1.978295
H	-1.107484	5.474544	2.098737
C	-4.493905	3.699785	1.435018
H	-3.325855	1.910641	1.123551
C	-4.471994	5.062542	1.739488
H	-3.229038	6.766447	2.208357
H	-5.445398	3.197300	1.243747
H	-5.405513	5.628625	1.784697
N	-0.734382	1.920828	0.422680
N	-0.762080	0.511781	2.080949
C	0.743720	-1.494105	-1.493514
C	1.180461	-0.681562	-2.668631
O	2.180275	0.002227	-2.654217
O	0.379747	-0.821226	-3.727929
Al	4.922399	1.825028	-0.483125
H	-2.868433	-3.335766	3.487306
C	-0.250592	-2.487248	-1.623992
C	-3.297502	-0.907807	2.329067
H	0.395019	1.902015	3.191730
C	1.719568	-0.460146	3.305403
H	1.305059	-2.901177	4.387645
C	-0.504518	-3.603019	-0.706668
H	-0.734643	-2.556018	-2.601714
C	0.484148	-4.124630	0.151863
C	-1.769400	-4.225410	-0.730424
C	1.402928	-1.168827	-0.276237
C	-4.044899	-0.900357	-1.604671
C	5.463815	2.592005	1.238199
C	6.052861	1.832093	-2.078892
H	5.512705	1.428235	-2.952065
H	6.962169	1.216952	-1.965584
H	6.395939	2.842527	-2.359227
H	6.468296	2.289154	1.579817
H	4.759633	2.297610	2.036453
H	5.463808	3.695913	1.224019
C	0.201933	-5.215182	0.970886
H	1.493854	-3.708065	0.140989
C	-2.047211	-5.306094	0.097102
H	-2.539393	-3.829923	-1.398465
C	-1.062783	-5.803439	0.955461
H	0.983295	-5.612530	1.623451
H	-3.037484	-5.767086	0.072189
H	-1.280286	-6.655959	1.603494
C	-2.876737	-0.945540	-1.200399
C	-5.401488	-0.822940	-2.038542
C	-5.885532	-1.633421	-3.087029
C	-6.299494	0.077170	-1.425218
C	-7.211224	-1.544183	-3.501356
H	-5.204044	-2.335508	-3.573671
C	-7.623504	0.160719	-1.844703
H	-5.938460	0.711355	-0.610873
C	-8.086517	-0.648359	-2.884317
H	-7.565338	-2.181321	-4.315756
H	-8.301561	0.864874	-1.355813
H	-9.126508	-0.581011	-3.212328
H	-3.082327	-0.304969	1.431534
H	1.637526	0.303965	2.517044
C	0.794352	-0.163864	-4.923601
H	-0.050493	-0.215937	-5.616462
H	1.661954	-0.677582	-5.359922
H	1.061535	0.881933	-4.730378
O	4.374610	0.112607	-0.132740
H	6.736368	-0.697577	1.159196
C	6.745745	-1.648524	0.605108
P	4.393147	-1.364405	-0.516281
H	7.305339	-2.388559	1.187656
H	7.254654	-1.503220	-0.360043
O	5.018679	-1.431571	-1.997137
O	5.426864	-2.157189	0.432253
O	3.086246	-2.144237	-0.404653
C	4.910161	-2.629739	-2.757629
H	5.310274	-3.496352	-2.209641

H	5.498119	-2.487068	-3.670772
H	3.864174	-2.831544	-3.032053
H	1.108387	-1.649426	0.656866
H	1.870958	-0.185308	-0.183524
C	1.933049	0.247744	4.643573
H	2.108475	-0.483388	5.448797
H	2.811296	0.909531	4.602312
H	1.070362	0.857373	4.948015
C	2.939448	-1.313803	2.976341
H	2.800895	-1.923715	2.072542
H	3.818586	-0.672683	2.809683
H	3.198331	-1.999466	3.797961
C	-4.311454	-1.964598	1.920701
H	-5.183858	-1.492879	1.446115
H	-3.895517	-2.685529	1.201261
H	-4.693289	-2.531740	2.783520
C	-3.895866	0.023768	3.381052
H	-4.826328	0.484347	3.015283
H	-4.140910	-0.527332	4.302805
H	-3.211995	0.837802	3.660848

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Scheme_S1_S.IV / electronic energy: -5345.96857494 a.u. / lowest freq: -259.11 cm-1

C	1.395866	-0.111912	-3.068825
H	0.620926	0.337368	-3.711373
C	1.182694	-1.623885	-2.918245
H	2.082533	-2.204549	-3.175914
C	0.873174	-0.642632	-0.821228
C	1.105746	1.721400	-1.329373
C	2.261565	2.366876	-0.875997
C	-0.092940	2.447206	-1.420129
C	2.224663	3.703648	-0.494226
H	3.186556	1.790820	-0.810663
C	-0.123715	3.794010	-1.042423
C	1.027500	4.415842	-0.571060
H	3.132945	4.187124	-0.128023
H	-1.061604	4.349073	-1.111971
H	0.987867	5.463683	-0.265319
C	0.633974	-3.091251	-0.928088
C	-0.578092	-3.749747	-1.227170
C	1.628621	-3.692928	-0.125182
C	-0.770863	-5.038950	-0.718055
C	1.376221	-4.978432	0.369893
C	0.194029	-5.650462	0.073786
H	0.025291	-6.656842	0.465359
S	-1.590790	1.788429	-2.153437
O	-2.647904	2.326464	-1.155813
O	-1.578099	0.320162	-2.133803
O	-1.714966	2.434139	-3.462298
Cu	0.767446	-0.184092	1.113665
C	2.759277	0.310518	-3.553997
C	2.895090	1.200802	-4.621886
C	3.909640	-0.148171	-2.897073
C	4.160697	1.619936	-5.036730
H	1.998779	1.572362	-5.127572
C	5.172394	0.269208	-3.308560
H	3.807508	-0.826524	-2.042470
C	5.299994	1.154396	-4.382419
H	4.254979	2.316975	-5.872888
H	6.062935	-0.093553	-2.788941
H	6.290688	1.483609	-4.705031
N	1.174051	0.345728	-1.674056
N	0.866150	-1.796387	-1.490601
C	-0.994117	-0.566943	2.159729
C	-0.963666	-2.003748	2.566404
O	-1.667772	-2.858112	2.073888
O	-0.074267	-2.243141	3.534026
Al	-4.495978	2.137053	-1.233226
H	2.132880	-5.468566	0.988057
C	-0.239643	0.396955	2.873621
C	2.972529	-3.041780	0.139402
H	0.358609	-1.992795	-3.544406
C	-1.669807	-3.109701	-2.059243
H	-1.703868	-5.564485	-0.940495
C	-0.384993	1.854004	2.821685
H	0.359893	0.014877	3.703275
C	0.681325	2.650948	3.288732
C	-1.557496	2.501001	2.381429
C	-1.769084	-0.282434	1.004869
C	3.744866	0.503644	1.933220
C	-5.073122	2.054647	-3.097168
C	-5.183029	3.415728	0.082381
H	-6.285724	3.452235	0.107892
H	-4.847623	4.448069	-0.116851

H	-4.861551	3.174252	1.110365
H	-4.873753	2.980724	-3.661298
H	-6.153581	1.853005	-3.196425
H	-4.554229	1.245513	-3.639319
C	0.593757	4.036922	3.282928
H	1.591256	2.159247	3.642413
C	-1.640486	3.891548	2.380331
H	-2.429828	1.914009	2.087603
C	-0.566592	4.664446	2.820927
H	1.435241	4.634642	3.641341
H	-2.560267	4.373065	2.039054
H	-0.636050	5.754997	2.815740
C	2.564011	0.230826	1.689484
C	5.116728	0.820463	2.155608
C	6.110162	0.360411	1.263845
C	5.523004	1.605255	3.255538
C	7.450569	0.674006	1.466255
H	5.810442	-0.249205	0.406658
C	6.865504	1.915931	3.450453
H	4.767507	1.969948	3.956030
C	7.835695	1.452995	2.559261
H	8.202935	0.307370	0.763300
H	7.158275	2.526503	4.308417
H	8.888670	1.699006	2.715827
H	2.874478	-1.959260	-0.039483
H	-1.401359	-2.054589	-2.219263
C	0.022222	-3.593893	3.978597
H	0.814967	-3.613424	4.731883
H	0.276738	-4.264548	3.147481
H	-0.924108	-3.925866	4.425539
O	-4.720665	0.438524	-0.559401
H	-7.336304	0.719666	0.121262
C	-7.308128	0.505205	1.199999
P	-4.798514	-0.176798	0.843684
H	-7.801571	-0.460305	1.383735
H	-7.855938	1.292623	1.729339
O	-5.261562	-1.687704	0.556175
O	-5.974821	0.500863	1.706688
O	-3.564682	-0.086571	1.739529
C	-5.213661	-2.649334	1.608910
H	-5.561465	-3.599669	1.189053
H	-5.874800	-2.365480	2.441921
H	-4.188330	-2.774938	1.985054
H	-2.020120	-1.111561	0.342496
H	-1.747944	0.703635	0.543363
C	-1.797097	-3.785079	-3.421853
H	-2.109535	-4.836247	-3.317436
H	-2.552673	-3.280499	-4.042111
H	-0.851326	-3.783552	-3.983542
C	-3.009830	-3.119071	-1.331392
H	-2.917747	-2.772747	-0.292333
H	-3.735596	-2.468072	-1.840588
H	-3.450403	-4.128054	-1.290254
C	4.013832	-3.577538	-0.840880
H	4.982714	-3.072544	-0.707421
H	4.181233	-4.656289	-0.693634
H	3.705897	-3.436116	-1.887706
C	3.436948	-3.209232	1.579512
H	4.368409	-2.650378	1.752014
H	2.692922	-2.832055	2.298033
H	3.646205	-4.259921	1.832682

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Scheme_S1_S.V / electronic energy: -5388.43148220 a.u. / lowest freq: -251.33 cm-1

C	0.509227	2.407840	1.631796
H	-0.394535	2.999043	1.830928
C	1.277019	2.957222	0.409839
H	2.337038	3.109794	0.673817
C	0.607178	0.736714	-0.045030
C	-0.653850	0.137610	1.931371
C	-0.002310	-0.937011	2.540823
C	-2.054067	0.240435	2.037794
C	-0.726229	-1.911412	3.226546
H	1.083712	-1.003348	2.451214
C	-2.773976	-0.730255	2.734954
C	-2.112261	-1.809233	3.320260
H	-0.200362	-2.750628	3.687542
H	-3.859608	-0.649240	2.802352
H	-2.688986	-2.568640	3.853009
C	1.838613	1.867629	-1.840070
C	1.018770	2.194842	-2.943642
C	3.224656	1.637684	-1.988430
C	1.616593	2.273786	-4.206999
C	3.772418	1.746430	-3.272698

C	2.980722	2.059587	-4.372525
H	3.430599	2.134822	-5.365765
S	-2.920681	1.595278	1.245522
O	-2.637713	2.810343	2.017141
O	-4.398699	1.211805	1.432172
O	-2.540890	1.598082	-0.174918
Cu	0.805710	-1.182895	-0.595972
C	1.312137	2.312098	2.904541
C	0.812577	2.854625	4.092335
C	2.545116	1.644874	2.926285
C	1.538171	2.748626	5.280140
H	-0.156098	3.363308	4.082873
C	3.271262	1.540347	4.110041
H	2.933791	1.192313	2.006647
C	2.768961	2.094312	5.290353
H	1.137891	3.179326	6.201152
H	4.234048	1.023224	4.113532
H	3.338636	2.011690	6.219147
N	0.105714	1.056954	1.158367
N	1.238342	1.802616	-0.541096
C	-0.692514	-2.158959	-1.684117
H	-0.765924	-1.748580	-2.694204
Al	-5.664607	0.478259	0.288762
H	4.843147	1.575924	-3.410937
C	0.318848	-3.112527	-1.407302
C	4.126508	1.282834	-0.823430
C	-0.474793	2.409207	-2.811477
H	0.997185	2.512389	-5.075627
C	1.334626	-3.387740	-2.446666
C	0.170164	-4.087510	-0.282426
C	1.710697	-2.394654	-3.375116
C	1.988992	-4.629754	-2.511979
C	-1.668378	-1.749418	-0.747577
C	-6.022458	1.689888	-1.202004
C	-7.090444	-0.130100	1.487050
H	-6.784413	-0.970095	2.134147
H	-8.003678	-0.455959	0.960716
H	-7.407316	0.680312	2.166578
H	-6.452526	2.650498	-0.870934
H	-6.737939	1.270309	-1.930197
H	-5.108414	1.937026	-1.767577
C	2.695653	-2.633656	-4.325218
H	1.250910	-1.402186	-3.319890
C	2.968875	-4.872443	-3.473085
H	1.725771	-5.422822	-1.809263
C	3.329255	-3.877967	-4.381224
H	2.979707	-1.838172	-5.018651
H	3.458706	-5.848476	-3.507836
H	4.105712	-4.066795	-5.126214
H	3.478071	0.940944	0.000524
C	4.918649	2.493048	-0.334542
C	5.079043	0.140726	-1.159074
H	-0.704963	2.567044	-1.748521
C	-1.228353	1.154554	-3.233069
C	-0.962572	3.631305	-3.576094
O	-4.728011	-0.955179	-0.370528
H	-5.029890	-5.009496	0.838690
C	-4.454316	-4.308946	1.462163
P	-4.497779	-2.466279	-0.402003
H	-3.382796	-4.533575	1.355327
H	-4.747516	-4.446832	2.508282
O	-5.607887	-3.206908	-1.293403
O	-4.733571	-2.953828	1.117877
O	-3.159046	-2.936617	-0.962726
C	-6.993198	-2.965016	-1.053362
H	-7.555007	-3.665226	-1.680676
H	-7.271249	-1.938719	-1.336535
H	-7.259230	-3.141681	-0.000513
H	-2.229695	-0.833056	-0.947418
H	-1.542620	-1.998667	0.309103
H	5.609630	-0.195488	-0.256264
H	5.848924	0.449059	-1.882807
H	4.554569	-0.730007	-1.579228
H	5.523508	2.234772	0.547920
H	4.276845	3.340931	-0.055429
H	5.609945	2.853239	-1.112949
H	-0.376107	4.530246	-3.334208
H	-2.013812	3.843088	-3.329073
H	-0.914604	3.487312	-4.666744
H	-0.934052	0.302749	-2.606293
H	-1.024339	0.888958	-4.283321
H	-2.314551	1.286659	-3.121786
H	-2.081673	6.068003	-0.677051

C	-1.020095	5.809868	-0.705021
H	-0.439116	7.635770	-1.707013
C	-0.101577	6.685762	-1.285311
C	0.763965	4.251370	-0.177886
C	1.248981	6.340972	-1.324491
C	1.675699	5.133386	-0.772088
H	1.977161	7.018335	-1.777112
H	2.738417	4.872825	-0.790053
C	-0.593929	4.599623	-0.160387
H	-1.332930	3.922663	0.276467
H	5.624252	-2.861132	4.910702
H	3.669217	-2.106408	3.585437
C	5.638972	-2.957022	3.821925
C	4.540846	-2.531634	3.080537
H	7.615459	-3.835622	3.767891
C	6.754060	-3.503664	3.183421
C	4.531073	-2.642802	1.673144
C	3.409123	-2.198115	0.914256
C	6.758895	-3.623278	1.792081
C	2.435662	-1.793577	0.265591
C	5.664246	-3.201356	1.043217
H	7.626508	-4.052096	1.283949
H	5.671165	-3.298544	-0.045663
H	-0.340683	-4.994455	-0.648780
H	-0.439627	-3.697802	0.541939
H	1.138196	-4.396007	0.131103

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Scheme_S1_S.VI / electronic energy: -5388.43068169 a.u. / lowest freq: -248.55 cm-1

C	-0.450498	2.739216	0.966088
H	-1.399190	3.058669	0.512571
C	0.724359	3.129896	0.038981
H	1.486002	3.693895	0.603019
C	0.652465	0.773303	0.225168
C	-1.144869	0.435333	1.812745
C	-0.457610	-0.400880	2.702526
C	-2.552678	0.421256	1.824358
C	-1.142558	-1.214860	3.598122
H	0.636325	-0.390463	2.683122
C	-3.234826	-0.396177	2.730402
C	-2.536227	-1.207813	3.618918
H	-0.582128	-1.848478	4.289137
H	-4.325384	-0.407235	2.714475
H	-3.083875	-1.837329	4.323062
C	2.591263	1.736501	-0.946174
C	2.676091	1.462782	-2.323792
C	3.739926	1.982039	-0.162870
C	3.947483	1.437964	-2.909894
C	4.985431	1.953631	-0.798080
C	5.091532	1.686199	-2.159366
H	6.074644	1.660790	-2.636417
S	-3.516960	1.417861	0.689111
O	-4.861389	0.675593	0.682446
O	-2.866481	1.336771	-0.631313
O	-3.669316	2.753543	1.268173
Cu	1.068672	-1.188258	-0.077592
C	-0.355522	3.333805	2.348035
C	-1.104714	4.475016	2.654724
C	0.512556	2.811105	3.315809
C	-0.977452	5.092428	3.898610
H	-1.796775	4.875822	1.909164
C	0.635963	3.424460	4.561418
H	1.092406	1.909477	3.097410
C	-0.106034	4.569874	4.854236
H	-1.567822	5.983749	4.124391
H	1.314508	3.004026	5.307883
H	-0.009087	5.051190	5.830404
N	-0.376828	1.255486	0.951352
N	1.310890	1.805052	-0.305999
C	-0.694076	-2.301202	-0.254166
H	-1.147786	-2.306078	0.741951
Al	-5.962012	0.103439	-0.704596
H	5.888969	2.133082	-0.207766
C	0.333119	-3.230090	-0.545320
C	3.671151	2.266395	1.324243
C	1.462673	1.123915	-3.161567
H	4.037892	1.212988	-3.976122
C	0.808660	-4.154056	0.504893
C	0.690541	-3.557559	-1.959044
C	0.648179	-3.856991	1.872162
C	1.453683	-5.358060	0.169007
C	-1.253978	-1.416191	-1.200608
C	-6.321840	1.601825	-1.906113
C	-7.382545	-0.861935	0.237218

H	-6.984598	-1.632016	0.920998
H	-8.106344	-1.366380	-0.424845
H	-7.977023	-0.177013	0.866837
H	-6.897654	2.406993	-1.418727
H	-6.895891	1.312370	-2.802603
H	-5.387616	2.063247	-2.268881
C	1.095277	-4.728093	2.857211
H	0.195300	-2.908651	2.166549
C	1.900509	-6.233046	1.157373
H	1.605532	-5.625068	-0.877992
C	1.723340	-5.925725	2.505025
H	0.965908	-4.466901	3.910515
H	2.395196	-7.163188	0.868043
H	2.079810	-6.609536	3.278809
H	2.614068	2.241879	1.623548
C	4.204160	3.656679	1.652737
C	4.379058	1.193473	2.143364
H	0.563482	1.353901	-2.566285
C	1.451059	-0.372835	-3.448323
C	1.387118	1.944446	-4.441326
O	-4.880709	-1.065556	-1.613510
H	-3.145982	-3.737988	1.609303
C	-3.548963	-3.882497	0.599358
P	-4.063116	-2.351741	-1.470846
H	-4.385472	-4.594920	0.649283
H	-2.760688	-4.307302	-0.040462
O	-4.845496	-3.596999	-2.114702
O	-4.000557	-2.615078	0.123167
O	-2.682196	-2.386189	-2.115415
C	-6.248266	-3.744605	-1.897934
H	-6.500064	-3.713749	-0.827389
H	-6.532443	-4.724115	-2.297325
H	-6.814185	-2.966539	-2.429518
H	-0.768409	-1.245122	-2.160662
H	-1.877848	-0.586557	-0.857557
H	4.316597	1.423808	3.218129
H	5.447302	1.116875	1.886502
H	3.931626	0.201000	1.985883
H	4.062221	3.888977	2.719073
H	3.695695	4.441830	1.072397
H	5.281341	3.739388	1.440810
H	1.442103	3.024097	-4.237262
H	0.442152	1.754901	-4.971736
H	2.202059	1.696560	-5.138657
H	1.472656	-0.950868	-2.508660
H	2.333645	-0.681684	-4.031252
H	0.556585	-0.669560	-4.018050
H	1.598990	6.509627	-3.061060
H	-0.469479	6.027769	-4.365514
C	0.925813	5.708385	-2.746724
C	-0.231747	5.438799	-3.476212
H	2.127092	5.173550	-1.030494
C	1.222160	4.958862	-1.607830
C	-1.086549	4.413699	-3.066076
C	0.366285	3.935071	-1.185018
C	-0.790194	3.664007	-1.929078
H	-1.469066	2.864301	-1.615095
H	-1.994381	4.196732	-3.634566
H	9.416448	-2.804687	-0.399142
H	8.254220	-2.837232	1.807167
C	8.340440	-2.623525	-0.341700
C	7.688196	-2.641240	0.892700
H	8.105944	-2.356423	-2.473932
C	7.605345	-2.372206	-1.502224
C	6.317787	-2.411254	0.970551
H	5.812795	-2.425894	1.939821
C	6.234855	-2.141826	-1.433414
C	5.560367	-2.154804	-0.192821
H	5.663707	-1.944993	-2.344543
C	4.159174	-1.905553	-0.117328
C	2.949444	-1.652984	-0.043467
H	0.330365	-2.820574	-2.681909
H	0.220150	-4.515530	-2.236763
H	1.773040	-3.680894	-2.097525

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Scheme_S2_S.VII / electronic energy: -5638.16611106 a.u. / lowest freq: -208.80 cm-1

C	-1.691561	-2.916424	-0.723052
H	-2.302365	-2.580663	-1.572332
C	-2.365824	-2.511578	0.608012
H	-2.344976	-3.360140	1.313269
C	-0.357470	-1.294413	0.353398
C	0.540924	-2.168723	-1.719235
C	1.840388	-2.549320	-1.364279

C	0.266646	-1.822941	-3.056178
C	2.850583	-2.623456	-2.318755
H	2.046703	-2.796929	-0.320475
C	1.282155	-1.922409	-4.009786
C	2.565481	-2.328868	-3.650645
H	3.854568	-2.922909	-2.011538
H	1.056434	-1.639903	-5.040137
H	3.346496	-2.393676	-4.412103
C	-1.756487	-0.634366	2.246429
C	-2.452478	0.537870	1.909666
C	-1.461757	-0.944282	3.592864
C	-2.893385	1.463967	2.857581
C	-1.911766	0.002883	4.529957
C	-2.600446	1.161138	4.192112
H	-2.909669	1.832792	4.995405
S	-1.324005	-1.170379	-3.598057
O	-1.020470	-0.372010	-4.821953
O	-1.768712	-0.266964	-2.491860
O	-2.206503	-2.327452	-3.834727
Cu	1.194527	-0.060783	0.584957
C	-1.443770	-4.394181	-0.875113
C	-2.219965	-5.138593	-1.769208
C	-0.458611	-5.045880	-0.121292
C	-2.026240	-6.514368	-1.897837
H	-2.974748	-4.627542	-2.372986
C	-0.259812	-6.418379	-0.254867
H	0.162270	-4.468529	0.570974
C	-1.046359	-7.156738	-1.141856
H	-2.639869	-7.085277	-2.599012
H	0.514757	-6.915347	0.334440
H	-0.889769	-8.233136	-1.246835
N	-0.440744	-2.125305	-0.694343
N	-1.426989	-1.472628	1.132151
C	1.183961	1.699748	-0.545345
C	1.555333	1.505052	-1.970026
O	0.764326	1.619084	-2.888955
O	2.849984	1.259235	-2.166040
Na	-1.345864	1.720739	-3.799435
C	2.193087	1.712337	0.483069
C	2.088284	2.389065	1.790062
H	3.219750	1.636283	0.114821
C	3.160757	3.205374	2.193728
C	1.002795	2.244216	2.678736
C	-0.181626	1.933027	-0.320584
C	3.129863	3.886893	3.407678
H	4.028161	3.302021	1.535809
C	0.975424	2.921108	3.894600
H	0.191778	1.547439	2.438568
C	2.034144	3.754510	4.260702
H	3.972727	4.521711	3.691857
H	0.125131	2.784901	4.568069
H	2.011751	4.284912	5.215525
C	2.573579	-0.929179	1.775211
C	3.282922	1.229452	-3.525992
H	4.329368	0.911000	-3.512936
H	3.206610	2.231564	-3.970314
H	2.681562	0.531547	-4.120969
O	-2.468996	3.044711	-2.314405
H	-3.897094	5.406175	-2.752763
C	-3.023062	6.069356	-2.666508
P	-1.440712	4.094669	-1.984422
H	-3.359301	7.048833	-2.305597
H	-2.580337	6.199224	-3.667088
O	-0.610977	4.258751	-3.403900
O	-2.077145	5.570736	-1.735111
O	-0.460573	3.910695	-0.824683
C	0.593914	5.000839	-3.424664
H	0.419441	6.061860	-3.182517
H	1.008761	4.940003	-4.438606
H	1.332940	4.599202	-2.713464
H	-0.554554	2.128439	0.682452
H	-0.914134	1.586735	-1.051634
C	-3.683308	2.699852	2.429430
C	-5.029904	2.240436	1.859380
H	-4.894823	1.587280	0.984186
H	-5.616720	1.681640	2.604752
H	-5.631940	3.104409	1.537941
C	-2.915757	3.457975	1.343648
H	-1.921165	3.779269	1.689621
H	-2.779897	2.857292	0.433272
H	-3.463953	4.363964	1.041723
C	-3.933734	3.642828	3.602569
H	-4.478072	4.534617	3.259496

H	-4.541224	3.177675	4.392895
H	-2.994737	3.990236	4.060507
C	-3.795409	-2.041089	0.509046
C	-4.699301	-2.393441	1.518576
C	-4.238626	-1.232547	-0.546823
C	-6.022074	-1.953431	1.477902
H	-4.360987	-3.026468	2.344801
C	-5.563200	-0.799644	-0.590577
H	-3.542012	-0.930161	-1.335791
C	-6.458233	-1.157799	0.418937
H	-6.715117	-2.240612	2.272492
H	-5.897302	-0.171275	-1.420138
H	-7.495450	-0.815499	0.380497
C	-0.720089	-2.165103	4.168601
H	-2.657437	0.703564	0.847579
H	-1.713303	-0.176923	5.589067
C	0.478035	-1.668603	4.991479
C	-0.183413	-3.158102	3.141877
C	-1.676922	-2.930142	5.093829
H	-2.046488	-2.310521	5.923057
H	-1.165142	-3.797609	5.537535
H	-2.553515	-3.309542	4.547553
H	1.186679	-1.102868	4.368656
H	1.024861	-2.522329	5.419441
H	0.182771	-1.021368	5.828906
H	0.512037	-2.696605	2.430166
H	-0.981218	-3.658232	2.579025
H	0.369696	-3.951641	3.666467
H	6.745245	-2.701959	-0.939405
C	6.982539	-2.052984	-0.084241
H	7.973281	-1.612862	-0.269125
H	7.923650	-0.851011	2.218197
H	5.348780	-0.967722	-2.011299
C	5.930839	-0.975930	0.064238
C	5.709617	-0.256627	-1.254833
H	6.635471	0.196646	-1.636665
C	6.170704	0.018985	1.248495
H	7.878716	1.102654	0.469629
C	6.873287	1.304220	0.867358
H	4.953773	0.534039	-1.151150
H	6.315399	1.874137	0.113230
H	6.990614	1.947634	1.750862
H	7.050918	-2.689731	0.806592
H	6.376218	-1.577493	2.716446
O	4.674215	-1.593776	0.433232
C	6.866974	-0.636205	2.430458
H	6.828627	0.036311	3.298526
B	4.011903	-0.728777	1.287631
O	4.822194	0.328215	1.666004
H	2.266161	-1.983588	1.815363
H	2.369167	-0.438030	2.739267

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Scheme_S2_S.VIII / electronic energy: -5638.16130781 a.u. / lowest freq: -250.09 cm-1

C	2.067406	0.938313	2.386721
H	1.670027	1.798922	2.945663
C	2.927079	1.411896	1.194976
H	3.935789	0.973670	1.253503
C	1.053807	0.211876	0.373373
C	-0.101587	-0.372055	2.438787
C	-0.208531	-1.766905	2.385774
C	-1.038988	0.365690	3.184844
C	-1.223859	-2.425961	3.076536
H	0.509651	-2.319046	1.771568
C	-2.042026	-0.306773	3.885477
C	-2.132545	-1.696216	3.841070
H	-1.302797	-3.514347	3.020041
H	-2.780503	0.280903	4.433851
H	-2.928701	-2.204952	4.388618
C	2.524507	1.226166	-1.297054
C	1.675882	2.233771	-1.787332
C	3.629397	0.770714	-2.042666
C	1.884081	2.869928	-3.007504
C	3.831499	1.440292	-3.266264
C	3.006108	2.450137	-3.737086
H	3.240086	2.913202	-4.699455
S	-1.121827	2.168318	3.136986
O	-2.523476	2.496221	3.521981
O	-0.910125	2.520311	1.694802
O	-0.088458	2.685384	4.051546
Cu	-0.289278	-0.618467	-0.901700
C	2.784493	0.026380	3.349285
C	3.128114	0.486203	4.624144
C	3.130442	-1.281266	2.979224

C	3.823442	-0.337737	5.510477
H	2.843426	1.499190	4.923464
C	3.823881	-2.103991	3.864470
H	2.844447	-1.658553	1.990903
C	4.175094	-1.632492	5.131455
H	4.086432	0.033166	6.504130
H	4.091285	-3.121197	3.567251
H	4.717140	-2.279418	5.825536
N	0.941914	0.251785	1.708191
N	2.215303	0.789884	0.030094
C	-2.340531	-0.073850	-0.981814
C	-2.587541	1.273553	-1.554280
O	-2.731109	2.288880	-0.893874
O	-2.698843	1.262604	-2.885106
Na	-3.173908	3.100517	1.240036
C	-1.985460	-1.181620	-1.838078
C	-2.336610	-2.599074	-1.644729
H	-1.852834	-0.911974	-2.889826
C	-1.862748	-3.535407	-2.586998
C	-3.180826	-3.074545	-0.619845
C	-2.547138	-0.180269	0.407404
C	-2.196654	-4.881790	-2.502961
H	-1.221920	-3.189568	-3.401533
C	-3.512654	-4.426580	-0.539107
H	-3.637822	-2.378952	0.086274
C	-3.020877	-5.339319	-1.472104
H	-1.809457	-5.579888	-3.249815
H	-4.180003	-4.764951	0.257829
H	-3.286943	-6.397169	-1.404595
C	0.881372	-1.706889	-2.102107
C	-3.196344	2.456017	-3.485976
H	-3.231656	2.266635	-4.562961
H	-2.548748	3.317184	-3.280295
H	-4.205890	2.672642	-3.110774
O	-5.146168	2.101469	1.008376
H	-7.908984	1.790998	1.555831
C	-7.960713	0.987125	0.806324
P	-5.380052	0.716497	0.477219
H	-8.058184	1.443830	-0.191865
H	-8.854968	0.382633	0.999653
O	-5.453277	0.844217	-1.155307
O	-6.837295	0.124531	0.886860
O	-4.432502	-0.441951	0.847665
C	-5.704552	-0.318839	-1.924457
H	-5.665312	-0.035607	-2.984029
H	-6.701575	-0.737506	-1.712314
H	-4.953222	-1.104521	-1.740809
H	-2.459079	0.726002	1.001308
H	-2.298034	-1.099425	0.930636
C	0.953524	3.953580	-3.545623
C	1.767695	5.171092	-3.993084
H	2.343974	5.598957	-3.158434
H	2.475132	4.931605	-4.799518
H	1.100802	5.959301	-4.374194
C	-0.049049	4.408388	-2.489007
H	-0.700056	3.591636	-2.146179
H	0.451764	4.822036	-1.600322
H	-0.700861	5.195770	-2.895629
C	0.196202	3.375919	-4.747325
H	-0.516817	4.108923	-5.156500
H	0.880912	3.092109	-5.560784
H	-0.370224	2.474595	-4.466234
C	3.090450	2.901830	1.019547
C	4.300700	3.395841	0.517614
C	2.039285	3.796067	1.255797
C	4.460226	4.753727	0.245377
H	5.126427	2.702473	0.331667
C	2.201638	5.155708	0.991101
H	1.078164	3.428464	1.626709
C	3.407340	5.638410	0.479932
H	5.411083	5.121838	-0.147613
H	1.372982	5.843407	1.179302
H	3.528035	6.703991	0.268990
H	0.845216	2.526643	-1.139910
C	4.615597	-0.368957	-1.716194
H	4.682631	1.149445	-3.886416
C	4.287539	-1.198236	-0.475703
C	6.016363	0.227900	-1.532614
C	4.646560	-1.351442	-2.899421
H	4.405338	-0.639315	0.459962
H	4.998452	-2.037220	-0.415847
H	3.277238	-1.627327	-0.499342
H	6.051041	0.921597	-0.679017

H	6.355714	0.778591	-2.421986
H	6.750733	-0.568523	-1.337625
H	3.663349	-1.821679	-3.059927
H	5.368331	-2.157286	-2.697075
H	4.948999	-0.881510	-3.844858
H	0.525256	-1.765234	-3.141112
H	1.765991	-1.052154	-2.090901
H	2.362404	-4.564363	2.106942
C	2.693220	-4.939555	1.127587
H	2.899509	-6.013967	1.240384
H	4.017636	-5.904056	-1.105127
H	-0.000577	-4.655966	1.509083
C	1.619253	-4.700147	0.089391
C	0.271616	-5.189080	0.588080
H	0.286810	-6.263098	0.820898
C	1.954163	-5.229682	-1.342312
H	1.835460	-7.358477	-0.971079
C	1.412036	-6.606604	-1.652825
H	-0.519514	-5.009895	-0.154715
H	0.318429	-6.647344	-1.571774
H	1.682405	-6.898930	-2.677144
H	3.633642	-4.433525	0.872015
H	3.846297	-4.157578	-1.409980
O	1.499948	-3.273681	-0.138434
C	3.439272	-5.149356	-1.656142
H	3.600075	-5.319308	-2.729909
B	1.201195	-3.078427	-1.478125
O	1.292732	-4.257746	-2.189513

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Scheme_S3_S.IX / electronic energy: -5695.09120238 a.u. / lowest freq: -189.12 cm-1

C	-0.548263	3.344496	0.030816
H	-1.027076	3.649028	-0.910280
C	0.845426	2.727471	-0.244508
H	1.610600	3.275599	0.328887
C	-0.528541	1.089384	0.751720
C	-2.630840	2.248676	1.039043
C	-2.878191	2.067321	2.405698
C	-3.712902	2.464674	0.167038
C	-4.176912	2.100224	2.905599
H	-2.027102	1.903118	3.071816
C	-5.012632	2.500065	0.679304
C	-5.247484	2.321901	2.040657
H	-4.348118	1.955637	3.974513
H	-5.840938	2.657280	-0.014350
H	-6.270315	2.350729	2.423278
S	-3.503196	2.700335	-1.602937
O	-4.833023	2.390479	-2.208605
O	-2.500140	1.677949	-2.035383
O	-3.072193	4.098383	-1.783864
Cu	-1.298793	-0.556838	1.607119
C	-0.563622	4.502637	0.994882
C	-1.262291	5.671066	0.674711
C	0.082708	4.411439	2.235927
C	-1.300792	6.739131	1.572644
H	-1.785300	5.730615	-0.283776
C	0.042932	5.476318	3.132187
H	0.618038	3.494245	2.505815
C	-0.647919	6.644572	2.800683
H	-1.847639	7.648356	1.311289
H	0.551243	5.395283	4.096059
H	-0.678387	7.479898	3.504565
N	-1.285281	2.177878	0.587016
N	0.709350	1.362572	0.304571
C	-2.622285	-2.142169	1.662597
C	-3.525631	-2.131508	2.809027
C	-3.221283	-2.917573	3.938051
C	-4.699424	-1.353914	2.841349
C	-4.050788	-2.919119	5.055531
C	-5.527355	-1.357441	3.959249
C	-5.206591	-2.136029	5.073698
H	-3.794320	-3.536884	5.919536
H	-6.434048	-0.746462	3.960271
H	-5.858464	-2.136775	5.950365
C	-2.818944	-1.408694	0.463343
C	-2.030191	-1.635140	-0.674460
H	-1.975203	-0.878068	-1.459222
H	-1.188651	-2.326568	-0.610712
H	-4.972455	-0.743142	1.977530
H	-3.624184	-0.668263	0.389563
P	-3.774493	-2.295742	-2.930167
O	-4.865919	-1.264704	-2.225658
O	-3.127212	-1.409262	-3.960526
O	-4.689699	-3.475757	-3.558684

O	-2.966642	-2.995988	-1.835490
Na	-4.013950	0.609085	-3.475506
H	-1.921091	-2.986203	1.615225
H	-2.317822	-3.533599	3.926559
C	-5.784672	-1.747492	-1.257299
H	-6.161692	-0.887650	-0.688600
H	-6.637837	-2.251760	-1.737131
H	-5.306069	-2.456564	-0.563801
C	-5.458742	-3.194182	-4.719957
H	-6.050682	-4.088915	-4.945030
H	-6.149911	-2.351489	-4.559306
H	-4.817620	-2.966437	-5.583871
C	1.767458	0.435457	0.218879
C	3.095698	0.876268	0.190802
C	1.492767	-0.927983	0.110561
C	4.142446	-0.044201	0.065314
C	2.521953	-1.862841	-0.001562
C	3.845608	-1.412130	-0.021043
H	4.661024	-2.134091	-0.134840
H	0.457448	-1.268393	0.070586
H	3.327301	1.941899	0.262760
C	2.163147	-3.300770	-0.164815
C	1.873829	-4.086246	0.977129
C	2.042355	-3.841718	-1.462958
C	1.489119	-5.418891	0.794000
C	1.654135	-5.182093	-1.598831
C	1.381809	-5.965651	-0.483442
H	1.266371	-6.041258	1.664294
H	1.552343	-5.611718	-2.599993
H	1.076628	-7.007994	-0.607448
C	5.558343	0.426910	0.030022
C	6.070976	1.042401	-1.141646
C	6.378770	0.255894	1.167247
C	7.403129	1.470780	-1.143338
C	7.704758	0.708507	1.119582
C	8.216169	1.307875	-0.023769
H	7.819245	1.941619	-2.036574
H	8.342303	0.592023	2.000832
H	9.252736	1.654192	-0.046325
C	5.868319	-0.356247	2.460335
H	4.856576	-0.751899	2.277494
C	5.747273	0.703052	3.550831
H	5.093345	1.533199	3.243454
H	5.331612	0.276640	4.476604
H	6.728424	1.135758	3.803038
C	6.733481	-1.523818	2.919575
H	6.821670	-2.300019	2.144637
H	7.754636	-1.203320	3.178264
H	6.311741	-1.998339	3.818152
C	5.218230	1.179536	-2.393883
H	4.194547	1.443421	-2.072431
C	5.123937	-0.154155	-3.132916
H	4.441582	-0.080178	-3.993949
H	6.109320	-0.465620	-3.515096
H	4.754161	-0.961225	-2.484789
C	5.687139	2.273833	-3.339583
H	4.977260	2.392371	-4.170436
H	5.777513	3.249538	-2.838931
H	6.662139	2.040828	-3.794025
C	2.285555	-3.013067	-2.712661
H	2.589899	-2.000695	-2.399236
C	2.022563	-3.504611	2.371503
H	1.781015	-2.430169	2.300358
C	1.071671	-4.105900	3.394235
H	0.027036	-4.085530	3.049247
H	1.319757	-5.151289	3.634607
H	1.117655	-3.544161	4.339174
C	3.468634	-3.608270	2.849974
H	3.780607	-4.660669	2.946492
H	4.167657	-3.123628	2.152507
H	3.595578	-3.134368	3.835819
C	1.010873	-2.860282	-3.536375
H	0.643159	-3.830973	-3.904613
H	0.193448	-2.403333	-2.957791
H	1.186494	-2.223931	-4.416891
C	3.419831	-3.586961	-3.553866
H	4.354205	-3.672310	-2.978678
H	3.176664	-4.591167	-3.934896
H	3.624909	-2.950736	-4.427651
H	0.177960	0.894262	-2.182215
H	0.803038	0.937886	-4.579305
C	0.803193	1.705201	-2.565428
C	1.151807	1.732429	-3.914617

C	1.242547	2.715471	-1.700679
C	1.937165	2.771836	-4.416086
H	2.210747	2.791438	-5.474032
C	2.038771	3.748017	-2.207739
C	2.378933	3.780607	-3.559829
H	2.393735	4.533737	-1.533464
H	3.003437	4.591316	-3.943473
C	-0.517571	-0.743530	3.420069
C	0.681745	-0.303493	3.657104
C	1.920279	0.141051	3.798281
H	-1.096267	-1.263410	4.201092
H	2.137992	1.151338	4.163617
H	2.783797	-0.495184	3.565603

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Scheme_S3_S.X / electronic energy: -5695.08952654 a.u. / lowest freq: -278.42 cm-1

C	-1.125573	3.122166	0.825389
H	-1.753980	3.573743	0.047593
C	0.285417	2.819813	0.261028
H	1.041463	3.333599	0.877463
C	-0.703238	0.800105	0.977002
C	-2.893202	1.520066	1.728883
C	-2.931930	0.854122	2.961115
C	-4.105327	1.897435	1.118538
C	-4.142585	0.549621	3.576044
H	-1.984643	0.580118	3.435013
C	-5.313996	1.604492	1.755932
C	-5.340241	0.932378	2.975111
H	-4.144628	0.028159	4.535765
H	-6.242608	1.896529	1.262288
H	-6.296651	0.709294	3.453054
S	-4.202276	2.705875	-0.489164
O	-5.586187	2.442907	-0.981324
O	-3.213229	1.981773	-1.349206
O	-3.902177	4.131054	-0.267033
Cu	-0.883069	-1.071498	1.655223
C	-1.124674	4.008273	2.043817
C	-1.624471	5.311350	1.964375
C	-0.596776	3.550267	3.258811
C	-1.587218	6.149729	3.079798
H	-2.052806	5.661231	1.021501
C	-0.565140	4.384770	4.373418
H	-0.209446	2.527857	3.328796
C	-1.058759	5.688608	4.284948
H	-1.979826	7.166956	3.007388
H	-0.153910	4.016749	5.316762
H	-1.034368	6.343563	5.159312
N	-1.624255	1.760750	1.139995
N	0.405794	1.363233	0.466401
C	-1.740307	-2.961520	1.749784
C	-0.912732	-4.103566	2.132431
C	-0.814369	-4.456628	3.492710
C	-0.230432	-4.896839	1.190196
C	-0.055923	-5.550468	3.897939
C	0.512784	-6.001057	1.597182
C	0.610419	-6.330349	2.950741
H	0.007042	-5.803515	4.959122
H	1.017272	-6.616120	0.847637
H	1.196398	-7.197399	3.264921
C	-1.879512	-2.452625	0.442062
C	-2.881056	-1.524606	0.083658
H	-2.732617	-0.892428	-0.794412
H	-3.521222	-1.107560	0.866009
H	-0.301030	-4.665174	0.124050
H	-1.217282	-2.816121	-0.351858
P	-4.931479	-1.947040	-1.946703
O	-6.031482	-0.812101	-1.473928
O	-4.110822	-1.195190	-2.959572
O	-5.823800	-3.147017	-2.564544
O	-4.293394	-2.583021	-0.702712
Na	-4.845751	0.943757	-2.645896
H	-2.513682	-2.678701	2.478210
H	-1.353710	-3.861617	4.235445
C	-6.960453	-1.093921	-0.439053
H	-7.540926	-0.182428	-0.254264
H	-7.651807	-1.899540	-0.731973
H	-6.449771	-1.392489	0.489012
C	-6.544262	-2.910934	-3.767036
H	-7.075837	-3.836262	-4.016898
H	-7.285038	-2.104801	-3.645722
H	-5.870686	-2.654294	-4.597627
C	1.560736	0.670758	0.044081
C	2.789418	1.340474	-0.025414
C	1.481310	-0.661459	-0.364752

C	3.928445	0.680552	-0.495491
C	2.612425	-1.340695	-0.825980
C	3.831114	-0.660249	-0.888675
H	4.719680	-1.170132	-1.273286
H	0.518926	-1.177365	-0.376690
H	2.869326	2.384459	0.287147
C	2.460118	-2.746677	-1.289042
C	3.052872	-3.809530	-0.559217
C	1.695322	-3.003304	-2.450595
C	2.830919	-5.119157	-0.997841
C	1.483876	-4.334835	-2.836074
C	2.041209	-5.384172	-2.115807
H	3.276838	-5.954600	-0.453913
H	0.884340	-4.546843	-3.726388
H	1.871842	-6.417293	-2.431203
C	5.245179	1.376515	-0.556839
C	5.509739	2.315407	-1.585979
C	6.224602	1.079451	0.416334
C	6.764398	2.934021	-1.617511
C	7.469178	1.720162	0.339856
C	7.738954	2.639302	-0.665933
H	6.990443	3.659129	-2.402365
H	8.234788	1.496748	1.089111
H	8.712850	3.133708	-0.711420
C	5.970869	0.110691	1.558922
H	4.937855	-0.263639	1.469526
C	6.079605	0.809056	2.910164
H	5.402416	1.673770	2.978664
H	5.825479	0.121835	3.731438
H	7.100367	1.176492	3.099544
C	6.896116	-1.099116	1.489486
H	6.800772	-1.637468	0.534174
H	7.953458	-0.809256	1.596480
H	6.673168	-1.811191	2.298486
C	4.482555	2.596744	-2.672210
H	3.486737	2.605640	-2.193220
C	4.471769	1.476049	-3.710828
H	3.678900	1.634344	-4.458150
H	5.430734	1.429942	-4.251129
H	4.305169	0.487769	-3.258295
C	4.665588	3.943276	-3.354548
H	3.839954	4.133562	-4.054971
H	4.689268	4.775987	-2.635686
H	5.592924	3.987513	-3.946030
C	1.131959	-1.889476	-3.321436
H	1.536816	-0.932305	-2.954751
C	3.880191	-3.534947	0.688999
H	4.533786	-2.676621	0.456688
C	3.008266	-3.112311	1.870243
H	2.334921	-2.280377	1.619550
H	2.380175	-3.945571	2.223485
H	3.629576	-2.786561	2.719792
C	4.786420	-4.687032	1.091497
H	4.214744	-5.561017	1.441561
H	5.434102	-5.021158	0.267548
H	5.439792	-4.387765	1.923536
C	-0.388260	-1.801895	-3.232268
H	-0.872290	-2.739326	-3.550137
H	-0.731206	-1.589648	-2.208433
H	-0.779069	-1.000177	-3.877231
C	1.586964	-2.027586	-4.770530
H	2.682852	-2.080634	-4.850221
H	1.175665	-2.927233	-5.253437
H	1.255510	-1.163310	-5.365709
H	-0.367736	1.394806	-1.993883
H	-0.078222	2.089746	-4.356895
C	0.073804	2.368595	-2.224474
C	0.231857	2.761825	-3.552153
C	0.474271	3.214318	-1.182933
C	0.780589	4.009552	-3.853574
H	0.905552	4.316804	-4.894952
C	1.031480	4.459602	-1.492158
C	1.176638	4.859222	-2.820424
H	1.355050	5.119974	-0.681282
H	1.615422	5.833631	-3.049614
C	0.211473	-1.112499	3.325787
C	1.194065	-0.278863	3.498646
C	2.198522	0.580196	3.571493
H	0.046410	-1.917776	4.059437
H	2.116609	1.537994	4.098901
H	3.172410	0.346779	3.124094

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Scheme_S3_S.XI / electronic energy: -5734.37462512 a.u. / lowest freq: -291.98 cm-1

C	-0.800838	3.089093	1.200559
H	-1.361786	3.737658	0.515546
C	0.555852	2.688628	0.586270
H	1.366403	3.120064	1.193658
C	-0.651025	0.731388	1.099969
C	-2.806542	1.609044	1.763035
C	-3.011066	0.888333	2.946912
C	-3.919643	2.134099	1.079283
C	-4.294099	0.684790	3.446391
H	-2.137061	0.491746	3.472219
C	-5.202863	1.926424	1.591973
C	-5.394814	1.205818	2.767987
H	-4.429271	0.122203	4.372998
H	-6.055280	2.331421	1.042595
H	-6.405376	1.054629	3.153238
S	-3.781269	3.112458	-0.422772
O	-5.081090	2.958707	-1.137273
O	-2.684382	2.485457	-1.226424
O	-3.493597	4.489404	0.021732
Cu	-1.197662	-1.169605	1.406703
C	-0.740510	3.729114	2.565352
C	-1.621289	4.769867	2.879288
C	0.135016	3.253240	3.551497
C	-1.617353	5.337020	4.154472
H	-2.316245	5.124714	2.112115
C	0.137757	3.819574	4.824317
H	0.820885	2.429327	3.325465
C	-0.737810	4.864614	5.127882
H	-2.306151	6.152615	4.388149
H	0.826467	3.442762	5.584514
H	-0.733642	5.309266	6.126084
N	-1.477441	1.765623	1.292701
N	0.551619	1.218023	0.735984
C	-2.206932	-2.897487	0.733395
C	-2.858287	-3.588140	1.867413
C	-2.565301	-4.932975	2.158132
C	-3.755227	-2.918327	2.723100
C	-3.150909	-5.579357	3.246831
C	-4.337909	-3.561979	3.807396
C	-4.039920	-4.900770	4.077232
H	-2.905553	-6.625518	3.445458
H	-5.024878	-3.011478	4.455502
H	-4.493703	-5.405834	4.933058
C	-2.783175	-1.720426	0.185771
C	-2.250201	-1.010732	-0.916301
H	-2.599285	0.013891	-1.081170
H	-1.231419	-1.197607	-1.253666
H	-3.979753	-1.862751	2.554024
H	-3.724414	-1.343524	0.600770
P	-3.607485	-0.850655	-3.475448
O	-4.866395	-0.103319	-2.709886
O	-2.852346	0.311636	-4.057083
O	-4.305492	-1.817818	-4.567918
O	-2.957354	-1.840816	-2.495649
Na	-3.978301	2.055399	-3.084414
C	-1.183902	-3.667108	-0.050071
H	-1.876345	-5.493553	1.523284
C	-5.853396	-0.862902	-2.027116
H	-6.272958	-0.236771	-1.229500
H	-6.664595	-1.155659	-2.710821
H	-5.422921	-1.771175	-1.580290
C	-4.910697	-1.227227	-5.711189
H	-5.353618	-2.037634	-6.301061
H	-5.710322	-0.523762	-5.430252
H	-4.172111	-0.698677	-6.330889
C	1.665344	0.454173	0.330697
C	2.933535	1.047638	0.292234
C	1.520671	-0.873314	-0.081837
C	4.046068	0.324571	-0.147803
C	2.621439	-1.614943	-0.514806
C	3.881982	-1.009879	-0.542306
H	4.747839	-1.573705	-0.904017
H	0.536244	-1.344471	-0.088600
H	3.068391	2.086985	0.599270
C	2.404313	-3.008648	-1.000988
C	2.490505	-4.093796	-0.096847
C	2.055868	-3.220179	-2.352631
C	2.238438	-5.385022	-0.572806
C	1.801733	-4.529846	-2.783606
C	1.893841	-5.603749	-1.905144
H	2.301130	-6.234896	0.112033
H	1.520658	-4.706802	-3.826235
H	1.691618	-6.618674	-2.257633

C	5.388864	0.973248	-0.192270
C	5.690706	1.906296	-1.217505
C	6.343657	0.663875	0.802333
C	6.955996	2.504130	-1.224324
C	7.595214	1.293586	0.756238
C	7.902223	2.203251	-0.247216
H	7.211366	3.221460	-2.007099
H	8.336596	1.072892	1.529318
H	8.882566	2.686382	-0.269572
C	6.036926	-0.274753	1.956407
H	5.113205	-0.824210	1.713956
C	5.767021	0.517234	3.232640
H	4.932892	1.224283	3.106629
H	5.513444	-0.150279	4.070408
H	6.650289	1.102063	3.535396
C	7.131514	-1.311676	2.172223
H	7.341317	-1.884582	1.256312
H	8.078770	-0.855060	2.497623
H	6.841623	-2.028963	2.954147
C	4.687218	2.216347	-2.318535
H	3.688301	2.271886	-1.849078
C	4.634371	1.087668	-3.346831
H	3.852008	1.276475	-4.097935
H	5.592679	0.994986	-3.882510
H	4.422490	0.112693	-2.885345
C	4.931450	3.547336	-3.012269
H	4.118447	3.765969	-3.719036
H	4.986947	4.385438	-2.301484
H	5.863132	3.546420	-3.598479
C	1.921024	-2.077641	-3.346081
H	2.223238	-1.144722	-2.841031
C	2.866212	-3.861224	1.355009
H	2.523280	-2.844806	1.613146
C	2.189757	-4.816830	2.326395
H	1.098180	-4.846313	2.188561
H	2.565469	-5.847402	2.231323
H	2.380457	-4.506053	3.364414
C	4.381012	-3.891727	1.539954
H	4.788324	-4.888998	1.307986
H	4.891567	-3.171240	0.884289
H	4.657239	-3.655898	2.579445
C	0.472383	-1.899713	-3.788353
H	0.090491	-2.792528	-4.308838
H	-0.201180	-1.715549	-2.938180
H	0.364529	-1.048685	-4.477944
C	2.847128	-2.261926	-4.542494
H	3.898929	-2.361463	-4.234633
H	2.589551	-3.159790	-5.125500
H	2.781697	-1.404894	-5.229126
H	-0.132738	1.331928	-1.723754
H	0.187502	2.085152	-4.059114
C	0.339197	2.299084	-1.919590
C	0.512965	2.725628	-3.235409
C	0.752162	3.106694	-0.853217
C	1.094429	3.966116	-3.501412
H	1.231906	4.297442	-4.533840
C	1.344177	4.344636	-1.128493
C	1.508096	4.776663	-2.443853
H	1.679415	4.975833	-0.299496
H	1.974935	5.744539	-2.643546
C	-0.176345	-1.964761	2.922219
C	0.935994	-1.444306	3.351414
C	2.081476	-0.875397	3.696934
H	-0.711898	-3.075960	-0.844653
H	-1.659414	-4.528020	-0.550759
H	-0.386997	-4.070280	0.590276
H	-0.561929	-2.882581	3.398006
H	3.028992	-1.168365	3.225852
H	2.140621	-0.110607	4.480392

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Scheme_S3_S.XII / electronic energy: -5734.37170022 a.u. / lowest freq: -269.37 cm-1

C	0.646695	-3.374360	0.938189
H	1.200408	-4.034714	0.258840
C	-0.703543	-2.947346	0.329203
H	-1.526410	-3.365717	0.930134
C	0.538043	-1.012092	0.876099
C	2.680086	-1.958052	1.521815
C	2.866436	-1.480242	2.823019
C	3.799339	-2.328982	0.754140
C	4.146242	-1.375825	3.364906
H	1.984627	-1.202637	3.408141
C	5.075155	-2.236925	1.311443
C	5.251766	-1.763690	2.611070

H	4.273535	-0.999464	4.382444
H	5.930868	-2.531309	0.701643
H	6.258084	-1.695581	3.030783
S	3.654781	-2.844702	-0.965965
O	5.057752	-2.925400	-1.472857
O	2.941337	-1.720420	-1.649955
O	2.939501	-4.132063	-0.973405
Cu	0.954673	0.818830	1.583626
C	0.584883	-3.978222	2.316932
C	1.444423	-5.026945	2.659669
C	-0.255152	-3.435953	3.298611
C	1.459314	-5.531412	3.960751
H	2.111439	-5.443010	1.898103
C	-0.239433	-3.936443	4.598133
H	-0.918485	-2.602427	3.044993
C	0.619014	-4.986908	4.931657
H	2.132626	-6.352850	4.217594
H	-0.897887	-3.502768	5.355361
H	0.632309	-5.380217	5.951050
N	1.358719	-2.061740	1.010421
N	-0.667885	-1.475601	0.493399
C	2.028715	2.637124	1.787132
C	1.210977	3.836580	2.090072
C	0.875588	4.165195	3.418216
C	0.809643	4.729486	1.077827
C	0.167250	5.325026	3.718610
C	0.119357	5.900520	1.382151
C	-0.209633	6.204946	2.702896
H	-0.084448	5.548030	4.758340
H	-0.152809	6.586755	0.576301
H	-0.751103	7.124062	2.940003
C	2.087275	2.144511	0.456960
C	3.011209	1.191556	-0.012521
H	2.811460	0.691001	-0.962042
H	3.627418	0.619965	0.684444
H	1.076403	4.533512	0.036857
H	1.412656	2.576908	-0.289469
P	5.233256	1.662432	-1.858555
O	6.107777	0.342504	-1.382266
O	4.477015	1.139607	-3.048880
O	6.351424	2.777308	-2.216468
O	4.519906	2.255194	-0.636435
Na	4.836078	-1.094252	-2.891087
C	3.109664	2.295280	2.772757
H	1.169669	3.502091	4.234188
C	6.968047	0.440226	-0.258115
H	7.431217	-0.541090	-0.102254
H	7.766022	1.179793	-0.429451
H	6.415042	0.729655	0.649246
C	7.184046	2.571553	-3.349739
H	7.916274	3.386990	-3.369497
H	7.728383	1.615996	-3.287757
H	6.604923	2.590821	-4.284573
C	-1.730891	-0.670298	0.038058
C	-3.033597	-1.180446	-0.013765
C	-1.481733	0.624953	-0.416154
C	-4.075508	-0.398062	-0.521846
C	-2.511131	1.426063	-0.912708
C	-3.806266	0.903315	-0.964733
H	-4.620393	1.508250	-1.375170
H	-0.460400	1.009089	-0.423872
H	-3.246560	-2.192307	0.339383
C	-2.173123	2.785529	-1.412837
C	-2.642037	3.934482	-0.725531
C	-1.348178	2.909889	-2.555078
C	-2.252553	5.193555	-1.194086
C	-0.971023	4.193966	-2.973988
C	-1.415268	5.325386	-2.300821
H	-2.600101	6.093078	-0.681556
H	-0.326293	4.305490	-3.850624
H	-1.115076	6.319817	-2.642179
C	-5.470227	-0.921455	-0.572671
C	-5.852889	-1.835473	-1.586484
C	-6.403087	-0.482025	0.391655
C	-7.177814	-2.284983	-1.612406
C	-7.719006	-0.960701	0.325511
C	-8.106038	-1.851806	-0.667334
H	-7.496429	-2.986864	-2.386245
H	-8.447868	-0.630331	1.071826
H	-9.135827	-2.216574	-0.706691
C	-6.025486	0.466476	1.516567
H	-4.961259	0.730487	1.402668
C	-6.178616	-0.207397	2.876004

H	-5.572496	-1.123379	2.946499
H	-5.864397	0.463609	3.689766
H	-7.224664	-0.489090	3.074920
C	-6.821608	1.764960	1.451480
H	-6.705302	2.271654	0.481316
H	-7.898995	1.591599	1.601529
H	-6.496120	2.466076	2.235006
C	-4.864986	-2.273270	-2.656735
H	-3.880193	-2.385585	-2.168506
C	-4.707411	-1.199846	-3.732439
H	-3.936296	-1.488667	-4.463570
H	-5.649442	-1.050456	-4.283808
H	-4.414118	-0.226306	-3.313559
C	-5.207704	-3.609145	-3.296930
H	-4.411163	-3.917564	-3.988902
H	-5.331148	-4.410833	-2.553275
H	-6.133714	-3.560719	-3.890071
C	-0.877664	1.707106	-3.361089
H	-1.432989	0.821549	-3.010588
C	-3.507332	3.800399	0.519490
H	-4.253503	3.014916	0.311086
C	-2.692297	3.328719	1.723151
H	-2.139078	2.398885	1.524110
H	-1.955172	4.089541	2.023571
H	-3.346268	3.145933	2.590588
C	-4.278443	5.062317	0.871364
H	-3.615173	5.873253	1.211345
H	-4.865602	5.446237	0.024021
H	-4.978714	4.865161	1.695678
C	0.606825	1.424250	-3.144878
H	1.231849	2.288971	-3.420624
H	0.830146	1.181591	-2.095286
H	0.941870	0.570611	-3.754237
C	-1.189455	1.860080	-4.845915
H	-2.255029	2.069878	-5.021663
H	-0.610743	2.671381	-5.313297
H	-0.942271	0.936374	-5.390502
H	0.378224	-1.788923	-1.909313
H	0.044132	-2.458435	-4.271063
C	-0.271062	-2.636435	-2.146414
C	-0.450104	-3.020553	-3.473992
C	-0.900384	-3.344085	-1.114741
C	-1.247881	-4.123462	-3.785153
H	-1.386790	-4.424250	-4.826736
C	-1.703698	-4.443843	-1.433364
C	-1.869653	-4.837956	-2.761102
H	-2.205860	-4.993694	-0.631109
H	-2.499079	-5.699648	-2.997272
C	0.018303	0.838490	3.338895
C	-1.178897	0.356625	3.496324
C	-2.406717	-0.135542	3.557086
H	3.656700	1.381521	2.511880
H	2.727110	2.164597	3.794208
H	3.848148	3.113975	2.814698
H	0.537553	1.289976	4.199686
H	-2.605347	-1.178747	3.832398
H	-3.283927	0.491781	3.360442

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Scheme_S3_S.XIII / electronic energy: -6103.58659718 a.u. / lowest freq: -223.58 cm-1

C	-0.740234	3.160606	-0.593492
H	-1.380733	3.301123	-1.474989
C	0.563083	2.427415	-1.017295
H	1.443918	3.005993	-0.690499
C	-0.640474	1.053308	0.470553
C	-2.603710	2.357088	0.974561
C	-2.593901	2.340005	2.375115
C	-3.826331	2.520427	0.299729
C	-3.774592	2.478545	3.099062
H	-1.635242	2.215628	2.886058
C	-5.005107	2.670599	1.034828
C	-4.984070	2.650657	2.427039
H	-3.744814	2.457205	4.190900
H	-5.945568	2.786132	0.492520
H	-5.915775	2.764953	2.985613
S	-3.948462	2.541921	-1.490955
O	-5.366643	2.193870	-1.808187
O	-3.046456	1.448988	-1.974766
O	-3.550483	3.897442	-1.908525
Cu	-1.366930	-0.457765	1.537458
C	-0.536357	4.494218	0.073402
C	-0.807299	5.668746	-0.636961
C	-0.060844	4.585130	1.388248
C	-0.591496	6.915616	-0.049898

H	-1.198403	5.597731	-1.655744
C	0.147993	5.831215	1.976960
H	0.143591	3.669547	1.954822
C	-0.114919	6.999062	1.257986
H	-0.806187	7.826157	-0.614555
H	0.514471	5.894176	3.004345
H	0.047014	7.974935	1.722241
N	-1.365823	2.162327	0.299894
N	0.497232	1.171180	-0.242578
C	-2.581366	-2.098265	1.698357
C	-3.397952	-2.076156	2.909317
C	-3.021744	-2.875534	4.005815
C	-4.527762	-1.246562	3.051343
C	-3.738152	-2.841107	5.198729
C	-5.239718	-1.211229	4.245927
C	-4.849064	-2.005651	5.326999
H	-3.426610	-3.470081	6.036234
H	-6.109855	-0.555243	4.334909
H	-5.409756	-1.974024	6.264076
C	-2.886529	-1.416251	0.491997
C	-2.176485	-1.627553	-0.706873
H	-2.242589	-0.871267	-1.492413
H	-1.254362	-2.212292	-0.688799
H	-4.849109	-0.612239	2.220772
H	-3.743806	-0.733941	0.450924
P	-4.103239	-2.486410	-2.706960
O	-5.251456	-1.635659	-1.871433
O	-3.722125	-1.525893	-3.799406
O	-4.875670	-3.810526	-3.224796
O	-3.070562	-3.038937	-1.714494
Na	-4.764500	0.373011	-3.140197
H	-1.844852	-2.912690	1.637404
H	-2.148740	-3.528151	3.909753
C	-5.949449	-2.244991	-0.794018
H	-6.375461	-1.448474	-0.171148
H	-6.769577	-2.879208	-1.164117
H	-5.279473	-2.862899	-0.176569
C	-5.807032	-3.682294	-4.291456
H	-6.245430	-4.672263	-4.461847
H	-6.618796	-2.980465	-4.043156
H	-5.317476	-3.345732	-5.216641
C	1.526108	0.208279	-0.299157
C	2.741359	0.504214	-0.934216
C	1.355755	-1.060450	0.262918
C	3.762877	-0.449091	-1.002623
C	2.372331	-2.017350	0.233714
C	3.578148	-1.703485	-0.400955
H	4.379921	-2.446651	-0.455018
H	0.412207	-1.335495	0.737112
H	2.909015	1.482555	-1.387868
C	2.090280	-3.343137	0.864043
C	2.336749	-3.529553	2.244909
C	1.493841	-4.369647	0.095337
C	1.976462	-4.747751	2.834387
C	1.153400	-5.573260	0.726690
C	1.386440	-5.761480	2.084976
H	2.160527	-4.905764	3.900081
H	0.693479	-6.375707	0.144120
H	1.108085	-6.704331	2.563079
C	5.030026	-0.141923	-1.729255
C	5.026377	-0.035943	-3.147664
C	6.229727	0.033741	-1.004351
C	6.237065	0.223760	-3.799236
C	7.416684	0.292587	-1.705039
C	7.425171	0.383123	-3.089281
H	6.259297	0.302266	-4.887632
H	8.347481	0.433220	-1.147604
H	8.357782	0.584174	-3.622966
C	6.293666	-0.001621	0.513040
H	5.279827	-0.198567	0.900997
C	6.739732	1.346658	1.070507
H	6.103892	2.169462	0.712428
H	6.706675	1.351642	2.170259
H	7.774994	1.583218	0.778424
C	7.202840	-1.120941	1.008071
H	6.887974	-2.105983	0.632211
H	8.244444	-0.967335	0.685099
H	7.211431	-1.169043	2.107377
C	3.754241	-0.243412	-3.959768
H	2.949983	0.333704	-3.467789
C	3.318789	-1.707173	-3.955099
H	2.374004	-1.838330	-4.505293
H	4.073818	-2.348200	-4.438119

H	3.162138	-2.094372	-2.939682
C	3.850623	0.260613	-5.391103
H	2.875564	0.171142	-5.890484
H	4.156788	1.315540	-5.448602
H	4.563825	-0.326537	-5.990204
C	1.273279	-4.214541	-1.398884
H	1.203898	-3.134017	-1.617380
C	3.045408	-2.467811	3.066041
H	2.802502	-1.483842	2.625358
C	2.622052	-2.428623	4.526762
H	1.530399	-2.372774	4.648779
H	2.972158	-3.311039	5.084408
H	3.053005	-1.548715	5.026094
C	4.556295	-2.658694	2.956461
H	4.856806	-3.645837	3.343139
H	4.903019	-2.596806	1.914750
H	5.099223	-1.899401	3.539600
C	-0.011573	-4.863440	-1.895323
H	0.046478	-5.962646	-1.880697
H	-0.889988	-4.570912	-1.302933
H	-0.213720	-4.572741	-2.936876
C	2.478723	-4.757703	-2.163342
H	3.414941	-4.262073	-1.866195
H	2.606904	-5.835755	-1.975696
H	2.358242	-4.623122	-3.248848
H	-0.505901	0.364903	-2.483664
H	-0.497890	0.104388	-4.947871
C	0.001235	1.106078	-3.106843
C	0.001936	0.963966	-4.493457
C	0.633019	2.201594	-2.507971
C	0.632976	1.915959	-5.295882
H	0.631566	1.804807	-6.383023
C	1.278528	3.143462	-3.316656
C	1.274956	3.004314	-4.704330
H	1.782651	3.996496	-2.851378
H	1.780479	3.747500	-5.326064
C	-0.640643	-0.470020	3.434293
H	-0.408345	-1.519727	3.680068
H	-1.497378	-0.140895	4.047999
C	0.484980	0.385156	3.521674
C	1.466945	1.136946	3.525382
Si	2.955814	2.202676	3.602610
C	3.336624	2.929753	1.913941
H	3.520002	2.140659	1.167332
H	2.517522	3.563152	1.539854
H	4.238361	3.561286	1.960103
C	2.649233	3.583911	4.835042
H	1.751532	4.169258	4.585629
H	2.507300	3.189437	5.852778
H	3.499666	4.283109	4.868031
C	4.423253	1.171626	4.154580
H	4.636237	0.367483	3.433176
H	5.328946	1.793374	4.236363
H	4.257760	0.706020	5.137953

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Scheme_S3_S.XIV / electronic energy: -6103.58384223 a.u. / lowest freq: -284.42 cm-1

C	-0.910201	-3.178462	-0.544848
H	-1.601095	-3.663911	0.155125
C	0.348689	-2.687235	0.202578
H	1.236436	-3.208238	-0.192055
C	-0.680469	-0.839298	-0.848941
C	-2.719332	-1.834892	-1.723317
C	-2.690609	-1.343030	-3.033529
C	-3.953602	-2.228801	-1.168841
C	-3.861375	-1.183869	-3.769281
H	-1.719525	-1.094862	-3.466125
C	-5.120847	-2.081732	-1.922535
C	-5.083934	-1.549661	-3.209279
H	-3.811571	-0.790282	-4.787100
H	-6.069014	-2.380321	-1.471522
H	-6.010303	-1.433674	-3.775934
S	-4.124830	-2.931576	0.479519
O	-5.556789	-2.747143	0.854278
O	-3.254741	-2.092234	1.361113
O	-3.712709	-4.342818	0.369074
Cu	-1.095422	0.960712	-1.674004
C	-0.651597	-4.105507	-1.705130
C	-1.222968	-5.381551	-1.725344
C	0.149214	-3.696851	-2.780504
C	-0.987763	-6.242727	-2.798837
H	-1.865176	-5.690489	-0.896156
C	0.380397	-4.554902	-3.852802
H	0.592538	-2.693894	-2.781704

C	-0.186805	-5.831794	-3.863324
H	-1.438992	-7.237971	-2.804607
H	1.004993	-4.225081	-4.686989
H	-0.006041	-6.503819	-4.705821
N	-1.493494	-1.895878	-1.008293
N	0.412783	-1.260092	-0.175183
C	-2.245151	2.679084	-1.854624
C	-1.633680	3.907862	-2.358728
C	-1.682092	4.184327	-3.739099
C	-1.012669	4.850816	-1.516697
C	-1.129979	5.350898	-4.259171
C	-0.471711	6.022545	-2.037873
C	-0.523068	6.278004	-3.409879
H	-1.180117	5.542499	-5.333803
H	-0.009831	6.747906	-1.363276
H	-0.097921	7.199561	-3.814512
C	-2.254695	2.272765	-0.503110
C	-3.129552	1.286846	-0.004009
H	-2.886547	0.786415	0.935552
H	-3.721453	0.697986	-0.711719
H	-0.968681	4.679713	-0.437662
H	-1.626092	2.801085	0.221680
P	-5.287415	1.615086	1.915102
O	-6.278088	0.401268	1.400183
O	-4.480211	0.939751	2.990154
O	-6.291220	2.765265	2.448534
O	-4.617982	2.268560	0.695856
Na	-5.016952	-1.252850	2.611295
H	-3.002972	2.230881	-2.513628
H	-2.166822	3.465118	-4.405640
C	-7.125052	0.585350	0.276457
H	-7.708243	-0.333464	0.144635
H	-7.819574	1.425162	0.434256
H	-6.544268	0.777720	-0.638381
C	-7.098171	2.494548	3.587715
H	-7.681682	3.398233	3.797106
H	-7.794911	1.662462	3.400642
H	-6.484716	2.255884	4.468846
C	1.450633	-0.444965	0.324169
C	2.627782	-1.030646	0.812008
C	1.290157	0.940712	0.426072
C	3.629673	-0.247109	1.398756
C	2.275775	1.734933	1.008056
C	3.446245	1.136605	1.487124
H	4.207057	1.754548	1.973087
H	0.361507	1.418278	0.110160
H	2.770595	-2.111520	0.762795
C	2.024071	3.192354	1.177701
C	2.532424	4.107744	0.228173
C	1.260292	3.632228	2.282240
C	2.260036	5.469396	0.401142
C	1.000384	5.003963	2.407119
C	1.496211	5.914411	1.478317
H	2.642930	6.193836	-0.322814
H	0.403680	5.365500	3.249234
H	1.286417	6.981257	1.594700
C	4.866920	-0.867777	1.960546
C	4.831871	-1.477355	3.240108
C	6.071701	-0.816467	1.223610
C	6.018026	-2.006252	3.762734
C	7.235611	-1.350924	1.793018
C	7.212850	-1.938454	3.051866
H	6.011504	-2.479904	4.746720
H	8.175238	-1.309203	1.236041
H	8.128870	-2.353190	3.480791
C	6.141981	-0.189075	-0.157924
H	5.116438	-0.168514	-0.568305
C	7.004347	-0.998895	-1.118384
H	6.720639	-2.061230	-1.135414
H	6.915701	-0.611817	-2.143083
H	8.072194	-0.948760	-0.856771
C	6.635452	1.253680	-0.087623
H	5.994701	1.883853	0.546234
H	7.654804	1.301793	0.327566
H	6.668073	1.711472	-1.088397
C	3.555061	-1.509401	4.064670
H	2.710709	-1.643111	3.364132
C	3.337962	-0.180162	4.786150
H	2.373611	-0.173402	5.317594
H	4.128467	-0.004576	5.533283
H	3.345168	0.676647	4.097170
C	3.503274	-2.657348	5.061317
H	2.516005	-2.703711	5.542383

H	3.687247	-3.632441	4.586251
H	4.239139	-2.537808	5.871327
C	0.705268	2.654453	3.307293
H	1.285456	1.719308	3.223498
C	3.279522	3.609150	-0.995960
H	3.769386	2.658692	-0.720055
C	2.289827	3.291013	-2.115231
H	1.500019	2.601734	-1.776714
H	1.795191	4.206697	-2.478505
H	2.791897	2.819022	-2.974158
C	4.366366	4.552953	-1.484643
H	3.953752	5.491141	-1.886314
H	5.077307	4.816578	-0.687372
H	4.939683	4.088242	-2.300426
C	-0.748967	2.297251	3.006332
H	-1.155627	1.609957	3.763912
H	-0.848654	1.800866	2.030032
H	-1.396428	3.189374	2.992958
C	0.860537	3.148197	4.739116
H	1.902692	3.412591	4.972649
H	0.239976	4.033180	4.946305
H	0.548475	2.370169	5.451273
H	-0.622102	-0.975154	2.144985
H	-0.837417	-1.424826	4.570614
C	-0.278070	-1.930395	2.550483
C	-0.406666	-2.186547	3.915015
C	0.269790	-2.894765	1.697828
C	0.003177	-3.412308	4.440861
H	-0.101585	-3.613958	5.509789
C	0.696042	-4.114677	2.235434
C	0.557148	-4.376123	3.597608
H	1.132470	-4.869997	1.574050
H	0.891130	-5.334331	4.003479
C	-0.215048	1.144757	-3.506802
H	0.047498	2.208944	-3.623871
H	-1.010112	0.901485	-4.232221
C	0.924019	0.312864	-3.632873
C	1.935629	-0.395520	-3.688649
Si	3.560228	-1.204485	-3.924416
C	3.886658	-2.466147	-2.573109
H	3.898690	-2.014858	-1.568399
H	3.117355	-3.254666	-2.571693
H	4.855485	-2.967361	-2.726564
C	4.848965	0.161476	-3.911090
H	4.612706	0.918919	-4.674769
H	5.854699	-0.225299	-4.137699
H	4.893857	0.679533	-2.940020
C	3.607660	-2.074294	-5.587790
H	2.853064	-2.871676	-5.660771
H	3.426987	-1.375253	-6.418473
H	4.591498	-2.540282	-5.756765

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Scheme_S3_XIVb / electronic energy: -6142.87107506 a.u. / lowest freq: -254.37 cm-1

C	0.671768	3.158881	0.873389
H	1.296098	3.242079	1.774049
C	-0.618393	2.362287	1.208886
H	-1.507650	2.955052	0.935444
C	0.634460	1.155328	-0.380831
C	2.577879	2.542938	-0.712503
C	2.586461	2.710030	-2.102802
C	3.786770	2.641943	-0.001592
C	3.770973	2.981970	-2.781030
H	1.638216	2.627736	-2.640735
C	4.970821	2.919155	-0.690124
C	4.966290	3.093099	-2.071792
H	3.756042	3.108710	-3.865996
H	5.901170	2.983135	-0.122316
H	5.900676	3.309293	-2.594605
S	3.879170	2.452506	1.781865
O	5.295691	2.078586	2.078404
O	2.978994	1.306902	2.124169
O	3.464877	3.749391	2.344495
Cu	1.425600	-0.228630	-1.568666
C	0.451489	4.537170	0.308683
C	0.712213	5.659489	1.101852
C	-0.023103	4.719637	-0.997259
C	0.487426	6.943798	0.605470
H	1.101702	5.519151	2.114168
C	-0.242314	6.002667	-1.494892
H	-0.218999	3.846380	-1.629679
C	0.010778	7.117783	-0.693416
H	0.695209	7.813000	1.234177
H	-0.609599	6.135008	-2.515492

H	-0.159071	8.123498	-1.085363
N	1.335181	2.252482	-0.085794
N	-0.523131	1.189359	0.310687
C	2.600670	-1.927176	-1.810820
C	3.599642	-1.713653	-2.881166
C	3.762375	-2.650740	-3.916925
C	4.414411	-0.562991	-2.908355
C	4.706505	-2.454724	-4.924813
C	5.352096	-0.366609	-3.914876
C	5.508117	-1.315377	-4.929945
H	4.814297	-3.204159	-5.712832
H	5.961998	0.540666	-3.913310
H	6.244357	-1.160206	-5.721967
C	2.825476	-1.338557	-0.528321
C	2.067700	-1.596271	0.632050
H	2.171703	-0.900189	1.467852
H	1.108739	-2.113956	0.578130
H	4.286410	0.209061	-2.143077
H	3.707985	-0.703316	-0.393048
P	3.895687	-2.700197	2.581594
O	5.117366	-1.884931	1.816607
O	3.547092	-1.772710	3.712366
O	4.565122	-4.098252	3.043557
O	2.855564	-3.130661	1.536723
Na	4.710846	0.093933	3.155939
C	1.664427	-3.093104	-1.945213
H	3.154159	-3.557072	-3.933218
C	5.801366	-2.493524	0.728479
H	6.251224	-1.700198	0.118693
H	6.601265	-3.157531	1.090060
H	5.114460	-3.080624	0.100076
C	5.462430	-4.096002	4.146900
H	5.822240	-5.123086	4.276290
H	6.330616	-3.443004	3.965416
H	4.962980	-3.773645	5.071764
C	-1.544216	0.217381	0.254962
C	-2.759205	0.448414	0.918618
C	-1.375612	-0.988958	-0.437376
C	-3.785497	-0.500516	0.894138
C	-2.394386	-1.945141	-0.483800
C	-3.599709	-1.691995	0.178274
H	-4.398089	-2.440607	0.162175
H	-0.438844	-1.218186	-0.953555
H	-2.923990	1.376872	1.467012
C	-2.130237	-3.232475	-1.195017
C	-2.330340	-3.324512	-2.592341
C	-1.620149	-4.333331	-0.469144
C	-2.013337	-4.524741	-3.240166
C	-1.320831	-5.516025	-1.158312
C	-1.510249	-5.612635	-2.532382
H	-2.165070	-4.610756	-4.319123
H	-0.928063	-6.374497	-0.606463
H	-1.267101	-6.541058	-3.055926
C	-5.056015	-0.260132	1.640175
C	-5.066458	-0.299551	3.061580
C	-6.247694	-0.006302	0.925300
C	-6.283989	-0.108307	3.724049
C	-7.442271	0.177628	1.636296
C	-7.465300	0.121940	3.022282
H	-6.316830	-0.140091	4.814560
H	-8.367325	0.373826	1.086122
H	-8.403668	0.266076	3.564201
C	-6.292641	0.119257	-0.587717
H	-5.269855	-0.014366	-0.979395
C	-6.760676	1.510114	-1.004658
H	-6.149572	2.301840	-0.547489
H	-6.707736	1.636002	-2.096328
H	-7.805829	1.692817	-0.709645
C	-7.170151	-0.959897	-1.211576
H	-6.837675	-1.971960	-0.936156
H	-8.218257	-0.863072	-0.887219
H	-7.164499	-0.893134	-2.310152
C	-3.800554	-0.580317	3.861136
H	-2.995075	0.044602	3.433777
C	-3.361234	-2.035650	3.718994
H	-2.416356	-2.217065	4.254744
H	-4.115940	-2.720265	4.138536
H	-3.203782	-2.323990	2.671289
C	-3.911376	-0.217314	5.333434
H	-2.941310	-0.353952	5.832026
H	-4.220101	0.826998	5.489516
H	-4.629601	-0.860502	5.865003
C	-1.422199	-4.280889	1.035363

H	-1.400026	-3.218711	1.336543
C	-2.954357	-2.184090	-3.375050
H	-2.701005	-1.240058	-2.859864
C	-2.447879	-2.069646	-4.805184
H	-1.348985	-2.057550	-4.859361
H	-2.801101	-2.896301	-5.440860
H	-2.809566	-1.139433	-5.266942
C	-4.474851	-2.324983	-3.351264
H	-4.787682	-3.286731	-3.788780
H	-4.872113	-2.287255	-2.326013
H	-4.961684	-1.527404	-3.932263
C	-0.108974	-4.906766	1.486735
H	-0.110901	-6.001459	1.370852
H	0.757124	-4.515109	0.934763
H	0.071280	-4.701922	2.552641
C	-2.604247	-4.935904	1.745462
H	-3.560706	-4.458117	1.485562
H	-2.685225	-5.999634	1.470018
H	-2.491583	-4.887876	2.839056
H	0.459639	0.170587	2.461493
H	0.467188	-0.331936	4.886373
C	-0.049891	0.841988	3.156192
C	-0.043362	0.563531	4.521788
C	-0.689599	1.986663	2.669264
C	-0.678106	1.427409	5.415506
H	-0.671966	1.210319	6.486498
C	-1.340042	2.839081	3.568190
C	-1.330953	2.563313	4.935290
H	-1.851360	3.730511	3.191255
H	-1.839987	3.237546	5.628595
C	0.770395	-0.032960	-3.486101
H	0.592731	-1.044629	-3.887905
H	1.617077	0.421405	-4.029292
C	-0.396328	0.771879	-3.487687
C	-1.414956	1.469969	-3.408371
Si	-2.943081	2.480418	-3.414377
C	-3.353846	3.107852	-1.692638
H	-3.512699	2.275022	-0.988959
H	-2.566483	3.754813	-1.276887
H	-4.280702	3.703349	-1.715950
C	-2.701329	3.938096	-4.571472
H	-1.836651	4.554693	-4.282509
H	-2.531995	3.607373	-5.607511
H	-3.586608	4.593587	-4.574904
C	-4.379761	1.425427	-4.001131
H	-4.584401	0.614607	-3.284798
H	-5.296144	2.030453	-4.089558
H	-4.193183	0.968751	-4.984826
H	0.843836	-3.069588	-1.216591
H	2.200025	-4.045441	-1.782365
H	1.211670	-3.146773	-2.944866

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Scheme_S3_XVb / electronic energy: -6142.86648284 a.u. / lowest freq: -294.57 cm-1

C	-0.846647	3.234821	-0.006945
H	-1.531683	3.482276	-0.829161
C	0.467670	2.650590	-0.584305
H	1.330151	3.188751	-0.156538
C	-0.616656	0.977179	0.685217
C	-2.566095	2.140071	1.531803
C	-2.440609	1.877010	2.901748
C	-3.837995	2.442625	1.007016
C	-3.552173	1.879489	3.739088
H	-1.441467	1.682170	3.298034
C	-4.946431	2.450610	1.858495
C	-4.811879	2.163734	3.214958
H	-3.427958	1.668301	4.803759
H	-5.925229	2.679214	1.432456
H	-5.692002	2.172464	3.861486
S	-4.122185	2.870516	-0.717983
O	-5.579203	2.654580	-0.956296
O	-3.325142	1.890600	-1.521929
O	-3.693994	4.273229	-0.861309
Cu	-1.043851	-0.715123	1.699365
C	-0.666150	4.453179	0.859790
C	-1.096457	5.700766	0.396081
C	-0.050087	4.366192	2.116169
C	-0.909002	6.846505	1.169416
H	-1.593385	5.763220	-0.574903
C	0.123663	5.509641	2.893947
H	0.291015	3.392349	2.488543
C	-0.302915	6.752602	2.421302
H	-1.248634	7.815518	0.795514
H	0.590255	5.434282	3.879082

H	-0.164831	7.647253	3.033366
N	-1.388914	2.073671	0.739250
N	0.458537	1.265952	-0.073614
C	-2.259435	-2.411124	2.048428
C	-1.595430	-3.616518	2.597096
C	-1.366470	-3.752946	3.980637
C	-1.218788	-4.691104	1.767295
C	-0.766813	-4.894332	4.505680
C	-0.634945	-5.839800	2.295894
C	-0.396755	-5.946186	3.666375
H	-0.592634	-4.964043	5.582256
H	-0.374896	-6.665279	1.628457
H	0.062051	-6.847542	4.079962
C	-2.176375	-2.137296	0.658473
C	-3.016567	-1.259880	-0.057453
H	-2.692217	-0.913639	-1.040800
H	-3.665669	-0.558851	0.472887
H	-1.417789	-4.649632	0.693752
H	-1.472655	-2.726612	0.061329
P	-5.277595	-1.784801	-1.816960
O	-6.196798	-0.563790	-1.192833
O	-4.662101	-1.140385	-3.028140
O	-6.331091	-2.965729	-2.149375
O	-4.422252	-2.385233	-0.689699
Na	-5.189588	1.044560	-2.631563
C	-3.375090	-1.813749	2.861783
H	-1.650898	-2.946795	4.659809
C	-6.840379	-0.714824	0.062302
H	-7.421523	0.195202	0.251518
H	-7.526784	-1.575885	0.058092
H	-6.112202	-0.853237	0.876571
C	-7.282455	-2.760648	-3.186186
H	-7.878068	-3.676779	-3.269039
H	-7.958638	-1.922744	-2.954696
H	-6.792593	-2.568294	-4.151871
C	1.471488	0.355561	-0.445588
C	2.751719	0.817167	-0.775122
C	1.181723	-1.005834	-0.559001
C	3.741622	-0.078766	-1.198525
C	2.159871	-1.916964	-0.956548
C	3.437245	-1.443457	-1.272657
H	4.198086	-2.145178	-1.626373
H	0.164581	-1.360625	-0.389593
H	2.987060	1.882238	-0.721739
C	1.805781	-3.357853	-1.088556
C	2.239148	-4.279701	-0.103157
C	1.028503	-3.783546	-2.188094
C	1.882863	-5.624555	-0.245845
C	0.680891	-5.139143	-2.279327
C	1.105893	-6.052491	-1.321494
H	2.208411	-6.352746	0.500815
H	0.072650	-5.482541	-3.121279
H	0.831585	-7.107186	-1.410838
C	5.097304	0.403245	-1.596429
C	5.267588	1.071426	-2.836827
C	6.206898	0.164013	-0.752486
C	6.552672	1.487883	-3.202958
C	7.475298	0.591367	-1.169739
C	7.650143	1.248030	-2.380889
H	6.704206	2.002790	-4.153862
H	8.342317	0.405176	-0.530703
H	8.646394	1.576670	-2.688241
C	6.080060	-0.561651	0.578188
H	5.016439	-0.542547	0.878879
C	6.882242	0.105771	1.689324
H	6.612141	1.163167	1.825243
H	6.717635	-0.408516	2.646664
H	7.965038	0.064061	1.498031
C	6.499202	-2.024541	0.446906
H	5.915856	-2.565443	-0.311965
H	7.559575	-2.105037	0.158825
H	6.379274	-2.556333	1.402900
C	4.104690	1.262882	-3.799355
H	3.204288	1.490472	-3.201127
C	3.820662	-0.030229	-4.562990
H	2.933749	0.077362	-5.206516
H	4.669936	-0.299992	-5.210954
H	3.640372	-0.881802	-3.890755
C	4.300213	2.414477	-4.773399
H	3.391252	2.566701	-5.372057
H	4.523102	3.362187	-4.260555
H	5.115893	2.222300	-5.486914
C	0.552953	-2.821052	-3.264448

H	1.070969	-1.859455	-3.112493
C	3.018000	-3.797299	1.109193
H	3.702884	-3.006479	0.758120
C	2.088012	-3.154296	2.138544
H	1.423986	-2.397973	1.690853
H	1.447085	-3.910834	2.619626
H	2.664269	-2.653550	2.932580
C	3.867993	-4.872233	1.766204
H	3.253080	-5.657061	2.234128
H	4.548904	-5.361413	1.053582
H	4.483150	-4.438267	2.567558
C	-0.943171	-2.552266	-3.133525
H	-1.293047	-1.833825	-3.890265
H	-1.193562	-2.139314	-2.145670
H	-1.535827	-3.472864	-3.258099
C	0.905718	-3.297113	-4.668383
H	1.982242	-3.496608	-4.776221
H	0.369641	-4.218457	-4.943383
H	0.635306	-2.534700	-5.414524
H	-0.487810	0.841021	-2.429879
H	-0.444176	1.045129	-4.897898
C	-0.026607	1.718747	-2.892655
C	-0.006094	1.834835	-4.281700
C	0.536767	2.718575	-2.089787
C	0.567492	2.955713	-4.883937
H	0.582915	3.046083	-5.972976
C	1.123605	3.832012	-2.701121
C	1.131092	3.954682	-4.090069
H	1.576097	4.611321	-2.079906
H	1.593137	4.829121	-4.555212
C	-0.136541	-0.708372	3.522152
H	0.195412	-1.743793	3.702888
H	-0.934294	-0.460672	4.244120
C	0.947684	0.201636	3.569939
C	1.904104	0.986145	3.559578
Si	3.413301	1.999226	3.774343
C	4.019605	2.657697	2.124160
H	4.278675	1.848014	1.425005
H	3.255479	3.285689	1.638592
H	4.916662	3.283261	2.258098
C	4.718372	0.908859	4.569286
H	4.425329	0.637287	5.595295
H	5.697377	1.409746	4.628862
H	4.851876	-0.031042	4.012985
C	3.038803	3.446625	4.906869
H	2.285691	4.120616	4.472501
H	2.659525	3.113847	5.884904
H	3.944495	4.045956	5.090657
H	-3.687446	-0.825013	2.499217
H	-3.111569	-1.699137	3.920883
H	-4.262328	-2.469540	2.823444

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Scheme_S4_XXII / electronic energy: -5523.50479848 a.u. / lowest freq: -321.98 cm-1

C	1.276246	-2.591188	0.106262
H	0.578327	-3.425104	0.253968
C	1.638707	-1.966847	1.478142
H	2.730742	-1.989342	1.618596
C	0.563966	-0.333990	0.145793
C	0.119796	-1.535287	-1.909944
C	0.622171	-0.588139	-2.813854
C	-0.815133	-2.484932	-2.367066
C	0.206584	-0.575997	-4.142428
H	1.359537	0.136392	-2.447423
C	-1.217050	-2.467675	-3.705323
C	-0.714652	-1.520295	-4.592489
H	0.613562	0.166205	-4.833691
H	-1.948752	-3.207116	-4.036202
H	-1.040515	-1.523348	-5.634766
C	1.222958	0.367481	2.383450
C	0.018843	0.964541	2.774912
C	2.422371	0.653037	3.060300
C	-0.046485	1.865617	3.839239
C	2.344355	1.535121	4.149673
C	1.149484	2.134310	4.524390
H	1.151335	2.833735	5.364530
S	-1.537095	-3.753619	-1.316119
O	-2.788713	-4.187362	-2.003762
O	-1.881743	-3.063649	-0.030700
O	-0.521821	-4.813162	-1.188736
Cu	-0.148231	1.437490	-0.480706
C	2.463215	-3.079535	-0.681709
C	2.723338	-4.452393	-0.753460
C	3.335492	-2.184434	-1.316221

C	3.842277	-4.925907	-1.437911
H	2.030929	-5.150012	-0.275524
C	4.448050	-2.660115	-2.008969
H	3.142292	-1.105749	-1.270332
C	4.705882	-4.030769	-2.068866
H	4.035159	-6.000486	-1.486093
H	5.120669	-1.956775	-2.506189
H	5.578596	-4.400505	-2.612830
N	0.570303	-1.473256	-0.567184
N	1.191836	-0.561413	1.308211
C	-1.999906	1.235475	-1.376674
Na	-4.162909	-3.416397	-0.250998
C	-1.585887	2.601250	-1.456333
C	-2.075752	3.689495	-0.575352
C	-1.018441	3.038734	-2.781787
C	-1.393970	4.924573	-0.536123
C	-3.265677	3.582906	0.170752
C	-2.584835	0.552879	-0.279147
C	-1.857288	5.983761	0.237545
H	-0.478646	5.056217	-1.117181
C	-3.728180	4.647390	0.943917
H	-3.865886	2.673814	0.113160
C	-3.027204	5.851060	0.988805
H	-1.300879	6.924440	0.250042
H	-4.658647	4.533027	1.506838
H	-3.392898	6.683820	1.594642
C	1.320529	2.772784	-0.095779
O	-5.123415	-1.621951	0.762798
H	-7.851016	-1.622735	0.300553
C	-7.806971	-1.092486	-0.661705
P	-5.238455	-0.654796	-0.380490
H	-8.739210	-0.533685	-0.800952
H	-7.715833	-1.831133	-1.473637
O	-4.815120	-1.577650	-1.675153
O	-6.741032	-0.150672	-0.691098
O	-4.436622	0.661911	-0.418528
C	-4.753500	-1.026957	-2.982769
H	-5.728335	-0.618646	-3.290282
H	-4.476905	-1.835865	-3.669029
H	-4.001487	-0.225965	-3.045502
H	-2.563596	1.002017	0.716311
H	-2.496268	-0.538795	-0.277864
C	0.984759	-2.625796	2.664490
C	1.753757	-3.359565	3.572822
C	-0.397698	-2.520419	2.869004
C	1.153406	-3.982178	4.668382
H	2.834034	-3.442125	3.417008
C	-0.996258	-3.135898	3.965447
H	-1.008292	-1.958607	2.156085
C	-0.221669	-3.868655	4.868187
H	1.764902	-4.553348	5.371233
H	-2.075048	-3.044923	4.116450
H	-0.692287	-4.349717	5.729155
H	-0.880735	0.682865	2.223508
H	3.264253	1.782393	4.686628
H	5.701994	2.077654	-1.291606
C	5.235786	2.831890	-1.940280
H	5.996238	3.172503	-2.657001
H	4.647741	4.138605	-4.672436
H	5.087735	0.385206	-2.960822
C	4.024571	2.232160	-2.637883
C	4.440670	1.075996	-3.520501
H	5.014933	1.430711	-4.389027
C	3.149088	3.317307	-3.344649
H	2.780140	2.368310	-5.277889
C	2.228474	2.722238	-4.395495
H	3.579555	0.502313	-3.889662
H	1.661305	1.877290	-3.981119
H	1.506479	3.479210	-4.732650
H	4.955222	3.686053	-1.307275
H	4.475126	5.031884	-3.141881
O	3.131065	1.747736	-1.611719
C	3.926368	4.482191	-3.916620
H	3.245329	5.191609	-4.407169
B	2.246195	2.782914	-1.303039
O	2.316897	3.787666	-2.259690
H	1.793020	2.359832	0.808950
H	0.858544	3.742518	0.144206
H	-1.862664	0.639640	-2.286242
H	-0.133967	3.681781	-2.678423
H	-1.766108	3.612355	-3.356319
H	-0.723706	2.174798	-3.394490
C	4.601297	-0.475545	3.564123

C	5.835909	-0.984327	3.163149
H	6.490853	-1.459051	3.898120
C	3.735535	0.122091	2.634692
C	6.231772	-0.894579	1.828032
H	7.197516	-1.296594	1.512281
C	5.388095	-0.281339	0.900375
C	4.151179	0.223104	1.296538
H	3.505671	0.709580	0.559040
H	5.694193	-0.194841	-0.146413
H	4.288694	-0.562146	4.608972
C	-1.345013	2.547948	4.264958
C	-1.210571	4.050347	3.991026
C	-1.586661	2.318080	5.760309
C	-2.546270	2.015205	3.491516
H	-0.780308	2.729792	6.383754
H	-1.674190	1.246273	5.994536
H	-2.521095	2.804946	6.077844
H	-0.383868	4.497823	4.562558
H	-2.132940	4.583688	4.269303
H	-1.020043	4.245156	2.923703
H	-2.459905	2.221040	2.414450
H	-3.468670	2.506586	3.834610
H	-2.681945	0.930340	3.622946

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Scheme_S4_XXIII / electronic energy: -5523.50179127 a.u. / lowest freq: -337.90 cm-1

C	0.023099	2.938392	-0.705289
H	0.818720	3.512655	-0.213263
C	-1.149682	2.697844	0.279447
H	-2.083356	3.073595	-0.168608
C	-0.248511	0.609486	-0.380374
C	1.531823	1.251944	-1.895563
C	1.232384	0.376424	-2.948300
C	2.841617	1.761951	-1.788385
C	2.202333	0.002083	-3.873151
H	0.212591	-0.006539	-3.028216
C	3.801953	1.395024	-2.735357
C	3.492762	0.518491	-3.771999
H	1.939977	-0.684650	-4.681299
H	4.812464	1.793717	-2.627364
H	4.261517	0.238098	-4.495681
S	3.380627	2.843925	-0.455667
O	4.865733	2.705550	-0.398730
O	2.773607	2.265748	0.786176
O	2.917463	4.201167	-0.792568
Cu	-0.208040	-1.362818	-0.715315
C	-0.386341	3.636040	-1.976165
C	0.069148	4.928091	-2.253455
C	-1.249353	3.006512	-2.883584
C	-0.339305	5.585535	-3.414939
H	0.758738	5.409601	-1.556086
C	-1.652842	3.660014	-4.045497
H	-1.605050	1.991127	-2.674105
C	-1.199181	4.953837	-4.312565
H	0.022077	6.595860	-3.622053
H	-2.324403	3.158478	-4.746940
H	-1.514436	5.467249	-5.224231
N	0.499125	1.555867	-0.971714
N	-1.203775	1.213611	0.343391
C	1.084230	-2.390513	0.511318
Na	4.795555	1.683684	1.730234
C	0.716156	-3.268761	-0.541233
C	1.536308	-3.476379	-1.761820
C	-0.269031	-4.353535	-0.220279
C	0.937559	-3.942556	-2.949383
C	2.933495	-3.300177	-1.761620
C	2.086836	-1.385721	0.519993
C	1.692197	-4.174878	-4.094860
H	-0.140373	-4.119188	-2.975831
C	3.688028	-3.534700	-2.910768
H	3.441678	-3.024183	-0.835540
C	3.073035	-3.962769	-4.086409
H	1.197911	-4.528859	-5.003124
H	4.772327	-3.393503	-2.877961
H	3.665081	-4.147428	-4.986109
C	-1.659237	-1.627419	-2.114429
O	4.342738	-0.234254	2.891779
H	6.188007	-1.978654	-0.449140
C	5.704131	-0.998409	-0.581996
P	4.672759	-1.279631	1.865014
H	4.805758	-1.122363	-1.205745
H	6.404425	-0.332003	-1.099659
O	5.790623	-2.349624	2.327603
O	5.384462	-0.403580	0.667908

O	3.588928	-2.189306	1.249112
C	6.942101	-1.889410	3.025037
H	7.524984	-2.773013	3.308372
H	6.668691	-1.336466	3.935254
H	7.568168	-1.245877	2.387290
H	1.992728	-0.594796	1.269046
H	2.545584	-1.062199	-0.419438
C	-0.991301	3.320240	1.641055
C	-1.852593	4.343276	2.048897
C	0.007109	2.876888	2.519015
C	-1.719377	4.919651	3.313241
H	-2.635760	4.688270	1.366300
C	0.135899	3.446434	3.783316
H	0.691043	2.084872	2.200432
C	-0.727384	4.469635	4.183480
H	-2.396857	5.720150	3.620392
H	0.916384	3.091481	4.461429
H	-0.625321	4.915472	5.175999
H	-1.890008	-0.609101	-2.470468
H	-1.174161	-2.185767	-2.930731
H	-4.498107	-6.043208	-1.330034
C	-5.078051	-5.109945	-1.364358
H	-6.009047	-5.278069	-0.803279
H	-6.811643	-3.006507	-1.930810
H	-3.075102	-5.208782	0.528213
C	-4.282907	-3.971731	-0.765129
C	-3.754208	-4.348654	0.610171
H	-4.564393	-4.629151	1.298364
C	-5.016662	-2.594694	-0.750553
H	-6.575735	-3.064329	0.673396
C	-5.794725	-2.305845	0.514350
H	-3.196015	-3.514506	1.063199
H	-5.151140	-2.285853	1.402761
H	-6.297030	-1.330246	0.440685
H	-5.338914	-4.920292	-2.413205
H	-5.367405	-2.628037	-2.902117
O	-3.144324	-3.692180	-1.612169
C	-5.902028	-2.390588	-1.971025
H	-6.213446	-1.337531	-2.023417
B	-2.886955	-2.327066	-1.536919
O	-3.913229	-1.673429	-0.863949
H	0.550292	-2.536470	1.457211
H	-0.853216	-4.108880	0.676361
H	0.258540	-5.304058	-0.029576
H	-0.983296	-4.537780	-1.032482
H	-5.060481	0.276017	2.687723
H	-3.853538	-1.159983	4.258001
C	-3.298618	-0.692802	3.441283
C	-1.918672	-0.913951	3.306979
C	-1.151270	-1.781444	4.306725
H	-6.298508	3.864499	-1.800605
C	-5.699057	3.234822	-1.138624
H	-6.520299	4.076752	0.674777
C	-5.824530	3.351228	0.245884
C	-4.804002	2.305688	-1.672677
C	-5.059087	2.545990	1.088057
C	-4.033096	1.506040	-0.832228
H	-5.149943	2.652795	2.173055
C	-4.145429	1.616916	0.563883
C	-3.353113	0.763779	1.474693
C	-3.984596	0.130566	2.557125
C	-1.972972	0.532934	1.327871
C	-1.284810	-0.288820	2.230435
H	-0.205279	-0.375364	2.098384
H	-4.709778	2.197764	-2.756653
H	-3.349560	0.766702	-1.253241
C	-1.667342	-1.540583	5.728539
C	0.346651	-1.469836	4.292163
C	-1.364909	-3.255229	3.940846
H	0.545685	-0.399432	4.459838
H	0.839547	-1.756263	3.351803
H	0.855931	-2.028482	5.090767
H	-1.582150	-0.482144	6.017834
H	-1.080629	-2.129561	6.448816
H	-2.716989	-1.838703	5.856334
H	-2.430337	-3.530136	3.973101
H	-0.829837	-3.914750	4.641556
H	-0.995135	-3.479390	2.928188

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Scheme_S5_XXIV / electronic energy: -4770.78820038 a.u. / lowest freq: -322.76 cm-1

C	-0.564695	3.197298	0.809182
H	0.336237	3.442984	1.384617
C	-1.710700	2.810413	1.756278

C	-1.308540	1.004504	0.325426
C	0.648703	1.697668	-0.893343
C	0.256028	1.324476	-2.184830
C	2.022587	1.772587	-0.593335
C	1.200981	1.045584	-3.166948
H	-0.814033	1.268054	-2.400782
C	2.965647	1.521897	-1.593766
C	2.559866	1.160530	-2.875822
H	0.871809	0.756722	-4.167791
H	4.027478	1.579726	-1.350002
H	3.309406	0.962556	-3.644865
C	-3.103271	0.675400	1.909909
C	-2.688135	-0.185702	2.944000
C	-4.439557	0.746683	1.478073
C	-3.659359	-0.997951	3.543651
C	-5.374130	-0.086691	2.104580
C	-4.987562	-0.950256	3.127243
H	-5.730091	-1.595522	3.603541
S	2.594448	2.120310	1.072683
O	4.023723	1.545049	1.078297
O	1.719737	1.384843	1.997288
O	2.669727	3.574242	1.235060
Cu	-1.562000	-0.757295	-0.522211
C	-0.850133	4.324156	-0.151818
C	-0.003709	5.436404	-0.191756
C	-1.938598	4.263518	-1.033427
C	-0.246313	6.479418	-1.086976
H	0.857667	5.474465	0.481029
C	-2.179452	5.302686	-1.929022
H	-2.597752	3.388410	-1.025546
C	-1.334746	6.415361	-1.955266
H	0.422354	7.343430	-1.108184
H	-3.029678	5.244608	-2.613015
H	-1.524657	7.229742	-2.658676
N	-0.358134	1.917793	0.072031
N	-2.123188	1.490203	1.264733
C	-0.344296	-2.192104	0.351868
H	-0.628212	-2.363876	1.395262
Al	4.747519	-0.118641	1.451605
C	-1.118158	-2.742806	-0.701782
C	-2.316250	-3.563623	-0.523900
H	-0.653003	-2.791359	-1.694753
C	-2.920754	-4.151174	-1.651197
C	-2.940756	-3.736679	0.725951
C	0.881184	-1.518038	0.110740
C	3.887046	-1.003861	2.970129
C	6.681127	0.124800	1.334343
H	7.222164	-0.836628	1.363719
H	7.090975	0.734197	2.157171
H	6.983341	0.624283	0.398010
H	4.297941	-2.017313	3.127869
H	2.800175	-1.126661	2.830080
H	4.017852	-0.466855	3.924839
C	-4.099722	-4.881637	-1.535728
H	-2.454424	-4.015897	-2.631553
C	-4.122016	-4.463990	0.838989
H	-2.503971	-3.288624	1.622593
C	-4.708962	-5.040956	-0.289615
H	-4.549874	-5.327713	-2.426199
H	-4.591146	-4.580938	1.819598
H	-5.637432	-5.609449	-0.197802
C	-3.062029	-0.729120	-1.795627
O	4.193741	-1.012193	-0.067371
H	5.106934	-3.007794	-2.903271
C	4.384798	-2.178470	-2.884322
P	3.572466	-2.372752	-0.388760
H	3.940179	-2.071128	-3.879485
H	4.912175	-1.250294	-2.622077
O	4.688305	-3.460197	-0.014078
O	3.321233	-2.452515	-1.972439
O	2.241418	-2.738939	0.275970
C	4.402126	-4.854862	-0.142944
H	3.716597	-5.186920	0.648170
H	5.353530	-5.387519	-0.043879
H	3.962871	-5.086018	-1.124171
H	1.253866	-0.828881	0.874417
H	1.090105	-1.214330	-0.920933
C	-1.263023	-0.224082	3.397043
C	-4.831666	1.670686	0.371776
H	-3.359120	-1.678293	4.345552
H	-6.417508	-0.053278	1.779538
H	-4.306946	1.420830	-0.564330
H	-4.579739	2.717242	0.601906

H	-5.909422	1.623366	0.172875
H	-0.551753	-0.244451	2.558451
H	-1.069707	-1.099463	4.030023
H	-1.001312	0.666267	3.991166
C	-3.147028	-0.377295	-3.090095
H	-3.995932	-1.143705	-1.358491
H	-2.259296	0.025679	-3.608306
C	-4.362560	-0.486705	-3.955335
H	-5.220847	-0.897805	-3.402983
H	-4.188917	-1.136481	-4.829865
H	-4.668323	0.489293	-4.368900
H	-2.550083	3.521262	1.721213
H	-1.376050	2.737610	2.802836

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Scheme_S5_XXV / electronic energy: -4770.78638982 a.u. / lowest freq: -290.46 cm-1

C	-2.554726	2.215080	0.805130
H	-1.881164	2.907032	1.331383
C	-3.270378	1.291000	1.802294
C	-1.919247	-0.039769	0.427659
C	-0.874454	1.585256	-1.024813
C	-1.178845	1.126504	-2.311780
C	0.283269	2.359588	-0.830513
C	-0.372625	1.461912	-3.395918
H	-2.073134	0.512121	-2.445749
C	1.069987	2.720087	-1.927800
C	0.742593	2.276953	-3.206683
H	-0.624147	1.092522	-4.392535
H	1.959244	3.332132	-1.769671
H	1.372828	2.558271	-4.053440
C	-3.200918	-1.237643	2.112205
C	-2.533828	-1.601419	3.296129
C	-4.245467	-2.011323	1.568765
C	-2.918130	-2.796277	3.920877
C	-4.595468	-3.194443	2.228750
C	-3.934004	-3.586161	3.391580
H	-4.215285	-4.516610	3.890981
S	0.794048	2.875530	0.810771
O	2.306556	3.091915	0.648652
O	0.509873	1.773705	1.737955
O	0.156723	4.164472	1.092048
Cu	-0.887331	-1.519035	-0.406063
C	-3.440526	3.002775	-0.126548
C	-3.205290	4.364603	-0.338600
C	-4.468440	2.369582	-0.838377
C	-3.993886	5.087310	-1.235679
H	-2.390820	4.856301	0.201553
C	-5.254075	3.088916	-1.735439
H	-4.648067	1.298886	-0.693236
C	-5.019572	4.451812	-1.933868
H	-3.802350	6.151830	-1.391123
H	-6.052891	2.584910	-2.285011
H	-5.636561	5.016342	-2.637262
N	-1.734758	1.230786	0.041032
N	-2.802942	-0.049919	1.427306
C	1.116914	-1.259753	0.039958
H	1.451290	-0.300235	-0.374544
Al	3.937256	2.224420	0.567078
C	0.907506	-2.376146	-0.816857
C	1.270584	-2.406313	-2.235945
H	0.809621	-3.358934	-0.337172
C	1.807606	-1.288373	-2.900913
C	1.105919	-3.595467	-2.972110
C	1.105345	-1.372306	1.451496
C	5.159859	3.313779	1.637797
C	4.350142	1.814563	-1.305308
H	3.619925	1.135867	-1.778123
H	5.330025	1.314311	-1.399518
H	4.406859	2.714705	-1.941879
H	6.216025	3.009925	1.540570
H	4.920984	3.284657	2.714742
H	5.121463	4.376982	1.344422
C	2.165098	-1.358045	-4.244824
H	1.955266	-0.350307	-2.360129
C	1.461764	-3.663380	-4.315480
H	0.689019	-4.474195	-2.471383
C	1.994643	-2.544531	-4.960510
H	2.585745	-0.475845	-4.735866
H	1.325317	-4.598399	-4.864746
H	2.277638	-2.598398	-6.014474
C	-2.040917	-2.749023	-1.412844
O	3.614072	0.650268	1.456681
H	6.257507	0.597317	2.779073
C	6.372552	-0.363958	2.259294

P	3.909318	-0.849096	1.511405
H	7.200654	-0.917982	2.713967
H	6.609924	-0.183465	1.199381
O	4.293436	-1.243018	-0.002190
O	5.197305	-1.161940	2.412205
O	2.812657	-1.748446	2.087029
C	4.581894	-2.599544	-0.332349
H	5.492437	-2.945953	0.179107
H	4.743777	-2.642081	-1.415065
H	3.746775	-3.263650	-0.065369
H	0.682716	-2.276015	1.897792
H	0.987662	-0.455009	2.030106
C	-4.960761	-1.574465	0.331110
C	-1.469504	-0.739651	3.897255
C	-2.445097	-3.949582	-0.964705
H	-2.444060	-2.435236	-2.396686
H	-2.072166	-4.315838	0.009026
C	-3.408346	-4.876117	-1.635901
H	-3.753276	-4.481650	-2.603505
H	-4.301606	-5.057130	-1.012893
H	-2.969913	-5.871857	-1.818537
H	-2.404514	-3.103375	4.836078
H	-5.396624	-3.814821	1.817466
H	-5.654914	-2.347530	-0.022104
H	-4.263345	-1.349176	-0.489702
H	-5.550478	-0.660489	0.506276
H	-0.985592	-0.080389	3.165187
H	-0.691883	-1.342554	4.385029
H	-1.887841	-0.086791	4.680228
H	-2.998972	1.512922	2.845246
H	-4.367487	1.351471	1.725883

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Scheme_S5_XXVI / electronic energy: -5040.93702353 a.u. / lowest freq: -360.75 cm-1

C	1.486936	-2.572529	-0.570652
H	0.758850	-3.202967	-0.042678
C	2.598215	-2.105281	0.393586
H	3.587210	-2.235022	-0.081630
C	1.361244	-0.220909	-0.318705
C	-0.265426	-1.172877	-1.815835
C	-0.092157	-0.467185	-3.010590
C	-1.539391	-1.678199	-1.496246
C	-1.158099	-0.282107	-3.887100
H	0.900128	-0.066837	-3.234187
C	-2.601505	-1.506833	-2.386792
C	-2.409851	-0.815349	-3.581515
H	-1.005335	0.271544	-4.816213
H	-3.587843	-1.888713	-2.119724
H	-3.247657	-0.684448	-4.269764
C	3.161701	0.254298	1.238484
C	2.755137	0.646236	2.528528
C	4.352472	0.731605	0.651571
C	3.559890	1.567714	3.214618
C	5.123180	1.646143	1.377750
C	4.728273	2.064702	2.646914
H	5.338100	2.785923	3.196976
S	-1.838803	-2.437851	0.100443
O	-3.366269	-2.303766	0.241893
O	-1.147300	-1.609833	1.103090
O	-1.459435	-3.852239	0.030284
Cu	0.884544	1.660123	-0.696185
C	1.964280	-3.320826	-1.787687
C	1.483026	-4.605151	-2.057613
C	2.871733	-2.729509	-2.677126
C	1.911641	-5.296279	-3.192059
H	0.763061	-5.061204	-1.372096
C	3.296621	-3.416666	-3.811395
H	3.239106	-1.716723	-2.479061
C	2.818571	-4.703998	-4.069567
H	1.531374	-6.300966	-3.391913
H	4.002804	-2.946816	-4.500220
H	3.152235	-5.243285	-4.959429
N	0.840720	-1.289246	-0.941146
N	2.340588	-0.639969	0.485488
C	-0.812118	2.386233	0.282818
C	-0.824683	2.429418	1.783239
Al	-4.364495	-1.619792	1.659141
C	-0.192718	3.367050	-0.554732
C	0.582192	4.528998	-0.084528
H	-0.638282	3.489845	-1.550736
C	0.305742	5.806486	-0.598818
C	1.637294	4.404102	0.838715
C	-1.721099	1.473088	-0.338139
C	-3.492539	-1.997444	3.368482

C	-6.202736	-2.172828	1.281177
H	-6.945247	-1.695748	1.943414
H	-6.335481	-3.260105	1.415617
H	-6.510792	-1.949252	0.245879
H	-2.983647	-2.976865	3.365575
H	-4.192194	-2.014668	4.221187
H	-2.717063	-1.250323	3.606917
C	1.036179	6.920695	-0.186794
H	-0.496594	5.922927	-1.332994
C	2.367070	5.514746	1.250041
H	1.912316	3.407736	1.201159
C	2.065943	6.781585	0.743202
H	0.800250	7.904835	-0.599772
H	3.188080	5.390191	1.961083
H	2.642721	7.653136	1.062036
C	2.321174	2.394418	-1.839535
O	-4.181977	0.191704	1.339437
H	-6.238376	1.745096	-2.042661
C	-5.418930	1.027233	-2.195335
P	-4.511853	1.225138	0.261202
H	-4.553336	1.557495	-2.617890
H	-5.752492	0.256734	-2.898616
O	-5.678432	2.214243	0.728011
O	-5.078005	0.366489	-0.977244
O	-3.375936	2.165827	-0.164005
C	-6.901587	1.683294	1.243996
H	-7.583057	2.529615	1.377964
H	-6.739790	1.198101	2.216762
H	-7.357259	0.965716	0.546172
H	-1.888423	0.523717	0.178263
H	-1.718558	1.407187	-1.430894
C	2.648536	-2.759286	1.753193
C	3.879072	-2.803121	2.422275
C	1.511122	-3.260231	2.399635
C	3.975383	-3.329153	3.709438
H	4.772890	-2.415133	1.923081
C	1.609648	-3.800125	3.681490
H	0.531211	-3.211971	1.918189
C	2.838465	-3.833757	4.341427
H	4.943100	-3.353362	4.216354
H	0.714029	-4.190758	4.170861
H	2.910543	-4.255016	5.347200
C	1.537278	0.088439	3.193208
C	4.785072	0.273146	-0.703573
H	3.255106	1.891165	4.213915
H	6.041688	2.037287	0.931637
H	3.950030	0.256782	-1.418808
H	5.203360	-0.746688	-0.675932
H	5.564605	0.926985	-1.115710
H	0.799484	-0.315442	2.488164
H	1.044366	0.845172	3.818401
H	1.814255	-0.735205	3.871314
C	2.408316	2.519007	-3.175442
H	3.200796	2.772110	-1.276982
H	1.569282	2.183257	-3.810937
C	3.566005	3.079785	-3.940024
H	4.384635	3.390415	-3.273156
H	3.280160	3.957537	-4.544439
H	3.981056	2.351233	-4.657412
H	-1.034458	1.435552	2.204336
H	-1.629942	3.098548	2.130889
H	0.106517	2.796375	2.229893

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Scheme_S5_XXVII / electronic energy: -5040.93573303 a.u. / lowest freq: -374.19 cm-1

C	2.792470	-0.771383	-0.990651
H	2.433885	-1.787800	-1.211583
C	3.250414	-0.666741	0.476236
H	4.170183	-0.056663	0.532006
C	1.297024	0.634569	0.193166
C	0.827111	0.338688	-2.160569
C	0.806362	1.592906	-2.779239
C	0.022348	-0.692547	-2.675520
C	0.025317	1.813098	-3.910413
H	1.421638	2.389634	-2.352777
C	-0.736288	-0.476768	-3.828639
C	-0.730664	0.770473	-4.447317
H	0.018360	2.798963	-4.380611
H	-1.361543	-1.282227	-4.217518
H	-1.332237	0.930564	-5.344382
C	2.191291	0.552210	2.457263
C	1.484620	-0.189743	3.422906
C	2.950502	1.692317	2.797708
C	1.527369	0.259326	4.751171

C	2.962657	2.099098	4.135886
C	2.254037	1.390835	5.104686
H	2.271097	1.724946	6.145090
S	-0.123134	-2.268843	-1.835166
O	-1.580561	-2.658096	-2.169628
O	0.014025	-2.033396	-0.388736
O	0.824529	-3.209320	-2.441160
Cu	-0.120264	1.984404	0.530510
C	3.839033	-0.408593	-2.011093
C	4.232929	-1.339623	-2.976400
C	4.421901	0.866148	-2.013607
C	5.204962	-1.009125	-3.922157
H	3.769147	-2.330630	-2.984458
C	5.388172	1.198441	-2.959473
H	4.108482	1.604329	-1.267686
C	5.784322	0.258789	-3.914607
H	5.508166	-1.746066	-4.669716
H	5.835634	2.195313	-2.953572
H	6.544084	0.519052	-4.655618
N	1.640781	0.161009	-1.015683
N	2.156424	0.140525	1.089742
C	-2.041368	1.153966	0.400609
C	-2.466088	0.728010	-0.976576
Al	-2.691890	-3.718702	-1.111730
C	-2.081885	2.493185	0.878511
C	-2.577941	3.713210	0.238098
H	-2.012147	2.585987	1.970376
C	-2.808378	3.877022	-1.142665
C	-2.788390	4.835953	1.065847
C	-1.772070	0.115170	1.357768
C	-1.637152	-5.231355	-0.462320
C	-4.350884	-3.875166	-2.133448
H	-4.712168	-2.887409	-2.466819
H	-5.174490	-4.329077	-1.556142
H	-4.236269	-4.489549	-3.042352
H	-2.220957	-5.963616	0.121034
H	-0.817242	-4.892428	0.194795
H	-1.161973	-5.796245	-1.282518
C	-3.236379	5.099491	-1.658046
H	-2.639550	3.053591	-1.835793
C	-3.215443	6.054427	0.550622
H	-2.599609	4.738626	2.139076
C	-3.443802	6.194781	-0.819856
H	-3.404966	5.195774	-2.733781
H	-3.368559	6.902655	1.222662
H	-3.777885	7.150495	-1.230639
C	0.713215	3.769322	0.710945
O	-3.002638	-2.628999	0.340175
H	-4.871937	-4.479391	1.436998
C	-5.534849	-3.683735	1.807940
P	-3.943988	-1.719549	1.120418
H	-6.061953	-4.047600	2.695698
H	-6.272919	-3.429948	1.033257
O	-4.995598	-1.159476	0.042518
O	-4.785321	-2.535053	2.210941
O	-3.286010	-0.588535	1.928831
C	-5.945719	-0.163496	0.423045
H	-6.669278	-0.561342	1.149716
H	-6.479122	0.134561	-0.485627
H	-5.449362	0.717393	0.855354
H	-1.416471	0.427241	2.343054
H	-1.309371	-0.798826	0.975822
C	3.513655	-1.956586	1.214267
C	4.441507	-1.941810	2.264749
C	2.833977	-3.149332	0.933991
C	4.683505	-3.085732	3.023566
H	4.982214	-1.016069	2.486740
C	3.084349	-4.297290	1.684783
H	2.085438	-3.187155	0.139435
C	4.004124	-4.269308	2.733554
H	5.410704	-3.054161	3.838597
H	2.547307	-5.220070	1.451129
H	4.195180	-5.170850	3.320917
C	3.738484	2.437584	1.768543
C	0.731618	-1.437606	3.086370
H	-1.882903	1.207471	-1.775038
H	-3.523450	0.970828	-1.170263
H	-2.349577	-0.357273	-1.103964
C	0.677868	4.794947	-0.158012
H	1.270910	3.978639	1.647095
H	0.130545	4.676360	-1.111750
C	1.282428	6.150774	0.025561
H	1.831466	6.231560	0.976201

H	0.512608	6.942248	0.018459
H	1.981951	6.412579	-0.786431
H	0.978794	-0.300066	5.514086
H	3.536691	2.987103	4.414125
H	4.000673	3.443895	2.119537
H	3.191747	2.544326	0.820339
H	4.688041	1.926913	1.536710
H	0.580772	-1.573127	2.008774
H	-0.250997	-1.458970	3.580023
H	1.273929	-2.324900	3.450954

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Scheme_S6_XXX / electronic energy: -5719.56183190 a.u. / lowest freq: -316.31 cm-1

C	-0.245364	2.640678	1.534989
H	-1.340136	2.751383	1.505132
C	0.380855	3.385737	0.342685
H	1.331299	3.855740	0.651409
C	0.601952	1.061105	-0.014538
C	-0.194919	0.186655	2.124184
C	0.875661	-0.480103	2.729930
C	-1.508157	-0.157061	2.490682
C	0.652492	-1.440281	3.712439
H	1.890781	-0.207270	2.429653
C	-1.727435	-1.106999	3.492985
C	-0.650579	-1.736079	4.111886
H	1.502225	-1.947824	4.175433
H	-2.751663	-1.361086	3.771611
H	-0.833760	-2.472620	4.897007
C	1.595099	2.518670	-1.705286
C	1.056999	2.695999	-2.996941
C	2.988908	2.596039	-1.466292
C	1.947470	2.922409	-4.054751
C	3.831751	2.815487	-2.560992
C	3.320285	2.972434	-3.845577
H	3.997032	3.141788	-4.686788
S	-2.928104	0.604212	1.706556
O	-3.962209	-0.539485	1.794859
O	-2.583716	0.883288	0.303642
O	-3.343042	1.747646	2.524413
Cu	0.879209	-0.817640	-0.672454
C	0.234824	3.088341	2.889144
C	-0.646159	3.740280	3.757904
C	1.560372	2.881409	3.293461
C	-0.207964	4.188052	5.004962
H	-1.685159	3.891171	3.451504
C	1.997176	3.321739	4.540430
H	2.254963	2.365544	2.622812
C	1.112977	3.979309	5.398761
H	-0.905506	4.698022	5.673729
H	3.032710	3.150840	4.844967
H	1.455288	4.325741	6.376948
N	0.094466	1.236579	1.217447
N	0.725678	2.270687	-0.588804
C	-1.004107	-1.682112	-0.908086
H	-1.514364	-1.584035	0.057198
Al	-5.446277	-0.760486	0.686190
H	4.911742	2.869783	-2.398577
C	0.027606	-2.644674	-1.076805
C	3.596552	2.518691	-0.076425
C	-0.427265	2.640018	-3.296707
H	1.549472	3.054355	-5.064857
C	0.383979	-3.666538	-0.095002
H	0.321841	-2.873672	-2.109241
C	-0.111379	-3.656052	1.220764
C	1.263725	-4.703153	-0.459952
C	-1.605916	-1.042656	-2.018991
C	-6.097090	1.006615	0.160381
C	-6.602738	-2.066108	1.574762
H	-6.057888	-2.781698	2.213008
H	-7.184137	-2.667142	0.853894
H	-7.345250	-1.576332	2.227828
H	-6.298327	1.646012	1.037316
H	-7.036783	0.973097	-0.416614
H	-5.366548	1.554188	-0.458645
C	0.250192	-4.648615	2.129356
H	-0.792052	-2.860597	1.536945
C	1.622143	-5.696198	0.445262
H	1.667653	-4.719355	-1.476226
C	1.114629	-5.675846	1.747051
H	-0.150117	-4.620224	3.146646
H	2.304064	-6.492081	0.135226
H	1.394943	-6.454723	2.460284
H	2.812210	2.186318	0.621261
C	4.075861	3.896161	0.377978

C	4.727100	1.504268	0.031816
H	-0.950703	2.388182	-2.359297
C	-0.755166	1.566973	-4.330360
C	-0.937140	3.993892	-3.779214
O	-4.640418	-1.534190	-0.762113
H	-3.275975	-5.070992	0.714883
C	-3.825730	-4.169648	0.422445
P	-4.005994	-2.575920	-1.671599
H	-3.705048	-3.409664	1.210469
H	-4.891078	-4.425734	0.321449
O	-5.226810	-3.278406	-2.435259
O	-3.270936	-3.717802	-0.809930
O	-2.977683	-2.074283	-2.691092
C	-4.976695	-4.300568	-3.400677
H	-4.454811	-3.894828	-4.278045
H	-5.950555	-4.692472	-3.711548
H	-4.382217	-5.119368	-2.970252
H	-1.066508	-1.057759	-2.967973
H	-2.209590	-0.151740	-1.837130
H	5.099309	1.455250	1.066691
H	5.585659	1.764618	-0.606699
H	4.392122	0.495905	-0.244196
H	4.442879	3.862272	1.414961
H	3.285167	4.659567	0.331103
H	4.906815	4.252448	-0.250718
H	-0.703362	4.804723	-3.075261
H	-2.028008	3.975280	-3.922081
H	-0.487209	4.261259	-4.748544
H	-0.320796	0.591422	-4.074302
H	-0.371227	1.837908	-5.326150
H	-1.842873	1.435633	-4.429520
C	4.584879	-2.568611	0.750025
C	5.739418	-2.210416	0.025971
C	4.751878	-3.433321	1.850780
C	6.990261	-2.717720	0.366828
H	5.662171	-1.500991	-0.802662
C	6.001222	-3.945921	2.189605
H	3.871667	-3.703757	2.443740
C	7.128973	-3.594971	1.445097
H	7.869245	-2.418725	-0.210439
H	6.097697	-4.622029	3.043314
H	8.112111	-3.991203	1.710816
C	2.756436	-1.488339	-0.687097
C	3.239968	-2.068849	0.435719
Si	3.509799	-1.385405	-2.397460
C	2.163030	-0.811617	-3.577146
C	4.147711	-3.054140	-2.990203
H	4.627489	-0.382993	-2.495990
H	3.330251	-3.791346	-3.017646
H	4.939697	-3.469023	-2.349451
H	4.551880	-2.981087	-4.012261
H	1.407087	-1.597078	-3.738934
H	2.549492	-0.525676	-4.568079
H	1.649264	0.068850	-3.159517
H	2.546863	-2.239900	1.282796
H	-0.328672	7.719008	-1.247174
H	-2.756466	7.313281	-1.641800
C	-0.763752	6.739391	-1.035169
C	-2.121347	6.511946	-1.256205
H	1.105677	5.896564	-0.350296
C	0.041978	5.716002	-0.533729
C	-2.666990	5.255756	-0.982586
C	-0.498355	4.457588	-0.246534
C	-1.862871	4.234228	-0.482525
H	-2.301484	3.253427	-0.270504
H	-3.729550	5.069758	-1.158026

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Scheme_S6_XXXI / electronic energy: -5719.56101765 a.u. / lowest freq: -331.11 cm-1

C	-0.409249	3.074093	0.536802
H	-1.245848	3.513171	-0.019172
C	0.899269	3.245869	-0.244998
H	1.640952	3.811074	0.342726
C	0.521446	0.924879	0.074932
C	-1.573175	0.979540	1.324264
C	-1.176623	0.299979	2.479918
C	-2.949383	1.101434	1.043241
C	-2.115335	-0.241640	3.353797
H	-0.106963	0.230764	2.696655
C	-3.886052	0.575988	1.935545
C	-3.474282	-0.089686	3.088617
H	-1.780174	-0.765080	4.252242
H	-4.949277	0.674549	1.712445
H	-4.221158	-0.495650	3.774287

C	2.659328	1.592365	-0.996681
C	2.697805	1.147896	-2.334494
C	3.848031	1.878144	-0.286636
C	3.949551	0.973811	-2.938995
C	5.070627	1.705081	-0.943036
C	5.126940	1.255904	-2.257808
H	6.092920	1.119289	-2.750540
S	-3.520505	1.826495	-0.502740
O	-3.363271	3.282947	-0.440685
O	-5.023830	1.499654	-0.514311
O	-2.808404	1.124981	-1.582270
Cu	0.748109	-1.090145	0.186639
C	-0.478796	3.597176	1.950824
C	-1.698462	4.105505	2.417619
C	0.589032	3.483228	2.848090
C	-1.846867	4.485701	3.751077
H	-2.540680	4.184626	1.723467
C	0.444338	3.864953	4.180812
H	1.545418	3.080000	2.507391
C	-0.776411	4.364337	4.637161
H	-2.805441	4.877861	4.099495
H	1.289197	3.767231	4.867379
H	-0.891755	4.659892	5.682785
N	-0.570661	1.581778	0.525995
N	1.395836	1.839317	-0.365405
C	-0.709202	-2.254225	-0.825273
H	-0.631034	-2.095841	-1.904849
Al	-5.995288	0.060256	-1.174769
H	5.998221	1.918236	-0.404815
C	0.234801	-3.067185	-0.151798
C	3.852369	2.361199	1.148259
C	1.459435	0.795179	-3.128353
H	3.994972	0.613723	-3.970375
C	1.258267	-3.898032	-0.786827
H	-0.032347	-3.375378	0.865544
C	1.429790	-3.970648	-2.180981
C	2.116081	-4.668520	0.022686
C	-1.913770	-1.837766	-0.200626
C	-5.855257	-0.103062	-3.114965
C	-7.724956	0.110243	-0.262163
H	-7.645421	0.378274	0.805291
H	-8.231212	-0.870802	-0.300564
H	-8.429036	0.832887	-0.708385
H	-6.345687	0.718694	-3.663363
H	-6.324991	-1.035200	-3.474810
H	-4.807189	-0.127624	-3.456815
C	2.429733	-4.765496	-2.738266
H	0.760522	-3.414825	-2.841531
C	3.109904	-5.465881	-0.533061
H	1.997969	-4.624203	1.109882
C	3.276783	-5.513767	-1.919664
H	2.541222	-4.807643	-3.824898
H	3.765055	-6.049191	0.118899
H	4.060182	-6.135851	-2.359385
H	2.827339	2.243525	1.530647
C	4.244394	3.832361	1.249436
C	4.748089	1.510385	2.037111
H	0.574154	1.132011	-2.564924
C	1.371805	-0.718960	-3.263071
C	1.428936	1.478281	-4.488728
O	-4.978565	-1.251809	-0.394856
H	-6.250316	-1.713418	1.994714
C	-6.080951	-2.799720	1.976515
P	-4.607448	-2.714645	-0.191168
H	-6.925359	-3.287057	1.466522
H	-6.025037	-3.171560	3.005027
O	-5.640343	-3.564542	-1.072037
O	-4.840449	-3.119346	1.345222
O	-3.159832	-3.098421	-0.522724
C	-5.535481	-4.989217	-1.137916
H	-6.418055	-5.349800	-1.675591
H	-5.519787	-5.436057	-0.133402
H	-4.631116	-5.289796	-1.683861
H	-2.443591	-0.996054	-0.652062
H	-1.956628	-1.878700	0.893601
H	4.693828	1.852719	3.081354
H	5.805263	1.563056	1.734976
H	4.444018	0.455810	2.009377
H	4.166648	4.190805	2.287033
H	3.616775	4.486342	0.626435
H	5.286753	3.985621	0.928617
H	1.587352	2.563360	-4.405058
H	0.458952	1.320161	-4.983007

H	2.201847	1.082100	-5.165228
H	1.400064	-1.198953	-2.272659
H	2.219069	-1.122279	-3.841490
H	0.443532	-1.029156	-3.767319
C	4.943787	-1.963187	0.418927
C	5.704409	-2.331828	-0.709851
C	5.600285	-1.957649	1.665073
C	7.041004	-2.704505	-0.599636
H	5.219020	-2.327314	-1.691974
C	6.938479	-2.326511	1.777603
H	5.064331	-1.635655	2.560672
C	7.667047	-2.706633	0.648349
H	7.600685	-2.990910	-1.494088
H	7.422193	-2.306473	2.757899
H	8.717968	-2.992059	0.739820
C	2.491306	-1.533363	1.078292
C	3.533518	-1.598128	0.216248
Si	2.348170	-1.923933	2.892978
C	0.693958	-2.742736	3.274691
C	2.473268	-0.349711	3.931864
H	3.380792	-2.892854	3.403806
H	2.104407	0.534073	3.387596
H	3.509506	-0.133082	4.230129
H	1.882653	-0.436786	4.858017
H	-0.157825	-2.219850	2.812691
H	0.520288	-2.759440	4.362791
H	0.658493	-3.788992	2.934440
H	3.341557	-1.402336	-0.857407
H	-1.400232	4.228381	-4.221861
C	-0.500413	4.375068	-3.619290
H	0.430601	5.709373	-5.043094
C	0.526009	5.200593	-4.080682
C	0.754161	3.914636	-1.593756
C	1.675501	5.369098	-3.309376
C	1.786229	4.729519	-2.074486
H	2.486837	6.009511	-3.663706
H	2.683540	4.874362	-1.464785
C	-0.385860	3.730242	-2.388980
H	-1.199763	3.082904	-2.049487

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Scheme_S6_XXXII / electronic energy: -5527.99348065 a.u. / lowest freq: -363.96 cm-1

C	-0.116953	-3.169756	-1.235469
H	0.901283	-3.503428	-1.469184
C	-0.730882	-2.440025	-2.424252
H	-1.550900	-2.998752	-2.896175
C	-0.766284	-0.972058	-0.601724
C	0.606832	-2.172475	1.005972
C	-0.137906	-2.072964	2.186459
C	2.004168	-2.330134	1.096070
C	0.480732	-2.116298	3.432167
H	-1.221735	-1.962642	2.102792
C	2.618482	-2.385895	2.350513
C	1.863051	-2.274624	3.514928
H	-0.122007	-2.033480	4.339942
H	3.701986	-2.501036	2.407130
H	2.359343	-2.314271	4.486642
C	-1.772729	-0.155494	-2.700840
C	-0.897596	0.618837	-3.497845
C	-3.174897	0.013266	-2.760966
C	-1.461877	1.561107	-4.367002
C	-3.681026	0.989906	-3.626836
C	-2.837231	1.750611	-4.430171
H	-3.256226	2.502820	-5.103569
S	3.036067	-2.490964	-0.363899
O	4.427497	-2.111934	0.170351
O	2.568428	-1.522748	-1.369334
O	3.031667	-3.905228	-0.750071
Cu	-1.074428	0.547754	0.680511
C	-0.888105	-4.334585	-0.666741
C	-0.194646	-5.413985	-0.106305
C	-2.286732	-4.327121	-0.618035
C	-0.888662	-6.468876	0.486628
H	0.899526	-5.418825	-0.138329
C	-2.981842	-5.379308	-0.025115
H	-2.838549	-3.483498	-1.041665
C	-2.283243	-6.453755	0.528364
H	-0.337057	-7.307893	0.917761
H	-4.074603	-5.357545	0.007328
H	-2.826756	-7.280400	0.992360
N	-0.060403	-2.061113	-0.236081
N	-1.214539	-1.171534	-1.851118
C	0.821303	1.213567	1.351177
H	1.320950	0.514821	2.032120

Al	5.541078	-0.681646	-0.219810
H	-4.760143	1.151209	-3.680178
C	-0.195477	2.067260	1.826394
C	-4.118530	-0.876440	-1.977189
H	0.018401	-2.236124	-3.202161
C	0.610733	0.454432	-3.467238
H	-0.802113	2.165860	-4.995757
C	-0.591197	2.223120	3.226247
H	-0.495390	2.894900	1.170237
C	0.013904	1.505102	4.274738
C	-1.607951	3.141241	3.553333
C	1.338588	1.326849	0.028711
C	5.882746	-0.591851	-2.142602
C	6.980960	-0.835700	1.095173
H	6.604026	-0.800312	2.132110
H	7.749208	-0.048242	1.013381
H	7.518354	-1.794715	0.996831
H	6.243522	-1.555243	-2.542786
H	6.643971	0.159661	-2.411534
H	4.973710	-0.338354	-2.713797
C	-0.392620	1.689413	5.593221
H	0.818261	0.797061	4.058293
C	-2.011228	3.326455	4.872008
H	-2.081314	3.713873	2.750353
C	-1.407546	2.598351	5.899831
H	0.092852	1.122502	6.391875
H	-2.801541	4.045748	5.101147
H	-1.722120	2.742926	6.936218
H	-3.600081	-1.151208	-1.042799
C	-4.415302	-2.160239	-2.752704
C	-5.433493	-0.206414	-1.606233
H	0.875138	-0.136440	-2.575575
C	1.350005	1.786761	-3.367531
C	1.115107	-0.299820	-4.697207
O	4.427236	0.698014	0.299346
H	6.342998	2.157697	2.072512
C	6.173874	3.003214	1.391459
P	4.112812	2.163889	0.005910
H	6.777629	2.865510	0.481734
H	6.487579	3.928723	1.885856
O	4.824903	2.485920	-1.398500
O	4.783367	3.135776	1.089098
O	2.631025	2.556871	-0.004840
C	4.694250	3.780860	-1.985213
H	5.101984	3.717418	-2.999530
H	5.261639	4.531627	-1.416067
H	3.640803	4.089442	-2.040892
H	0.723578	1.861733	-0.696454
H	1.880084	0.470961	-0.386760
H	-5.996951	-0.837533	-0.902804
H	-6.083202	-0.064684	-2.483577
H	-5.290045	0.775768	-1.135427
H	-5.025628	-2.852532	-2.151793
H	-3.508367	-2.697881	-3.060169
H	-4.981982	-1.936432	-3.670359
H	0.611942	-1.264758	-4.850149
H	2.194851	-0.497476	-4.618699
H	0.954482	0.292584	-5.611816
H	0.937727	2.452898	-2.596399
H	1.322186	2.341882	-4.318027
H	2.411392	1.617381	-3.127905
C	-3.307101	3.035162	-0.447633
C	-4.241294	4.042933	-0.763176
C	-2.053440	3.103440	-1.084070
C	-3.936100	5.072020	-1.650232
H	-5.228923	4.006533	-0.291633
C	-1.740203	4.134721	-1.964024
H	-1.318302	2.314769	-0.898882
C	-2.678144	5.129243	-2.252445
H	-4.684696	5.837506	-1.871442
H	-0.757474	4.156694	-2.444424
H	-2.432013	5.936790	-2.946323
C	-2.990008	0.950876	1.022024
C	-3.699044	1.985901	0.502990
Si	-3.886316	-0.206885	2.191537
C	-3.016950	-0.282088	3.860448
C	-3.913792	-1.958024	1.482220
C	-5.664750	0.325458	2.518504
H	-2.974569	-2.203373	0.962392
H	-4.728841	-2.102174	0.754721
H	-4.052216	-2.714015	2.272694
H	-5.715638	1.306932	3.016309
H	-6.165979	-0.396828	3.182982

H	-6.268380	0.390758	1.599751
H	-1.949988	-0.537181	3.778538
H	-3.484260	-1.040975	4.509487
H	-3.077737	0.681122	4.391761
H	-4.758228	2.114209	0.800026

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Scheme_S6_XXXIII / electronic energy: -5527.98798981 a.u. / lowest freq: -290.69 cm-1

C	2.156869	2.759806	-1.077579
H	1.403131	3.315778	-1.659818
C	2.930199	1.792019	-1.964174
H	4.007210	1.809064	-1.741799
C	1.517274	0.525717	-0.575390
C	0.612987	2.329306	0.845702
C	1.127896	2.368825	2.146196
C	-0.634555	2.921429	0.592164
C	0.426880	2.992872	3.172633
H	2.099868	1.906119	2.330494
C	-1.325516	3.568862	1.621704
C	-0.795486	3.610062	2.906146
H	0.843452	3.006776	4.182223
H	-2.295603	4.026321	1.410585
H	-1.346163	4.113395	3.703716
C	2.707545	-0.711601	-2.357913
C	1.772551	-1.278747	-3.260950
C	3.995938	-1.268137	-2.191369
C	2.121478	-2.473830	-3.900590
C	4.294794	-2.458562	-2.867343
C	3.361564	-3.071382	-3.693345
H	3.609149	-4.006486	-4.201881
S	-1.474632	2.881046	-0.990440
O	-1.779865	4.268117	-1.356153
O	-2.760834	2.127533	-0.577476
O	-0.710307	2.086913	-1.959273
Cu	0.539943	-0.952716	0.407798
C	2.964962	3.730474	-0.258006
C	2.519244	5.047262	-0.104860
C	4.095420	3.307935	0.453509
C	3.192741	5.930301	0.739539
H	1.623954	5.373538	-0.644015
C	4.768258	4.187349	1.298717
H	4.440982	2.272302	0.360092
C	4.317289	5.501359	1.443813
H	2.834295	6.956458	0.850504
H	5.646478	3.845512	1.851995
H	4.843741	6.190490	2.108644
N	1.427909	1.807635	-0.192204
N	2.350922	0.476267	-1.634715
C	-0.943676	-1.904981	-0.761797
H	-0.453095	-2.365678	-1.622999
Al	-4.420840	2.092150	-1.413433
H	5.283255	-2.907920	-2.742887
C	-0.819686	-2.502101	0.518257
C	5.090658	-0.580991	-1.397252
H	2.821017	2.014588	-3.033333
C	0.471366	-0.580414	-3.605911
H	1.412121	-2.939511	-4.588015
C	-0.203654	-3.806871	0.764202
H	-1.505996	-2.158281	1.301681
C	0.402461	-4.567929	-0.253377
C	-0.229958	-4.343776	2.066027
C	-1.837761	-0.834782	-1.003167
C	-4.103839	1.974197	-3.342168
C	-5.530465	3.448168	-0.550119
H	-5.550544	3.307696	0.545231
H	-6.581630	3.452898	-0.883503
H	-5.143915	4.467414	-0.723300
H	-3.519246	2.830723	-3.720316
H	-5.027153	1.938452	-3.944889
H	-3.528436	1.069231	-3.606597
C	0.955440	-5.815317	0.022163
H	0.439206	-4.184825	-1.276547
C	0.325793	-5.589424	2.340343
H	-0.703100	-3.766164	2.865551
C	0.922698	-6.332586	1.318866
H	1.417362	-6.390248	-0.784440
H	0.291047	-5.986688	3.357983
H	1.357576	-7.312060	1.531970
H	4.614617	0.145927	-0.719638
C	6.014793	0.183105	-2.347495
C	5.912552	-1.526716	-0.534217
H	0.082015	-0.138732	-2.677039
C	-0.592180	-1.495022	-4.198751
C	0.710595	0.580970	-4.569367

O	-4.976890	0.459016	-0.772027
H	-5.867094	-0.377077	1.650345
C	-5.682646	-1.452021	1.511124
P	-4.709929	-1.043200	-0.900873
H	-6.615752	-1.937079	1.187775
H	-5.365151	-1.889727	2.463505
O	-6.014647	-1.641258	-1.611497
O	-4.635936	-1.685531	0.570246
O	-3.448972	-1.508713	-1.635256
C	-6.082965	-3.036642	-1.910824
H	-7.123633	-3.259082	-2.168762
H	-5.790836	-3.650620	-1.046424
H	-5.437849	-3.285050	-2.764346
H	-1.700746	-0.194587	-1.873645
H	-2.234752	-0.308666	-0.131440
H	6.631189	-0.959681	0.075392
H	6.502127	-2.231076	-1.139855
H	5.287613	-2.116678	0.147776
H	6.742096	0.790823	-1.788158
H	5.471085	0.853331	-3.028290
H	6.586505	-0.516755	-2.976960
H	1.405491	1.329168	-4.169011
H	-0.234275	1.102015	-4.782421
H	1.120813	0.224247	-5.527416
H	-0.756821	-2.416530	-3.622163
H	-0.339783	-1.799870	-5.226218
H	-1.555966	-0.968648	-4.258635
C	-0.972804	-0.330096	3.534105
C	-1.625539	-0.319671	4.782707
C	-1.664039	0.225369	2.442843
C	-2.911670	0.196867	4.925074
H	-1.104528	-0.730826	5.653460
C	-2.952979	0.730829	2.574114
H	-1.153506	0.283537	1.476662
C	-3.586345	0.720020	3.819965
H	-3.392860	0.190928	5.906840
H	-3.457262	1.152132	1.698461
H	-4.596103	1.124348	3.929362
C	1.112589	-1.167958	2.317010
C	0.379159	-0.889795	3.424042
Si	2.853498	-1.801338	2.539902
C	3.218817	-3.202318	1.340071
C	3.169106	-2.455357	4.279108
C	4.025885	-0.358210	2.227380
H	2.472829	-3.269637	4.537780
H	3.069340	-1.677500	5.051983
H	4.189217	-2.863147	4.365671
H	3.841310	0.101410	1.243197
H	5.084599	-0.660393	2.263201
H	3.890143	0.429718	2.986133
H	2.591488	-4.077348	1.570303
H	4.264898	-3.539107	1.416077
H	3.031097	-2.931785	0.287225
H	0.803678	-1.109222	4.423494

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Scheme_S7_S.XV / electronic energy: -4351.35404269 a.u. / lowest freq: -333.86 cm-1

C	-2.279831	1.408442	-0.018272
H	-2.456577	1.647772	1.038256
C	-2.874594	0.028436	-0.375741
H	-3.593018	0.122494	-1.207758
C	-0.539765	-0.026956	-0.750562
C	0.179471	2.177565	-0.106895
C	0.626799	2.793065	-1.280169
C	0.771923	2.537133	1.115836
C	1.632015	3.756907	-1.241174
H	0.170483	2.499191	-2.229371
C	1.777579	3.503236	1.153478
C	2.205596	4.115290	-0.022764
H	1.968234	4.226390	-2.168267
H	2.227083	3.758132	2.115019
H	2.993795	4.870198	0.016089
C	-1.726223	-2.058446	-1.349900
C	-1.341850	-3.113504	-0.498875
C	-2.125512	-2.285178	-2.683421
C	-1.366139	-4.415179	-1.022108
C	-2.148924	-3.601938	-3.153852
C	-1.770865	-4.660116	-2.329656
H	-1.784950	-5.682919	-2.714022
S	0.304250	1.755225	2.655652
O	1.160122	2.302921	3.712619
O	0.640807	0.268869	2.398841
O	-1.142605	1.931456	2.817812
Cu	1.264567	-0.630681	-1.118961

C	-2.737312	2.575074	-0.855878
C	-2.975652	3.810099	-0.243021
C	-2.852037	2.476274	-2.248492
C	-3.328890	4.924576	-1.004227
H	-2.874899	3.895367	0.843474
C	-3.205974	3.587691	-3.010688
H	-2.653135	1.520321	-2.742729
C	-3.445561	4.815212	-2.389432
H	-3.513656	5.882114	-0.511396
H	-3.294144	3.497068	-4.096173
H	-3.722591	5.686827	-2.987348
N	-0.817272	1.167425	-0.200574
N	-1.680986	-0.710963	-0.877707
C	2.899283	-0.862698	0.113929
C	2.516654	-1.998299	0.821404
O	2.141388	-2.094404	2.048146
C	2.611290	-3.211852	-0.064464
Al	1.941487	-0.747388	3.288662
H	-2.452138	-3.791032	-4.187028
C	3.264228	-1.230352	-1.282575
C	-2.472216	-1.144352	-3.583882
C	-0.937693	-2.902558	0.925694
H	-1.062286	-5.245436	-0.378276
H	-1.665634	-0.394759	-3.612998
H	-3.381561	-0.615826	-3.256865
H	-2.648509	-1.486491	-4.611014
H	-0.572006	-1.888489	1.135589
H	-0.154957	-3.612529	1.225298
H	-1.788823	-3.082821	1.601732
C	3.468843	-2.739460	-1.232747
H	1.598941	-3.516832	-0.389280
H	3.027137	-4.071388	0.480948
H	4.533803	-2.916147	-1.014148
H	3.253644	-3.248795	-2.181378
H	3.016137	0.135975	0.542697
C	1.066754	-1.529574	4.852439
C	3.640323	0.231939	3.407197
H	3.714146	1.063751	2.685991
H	4.510998	-0.421204	3.219487
H	3.797843	0.681653	4.402096
H	1.729555	-2.161418	5.467847
H	0.207824	-2.163152	4.568611
H	0.666790	-0.753665	5.528409
C	-3.549376	-0.724691	0.745314
C	-4.592213	-1.607155	0.436988
C	-3.112707	-0.628186	2.072781
C	-5.190293	-2.379352	1.432128
H	-4.937314	-1.688346	-0.598920
C	-3.719385	-1.390564	3.069927
H	-2.287005	0.039150	2.335503
C	-4.756300	-2.269462	2.753678
H	-6.003326	-3.062860	1.175421
H	-3.371706	-1.302065	4.102312
H	-5.227648	-2.867517	3.537534
C	4.378282	-0.425666	-1.875124
O	5.359074	-0.894311	-2.405805
O	4.164189	0.890811	-1.741635
C	5.179690	1.741920	-2.266303
H	4.842872	2.769120	-2.099695
H	6.135123	1.578934	-1.750422
H	5.323803	1.567208	-3.340792
C	2.117771	-1.060784	-2.977713
H	1.817245	-0.073597	-3.363029
H	2.992967	-1.403344	-3.537549
H	1.318566	-1.806003	-3.126022

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Scheme_S7_S.XVI / electronic energy: -4351.35275204 a.u. / lowest freq: -327.80 cm-1

C	2.588657	-0.420911	-0.159422
H	2.564125	-0.955915	0.803109
C	2.571340	1.102187	0.074518
H	3.230455	1.599560	-0.660271
C	0.481856	0.433043	-0.804403
C	0.819177	-1.937338	-1.178969
C	0.789815	-2.310005	-2.526431
C	0.375774	-2.850379	-0.205983
C	0.334905	-3.569815	-2.906693
H	1.135043	-1.589468	-3.271754
C	-0.073633	-4.115547	-0.591808
C	-0.092260	-4.475310	-1.936505
H	0.318548	-3.844775	-3.963402
H	-0.427465	-4.813037	0.169932
H	-0.447975	-5.466485	-2.225079
C	0.670702	2.791717	-0.257134

C	-0.072335	3.253098	0.844942
C	0.927367	3.607675	-1.379726
C	-0.548472	4.572485	0.803587
C	0.436456	4.916832	-1.371921
C	-0.295171	5.396867	-0.286654
H	-0.675694	6.421313	-0.296412
S	0.390448	-2.444088	1.543501
O	1.685775	-2.872991	2.077810
O	-0.728468	-3.334654	2.112235
O	0.046638	-1.021995	1.686760
Cu	-1.429646	0.511763	-1.124117
C	3.759212	-0.936933	-0.952458
C	4.606823	-1.903505	-0.402639
C	4.008753	-0.470386	-2.250076
C	5.693487	-2.388924	-1.131736
H	4.407068	-2.278362	0.605733
C	5.090017	-0.956997	-2.980320
H	3.343305	0.278299	-2.692510
C	5.937098	-1.916606	-2.420385
H	6.350443	-3.142234	-0.690466
H	5.274646	-0.587656	-3.992042
H	6.786333	-2.297595	-2.992738
N	1.290846	-0.639855	-0.843125
N	1.166225	1.450635	-0.271113
C	-3.041032	-0.180540	-0.011441
C	-3.088845	-1.530947	-0.335415
O	-2.857109	-2.558901	0.401800
C	-3.515093	-1.704020	-1.768984
Al	-2.565143	-2.978129	2.159088
H	0.622736	5.559289	-2.236798
C	-3.509119	0.637070	-1.174438
C	1.674437	3.077437	-2.561227
C	-0.359150	2.394544	2.034444
H	-1.129115	4.949252	1.650252
H	1.254941	2.122360	-2.914503
H	2.735766	2.888521	-2.334636
H	1.646989	3.785431	-3.398607
H	-0.191285	1.327358	1.844390
H	-1.396319	2.525537	2.375975
H	0.279408	2.680194	2.885948
C	-4.169757	-0.371196	-2.107844
H	-4.179211	-2.572441	-1.884308
H	-2.630428	-1.909957	-2.399952
H	-4.110320	-0.098358	-3.169693
H	-5.240408	-0.405201	-1.850394
H	-2.855550	0.212572	0.989952
C	-2.949730	-1.480039	3.363893
C	-3.358510	-4.741972	2.459598
H	-3.064104	-5.465275	1.679505
H	-4.461802	-4.729023	2.469450
H	-3.048655	-5.182453	3.422717
H	-3.949207	-1.039993	3.201507
H	-2.219385	-0.659193	3.269752
H	-2.927377	-1.793524	4.422331
C	-2.404740	1.736615	-2.498079
H	-1.921292	2.652299	-2.123531
H	-1.775017	1.230865	-3.249943
H	-3.346497	2.002083	-2.986605
C	-4.324710	1.840723	-0.815841
O	-3.751074	2.553266	0.163424
O	-5.372383	2.143238	-1.340042
C	-4.435800	3.737295	0.560239
H	-5.487884	3.527212	0.791429
H	-3.928508	4.108345	1.455484
H	-4.391598	4.497679	-0.232155
C	2.964538	1.583663	1.449430
C	2.659937	0.866508	2.614223
C	3.605313	2.823782	1.569064
C	3.000644	1.377653	3.865685
H	2.130226	-0.087437	2.553972
C	3.933919	3.341416	2.821118
H	3.847601	3.390607	0.664539
C	3.634824	2.615857	3.974331
H	2.760439	0.804946	4.764794
H	4.432318	4.311006	2.895159
H	3.897455	3.013890	4.957627

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Scheme_S7_S.XVII / electronic energy: -5848.15114599 a.u. / lowest freq: -335.15 cm-1

C	0.541258	0.472984	-0.717932
N	1.390800	-0.561723	-0.646460
C	1.037807	-1.873149	-1.065922
C	1.109049	-2.192544	-2.425784
N	1.177326	1.568303	-0.280353

Cu	-1.341519	0.358588	-1.151321
C	-3.395462	0.190574	-1.531231
C	-3.011654	-0.444896	-0.234776
C	-2.849577	-1.825428	-0.397099
C	2.725694	-0.207751	-0.092371
H	2.851830	-0.749785	0.857254
C	2.572096	1.308024	0.167731
C	0.598031	-2.847462	-0.155366
C	0.756242	-3.463337	-2.875130
H	1.448701	-1.424863	-3.125893
C	0.234087	-4.114963	-0.609982
C	0.319058	-4.425365	-1.965459
H	0.819915	-3.699374	-3.939596
H	-0.130314	-4.846915	0.112786
H	0.033911	-5.421413	-2.311067
C	0.569518	2.859848	-0.249058
C	-0.440721	3.140381	0.693161
C	0.974281	3.815693	-1.206633
C	-1.032784	4.411923	0.658593
C	0.362595	5.073245	-1.190339
C	-0.634202	5.371762	-0.264149
H	-1.108356	6.356334	-0.269269
S	0.494658	-2.504832	1.602510
O	1.877759	-2.407426	2.090784
O	-0.320216	-3.605519	2.192359
O	-0.294088	-1.224299	1.733770
C	3.828351	-0.624491	-1.030518
C	4.604861	-1.748247	-0.727870
C	4.040436	0.039106	-2.245905
C	5.581243	-2.196931	-1.617877
H	4.429963	-2.279166	0.213051
C	5.015594	-0.406287	-3.135533
H	3.426916	0.908370	-2.502964
C	5.789120	-1.526328	-2.822584
H	6.180554	-3.075985	-1.368765
H	5.172634	0.120899	-4.079823
O	-2.608675	-2.713241	0.484566
C	-3.028507	-2.177768	-1.854815
H	0.663779	5.817231	-1.932742
C	1.992874	3.488518	-2.250576
C	-0.894313	2.157958	1.727216
H	-1.818351	4.643441	1.383530
C	-2.246118	1.254147	-2.825255
H	1.800498	2.508580	-2.713174
H	3.017892	3.452058	-1.848139
H	1.994627	4.241356	-3.048517
H	-0.581507	1.125147	1.530766
H	-1.990802	2.172363	1.819388
H	-0.504061	2.433010	2.720567
C	-4.383851	1.308272	-1.414656
C	-3.794325	-0.986044	-2.417385
O	-4.011334	2.197630	-0.481378
H	-3.541255	-3.142593	-1.977042
H	-2.034553	-2.293268	-2.327381
H	-3.629087	-0.811189	-3.489099
H	-4.877011	-1.142800	-2.286147
H	-3.050464	0.058066	0.735962
C	-2.725303	-1.814968	4.198256
H	-3.146337	-0.806848	4.346576
H	-1.832543	-1.892583	4.840579
H	-3.466737	-2.535679	4.579090
H	4.233936	4.283805	3.366663
C	3.666766	3.370235	3.171996
H	3.236919	3.000906	5.257430
C	3.503480	2.919632	1.861771
C	3.108393	2.652815	4.229490
C	2.783544	1.749993	1.594270
C	2.386491	1.485886	3.970452
C	2.220247	1.037532	2.661671
H	1.945764	0.920029	4.795101
H	1.642151	0.128405	2.469616
H	3.941809	3.481644	1.030873
H	6.553571	-1.876575	-3.520445
H	3.261615	1.877976	-0.476638
H	-3.134370	1.381141	-3.451350
H	-1.489751	0.721401	-3.425555
H	-1.880763	2.249003	-2.523808
C	-4.870965	3.317423	-0.298996
H	-4.498300	3.857230	0.576799
H	-5.906867	2.998991	-0.124725
H	-4.846069	3.978053	-1.177004
O	-5.395174	1.411264	-2.070793
Zn	-2.208101	-2.155048	2.335201

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Scheme_S7_S.XVIII / electronic energy: -5848.14566459 a.u. / lowest freq: -345.29 cm-1

C	-2.871975	0.573436	0.030162
Zn	-2.347318	-0.018374	3.210379
C	-2.753188	1.659026	0.906035
Cu	-1.148189	0.712025	-1.068385
C	-3.207580	1.051552	-1.341493
H	3.098789	-0.856365	-2.782298
N	1.033500	-1.048312	-0.387810
C	0.682759	0.200514	-0.733055
C	0.132778	-2.140787	-0.527348
C	-0.145537	-2.624326	-1.809996
N	1.771108	0.977825	-0.667002
C	2.492408	-1.206614	-0.122139
H	2.607675	-1.595392	0.898824
C	2.991801	0.251413	-0.215159
H	3.761907	0.344188	-0.999586
C	-0.505263	-2.726199	0.577930
C	-1.032100	-3.682483	-1.995611
H	0.346935	-2.153810	-2.665156
C	-1.395331	-3.783717	0.386993
C	-1.655023	-4.265761	-0.894181
H	-1.239143	-4.046123	-3.004333
H	-1.886583	-4.216944	1.260091
H	-2.353533	-5.094275	-1.029704
C	1.733857	2.380481	-0.930441
C	1.168383	3.255893	0.018503
C	2.227170	2.844938	-2.167336
C	1.119726	4.621118	-0.299264
C	2.171136	4.217784	-2.431557
C	1.622856	5.100699	-1.504311
H	1.577378	6.169246	-1.728737
S	-0.248161	-2.129298	2.252494
O	-1.123807	-2.934126	3.116454
O	-0.693919	-0.672590	2.188645
O	1.196827	-2.240580	2.521673
C	3.104441	-2.193525	-1.083092
C	3.372783	-3.497498	-0.652026
C	3.323341	-1.866709	-2.427328
C	3.854556	-4.455858	-1.543981
H	3.189246	-3.762756	0.393909
C	3.806677	-2.821393	-3.319770
C	4.073027	-4.119468	-2.879588
H	4.059221	-5.470462	-1.193585
H	3.973510	-2.552853	-4.365879
H	4.450294	-4.868959	-3.579552
O	-2.527090	1.669330	2.157448
C	-2.972319	2.940318	0.132326
H	2.546688	4.588632	-3.389102
C	2.749899	1.894039	-3.195004
C	0.648930	2.784313	1.339544
H	0.678697	5.313379	0.423436
H	2.031704	1.083312	-3.395317
H	3.691072	1.412936	-2.885584
H	2.949462	2.405927	-4.144333
H	0.231183	1.767704	1.312019
H	-0.128970	3.458596	1.721314
H	1.451444	2.777805	2.094770
C	-3.695553	2.480066	-1.126779
H	-1.996058	3.405722	-0.101385
H	-3.529592	3.677261	0.728301
H	-4.779139	2.435297	-0.933406
H	-3.554685	3.138326	-1.994611
H	-2.867607	-0.477342	0.334314
C	-3.462268	-0.986113	4.517603
H	-3.978583	-1.821375	4.016612
H	-4.233456	-0.360574	4.995954
H	-2.846647	-1.428527	5.317038
C	3.543932	0.854496	1.054175
C	3.050675	0.505329	2.318260
C	4.526840	1.847649	0.959352
C	3.548812	1.128481	3.462051
H	2.267493	-0.253353	2.415899
C	5.014619	2.479789	2.102416
H	4.914123	2.126549	-0.025970
C	4.528478	2.117271	3.358814
H	3.162374	0.841867	4.443447
H	5.782601	3.251876	2.011978
H	4.915105	2.603816	4.257824
C	-1.953286	1.347841	-2.910126
H	-2.819445	1.641150	-3.510972
H	-1.279259	2.218890	-2.849270
H	-1.456869	0.499576	-3.407777

O	-3.819278	-1.114626	-2.168338
C	-4.032614	0.076190	-2.119487
O	-5.040712	0.674328	-2.768913
C	-5.867429	-0.180025	-3.554858
H	-6.346186	-0.946104	-2.931070
H	-6.630771	0.458550	-4.008880
H	-5.283735	-0.677605	-4.340790

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Scheme_S7_S.XIX / electronic energy: -6080.42219364 a.u. / lowest freq: -346.68 cm-1

C	-1.354679	0.360818	-0.494402
N	-0.632873	1.480447	-0.669261
C	0.321645	1.593834	-1.714398
C	-0.128413	1.492073	-3.036544
N	-2.316498	0.615619	0.403730
Cu	-0.926903	-1.381081	-1.218903
C	-0.383808	-3.305184	-1.867509
C	0.512886	-2.787823	-0.796298
C	1.676767	-2.236166	-1.355661
C	-1.156630	2.648586	0.101543
H	-0.339399	3.040563	0.720940
C	-2.238510	1.989225	0.978411
C	1.692930	1.782294	-1.471515
C	0.759723	1.588895	-4.104631
H	-1.198018	1.347480	-3.212197
C	2.577454	1.882626	-2.547251
C	2.116645	1.791656	-3.858912
H	0.387731	1.512859	-5.128736
H	3.639351	2.021803	-2.336297
H	2.822537	1.873603	-4.688290
C	-3.214499	-0.383390	0.885770
C	-2.749024	-1.391159	1.752024
C	-4.556589	-0.344162	0.449425
C	-3.668492	-2.358619	2.184901
C	-5.436257	-1.326293	0.914254
C	-4.996769	-2.327424	1.778397
H	-5.694773	-3.091426	2.129824
S	2.375616	1.877735	0.191533
O	1.822397	3.099487	0.808194
O	3.837792	1.872749	0.025285
O	1.851680	0.639524	0.885705
C	-1.603105	3.741707	-0.836682
C	-0.740447	4.816137	-1.086313
C	-2.814758	3.670226	-1.535091
C	-1.085598	5.803792	-2.008845
H	0.214388	4.864675	-0.553598
C	-3.162347	4.657613	-2.455175
H	-3.493491	2.830202	-1.362660
C	-2.298086	5.727613	-2.694114
H	-0.403852	6.637914	-2.192002
H	-4.113062	4.591393	-2.990041
O	2.690846	-1.751765	-0.765070
C	1.586816	-2.306012	-2.862471
H	-6.475905	-1.309057	0.576223
C	-5.022398	0.691060	-0.521740
C	-1.337972	-1.471187	2.242527
H	-3.319960	-3.147047	2.858046
C	-2.087503	-2.463889	-2.609123
H	-4.383539	0.722881	-1.418197
H	-5.015000	1.705154	-0.092152
H	-6.049378	0.491014	-0.851108
H	-0.629688	-0.844842	1.684012
H	-0.978536	-2.509910	2.201394
H	-1.274522	-1.169555	3.300523
C	-1.102760	-4.575434	-1.539481
C	0.490272	-3.331862	-3.118389
O	-1.712699	-4.509664	-0.346554
H	2.558064	-2.565648	-3.307747
H	1.326783	-1.306581	-3.257637
H	-0.067278	-3.169169	-4.050833
H	0.927593	-4.340442	-3.187844
H	0.391063	-2.993652	0.270917
C	2.077402	-2.079714	2.931568
H	1.339079	-2.897150	2.874854
H	1.657687	-1.322418	3.617016
H	2.963553	-2.502861	3.436349
H	-3.646178	1.815033	5.423652
C	-2.799836	1.806855	4.732430
H	-1.320789	1.579371	6.292218
C	-3.020202	1.937640	3.361738
C	-1.498552	1.675098	5.218155
C	-1.948758	1.930020	2.459839
C	-0.424780	1.670169	4.326573
C	-0.645240	1.789103	2.954850

H	0.597161	1.567310	4.700375
H	0.207657	1.760841	2.270276
H	-4.040696	2.046918	2.980496
H	-2.570835	6.502168	-3.415089
H	-3.213039	2.485181	0.836804
H	-2.981210	-2.402094	-1.967981
H	-2.184432	-3.333904	-3.265906
H	-2.003675	-1.573305	-3.254294
C	-2.445048	-5.668394	0.038244
H	-2.834460	-5.474101	1.041813
H	-1.800525	-6.557077	0.057451
H	-3.279234	-5.852182	-0.652726
O	-1.138114	-5.552998	-2.252251
Zn	2.569912	-1.274456	1.182837
O	4.628882	-0.789706	1.177534
C	5.487489	-0.668120	0.024668
C	5.147334	-0.019158	2.272482
C	6.615942	0.133655	1.958508
H	4.932896	-0.563994	3.203382
H	4.630303	0.955547	2.306719
C	6.593927	0.279503	0.443567
H	4.891997	-0.302236	-0.821944
H	5.860712	-1.676364	-0.221993
H	6.326339	1.309829	0.168733
H	7.553432	0.039011	-0.033546
H	7.166032	-0.772965	2.257468
H	7.072376	0.987798	2.475855

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Scheme_S7_S.XX / electronic energy: -6080.42012747 a.u. / lowest freq: -348.70 cm-1

C	-1.984666	2.177576	0.815534
Zn	-3.303815	-0.085665	-1.026121
O	-3.337470	-2.228480	-0.693091
C	-2.649203	1.130162	1.472741
Cu	-0.045074	1.644975	1.180646
C	-1.406501	3.125025	1.808588
H	4.562447	0.357258	0.627512
N	1.711936	0.291946	-0.683270
C	1.176366	0.294448	0.547128
C	1.460929	1.338463	-1.613019
C	2.234911	2.501147	-1.553032
N	1.616581	-0.790337	1.195856
C	2.641052	-0.843847	-0.933839
H	2.226017	-1.441994	-1.757690
C	2.567262	-1.616390	0.402092
H	3.545914	-1.588252	0.912661
C	0.427213	1.250314	-2.560765
C	1.991603	3.563018	-2.421983
H	3.028750	2.563291	-0.804005
C	0.185003	2.316839	-3.426480
C	0.966379	3.469049	-3.361316
H	2.603638	4.465676	-2.360894
H	-0.628061	2.228794	-4.149605
H	0.767255	4.297454	-4.044930
C	1.238414	-1.106013	2.534885
C	0.018675	-1.766325	2.780303
C	2.102700	-0.721455	3.582285
C	-0.307746	-2.054218	4.114755
C	1.731666	-1.028278	4.895094
C	0.536947	-1.696522	5.159286
H	0.259058	-1.929290	6.190328
S	-0.622001	-0.204571	-2.686261
O	-1.596633	0.075867	-3.751543
O	-1.276268	-0.301164	-1.318110
O	0.281463	-1.344239	-2.934798
C	4.005937	-0.349918	-1.340280
C	4.397727	-0.432744	-2.680658
C	4.864892	0.266334	-0.420772
C	5.626716	0.080778	-3.095781
H	3.722850	-0.899670	-3.404926
C	6.093303	0.778995	-0.832331
C	6.477351	0.686807	-2.172030
H	5.919553	0.007633	-4.145957
H	6.754772	1.256409	-0.105135
H	7.440838	1.088854	-2.494694
O	-3.289389	0.154561	0.974798
C	-2.513406	1.327372	2.967757
H	2.388190	-0.729394	5.716831
C	3.369154	0.020118	3.297422
C	-0.933370	-2.151954	1.692463
H	-1.252218	-2.564382	4.324933
H	3.201166	0.870167	2.618294
H	4.126818	-0.619482	2.816066
H	3.819151	0.409175	4.219269

H	-0.734679	-1.656955	0.733216
H	-1.966634	-1.902352	1.971537
H	-0.913296	-3.241006	1.519022
C	-2.138860	2.797983	3.104143
H	-1.718404	0.662649	3.356659
H	-3.435804	1.046175	3.496269
H	-3.050597	3.416120	3.130547
H	-1.566930	3.037007	4.011142
H	-2.010180	2.343153	-0.266058
C	-4.693513	0.361414	-2.368888
H	-4.471226	1.285794	-2.927445
H	-5.703110	0.483743	-1.939739
H	-4.758538	-0.446278	-3.119002
C	2.128151	-3.058511	0.329060
C	1.185748	-3.500556	-0.607873
C	2.625907	-3.967892	1.270942
C	0.765983	-4.830558	-0.608653
H	0.770335	-2.799938	-1.340199
C	2.193656	-5.293555	1.280585
H	3.362104	-3.628086	2.006685
C	1.264009	-5.729477	0.335835
H	0.039252	-5.166793	-1.353267
H	2.590854	-5.990265	2.022884
H	0.931187	-6.770433	0.333566
C	-2.651726	-3.062089	-1.642699
H	-1.584252	-3.074389	-1.380994
H	-2.743761	-2.613771	-2.649781
C	-3.343602	-4.402773	-1.550387
H	-3.236351	-4.998076	-2.466769
H	-2.925781	-4.991354	-0.717114
C	-4.777085	-3.995717	-1.243345
H	-5.280472	-3.651611	-2.160899
H	-5.386090	-4.799906	-0.810087
C	-4.574260	-2.838000	-0.290262
H	-5.370417	-2.077982	-0.327538
H	-4.477286	-3.173298	0.757661
C	0.497545	3.208314	2.505202
H	0.224422	4.112800	3.058308
H	0.774343	2.440055	3.245187
H	1.348058	3.447449	1.847317
O	-1.847752	5.475451	2.030298
C	-1.400413	4.556845	1.381654
O	-0.839303	4.710238	0.171817
C	-0.812992	6.042568	-0.331417
H	-0.186641	6.689437	0.297839
H	-0.391920	5.988274	-1.339344
H	-1.824641	6.466602	-0.377346

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Scheme_S8_XXXIV / electronic energy: -4417.90758076 a.u. / lowest freq: -197.45 cm-1

C	2.339283	-1.053109	1.802031
H	2.238982	-2.102933	2.114356
C	1.634119	-0.115423	2.786538
H	2.318082	0.624208	3.231139
C	0.538653	0.054591	0.708912
C	1.687694	-1.742200	-0.532006
C	2.751498	-1.523888	-1.413678
C	0.861602	-2.862512	-0.733059
C	2.967178	-2.374407	-2.495050
H	3.406375	-0.667438	-1.245895
C	1.072899	-3.706199	-1.824704
C	2.119438	-3.459171	-2.709858
H	3.798659	-2.180961	-3.176418
H	0.416499	-4.567939	-1.959344
H	2.278081	-4.125640	-3.560182
C	-0.260585	1.548620	2.456327
C	-1.537085	1.165731	2.911240
C	0.169871	2.888580	2.467098
C	-2.386251	2.170225	3.393917
C	-0.717254	3.859210	2.948681
C	-1.982260	3.503218	3.411618
H	-2.661063	4.272904	3.787394
S	-0.453608	-3.302923	0.401406
O	-0.819173	-4.695223	0.113535
O	-1.590104	-2.354186	-0.038067
O	-0.013096	-2.995276	1.765179
Cu	-0.797794	0.841481	-0.494169
C	3.785582	-0.747023	1.509496
C	4.188755	0.562144	1.214663
C	4.726636	-1.778170	1.434989
C	5.504099	0.833417	0.846407
H	3.455267	1.373366	1.254753
C	6.046715	-1.509207	1.069730
H	4.415556	-2.803944	1.654924

C	6.436695	-0.204259	0.770889
H	5.803684	1.858027	0.611659
H	6.772471	-2.324268	1.014072
H	7.468612	0.006946	0.480001
N	1.504623	-0.872420	0.573010
N	0.620071	0.541979	1.956526
C	-2.646583	0.282685	-1.327362
C	-3.551482	0.047918	-0.300882
O	-4.025604	-1.070299	0.129841
C	-4.055749	1.342772	0.258733
Al	-3.409068	-2.784010	-0.037846
H	-0.404659	4.907379	2.954772
C	-2.402857	1.729120	-1.509193
C	1.525352	3.262053	1.961371
H	1.153806	-0.660524	3.613513
C	-1.970535	-0.264106	2.867682
H	-3.380459	1.892988	3.755341
C	-0.386045	2.560870	-1.465129
H	1.696652	2.881927	0.941052
H	2.327438	2.848152	2.592528
H	1.660687	4.350516	1.944383
H	-1.872705	-0.694730	1.858259
H	-3.014020	-0.374842	3.188949
H	-1.350863	-0.901690	3.517225
C	-2.634895	2.274310	-2.893032
C	-3.156967	2.410419	-0.360212
H	-2.040534	1.755449	-3.657541
H	-2.429753	3.350400	-2.969671
H	-3.694469	2.113626	-3.157806
H	-4.065596	1.340538	1.359836
H	-5.110256	1.453130	-0.048101
H	-3.708241	3.294622	-0.712683
H	-2.458189	2.781708	0.408007
H	-2.324800	-0.486733	-2.035193
C	-0.430292	3.795504	-0.932001
Si	0.817458	2.001197	-2.806979
H	-1.173938	4.030620	-0.151445
C	0.431152	4.965711	-1.279079
C	0.383919	0.251076	-3.349369
C	2.528451	1.981931	-2.020277
C	0.815356	3.093495	-4.339221
H	1.288591	4.710284	-1.916227
H	0.823000	5.454859	-0.372950
H	-0.148014	5.744819	-1.804987
H	2.510589	1.408668	-1.079182
H	2.884722	2.995096	-1.776082
H	3.283973	1.521218	-2.677501
H	-0.184900	3.152023	-4.795657
H	1.495351	2.684075	-5.103995
H	1.140900	4.124162	-4.135351
H	0.250969	-0.433437	-2.494359
H	1.187051	-0.167834	-3.977086
H	-0.538373	0.204680	-3.948778
C	-3.824265	-3.705682	1.641853
C	-3.883974	-3.535529	-1.784743
H	-3.578509	-2.890768	-2.627028
H	-4.967907	-3.704887	-1.904393
H	-3.402634	-4.514568	-1.953989
H	-4.876473	-3.591620	1.954711
H	-3.209727	-3.315175	2.472324
H	-3.628939	-4.790588	1.600204

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Scheme_S8_XXXV / electronic energy: -4417.90212278 a.u. / lowest freq: -212.38 cm-1

C	1.393833	2.223804	1.343148
H	2.378275	1.977092	1.756110
C	0.305759	2.096939	2.403444
H	-0.172250	3.056733	2.650682
C	-0.223280	0.609767	0.660746
C	1.652842	0.955849	-0.847368
C	0.987579	1.357303	-2.011117
C	2.953572	0.426866	-0.958614
C	1.593817	1.245945	-3.260183
H	-0.017620	1.776648	-1.915461
C	3.560018	0.327416	-2.212204
C	2.887610	0.738911	-3.360894
H	1.054727	1.570889	-4.153353
H	4.562306	-0.099482	-2.275704
H	3.376707	0.655908	-4.333533
C	-1.769692	0.693687	2.566367
C	-1.673007	-0.573785	3.177331
C	-2.895330	1.520709	2.737611
C	-2.768491	-1.029143	3.919633
C	-3.966461	1.021475	3.489996

C	-3.908950	-0.243475	4.067988
H	-4.756179	-0.616357	4.648930
S	3.872041	-0.238315	0.434278
O	5.065269	-0.889017	-0.111217
O	2.879543	-1.267475	1.014088
O	4.102425	0.832944	1.408755
Cu	-1.051367	-0.768642	-0.484241
C	1.490089	3.529857	0.596953
C	2.744699	3.965981	0.153757
C	0.352831	4.266435	0.243798
C	2.862714	5.119548	-0.620970
H	3.632709	3.383052	0.417934
C	0.469042	5.421243	-0.528231
H	-0.636825	3.930886	0.569020
C	1.724586	5.850019	-0.962972
H	3.848328	5.449608	-0.958128
H	-0.425762	5.989581	-0.793707
H	1.815049	6.755284	-1.568240
N	0.997773	1.124398	0.398474
N	-0.660130	1.166361	1.803381
C	-0.995308	-2.894128	-0.384784
C	0.388275	-3.005579	-0.314787
O	1.076014	-3.368323	0.714462
C	1.004716	-2.683005	-1.651350
Al	2.852226	-3.132291	1.105013
H	-4.856331	1.643892	3.619531
C	-1.438238	-2.485532	-1.729967
C	-2.950101	2.898464	2.161745
H	0.692059	1.671180	3.342689
C	-0.436025	-1.401602	3.044501
H	-2.713628	-2.012331	4.394864
C	-2.337914	-0.549771	-2.040960
H	-2.465457	2.959534	1.178455
H	-2.437253	3.627366	2.810657
H	-3.984531	3.248870	2.054450
H	-0.301806	-1.786992	2.022681
H	-0.463068	-2.266522	3.719189
H	0.472230	-0.821603	3.269544
C	-2.659024	-3.178900	-2.272724
C	-0.186254	-2.581740	-2.599808
H	-3.532381	-3.080668	-1.615754
H	-2.938725	-2.828857	-3.275533
H	-2.441695	-4.258310	-2.341077
H	1.716006	-3.471716	-1.942074
H	1.602035	-1.756240	-1.590740
H	-0.088134	-1.774993	-3.338535
H	-0.275232	-3.506747	-3.193192
H	-1.670333	-3.183565	0.425705
C	-1.955695	0.002141	-3.207904
Si	-4.048150	-0.306757	-1.265909
H	-0.937392	-0.179678	-3.589727
C	-2.749270	0.892418	-4.105094
C	-4.095371	-1.195907	0.389409
C	-5.465040	-0.935392	-2.334943
C	-4.286445	1.538305	-0.966090
H	-2.262896	1.877181	-4.211249
H	-2.804469	0.482272	-5.127294
H	-3.776570	1.068265	-3.760004
H	-5.492833	-2.033674	-2.390117
H	-5.418545	-0.557116	-3.367619
H	-6.430263	-0.609444	-1.914335
H	-3.351438	2.022897	-0.645200
H	-5.044598	1.726219	-0.188755
H	-4.623163	2.062013	-1.873872
H	-4.139284	-2.291283	0.293421
H	-4.978236	-0.891826	0.973846
H	-3.205142	-0.957235	0.994410
C	3.088861	-3.648989	2.977272
C	3.987283	-3.922017	-0.287949
H	4.020744	-3.328514	-1.216780
H	3.658981	-4.938455	-0.569068
H	5.034957	-4.019504	0.044632
H	2.868165	-4.716645	3.149554
H	2.439012	-3.082587	3.665415
H	4.123034	-3.492071	3.329023

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Scheme_S9_XXXVI / electronic energy: -4076.36248646 a.u. / lowest freq: -224.30 cm-1

N	-0.713650	0.110230	1.014039
C	0.374509	0.442252	0.301467
N	0.167897	1.643769	-0.254831
C	-0.767858	-1.039019	1.841505
C	0.288034	-1.239976	2.741450
H	1.107664	-0.515356	2.753137

C	3.761236	-0.338720	0.792017
C	1.419046	-2.532094	-1.700445
C	2.581261	-1.764362	-1.719142
C	3.641640	-1.858383	-0.701938
H	5.787463	-1.539731	-0.475119
C	5.011397	-1.556262	-1.252149
H	5.042558	-0.604105	-1.797468
O	0.539762	-2.428418	-2.647400
Al	-1.282726	-2.569067	-2.682843
Cu	1.979577	-0.587071	-0.113934
C	-1.146047	2.239379	0.084536
C	-1.348946	1.884135	3.311532
C	3.970635	-0.754305	2.113617
H	-0.277032	1.763435	3.124720
C	-1.792675	1.121964	0.942013
H	-2.653599	0.700282	0.399167
H	-0.974458	3.140510	0.698415
C	-1.862622	-1.928400	1.815572
C	0.289182	-2.322347	3.614356
C	-1.846182	-2.998646	2.727393
C	-0.790351	-3.205324	3.610558
H	1.123190	-2.463801	4.306287
H	-2.686713	-3.698070	2.715837
H	-0.812597	-4.055862	4.295840
C	1.185646	2.337467	-0.981168
C	1.411604	2.029597	-2.336948
C	1.969632	3.286215	-0.291888
C	2.440354	2.714090	-3.000617
C	2.966675	3.961916	-1.004266
C	3.200472	3.679675	-2.347999
H	3.991458	4.207255	-2.886797
C	-2.265095	1.576171	2.297311
C	-3.632503	1.731282	2.545956
C	-4.079114	2.190997	3.785559
H	-4.350504	1.489962	1.755970
C	-1.793691	2.337028	4.551508
C	-3.160968	2.492255	4.790877
H	-5.150073	2.309439	3.967316
H	-1.070450	2.569580	5.336920
H	-3.509491	2.846621	5.763998
C	1.214144	-3.586871	-0.646810
H	3.583288	4.699125	-0.482418
C	1.784960	3.526335	1.172188
C	0.581381	1.030680	-3.076732
H	2.633761	2.483311	-4.051899
H	1.768534	2.582004	1.739272
H	0.841877	4.047252	1.401707
H	2.596955	4.143053	1.577588
H	0.157109	0.254789	-2.424980
H	1.162172	0.529701	-3.863141
H	-0.262382	1.526057	-3.584131
C	3.577030	-3.135231	0.108155
H	2.732103	-1.093565	-2.572871
C	-1.881028	-4.448823	-2.622710
H	-1.720075	-4.916025	-1.634609
H	-1.370025	-5.096121	-3.357371
H	-2.960901	-4.552405	-2.832331
C	-1.934658	2.639254	-1.136389
C	-2.511269	1.672093	-1.970709
C	-2.075204	3.990782	-1.468133
C	-3.233962	2.052208	-3.099121
H	-2.373782	0.608316	-1.749172
C	-2.787993	4.373158	-2.605152
H	-1.619998	4.750080	-0.824495
C	-3.374509	3.404487	-3.419057
H	-3.684194	1.287015	-3.737516
H	-2.890025	5.432705	-2.852135
H	-3.941063	3.701782	-4.304844
C	-3.024568	-1.778702	0.910984
C	-5.314151	-1.530229	-0.703597
C	-4.310778	-1.723663	1.468568
H	-6.195034	-1.425788	-1.343240
H	-4.402573	-1.762357	2.558919
C	-5.454997	-1.593245	0.684151
H	-6.441097	-1.537526	1.150453
O	-1.686111	-1.808124	-1.067906
C	-4.052381	-1.604269	-1.283564
H	-3.947130	-1.559009	-2.372769
C	-2.878724	-1.731839	-0.505208
C	-1.828212	-1.479526	-4.233841
H	-2.858131	-1.674442	-4.581425
H	-1.175088	-1.674165	-5.103957
H	-1.762724	-0.393614	-4.047633

C	5.336308	1.198749	2.551428
H	5.948550	1.792858	3.234517
H	3.508835	-1.675347	2.486896
C	4.749789	0.009699	2.987641
H	4.896264	-0.326407	4.018265
H	4.239554	1.189419	-0.672624
C	5.140610	1.619755	1.233710
H	5.592851	2.551823	0.881237
C	4.369530	0.850538	0.362211
C	2.163732	-3.477995	0.537089
H	1.332866	-4.559650	-1.159931
H	0.161870	-3.563817	-0.318201
H	4.259585	-3.086118	0.968935
H	3.977386	-3.934664	-0.543193
H	2.145615	-4.407482	1.125284
H	1.800913	-2.689853	1.222283
H	5.273530	-2.347419	-1.974267

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Scheme_S9_XXXVII / electronic energy: -4076.36015978 a.u. / lowest freq: -228.84 cm-1

C	3.718231	-0.401401	1.083963
Cu	1.902260	-0.825099	0.333562
C	3.514837	-2.233044	0.050927
H	3.154204	-1.282756	2.985953
C	2.176167	-2.837489	-0.122936
C	1.481968	-2.860937	-1.329171
C	0.119003	-0.966172	2.869790
Al	-1.324750	-3.126676	-2.043326
C	-2.103884	-1.562935	2.063275
C	-0.927089	-0.792080	1.951260
N	-0.768336	0.219855	0.971219
C	0.380690	0.405870	0.296218
N	0.247482	1.489427	-0.482524
C	-1.809980	1.213867	0.638639
C	-2.409319	1.889979	1.842747
C	-1.634456	2.219414	2.962005
H	-0.573733	1.951866	2.985757
H	-2.624403	0.717283	0.090888
C	-1.068579	2.162154	-0.334233
H	-0.896524	3.148441	0.133007
C	0.028441	-1.899849	3.895559
H	1.001388	-0.326053	2.776723
C	-2.185287	-2.465935	3.138505
C	-1.141639	-2.645678	4.040572
H	0.856454	-2.019003	4.598758
H	-3.093818	-3.066648	3.235672
H	-1.240202	-3.370786	4.851594
C	1.357331	2.171262	-1.076424
C	1.627864	2.037711	-2.450460
C	2.147290	2.988045	-0.238595
C	2.702676	2.766506	-2.981212
C	3.200083	3.705174	-0.815220
C	3.472459	3.600809	-2.177987
H	4.300334	4.165530	-2.614042
C	-3.767131	2.228666	1.831813
C	-4.341905	2.888811	2.917323
H	-4.376551	1.963916	0.961677
C	-2.210361	2.872459	4.050746
C	-3.564716	3.209903	4.030507
H	-5.403632	3.146389	2.896306
H	-1.598276	3.117050	4.922329
H	-4.015389	3.719172	4.885816
O	0.359778	-3.497197	-1.448040
C	2.077185	-2.243660	-2.563943
H	3.817624	4.344107	-0.177821
C	1.893991	3.047870	1.233107
C	0.831298	1.134405	-3.333657
H	2.931470	2.667479	-4.046050
H	2.070253	2.066831	1.707195
H	0.855549	3.324865	1.471521
H	2.554918	3.773437	1.723582
H	0.303919	0.359003	-2.762939
H	1.474741	0.643079	-4.077555
H	0.068464	1.688837	-3.903102
C	4.200634	-1.943484	-1.268961
H	1.742621	-3.396069	0.715451
C	-2.347976	-4.798088	-1.865995
H	-2.423038	-5.121369	-0.812341
H	-1.891963	-5.642182	-2.412819
H	-3.385015	-4.723135	-2.237155
C	-1.764162	2.372734	-1.655120
C	-2.316653	1.292225	-2.357593
C	-1.834079	3.651894	-2.215354
C	-2.942367	1.493281	-3.584984

H	-2.232775	0.277131	-1.953628
C	-2.452220	3.854026	-3.450504
H	-1.397307	4.497595	-1.675162
C	-3.012754	2.775800	-4.134558
H	-3.371145	0.641763	-4.120009
H	-2.501013	4.859363	-3.875867
H	-3.504890	2.932967	-5.097500
C	4.373159	-3.002901	1.022980
C	-3.240807	-1.484537	1.119900
C	-5.452282	-1.401039	-0.611210
C	-4.533882	-1.244296	1.604139
H	-6.304547	-1.363417	-1.295557
H	-4.662448	-1.072322	2.677847
C	-5.640125	-1.193461	0.757213
H	-6.634711	-0.988559	1.159558
O	-1.842718	-1.960476	-0.743693
C	-4.181637	-1.662225	-1.114536
H	-4.036890	-1.829895	-2.187339
C	-3.048855	-1.714612	-0.272045
C	-1.319115	-2.250182	-3.815921
H	-0.723674	-2.806236	-4.562528
H	-0.937914	-1.213978	-3.832143
H	-2.341607	-2.200465	-4.233891
C	5.294505	1.342390	2.644232
C	3.741872	-0.505611	2.484797
H	5.908205	2.016388	3.247152
C	4.510424	0.363273	3.259605
H	4.503483	0.270447	4.349395
H	4.518358	0.703900	-0.608160
C	5.293336	1.446968	1.253040
H	5.900556	2.212038	0.759934
C	4.513285	0.582184	0.480327
C	3.258034	-1.328523	-2.287059
H	1.282960	-1.728617	-3.125997
H	2.381172	-3.084297	-3.214753
H	4.566691	-2.915769	-1.648545
H	5.099601	-1.329329	-1.118280
H	2.891047	-0.356404	-1.902647
H	3.789166	-1.094237	-3.222047
H	3.872225	-3.162937	1.986450
H	5.342116	-2.520201	1.209353
H	4.568635	-4.000379	0.595820

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Scheme_S9_XXXVIII / electronic energy: -4162.96234452 a.u. / lowest freq: -231.19 cm-1

H	-6.234774	-0.551255	2.714021
H	-4.172487	-0.837323	4.092884
C	-5.286568	-0.121843	2.381022
C	-4.132793	-0.277379	3.154157
H	-6.113766	0.709624	0.565388
C	-5.218461	0.589196	1.182771
C	-2.929873	0.289639	2.734933
H	-2.041162	0.176666	3.367286
C	-4.008243	1.146578	0.759199
C	-2.846490	1.004098	1.528010
H	-3.028902	3.177764	3.036296
H	-3.981630	1.679986	-0.197193
H	-1.583181	2.388619	3.716656
C	-1.939549	3.075009	2.937928
H	-3.139792	3.534382	0.426940
Cu	-1.048126	0.739711	0.696255
C	-1.516913	2.643631	1.554212
H	-1.487228	4.058824	3.146076
C	-2.041287	3.550656	0.457991
H	-1.716758	2.216890	-1.202168
C	-0.056651	2.421540	1.461165
H	0.477867	2.106403	2.365448
H	-1.771486	4.581548	0.754245
C	-1.433165	3.243447	-0.898183
H	-1.852781	3.902074	-1.673048
C	0.717840	2.806991	0.372389
C	0.082281	3.371936	-0.865066
O	2.010780	2.758560	0.435295
H	0.551056	2.901207	-1.743910
H	0.382333	4.434899	-0.917972
C	-0.465877	-0.834633	-0.300629
N	0.671431	-1.494354	-0.030005
C	1.536739	-1.100803	1.020993
N	-0.985786	-1.345395	-1.420515
C	-0.170829	-2.420742	-2.001304
C	1.020437	-2.531140	-1.037348
H	-2.994369	-1.894372	0.536930
C	0.171692	-4.506421	0.289657
C	1.156435	-1.369763	2.340225

O	2.052855	0.366230	-1.665116
Al	3.507634	3.037161	-0.556814
H	-0.812879	-4.027875	0.319910
H	1.953029	-2.237378	-1.541849
C	2.735025	-0.408234	0.779686
C	1.958850	-0.972814	3.405917
H	0.216239	-1.901006	2.510672
C	3.546176	-0.028747	1.851951
C	3.161417	-0.310292	3.159770
H	1.648137	-1.189425	4.430257
H	4.471474	0.515865	1.654562
H	3.801452	-0.001788	3.988934
C	-2.202927	-0.893460	-2.015153
C	-2.148668	0.027789	-3.078186
C	-3.422562	-1.392289	-1.517711
C	-3.361717	0.444590	-3.643895
C	-4.607220	-0.954188	-2.119694
C	-4.577466	-0.045539	-3.175462
H	-5.512090	0.289537	-3.632273
C	1.225904	-3.872247	-0.380929
C	2.486234	-4.477264	-0.391424
C	2.687813	-5.703743	0.244204
H	3.316249	-3.976726	-0.899241
C	0.371065	-5.729299	0.925219
C	1.631136	-6.332488	0.901106
H	3.676945	-6.167814	0.227237
H	-0.458606	-6.215291	1.444501
H	1.788196	-7.291982	1.399910
H	-5.563106	-1.330261	-1.744643
C	-3.444935	-2.342167	-0.364794
C	-0.847507	0.556459	-3.589686
H	-3.341274	1.167429	-4.464354
H	-2.873125	-3.258691	-0.577300
H	-4.469611	-2.641496	-0.111516
H	-0.075091	0.607504	-2.810598
H	-0.969696	1.556187	-4.028058
H	-0.438048	-0.083820	-4.388029
C	4.810924	3.946687	0.590473
H	4.862465	3.508288	1.602145
H	4.588458	5.018517	0.731882
H	5.834897	3.900613	0.181026
C	3.194981	3.698575	-2.378447
H	4.151834	3.863619	-2.904903
H	2.657331	4.661357	-2.420510
H	2.623157	2.988694	-3.000054
H	0.141128	-2.156915	-3.022688
H	-0.754344	-3.353657	-2.062662
S	3.252574	0.024739	-0.885394
O	4.083373	-1.075182	-1.382002
O	4.126517	1.271681	-0.657368

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Scheme_S9_XXXIX / electronic energy: -4162.96147012 a.u. / lowest freq: -220.73 cm-1

H	-5.901907	-0.326017	-2.840319
H	-3.874256	0.152042	-4.211043
C	-4.917003	-0.652572	-2.497278
C	-3.781751	-0.389262	-3.265062
H	-5.665009	-1.544000	-0.672531
C	-4.783595	-1.338117	-1.287546
C	-2.522376	-0.813930	-2.831666
H	-1.648533	-0.582235	-3.450056
C	-3.526087	-1.764322	-0.859401
C	-2.376033	-1.502778	-1.620258
H	-0.904127	-2.642829	-3.656966
H	-2.617186	-4.084216	-2.284973
H	-3.446105	-2.307475	0.089457
H	0.518992	-0.846205	-2.575814
C	-0.179895	-2.861509	-2.859475
Cu	-0.784495	-1.152440	-0.440072
C	0.942411	-1.840866	-2.819215
C	-1.871559	-4.142197	-1.480451
C	-0.878362	-3.009021	-1.523263
H	0.238446	-3.855722	-3.104270
H	-2.400283	-4.198612	-0.520119
H	-1.320820	-5.090163	-1.597571
C	1.982079	-2.217869	-1.777838
C	0.057486	-3.029459	-0.379636
C	1.393169	-2.641787	-0.461222
H	-0.282743	-3.467455	0.566716
O	2.177368	-2.739293	0.565477
N	0.168497	1.586261	0.189339
C	-0.638819	0.556106	0.480448
N	-1.282055	0.845207	1.617856
C	-0.878781	2.128432	2.205958

C	0.171154	2.659468	1.220349
C	1.085470	1.587328	-0.890285
C	0.633824	1.976097	-2.157614
H	-0.418720	2.248357	-2.271427
Al	3.891538	-2.256682	0.967547
C	-1.351491	4.319460	0.063222
H	-2.172282	3.599961	0.149265
H	1.167942	2.678026	1.689792
C	2.432796	1.231688	-0.722364
C	1.504048	2.013213	-3.241863
C	3.307558	1.286417	-1.812784
C	2.846136	1.671771	-3.066994
H	1.135971	2.315601	-4.224546
H	4.354068	1.006408	-1.672693
H	3.538641	1.704736	-3.910677
C	-2.248453	-0.027490	2.202792
C	-1.800791	-1.147503	2.931457
C	-3.615628	0.238990	2.001493
C	-2.769102	-2.009490	3.462522
C	-4.546631	-0.642881	2.564625
C	-4.128243	-1.756932	3.287542
H	-4.867984	-2.438461	3.714955
C	-0.092684	4.003059	0.590648
C	0.952388	4.921792	0.448902
C	0.744051	6.139536	-0.199933
H	1.941747	4.670181	0.844314
C	-1.561742	5.534674	-0.584452
C	-0.513625	6.448628	-0.716173
H	1.569055	6.848512	-0.303546
H	-2.547926	5.770641	-0.991931
H	-0.678632	7.401075	-1.225788
H	-5.613286	-0.454573	2.413241
C	-4.060475	1.405159	1.179127
C	-0.342337	-1.407165	3.129864
H	-2.442965	-2.885319	4.030254
H	-3.536987	1.444212	0.211090
H	-3.866202	2.366831	1.680349
H	-5.138038	1.362601	0.976287
H	0.198015	-1.513911	2.176690
H	-0.177436	-2.319666	3.716743
H	0.155639	-0.575430	3.650010
C	5.161314	-3.166096	-0.224150
H	5.182518	-2.730444	-1.238078
H	4.928931	-4.237806	-0.353566
H	6.199626	-3.124050	0.147915
O	2.076481	0.327983	1.777727
C	4.057180	-2.387733	2.913959
H	4.977558	-1.911645	3.294012
H	4.081121	-3.430221	3.275638
H	3.216485	-1.894979	3.431748
H	2.587872	-3.073255	-2.132075
H	2.707676	-1.405973	-1.611343
H	1.412503	-1.731413	-3.807570
S	3.140340	0.746939	0.858391
O	3.994373	1.861488	1.271475
O	4.003084	-0.465651	0.441974
H	-0.462674	1.972316	3.212029
H	-1.742924	2.803675	2.308628

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Scheme_S10_XL / electronic energy: -5439.94152073 a.u. / lowest freq: -268.63 cm-1

C	-1.348166	-2.528229	-2.206018
H	-1.709987	-3.489250	-1.814702
C	0.149602	-2.332711	-1.870705
H	0.707984	-2.098142	-2.791470
C	-1.102513	-0.657670	-0.764997
C	-3.371164	-1.146782	-1.477563
C	-3.810973	-0.204408	-2.411861
C	-4.314845	-1.791505	-0.660069
C	-5.168571	0.078003	-2.549633
H	-3.070009	0.299085	-3.037701
C	-5.673461	-1.507070	-0.801506
C	-6.101133	-0.579578	-1.749882
H	-5.495554	0.816366	-3.285045
H	-6.387888	-2.015596	-0.151431
H	-7.167072	-0.366756	-1.855636
S	-3.826204	-2.949208	0.620337
O	-5.058428	-3.445659	1.244070
O	-3.054525	-2.050920	1.615865
O	-2.922921	-3.933716	0.024788
Cu	-1.637013	0.942770	0.186100
C	-1.717958	-2.410787	-3.661105
C	-2.644322	-3.301755	-4.212651
C	-1.210815	-1.377054	-4.459912

C	-3.053316	-3.169420	-5.539889
H	-3.051545	-4.102517	-3.587715
C	-1.617788	-1.243321	-5.785402
H	-0.501682	-0.657687	-4.037084
C	-2.540606	-2.140115	-6.328438
H	-3.776149	-3.873816	-5.958378
H	-1.215761	-0.433130	-6.398563
H	-2.859160	-2.035125	-7.368352
N	-1.980850	-1.444667	-1.397796
N	0.132408	-1.135871	-0.996151
C	-2.856639	1.419645	1.820674
C	-2.142214	0.899371	2.900437
O	-2.534019	-0.139877	3.563743
C	-0.887568	1.545372	3.395751
Al	-3.798607	-1.428108	3.223220
C	-2.484636	2.647078	1.092144
C	-3.593735	3.445664	0.499748
H	-1.772939	3.274089	1.638910
C	-4.727511	2.837741	-0.061023
C	-3.500016	4.844970	0.465626
H	-3.819575	0.949452	1.600316
C	-0.188217	3.400220	-0.514867
H	0.443901	3.232855	0.369274
C	-3.587368	-2.804550	4.594810
C	-5.557745	-0.608884	2.897012
H	-5.706633	-0.242425	1.865773
H	-5.733478	0.262195	3.553687
H	-6.385390	-1.313076	3.089229
H	-3.860930	-2.454068	5.604833
H	-2.552104	-3.179504	4.665342
H	-4.222844	-3.684101	4.393437
C	-5.741330	3.607784	-0.627038
H	-4.818609	1.747477	-0.065449
C	-4.517548	5.615841	-0.092408
H	-2.612087	5.329503	0.883167
C	-5.642735	5.000114	-0.642440
H	-6.616720	3.115295	-1.058857
H	-4.429700	6.705026	-0.100391
H	-6.439621	5.603269	-1.083916
H	-1.128264	2.386898	4.065740
H	-0.269545	1.948838	2.581589
H	-0.291757	0.828380	3.973857
C	-1.359603	2.732487	-0.614882
H	-2.022061	2.922318	-1.472500
C	0.368494	4.340905	-1.483420
C	1.709891	4.752167	-1.354426
C	-0.383470	4.873139	-2.550550
C	2.278876	5.650644	-2.253882
H	2.307951	4.348090	-0.530590
C	0.186459	5.769243	-3.448043
H	-1.433279	4.588877	-2.666287
C	1.520701	6.162854	-3.307671
H	3.321966	5.954945	-2.132088
H	-0.417723	6.173063	-4.264553
H	1.963100	6.869988	-4.013278
H	3.124931	-5.940907	-1.784268
H	2.520770	-6.535795	0.558393
C	2.376470	-5.355087	-1.245200
C	2.038868	-5.687281	0.066199
C	1.769536	-4.263380	-1.867034
C	1.081357	-4.933395	0.748557
H	0.807640	-5.195130	1.773751
C	0.806675	-3.507616	-1.191491
C	0.463084	-3.853158	0.122173
H	-0.302663	-3.278643	0.652814
H	2.046292	-3.990360	-2.890189
H	8.458034	-0.777443	-2.962373
H	7.111461	1.277897	-3.273329
H	5.711871	2.790593	-3.908475
H	6.260656	3.193352	-1.377809
C	7.488370	-0.680472	-2.466988
C	6.730233	0.472675	-2.639549
C	4.714267	2.437789	-3.605648
C	5.199896	2.956764	-1.197076
C	7.007974	-1.716330	-1.670449
H	7.608617	-2.621464	-1.552578
H	4.633618	3.895760	-1.290782
C	5.486441	0.616559	-2.011593
C	4.698447	1.903343	-2.180365
H	5.114876	2.613280	-0.155458
H	5.453515	-4.284060	-1.698944
C	5.769391	-1.617775	-1.024268
C	5.016513	-0.430821	-1.189002

H	3.646720	1.687984	-1.922825
H	6.784780	-4.288309	-0.525609
C	5.701804	-4.127042	-0.638734
C	5.272583	-2.753147	-0.143219
C	3.710540	-0.287691	-0.482457
H	5.206496	-4.918778	-0.058443
H	4.167623	-2.726817	-0.159282
H	4.387197	4.533112	1.642472
H	1.871672	5.082699	1.733113
H	6.801822	-2.579765	1.401345
C	5.704223	-2.559195	1.308887
C	3.656217	0.266504	0.801357
H	2.643161	2.788864	1.320048
C	4.223917	3.746598	2.395225
H	4.581004	0.596453	1.284147
H	4.975608	2.960874	2.229587
C	1.790280	4.330006	2.531833
H	5.357945	-1.601741	1.724391
C	2.799907	3.203421	2.332307
H	5.303410	-3.361796	1.946673
H	4.432143	4.192429	3.380698
C	2.449018	0.336300	1.509923
H	0.752486	3.963628	2.537444
H	1.951794	4.858729	3.483701
C	2.602684	2.080610	3.335804
C	2.434536	0.732135	2.947593
C	2.576729	2.400447	4.699106
H	2.705584	3.441913	5.007930
C	2.248028	-0.276588	3.925314
C	2.034049	-1.739289	3.567833
H	3.964369	-2.390720	4.368242
C	2.388098	1.417861	5.664981
C	2.902936	-2.677051	4.397892
C	2.225601	0.092112	5.276158
H	2.827087	-3.707578	4.019445
H	2.367279	1.685608	6.724562
H	2.596737	-2.703258	5.454711
H	2.074387	-0.676778	6.039038
H	4.033468	3.296137	-3.703778
H	4.396126	1.679016	-4.335693
H	2.572386	-1.188203	-2.077507
C	2.529943	-0.742502	-1.080774
C	1.311091	-0.637015	-0.405318
C	1.277479	-0.104808	0.889452
H	0.335536	-0.110002	1.445447
H	2.323169	-1.884739	2.513164
H	-0.090743	-1.527496	3.036347
C	0.558811	-2.113770	3.703686
H	0.391976	-3.177677	3.477019
H	0.200727	-1.938853	4.731190

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Scheme_S10_XLI / electronic energy: -5439.94245882 a.u. / lowest freq: -243.82 cm-1

C	1.555632	-2.153720	2.092411
O	2.836158	-1.933773	2.176467
C	1.053020	3.248559	-0.262252
H	1.098340	3.440004	0.827185
C	-0.389629	2.892307	-0.657151
H	-0.549699	3.126627	-1.725475
C	0.878461	0.918457	-0.488629
C	3.136883	1.804776	-0.321799
C	3.974660	1.915292	-1.434787
C	3.700246	1.565998	0.943504
C	5.355092	1.802300	-1.300824
H	3.518129	2.076485	-2.414220
C	5.088932	1.466047	1.073440
C	5.912405	1.578355	-0.042941
H	5.994868	1.877121	-2.183336
H	5.523099	1.295320	2.060111
H	6.994678	1.485367	0.073150
S	2.729701	1.535058	2.457597
O	3.539104	0.595179	3.367787
O	1.399365	0.973506	2.179240
O	2.769201	2.895018	2.996961
Cu	1.449618	-0.947433	-0.356504
C	1.671347	4.407809	-0.988680
C	2.259036	5.448450	-0.262079
C	1.700759	4.454182	-2.389190
C	2.857758	6.522997	-0.920447
H	2.251110	5.407585	0.831293
C	2.300141	5.525423	-3.047251
H	1.262158	3.636517	-2.970014
C	2.878415	6.563853	-2.313643
H	3.312575	7.329554	-0.340543

H	2.319080	5.550410	-4.139533
H	3.348300	7.403933	-2.830682
N	1.734938	1.952396	-0.509893
N	-0.366073	1.417618	-0.499741
C	0.995765	-2.592325	0.897027
C	0.715388	-1.970534	3.307869
Al	3.947548	-1.224438	3.444483
C	1.817452	-2.978692	-0.262667
C	1.128539	-3.765202	-1.315879
H	2.797245	-3.364700	0.030432
C	-0.078353	-3.305901	-1.868428
C	1.660720	-4.975468	-1.779112
H	-0.085186	-2.760210	0.867504
C	4.153925	-1.606189	-1.328660
H	4.486928	-1.642504	-0.280316
C	3.539082	-1.801225	5.273626
C	5.765504	-1.494601	2.761404
H	5.868903	-1.289248	1.682341
H	6.094372	-2.538988	2.906507
H	6.517761	-0.869382	3.272845
H	3.460920	-2.898766	5.364108
H	2.603442	-1.384164	5.681112
H	4.339567	-1.500442	5.972186
C	-0.746492	-4.047581	-2.838213
H	-0.490286	-2.347144	-1.524961
C	0.990889	-5.720261	-2.750328
H	2.607420	-5.336686	-1.367375
C	-0.215140	-5.261611	-3.280541
H	-1.690258	-3.681044	-3.250693
H	1.415738	-6.665916	-3.096118
H	-0.739010	-5.844902	-4.041563
H	0.959994	-2.747352	4.050465
H	-0.357331	-2.044510	3.086878
H	0.918843	-0.997787	3.778448
C	2.828420	-1.657728	-1.577481
H	2.453303	-1.740183	-2.609668
C	5.237128	-1.479172	-2.301402
C	6.571549	-1.523876	-1.852398
C	5.014668	-1.274189	-3.677647
C	7.637226	-1.376664	-2.736687
H	6.764408	-1.673415	-0.785571
C	6.079244	-1.127068	-4.560448
H	3.990540	-1.218304	-4.056882
C	7.397436	-1.175691	-4.096785
H	8.663009	-1.417217	-2.361229
H	5.880939	-0.966621	-5.623430
H	8.230971	-1.055310	-4.792958
H	-3.768634	6.065948	-0.122918
H	-2.059419	4.858557	-1.468672
C	-3.173696	5.273592	0.337930
C	-2.215829	4.597115	-0.417431
H	-4.135166	5.450980	2.264636
C	-3.378230	4.929379	1.673447
C	-1.443391	3.583919	0.158973
C	-2.615343	3.913304	2.253435
C	-1.647378	3.246971	1.504160
H	-2.771611	3.644351	3.301283
H	-1.039996	2.458685	1.962898
H	-8.159209	0.774748	-4.112453
H	-6.561915	-1.053840	-4.591211
H	-3.616258	-0.737349	-5.201758
H	-5.274934	-2.728250	-4.893105
C	-7.270795	0.650053	-3.487786
C	-6.373304	-0.379598	-3.751966
C	-3.162340	-1.067745	-4.254057
C	-4.844111	-2.897763	-3.894767
C	-7.036405	1.524111	-2.430385
H	-7.749767	2.328067	-2.235532
H	-4.085292	-3.685363	-4.012775
C	-5.231732	-0.559694	-2.960857
C	-4.220720	-1.638356	-3.311914
H	-5.641345	-3.301149	-3.253043
H	-5.930529	4.175556	-1.571215
C	-5.906596	1.386256	-1.614468
C	-5.004553	0.330436	-1.885666
H	-3.705436	-1.932379	-2.380221
H	-7.382439	3.689927	-0.671078
C	-6.282313	3.706086	-0.640141
C	-5.690847	2.319673	-0.433851
C	-3.813701	0.127825	-1.011719
H	-6.004939	4.369508	0.191376
H	-4.600113	2.444536	-0.306434
H	-3.827927	-4.827831	-1.094581

H	-1.481368	-5.569769	-0.469558
H	-7.316210	1.549055	0.798935
C	-6.226384	1.700439	0.856224
C	-3.863049	-0.824859	0.014434
H	-2.153676	-3.257333	-0.135762
C	-3.962944	-4.388639	-0.093696
H	-4.794498	-1.373376	0.182176
H	-4.637335	-3.526588	-0.196144
C	-1.698206	-5.225444	0.552539
H	-5.771255	0.722278	1.069810
C	-2.618351	-4.011327	0.524891
H	-6.027670	2.353599	1.719995
H	-4.483566	-5.137641	0.524072
C	-2.771499	-1.050604	0.860182
H	-0.736288	-5.012714	1.043762
H	-2.155344	-6.077107	1.079176
C	-2.796458	-3.364364	1.887420
C	-2.890089	-1.959531	2.037266
C	-2.884932	-4.168899	3.029887
H	-2.808840	-5.254613	2.930779
C	-3.086506	-1.384712	3.314891
C	-3.184974	0.117351	3.529910
H	-5.335903	0.107267	3.931478
C	-3.062950	-3.610232	4.292203
C	-4.403244	0.502114	4.361223
C	-3.163906	-2.230500	4.429175
H	-4.504112	1.596218	4.419099
H	-3.123131	-4.254965	5.172855
H	-4.335002	0.133922	5.396327
H	-3.301260	-1.796362	5.423561
H	-2.394808	-1.816689	-4.501063
H	-2.649218	-0.197977	-3.817045
H	-2.589750	1.627372	-1.980594
C	-2.640918	0.867934	-1.195186
C	-1.538682	0.639965	-0.367669
C	-1.602100	-0.309829	0.655535
H	-0.745038	-0.417071	1.325768
H	-3.301487	0.602876	2.545804
H	-1.025770	0.491929	3.506774
C	-1.900328	0.656073	4.153563
H	-1.970137	1.737400	4.346102
H	-1.689066	0.168578	5.119112

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Scheme_S10_XLII / electronic energy: -4550.91934608 a.u. / lowest freq: -231.04 cm-1

C	-0.285269	-0.771213	-3.170293
O	0.535521	0.227007	-3.300355
C	2.403329	-1.301783	1.883929
H	3.160233	-1.707168	1.188088
C	1.393966	-2.384411	2.259553
H	1.044189	-2.293736	3.302347
C	0.376168	-0.941684	0.726069
C	2.007807	0.861034	0.605714
C	1.673559	2.026717	1.302414
C	2.818973	0.948512	-0.535217
C	2.158926	3.263504	0.888380
H	1.021329	1.940692	2.175868
C	3.313209	2.191862	-0.941338
C	2.985949	3.343899	-0.232143
H	1.893853	4.165034	1.444768
H	3.949856	2.253736	-1.826214
H	3.376973	4.308976	-0.561539
C	-0.936078	-2.884723	1.402246
C	-1.203885	-3.885715	0.442182
C	-1.837873	-2.577889	2.441786
C	-2.386694	-4.620544	0.594787
C	-3.003312	-3.346274	2.549881
C	-3.267111	-4.367599	1.644581
H	-4.179718	-4.961150	1.741721
S	3.329096	-0.497817	-1.472238
O	3.390674	0.048514	-2.911661
O	2.306743	-1.544808	-1.352979
O	4.680773	-0.833076	-1.021263
Cu	-0.794506	-0.120119	-0.604899
C	3.102598	-0.592439	3.012786
C	4.469360	-0.310526	2.912948
C	2.395583	-0.131527	4.131544
C	5.121806	0.407931	3.915303
H	5.021739	-0.651314	2.032041
C	3.045565	0.585627	5.133463
H	1.321375	-0.326739	4.216832
C	4.411414	0.856229	5.027978
H	6.189692	0.620239	3.824060
H	2.482668	0.938543	6.000978

H	4.920173	1.419517	5.814002
N	1.532637	-0.379764	1.102760
N	0.282262	-2.137533	1.325573
C	-1.510675	-0.639486	-2.517977
C	0.111429	-2.077434	-3.768481
Al	2.110266	0.622470	-4.136116
H	-3.721183	-3.126660	3.344901
C	-2.138125	0.634033	-2.065700
C	-1.627962	-1.387169	3.357983
H	1.796691	-3.398242	2.144887
C	-0.276515	-4.114329	-0.739924
H	-2.632660	-5.404700	-0.123340
H	-0.575847	-1.075810	3.284553
H	-0.023231	-3.109139	-1.130582
C	-3.528948	0.429430	-1.531833
C	-1.972618	1.798438	-3.017669
C	-3.803996	-0.590830	-0.602550
C	-4.593240	1.255402	-1.922939
H	-2.119557	-1.545654	-2.452733
C	-2.156530	2.425193	0.304369
H	-3.037882	1.878870	0.670519
C	2.444374	-0.404958	-5.772448
C	2.134244	2.584145	-4.196709
H	1.760976	3.046524	-3.265837
H	1.491148	2.970928	-5.007367
H	3.135601	3.011656	-4.378013
H	1.615568	-0.366787	-6.500248
H	2.651799	-1.471591	-5.583064
H	3.329228	-0.012525	-6.303999
C	-5.082573	-0.773435	-0.082815
H	-2.995791	-1.251231	-0.262580
C	-5.877209	1.068832	-1.409935
H	-4.427492	2.057834	-2.643517
C	-6.129470	0.057328	-0.485412
H	-5.262195	-1.569971	0.643762
H	-6.686881	1.725357	-1.738309
H	-7.134230	-0.084784	-0.080534
H	-2.484998	1.557952	-3.963887
H	-0.921857	1.979871	-3.259317
H	-2.400653	2.731224	-2.629410
H	0.249729	-1.954852	-4.853770
H	-0.638985	-2.858692	-3.608410
H	1.077902	-2.407826	-3.357342
C	1.038957	-4.782817	-0.352440
H	0.868175	-5.776198	0.091333
H	1.671529	-4.921254	-1.241659
H	1.625735	-4.191811	0.359776
C	-0.932704	-4.901626	-1.863244
H	-0.264752	-4.953278	-2.734456
H	-1.140463	-5.941731	-1.568248
H	-1.883288	-4.457594	-2.195189
C	-1.902641	-1.697215	4.821606
H	-1.302063	-2.545497	5.182178
H	-1.661981	-0.829181	5.452777
H	-2.960129	-1.939436	5.005336
C	-2.457404	-0.206421	2.860689
H	-2.252610	0.701699	3.449278
H	-2.224856	0.021311	1.808402
H	-3.538310	-0.410390	2.926450
C	-1.282100	1.787272	-0.498686
H	-0.428633	2.337859	-0.929042
C	-2.058757	3.801830	0.785671
C	-2.914845	4.234213	1.817676
C	-1.141144	4.734160	0.259308
C	-2.849430	5.533941	2.313371
H	-3.640846	3.527007	2.230899
C	-1.078650	6.032671	0.753791
H	-0.479205	4.436790	-0.559618
C	-1.928682	6.440641	1.786069
H	-3.524158	5.843135	3.115877
H	-0.363093	6.739624	0.325392
H	-1.877557	7.462189	2.170359

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Scheme_S10_XLIII / electronic energy: -4550.91984075 a.u. / lowest freq: -237.83 cm-1

C	-0.101207	-1.956437	2.457219
H	0.485506	-1.836732	3.378907
C	0.544392	-2.978641	1.515581
H	-0.055450	-3.893931	1.406314
C	0.376061	-0.948347	0.367892
C	-0.166411	0.576190	2.184017
C	-1.457982	1.064146	2.402654
C	0.938565	1.378328	2.528424
C	-1.650730	2.333323	2.946093

H	-2.310939	0.437269	2.132536
C	0.740080	2.649100	3.068668
C	-0.553215	3.125204	3.277910
H	-2.666179	2.704168	3.105061
H	1.610260	3.252309	3.334568
H	-0.699870	4.119148	3.705986
C	1.222947	-2.848273	-0.929266
C	2.622683	-3.026102	-0.959634
C	0.399565	-3.237874	-2.009079
C	3.183114	-3.644330	-2.084567
C	1.014184	-3.835368	-3.115894
C	2.389733	-4.048295	-3.151523
H	2.844888	-4.525028	-4.023314
S	2.629494	0.783345	2.378325
O	3.484220	1.763804	3.056994
O	2.902821	0.797352	0.860064
O	2.650551	-0.595899	2.875334
Cu	0.177276	0.487573	-0.923739
C	-1.549220	-2.214131	2.794746
C	-1.978969	-2.261408	4.123051
C	-2.493001	-2.363345	1.768386
C	-3.328436	-2.457811	4.424234
H	-1.248627	-2.136118	4.927886
C	-3.838217	-2.562626	2.065690
H	-2.168757	-2.301851	0.723807
C	-4.259515	-2.608468	3.397701
H	-3.652773	-2.489473	5.467291
H	-4.563785	-2.678090	1.255942
H	-5.315773	-2.760109	3.633030
N	0.028947	-0.720055	1.644585
N	0.633993	-2.256613	0.234651
C	1.130341	2.039534	-1.891656
C	2.193971	1.214690	-2.257988
O	3.383914	1.422977	-1.765472
C	2.112500	0.091085	-3.245532
Al	3.882980	2.061034	-0.118465
H	0.403986	-4.147336	-3.966229
C	-0.302619	2.055993	-2.307361
C	-1.105845	-3.052580	-1.972253
H	1.547882	-3.272089	1.858448
C	3.527694	-2.566641	0.164088
H	4.265231	-3.798130	-2.123095
H	-1.311649	-2.158462	-1.356731
H	2.934286	-1.956192	0.860085
C	-0.973249	3.278717	-1.745126
C	-0.605357	1.767444	-3.759678
C	-0.814627	3.608176	-0.388368
C	-1.754823	4.127844	-2.539315
H	1.414476	2.825753	-1.187929
C	-2.747984	1.036002	-0.888275
H	-2.614347	1.845615	-0.157175
C	5.813833	1.773314	0.054864
C	3.173256	3.844179	0.326503
H	2.123008	3.834920	0.669708
H	3.208936	4.553111	-0.519874
H	3.753965	4.313019	1.140478
H	6.213126	0.986851	-0.606834
H	6.095909	1.493190	1.084939
H	6.386365	2.689662	-0.172483
C	-1.404059	4.746863	0.152320
H	-0.229387	2.943602	0.259193
C	-2.346946	5.270493	-1.998561
H	-1.902798	3.911362	-3.598695
C	-2.174414	5.587922	-0.653283
H	-1.261856	4.979141	1.210938
H	-2.945098	5.920135	-2.642469
H	-2.636181	6.484172	-0.232381
H	-0.103772	2.512788	-4.397463
H	-1.681384	1.808763	-3.974183
H	-0.253443	0.781403	-4.078883
H	2.291646	0.456988	-4.269094
H	1.135472	-0.412127	-3.241448
H	2.889560	-0.652414	-3.024920
C	4.098773	-3.752715	0.936252
H	4.774495	-4.352630	0.305947
H	4.679151	-3.408744	1.805500
H	3.317413	-4.432434	1.307753
C	4.649324	-1.667381	-0.339392
H	4.262861	-0.818973	-0.922935
H	5.211234	-1.253163	0.511210
H	5.369882	-2.211980	-0.970101
C	-1.709062	-2.809732	-3.347958
H	-1.627422	-3.691520	-4.000684

H	-2.782458	-2.588195	-3.267014
H	-1.230148	-1.969075	-3.874085
C	-1.781672	-4.241626	-1.293007
H	-2.867680	-4.082603	-1.203475
H	-1.628319	-5.165698	-1.872330
H	-1.388814	-4.421692	-0.281976
C	-1.682290	0.635257	-1.611970
H	-1.815639	-0.124758	-2.397547
C	-4.097539	0.474860	-0.909831
C	-5.029746	0.890883	0.060704
C	-4.511798	-0.493062	-1.845904
C	-6.314094	0.353086	0.104251
H	-4.729399	1.648843	0.791299
C	-5.794161	-1.028631	-1.803344
H	-3.816418	-0.817044	-2.624563
C	-6.702925	-0.612527	-0.825136
H	-7.017648	0.691906	0.869061
H	-6.093296	-1.775724	-2.543404
H	-7.709921	-1.035262	-0.793381

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Scheme_S11_S.XXI / electronic energy: -4776.97951262 a.u. / lowest freq: -249.48 cm-1

C	-1.903906	-1.059563	1.758714
H	-1.857602	-2.132862	2.007796
C	-2.688338	-0.834444	0.437649
C	-0.422750	-0.248290	0.095080
C	0.601178	-0.719666	2.226325
C	0.858119	0.274549	3.173504
C	1.503417	-1.790076	2.086202
C	2.007789	0.221176	3.959861
H	0.149550	1.099295	3.276372
C	2.656545	-1.834908	2.870248
C	2.911540	-0.826670	3.798741
H	2.198689	1.007469	4.693138
H	3.351446	-2.667905	2.756266
H	3.819105	-0.869907	4.404242
S	1.098043	-3.186594	1.026371
O	2.382558	-4.032266	1.059893
O	0.841677	-2.725319	-0.350433
O	-0.000103	-3.882747	1.700586
Cu	1.236377	0.413477	-0.689503
C	-2.423518	-0.289766	2.943831
C	-2.646469	-0.925780	4.167755
C	-2.636481	1.092068	2.846068
C	-3.078104	-0.194099	5.275942
H	-2.474026	-2.002670	4.252362
C	-3.065893	1.823967	3.949144
H	-2.450037	1.599643	1.893834
C	-3.287734	1.180009	5.169586
H	-3.249422	-0.702573	6.227804
H	-3.227288	2.901664	3.858155
H	-3.623985	1.752105	6.037680
N	-0.536904	-0.617795	1.378939
N	-1.622614	-0.354685	-0.486027
C	3.312085	0.221707	-0.537677
C	3.383712	-1.068111	-1.056358
O	3.816054	-2.032545	-0.299154
C	3.042419	-1.410754	-2.470821
Al	3.780487	-3.847765	-0.190247
C	2.992376	1.451624	-1.293948
C	3.611869	2.711592	-0.800199
H	3.129468	1.336420	-2.374401
C	3.734253	2.999330	0.567606
C	4.040983	3.675976	-1.724316
H	3.633752	0.319099	0.504738
C	0.760484	2.203591	-2.854354
H	1.160146	1.453289	-3.545975
C	3.265436	-4.789306	-1.833290
C	5.381637	-4.413454	0.787431
H	5.639070	-3.733097	1.617264
H	6.279734	-4.472686	0.148767
H	5.261667	-5.415544	1.234417
H	3.919630	-4.578905	-2.696785
H	2.233825	-4.564204	-2.152342
H	3.307467	-5.882679	-1.682741
C	4.266474	4.214279	0.995461
H	3.389185	2.275635	1.311496
C	4.582878	4.886403	-1.298000
H	3.936185	3.470541	-2.794295
C	4.693538	5.162924	0.065702
H	4.343719	4.423201	2.065582
H	4.917468	5.620712	-2.035083
H	5.110335	6.115057	0.402825
H	3.932694	-1.802917	-2.986877

H	2.655475	-0.561817	-3.048685
H	2.290793	-2.212853	-2.483290
C	1.125059	2.251424	-1.559536
H	0.017401	2.895017	-3.274406
C	0.703454	3.322470	-0.643487
C	0.483691	3.081760	0.725114
C	0.527677	4.638143	-1.112692
C	0.068329	4.098129	1.582142
H	0.646570	2.073116	1.119988
C	0.117505	5.656912	-0.256736
H	0.728174	4.858289	-2.165265
C	-0.117455	5.392420	1.094239
H	-0.102213	3.879920	2.640235
H	-0.012538	6.670074	-0.645678
H	-0.433039	6.194859	1.765464
H	-6.546990	-3.124960	-0.879029
H	-5.259105	-5.157363	-1.526287
C	-5.460621	-3.146407	-0.763047
C	-4.739941	-4.283774	-1.124316
C	-4.794205	-2.030446	-0.254011
C	-3.351353	-4.303685	-0.972500
H	-2.782249	-5.193415	-1.252951
C	-3.404869	-2.044967	-0.097964
C	-2.685835	-3.192088	-0.461671
H	-1.597923	-3.212119	-0.341374
H	-5.356728	-1.134322	0.026410
C	-2.950540	0.498324	-3.854315
C	-2.105095	-0.261006	-4.656575
H	-2.244869	-0.257041	-5.741112
C	-1.074505	-1.028332	-4.095494
C	-0.136619	-1.820182	-4.948465
C	-2.804674	0.543206	-2.459220
C	-1.795032	-0.258166	-1.893630
C	-0.951161	-1.026349	-2.702358
H	-0.203722	-1.655804	-2.208039
H	-0.598608	-2.113538	-5.900345
H	0.210403	-2.730611	-4.441039
H	0.763597	-1.236740	-5.202523
H	-3.729413	1.110077	-4.318078
H	-1.986977	2.371557	-0.630902
H	-3.404655	3.909019	0.705807
C	-3.075558	2.346663	-0.742499
C	-3.872351	3.211336	0.005380
C	-3.653745	1.444797	-1.651384
C	-5.260893	3.187178	-0.135929
H	-5.885353	3.860235	0.456464
C	-5.049549	1.443645	-1.798581
C	-5.846155	2.302686	-1.042897
H	-5.512419	0.743131	-2.499881
H	-6.932331	2.278677	-1.161217
H	-3.423449	-0.023526	0.578096

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Scheme_S11_S.XXII / electronic energy: -4776.97661758 a.u. / lowest freq: -269.78 cm-1

C	2.152584	-0.226337	-2.461585
O	2.295962	-1.493398	-2.192580
C	-2.933997	-0.475358	0.073131
H	-3.358658	-1.074917	-0.743072
C	-2.851905	1.005163	-0.335351
H	-3.412811	1.653057	0.358741
C	-0.654481	0.202801	0.044388
C	-1.080604	-2.058402	0.819336
C	-0.757397	-2.024393	2.179976
C	-1.064247	-3.291528	0.148041
C	-0.461025	-3.195355	2.871748
H	-0.760879	-1.058641	2.693676
C	-0.771715	-4.465263	0.844089
C	-0.483780	-4.419702	2.206421
H	-0.211835	-3.148439	3.934401
H	-0.761684	-5.410958	0.299071
H	-0.259745	-5.343896	2.743603
C	-0.863331	2.572090	-0.510533
C	-0.339443	2.768959	-1.789172
C	-0.959275	3.638245	0.405275
C	0.109479	4.023948	-2.215114
C	-0.528601	4.899280	-0.036184
C	-0.006518	5.089668	-1.312221
H	0.321670	6.087872	-1.615082
S	-1.376173	-3.413866	-1.612485
O	-0.289211	-2.499278	-2.221038
O	-2.700078	-2.846330	-1.885592
O	-1.152738	-4.810716	-1.996781
Cu	1.299625	0.340005	-0.063180
C	-3.674985	-0.808523	1.341707

C	-4.267693	-2.073271	1.455688
C	-3.702260	0.053067	2.443595
C	-4.866653	-2.472654	2.648984
H	-4.243671	-2.751262	0.596499
C	-4.302717	-0.344014	3.638056
H	-3.242356	1.042953	2.376108
C	-4.882248	-1.608963	3.745041
H	-5.323890	-3.462280	2.723126
H	-4.317218	0.339682	4.490854
H	-5.350874	-1.919788	4.681935
N	-1.477692	-0.849806	0.183731
N	-1.397865	1.292204	-0.183161
C	2.648848	0.754808	-1.610552
C	1.481018	0.151424	-3.740899
Al	1.426983	-2.996307	-2.783627
H	-0.588287	5.745196	0.654051
C	3.394677	0.473042	-0.371163
C	0.691096	4.205400	-3.579636
C	4.391996	1.500034	0.027003
H	3.804575	-0.544646	-0.360170
C	4.125712	2.874613	-0.075136
C	5.639344	1.096726	0.526000
H	2.549940	1.791737	-1.941046
C	2.404311	1.349866	2.268906
H	2.398138	1.324582	3.366894
C	1.382667	-3.171682	-4.736876
C	2.116743	-4.473429	-1.697272
H	1.606063	-4.550471	-0.722460
H	3.194982	-4.372512	-1.483316
H	1.984422	-5.452978	-2.187000
H	2.375021	-3.067686	-5.209118
H	0.718814	-2.446887	-5.237092
H	1.015178	-4.172506	-5.025576
C	5.076254	3.814676	0.316857
H	3.153975	3.216693	-0.445611
C	6.593076	2.036935	0.910290
H	5.858298	0.028122	0.612673
C	6.314879	3.400715	0.810001
H	4.847237	4.880375	0.236740
H	7.561135	1.701488	1.290809
H	7.060807	4.138855	1.114281
H	2.020842	-0.290336	-4.592324
H	1.437331	1.236792	-3.890356
H	0.455609	-0.250145	-3.779096
C	2.556759	0.243924	1.521607
H	2.267959	2.340660	1.821701
C	2.866386	-1.091057	2.043635
C	3.433517	-1.258488	3.322595
C	2.625235	-2.241861	1.269978
C	3.712777	-2.527256	3.820156
H	3.665561	-0.377393	3.926842
C	2.911865	-3.511444	1.768138
H	2.203235	-2.122075	0.262901
C	3.451676	-3.660246	3.045889
H	4.151063	-2.633247	4.815953
H	2.714274	-4.392828	1.153305
H	3.681537	-4.656212	3.432343
H	-2.845537	0.203954	-4.947370
H	-4.022472	2.347445	-5.432816
C	-3.153571	0.858247	-4.127779
C	-3.813632	2.058892	-4.399736
C	-2.883961	0.488800	-2.811549
C	-4.210072	2.885039	-3.348492
H	-4.731338	3.823181	-3.554110
C	-3.271680	1.318966	-1.750509
C	-3.937876	2.516142	-2.030703
H	-4.232463	3.171697	-1.204739
H	-2.361581	-0.452685	-2.610055
H	1.743951	3.880757	-3.615664
H	0.672574	5.256437	-3.895378
H	0.153216	3.613165	-4.333600
H	-0.311240	1.915458	-2.472164
H	-3.634332	4.888216	4.010429
C	-2.434441	4.334564	2.307644
C	-2.871723	4.206771	3.625466
C	-1.463760	3.464762	1.785575
C	-2.335271	3.218243	4.451470
H	-2.671947	3.124952	5.486864
C	-0.942355	2.465316	2.624347
C	-1.365121	2.351046	3.946808
H	-0.175432	1.786630	2.239136
H	-0.934988	1.574805	4.586072
H	-2.855235	5.115071	1.667005

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Scheme_S11_S.XXIII / electronic energy: -4393.80164026 a.u. / lowest freq: -239.66 cm-1

C	2.941350	-2.005941	-0.190359
O	3.364082	-1.137974	-1.071630
C	-1.118352	2.492746	1.913821
H	-0.496148	3.382140	2.092007
C	-0.950242	1.466735	3.038173
H	-1.890145	1.264973	3.573862
C	-0.178244	0.488804	1.047445
C	-0.308412	2.407356	-0.481667
C	-1.371727	2.588634	-1.370756
C	0.955570	2.923470	-0.816717
C	-1.180109	3.262786	-2.575307
H	-2.352690	2.183012	-1.113018
C	1.143773	3.600967	-2.020989
C	0.076147	3.770409	-2.900627
H	-2.019757	3.385246	-3.263300
H	2.133567	3.996111	-2.256736
H	0.230011	4.302852	-3.841595
C	-0.178362	-0.950539	3.023999
C	1.152173	-1.198305	3.413770
C	-1.220117	-1.854956	3.301449
C	1.428558	-2.403976	4.070701
C	-0.897291	-3.045524	3.964738
C	0.415156	-3.320865	4.340579
H	0.649219	-4.255984	4.855360
S	2.370858	2.715142	0.261721
O	2.717293	1.219028	0.064740
O	1.938209	2.949642	1.640241
O	3.454709	3.549609	-0.269283
Cu	0.569473	-0.838269	-0.202395
C	-2.533340	2.915937	1.612781
C	-2.837271	4.260795	1.383345
C	-3.548928	1.958576	1.484192
C	-4.132243	4.645631	1.032172
H	-2.045608	5.010978	1.471793
C	-4.841056	2.339254	1.131175
H	-3.317056	0.901083	1.649520
C	-5.135166	3.685855	0.902922
H	-4.356794	5.700232	0.855007
H	-5.623761	1.583024	1.030811
H	-6.148533	3.985419	0.624969
N	-0.527170	1.751651	0.758231
N	-0.473733	0.266280	2.336467
C	1.703993	-2.626036	-0.292171
C	3.871819	-2.356973	0.923696
Al	4.136534	0.508508	-0.928289
H	-1.692815	-3.764156	4.180616
C	0.781286	-2.587794	-1.470126
C	-2.624673	-1.568531	2.878350
H	-0.205319	1.783973	3.784057
C	2.225510	-0.201200	3.127742
H	2.456572	-2.615842	4.377825
C	-0.106072	-0.730746	-2.104852
H	-2.698065	-1.390877	1.793276
H	-3.028070	-0.668382	3.367527
H	-3.296051	-2.399327	3.127775
H	1.980208	0.792514	3.530778
H	2.361147	-0.044246	2.045820
H	3.186802	-0.512542	3.555524
C	-0.456866	-3.409506	-1.256494
C	1.490581	-2.823249	-2.784799
C	-1.049768	-3.510173	0.015287
C	-1.089301	-4.076922	-2.317937
H	1.462910	-3.334416	0.504804
C	0.735635	0.034322	-2.819341
H	1.820668	-0.034432	-2.702146
H	0.367720	0.776993	-3.541611
C	5.743442	0.550339	0.198872
C	4.214781	1.267265	-2.736675
H	3.288329	1.784524	-3.039745
H	4.403657	0.499785	-3.508189
H	5.024860	2.010056	-2.836604
H	6.463040	-0.255465	-0.028149
H	5.523803	0.479177	1.278394
H	6.293559	1.498547	0.063717
C	-1.552947	-0.768578	-2.329268
C	-2.463657	-0.868263	-1.262134
C	-2.074925	-0.709761	-3.636257
C	-3.837742	-0.880613	-1.483415
C	-3.449620	-0.721417	-3.859230
C	-4.337972	-0.807662	-2.784966
H	-3.832577	-0.671786	-4.881851

H	-5.415890	-0.826762	-2.962984
H	-2.066331	-0.933232	-0.244704
H	-4.524590	-0.957342	-0.635325
H	-1.382967	-0.657906	-4.482247
C	-2.213374	-4.246571	0.220038
H	-0.604450	-2.977583	0.862909
C	-2.258935	-4.809519	-2.117478
H	-0.670130	-4.025751	-3.324380
C	-2.827460	-4.902117	-0.847957
H	-2.646036	-4.305157	1.222473
H	-2.727371	-5.315314	-2.965609
H	-3.741958	-5.479063	-0.690921
H	1.854565	-3.864575	-2.799857
H	2.363176	-2.171282	-2.888025
H	0.852136	-2.674306	-3.663951
H	4.765002	-2.847030	0.504543
H	3.422863	-3.036760	1.657610
H	4.234275	-1.457004	1.439861

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Scheme_S11_S.XXIV / electronic energy: -4393.79583611 a.u. / lowest freq: -258.44 cm-1

C	1.164032	-3.092130	0.565535
H	0.615733	-3.942528	0.135910
C	0.778636	-2.870137	2.030955
H	1.632314	-2.988255	2.715817
C	0.166392	-0.949081	0.824468
C	0.576073	-1.720227	-1.476611
C	1.731007	-1.378645	-2.188959
C	-0.605845	-1.988568	-2.191505
C	1.706505	-1.269759	-3.577517
H	2.655120	-1.195847	-1.637358
C	-0.628786	-1.871210	-3.582064
C	0.523711	-1.507134	-4.274713
H	2.617387	-0.992825	-4.113309
H	-1.557800	-2.083915	-4.114460
H	0.496286	-1.418294	-5.362819
C	-0.180239	-0.855057	3.240562
C	-1.560179	-0.865957	3.522442
C	0.754600	-0.249315	4.100390
C	-1.991483	-0.251355	4.705204
C	0.277835	0.349699	5.272649
C	-1.082171	0.346855	5.574154
H	-1.437448	0.818221	6.493941
S	-2.106936	-2.544425	-1.381666
O	-3.011858	-3.010119	-2.438969
O	-2.657388	-1.254898	-0.741082
O	-1.727246	-3.501600	-0.340442
Cu	-0.458421	0.878485	0.523706
C	2.637269	-3.241290	0.281666
C	3.094426	-4.239513	-0.583544
C	3.559886	-2.330420	0.814390
C	4.447770	-4.327012	-0.914509
H	2.378245	-4.948592	-1.009394
C	4.909934	-2.412793	0.483056
H	3.211390	-1.537361	1.483214
C	5.357007	-3.412243	-0.385215
H	4.791792	-5.111321	-1.593157
H	5.617549	-1.691759	0.900214
H	6.415837	-3.476572	-0.647472
N	0.630577	-1.846385	-0.064276
N	0.281344	-1.487821	2.046300
C	-1.998244	1.999066	-0.316021
C	-3.041493	1.645146	0.536888
O	-4.039554	0.929148	0.106687
C	-3.159089	2.026400	1.977572
Al	-4.188339	-0.304043	-1.234596
H	0.989714	0.831234	5.948787
C	-0.856445	2.945409	-0.116567
C	2.205926	-0.211934	3.749193
H	-0.013041	-3.558986	2.363845
C	-2.530048	-1.485334	2.570791
H	-3.059519	-0.248944	4.940820
C	0.771425	2.438061	1.120201
H	2.363771	0.207183	2.742539
H	2.660094	-1.215206	3.747245
H	2.773745	0.401284	4.460089
H	-2.251387	-2.513598	2.296781
H	-2.566617	-0.936892	1.615964
H	-3.545431	-1.505967	2.986940
C	-0.116108	3.167905	-1.408869
C	-1.210331	4.214245	0.626100
C	0.092275	2.111157	-2.314231
C	0.407706	4.423883	-1.749846
H	-2.138525	1.639818	-1.339383

C	0.597257	2.698892	2.428101
H	-0.381555	2.729003	2.915446
H	1.454269	2.877849	3.092512
C	-5.781577	-1.360499	-0.816956
C	-3.913777	0.437236	-3.036552
H	-2.855174	0.641515	-3.277796
H	-4.448008	1.391060	-3.192369
H	-4.278191	-0.247954	-3.822123
H	-6.718920	-0.781612	-0.883286
H	-5.740656	-1.763930	0.210093
H	-5.905176	-2.227454	-1.487702
C	2.093274	2.537954	0.490795
C	2.565783	1.544465	-0.382679
C	2.924021	3.646437	0.742254
C	3.826457	1.634622	-0.965511
C	4.182866	3.743091	0.153185
C	4.639994	2.738852	-0.702717
H	4.811526	4.612966	0.360638
H	5.624985	2.820102	-1.168749
H	1.913749	0.690587	-0.589147
H	4.174426	0.843953	-1.637093
H	2.565121	4.440965	1.403803
C	0.779032	2.304222	-3.509574
H	-0.272686	1.106227	-2.066737
C	1.104327	4.617988	-2.942606
H	0.276467	5.274763	-1.079785
C	1.290091	3.562000	-3.831931
H	0.920074	1.463126	-4.192825
H	1.498525	5.609789	-3.178206
H	1.829838	3.715724	-4.769330
H	-1.927264	4.787686	0.015147
H	-0.343137	4.854181	0.828281
H	-1.693636	4.021503	1.587383
H	-3.802337	2.914039	2.086113
H	-2.198661	2.242120	2.455944
H	-3.652499	1.215573	2.529120

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Scheme_S12_XLIV / electronic energy: -4409.29483899 a.u. / lowest freq: -120.00 cm-1

C	-2.022150	0.389869	1.585978
H	-2.040953	-0.539645	2.172899
C	-2.814668	0.209327	0.279839
H	-3.356306	1.142492	0.029280
C	-0.507292	0.329883	-0.227360
C	0.458718	0.760801	1.957823
C	1.157708	1.971094	1.909019
C	0.871761	-0.249674	2.845236
C	2.244371	2.198653	2.750085
H	0.829682	2.736221	1.198403
C	1.952301	-0.001896	3.694293
C	2.633230	1.213284	3.655960
H	2.777322	3.151029	2.701326
H	2.272287	-0.799325	4.368877
H	3.479084	1.383631	4.326806
C	-2.017298	0.001321	-2.116600
C	-2.046426	-1.244980	-2.775685
C	-2.277844	1.209561	-2.799451
C	-2.335520	-1.257246	-4.145964
C	-2.569506	1.142937	-4.166836
C	-2.598194	-0.077423	-4.836109
H	-2.824639	-0.108521	-5.905113
S	0.109334	-1.895730	2.910982
O	1.154325	-2.762757	3.503927
O	-0.230584	-2.228359	1.501590
O	-1.086361	-1.746705	3.782106
Cu	1.137733	0.281562	-1.207971
C	-2.493243	1.513043	2.472540
C	-2.888469	1.242006	3.786565
C	-2.531552	2.836118	2.011214
C	-3.329305	2.271071	4.620615
H	-2.830779	0.212957	4.153105
C	-2.966646	3.864676	2.843565
H	-2.208760	3.061354	0.989076
C	-3.370933	3.583126	4.151005
H	-3.635978	2.045546	5.645118
H	-2.989052	4.892493	2.472571
H	-3.712658	4.389997	4.804254
N	-0.647719	0.595097	1.084269
N	-1.730237	0.041418	-0.718721
H	-2.773356	2.067119	-4.716002
C	-2.245091	2.559042	-2.108309
C	-1.709770	-2.532663	-2.055416
H	-2.349776	-2.210851	-4.681129
H	-1.927696	2.397684	-1.066708

H	-1.748691	-2.326686	-0.974855
C	-2.700027	-3.648676	-2.353717
H	-2.646505	-3.986200	-3.400814
H	-2.493002	-4.527751	-1.725260
H	-3.738383	-3.340021	-2.158268
C	-0.275863	-2.945485	-2.367274
H	0.015282	-3.837068	-1.792021
H	-0.141192	-3.175981	-3.437457
H	0.430184	-2.144896	-2.100586
C	-3.624235	3.208184	-2.077438
H	-4.377839	2.559926	-1.605453
H	-3.602498	4.153643	-1.514467
H	-3.983930	3.442674	-3.091683
C	-1.209592	3.483840	-2.735351
H	-1.144650	4.432937	-2.181770
H	-0.212564	3.021617	-2.718861
H	-1.452926	3.730235	-3.780781
C	2.193463	1.582600	-2.478233
H	1.633671	1.841885	-3.385690
C	-3.820455	-0.916685	0.277606
C	-5.048265	-0.738002	-0.370803
C	-3.549964	-2.151319	0.886840
C	-5.994806	-1.762788	-0.407742
H	-5.265266	0.222185	-0.849637
C	-4.497766	-3.172901	0.853630
H	-2.584186	-2.319224	1.375797
C	-5.722531	-2.982600	0.210110
H	-6.949345	-1.603638	-0.915697
H	-4.275737	-4.129092	1.334653
H	-6.463475	-3.785971	0.190023
C	2.721805	0.213053	-2.409709
H	3.772068	0.151425	-2.075607
O	3.294735	-0.819439	0.361350
B	2.569608	-1.108238	-0.780454
O	2.852740	-2.375123	-1.248458
C	3.650839	-3.063035	-0.248828
C	4.271765	-1.875619	0.559584
C	4.663929	-3.935107	-0.960092
H	5.344235	-4.414411	-0.240316
H	4.152924	-4.736164	-1.512824
H	5.269514	-3.370042	-1.680185
C	2.703791	-3.915386	0.576781
H	2.187603	-4.627992	-0.082213
H	3.240446	-4.499168	1.338617
H	1.938440	-3.312069	1.083398
C	4.413541	-2.135079	2.042858
H	3.443694	-2.346855	2.513764
H	5.084606	-2.987641	2.228452
H	4.851010	-1.258046	2.541747
C	5.579317	-1.373865	-0.029770
H	5.869228	-0.434716	0.463188
H	6.399910	-2.091644	0.112533
H	5.489307	-1.171225	-1.107583
C	2.449709	-0.621323	-3.641300
H	2.672253	-1.685241	-3.493064
H	1.395636	-0.540107	-3.953195
H	3.056443	-0.263020	-4.489807
C	2.775889	2.681136	-1.747958
C	3.658806	2.480192	-0.651958
C	2.497298	4.031698	-2.090179
C	4.216664	3.552192	0.038324
H	3.880427	1.459152	-0.324260
C	3.051740	5.095537	-1.389113
H	1.832809	4.232452	-2.937198
C	3.921858	4.873257	-0.313516
H	4.889631	3.350310	0.878291
H	2.809451	6.119652	-1.690576
H	4.361645	5.711167	0.233111

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Scheme_S12_XLV / electronic energy: -4409.29464501 a.u. / lowest freq: -123.29 cm-1

C	-2.362187	1.382879	-0.176339
H	-2.294928	2.021491	0.716223
C	-2.739992	-0.052534	0.221322
H	-3.415811	-0.490343	-0.538780
C	-0.486920	-0.025016	-0.499321
C	-0.212449	2.303991	-1.140370
C	0.148647	2.376576	-2.490020
C	0.218095	3.302163	-0.247824
C	0.915357	3.436865	-2.966878
H	-0.189526	1.580835	-3.160418
C	0.970704	4.369955	-0.742770
C	1.314296	4.445686	-2.090779
H	1.192585	3.476858	-4.023052

H	1.311635	5.131720	-0.037937
H	1.908840	5.287688	-2.453995
C	-1.373078	-2.182096	0.236084
C	-0.926840	-2.733292	1.454485
C	-1.775009	-2.993015	-0.846281
C	-0.871448	-4.127330	1.562998
C	-1.712570	-4.381969	-0.683454
C	-1.262741	-4.945277	0.506971
H	-1.207573	-6.032537	0.609228
S	-0.109439	3.262282	1.538963
O	0.958966	4.101367	2.129697
O	-0.039873	1.827692	1.924999
O	-1.467172	3.846510	1.702089
Cu	1.318399	-0.495674	-0.993974
C	-3.294229	2.043417	-1.158935
C	-3.904336	3.258919	-0.833130
C	-3.549829	1.470772	-2.412427
C	-4.766106	3.884079	-1.736309
H	-3.685243	3.717476	0.135638
C	-4.406273	2.094517	-3.316283
H	-3.063925	0.527027	-2.682449
C	-5.019971	3.303293	-2.978095
H	-5.237534	4.833138	-1.468988
H	-4.595790	1.637138	-4.290723
H	-5.692547	3.793175	-3.686686
N	-1.002108	1.200611	-0.721756
N	-1.438330	-0.761104	0.106566
H	-2.012357	-5.032423	-1.510881
C	-2.262749	-2.416946	-2.161959
C	-0.460288	-1.848496	2.589593
H	-0.505980	-4.578616	2.489817
H	-2.163614	-1.321416	-2.109153
H	-0.887507	-0.849031	2.420360
C	-0.932448	-2.330684	3.953177
H	-0.445838	-3.271223	4.256274
H	-0.695499	-1.586238	4.728016
H	-2.019969	-2.498024	3.978481
C	1.053606	-1.680536	2.544383
H	1.391913	-0.981614	3.324173
H	1.573907	-2.640104	2.700682
H	1.385267	-1.275638	1.576080
C	-3.734499	-2.736940	-2.401433
H	-4.375296	-2.382595	-1.579762
H	-4.096160	-2.266168	-3.328380
H	-3.901546	-3.821049	-2.500907
C	-1.400815	-2.872371	-3.332516
H	-1.745161	-2.414185	-4.272149
H	-0.350692	-2.581893	-3.182928
H	-1.434763	-3.964284	-3.471136
C	2.249982	-1.912391	-2.244232
H	1.927442	-1.927282	-3.292379
C	-3.412881	-0.205893	1.564383
C	-4.433514	-1.152945	1.711708
C	-3.033176	0.557450	2.678887
C	-5.071063	-1.335700	2.939315
H	-4.735260	-1.751955	0.846591
C	-3.674318	0.378241	3.903500
H	-2.218365	1.283895	2.591951
C	-4.694591	-0.565557	4.038960
H	-5.867933	-2.077655	3.033203
H	-3.371073	0.982170	4.762685
H	-5.195683	-0.699359	5.001114
C	3.110649	-0.790926	-1.837317
H	4.011236	-1.098431	-1.280077
O	3.323309	1.740847	-0.383796
B	2.926929	0.443326	-0.149288
O	3.578960	-0.085819	0.955921
C	4.249386	1.001118	1.644817
C	4.430487	2.053035	0.501627
C	5.544231	0.476147	2.227304
H	6.128428	1.288825	2.684289
H	5.333488	-0.260625	3.015267
H	6.171763	-0.015906	1.473315
C	3.327281	1.483230	2.751172
H	3.121690	0.654698	3.443151
H	3.787021	2.293922	3.335034
H	2.363648	1.843093	2.364076
C	4.302389	3.493824	0.944197
H	3.311958	3.700707	1.372216
H	5.067825	3.744067	1.694399
H	4.449355	4.167884	0.087602
C	5.704896	1.842975	-0.299433
H	5.691027	2.485296	-1.191536

H	6.602990	2.100564	0.280187
H	5.806230	0.801070	-0.638192
C	3.421247	0.173052	-2.962032
H	3.868221	1.113844	-2.618529
H	4.116954	-0.292315	-3.680067
H	2.511742	0.430814	-3.526438
C	2.254854	-3.177193	-1.552582
C	1.740112	-4.357875	-2.152028
C	2.771953	-3.315134	-0.234875
C	1.740402	-5.578219	-1.488960
H	1.346392	-4.298866	-3.172173
C	2.762937	-4.541572	0.423735
H	3.173329	-2.433484	0.276943
C	2.248519	-5.688941	-0.188135
H	1.336249	-6.462257	-1.993281
H	3.166063	-4.602450	1.440116
H	2.246497	-6.649347	0.333794

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Scheme_S12_XLVI / electronic energy: -4409.29233449 a.u. / lowest freq: -111.38 cm-1

C	-1.962808	-1.241240	1.179587
H	-1.962989	-2.325064	0.996546
C	-2.745559	-0.498196	0.071786
H	-3.520091	0.146262	0.525012
C	-0.486562	0.228616	0.056308
C	0.490918	-1.101855	1.836509
C	1.172256	-0.091590	2.530476
C	0.915210	-2.437306	1.973287
C	2.235933	-0.391537	3.375209
H	0.839964	0.943265	2.402193
C	1.967895	-2.725192	2.846245
C	2.624263	-1.718923	3.550445
H	2.750349	0.413940	3.904616
H	2.290985	-3.765253	2.926653
H	3.448818	-1.971216	4.221687
C	-2.046613	1.431787	-1.410854
C	-1.848447	1.254324	-2.793917
C	-2.617842	2.614534	-0.888227
C	-2.237646	2.292304	-3.651775
C	-2.994159	3.618379	-1.786173
C	-2.809814	3.459202	-3.157769
H	-3.108550	4.255251	-3.844761
S	0.263479	-3.807801	0.976510
O	1.291215	-4.865969	1.080813
O	0.127815	-3.231244	-0.389353
O	-1.034750	-4.186911	1.591840
Cu	1.154046	1.048302	-0.526885
C	-2.516618	-0.988440	2.559893
C	-3.383377	-1.921679	3.139061
C	-2.230196	0.193852	3.255717
C	-3.965850	-1.672083	4.381968
H	-3.596525	-2.853244	2.606861
C	-2.809523	0.443123	4.498908
H	-1.538708	0.922525	2.821614
C	-3.682243	-0.488652	5.064170
H	-4.640314	-2.410385	4.823019
H	-2.574959	1.368446	5.031673
H	-4.135458	-0.295069	6.039649
N	-0.593117	-0.717047	1.011164
N	-1.701835	0.385301	-0.503024
H	-3.426964	4.546661	-1.403188
C	-2.744726	2.838944	0.604812
C	-1.185355	0.021303	-3.369210
H	-2.083597	2.179571	-4.728922
H	-2.693648	1.858333	1.098673
H	-1.050962	-0.706433	-2.552598
C	-2.039383	-0.639890	-4.442660
H	-2.140219	-0.006463	-5.338182
H	-1.588710	-1.589172	-4.768416
H	-3.053962	-0.861575	-4.078490
C	0.202315	0.372533	-3.893681
H	0.717816	-0.517220	-4.282994
H	0.153110	1.117206	-4.704997
H	0.834751	0.783033	-3.090603
C	-4.065414	3.474606	1.011117
H	-4.928609	2.905947	0.633036
H	-4.152165	3.515949	2.107143
H	-4.164062	4.508080	0.645554
C	-1.549288	3.639690	1.111138
H	-1.562269	3.733956	2.208723
H	-0.599930	3.157762	0.825002
H	-1.544018	4.659294	0.692704
C	1.890845	3.022608	-0.742042
C	-3.436157	-1.356593	-0.960718

C	-4.677729	-0.944229	-1.461393
C	-2.867333	-2.543417	-1.444515
C	-5.350574	-1.703626	-2.418845
H	-5.126378	-0.018962	-1.084413
C	-3.543650	-3.302975	-2.399062
H	-1.890498	-2.876291	-1.072101
C	-4.785388	-2.889635	-2.886633
H	-6.322052	-1.370851	-2.793173
H	-3.095052	-4.230128	-2.765557
H	-5.312027	-3.492434	-3.631039
C	2.735227	1.954669	-1.288392
H	2.763691	1.911958	-2.384770
O	3.652792	-0.572564	-0.142566
B	2.727204	-0.130835	-1.073154
O	2.922546	-0.728213	-2.301717
C	4.194597	-1.425880	-2.261667
C	4.382509	-1.683887	-0.732750
C	5.234430	-0.475334	-2.831925
H	6.227765	-0.941602	-2.898953
H	4.938274	-0.169953	-3.845625
H	5.326972	0.436044	-2.223344
C	4.090260	-2.674462	-3.108397
H	3.954127	-2.406413	-4.165868
H	5.005412	-3.280610	-3.035303
H	3.238876	-3.298877	-2.810611
C	3.717917	-2.966598	-0.270780
H	2.662543	-3.017777	-0.573016
H	4.232829	-3.857599	-0.658288
H	3.746040	-3.020988	0.824968
C	5.816075	-1.623438	-0.251643
H	5.857540	-1.801442	0.832537
H	6.428375	-2.398360	-0.736538
H	6.280530	-0.647842	-0.445084
H	3.745892	1.868802	-0.866239
C	2.186178	3.546822	0.575405
C	2.995862	2.835421	1.507391
C	1.686996	4.802703	1.016053
C	3.264129	3.338431	2.774831
H	3.396666	1.854031	1.230391
C	1.958262	5.295473	2.288652
H	1.069721	5.399242	0.338877
C	2.749013	4.573568	3.188421
H	3.889981	2.754836	3.457629
H	1.550676	6.268317	2.582061
H	2.963848	4.964034	4.186122
C	1.075121	3.852198	-1.696997
H	0.097606	4.156675	-1.284691
H	1.581054	4.791319	-2.001714
H	0.863480	3.299550	-2.625501

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Scheme_S12_XLVII / electronic energy: -4409.29204653 a.u. / lowest freq: -46.64 cm-1

C	2.225168	-1.498558	-0.211866
H	2.209504	-2.342352	0.491980
C	2.633610	-0.194462	0.509368
H	3.441805	0.308525	-0.052225
C	0.421574	0.038898	-0.323586
C	0.052534	-2.114297	-1.381911
C	-0.446784	-1.689439	-2.621018
C	-0.277246	-3.398082	-0.909770
C	-1.251633	-2.518288	-3.395881
H	-0.188542	-0.681591	-2.960615
C	-1.069089	-4.228621	-1.708500
C	-1.552441	-3.802614	-2.943155
H	-1.631388	-2.164468	-4.357539
H	-1.330433	-5.214126	-1.317197
H	-2.175203	-4.469532	-3.544273
C	1.439660	2.023886	0.701828
C	0.901604	2.456536	1.930595
C	2.044917	2.924090	-0.202052
C	0.945541	3.826100	2.219266
C	2.067195	4.281342	0.134891
C	1.517947	4.731947	1.331751
H	1.533887	5.798165	1.573319
S	0.169086	-4.006314	0.740829
O	-0.772428	-5.120414	0.992996
O	-0.027607	-2.830910	1.629324
O	1.584489	-4.446645	0.642788
Cu	-1.376376	0.639066	-0.753180
C	3.140415	-1.848892	-1.358799
C	4.154239	-2.795391	-1.173476
C	3.038020	-1.200921	-2.597275
C	5.058626	-3.076155	-2.198032
H	4.226768	-3.317410	-0.215192

C	3.938885	-1.482642	-3.622745
H	2.236458	-0.473833	-2.762246
C	4.954916	-2.419530	-3.424427
H	5.845050	-3.818289	-2.039265
H	3.844647	-0.970980	-4.584129
H	5.660397	-2.642642	-4.228724
N	0.850039	-1.199447	-0.651817
N	1.410898	0.635216	0.370955
H	2.517423	4.996853	-0.559990
C	2.667210	2.465045	-1.505599
C	0.252262	1.496654	2.904438
H	0.515064	4.188402	3.157483
H	2.565729	1.372605	-1.558256
H	0.496704	0.475263	2.574389
C	0.782961	1.661799	4.322075
H	0.492567	2.627668	4.764672
H	0.382888	0.876336	4.980586
H	1.881142	1.598153	4.359724
C	-1.263694	1.627973	2.848046
H	-1.751187	0.891754	3.505307
H	-1.599081	2.631457	3.158902
H	-1.633989	1.444609	1.828984
C	4.155776	2.785826	-1.566731
H	4.704721	2.361377	-0.712517
H	4.606292	2.377272	-2.484304
H	4.341342	3.871407	-1.569424
C	1.925361	3.021653	-2.711676
H	2.351040	2.630821	-3.649149
H	0.863355	2.740110	-2.679935
H	1.976044	4.121007	-2.758684
C	-2.131876	2.031241	-2.217619
C	3.110451	-0.336093	1.935275
C	4.143968	0.491490	2.391843
C	2.537078	-1.258646	2.822125
C	4.609241	0.397412	3.704040
H	4.596130	1.212442	1.702883
C	3.004173	-1.352120	4.132628
H	1.717543	-1.905379	2.485768
C	4.041369	-0.529571	4.577443
H	5.421589	1.046253	4.041146
H	2.553045	-2.078297	4.814054
H	4.406085	-0.611518	5.604621
C	-3.100573	1.151351	-1.584292
H	-3.507750	0.366011	-2.233967
O	-3.462793	-1.510738	-0.344767
B	-2.985980	-0.284871	0.082913
O	-3.706829	0.172462	1.173469
C	-4.845211	-0.711686	1.357693
C	-4.337992	-2.026908	0.691700
C	-6.017976	-0.093845	0.614797
H	-6.947776	-0.659610	0.771455
H	-6.185479	0.931560	0.974456
H	-5.829875	-0.042708	-0.467397
C	-5.144797	-0.818647	2.835838
H	-5.489163	0.149652	3.226614
H	-5.940308	-1.554392	3.026643
H	-4.259431	-1.113415	3.413044
C	-3.489850	-2.864331	1.632604
H	-2.724378	-2.257035	2.135442
H	-4.102878	-3.358231	2.400798
H	-2.954134	-3.644904	1.075182
C	-5.409338	-2.872823	0.040369
H	-4.956669	-3.764322	-0.417388
H	-6.145669	-3.219488	0.780790
H	-5.944133	-2.330078	-0.749657
C	-1.911644	3.349226	-1.643895
C	-2.277732	3.650263	-0.302148
C	-1.337242	4.412222	-2.387808
C	-2.068310	4.908742	0.248711
H	-2.715593	2.863273	0.321448
C	-1.137864	5.672572	-1.830887
H	-1.044218	4.242050	-3.427367
C	-1.497930	5.939747	-0.507087
H	-2.353828	5.089788	1.290044
H	-0.694400	6.463119	-2.444821
H	-1.336591	6.928935	-0.071177
H	-3.882289	1.614521	-0.967830
C	-1.788493	1.796764	-3.663654
H	-2.406440	2.410593	-4.349211
H	-0.740778	2.026050	-3.918766
H	-1.963303	0.749307	-3.949124

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Scheme_S13_S.XXV / electronic energy: -4451.87872350 a.u. / lowest freq: -299.91 cm-1

C	0.166455	-2.754844	1.044974
H	-0.671941	-3.453906	0.926983
C	0.044453	-1.973792	2.356170
H	0.786789	-2.281557	3.106602
C	0.189643	-0.437420	0.597757
C	-0.131821	-1.877896	-1.331095
C	0.875207	-1.484496	-2.216953
C	-1.318570	-2.435876	-1.841456
C	0.714219	-1.632047	-3.591228
H	1.786484	-1.046312	-1.807614
C	-1.463811	-2.599472	-3.221643
C	-0.455724	-2.198289	-4.095324
H	1.509226	-1.302768	-4.264311
H	-2.393998	-3.023583	-3.604575
H	-0.590952	-2.323167	-5.171910
C	0.168098	0.535899	2.829992
C	-1.093654	0.912032	3.342918
C	1.343353	1.255660	3.148373
C	-1.149263	2.001859	4.221098
C	1.225607	2.348695	4.015060
C	-0.004465	2.714803	4.554711
H	-0.069311	3.567631	5.235140
S	-2.690855	-2.953895	-0.797361
O	-3.897775	-2.849150	-1.673648
O	-2.793799	-1.940551	0.303001
O	-2.381225	-4.320279	-0.344113
Cu	0.357101	1.287473	-0.286934
C	1.467932	-3.496622	0.854090
C	1.479388	-4.888827	0.729527
C	2.682099	-2.798512	0.790620
C	2.683232	-5.575535	0.561084
H	0.533124	-5.437239	0.759764
C	3.884200	-3.482098	0.625561
H	2.681251	-1.705052	0.865679
C	3.887333	-4.874702	0.512429
H	2.678194	-6.663893	0.462897
H	4.824886	-2.926393	0.582153
H	4.829859	-5.411334	0.379343
N	0.052401	-1.657337	0.054434
N	0.253587	-0.580628	1.934259
H	2.114279	2.926672	4.275741
C	2.698076	0.844935	2.600301
C	-2.374304	0.185286	2.981343
H	-2.114787	2.303376	4.636313
H	2.543835	0.543136	1.548307
H	-2.172946	-0.439651	2.097250
C	-2.829055	-0.729527	4.117951
H	-3.133706	-0.141835	4.998493
H	-3.694840	-1.336641	3.812374
H	-2.041475	-1.420302	4.451164
C	-3.508070	1.136893	2.609146
H	-4.360793	0.575171	2.196338
H	-3.891359	1.685205	3.483296
H	-3.212254	1.887254	1.861949
C	3.252385	-0.357468	3.360692
H	2.564103	-1.214080	3.359171
H	4.203477	-0.697599	2.922371
H	3.449562	-0.099775	4.413469
C	3.715450	1.974455	2.597354
H	4.625919	1.666023	2.065149
H	3.337498	2.874768	2.093507
H	4.022958	2.255064	3.616739
C	-1.235022	2.609877	-0.194849
H	-1.389737	2.924336	0.846248
H	-0.954173	-2.094017	2.801517
C	-0.097835	3.134311	-0.901432
H	-0.155710	3.100914	-1.999169
Na	-4.724545	-0.988825	-0.561894
O	3.289610	2.079714	-0.553214
B	2.147737	1.609208	-1.166934
O	2.376759	1.329228	-2.500931
C	3.706841	1.810463	-2.843517
C	4.407952	1.833919	-1.450178
C	3.536147	3.194617	-3.444685
H	4.490422	3.611215	-3.796926
H	2.856889	3.138940	-4.306597
H	3.100035	3.899288	-2.722174
C	4.322918	0.863869	-3.849422
H	3.773000	0.907009	-4.800218
H	5.367154	1.138230	-4.060580
H	4.307264	-0.177453	-3.502225
C	4.988932	0.482502	-1.065203
H	4.257103	-0.325374	-1.214841

H	5.889668	0.238690	-1.646172
H	5.268756	0.487124	-0.001769
C	5.431232	2.931423	-1.269808
H	5.878806	2.875545	-0.267455
H	6.246530	2.834320	-2.001868
H	4.987423	3.928936	-1.380793
C	0.658555	4.298148	-0.337001
H	1.653563	4.413434	-0.787461
H	0.110666	5.240542	-0.508689
H	0.799198	4.204234	0.750607
C	-2.205213	1.775845	-0.786600
H	-2.811387	1.135714	-0.144901
H	-1.988010	1.348307	-1.771383
H	-7.144030	1.709517	-2.470557
O	-3.635150	2.823452	-1.377922
C	-4.771893	2.255805	-1.356073
O	-5.041050	1.091677	-1.031299
C	-7.068187	2.565261	-1.784444
H	-7.405533	2.245760	-0.787789
O	-5.756079	3.097643	-1.751244
H	-7.721089	3.369288	-2.141533

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Scheme_S13_S.XXVI / electronic energy: -4451.87751112 a.u. / lowest freq: -312.00 cm-1

C	-1.675031	-2.669629	0.820655
H	-2.548006	-2.319369	1.390123
C	-0.438709	-2.721683	1.720434
H	0.097853	-3.683283	1.663271
C	-0.101872	-1.019092	0.140245
C	-2.147709	-1.126985	-1.153914
C	-1.784053	-1.345136	-2.486804
C	-3.327929	-0.421569	-0.865889
C	-2.582536	-0.878213	-3.526536
H	-0.857242	-1.889439	-2.688436
C	-4.127696	0.039811	-1.914982
C	-3.760432	-0.188553	-3.238967
H	-2.285101	-1.055023	-4.562511
H	-5.033637	0.602076	-1.679441
H	-4.394642	0.181371	-4.047443
C	1.715706	-1.427636	1.752351
C	1.887193	-0.460166	2.762810
C	2.779310	-2.233744	1.298844
C	3.170788	-0.288183	3.292397
C	4.041728	-2.032568	1.869289
C	4.238077	-1.066819	2.852199
H	5.232629	-0.920291	3.281804
S	-3.875828	-0.068275	0.813673
O	-4.675793	1.189574	0.704109
O	-2.646670	0.204551	1.628561
O	-4.645132	-1.246489	1.251731
Cu	0.615235	0.532845	-0.864618
C	-2.059531	-3.931518	0.088634
C	-3.416532	-4.225060	-0.093356
C	-1.101260	-4.779189	-0.481357
C	-3.808054	-5.347450	-0.823581
H	-4.165085	-3.553221	0.338657
C	-1.491072	-5.901233	-1.210215
H	-0.035946	-4.560698	-0.358444
C	-2.846458	-6.188855	-1.382420
H	-4.870677	-5.565430	-0.956256
H	-0.732390	-6.555168	-1.647465
H	-3.151307	-7.068891	-1.954049
N	-1.283958	-1.594947	-0.135154
N	0.411547	-1.638954	1.210040
H	4.884483	-2.643825	1.532467
C	2.589933	-3.301800	0.240234
C	0.732747	0.407574	3.219252
H	3.337814	0.468356	4.063639
H	1.549446	-3.238444	-0.114334
H	-0.199411	-0.118781	2.957802
C	0.719365	0.648438	4.721675
H	1.566768	1.266102	5.055526
H	-0.195775	1.182058	5.017592
H	0.749989	-0.292629	5.290226
C	0.731608	1.725326	2.449909
H	-0.137316	2.346462	2.722523
H	1.637926	2.314919	2.660826
H	0.710264	1.555345	1.360376
C	2.799783	-4.697739	0.817598
H	2.132641	-4.900778	1.668764
H	2.612967	-5.471435	0.057721
H	3.833042	-4.835048	1.173040
C	3.481832	-3.068743	-0.971918
H	3.268485	-3.808745	-1.757789

H	3.329413	-2.067982	-1.401707
H	4.548931	-3.166013	-0.717847
C	-0.715672	1.990760	-1.641780
H	-0.682665	-2.548153	2.779237
C	0.681458	2.227311	-1.915130
H	1.152923	3.011167	-1.303209
Na	-3.193055	2.410836	2.065424
O	3.258942	1.575830	-0.032163
B	2.622001	0.840963	-1.014063
O	3.485369	0.535121	-2.046359
C	4.823903	0.981446	-1.682386
C	4.530456	2.033559	-0.564246
C	5.496745	1.542347	-2.916175
H	6.479532	1.969071	-2.666494
H	5.661676	0.745119	-3.654439
H	4.897714	2.324625	-3.398912
C	5.585904	-0.227015	-1.172015
H	5.601985	-1.006911	-1.945912
H	6.628386	0.023160	-0.928100
H	5.112158	-0.649093	-0.274559
C	5.545530	2.073091	0.556250
H	5.637236	1.106838	1.067795
H	6.538521	2.359472	0.179287
H	5.249718	2.819189	1.307687
C	4.294300	3.430047	-1.116213
H	3.892209	4.076020	-0.322937
H	5.221365	3.890286	-1.486404
H	3.565726	3.421725	-1.939840
C	-1.393986	2.532553	-0.532947
C	1.130427	2.191064	-3.347473
H	0.720467	1.316188	-3.875252
H	0.767599	3.085278	-3.882427
H	2.221310	2.155957	-3.456367
H	-1.329322	1.563396	-2.445149
H	-2.400686	2.155004	-0.334926
H	-0.814010	2.788051	0.358225
H	-4.431241	6.390969	1.060645
O	-1.902721	4.254625	-0.892771
C	-2.478627	4.833181	0.086233
O	-2.748909	4.357570	1.196083
C	-3.462237	6.843913	0.807197
H	-2.859282	6.914623	1.723568
O	-2.792713	6.113990	-0.207044
H	-3.628900	7.849786	0.406858

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Scheme_S13_S.XXVII / electronic energy: -4564.91431346 a.u. / lowest freq: -301.63 cm-1

C	0.366911	-2.685196	-0.775976
H	-0.528816	-3.213889	-1.130893
C	0.543857	-2.857581	0.749077
H	1.544731	-3.265074	0.974235
C	0.273679	-0.557418	0.259416
C	-0.036656	-0.554114	-2.139717
C	1.025725	0.194926	-2.653069
C	-1.251880	-0.595581	-2.844462
C	0.891933	0.892907	-3.850647
H	1.958872	0.232686	-2.087462
C	-1.374786	0.090084	-4.054417
C	-0.307543	0.831928	-4.557629
H	1.729771	1.483792	-4.228063
H	-2.327504	0.050895	-4.585340
H	-0.420583	1.370288	-5.501236
C	0.637844	-1.065670	2.600062
C	-0.509737	-0.762267	3.358718
C	1.936086	-0.960675	3.141426
C	-0.325324	-0.349438	4.686609
C	2.068770	-0.553105	4.472758
C	0.946236	-0.249997	5.240739
H	1.065772	0.073937	6.277669
S	-2.687421	-1.466472	-2.202166
O	-3.837162	-0.974953	-3.021976
O	-2.852082	-0.991270	-0.790255
O	-2.415839	-2.908851	-2.335161
Cu	0.362472	1.360763	0.581572
C	1.538529	-3.101552	-1.628653
C	1.323919	-3.836169	-2.799231
C	2.841547	-2.694745	-1.312102
C	2.392645	-4.170502	-3.632405
H	0.305555	-4.139805	-3.060043
C	3.909570	-3.026533	-2.142433
H	3.017525	-2.102558	-0.408153
C	3.686613	-3.767068	-3.305733
H	2.211422	-4.746261	-4.543322
H	4.921302	-2.703622	-1.883278

H	4.523790	-4.027494	-3.957975
N	0.133652	-1.219373	-0.898356
N	0.499539	-1.450086	1.231579
H	3.070269	-0.461218	4.901600
H	-1.205239	-0.105183	5.288522
C	-1.189821	2.401830	1.478381
H	-1.298816	2.063973	2.516569
C	-0.054617	3.241785	1.171212
Na	-4.724068	0.294165	-1.298828
O	3.315728	1.937547	0.991081
B	2.222834	2.033963	0.149912
O	2.571970	2.616481	-1.053363
C	3.932450	3.118287	-0.941397
C	4.508023	2.240913	0.214285
C	3.839427	4.589970	-0.576901
H	4.830207	5.063693	-0.526958
H	3.254127	5.122797	-1.339377
H	3.341938	4.737832	0.392630
C	4.622882	2.946813	-2.276274
H	4.154269	3.593463	-3.031547
H	5.684039	3.229881	-2.212152
H	4.566758	1.913729	-2.642861
C	5.067480	0.917065	-0.281826
H	4.347842	0.395335	-0.930509
H	5.999558	1.053582	-0.848493
H	5.290655	0.261497	0.571310
C	5.506910	2.940257	1.107983
H	5.853691	2.258340	1.897112
H	6.390418	3.262089	0.537125
H	5.074990	3.821903	1.598051
C	0.740469	3.743530	2.346071
H	1.737890	4.098933	2.050406
H	0.222694	4.592180	2.828691
H	0.880271	2.967545	3.113610
C	-2.256607	2.128466	0.598486
H	-2.927716	1.306211	0.854115
H	-2.118626	2.265597	-0.478106
H	-6.728022	4.063430	-1.279773
O	-3.519879	3.482997	0.773219
C	-4.633372	3.255568	0.203966
O	-4.957746	2.269147	-0.469808
C	-6.792509	4.114064	-0.183238
H	-7.310883	3.214776	0.178923
O	-5.515542	4.260472	0.412751
H	-7.371116	5.000192	0.100113
C	3.137657	-1.254423	2.304865
H	4.057892	-0.924291	2.803304
H	3.247677	-2.331556	2.097035
H	3.078683	-0.739784	1.334951
C	-1.897000	-0.883784	2.812569
H	-1.938559	-0.895895	1.715559
H	-2.372185	-1.813366	3.165664
H	-2.533606	-0.063226	3.173523
C	-0.139331	4.196145	0.010286
H	-0.773487	5.061694	0.272819
H	0.851413	4.581277	-0.266096
H	-0.570846	3.743813	-0.894255
C	-0.480920	-3.718237	1.448266
C	-0.102011	-4.432671	2.591504
C	-1.815918	-3.773147	1.026471
C	-1.033912	-5.187576	3.303141
H	0.939771	-4.395107	2.925959
C	-2.744930	-4.537233	1.731190
H	-2.141481	-3.206053	0.149761
C	-2.359250	-5.243997	2.871290
H	-0.721855	-5.740043	4.192789
H	-3.782062	-4.575779	1.388402
H	-3.090882	-5.840862	3.421622

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Scheme_S13_S.XXVIII / electronic energy: -4564.91486367 a.u. / lowest freq: -281.95 cm-1

C	-0.567467	-2.704653	-0.440124
H	-1.619579	-2.866262	-0.715357
C	-0.399693	-2.680993	1.096614
H	0.465785	-3.301853	1.390854
C	0.119505	-0.543023	0.236217
C	-0.152907	-0.831696	-2.140539
C	1.087980	-0.503647	-2.694731
C	-1.324130	-0.591469	-2.879199
C	1.173962	0.045034	-3.971449
H	1.986580	-0.667486	-2.095980
C	-1.229590	-0.057018	-4.166279
C	0.012778	0.258618	-4.712955
H	2.152258	0.307169	-4.381614

H	-2.148723	0.134237	-4.722979
H	0.068996	0.684332	-5.717241
C	0.332255	-0.756336	2.639331
C	-0.621251	-0.099804	3.439538
C	1.676319	-0.896716	3.044247
C	-0.192791	0.425968	4.667607
C	2.056878	-0.355430	4.275761
C	1.128883	0.301386	5.081943
H	1.442271	0.724404	6.039667
S	-2.963353	-0.869149	-2.191711
O	-3.877431	-0.047626	-3.043769
O	-2.924199	-0.287348	-0.810036
O	-3.221040	-2.318388	-2.237699
Cu	0.780635	1.284694	0.010767
C	0.278027	-3.721309	-1.163467
C	-0.317165	-4.680172	-1.988316
C	1.675000	-3.695169	-1.048641
C	0.468106	-5.607113	-2.676350
H	-1.405705	-4.692613	-2.095047
C	2.459952	-4.615655	-1.737860
H	2.149051	-2.936400	-0.416913
C	1.856272	-5.576941	-2.552661
H	-0.008944	-6.352979	-3.316837
H	3.548282	-4.583217	-1.642430
H	2.471123	-6.299754	-3.094534
N	-0.180997	-1.324675	-0.811341
N	-0.041166	-1.258589	1.354956
H	3.098872	-0.444010	4.595550
H	-0.917995	0.945447	5.300189
C	-0.591420	2.782195	-0.377877
C	0.760523	3.279173	-0.267037
Na	-4.214931	1.566962	-1.422527
O	3.629166	1.515599	1.038047
B	2.802510	1.354866	-0.055649
O	3.536712	1.228829	-1.221266
C	4.934838	1.061817	-0.861512
C	4.988490	1.714369	0.556681
C	5.791520	1.741786	-1.906275
H	6.854052	1.718242	-1.622627
H	5.695833	1.224444	-2.871239
H	5.500957	2.788445	-2.061877
C	5.209247	-0.433290	-0.840866
H	4.956726	-0.867145	-1.819223
H	6.266834	-0.656767	-0.640521
H	4.601530	-0.945425	-0.080411
C	5.949734	1.059257	1.522981
H	5.718769	-0.000573	1.686960
H	6.984776	1.131035	1.157374
H	5.908381	1.563639	2.498647
C	5.226614	3.213813	0.506643
H	5.058458	3.647878	1.502231
H	6.256073	3.456118	0.206750
H	4.540747	3.708573	-0.196103
C	-1.469673	2.614303	0.710403
C	1.391470	3.814053	-1.522357
H	1.126571	3.218450	-2.408091
H	1.051561	4.848514	-1.710807
H	2.488282	3.842193	-1.456607
H	-0.993241	2.623808	-1.388307
H	-2.341185	1.970290	0.589579
H	-1.062592	2.626934	1.723310
H	-5.075338	5.726751	-1.325277
O	-2.449051	4.186552	1.037242
C	-3.487588	4.309293	0.315912
O	-3.968813	3.493629	-0.482313
C	-5.265603	5.750573	-0.242647
H	-6.052096	5.018559	-0.009170
O	-4.085692	5.509867	0.503061
H	-5.613304	6.750796	0.038645
C	1.190579	3.969384	1.000958
H	2.281375	4.096743	1.031901
H	0.734865	4.973621	1.069435
H	0.907373	3.425354	1.913935
C	2.668167	-1.587671	2.166649
H	3.689733	-1.470048	2.548444
H	2.469771	-2.669247	2.093134
H	2.640621	-1.185785	1.141617
C	-2.052679	0.037450	3.030148
H	-2.201378	-0.085413	1.949663
H	-2.676809	-0.720067	3.531124
H	-2.458595	1.014113	3.328803
C	-1.590403	-3.134624	1.904043
C	-1.372604	-3.795595	3.119021

C	-2.907334	-2.873420	1.501471
C	-2.444050	-4.190151	3.919810
H	-0.345846	-4.002894	3.437676
C	-3.978669	-3.276951	2.296671
H	-3.100987	-2.332766	0.569915
C	-3.751605	-3.934402	3.507116
H	-2.256616	-4.706891	4.864262
H	-5.001180	-3.071326	1.969954
H	-4.594402	-4.249213	4.127562

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Scheme_S14_LX / electronic energy: -5327.02819082 a.u. / lowest freq: -134.97 cm-1

Cu	-1.646252	0.686582	-1.304551
C	-1.303735	1.697511	-3.018248
C	-2.078371	2.484240	-2.022293
O	-3.829133	1.899823	0.363945
B	-2.508142	1.969780	-0.011658
O	-1.766943	2.753742	0.847514
C	-2.571877	3.000795	2.031339
C	-4.029863	2.797965	1.492863
C	-2.270877	4.397751	2.530877
H	-2.919586	4.659675	3.380030
H	-1.229728	4.454334	2.879970
H	-2.399981	5.159803	1.751606
C	-2.164263	1.969970	3.068506
H	-1.085617	2.070277	3.260171
H	-2.687675	2.122073	4.023936
H	-2.350979	0.940201	2.729348
C	-4.972657	2.132881	2.470370
H	-4.628710	1.129569	2.756532
H	-5.081536	2.738696	3.382529
H	-5.971212	2.027935	2.021576
C	-4.637549	4.075073	0.938218
H	-5.562863	3.839252	0.393354
H	-4.893533	4.785778	1.737236
H	-3.955141	4.581335	0.239834
C	0.092333	2.057163	-3.230632
H	-1.816810	1.471171	-3.959027
F	0.751927	1.169000	-4.020235
F	0.809379	2.153739	-2.076126
F	0.315513	3.274737	-3.845811
C	-3.483200	2.805102	-2.469870
H	-1.555536	3.372230	-1.633607
C	-1.372692	-3.363781	-0.278743
H	-1.615286	-3.526568	0.784139
C	0.119398	-2.995217	-0.421027
H	0.493558	-3.339686	-1.403930
C	-1.182751	-1.063237	-0.730264
C	-3.428517	-1.896017	-0.665607
C	-4.121295	-1.690672	-1.862284
C	-4.108064	-1.802974	0.563199
C	-5.486143	-1.410657	-1.853387
H	-3.565183	-1.744462	-2.802046
C	-5.479118	-1.536134	0.556601
C	-6.167889	-1.343681	-0.639121
H	-6.014731	-1.246894	-2.795418
H	-5.993606	-1.451319	1.516360
H	-7.238799	-1.127226	-0.619969
S	-3.290836	-1.974188	2.177955
O	-4.204434	-1.306820	3.132650
O	-1.975121	-1.294701	2.026667
O	-3.174493	-3.438211	2.394380
C	-1.805310	-4.567151	-1.069569
C	-2.339227	-5.681086	-0.413578
C	-1.687326	-4.592659	-2.466395
C	-2.735660	-6.807004	-1.137484
H	-2.448173	-5.654729	0.674577
C	-2.085777	-5.713913	-3.189941
H	-1.283912	-3.719784	-2.990028
C	-2.609439	-6.826058	-2.525798
H	-3.150214	-7.671679	-0.613213
H	-1.989979	-5.721336	-4.278684
H	-2.921701	-7.706055	-3.093783
N	-2.023036	-2.115118	-0.729117
N	0.049931	-1.519275	-0.439954
C	1.155213	-0.676817	-0.205109
C	2.392694	-0.940097	-0.794828
C	1.004757	0.396781	0.681372
C	3.489720	-0.114955	-0.520036
C	2.097545	1.211017	0.990482
C	3.327723	0.955371	0.367545
H	4.187497	1.590874	0.604052
H	0.033693	0.559310	1.160011
H	2.504943	-1.787666	-1.477100

C	1.973286	2.263813	2.040316
C	1.958368	3.635839	1.697823
C	1.871393	1.865163	3.395908
C	1.788825	4.584527	2.714387
C	1.697280	2.849307	4.377392
C	1.646097	4.199032	4.043356
H	1.760612	5.647313	2.454172
H	1.605283	2.550153	5.425753
H	1.504826	4.952889	4.822719
C	4.813822	-0.368666	-1.159678
C	5.747202	-1.220149	-0.525001
C	5.118887	0.244162	-2.397592
C	7.004808	-1.394987	-1.117278
C	6.387375	0.038946	-2.953884
C	7.328389	-0.762774	-2.314394
H	7.742791	-2.042659	-0.636961
H	6.640640	0.510746	-3.907104
H	8.315639	-0.909173	-2.760820
C	4.099252	1.120565	-3.103404
H	3.103271	0.776363	-2.781734
C	4.145445	1.007884	-4.620070
H	4.072722	-0.035553	-4.961248
H	3.308269	1.560982	-5.069687
H	5.068905	1.431212	-5.044431
C	4.226312	2.577978	-2.669397
H	4.177419	2.684372	-1.576475
H	5.185699	3.009854	-2.997879
H	3.418556	3.190657	-3.100001
C	5.406869	-1.923620	0.778770
H	4.310845	-2.061964	0.798695
C	5.770294	-1.067428	1.988962
H	5.454666	-1.556940	2.923515
H	6.858454	-0.904288	2.048652
H	5.291726	-0.078026	1.955497
C	6.039301	-3.303319	0.894820
H	5.669421	-3.823620	1.790179
H	5.814836	-3.937472	0.024018
H	7.134514	-3.252276	0.993549
C	1.966115	0.410635	3.830054
H	2.312764	-0.181385	2.966135
C	2.110110	4.121396	0.268015
H	2.272673	3.242381	-0.372407
C	0.839070	4.803294	-0.225130
H	-0.035317	4.147184	-0.108470
H	0.635074	5.731842	0.333275
H	0.923047	5.073424	-1.289668
C	3.323608	5.031351	0.111593
H	3.220345	5.956413	0.700829
H	4.253906	4.540550	0.436348
H	3.457872	5.334041	-0.938060
C	0.604854	-0.137154	4.246612
H	0.172691	0.455499	5.069606
H	-0.120981	-0.134904	3.420980
H	0.687064	-1.173891	4.607013
C	2.992168	0.216466	4.941856
H	3.970994	0.645934	4.681224
H	2.671718	0.677859	5.888804
H	3.145275	-0.854334	5.145505
H	0.040178	-2.452470	2.243509
H	1.540109	-3.368197	4.020825
C	0.839355	-3.160113	1.991798
C	1.674644	-3.677231	2.980850
C	1.007660	-3.553388	0.656268
C	2.674015	-4.596711	2.652663
H	3.325349	-5.000357	3.432356
C	2.009662	-4.474057	0.333744
C	2.835869	-5.000057	1.327750
H	2.142189	-4.778976	-0.709261
H	3.614262	-5.720493	1.063726
O	-3.426291	3.612380	-3.627469
H	-4.053939	3.326029	-1.679739
H	-4.041141	1.867528	-2.683057
C	-4.694093	4.014204	-4.050012
H	-5.347111	3.155989	-4.303150
H	-4.578282	4.631492	-4.950813
H	-5.224090	4.615661	-3.285363

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Scheme_S14_LXI / electronic energy: -5327.02122721 a.u. / lowest freq: -118.63 cm-1

Cu	-1.850432	-1.179927	-0.177566
C	-2.709549	-2.406463	-1.530551
C	-2.467076	-3.059670	-0.226877
O	-0.187624	-2.799013	1.688230
B	-1.407022	-2.187807	1.497612

O	-2.096418	-2.040032	2.686438
C	-1.139759	-2.255371	3.760859
C	-0.097960	-3.200190	3.081982
C	-1.862213	-2.850771	4.947604
H	-1.154790	-3.114154	5.747634
H	-2.574732	-2.124461	5.362924
H	-2.426484	-3.752273	4.677473
C	-0.559423	-0.894534	4.113554
H	-1.374995	-0.211397	4.390543
H	0.133579	-0.951052	4.965377
H	-0.020479	-0.450143	3.262600
C	1.328938	-3.000651	3.543428
H	1.690637	-1.995795	3.288929
H	1.420970	-3.142573	4.630756
H	1.995661	-3.727450	3.056667
C	-0.501252	-4.662096	3.156629
H	0.142796	-5.259230	2.497375
H	-0.401469	-5.062916	4.175469
H	-1.540498	-4.811593	2.829749
C	-1.942775	-2.881027	-2.678311
H	-3.757821	-2.217780	-1.790786
F	-2.081122	-2.098170	-3.774951
F	-2.281876	-4.141152	-3.120860
F	-0.605363	-2.976182	-2.435077
C	-3.708756	-3.461455	0.527425
H	-1.704244	-3.852927	-0.241744
C	-1.837905	2.949812	0.519213
H	-2.156551	3.626609	-0.287834
C	-0.309833	2.724132	0.473750
H	0.125874	2.957482	1.459619
C	-1.399849	0.663707	0.064805
C	-3.736336	1.282984	0.166612
C	-4.240508	0.379547	1.110826
C	-4.590346	1.825079	-0.809538
C	-5.583010	0.010065	1.093095
H	-3.553254	-0.039564	1.853219
C	-5.936469	1.450788	-0.808405
C	-6.435946	0.553144	0.132770
H	-5.959842	-0.699793	1.833698
H	-6.581671	1.862678	-1.587508
H	-7.491513	0.271468	0.109296
S	-4.024323	2.951237	-2.117007
O	-5.080298	2.879949	-3.148849
O	-2.710776	2.413514	-2.541544
O	-3.937266	4.285160	-1.460146
C	-2.391030	3.448636	1.831450
C	-3.447282	4.366992	1.829985
C	-1.927161	2.947003	3.054898
C	-4.016494	4.789727	3.032270
H	-3.824099	4.729802	0.868329
C	-2.495019	3.369186	4.255129
H	-1.116864	2.210928	3.070583
C	-3.541323	4.294343	4.246347
H	-4.838851	5.509701	3.019287
H	-2.122304	2.971448	5.202777
H	-3.986572	4.626489	5.187609
N	-2.352200	1.592859	0.221704
N	-0.199754	1.274878	0.220847
C	1.051543	0.657400	0.060776
C	2.188704	1.222856	0.655818
C	1.191221	-0.479293	-0.744552
C	3.452098	0.659960	0.453484
C	2.451245	-1.030383	-0.984708
C	3.573853	-0.467403	-0.367547
H	4.566409	-0.884602	-0.563127
H	0.321017	-0.901387	-1.252104
H	2.101259	2.119330	1.274402
C	2.598578	-2.121465	-1.989153
C	2.795762	-3.457626	-1.578414
C	2.519562	-1.792654	-3.363128
C	2.930055	-4.450373	-2.557021
C	2.643234	-2.820375	-4.306161
C	2.853248	-4.137604	-3.910616
H	3.088397	-5.489193	-2.253957
H	2.570752	-2.584351	-5.371549
H	2.949889	-4.926087	-4.661767
C	4.661803	1.263034	1.085033
C	5.260978	2.410791	0.507200
C	5.201097	0.681981	2.254650
C	6.404363	2.943730	1.113609
C	6.343911	1.255395	2.829415
C	6.945001	2.372835	2.263238
H	6.884502	3.824739	0.682330

H	6.762525	0.822606	3.742670
H	7.836995	2.808253	2.721501
C	4.535784	-0.494364	2.949075
H	3.820185	-0.946296	2.242234
C	3.740187	-0.009304	4.158624
H	2.942215	0.692543	3.871540
H	3.269601	-0.848928	4.692348
H	4.390825	0.510660	4.879747
C	5.519001	-1.586421	3.349553
H	6.122788	-1.932617	2.497718
H	6.216482	-1.254021	4.133667
H	4.982454	-2.458521	3.753163
C	4.707858	3.029530	-0.767839
H	3.605488	2.963934	-0.715106
C	5.145483	2.240855	-2.001017
H	4.673431	2.642807	-2.910925
H	6.237229	2.297642	-2.138653
H	4.878548	1.176603	-1.933912
C	5.065885	4.498105	-0.938322
H	4.550481	4.917766	-1.813880
H	4.782839	5.104653	-0.065006
H	6.143244	4.645607	-1.111227
C	2.257509	-0.373222	-3.841705
H	2.470385	0.313608	-3.004645
C	2.861183	-3.831172	-0.109441
H	2.423824	-2.996164	0.464112
C	2.033439	-5.068253	0.208880
H	0.987744	-4.948811	-0.110824
H	2.431336	-5.972705	-0.276190
H	2.033936	-5.267704	1.290885
C	4.304458	-4.006247	0.353242
H	4.794914	-4.839784	-0.175234
H	4.909011	-3.105858	0.169939
H	4.353627	-4.227910	1.430641
C	0.788207	-0.195250	-4.218948
H	0.496419	-0.892252	-5.020935
H	0.112475	-0.380978	-3.371663
H	0.589333	0.824841	-4.581302
C	3.167372	0.038730	-4.992382
H	4.230802	-0.109845	-4.751718
H	2.955667	-0.522175	-5.915623
H	3.028847	1.103737	-5.231834
H	-0.031517	2.204552	-2.205095
H	1.127882	3.597062	-3.902845
C	0.450553	3.139461	-1.907734
C	1.097278	3.925349	-2.860492
C	0.405173	3.548627	-0.569657
C	1.692963	5.132465	-2.490705
H	2.196953	5.748183	-3.240163
C	1.014301	4.753655	-0.203184
C	1.647611	5.547090	-1.159491
H	0.988795	5.071876	0.844058
H	2.118949	6.487090	-0.860951
H	-4.349362	-2.571895	0.705850
H	-3.467694	-3.871156	1.528678
O	-4.414788	-4.420714	-0.229959
C	-5.623487	-4.779873	0.366446
H	-6.306538	-3.915408	0.485298
H	-5.486392	-5.231742	1.368717
H	-6.118414	-5.520532	-0.275694

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Scheme_S14_LXII / electronic energy: -5325.16005931 a.u. / lowest freq: -130.00 cm-1

C	-2.298418	-2.598753	-0.454421
H	-2.541890	-3.011782	0.537773
C	-0.768800	-2.577574	-0.654659
H	-0.522674	-2.770896	-1.715737
C	-1.535659	-0.364942	-0.314107
C	-3.939191	-0.659721	-0.338746
C	-4.441179	0.121413	-1.385967
C	-4.732328	-0.902092	0.795898
C	-5.735288	0.634363	-1.332078
H	-3.794067	0.314306	-2.246908
C	-6.034559	-0.397235	0.828875
C	-6.541116	0.356685	-0.227713
H	-6.114132	1.243629	-2.156595
H	-6.631893	-0.575104	1.725672
H	-7.561435	0.744853	-0.178644
S	-4.108745	-1.731516	2.289723
O	-4.998731	-1.245522	3.365631
O	-2.700807	-1.269845	2.418865
O	-4.233129	-3.187422	2.022414
C	-3.064225	-3.363799	-1.499078
C	-3.858014	-4.452572	-1.124464

C	-3.003576	-2.997634	-2.850984
C	-4.566804	-5.174743	-2.086154
H	-3.927301	-4.714796	-0.065223
C	-3.714863	-3.714422	-3.810268
H	-2.396433	-2.137240	-3.151634
C	-4.496033	-4.808544	-3.429588
H	-5.183292	-6.024342	-1.781850
H	-3.661466	-3.418897	-4.861169
H	-5.053816	-5.371518	-4.182242
N	-2.615787	-1.155807	-0.452099
N	-0.449079	-1.170222	-0.340322
C	0.875407	-0.717154	-0.175867
C	1.886946	-1.087944	-1.064786
C	1.173455	0.074520	0.933666
C	3.196468	-0.637759	-0.855330
C	2.472331	0.535893	1.162104
C	3.472520	0.179470	0.247856
H	4.498101	0.524433	0.412334
H	0.377038	0.286484	1.646622
H	1.659390	-1.725400	-1.923692
C	2.775046	1.325685	2.389736
C	3.181314	2.679579	2.295873
C	2.622116	0.717314	3.660527
C	3.410343	3.401944	3.473314
C	2.852593	1.483931	4.809806
C	3.239679	2.816924	4.723639
H	3.719200	4.449495	3.405102
H	2.731144	1.021004	5.793763
H	3.413679	3.398983	5.632547
C	4.296730	-1.037191	-1.779794
C	5.100528	-2.153930	-1.457646
C	4.529910	-0.293251	-2.960991
C	6.159583	-2.487243	-2.313066
C	5.595331	-0.666869	-3.788573
C	6.409881	-1.749081	-3.465022
H	6.797567	-3.342429	-2.073556
H	5.792891	-0.102228	-4.703269
H	7.240555	-2.024052	-4.120594
C	3.671895	0.912858	-3.302143
H	2.667202	0.729089	-2.886336
C	3.511742	1.145043	-4.796864
H	3.158406	0.245478	-5.322408
H	2.782744	1.945552	-4.984915
H	4.452915	1.459597	-5.273428
C	4.206190	2.167804	-2.615737
H	4.316658	2.020225	-1.532161
H	5.196123	2.447726	-3.011378
H	3.529042	3.023914	-2.766061
C	4.855262	-2.975451	-0.202295
H	3.819598	-2.783841	0.129273
C	5.778827	-2.534473	0.929854
H	5.583986	-3.111751	1.846487
H	6.837215	-2.685453	0.663188
H	5.651249	-1.470031	1.176316
C	4.979272	-4.473836	-0.444864
H	4.699429	-5.036257	0.457913
H	4.329691	-4.813933	-1.265148
H	6.009242	-4.771941	-0.693789
C	2.248439	-0.745656	3.838635
H	2.206044	-1.217866	2.844227
C	3.363618	3.389890	0.966809
H	3.045035	2.703521	0.169530
C	2.491823	4.635950	0.854436
H	1.431133	4.415041	1.044286
H	2.798041	5.419554	1.565260
H	2.561620	5.069842	-0.154775
C	4.829298	3.732862	0.720147
H	5.214756	4.429828	1.481564
H	5.473233	2.840512	0.741576
H	4.963800	4.216473	-0.259516
C	0.872218	-0.893735	4.477885
H	0.846574	-0.446114	5.484173
H	0.085269	-0.404438	3.885706
H	0.592473	-1.952066	4.587487
C	3.306540	-1.500162	4.637154
H	4.308769	-1.386986	4.197703
H	3.363884	-1.154669	5.681192
H	3.078522	-2.576672	4.666089
H	-0.717349	-2.676853	2.056917
H	0.568587	-4.256751	3.496460
C	-0.084450	-3.450742	1.606256
C	0.628792	-4.339415	2.408060
C	-0.013214	-3.551382	0.209174

C	1.410644	-5.341510	1.827233
H	1.965514	-6.039355	2.459706
C	0.770606	-4.555672	-0.365997
C	1.473806	-5.453521	0.439079
H	0.829293	-4.633396	-1.456310
H	2.078034	-6.239017	-0.021650
Cu	-1.584488	1.529587	-0.541891
C	-1.207379	2.805893	-2.043005
C	-1.852327	3.548124	-0.899836
C	0.205726	3.053624	-2.279496
H	-1.771610	2.856916	-2.981373
F	0.668249	2.412241	-3.382253
F	1.019962	2.672512	-1.245855
F	0.573954	4.374366	-2.482788
C	-3.277283	3.923248	-1.246908
H	-1.284007	4.445131	-0.596688
Si	-2.112835	3.101077	1.283322
C	-0.682077	2.526227	2.372797
H	0.278472	2.529209	1.836392
H	-0.564560	3.188236	3.248230
H	-0.859114	1.506368	2.745532
C	-3.734851	2.307418	1.833228
H	-4.169254	2.841446	2.695569
H	-4.498571	2.304612	1.039306
H	-3.571842	1.262023	2.138789
C	-2.217755	4.951977	1.665513
H	-2.542075	5.082376	2.711059
H	-1.227269	5.426885	1.580299
H	-2.911056	5.530474	1.036751
O	-3.269882	4.951484	-2.210001
H	-3.869432	4.248012	-0.366892
H	-3.804088	3.028185	-1.644376
C	-4.559792	5.312768	-2.605235
H	-5.170610	5.686467	-1.760488
H	-5.110867	4.467732	-3.062720
H	-4.481478	6.113788	-3.352014

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Scheme_S14_LXIII / electronic energy: -5325.16294218 a.u. / lowest freq: -120.28 cm-1

C	2.507214	2.401136	-0.088876
H	2.766523	2.638672	0.955056
C	0.980481	2.528947	-0.285162
H	0.762883	2.913176	-1.300294
C	1.574279	0.241853	-0.287417
C	3.985402	0.330902	-0.165645
C	4.548329	-0.274994	-1.292014
C	4.653368	0.266107	1.071833
C	5.771543	-0.936039	-1.207988
H	4.000832	-0.229805	-2.236095
C	5.880200	-0.397767	1.140065
C	6.442365	-0.991872	0.011924
H	6.200605	-1.402305	-2.097515
H	6.375952	-0.458191	2.111177
H	7.402742	-1.507483	0.090420
S	3.995628	0.965818	2.615002
O	4.738039	0.266026	3.684304
O	2.541926	0.664229	2.586217
O	4.305267	2.417899	2.532736
C	3.334530	3.263385	-1.001831
C	4.128283	4.282807	-0.466247
C	3.321937	3.068522	-2.390087
C	4.886179	5.103865	-1.302838
H	4.155078	4.416848	0.618862
C	4.082357	3.883859	-3.225217
H	2.714561	2.263719	-2.817954
C	4.864431	4.906754	-2.682888
H	5.501860	5.897487	-0.872054
H	4.067337	3.720863	-4.305883
H	5.460620	5.546437	-3.338518
N	2.714612	0.956935	-0.309027
N	0.549387	1.119851	-0.204237
C	-0.801738	0.752582	-0.068463
C	-1.803365	1.496398	-0.703335
C	-1.143000	-0.342112	0.729663
C	-3.146690	1.139470	-0.548253
C	-2.482036	-0.703062	0.914174
C	-3.470598	0.046990	0.265851
H	-4.523203	-0.216855	0.403068
H	-0.346953	-0.909895	1.220643
H	-1.537786	2.351429	-1.331619
C	-2.825757	-1.839238	1.812007
C	-3.533060	-2.965583	1.318583
C	-2.402714	-1.804753	3.165674
C	-3.774842	-4.041375	2.180994

C	-2.650757	-2.915709	3.980828
C	-3.326999	-4.029713	3.497426
H	-4.314198	-4.915907	1.806053
H	-2.312553	-2.900061	5.021154
H	-3.510368	-4.888488	4.148576
C	-4.227939	1.877259	-1.263552
C	-4.685679	3.125031	-0.776518
C	-4.798086	1.302227	-2.424333
C	-5.718910	3.773189	-1.465358
C	-5.827215	1.988759	-3.080917
C	-6.287279	3.212257	-2.605556
H	-6.090932	4.734528	-1.104010
H	-6.272942	1.560051	-3.982277
H	-7.093045	3.734989	-3.127849
C	-4.260700	0.004593	-3.003949
H	-3.861977	-0.593452	-2.167365
C	-3.092904	0.290124	-3.946477
H	-2.277741	0.830698	-3.441072
H	-2.669388	-0.640903	-4.354131
H	-3.416191	0.908095	-4.799614
C	-5.316102	-0.846089	-3.695044
H	-6.209419	-0.989051	-3.069529
H	-5.647996	-0.410641	-4.650364
H	-4.911375	-1.842965	-3.927783
C	-4.110049	3.726828	0.495698
H	-3.031112	3.489137	0.513099
C	-4.728475	3.083531	1.735652
H	-4.276294	3.486595	2.654826
H	-5.811682	3.278688	1.785227
H	-4.588354	1.993047	1.753604
C	-4.241084	5.240378	0.567756
H	-3.713164	5.628578	1.450461
H	-3.820254	5.739509	-0.318230
H	-5.288854	5.563796	0.665392
C	-1.726599	-0.596659	3.796845
H	-1.748273	0.231381	3.071155
C	-4.024151	-3.078719	-0.116310
H	-3.552529	-2.273993	-0.702214
C	-3.619028	-4.397513	-0.768066
H	-2.540500	-4.592816	-0.677425
H	-4.146500	-5.257254	-0.326876
H	-3.868075	-4.391019	-1.840531
C	-5.536297	-2.892382	-0.203683
H	-6.066568	-3.662659	0.379050
H	-5.863947	-1.914815	0.180690
H	-5.886813	-2.975179	-1.243621
C	-0.266183	-0.873311	4.137091
H	-0.171165	-1.711700	4.845918
H	0.333465	-1.126693	3.251692
H	0.204908	0.004533	4.604606
C	-2.489374	-0.112539	5.026611
H	-3.544447	0.099951	4.796877
H	-2.470857	-0.848662	5.845116
H	-2.044546	0.814431	5.418966
H	0.624283	2.032662	2.360866
H	-0.483700	3.496799	4.046675
C	0.207462	3.002191	2.066362
C	-0.398029	3.830266	3.008909
C	0.316709	3.418419	0.731804
C	-0.880071	5.087824	2.636269
H	-1.351308	5.737073	3.378991
C	-0.168825	4.676284	0.363717
C	-0.756546	5.512845	1.314020
H	-0.083956	5.001724	-0.678222
H	-1.128477	6.496603	1.016427
Cu	1.544869	-1.656010	-0.402930
C	1.842107	-3.453653	0.376362
C	1.649116	-3.612637	-1.118919
C	0.851969	-4.099671	1.225118
H	2.854865	-3.691420	0.724874
F	1.019716	-3.845039	2.544904
F	0.831072	-5.486590	1.159049
F	-0.435988	-3.761679	0.927248
C	2.907183	-4.009736	-1.875537
H	0.814100	-4.303708	-1.336870
Si	0.659543	-2.295064	-2.606354
C	0.672490	-3.622004	-3.957139
H	0.394879	-4.622643	-3.589558
H	-0.075735	-3.345240	-4.718880
H	1.639625	-3.706103	-4.474627
C	1.090388	-0.704388	-3.549481
H	0.526256	-0.668902	-4.498760
H	0.835120	0.203330	-2.980921

H	2.159366	-0.659216	-3.808421
C	-1.147284	-2.183278	-2.041350
H	-1.286460	-2.629310	-1.047179
H	-1.495990	-1.140698	-1.979780
H	-1.814605	-2.718546	-2.738581
H	2.714122	-4.881949	-2.532129
H	3.708839	-4.316031	-1.174054
O	3.367332	-2.925602	-2.660609
C	4.432353	-3.269741	-3.497377
H	4.159745	-4.076993	-4.204801
H	5.318171	-3.613607	-2.930823
H	4.713089	-2.382008	-4.080806

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Scheme_S15_ts(CuXadd)_Bpin / electronic energy: -4211.98699480 a.u. / lowest freq: -185.43 cm-1

C	0.001788	-3.866998	1.571502
C	0.358644	-3.204978	2.892628
C	0.911124	-1.735470	1.167842
C	-0.137774	-2.774687	-0.742056
C	0.873676	-2.671075	-1.706901
C	-1.481542	-2.783766	-1.163851
C	0.568559	-2.608132	-3.063567
H	1.912854	-2.641737	-1.368571
C	-1.777258	-2.741209	-2.528895
C	-0.761445	-2.657453	-3.477866
H	1.374148	-2.526412	-3.797021
H	-2.824765	-2.738694	-2.834858
H	-1.012859	-2.616256	-4.539963
S	-2.869262	-2.731755	-0.013701
O	-4.024747	-2.258532	-0.839638
O	-2.523302	-1.682229	0.995593
O	-3.040007	-4.087881	0.534984
Cu	1.145697	-0.117060	0.211879
N	0.231840	-2.772785	0.619790
N	1.102533	-2.020695	2.466348
C	1.202100	1.615866	-0.818886
C	-0.185533	1.236474	-0.408669
C	-0.867717	1.907370	0.695880
H	-1.568523	1.251292	1.242808
H	-0.167535	2.312026	1.441295
H	-0.833030	0.855391	-1.210250
P	-3.174928	2.803325	-0.101144
O	-3.692674	4.284007	-0.403104
O	-3.456536	1.753303	-1.126888
O	-3.955533	2.277249	1.232241
O	-1.683328	3.106403	0.312347
Na	-4.007456	-0.122528	0.029698
C	-4.995234	4.462537	-0.967486
H	-5.193041	5.539121	-0.974522
H	-5.033485	4.080778	-1.996547
H	-5.766490	3.961715	-0.364219
C	-3.893957	3.012947	2.454676
H	-4.493565	2.468873	3.191830
H	-2.860393	3.092341	2.820799
H	-4.311191	4.022353	2.329605
C	1.615610	-1.080201	3.421275
H	1.537467	2.544415	-0.327441
C	1.410080	1.662092	-2.320983
H	0.968048	-3.844045	3.547508
H	-0.535081	-2.897469	3.465544
H	1.176609	0.692978	-2.786886
H	2.436078	1.921002	-2.613826
H	0.729047	2.404150	-2.767988
H	2.280776	-1.578323	4.141214
H	0.807407	-0.588665	3.989992
H	2.187741	-0.305989	2.892716
H	-1.033460	-4.226631	1.526182
H	0.669480	-4.712556	1.332487
H	6.189515	0.157040	-2.468405
H	5.491111	-1.498001	-0.776937
C	6.079394	0.995892	-1.767084
H	7.079920	1.234512	-1.377283
H	5.717321	1.860629	-2.337543
H	6.577347	-0.678096	0.362612
C	5.547139	-0.703387	-0.019888
O	3.804802	0.440349	-1.188742
C	5.138236	0.620802	-0.644953
H	4.876430	-0.982865	0.806071
H	5.939009	3.447166	-0.475932
H	4.283704	3.195466	-1.082162
B	2.906430	0.805943	-0.203072
C	4.905821	1.741125	0.415715
H	6.867503	1.760684	1.331521
C	4.924647	3.134481	-0.190280

C	5.811300	1.667714	1.624355
H	5.687578	0.725972	2.173980
O	3.539032	1.480337	0.831325
H	4.545269	3.859556	0.543285
H	5.587636	2.489960	2.318501

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Scheme_S15_pc_Bpin / electronic energy: -4212.00418535 a.u. / lowest freq: 19.03 cm-1

C	0.132547	2.834983	2.276831
C	0.211574	1.848159	3.428089
C	-0.642540	0.734515	1.559675
C	-0.267933	2.342965	-0.202568
C	-1.473313	2.193326	-0.903438
C	0.868576	2.801591	-0.897067
C	-1.559177	2.494972	-2.258575
H	-2.345174	1.814991	-0.364847
C	0.766512	3.123342	-2.253700
C	-0.438132	2.973622	-2.936134
H	-2.509076	2.355636	-2.781318
H	1.661962	3.464428	-2.776710
H	-0.494475	3.220348	-3.998637
S	2.496356	2.932451	-0.140677
O	3.461389	2.844992	-1.281708
O	2.649833	1.720651	0.726351
O	2.536006	4.215560	0.581969
Cu	-1.258680	-0.670509	0.321214
N	-0.228933	1.955639	1.153392
N	-0.476096	0.675717	2.885778
C	-0.603032	-2.017610	-1.048503
C	0.503185	-1.319618	-0.513525
C	1.325966	-1.873033	0.580205
H	1.819307	-1.091076	1.179436
H	0.744213	-2.512568	1.258178
H	0.940963	-0.495809	-1.094450
P	3.756395	-2.200301	-0.439247
O	4.560487	-3.564434	-0.646737
O	3.744472	-1.231634	-1.575539
O	4.463105	-1.394563	0.785237
O	2.399962	-2.801742	0.105792
Na	4.261374	0.776711	-0.657024
C	5.835232	-3.533634	-1.294410
H	6.198337	-4.565555	-1.327405
H	5.749621	-3.147841	-2.319069
H	6.553958	-2.919772	-0.732255
C	4.674201	-2.016312	2.054899
H	4.983864	-1.232016	2.753180
H	3.753155	-2.486571	2.427285
H	5.465169	-2.776889	1.991132
C	-0.669882	-0.508646	3.672644
H	-0.804741	-3.016489	-0.635635
C	-1.101144	-1.781579	-2.439774
H	-0.279150	2.207747	4.343654
H	1.251127	1.580309	3.689117
H	-0.981346	-0.730678	-2.743923
H	-2.164795	-2.033917	-2.550740
H	-0.544251	-2.392748	-3.172101
H	-1.250251	-0.288081	4.580616
H	0.290696	-0.951583	3.985657
H	-1.222111	-1.247578	3.077207
H	1.069849	3.371192	2.091246
H	-0.663909	3.584510	2.420989
H	-5.913574	0.370709	-2.707006
H	-5.372330	1.872801	-0.836197
C	-6.082017	-0.485324	-2.037998
H	-7.167558	-0.571294	-1.879264
H	-5.739459	-1.386020	-2.563200
H	-6.774113	1.205562	0.023977
C	-5.694018	1.082845	-0.142025
O	-3.925718	-0.284832	-0.977385
C	-5.351730	-0.278214	-0.728681
H	-5.177760	1.250347	0.814456
H	-6.646643	-2.915283	-0.848652
H	-4.887608	-2.963821	-1.127526
B	-3.278675	-0.855964	0.118795
C	-5.509643	-1.439969	0.298629
H	-7.584352	-1.141984	0.854025
C	-5.664869	-2.797969	-0.367569
C	-6.596416	-1.229994	1.330667
H	-6.424979	-0.327706	1.931247
O	-4.220377	-1.437949	0.962919
H	-5.565548	-3.591309	0.386559
H	-6.638418	-2.084360	2.021164

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Scheme_S15_ts(oa)_Bpin / electronic energy: -4211.99903517 a.u. / lowest freq: -366.39 cm-1

C	0.087590	-2.982415	-2.151979
C	0.074162	-2.067503	-3.364998
C	-0.707420	-0.864539	-1.527068
C	-0.234281	-2.349561	0.313356
C	-1.426302	-2.200620	1.035464
C	0.939207	-2.711357	1.002506
C	-1.462147	-2.402314	2.411546
H	-2.328466	-1.906320	0.494307
C	0.888444	-2.933408	2.381309
C	-0.302287	-2.779096	3.087543
H	-2.402478	-2.265085	2.951554
H	1.811348	-3.198602	2.900300
H	-0.318260	-2.945233	4.166867
S	2.544778	-2.835494	0.198995
O	3.543584	-2.700502	1.304524
O	2.642219	-1.647574	-0.707841
O	2.583298	-4.139139	-0.486084
Cu	-1.263784	0.591333	-0.330342
N	-0.247978	-2.046282	-1.066192
N	-0.613334	-0.878136	-2.858931
C	-0.783160	2.072175	0.943536
C	0.406809	1.355845	0.613133
C	1.184126	1.626548	-0.549501
H	1.803306	0.807804	-0.931259
H	0.707170	2.209617	-1.342865
H	0.799230	0.622974	1.330971
P	3.759638	2.264803	0.344690
O	4.666485	3.588725	0.497651
O	3.750112	1.353478	1.536671
O	4.514533	1.355213	-0.803412
O	2.450428	2.835058	-0.250170
Na	4.309089	-0.643934	0.624999
C	5.962385	3.468776	1.076623
H	6.385560	4.477473	1.135997
H	5.911822	3.043746	2.089163
H	6.623128	2.844125	0.455731
C	4.609845	1.825621	-2.142689
H	5.333068	1.191041	-2.667426
H	3.640122	1.761240	-2.658425
H	4.963493	2.866828	-2.176882
C	-0.862965	0.257313	-3.701302
H	-0.964078	2.995533	0.373941
C	-1.336422	2.060927	2.332829
H	-0.456913	-2.494904	-4.227169
H	1.089052	-1.790964	-3.701483
H	-1.240954	1.071804	2.804376
H	-2.398523	2.337670	2.360990
H	-0.796359	2.777513	2.975768
H	-1.477948	-0.024088	-4.568322
H	0.076201	0.694810	-4.079576
H	-1.400784	1.021515	-3.125227
H	1.052145	-3.473118	-1.980034
H	-0.687492	-3.765101	-2.206637
H	-5.941703	-0.194685	2.754901
H	-5.398599	-1.819931	0.988732
C	-6.078159	0.623669	2.033904
H	-7.158696	0.730571	1.856502
H	-5.715225	1.545054	2.506922
H	-6.782295	-1.184223	0.076542
C	-5.701750	-1.070255	0.243842
O	-3.915398	0.313475	1.011747
C	-5.342846	0.318312	0.747817
H	-5.181421	-1.304860	-0.696182
H	-6.583055	2.984289	0.682047
H	-4.826464	3.018356	0.975310
B	-3.264383	0.799872	-0.110601
C	-5.468594	1.416279	-0.353378
H	-7.540492	1.122491	-0.912212
C	-5.599650	2.817371	0.220064
C	-6.547007	1.161501	-1.383053
H	-6.387696	0.220517	-1.924460
O	-4.169242	1.345742	-1.004496
H	-5.478715	3.556579	-0.584025
H	-6.564787	1.972194	-2.124967

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Scheme_S15_pa_Bpin / electronic energy: -4212.03162404 a.u. / lowest freq: -45.91 cm-1

C	-0.826627	2.637093	1.838319
C	-0.937941	1.659907	2.999138
C	-0.975277	0.457752	1.012143
C	-0.389551	2.138266	-0.633248
C	-1.314781	1.905842	-1.658768
C	0.852940	2.720462	-0.944116
C	-1.019045	2.252756	-2.974555

H	-2.273845	1.445945	-1.404590
C	1.130025	3.082809	-2.264629
C	0.201162	2.855423	-3.277054
H	-1.752137	2.061803	-3.761738
H	2.103750	3.520725	-2.492481
H	0.438809	3.138951	-4.304570
S	2.152910	2.975342	0.279167
O	3.420427	2.952803	-0.510863
O	2.098376	1.783888	1.182063
O	1.868560	4.261545	0.938376
Cu	-1.131938	-0.965857	-0.283427
N	-0.717136	1.732009	0.681526
N	-1.182416	0.382981	2.324187
C	-1.681885	-2.507270	-1.515102
C	-0.301843	-2.138994	-1.766368
C	0.687789	-2.148742	-0.809455
H	1.690401	-1.759101	-1.011959
H	0.567717	-2.723760	0.117131
H	-0.095218	-1.620038	-2.713522
P	4.431878	-2.099035	-0.029316
O	5.879827	-2.676645	-0.550294
O	3.886325	-1.077264	-1.010390
O	4.917914	-1.080159	1.222638
O	3.659379	-3.260625	0.499615
Na	3.978723	0.805405	0.210485
C	6.791225	-1.784064	-1.150971
H	7.708400	-2.341373	-1.383929
H	6.397391	-1.358306	-2.087770
H	7.061154	-0.949889	-0.480343
C	5.502410	-1.661406	2.369461
H	5.531063	-0.907891	3.167207
H	4.917578	-2.525600	2.720965
H	6.533341	-1.999033	2.171135
C	-1.387415	-0.835740	3.056477
H	-1.819233	-3.315876	-0.781691
C	-2.636741	-2.524984	-2.671050
H	-1.760743	1.897386	3.688577
H	-0.011493	1.590595	3.593059
H	-2.556852	-1.612876	-3.279618
H	-3.682695	-2.622368	-2.353333
H	-2.421238	-3.379384	-3.333054
H	-2.296594	-0.778623	3.672880
H	-0.534003	-1.045075	3.719985
H	-1.497871	-1.664129	2.346540
H	0.040658	3.304350	1.907153
H	-1.728295	3.260259	1.719246
H	-6.215055	1.131792	-1.654134
H	-4.720029	2.122382	0.053662
C	-6.310327	0.186830	-1.102219
H	-7.265594	0.214035	-0.558604
H	-6.353780	-0.627699	-1.835733
H	-5.871919	1.526468	1.264270
C	-4.963255	1.269542	0.702721
O	-3.923160	-0.152545	-0.913113
C	-5.158430	0.022915	-0.141145
H	-4.140660	1.146021	1.423426
H	-6.918245	-2.333458	-0.108325
H	-5.416237	-2.582065	-1.027636
B	-3.129304	-0.974850	-0.170978
C	-5.197472	-1.287343	0.711646
H	-6.844513	-0.802860	2.018234
C	-5.830360	-2.456157	-0.017515
C	-5.795407	-1.124305	2.088866
H	-5.252663	-0.388525	2.694663
O	-3.769697	-1.598672	0.854950
H	-5.643072	-3.383242	0.540896
H	-5.778180	-2.081940	2.626715

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Scheme_S15_ts(cc)_Bpin / electronic energy: -4212.03162404 a.u. / lowest freq: -45.91 cm-1

C	-0.826627	2.637093	1.838319
C	-0.937941	1.659907	2.999138
C	-0.975277	0.457752	1.012143
C	-0.389551	2.138266	-0.633248
C	-1.314781	1.905842	-1.658768
C	0.852940	2.720462	-0.944116
C	-1.019045	2.252756	-2.974555
H	-2.273845	1.445945	-1.404590
C	1.130025	3.082809	-2.264629
C	0.201162	2.855423	-3.277054
H	-1.752137	2.061803	-3.761738
H	2.103750	3.520725	-2.492481
H	0.438809	3.138951	-4.304570
S	2.152910	2.975342	0.279167

O	3.420427	2.952803	-0.510863
O	2.098376	1.783888	1.182063
O	1.868560	4.261545	0.938376
Cu	-1.131938	-0.965857	-0.283427
N	-0.717136	1.732009	0.681526
N	-1.182416	0.382981	2.324187
C	-1.681885	-2.507270	-1.515102
C	-0.301843	-2.138994	-1.766368
C	0.687789	-2.148742	-0.809455
H	1.690401	-1.759101	-1.011959
H	0.567717	-2.723760	0.117131
H	-0.095218	-1.620038	-2.713522
P	4.431878	-2.099035	-0.029316
O	5.879827	-2.676645	-0.550294
O	3.886325	-1.077264	-1.010390
O	4.917914	-1.080159	1.222638
O	3.659379	-3.260625	0.499615
Na	3.978723	0.805405	0.210485
C	6.791225	-1.784064	-1.150971
H	7.708400	-2.341373	-1.383929
H	6.397391	-1.358306	-2.087770
H	7.061154	-0.949889	-0.480343
C	5.502410	-1.661406	2.369461
H	5.531063	-0.907891	3.167207
H	4.917578	-2.525600	2.720965
H	6.533341	-1.999033	2.171135
C	-1.387415	-0.835740	3.056477
H	-1.819233	-3.315876	-0.781691
C	-2.636741	-2.524984	-2.671050
H	-1.760743	1.897386	3.688577
H	-0.011493	1.590595	3.593059
H	-2.556852	-1.612876	-3.279618
H	-3.682695	-2.622368	-2.353333
H	-2.421238	-3.379384	-3.333054
H	-2.296594	-0.778623	3.672880
H	-0.534003	-1.045075	3.719985
H	-1.497871	-1.664129	2.346540
H	0.040658	3.304350	1.907153
H	-1.728295	3.260259	1.719246
H	-6.215055	1.131792	-1.654134
H	-4.720029	2.122382	0.053662
C	-6.310327	0.186830	-1.102219
H	-7.265594	0.214035	-0.558604
H	-6.353780	-0.627699	-1.835733
H	-5.871919	1.526468	1.264270
C	-4.963255	1.269542	0.702721
O	-3.923160	-0.152545	-0.913113
C	-5.158430	0.022915	-0.141145
H	-4.140660	1.146021	1.423426
H	-6.918245	-2.333458	-0.108325
H	-5.416237	-2.582065	-1.027636
B	-3.129304	-0.974850	-0.170978
C	-5.197472	-1.287343	0.711646
H	-6.844513	-0.802860	2.018234
C	-5.830360	-2.456157	-0.017515
C	-5.795407	-1.124305	2.088866
H	-5.252663	-0.388525	2.694663
O	-3.769697	-1.598672	0.854950
H	-5.643072	-3.383242	0.540896
H	-5.778180	-2.081940	2.626715

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Scheme_S15_prod_Bpin / electronic energy: -4212.10124845 a.u. / lowest freq: 19.21 cm-1

C	-0.154194	2.525603	1.216677
C	-0.633419	1.700439	2.397726
C	-0.329089	0.270261	0.571536
C	0.829113	1.710074	-0.993051
C	0.197554	1.339321	-2.188903
C	2.131343	2.242167	-1.045366
C	0.835560	1.493846	-3.414868
H	-0.812205	0.923547	-2.131672
C	2.756600	2.407763	-2.284639
C	2.117478	2.040761	-3.465203
H	0.324245	1.195448	-4.332872
H	3.773930	2.803275	-2.305647
H	2.627226	2.171224	-4.422201
S	3.093890	2.682953	0.416019
O	4.514330	2.473620	0.005680
O	2.725199	1.688392	1.470629
O	2.747075	4.077708	0.741742
Cu	-0.160727	-1.365392	-0.546247
N	0.152030	1.481320	0.224233
N	-0.856988	0.383488	1.795635
C	-3.028861	-2.314018	-0.482960

C	-1.905372	-2.126700	-1.466288
C	-0.831190	-2.974394	-1.626724
H	-0.209762	-2.940837	-2.526072
H	-0.686313	-3.840633	-0.969231
H	-2.109802	-1.408407	-2.273694
P	3.126151	-1.981490	-0.086526
O	3.432538	-3.580762	0.020067
O	4.326325	-1.197326	-0.546883
O	2.992861	-1.522081	1.499978
O	1.787530	-1.895745	-0.782021
Na	4.566111	0.344950	1.074993
C	4.674522	-3.999728	0.554094
H	4.680990	-5.096799	0.562556
H	5.521333	-3.648301	-0.055002
H	4.818152	-3.645793	1.588580
C	1.909915	-1.979243	2.282486
H	1.733367	-1.251745	3.086592
H	0.989775	-2.069591	1.678510
H	2.127026	-2.960375	2.736007
C	-1.402865	-0.697162	2.566699
H	-2.646204	-2.789583	0.436918
C	-4.093969	-3.254702	-1.074745
H	-1.558081	2.086323	2.852993
H	0.123737	1.616447	3.196911
H	-4.522234	-2.845864	-2.003206
H	-4.925552	-3.414644	-0.371957
H	-3.669188	-4.240597	-1.317523
H	-2.429853	-0.475758	2.893379
H	-0.795507	-0.895794	3.464642
H	-1.424096	-1.604095	1.948325
H	0.719162	3.146894	1.441698
H	-0.941279	3.184446	0.812795
H	-4.985848	2.255382	-2.201569
H	-2.937962	2.427318	-0.818244
C	-5.552673	1.771328	-1.394426
H	-6.162861	2.545634	-0.907814
H	-6.228033	1.039099	-1.853490
H	-3.986128	3.025836	0.485982
C	-3.546447	2.120719	0.044239
O	-3.909234	0.036831	-1.058008
C	-4.606876	1.132651	-0.403512
H	-2.876704	1.665430	0.785786
H	-7.416204	0.597453	0.279279
H	-6.596357	-0.775396	-0.501524
B	-3.753183	-0.963076	-0.135031
C	-5.305641	0.407849	0.796295
H	-6.016693	2.133984	1.884519
C	-6.654664	-0.181358	0.422137
C	-5.412983	1.231753	2.058822
H	-4.431603	1.545925	2.436014
O	-4.414936	-0.719379	1.038471
H	-7.001130	-0.845810	1.225628
H	-5.905908	0.651649	2.851088

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Scheme_S15_ts(CuXadd)_H / electronic energy: -3801.64295456 a.u. / lowest freq: -899.31 cm-1

C	3.412237	0.517507	-1.896450
C	2.877789	-0.339452	-3.031687
C	2.224502	-1.311902	-1.008582
C	2.752277	0.434079	0.573990
C	3.327436	-0.305077	1.617233
C	2.101181	1.645687	0.879340
C	3.289789	0.154430	2.929994
H	3.810310	-1.254030	1.371926
C	2.082328	2.106992	2.198790
C	2.676209	1.372320	3.221476
H	3.747727	-0.438625	3.725081
H	1.562315	3.041630	2.416031
H	2.646169	1.746283	4.247164
S	1.188755	2.604789	-0.342775
O	0.241540	3.440332	0.460964
O	0.409633	1.609806	-1.145580
O	2.171052	3.388656	-1.111100
Cu	1.136723	-2.216214	0.255486
N	2.781693	-0.107844	-0.727279
N	2.361525	-1.513647	-2.330140
C	-0.339308	-2.835590	1.561056
C	-0.730068	-1.629534	0.851462
C	-1.614652	-1.655084	-0.315499
H	-1.384708	-0.871887	-1.058356
H	-1.588215	-2.619791	-0.841902
H	-0.623335	-0.673240	1.380484
P	-3.590312	-0.005347	0.156828
O	-5.152687	-0.280287	0.345491

O	-2.931798	0.910571	1.136728
O	-3.398811	0.747969	-1.278912
O	-3.074125	-1.485812	-0.013363
Na	-1.624602	2.253359	-0.157882
C	-6.017923	0.811733	0.670953
H	-7.030159	0.402291	0.746862
H	-5.738479	1.264618	1.631609
H	-6.001153	1.580827	-0.115092
C	-3.868299	0.149783	-2.488591
H	-3.819817	0.914875	-3.270514
H	-3.237471	-0.702392	-2.778601
H	-4.908567	-0.189797	-2.384859
C	1.713195	-2.574622	-3.046171
H	-0.875373	-3.742715	1.245377
H	1.042870	-3.484710	1.254043
C	-0.154647	-2.745685	3.053119
H	3.648939	-0.618957	-3.763878
H	2.057172	0.153406	-3.583810
H	0.469976	-1.882165	3.324735
H	0.316152	-3.643194	3.478814
H	-1.129675	-2.606099	3.546341
H	2.400079	-3.050324	-3.761735
H	0.838475	-2.207549	-3.610185
H	1.370142	-3.332843	-2.330267
H	3.144058	1.577341	-1.982649
H	4.509598	0.450915	-1.801509

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Scheme_S15_pc_H / electronic energy: -3801.67163517 a.u. / lowest freq: 25.17 cm-1

C	2.796650	0.731149	-2.158374
C	2.243827	-0.207773	-3.214974
C	2.005179	-1.225532	-1.126377
C	2.529641	0.580947	0.383823
C	3.219493	-0.179802	1.339986
C	1.946070	1.800061	0.783201
C	3.350201	0.260430	2.652827
H	3.648443	-1.135847	1.028951
C	2.100101	2.242001	2.100612
C	2.801460	1.484273	3.034283
H	3.890733	-0.354283	3.376438
H	1.628827	3.182398	2.392012
H	2.905084	1.844078	4.060157
S	0.902194	2.792868	-0.295571
O	0.033627	3.585544	0.630454
O	0.054122	1.814530	-1.049198
O	1.789957	3.616230	-1.134166
Cu	1.416612	-2.445762	0.319173
N	2.391054	0.052673	-0.915160
N	1.985603	-1.426778	-2.446669
C	-0.130676	-2.758905	1.640184
C	-0.383660	-1.629035	0.852322
C	-1.239358	-1.688847	-0.360359
H	-0.993844	-0.895167	-1.084790
H	-1.160609	-2.657629	-0.871859
H	-0.195132	-0.630738	1.272622
P	-3.341284	-0.182404	0.243716
O	-4.852466	-0.663150	0.413066
O	-2.769593	0.702731	1.300429
O	-3.252483	0.695796	-1.122082
O	-2.682598	-1.592552	-0.050479
Na	-1.882877	2.432317	0.098585
C	-5.835401	0.257443	0.898302
H	-6.778348	-0.294145	0.963388
H	-5.566100	0.633502	1.894113
H	-5.962929	1.104300	0.208487
C	-3.741667	0.193096	-2.368205
H	-3.376050	0.862727	-3.153459
H	-3.370754	-0.823102	-2.560713
H	-4.840438	0.186448	-2.379845
C	1.478735	-2.614613	-3.074185
H	-0.589574	-3.706884	1.326729
H	2.375747	-3.702739	0.640332
C	0.305930	-2.675307	3.066198
H	2.945044	-0.398369	-4.039376
H	1.299129	0.157380	-3.656373
H	0.838170	-1.736048	3.275988
H	0.966106	-3.506522	3.349730
H	-0.560196	-2.712572	3.749669
H	2.163565	-2.968517	-3.858478
H	0.494302	-2.438657	-3.539441
H	1.377657	-3.403132	-2.317386
H	2.397507	1.748783	-2.222162
H	3.897438	0.794730	-2.188757

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Scheme_S15_ts(oa)_H / electronic energy: -3801.66029997 a.u. / lowest freq: -291.37 cm-1

C	2.851381	1.185682	-1.966314
C	2.490193	0.294690	-3.141558
C	2.162475	-0.908967	-1.173743
C	2.409991	0.792182	0.525951
C	3.143414	0.045790	1.460360
C	1.654153	1.892436	0.977351
C	3.137898	0.380603	2.810770
H	3.715704	-0.813784	1.100858
C	1.671548	2.230793	2.333158
C	2.408331	1.484578	3.249171
H	3.714551	-0.219057	3.518734
H	1.068794	3.078145	2.664674
H	2.402499	1.761709	4.305431
S	0.589469	2.867581	-0.099483
O	-0.401098	3.511209	0.816722
O	-0.111762	1.880035	-0.980625
O	1.454083	3.824406	-0.811297
Cu	1.640975	-2.326765	0.105416
N	2.409466	0.368539	-0.821038
N	2.271315	-1.002719	-2.498424
C	0.262449	-3.202602	1.332698
C	-0.187441	-1.914312	0.967574
C	-0.755145	-1.627294	-0.299849
H	-0.720476	-0.595986	-0.663758
H	-0.719826	-2.393774	-1.077521
H	-0.110568	-1.093232	1.691922
P	-3.357847	-0.470733	0.191979
O	-4.895560	-0.935421	0.373836
O	-2.842568	0.432280	1.277248
O	-3.384342	0.532240	-1.122601
O	-2.645989	-1.780043	-0.184587
Na	-2.184498	2.250773	0.099494
C	-5.878204	0.046948	0.675348
H	-6.824546	-0.478788	0.845805
H	-5.620017	0.613385	1.582169
H	-6.014022	0.750485	-0.161005
C	-3.641515	0.000530	-2.414285
H	-3.775440	0.843472	-3.102180
H	-2.801083	-0.615939	-2.767393
H	-4.557615	-0.609644	-2.424488
C	1.930905	-2.172502	-3.258951
H	-0.058886	-4.038624	0.696068
H	2.756409	-3.434824	0.258231
C	0.651948	-3.545941	2.729254
H	3.282527	0.230984	-3.900271
H	1.563802	0.613365	-3.650893
H	1.093026	-2.688538	3.256798
H	1.370108	-4.374892	2.765763
H	-0.230573	-3.863365	3.310387
H	2.712384	-2.401729	-3.997463
H	0.980106	-2.038561	-3.800673
H	1.833295	-3.025215	-2.575189
H	2.357544	2.162578	-1.985091
H	3.937855	1.355133	-1.885318

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Scheme_S15_pa_H / electronic energy: -3801.67476642 a.u. / lowest freq: 12.08 cm-1

C	2.888305	1.480098	-1.903729
C	2.542248	0.674519	-3.147449
C	2.228850	-0.668881	-1.286696
C	2.448023	0.877377	0.556919
C	3.233471	0.117675	1.433787
C	1.602048	1.872464	1.081404
C	3.189595	0.337600	2.807571
H	3.883157	-0.653946	1.013013
C	1.578887	2.096685	2.460243
C	2.366743	1.337826	3.322638
H	3.808922	-0.268147	3.472869
H	0.905784	2.861632	2.851830
H	2.328836	1.524536	4.397861
S	0.481144	2.844456	0.058792
O	-0.586997	3.303975	0.995892
O	-0.093355	1.879184	-0.930296
O	1.278725	3.931805	-0.532946
Cu	1.720463	-2.121768	-0.093606
N	2.485895	0.562384	-0.822164
N	2.319139	-0.671585	-2.609648
C	0.696165	-3.429156	1.148740
C	0.120150	-2.136796	1.226144
C	-0.275995	-1.464943	0.071388
H	-0.517426	-0.400671	0.091635
H	-0.591594	-2.019771	-0.818841
H	0.255463	-1.560639	2.151399

P	-3.639068	-0.723485	0.201396
O	-5.281331	-0.699805	0.270546
O	-3.048668	0.116346	1.316714
O	-3.351027	0.288688	-1.114853
O	-3.242986	-2.127746	-0.119015
Na	-2.197668	1.848029	0.175085
C	-5.934925	0.511234	0.576169
H	-7.015479	0.317090	0.600896
H	-5.631763	0.909283	1.557807
H	-5.747794	1.287912	-0.186017
C	-3.699865	-0.161695	-2.405094
H	-3.443567	0.624427	-3.127452
H	-3.155485	-1.080503	-2.676138
H	-4.780519	-0.367043	-2.485733
C	1.991705	-1.786188	-3.455256
H	0.376609	-4.057915	0.304604
H	2.936837	-3.045284	-0.035370
C	1.252498	-4.134164	2.331717
H	3.345250	0.665609	-3.897196
H	1.621620	1.024966	-3.643347
H	1.710028	-3.440586	3.049760
H	1.996815	-4.887875	2.049015
H	0.444819	-4.667210	2.859861
H	2.789625	-1.967210	-4.188991
H	1.054128	-1.607212	-4.004585
H	1.873848	-2.682637	-2.834586
H	2.355222	2.435068	-1.835026
H	3.967746	1.682956	-1.816888

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Scheme_S15_ts(cc)_H / electronic energy: -3801.67381837 a.u. / lowest freq: -291.80 cm-1

C	3.007902	-1.478417	1.900834
C	2.523397	-0.782625	3.165704
C	2.126443	0.616927	1.354722
C	2.572615	-0.804775	-0.540151
C	3.348417	0.003420	-1.380458
C	1.744606	-1.791765	-1.105160
C	3.321250	-0.171660	-2.761586
H	3.978295	0.772688	-0.926227
C	1.734819	-1.968483	-2.490778
C	2.520047	-1.167975	-3.317618
H	3.934118	0.467185	-3.401406
H	1.075257	-2.727595	-2.915759
H	2.495351	-1.317920	-4.399015
S	0.622565	-2.803328	-0.120133
O	-0.441772	-3.229156	-1.076928
O	0.041018	-1.878644	0.902491
O	1.423119	-3.909591	0.431823
Cu	1.494233	2.047557	0.198770
N	2.580571	-0.539365	0.849951
N	2.142401	0.547516	2.680953
C	0.773694	3.587962	-0.935729
C	0.172169	2.353618	-1.362291
C	-0.497571	1.518282	-0.490190
H	-0.820080	0.528323	-0.818981
H	-0.922353	1.891419	0.447880
H	0.471655	1.954240	-2.340426
P	-3.827670	0.541530	-0.407513
O	-5.422875	0.377217	-0.046970
O	-3.394365	-0.515784	-1.403469
O	-3.105752	-0.061812	0.990071
O	-3.563659	2.005430	-0.543617
Na	-2.064642	-1.827588	-0.161042
C	-5.965923	-0.920002	0.054926
H	-7.038839	-0.824218	0.268178
H	-5.846656	-1.491771	-0.879078
H	-5.507131	-1.499216	0.875481
C	-3.242106	0.657887	2.194729
H	-2.389186	0.421615	2.847193
H	-3.254257	1.743888	2.010945
H	-4.170200	0.387251	2.725799
C	1.636344	1.556206	3.569491
H	0.252329	4.116922	-0.125785
H	2.403191	3.270574	0.257671
C	1.501950	4.444921	-1.915471
H	3.297838	-0.705004	3.941790
H	1.644685	-1.272205	3.617346
H	2.153145	3.852214	-2.572194
H	2.111437	5.213025	-1.425858
H	0.775327	4.964166	-2.560431
H	2.381644	1.817014	4.334524
H	0.726060	1.210720	4.083952
H	1.395450	2.456325	2.991073
H	2.566521	-2.470667	1.748877

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 H      4.103884     -1.583829      1.867032
54
Scheme_S15_prod_H / electronic energy: -3801.73523435 a.u. / lowest freq: 15.68 cm-1
 C      3.224078      0.348559      2.050987
 C      2.336512      0.696364      3.239519
 C      1.290583      1.449238      1.293652
 C      2.724163      0.569267     -0.443552
 C      2.999243      1.663542     -1.273005
 C      2.707757     -0.724850     -0.991981
 C      3.272413      1.481412     -2.625448
 H      3.003121      2.662868     -0.830987
 C      2.991808     -0.898302     -2.349765
 C      3.277106      0.194716     -3.163785
 H      3.488775      2.345915     -3.256909
 H      2.959324     -1.906906     -2.766608
 H      3.494145      0.040229     -4.222881
 S      2.288893     -2.195998     -0.034947
 O      1.679475     -3.123544     -1.035315
 O      1.250511     -1.767368      0.950431
 O      3.546986     -2.672939      0.562869
Cu     -0.043359      1.940105     -0.050580
 N      2.414606      0.816850      0.915763
 N      1.239715      1.449334      2.624114
 C     -2.705232      3.266246     -0.392734
 C     -1.464944      3.037439     -1.198498
 C     -1.154273      1.849901     -1.803605
 H     -0.336200      1.784081     -2.530488
 H     -1.838518      0.993640     -1.712090
 H     -0.861850      3.928869     -1.429699
 P     -3.193609     -1.427985     -0.512335
 O     -4.454372     -2.011691      0.361931
 O     -2.529249     -2.535926     -1.302449
 O     -2.038327     -1.184171      0.681008
 O     -3.642359     -0.118644     -1.082359
Na     -0.518875     -2.704609     -0.305954
 C     -4.330919     -3.276584      0.974450
 H     -5.280188     -3.502991      1.477577
 H     -4.127489     -4.073110      0.241302
 H     -3.531131     -3.290407      1.735068
 C     -2.193731     -0.129450      1.598047
 H     -1.955010      0.849849      1.139580
 H     -3.219801     -0.077208      1.999396
 H     -1.502537     -0.296924      2.436064
 C      0.187421      2.014157      3.420356
 H     -3.213152      2.301065     -0.234870
 H     -2.432405      3.654576      0.604988
 C     -3.645853      4.253284     -1.065213
 H      2.846708      1.305953      3.999679
 H      1.927964     -0.193488      3.746215
 H     -3.168504      5.232079     -1.221635
 H     -4.544451      4.418367     -0.455338
 H     -3.975529      3.885811     -2.047678
 H      0.569730      2.808323      4.079854
 H     -0.284452      1.248794      4.055090
 H     -0.573795      2.445245      2.758538
 H      3.437972     -0.724956      1.965683
 H      4.185786      0.885074      2.062012
66
Scheme_S15_ts(CuXadd)_SiMe3 / electronic energy: -4210.12384995 a.u. / lowest freq: -159.19 cm-1
 C      3.209116      2.843197     -0.744845
 C      3.626341      2.241067     -2.073194
 C      2.531746      0.593305     -0.835060
 C      1.673472      1.871578      1.029909
 C      2.268472      1.251253      2.134317
 C      0.432989      2.513546      1.189068
 C      1.658010      1.282187      3.386240
 H      3.224918      0.740478      1.991730
 C     -0.168989      2.548947      2.448650
 C      0.439917      1.940414      3.544792
 H      2.136588      0.792128      4.237327
 H     -1.132196      3.051081      2.553955
 H     -0.045943      1.974762      4.522486
 S     -0.463320      3.210610     -0.211477
 O     -1.731150      3.746815      0.379887
 O     -0.797473      2.053762     -1.099584
 O      0.406563      4.227913     -0.821702
Cu      1.471639     -0.869567     -0.226231
 N      2.321980      1.793339     -0.228104
 N      3.366959      0.816000     -1.864213
 C      0.419834     -2.374693      0.851067
 C     -0.407584     -1.306255      0.188730
 C     -1.346147     -1.623162     -0.882543
 H     -1.547781     -0.767619     -1.549703
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H	-1.012491	-2.458606	-1.515566
H	-0.754668	-0.515527	0.870316
P	-3.758478	-0.963547	-0.092908
O	-5.032172	-1.879740	0.221451
O	-3.437116	0.117960	0.887752
O	-4.081732	-0.156445	-1.476924
O	-2.700683	-2.080580	-0.428669
Na	-3.004323	1.965981	-0.390102
C	-6.218067	-1.269413	0.735139
H	-6.991606	-2.043980	0.754357
H	-6.059054	-0.892011	1.754331
H	-6.557890	-0.443840	0.092513
C	-4.465978	-0.858780	-2.658811
H	-4.455993	-0.138605	-3.483714
H	-3.764779	-1.674531	-2.885308
H	-5.479274	-1.273053	-2.555732
C	3.687723	-0.146113	-2.878369
H	0.114058	-3.371396	0.480167
C	0.397160	-2.326045	2.365496
H	4.680709	2.420592	-2.325885
H	3.010743	2.612922	-2.912659
H	0.713665	-1.335843	2.728514
H	1.049134	-3.070744	2.846884
H	-0.627174	-2.484650	2.744255
H	4.759331	-0.112025	-3.123794
H	3.121220	0.032958	-3.807965
H	3.444271	-1.151083	-2.514070
H	2.677363	3.796925	-0.837523
H	4.065989	2.978526	-0.060082
H	1.676316	-2.585858	-2.136691
H	4.517053	-1.704658	-0.153096
C	2.112745	-3.442489	-1.592679
H	3.040515	-3.727205	-2.114347
H	1.404987	-4.279915	-1.705551
H	4.892778	-3.337983	0.461107
C	4.190818	-2.489036	0.545977
Si	2.402719	-3.061896	0.241358
H	4.309256	-2.082860	1.563751
C	2.334439	-4.702221	1.176112
H	2.987809	-5.431827	0.669347
H	1.327587	-5.145239	1.221072
H	2.708229	-4.616239	2.208170

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Scheme_S15_pc_SiMe3 / electronic energy: -4210.15887996 a.u. / lowest freq: 16.39 cm-1

C	-0.982660	2.890904	1.940365
C	-1.122408	1.996469	3.158250
C	-1.563304	0.721332	1.251300
C	-0.871916	2.210872	-0.523118
C	-1.903920	1.929277	-1.430610
C	0.347926	2.711188	-1.021136
C	-1.744398	2.144703	-2.795398
H	-2.841696	1.529782	-1.035156
C	0.491369	2.942396	-2.392251
C	-0.545185	2.665628	-3.279740
H	-2.565385	1.912370	-3.478178
H	1.449059	3.317041	-2.757871
H	-0.409505	2.847694	-4.347933
S	1.797058	2.987107	0.011159
O	2.956166	2.949860	-0.934645
O	1.871810	1.808003	0.931931
O	1.617758	4.286012	0.682220
Cu	-1.936226	-0.815369	0.074056
N	-1.080297	1.916034	0.839933
N	-1.674406	0.769471	2.583300
C	-1.081226	-2.208702	-1.139198
C	-0.069658	-1.384627	-0.603830
C	0.704317	-1.762025	0.597663
H	1.096409	-0.885951	1.139294
H	0.118161	-2.369011	1.301702
H	0.353206	-0.586441	-1.229460
P	3.223479	-1.993701	-0.178469
O	4.071079	-3.325119	-0.418196
O	3.225358	-0.964565	-1.259462
O	3.872591	-1.234828	1.108924
O	1.863890	-2.652353	0.286696
Na	3.767453	0.954016	-0.153736
C	5.382514	-3.223964	-0.981901
H	5.783476	-4.240882	-1.034389
H	5.344570	-2.798359	-1.993488
H	6.041403	-2.611132	-0.349530
C	3.982773	-1.890753	2.375048
H	4.614305	-1.262809	3.011762
H	2.996052	-2.003438	2.845306

H	4.450149	-2.879615	2.268330
C	-1.997030	-0.362758	3.404779
H	-1.247265	-3.180581	-0.651895
C	-1.504635	-2.122696	-2.571917
H	-1.789162	2.409453	3.928156
H	-0.152339	1.776403	3.639118
H	-1.423970	-1.097055	-2.962680
H	-2.540597	-2.457203	-2.724699
H	-0.868902	-2.758415	-3.213319
H	-2.774119	-0.109541	4.141327
H	-1.113432	-0.727447	3.954959
H	-2.369988	-1.171674	2.762220
H	-0.042282	3.451077	1.909704
H	-1.811220	3.614111	1.855389
H	-4.155389	-3.918331	0.355222
H	-5.045670	-1.627628	2.253189
C	-4.550237	-3.277514	-0.451097
H	-5.632476	-3.485890	-0.522861
H	-4.093551	-3.637579	-1.387797
H	-6.370042	-1.195548	1.162174
C	-5.300400	-1.015169	1.372078
Si	-4.194169	-1.428063	-0.132979
H	-5.206586	0.039119	1.683085
C	-5.053234	-0.527814	-1.586796
H	-6.068856	-0.921968	-1.770086
H	-4.496763	-0.621304	-2.534615
H	-5.164182	0.551858	-1.390623

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Scheme_S15_ts(oa)_SiMe3 / electronic energy: -4210.15329254 a.u. / lowest freq: -364.65 cm-1

C	-1.360213	-2.855539	-1.948388
C	-1.392238	-1.962735	-3.177611
C	-1.648003	-0.622496	-1.287385
C	-1.186045	-2.160499	0.514102
C	-2.236044	-1.843860	1.385909
C	0.007476	-2.685089	1.045769
C	-2.115051	-2.041002	2.758413
H	-3.155115	-1.435972	0.957373
C	0.112483	-2.899885	2.422234
C	-0.939377	-2.580584	3.278134
H	-2.945729	-1.781031	3.419028
H	1.049631	-3.295719	2.817278
H	-0.834040	-2.747056	4.352320
S	1.460881	-3.011178	0.034168
O	2.595412	-3.102137	1.004989
O	1.635401	-1.797317	-0.825210
O	1.206808	-4.260654	-0.703242
Cu	-1.786984	0.933656	-0.096039
N	-1.343135	-1.864094	-0.858781
N	-1.765547	-0.662913	-2.616835
C	-0.982847	2.345917	1.084547
C	0.054423	1.443965	0.697076
C	0.787910	1.567376	-0.516205
H	1.259999	0.659024	-0.905732
H	0.362264	2.203665	-1.297825
H	0.382252	0.677929	1.412717
P	3.491316	1.814447	0.179983
O	4.591494	2.986676	0.302048
O	3.420198	0.873758	1.347105
O	4.032385	0.842182	-1.036713
O	2.245363	2.585709	-0.313182
Na	3.599836	-1.151653	0.342566
C	5.900976	2.656171	0.754320
H	6.486257	3.582337	0.754767
H	5.881161	2.246332	1.774256
H	6.388069	1.931387	0.083916
C	4.128781	1.343699	-2.364676
H	4.664101	0.598143	-2.963483
H	3.133239	1.504877	-2.804252
H	4.689135	2.290134	-2.395110
C	-1.922740	0.495490	-3.450081
H	-1.059716	3.277992	0.504966
C	-1.428169	2.440634	2.509017
H	-2.117607	-2.290588	-3.935311
H	-0.407580	-1.881282	-3.670913
H	-1.428740	1.458222	3.004731
H	-2.436551	2.866945	2.606990
H	-0.752437	3.091118	3.091290
H	-2.720744	0.343875	-4.191635
H	-0.992910	0.730000	-3.994537
H	-2.186031	1.355948	-2.820435
H	-0.486522	-3.515651	-1.903613
H	-2.265922	-3.477989	-1.856708
H	-3.826413	4.040904	-0.746980

H	-4.838109	1.513024	-2.246338
C	-4.219072	3.566821	0.167488
H	-5.285835	3.841841	0.236655
H	-3.708058	4.046114	1.017703
H	-6.174890	1.365428	-1.093742
C	-5.122917	1.081504	-1.273165
Si	-3.993751	1.680471	0.138028
H	-5.102011	-0.014574	-1.390304
C	-4.811769	1.021743	1.725768
H	-5.797511	1.492709	1.885412
H	-4.214763	1.208234	2.632611
H	-4.986960	-0.065108	1.674346

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Scheme_S15_pa_SiMe3 / electronic energy: -4210.18056310 a.u. / lowest freq: 15.36 cm-1

C	-1.374028	-2.532161	-2.153320
C	-1.211956	-1.523985	-3.284176
C	-1.515067	-0.361284	-1.296389
C	-1.382984	-2.091096	0.378896
C	-2.486535	-1.838025	1.201773
C	-0.232002	-2.679438	0.932399
C	-2.454349	-2.147775	2.558596
H	-3.377171	-1.394758	0.749241
C	-0.214724	-3.004627	2.291096
C	-1.314633	-2.737529	3.103773
H	-3.324774	-1.936653	3.184326
H	0.690552	-3.447997	2.710376
H	-1.277053	-2.989114	4.165778
S	1.248302	-3.022901	-0.036318
O	2.356633	-3.067708	0.964116
O	1.431737	-1.846512	-0.940945
O	0.997015	-4.299015	-0.727582
Cu	-1.635230	1.020751	0.055985
N	-1.439422	-1.660314	-0.969005
N	-1.455306	-0.241090	-2.617979
C	-1.531181	2.558201	1.395470
C	-0.376505	1.717907	1.561706
C	0.505053	1.431398	0.541349
H	1.277547	0.672771	0.670926
H	0.596328	2.081315	-0.335578
H	-0.334200	1.097502	2.468416
P	4.046113	1.792808	0.461829
O	5.570213	2.240192	0.035277
O	4.088989	0.656040	1.464265
O	3.549500	0.949227	-0.907564
O	3.256715	3.049957	0.623191
Na	3.312257	-1.070622	0.263505
C	6.549264	1.241533	-0.138009
H	7.508886	1.736047	-0.339963
H	6.665167	0.615177	0.761073
H	6.322137	0.580515	-0.992989
C	3.278363	1.652722	-2.097512
H	2.530870	1.092209	-2.678205
H	2.879243	2.657115	-1.884732
H	4.184170	1.766520	-2.716821
C	-1.420358	1.002525	-3.335342
H	-1.424630	3.364871	0.652766
C	-2.382930	2.885870	2.577489
H	-1.928455	-1.674685	-4.104378
H	-0.199251	-1.523592	-3.720143
H	-2.485015	2.028428	3.258192
H	-3.391279	3.225256	2.304076
H	-1.927022	3.704289	3.158804
H	-2.176268	1.018216	-4.134103
H	-0.434921	1.168658	-3.798028
H	-1.623932	1.827500	-2.639628
H	-0.542153	-3.243027	-2.076128
H	-2.309811	-3.108890	-2.228842
H	-3.638943	3.630710	-1.405565
H	-4.206130	0.840805	-2.529836
C	-4.201485	3.328081	-0.508691
H	-5.268613	3.502071	-0.726466
H	-3.918034	4.011799	0.303807
H	-5.714650	0.676931	-1.614705
C	-4.623007	0.523938	-1.562477
Si	-3.932118	1.510101	-0.111349
H	-4.452602	-0.559415	-1.460779
C	-4.893722	0.969995	1.418570
H	-5.783896	1.609203	1.539529
H	-4.334555	1.015516	2.362781
H	-5.256154	-0.062481	1.298807

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Scheme_S15_ts(cc)_SiMe3 / electronic energy: -4210.17500778 a.u. / lowest freq: -116.91 cm-1

C	-0.829125	2.551754	2.397600

C	-0.491548	1.480425	3.428436
C	-1.104030	0.424416	1.442617
C	-1.289894	2.261417	-0.104223
C	-2.526140	2.097054	-0.742140
C	-0.228420	2.859536	-0.805899
C	-2.716642	2.528362	-2.052234
H	-3.340047	1.624637	-0.185033
C	-0.432627	3.300525	-2.116384
C	-1.668071	3.140439	-2.738486
H	-3.688223	2.394136	-2.533330
H	0.405294	3.748661	-2.654303
H	-1.807224	3.486553	-3.764918
S	1.423939	3.058303	-0.111176
O	2.335573	2.980482	-1.292914
O	1.650369	1.875924	0.773678
O	1.421595	4.356262	0.583742
Cu	-1.438218	-0.810030	-0.015336
N	-1.131488	1.746878	1.204935
N	-0.789454	0.231471	2.720691
C	-2.107834	-2.372035	-1.318140
C	-1.001173	-1.565190	-1.870913
C	0.265281	-1.502828	-1.366233
H	1.007808	-0.844935	-1.827033
H	0.647650	-2.226368	-0.638261
H	-1.267142	-0.886896	-2.694909
P	3.732151	-2.065781	-0.595619
O	5.194884	-2.499512	0.018470
O	3.906172	-1.041299	-1.700249
O	3.140767	-1.071421	0.622841
O	2.919909	-3.315178	-0.696539
Na	3.102208	0.824244	-0.725675
C	6.181942	-1.507571	0.186578
H	7.086736	-1.990792	0.578861
H	6.438703	-1.013078	-0.763986
H	5.872476	-0.731304	0.908218
C	2.723629	-1.624563	1.846264
H	2.334057	-0.811297	2.474214
H	1.933607	-2.381503	1.707285
H	3.559099	-2.105243	2.384038
C	-0.685168	-1.041095	3.377465
H	-1.729849	-3.229873	-0.737136
C	-3.063720	-2.811271	-2.412787
H	-1.096665	1.555678	4.344097
H	0.568600	1.490388	3.730003
H	-3.385576	-1.966153	-3.035945
H	-3.960370	-3.331403	-2.056307
H	-2.533838	-3.513006	-3.075353
H	-1.406614	-1.120966	4.205627
H	0.321752	-1.191835	3.795475
H	-0.888455	-1.843558	2.656385
H	-0.001420	3.246652	2.204656
H	-1.713973	3.147070	2.672853
H	-3.451545	-3.738519	1.440222
H	-3.336403	-1.079172	2.568495
C	-4.148571	-3.426787	0.645896
H	-5.159188	-3.462811	1.083117
H	-4.105067	-4.185431	-0.146031
H	-5.029601	-0.895354	2.076145
C	-3.985999	-0.717087	1.759633
Si	-3.757351	-1.664591	0.134238
H	-3.850351	0.370317	1.672091
C	-4.962503	-0.874038	-1.075346
H	-5.533687	-1.604176	-1.665057
H	-4.463399	-0.201890	-1.789545
H	-5.689380	-0.265481	-0.515526

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Scheme_S15_prod_SiMe3 / electronic energy: -4210.23135804 a.u. / lowest freq: 20.51 cm-1

C	0.192600	-2.364213	-2.403243
C	0.032219	-1.179500	-3.345379
C	-0.386677	-0.445012	-1.158300
C	0.157703	-2.445036	0.118558
C	-0.921725	-2.886314	0.889933
C	1.467927	-2.683837	0.569358
C	-0.716244	-3.545183	2.098634
H	-1.931460	-2.694464	0.519025
C	1.667629	-3.353565	1.780208
C	0.584472	-3.780447	2.544073
H	-1.573269	-3.875130	2.691119
H	2.689832	-3.520603	2.126887
H	0.758782	-4.297206	3.490439
S	2.943830	-2.218718	-0.358137
O	3.948749	-1.866323	0.691223
O	2.603320	-0.998765	-1.151032

O	3.285676	-3.400477	-1.167737
Cu	-0.839261	0.746403	0.361903
N	-0.102896	-1.762732	-1.094926
N	-0.332848	-0.087372	-2.442860
C	-3.808881	0.134615	1.457027
C	-2.349643	0.185597	1.827174
C	-1.641164	1.321964	2.151734
H	-0.685969	1.251316	2.684206
H	-2.098496	2.316728	2.104006
H	-1.897994	-0.779420	2.093447
P	1.603903	2.548103	0.612153
O	1.877718	4.051744	1.175667
O	2.107622	1.472433	1.542186
O	2.654949	2.430556	-0.665708
O	0.172312	2.572871	0.110565
Na	3.683621	0.439216	0.297380
C	3.109912	4.320079	1.821584
H	3.130905	5.389347	2.064870
H	3.213323	3.744888	2.754055
H	3.973845	4.097279	1.174148
C	2.546653	3.337985	-1.749255
H	2.958418	2.856955	-2.645558
H	1.498719	3.608978	-1.945918
H	3.115279	4.260702	-1.553567
C	-0.541338	1.239496	-2.949272
H	-4.302710	0.971623	1.988244
C	-4.442899	-1.173081	1.927011
H	-0.756961	-1.331758	-4.099406
H	0.958309	-0.924938	-3.885335
H	-4.017742	-2.043889	1.402332
H	-5.528628	-1.192867	1.752225
H	-4.287783	-1.344065	3.004328
H	-1.479186	1.317627	-3.524328
H	0.285056	1.523814	-3.618797
H	-0.568146	1.946637	-2.111134
H	1.204580	-2.794747	-2.413719
H	-0.521191	-3.177665	-2.608770
H	-6.485915	1.502794	0.242276
H	-3.887717	2.947529	-0.275231
C	-6.140873	0.705575	-0.434844
H	-6.467663	0.982445	-1.449790
H	-6.682862	-0.213578	-0.165186
H	-3.794496	2.363211	-1.942668
C	-3.512064	2.124788	-0.904799
Si	-4.275203	0.495418	-0.366908
H	-2.411839	2.162042	-0.854303
C	-3.790334	-0.941819	-1.478612
H	-4.519708	-1.762704	-1.390043
H	-2.801687	-1.357806	-1.235847
H	-3.770081	-0.646186	-2.540127

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Scheme_S15_ts(CuXadd)_Me / electronic energy: -3840.89997454 a.u. / lowest freq: -447.59 cm-1

C	-3.912731	-1.233701	-1.089792
C	-3.861760	-0.552559	-2.442690
C	-2.633560	0.735624	-0.928095
C	-2.443475	-0.786474	0.946237
C	-2.904348	-0.017104	2.020996
C	-1.501536	-1.803617	1.188699
C	-2.460621	-0.260515	3.318821
H	-3.627676	0.777095	1.819237
C	-1.072388	-2.052645	2.494166
C	-1.549267	-1.287847	3.557069
H	-2.831759	0.351659	4.144157
H	-0.339450	-2.843773	2.661009
H	-1.199635	-1.492118	4.571539
S	-0.721940	-2.717958	-0.155311
O	0.293621	-3.592214	0.514761
O	-0.011306	-1.691064	-0.979724
O	-1.778937	-3.456268	-0.864542
Cu	-1.340669	1.882584	-0.116891
N	-2.886286	-0.476609	-0.361082
N	-3.276844	0.746706	-2.110815
C	0.183843	2.971245	0.960581
C	0.585453	1.676780	0.400566
C	1.465929	1.580164	-0.759470
H	1.320567	0.653194	-1.338687
H	1.351819	2.425169	-1.453476
H	0.608111	0.823772	1.093736
P	3.627626	0.257284	-0.079883
O	5.134395	0.761920	0.106415
O	3.067233	-0.620453	0.992179
O	3.600108	-0.688989	-1.413579
O	2.932615	1.619904	-0.447616

Na	2.086891	-2.317220	-0.185190
C	6.121590	-0.150679	0.591113
H	7.059377	0.408388	0.671375
H	5.848677	-0.541899	1.580499
H	6.265487	-0.989877	-0.105502
C	4.037009	-0.184408	-2.675680
H	4.003399	-1.014716	-3.388793
H	3.379104	0.621016	-3.031819
H	5.067953	0.192740	-2.614255
C	-3.094897	1.749224	-3.120623
H	0.707086	3.815220	0.488203
C	-1.585323	3.887113	0.647638
C	0.188161	3.050823	2.465255
H	-4.847217	-0.439507	-2.915810
H	-3.204405	-1.087044	-3.154072
H	-1.931507	4.120698	-0.375396
H	-1.158605	4.809838	1.055883
H	-2.453285	3.618566	1.273974
H	-0.432022	2.254835	2.905565
H	-0.177097	4.010185	2.858544
H	1.211705	2.898796	2.844070
H	-4.059014	2.061124	-3.548898
H	-2.460465	1.385347	-3.946596
H	-2.608721	2.626141	-2.675550
H	-3.672255	-2.301699	-1.122414
H	-4.892315	-1.102499	-0.594993

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Scheme_S15_pc_Me / electronic energy: -3840.95167061 a.u. / lowest freq: 21.13 cm-1

C	-2.538190	1.410853	2.114028
C	-2.117775	0.462685	3.220883
C	-2.058107	-0.697022	1.191608
C	-2.310172	1.090611	-0.413193
C	-3.137381	0.419558	-1.326257
C	-1.527183	2.167513	-0.874691
C	-3.199939	0.806653	-2.660694
H	-3.733849	-0.420030	-0.960033
C	-1.611202	2.559851	-2.213794
C	-2.441986	1.888957	-3.106699
H	-3.851647	0.265237	-3.350535
H	-0.985099	3.387183	-2.552647
H	-2.487808	2.206428	-4.150604
S	-0.339831	3.039933	0.158512
O	0.650251	3.624072	-0.799676
O	0.335292	1.990223	0.986914
O	-1.090720	4.045794	0.929470
Cu	-1.694523	-2.135849	-0.130503
N	-2.247933	0.611852	0.910604
N	-2.059974	-0.822653	2.523509
C	-0.248990	-2.878726	-1.354447
C	0.209128	-1.697072	-0.744407
C	1.065655	-1.717569	0.462600
H	0.949445	-0.810988	1.078459
H	0.868906	-2.592827	1.096482
H	0.197997	-0.760305	-1.319298
P	3.352925	-0.585904	-0.262855
O	4.760233	-1.294449	-0.521147
O	2.839824	0.342859	-1.312328
O	3.522719	0.345909	1.061994
O	2.513764	-1.862751	0.144221
Na	2.359182	2.238307	-0.141900
C	5.861159	-0.502275	-0.977612
H	6.713244	-1.179542	-1.090709
H	5.638303	-0.037641	-1.947538
H	6.118505	0.278892	-0.247652
C	3.959346	-0.206029	2.307114
H	4.145307	0.632756	2.985498
H	3.187544	-0.856659	2.741214
H	4.888255	-0.779411	2.180635
C	-1.735450	-2.036153	3.218555
H	0.057750	-3.831337	-0.898662
C	-3.183957	-3.460999	-0.386759
C	-0.669766	-2.946846	-2.786357
H	-2.827831	0.428838	4.059139
H	-1.122171	0.705153	3.634316
H	-3.972894	-3.424075	0.388777
H	-2.847649	-4.514471	-0.435733
H	-3.695637	-3.270559	-1.351097
H	-1.059684	-1.982548	-3.144950
H	-1.445527	-3.707055	-2.957693
H	0.178097	-3.212197	-3.442247
H	-0.731481	-1.987717	3.672840
H	-1.762663	-2.871690	2.506422
H	-2.458860	-2.236290	4.022535

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 H    -1.995812     2.361988     2.118264
 H    -3.617855     1.635158     2.143268
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Scheme_S15_ts(oa)_Me / electronic energy: -3840.94344163 a.u. / lowest freq: -330.00 cm-1
 C    -2.482162    -1.868772    -1.863614
 C    -2.366063    -0.959434    -3.073142
 C    -2.210114     0.347857    -1.148725
 C    -2.024732    -1.315205     0.594245
 C    -2.838226    -0.681410     1.545751
 C    -1.063650    -2.245892     1.037264
 C    -2.713047    -0.962177     2.902342
 H    -3.577006     0.043638     1.192941
 C    -0.958572    -2.533226     2.401129
 C    -1.775953    -1.900003     3.333387
 H    -3.358519    -0.452595     3.621525
 H    -0.198294    -3.246501     2.724241
 H    -1.673043    -2.134910     4.394887
 S     0.107548    -3.059361    -0.062385
 O     1.239917    -3.475496     0.821255
 O     0.576310    -2.002167    -1.013719
 O    -0.602207    -4.185083    -0.694091
Cu    -1.971278     1.919954     0.047915
 N    -2.162480    -0.943571    -0.760115
 N    -2.405553     0.373528    -2.468271
 C    -0.783231     3.068148     1.208227
 C    -0.104486     1.854633     0.936580
 C     0.579473     1.614296    -0.285543
 H     0.730522     0.573302    -0.588362
 H     0.393899     2.297031    -1.119129
 H    -0.051461     1.079363     1.712070
 P     3.312587     0.971777     0.164191
 O     4.723341     1.740425     0.322798
 O     3.021755    -0.049045     1.225846
 O     3.488475     0.043296    -1.190716
 O     2.336403     2.125062    -0.141402
Na     2.725750    -1.932759     0.000885
 C     5.888076     0.982537     0.629241
 H     6.714475     1.691230     0.752862
 H     5.765149     0.414534     1.562608
 H     6.140891     0.286002    -0.185242
 C     3.637259     0.663231    -2.462043
 H     3.915367    -0.114084    -3.182616
 H     2.697531     1.132911    -2.789058
 H     4.428210     1.428223    -2.444276
 C    -2.358485     1.563224    -3.271984
 H    -0.571364     3.912189     0.536019
 C    -3.619199     3.040249     0.129348
 C    -1.280476     3.428328     2.566460
 H    -3.181458    -1.090192    -3.797904
 H    -1.412097    -1.089606    -3.614234
 H    -4.375483     2.728228    -0.612419
 H    -3.420402     4.115071    -0.027426
 H    -4.077796     2.941248     1.130148
 H    -1.590943     2.543097     3.140556
 H    -2.133529     4.119670     2.520674
 H    -0.497200     3.935947     3.155123
 H    -3.216894     1.610582    -3.957634
 H    -1.438070     1.602564    -3.877664
 H    -2.383436     2.441160    -2.613428
 H    -1.802045    -2.726101    -1.889642
 H    -3.506939    -2.251147    -1.723221
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Scheme_S15_pa_Me / electronic energy: -3840.96546396 a.u. / lowest freq: 28.92 cm-1
 C    -2.326294    -1.200569    -2.456464
 C    -1.441426    -0.466581    -3.458341
 C    -1.404869     0.697610    -1.447625
 C    -2.633962    -0.756641     0.039893
 C    -3.587927     0.060211     0.658019
 C    -2.122378    -1.869732     0.727575
 C    -4.048428    -0.232369     1.938884
 H    -3.964188     0.928984     0.110930
 C    -2.599997    -2.161744     2.007888
 C    -3.560818    -1.353392     2.610732
 H    -4.792556     0.413714     2.409779
 H    -2.181039    -3.016936     2.542317
 H    -3.918275    -1.594319     3.614158
 S    -0.799920    -2.910866     0.075905
 O    -0.027073    -3.325931     1.286206
 O     0.053681    -2.027828    -0.775540
 O    -1.464561    -4.008175    -0.645857
Cu    -1.016334     2.006035    -0.043703
 N    -2.161598    -0.386771    -1.241351
 N    -1.004966     0.719172    -2.713003
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C	-0.270152	3.146412	1.529066
C	-0.431252	1.809343	1.959751
C	0.140584	0.762319	1.240616
H	-0.131953	-0.269299	1.474648
H	1.051940	0.938564	0.656789
H	-1.224161	1.589991	2.686979
P	3.668173	0.333112	0.594649
O	5.247104	0.284265	0.152450
O	3.384341	-0.662534	1.701612
O	2.921148	-0.446337	-0.693419
O	3.266732	1.774572	0.620060
Na	1.877875	-2.022128	0.707543
C	5.894202	-0.967145	0.072842
H	6.947295	-0.787274	-0.180307
H	5.854337	-1.514047	1.028153
H	5.458419	-1.608586	-0.712319
C	2.770708	0.225328	-1.921369
H	2.138192	-0.390332	-2.575609
H	2.301190	1.214107	-1.788228
H	3.741493	0.377650	-2.424029
C	-0.234919	1.758291	-3.339250
H	0.647194	3.364972	0.960595
C	-1.941900	3.588555	-0.768199
C	-0.948469	4.298981	2.167472
H	-1.978631	-0.165788	-4.369739
H	-0.561391	-1.052540	-3.768190
H	-2.382586	3.352959	-1.747400
H	-1.242667	4.431867	-0.870267
H	-2.737685	3.854757	-0.055276
H	-1.896479	4.011486	2.642019
H	-1.146113	5.108084	1.451203
H	-0.303670	4.732294	2.949391
H	-0.823559	2.274590	-4.113423
H	0.664619	1.345306	-3.818376
H	0.071004	2.491020	-2.583040
H	-2.011289	-2.236710	-2.274795
H	-3.387506	-1.213249	-2.748344

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Scheme_S15_ts(cc)_Me / electronic energy: -3840.94348055 a.u. / lowest freq: -352.34 cm-1

C	-2.984634	-1.996230	-1.597999
C	-2.852657	-1.331349	-2.960011
C	-2.398727	0.261777	-1.319572
C	-2.368247	-1.050074	0.703011
C	-3.137447	-0.234367	1.543484
C	-1.402522	-1.899912	1.273970
C	-2.964188	-0.258890	2.924474
H	-3.884637	0.420271	1.088372
C	-1.250080	-1.932706	2.662872
C	-2.023659	-1.119925	3.488075
H	-3.574416	0.388167	3.559171
H	-0.486221	-2.586987	3.086983
H	-1.882317	-1.153996	4.570388
S	-0.272708	-2.897616	0.285095
O	0.880487	-3.169784	1.195196
O	0.164373	-2.004665	-0.832499
O	-1.010852	-4.100810	-0.134433
Cu	-1.685371	1.776149	-0.279684
N	-2.546325	-0.921479	-0.693187
N	-2.636394	0.077553	-2.616922
C	-0.898011	3.387533	0.852127
C	-0.005310	2.225441	0.800476
C	0.528553	1.731078	-0.359058
H	1.119518	0.814837	-0.368125
H	0.530625	2.316304	-1.286050
H	0.104398	1.635382	1.721332
P	3.921381	0.845075	0.106582
O	5.550958	0.631731	0.062690
O	3.315165	0.065927	1.256856
O	3.430643	-0.121516	-1.188562
O	3.664116	2.285280	-0.187844
Na	2.266435	-1.608168	0.192707
C	6.080568	-0.643386	0.346064
H	7.174906	-0.579577	0.280134
H	5.814660	-0.987340	1.358495
H	5.741745	-1.404378	-0.378784
C	3.720465	0.312871	-2.499213
H	3.276773	-0.399448	-3.207360
H	3.303793	1.314027	-2.693883
H	4.807397	0.352003	-2.682953
C	-2.463977	1.068796	-3.641874
H	-0.679603	4.130099	0.073202
C	-2.961226	3.266257	0.421841
C	-1.099652	3.969491	2.217386

H	-3.745759	-1.448070	-3.590189
H	-1.988304	-1.702837	-3.536113
H	-3.584191	2.941732	-0.427204
H	-2.922940	4.358300	0.393577
H	-3.403659	2.926853	1.366640
H	-1.435777	3.208000	2.935711
H	-1.817108	4.798519	2.230689
H	-0.137939	4.358105	2.585826
H	-3.365186	1.150540	-4.266962
H	-1.616877	0.817210	-4.299519
H	-2.268830	2.043007	-3.178026
H	-2.363621	-2.892856	-1.483828
H	-4.024402	-2.270858	-1.357500

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Scheme_S15_prod_Me / electronic energy: -3841.01738783 a.u. / lowest freq: 18.95 cm-1

C	3.330604	0.001795	2.042541
C	2.493973	0.227751	3.296417
C	1.344369	1.127374	1.473179
C	2.752872	0.509364	-0.390216
C	3.006266	1.692445	-1.094963
C	2.705415	-0.711244	-1.085267
C	3.231996	1.669312	-2.468050
H	3.029324	2.633663	-0.540173
C	2.947232	-0.726389	-2.462308
C	3.214702	0.453400	-3.151794
H	3.429352	2.601203	-3.002564
H	2.892243	-1.678637	-2.993612
H	3.397405	0.422966	-4.228067
S	2.267252	-2.274323	-0.297769
O	1.616138	-3.060869	-1.388835
O	1.254495	-1.935711	0.748408
O	3.518920	-2.851658	0.218582
Cu	-0.012499	1.661620	0.157333
N	2.487029	0.600474	0.998368
N	1.331913	0.967807	2.794562
C	-2.232933	3.527430	-0.572717
C	-1.114224	2.804295	-1.270574
C	-1.132431	1.477285	-1.596562
H	-0.361262	1.052945	-2.251556
H	-2.014643	0.857180	-1.378262
H	-0.295996	3.439856	-1.646926
P	-3.301672	-1.514833	-0.493257
O	-4.425124	-2.262858	0.441140
O	-2.638172	-2.508739	-1.424307
O	-2.054872	-1.268809	0.606977
O	-3.891554	-0.203738	-0.907481
Na	-0.557290	-2.650100	-0.582791
C	-4.177224	-3.581307	0.878015
H	-5.022236	-3.892842	1.506060
H	-4.091023	-4.285902	0.035967
H	-3.258554	-3.652757	1.485774
C	-2.182746	-0.288037	1.605930
H	-1.422206	-0.482613	2.374838
H	-2.024876	0.734025	1.206489
H	-3.173917	-0.315650	2.088644
C	0.296334	1.398174	3.690485
H	-2.950785	2.765688	-0.218311
C	-1.709597	4.307001	0.625554
C	-2.953742	4.438252	-1.559914
H	3.016853	0.812568	4.068345
H	2.156127	-0.710155	3.765532
H	-1.189518	3.645645	1.339529
H	-2.523590	4.808842	1.168067
H	-0.990354	5.081704	0.315895
H	-2.273556	5.200350	-1.971285
H	-3.783427	4.967331	-1.069234
H	-3.370858	3.872943	-2.404914
H	0.671792	2.149988	4.401920
H	-0.094851	0.550924	4.273937
H	-0.526348	1.840459	3.116608
H	3.516731	-1.059729	1.828601
H	4.303430	0.515490	2.074992

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Scheme_S15_ts(CuXadd)_Ph / electronic energy: -4032.49730588 a.u. / lowest freq: -323.69 cm-1

C	-1.513526	3.259879	1.799579
C	-1.534133	2.465021	3.093745
C	-1.841617	0.975492	1.317150
C	-1.327271	2.364540	-0.588483
C	-2.343718	1.972706	-1.471966
C	-0.112613	2.840226	-1.121040
C	-2.179286	2.075735	-2.849752
H	-3.277239	1.593844	-1.048556
C	0.036903	2.955653	-2.506363

C	-0.988408	2.581671	-3.370585
H	-2.988525	1.767777	-3.516445
H	0.989499	3.315574	-2.899093
H	-0.850315	2.674367	-4.449992
S	1.324662	3.220778	-0.102914
O	2.489516	3.115255	-1.037181
O	1.408396	2.126005	0.914625
O	1.123657	4.569836	0.453547
Cu	-1.571347	-0.605808	0.269752
N	-1.538928	2.190803	0.793391
N	-1.957077	1.137941	2.646800
C	-0.952522	-2.251517	-0.962082
C	0.132400	-1.433032	-0.393355
C	0.974071	-1.927410	0.695810
H	1.372719	-1.128613	1.345177
H	0.447713	-2.639499	1.347913
H	0.600412	-0.711091	-1.076722
P	3.451889	-1.884889	-0.166696
O	4.483746	-3.081066	-0.406790
O	3.349517	-0.847103	-1.237275
O	3.960176	-1.056178	1.144745
O	2.178895	-2.709375	0.263457
Na	3.270874	1.144159	-0.137502
C	5.754561	-2.800447	-0.999689
H	6.285949	-3.754344	-1.076374
H	5.637521	-2.370283	-2.003356
H	6.343191	-2.112802	-0.374807
C	4.193075	-1.725808	2.384911
H	4.458382	-0.961623	3.122645
H	3.293902	-2.258566	2.725829
H	5.022447	-2.441631	2.293623
C	-2.061928	0.050872	3.577273
H	-0.944112	-3.281255	-0.577611
C	-1.071705	-2.195359	-2.463005
H	-2.227646	2.872828	3.843235
H	-0.536658	2.397895	3.564639
H	-1.212869	-1.162411	-2.817101
H	-1.894920	-2.802876	-2.862846
H	-0.134327	-2.556682	-2.913923
H	-2.765009	0.293283	4.387202
H	-1.087322	-0.190095	4.036905
H	-2.428935	-0.841048	3.054430
H	-0.629310	3.899497	1.691037
H	-2.408547	3.894829	1.683140
H	-3.583868	-1.123000	-2.200809
H	-5.887809	-1.984510	-1.965349
C	-3.826758	-1.771630	-1.351313
C	-5.130993	-2.254701	-1.222624
C	-2.836505	-2.090161	-0.407885
C	-5.473680	-3.078420	-0.148437
H	-6.493250	-3.459663	-0.049291
C	-3.195503	-2.944064	0.650402
C	-4.497112	-3.423618	0.790690
H	-4.752827	-4.075690	1.631312
H	-2.433305	-3.244611	1.381748

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Scheme_S15_pc_Ph / electronic energy: -4032.54192279 a.u. / lowest freq: 15.99 cm-1

C	-0.569389	2.614829	2.330629
C	-0.530156	1.553870	3.414726
C	-1.306665	0.567366	1.443152
C	-0.862941	2.290524	-0.189440
C	-2.030055	2.162055	-0.956559
C	0.289234	2.832914	-0.792111
C	-2.064949	2.573611	-2.285220
H	-2.916336	1.733217	-0.481582
C	0.238836	3.257312	-2.123009
C	-0.929502	3.133895	-2.869936
H	-2.987624	2.465177	-2.860364
H	1.146226	3.662467	-2.574790
H	-0.947819	3.466814	-3.909857
S	1.877739	2.947494	0.045465
O	2.893430	2.963889	-1.053686
O	2.022925	1.680925	0.831534
O	1.852223	4.177521	0.855459
Cu	-1.850586	-0.799017	0.099849
N	-0.875061	1.809617	1.135410
N	-1.190156	0.419441	2.766416
C	-1.010636	-2.068729	-1.286143
C	-0.006559	-1.325627	-0.651426
C	0.775905	-1.871926	0.484764
H	1.184878	-1.080189	1.132981
H	0.179261	-2.552757	1.106855
H	0.418597	-0.453708	-1.168349

P	3.258345	-2.063106	-0.434785
O	4.119251	-3.393141	-0.623250
O	3.245918	-1.078419	-1.556223
O	3.880190	-1.247579	0.825888
O	1.905176	-2.727574	0.050253
Na	3.744825	0.893542	-0.533648
C	5.414809	-3.305141	-1.225772
H	5.816211	-4.322533	-1.260899
H	5.349249	-2.907405	-2.247201
H	6.089327	-2.674133	-0.629048
C	4.072477	-1.874554	2.096785
H	4.111229	-1.081457	2.851197
H	3.243799	-2.555643	2.335143
H	5.016545	-2.436254	2.110192
C	-1.413178	-0.811238	3.469922
H	-1.210323	-3.079070	-0.901953
C	-1.475621	-1.793222	-2.677509
H	-1.057933	1.848652	4.332629
H	0.499615	1.269027	3.696278
H	-1.319115	-0.741875	-2.962279
H	-2.540847	-2.027521	-2.816918
H	-0.921689	-2.407720	-3.408138
H	-0.469342	-1.227924	3.859343
H	-1.862377	-1.539582	2.783237
H	-2.093771	-0.665612	4.321947
H	0.368308	3.170070	2.223152
H	-1.380475	3.345326	2.487977
H	-4.029423	-0.033330	-1.918774
H	-6.438518	-0.415316	-2.174731
C	-4.538805	-0.645582	-1.160697
C	-5.911811	-0.857606	-1.322279
C	-3.796736	-1.180504	-0.083983
C	-6.612873	-1.635545	-0.399156
H	-7.686360	-1.808450	-0.517799
C	-4.546278	-1.960766	0.823616
C	-5.918502	-2.190269	0.677470
H	-6.451896	-2.805426	1.410191
H	-4.050474	-2.418010	1.690852

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Scheme_S15_ts(oa)_Ph / electronic energy: -4032.53119545 a.u. / lowest freq: -311.05 cm-1

C	-0.649965	-2.663894	-2.223022
C	-0.671757	-1.643697	-3.346872
C	-1.343590	-0.590182	-1.379908
C	-0.812511	-2.237072	0.300041
C	-1.940919	-2.075937	1.116065
C	0.372360	-2.743832	0.868287
C	-1.904826	-2.415244	2.465235
H	-2.855296	-1.682119	0.664541
C	0.391652	-3.099420	2.219792
C	-0.737365	-2.939350	3.018756
H	-2.797774	-2.281351	3.080460
H	1.323277	-3.477850	2.644302
H	-0.699980	-3.216902	4.074241
S	1.915455	-2.893063	-0.045949
O	2.984012	-2.888899	1.000209
O	2.020004	-1.648774	-0.873109
O	1.840606	-4.143540	-0.820655
Cu	-1.858305	0.797239	-0.047077
N	-0.894085	-1.814673	-1.043466
N	-1.298636	-0.483961	-2.708071
C	-1.244947	2.222792	1.284205
C	-0.133539	1.430989	0.915615
C	0.561739	1.594641	-0.309788
H	1.135492	0.746316	-0.694276
H	0.125074	2.238877	-1.076299
H	0.233812	0.667799	1.614272
P	3.313148	2.098899	0.367612
O	4.325738	3.348457	0.521432
O	3.346766	1.117697	1.505249
O	3.930280	1.213516	-0.883612
O	2.008471	2.776793	-0.086370
Na	3.814792	-0.825356	0.436182
C	5.672900	3.101055	0.904037
H	6.154513	4.074455	1.050777
H	5.729125	2.532355	1.843749
H	6.218930	2.554364	0.119305
C	3.878776	1.721106	-2.209237
H	4.520854	1.090100	-2.834901
H	2.854002	1.690115	-2.609924
H	4.247703	2.756765	-2.259010
C	-1.541742	0.728973	-3.436885
H	-1.422466	3.134126	0.695703
C	-1.818614	2.208948	2.657746

H	-1.246987	-1.972148	-4.223421
H	0.340161	-1.366948	-3.691959
H	-1.696959	1.231692	3.147417
H	-2.887064	2.464778	2.660931
H	-1.315074	2.954295	3.296412
H	-2.283471	0.575113	-4.234388
H	-0.615711	1.104403	-3.902323
H	-1.921193	1.491521	-2.745599
H	0.294147	-3.212726	-2.143316
H	-1.466635	-3.399944	-2.306960
H	-4.043120	0.155767	2.007846
H	-6.481841	0.436006	2.127457
C	-4.553412	0.645969	1.167972
C	-5.940489	0.804729	1.250207
C	-3.809122	1.095881	0.060780
C	-6.635086	1.437271	0.217796
H	-7.719024	1.568548	0.277455
C	-4.539712	1.728522	-0.962950
C	-5.925979	1.902088	-0.890511
H	-6.456145	2.402974	-1.706996
H	-4.025793	2.106548	-1.855825

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Scheme_S15_pa_Ph / electronic energy: -4032.54742087 a.u. / lowest freq: 25.49 cm-1

C	-0.788988	2.339519	2.495986
C	-0.568425	1.154110	3.426820
C	-1.207842	0.351782	1.345525
C	-1.067578	2.306100	-0.058958
C	-2.247230	2.269595	-0.810582
C	0.090087	2.878195	-0.617064
C	-2.290012	2.800162	-2.097330
H	-3.135043	1.822382	-0.357177
C	0.032879	3.421320	-1.903329
C	-1.147431	3.384771	-2.642515
H	-3.220842	2.765138	-2.668353
H	0.941512	3.850822	-2.329980
H	-1.169877	3.809294	-3.648352
S	1.674925	2.935459	0.241216
O	2.697117	2.949832	-0.848140
O	1.782944	1.656997	1.010147
O	1.642931	4.151278	1.071283
Cu	-1.635808	-0.788799	-0.194907
N	-1.060872	1.676614	1.209320
N	-0.981989	0.009589	2.606192
C	-1.487723	-2.005156	-1.888867
C	-0.451159	-1.044194	-1.888168
C	0.384098	-0.901484	-0.781661
H	1.034459	-0.031816	-0.676198
H	0.603136	-1.757984	-0.134992
H	-0.496360	-0.232229	-2.626384
P	3.633709	-2.137023	-0.635518
O	5.009704	-2.942387	-0.236242
O	3.938804	-1.014901	-1.608246
O	3.348420	-1.242228	0.758624
O	2.569498	-3.170028	-0.822073
Na	3.534994	0.814495	-0.368464
C	6.199597	-2.208426	-0.056259
H	6.998058	-2.914479	0.207921
H	6.499032	-1.673949	-0.972034
H	6.114672	-1.470836	0.760977
C	2.891597	-1.885151	1.924371
H	2.461309	-1.127164	2.594454
H	2.123845	-2.641988	1.694312
H	3.714009	-2.390508	2.459611
C	-0.972319	-1.333304	3.117596
H	-1.323202	-2.908815	-1.283183
C	-2.495516	-2.103147	-2.972398
H	-1.170809	1.207828	4.344269
H	0.485841	1.028043	3.721934
H	-2.747904	-1.120664	-3.395432
H	-3.418929	-2.588515	-2.631802
H	-2.099274	-2.720653	-3.795489
H	-1.795148	-1.502922	3.828579
H	-0.025063	-1.539289	3.636965
H	-1.073230	-2.038588	2.283562
H	0.078604	3.006432	2.422062
H	-1.663236	2.945852	2.780270
H	-4.261792	0.125740	-1.524930
H	-6.638208	-0.423538	-1.181692
C	-4.527871	-0.607003	-0.754513
C	-5.878224	-0.921165	-0.572129
C	-3.534366	-1.225117	0.015522
C	-6.255468	-1.871216	0.377639
H	-7.310208	-2.121425	0.517909

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 C    -3.925445    -2.180835     0.962605
 C    -5.274828    -2.504219     1.141292
 H    -5.558339    -3.256642     1.883105
 H    -3.180264    -2.698534     1.575885
64
Scheme_S15_ts(cc)_Ph / electronic energy: -4032.54422109 a.u. / lowest freq: -187.76 cm-1
 C    -1.927452    -2.208982     2.368736
 C    -0.834238    -1.767868     3.327446
 C    -0.052368    -1.485561     1.142609
 C    -2.054117    -2.047146    -0.143550
 C    -1.700099    -3.037536    -1.065942
 C    -3.116533    -1.176611    -0.439641
 C    -2.397891    -3.178060    -2.262004
 H    -0.864133    -3.699681    -0.824860
 C    -3.825709    -1.337802    -1.633162
 C    -3.473777    -2.334201    -2.539998
 H    -2.106339    -3.954160    -2.973278
 H    -4.639456    -0.645604    -1.859968
 H    -4.033417    -2.442898    -3.471559
 S    -3.578833     0.214895     0.611756
 O    -4.022423     1.269050    -0.351575
 O    -2.327839     0.661046     1.295963
 O    -4.632957    -0.281103     1.511999
Cu     0.981706    -0.970243    -0.494903
 N    -1.316839    -1.937865     1.058428
 N     0.277027    -1.429996     2.433051
 C     2.114058    -0.557865    -2.218247
 C     0.726632    -0.818686    -2.564287
 C    -0.310108    -0.031424    -2.136888
 H    -1.346104    -0.292947    -2.363919
 H    -0.107420     0.970100    -1.737940
 H     0.498632    -1.769289    -3.066450
 P     0.744908     3.312213    -0.552021
 O     1.475168     4.708220    -0.111310
 O    -0.522847     3.589346    -1.334554
 O     0.105989     2.764143     0.894880
 O     1.826235     2.379739    -1.012599
Na    -2.083126     2.578997    -0.049681
 C     0.673373     5.802403     0.283070
 H     1.340892     6.642980     0.512491
 H    -0.019045     6.113059    -0.514703
 H     0.084397     5.576668     1.187864
 C     0.880964     1.921287     1.715739
 H     0.267098     1.635182     2.580408
 H     1.184811     1.006960     1.173829
 H     1.793639     2.423771     2.080649
 C     1.547276    -1.064918     2.994654
 H     2.318266     0.499719    -1.999263
 C     3.161346    -1.291857    -2.992656
 H    -0.530220    -2.554707     4.033578
 H    -1.109335    -0.879322     3.919350
 H     2.987170    -2.377143    -3.005461
 H     4.174855    -1.108007    -2.616201
 H     3.131582    -0.949911    -4.040329
 H     2.011647    -1.922544     3.507411
 H     1.426770    -0.259252     3.734648
 H     2.224911    -0.723417     2.206558
 H    -2.863080    -1.644602     2.483625
 H    -2.167505    -3.280660     2.448607
 H     2.792892    -3.355322    -0.419550
 H     4.926103    -3.770519     0.764218
 C     3.383511    -2.505438    -0.060755
 C     4.589440    -2.742353     0.603200
 C     2.934683    -1.193980    -0.244982
 C     5.363249    -1.672331     1.058289
 H     6.310036    -1.859783     1.571009
 C     3.720676    -0.119248     0.184186
 C     4.928939    -0.363079     0.842821
 H     5.538569     0.478970     1.182937
 H     3.383337     0.907970     0.002593
64
Scheme_S15_prod_Ph / electronic energy: -4032.60724620 a.u. / lowest freq: 18.71 cm-1
 C    -2.595653    -1.912760     2.262221
 C    -1.501718    -1.683227     3.298153
 C    -0.516853    -1.716508     1.182001
 C    -2.430265    -1.803607    -0.286488
 C    -2.119835    -2.827624    -1.191021
 C    -3.238417    -0.734128    -0.709931
 C    -2.624519    -2.811788    -2.487882
 H    -1.478599    -3.644629    -0.850109
 C    -3.754260    -0.735399    -2.009562
 C    -3.456425    -1.768175    -2.894590
 H    -2.373973    -3.620220    -3.178433
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H	-4.368957	0.108457	-2.329428
H	-3.864056	-1.749142	-3.907546
S	-3.591210	0.703309	0.321864
O	-3.757856	1.825232	-0.651514
O	-2.365114	0.933947	1.144554
O	-4.800045	0.373519	1.095524
Cu	0.654824	-1.434015	-0.368325
N	-1.843422	-1.844309	1.000052
N	-0.278633	-1.672783	2.490716
C	2.912011	-0.607031	-1.982563
C	1.476163	-0.978508	-2.267240
C	0.415984	-0.146997	-2.029689
H	-0.593279	-0.397790	-2.372871
H	0.597443	0.873733	-1.670856
H	1.298918	-1.931352	-2.789650
P	1.218837	3.384839	-0.460681
O	2.009483	4.533509	0.402860
O	-0.011365	3.965346	-1.128036
O	0.493715	2.479971	0.751907
O	2.266312	2.571490	-1.154595
Na	-1.668278	2.792324	-0.126836
C	1.256421	5.495960	1.108473
H	1.959376	6.190692	1.586591
H	0.596062	6.072697	0.441835
H	0.637636	5.038396	1.899297
C	1.235013	1.517159	1.457902
H	0.648807	1.215358	2.337095
H	1.426828	0.616187	0.841137
H	2.205334	1.909796	1.806942
C	1.017214	-1.534463	3.093384
H	2.942066	0.484288	-1.829571
C	3.824760	-0.982264	-3.143873
H	-1.455995	-2.473562	4.061967
H	-1.600428	-0.719397	3.824358
H	3.816624	-2.068124	-3.326157
H	4.864112	-0.687143	-2.942510
H	3.509775	-0.484741	-4.072252
H	1.320966	-2.453260	3.620442
H	1.021409	-0.711460	3.823657
H	1.757656	-1.318096	2.311798
H	-3.388782	-1.154288	2.290348
H	-3.070830	-2.902076	2.353371
H	2.502861	-3.193243	-1.116324
H	3.273946	-4.231836	0.998278
C	3.062654	-2.591643	-0.390788
C	3.510791	-3.184717	0.793126
C	3.364057	-1.249099	-0.684088
C	4.262016	-2.444331	1.704672
H	4.615563	-2.906414	2.629586
C	4.098902	-0.511812	0.254956
C	4.547416	-1.103996	1.435254
H	5.125179	-0.513729	2.151275
H	4.312892	0.541523	0.049217

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Scheme_S16_NHC(S)-1b-Cu-Me / electronic energy: -3689.54478686 a.u. / lowest freq: 10.62 cm-1

C	-1.027231	0.617857	1.003016
H	-1.517373	1.575263	0.785640
C	0.492375	0.801526	1.214823
H	0.776024	0.440439	2.218907
C	0.125734	-0.719119	-0.574209
C	-2.292162	-0.773763	-0.714304
C	-2.416994	-2.168482	-0.816570
C	-3.354511	0.044581	-1.143305
C	-3.571883	-2.751439	-1.327378
H	-1.575620	-2.788040	-0.490815
C	-4.515709	-0.558004	-1.637260
C	-4.634567	-1.942195	-1.727823
H	-3.642859	-3.839341	-1.399234
H	-5.320055	0.094836	-1.982106
H	-5.551198	-2.386700	-2.123077
C	2.451865	-0.373545	0.062649
C	3.153089	0.276763	-0.972753
C	3.097165	-1.248463	0.964369
C	4.528978	0.035300	-1.082701
C	4.474008	-1.444911	0.820703
C	5.186037	-0.806978	-0.192825
H	6.261278	-0.976117	-0.293144
S	-3.273208	1.858371	-1.206392
O	-4.353892	2.245698	-2.137195
O	-1.907331	2.141098	-1.717588
O	-3.498951	2.326875	0.185815
Cu	0.551932	-2.115565	-1.837428
C	-1.717255	-0.022145	2.182407

C	-2.582976	0.725256	2.986408
C	-1.474764	-1.363831	2.508124
C	-3.180220	0.147771	4.108181
H	-2.795099	1.762564	2.715185
C	-2.071053	-1.941823	3.626535
H	-0.818279	-1.962883	1.868166
C	-2.923811	-1.184076	4.432801
H	-3.856406	0.741557	4.728568
H	-1.873780	-2.989523	3.868473
H	-3.394608	-1.636213	5.309356
N	-1.080674	-0.257706	-0.191988
N	1.050727	-0.145268	0.212962
H	4.996513	-2.120904	1.502180
C	2.301359	-2.035093	1.986758
C	2.469744	1.178684	-1.980244
H	5.093343	0.520551	-1.884032
H	1.425668	-1.428925	2.268048
H	1.446962	1.376642	-1.622246
C	3.174924	2.521963	-2.113540
H	4.170064	2.422055	-2.574717
H	2.593631	3.206053	-2.749530
H	3.310528	3.010488	-1.136785
C	2.347956	0.477543	-3.329469
H	1.814414	1.108458	-4.056011
H	3.337369	0.242805	-3.753959
H	1.791055	-0.471214	-3.236468
C	3.067442	-2.332321	3.266012
H	3.489081	-1.421106	3.716292
H	2.403742	-2.792294	4.012604
H	3.896387	-3.037722	3.103664
C	1.769935	-3.317757	1.350138
H	1.113017	-3.866365	2.043009
H	1.199766	-3.111304	0.426144
H	2.596340	-3.991468	1.072666
C	1.041775	2.202366	1.077406
C	2.184259	2.548770	1.811655
C	0.463929	3.157868	0.230300
C	2.735702	3.826208	1.716970
H	2.638627	1.805876	2.476187
C	1.012669	4.437862	0.143274
H	-0.417493	2.902045	-0.370346
C	2.144917	4.777850	0.885262
H	3.622896	4.080889	2.302275
H	0.548728	5.177382	-0.514821
H	2.567261	5.783591	0.815202
C	1.025992	-3.608127	-3.005889
H	0.580390	-3.529158	-4.017342
H	0.707206	-4.596401	-2.619440
H	2.118455	-3.693484	-3.172996

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Scheme_S16_NHC(S)-1a-Cu-Me / electronic energy: -3571.70652471 a.u. / lowest freq: 23.10 cm-1

C	0.893453	-1.167985	0.397443
H	1.263926	-1.644011	-0.521490
C	-0.629351	-1.357776	0.548382
H	-0.859197	-1.774910	1.543375
C	-0.155805	0.961272	0.333670
C	2.256915	0.970666	0.133406
C	2.585066	1.925368	1.105940
C	3.149244	0.725903	-0.926661
C	3.793609	2.612852	1.053631
H	1.864661	2.114635	1.906553
C	4.366136	1.413613	-0.957160
C	4.696985	2.342797	0.025716
H	4.030754	3.352814	1.821622
H	5.037429	1.226342	-1.797568
H	5.653261	2.869349	-0.021954
C	-2.517918	0.353790	0.466605
C	-3.079680	0.904652	-0.706043
C	-3.318067	0.075773	1.591927
C	-4.454642	1.159451	-0.720881
C	-4.690429	0.339468	1.517914
C	-5.282155	0.877367	0.371610
C	-6.755839	1.124383	0.302133
S	2.750034	-0.327590	-2.353181
O	3.703729	0.095632	-3.399433
O	1.332733	-0.001082	-2.655654
O	2.952275	-1.733288	-1.910375
Cu	-0.362402	2.869053	0.202567
C	1.723808	-1.657274	1.558934
C	2.880106	-2.409651	1.324918
C	1.389073	-1.318835	2.877372
C	3.677127	-2.830610	2.391023
H	3.155050	-2.642158	0.291892

C	2.184579	-1.737444	3.941574
H	0.499216	-0.710830	3.071679
C	3.330801	-2.498652	3.700194
H	4.577562	-3.418702	2.195651
H	1.911929	-1.466383	4.964679
H	3.955843	-2.827429	4.534362
N	1.012932	0.305191	0.254432
N	-1.128693	0.045473	0.501114
H	-5.311906	0.131930	2.395203
C	-2.730203	-0.467642	2.854938
C	-2.249600	1.233978	-1.904327
H	-4.896191	1.586600	-1.627155
C	-1.306379	-2.224240	-0.485181
C	-2.375311	-3.042228	-0.099025
C	-0.939346	-2.177228	-1.837180
C	-3.072697	-3.798149	-1.041054
H	-2.661665	-3.086350	0.956905
C	-1.636466	-2.935690	-2.777450
H	-0.107984	-1.538326	-2.159917
C	-2.704597	-3.744557	-2.385280
H	-3.904169	-4.432296	-0.723261
H	-1.341513	-2.892585	-3.829211
H	-3.247724	-4.335742	-3.127102
C	-0.556835	4.806109	0.080523
H	-0.018015	5.236725	-0.786606
H	-0.161520	5.342688	0.965792
H	-1.606388	5.145009	-0.026374
H	-3.371131	-0.244533	3.717709
H	-1.734249	-0.049024	3.056939
H	-2.614684	-1.563806	2.826818
H	-2.867871	1.301643	-2.809295
H	-1.451484	0.499782	-2.083550
H	-1.738259	2.206095	-1.778643
H	-6.993003	2.038305	-0.259881
H	-7.205866	1.212135	1.299975
H	-7.276732	0.300308	-0.211483

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Scheme_S16_NHC(S)-2c-Cu-Me / electronic energy: -3458.67482873 a.u. / lowest freq: 25.35 cm-1

C	-1.047494	0.774857	-1.211854
H	-1.801837	0.358505	-1.889115
C	0.358166	0.622971	-1.792221
H	0.760828	1.558811	-2.207541
C	0.347694	-0.295320	0.364449
C	-2.031261	-0.364940	0.846554
C	-1.939167	-0.039831	2.209108
C	-3.187909	-1.010245	0.367542
C	-2.974063	-0.338621	3.089143
H	-1.025199	0.446802	2.564038
C	-4.224670	-1.289330	1.263410
C	-4.129862	-0.956703	2.612177
H	-2.878922	-0.076549	4.145587
H	-5.104885	-1.807268	0.876610
H	-4.953220	-1.190943	3.291373
C	2.531504	-0.068439	-0.698518
C	2.995522	-1.351751	-1.048209
C	3.413455	1.000797	-0.434024
C	4.381615	-1.547510	-1.114503
C	4.787268	0.759020	-0.527474
C	5.268061	-0.505445	-0.863709
H	6.345447	-0.679312	-0.926241
S	-3.404004	-1.576705	-1.347902
O	-4.445742	-2.622906	-1.261326
O	-2.071696	-2.079580	-1.761598
O	-3.844704	-0.368054	-2.095531
Cu	1.071880	-0.981872	2.013097
C	-1.422554	2.196539	-0.860844
C	-2.341292	2.891688	-1.654682
C	-0.844140	2.851898	0.234898
C	-2.660368	4.220801	-1.373402
H	-2.814270	2.376503	-2.495325
C	-1.159692	4.180000	0.516072
H	-0.144844	2.312113	0.881831
C	-2.067455	4.869631	-0.290271
H	-3.382832	4.749963	-2.000119
H	-0.699877	4.677540	1.374224
H	-2.320050	5.909198	-0.066961
N	-0.932572	-0.059392	0.010338
N	1.127817	0.174828	-0.627854
H	5.493846	1.567014	-0.322012
C	2.871422	2.335503	0.035056
C	2.055720	-2.511869	-1.312924
H	4.769869	-2.537695	-1.369848
H	1.894765	2.483960	-0.457165

H	1.027333	-2.120553	-1.365356
C	2.347420	-3.194531	-2.643342
H	3.336050	-3.678980	-2.652924
H	1.603556	-3.978214	-2.848163
H	2.318365	-2.484976	-3.483684
C	2.097442	-3.504789	-0.155828
H	1.381205	-4.325287	-0.311542
H	3.097854	-3.952085	-0.041491
H	1.840132	-3.011977	0.798203
C	3.748944	3.522307	-0.327893
H	3.982725	3.553749	-1.402237
H	3.242529	4.464762	-0.072937
H	4.703064	3.519164	0.220811
C	2.615781	2.284112	1.540425
H	2.138432	3.209515	1.898416
H	1.969037	1.433074	1.821124
H	3.560427	2.162360	2.094354
H	0.396883	-0.144415	-2.585476
C	1.876126	-1.567981	3.694548
H	1.605913	-2.609279	3.960441
H	1.586207	-0.955230	4.571036
H	2.984163	-1.549320	3.674835

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Scheme_S16_NHC(S)-2a-Cu-Me / electronic energy: -3340.83727707 a.u. / lowest freq: 29.36 cm-1

C	-0.894777	1.133640	-0.988969
H	-1.514160	0.790233	-1.826529
C	0.557141	1.324709	-1.418686
H	0.854262	2.383014	-1.469357
C	0.525599	-0.202860	0.362002
C	-1.847518	-0.617417	0.611821
C	-1.908822	-0.626470	2.013555
C	-2.848972	-1.272574	-0.129150
C	-2.955212	-1.255611	2.679674
H	-1.110071	-0.126885	2.568769
C	-3.900516	-1.889601	0.556121
C	-3.964813	-1.880105	1.946806
H	-2.984303	-1.249561	3.771852
H	-4.657762	-2.410237	-0.034016
H	-4.795701	-2.372567	2.457769
C	2.724332	0.421716	-0.480131
C	3.244764	-0.788343	-0.982908
C	3.573529	1.476070	-0.095675
C	4.634699	-0.913993	-1.088891
C	4.954823	1.301882	-0.227849
C	5.508002	0.115035	-0.721396
C	6.990181	-0.062271	-0.821966
S	-2.829057	-1.441557	-1.939681
O	-3.670300	-2.628012	-2.205025
O	-1.401480	-1.613032	-2.300176
O	-3.422292	-0.175678	-2.454007
Cu	1.127782	-1.476059	1.670872
C	-1.569801	2.312315	-0.328469
C	-2.945236	2.503388	-0.510127
C	-0.870993	3.177539	0.523358
C	-3.605303	3.548139	0.138295
H	-3.487860	1.813072	-1.164831
C	-1.529837	4.221970	1.169857
H	0.201020	3.029806	0.684901
C	-2.899955	4.410735	0.977500
H	-4.678693	3.688883	-0.013225
H	-0.971610	4.891545	1.829364
H	-3.416684	5.229886	1.484034
N	-0.748605	0.024986	-0.002275
N	1.312136	0.595347	-0.389185
H	5.618395	2.118921	0.073531
C	3.016994	2.739830	0.476598
C	2.356303	-1.925392	-1.373151
H	5.046942	-1.848711	-1.482900
H	0.753236	0.876546	-2.406903
C	1.787221	-2.754171	2.989494
H	1.217276	-3.704176	3.006821
H	1.748629	-2.371677	4.028764
H	2.842876	-3.046086	2.820968
H	3.816116	3.412311	0.812720
H	2.365552	2.535680	1.340288
H	2.406463	3.299355	-0.249363
H	2.876221	-2.627541	-2.037912
H	1.430553	-1.599349	-1.868402
H	2.033668	-2.491142	-0.480228
H	7.268383	-0.725180	-1.652544
H	7.401884	-0.517705	0.093092
H	7.511450	0.894655	-0.959444

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Scheme_S16_NHC(S)-4d-Cu-Me / electronic energy: -3838.24574694 a.u. / lowest freq: 17.43 cm-1

C	1.202147	0.879319	0.721863
H	1.535859	0.339191	1.621257
C	-0.319991	1.127421	0.776627
H	-0.554176	2.137419	0.392064
C	0.149394	-0.498677	-0.890648
C	2.567493	-0.560378	-0.879467
C	3.004063	-0.221081	-2.164558
C	3.345346	-1.418802	-0.082314
C	4.211203	-0.707508	-2.658304
H	2.374642	0.435939	-2.770598
C	4.559309	-1.892704	-0.586601
C	4.997775	-1.537540	-1.860068
H	4.537228	-0.433789	-3.664344
H	5.142655	-2.574029	0.036445
H	5.949331	-1.922545	-2.234642
S	2.818120	-2.021076	1.548131
O	3.630048	-3.234036	1.773189
O	1.362521	-2.287354	1.393740
O	3.118518	-0.919989	2.500219
Cu	-0.208030	-1.895264	-2.160118
C	2.050036	2.113123	0.559158
C	3.119644	2.354792	1.427305
C	1.801555	3.017602	-0.481448
C	3.913705	3.492502	1.268687
H	3.329596	1.630503	2.219801
C	2.591979	4.152355	-0.641334
H	0.979539	2.822689	-1.176960
C	3.650224	4.394677	0.238335
H	4.745889	3.672618	1.953969
H	2.382887	4.850899	-1.456364
H	4.272056	5.285148	0.115836
N	1.323284	-0.035090	-0.439747
N	-0.824975	0.122879	-0.194676
C	-0.951295	0.977674	2.135759
C	-1.821125	1.963251	2.614205
C	-0.711303	-0.161830	2.917980
C	-2.447406	1.819195	3.852939
H	-2.005545	2.854860	2.006089
C	-1.340732	-0.305370	4.153105
H	-0.024149	-0.936113	2.555543
C	-2.210032	0.681671	4.623529
H	-3.122649	2.598141	4.216113
H	-1.148829	-1.196823	4.755796
H	-2.700632	0.563612	5.593132
H	-4.048276	-5.071152	0.696893
H	-1.630183	-4.546511	1.046021
C	-3.675745	-4.063848	0.494589
C	-2.308361	-3.768766	0.686172
H	-5.603129	-3.288561	-0.067155
C	-4.538690	-3.078426	0.068682
C	-1.813761	-2.508067	0.425315
C	-4.069209	-1.766337	-0.198592
C	-2.673682	-1.477238	-0.043629
H	-6.013959	-0.948075	-0.695810
C	-4.947312	-0.728740	-0.599708
C	-2.203894	-0.165566	-0.367975
C	-4.468612	0.528600	-0.875916
C	-3.081706	0.825975	-0.802746
H	-5.152139	1.314779	-1.207426
C	-2.615590	2.161552	-1.239381
H	-3.994750	3.241731	0.026012
H	-1.152699	1.391722	-2.633867
C	-3.202889	3.327869	-0.723961
C	-1.603505	2.291722	-2.204830
C	-2.770854	4.587303	-1.137406
C	-1.184792	3.551158	-2.629523
H	-3.229081	5.483704	-0.712013
C	-1.757095	4.703938	-2.088999
H	-1.419546	5.690766	-2.415133
H	-0.752534	-2.306081	0.588611
H	-0.400004	3.632177	-3.386363
C	-0.673606	-3.339577	-3.386963
H	-0.608140	-3.088185	-4.463796
H	-1.715831	-3.683802	-3.225644
H	-0.043452	-4.241310	-3.255639

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Scheme_S16_NHC(S)-3b-Cu-Me / electronic energy: -3768.10570677 a.u. / lowest freq: 16.21 cm-1

O	4.482316	-1.068620	3.128914
O	2.121622	-0.592381	2.513430
S	3.557997	-0.340245	2.235148
O	3.893765	1.100975	2.089060
H	5.699007	-1.904104	1.252705

H	0.494681	0.961769	2.456924
C	-0.072596	1.886064	2.294101
C	4.997515	-1.837093	0.418512
C	3.835186	-1.080950	0.598479
H	2.119262	1.447221	0.824366
H	6.153223	-3.105276	-0.887389
H	3.939415	2.679929	0.202867
C	5.238731	-2.518426	-0.771564
C	-0.301446	2.336592	0.986779
C	2.907723	-1.003002	-0.455269
N	1.708760	-0.248873	-0.358729
C	1.695901	1.218388	-0.165159
C	0.495017	-0.813022	-0.409648
C	0.183431	1.530900	-0.193146
C	3.653908	2.646136	-0.852174
Cu	0.261611	-2.699877	-0.745807
N	-0.417041	0.176365	-0.261389
C	4.302199	-2.463058	-1.804010
C	-1.810306	-0.032052	-0.254143
C	3.145622	-1.706547	-1.643135
C	2.513675	1.923118	-1.217043
C	4.422424	3.289774	-1.823897
H	-0.073617	2.074742	-1.119656
H	-0.079060	-5.255147	-0.378538
H	1.179283	-4.960305	-1.577945
H	4.471388	-3.005588	-2.737046
C	0.195447	-4.592560	-1.223389
H	2.398652	-1.648913	-2.439214
C	2.166081	1.837119	-2.572501
C	4.064218	3.208190	-3.168909
H	1.286480	1.256115	-2.870106
H	-0.522061	-4.836656	-2.031813
H	-2.262023	1.931060	-1.021102
C	2.934878	2.475441	-3.542640
H	4.667299	3.710695	-3.929392
H	2.654358	2.400529	-4.596340
C	-2.678722	0.985468	-0.676914
C	-2.331587	-1.252137	0.180229
H	-1.639144	-2.020441	0.537408
H	5.309843	3.854746	-1.527506
H	-1.593783	4.399036	4.029305
H	-0.352247	2.270372	4.395759
C	-1.230020	3.822573	3.174897
C	-0.537086	2.627103	3.379257
H	-1.982493	5.221099	1.707397
C	-1.448605	4.282341	1.876627
C	-0.984284	3.540864	0.789764
H	-1.152316	3.899991	-0.230864
C	-4.060959	0.789058	-0.669173
C	-3.711420	-1.489385	0.167689
C	-4.556944	-0.457223	-0.250630
H	-5.637670	-0.612765	-0.244095
C	-4.224432	-2.859613	0.617244
C	-5.041969	1.891076	-1.078035
C	-4.328156	3.138738	-1.591211
C	-5.875900	2.281384	0.148214
C	-5.973193	1.378174	-2.181427
H	-5.236469	2.654753	0.963036
H	-6.452247	1.431258	0.542019
H	-6.593355	3.077589	-0.104608
H	-3.690373	3.598229	-0.821529
H	-5.064857	3.897408	-1.893662
H	-3.699071	2.927524	-2.469159
H	-5.411230	1.081500	-3.079983
H	-6.686309	2.161616	-2.480724
H	-6.564183	0.508899	-1.859277
C	-5.745452	-2.956840	0.548651
C	-3.781495	-3.119101	2.061498
C	-3.620325	-3.933839	-0.294761
H	-3.938979	-3.800213	-1.340161
H	-3.934575	-4.940127	0.023075
H	-2.519707	-3.909739	-0.283238
H	-4.180651	-2.358261	2.749340
H	-2.686812	-3.117393	2.165285
H	-4.139341	-4.101049	2.407434
H	-6.239791	-2.226778	1.207097
H	-6.075046	-3.956623	0.867813
H	-6.126141	-2.800492	-0.471807

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Scheme_S16_NHC(S)-3a-Cu-Me / electronic energy: -4386.96712820 a.u. / lowest freq: 11.53 cm-1

O	-6.503553	2.293524	1.607291
O	-4.023791	2.136750	1.681141
S	-5.313053	1.423798	1.506178

O	-5.423890	0.187008	2.327521
H	-7.285793	1.602058	-0.491180
H	-2.458845	1.003625	2.646337
C	-1.608765	0.515564	3.139885
C	-6.430885	1.146203	-0.994488
C	-5.289012	0.887181	-0.230701
H	-3.558005	-0.715427	1.767647
H	-7.373843	1.083431	-2.933396
H	-5.445051	-2.009231	1.417980
C	-6.469599	0.868780	-2.358632
C	-1.026644	-0.629878	2.581842
C	-4.164393	0.319442	-0.858603
N	-2.979779	-0.013639	-0.153336
C	-2.969752	-1.067533	0.908611
C	-1.750179	0.284422	-0.613550
C	-1.473354	-1.173183	1.246463
C	-4.911658	-2.658123	0.716283
Cu	-1.256018	1.109936	-2.287217
N	-0.863327	-0.381590	0.149316
C	-5.345918	0.330722	-2.984450
C	0.533974	-0.216448	0.028231
C	-4.207739	0.051404	-2.234717
C	-3.597847	-2.328149	0.364122
C	-5.531117	-3.778979	0.161078
H	-1.130694	-2.218193	1.162774
H	0.206965	1.665327	-4.400146
H	-1.311063	2.572106	-4.434059
H	-5.355633	0.113647	-4.055234
C	-0.867744	1.600945	-4.137677
H	-3.320948	-0.383561	-2.705741
C	-2.920817	-3.130446	-0.565108
C	-4.847112	-4.577657	-0.754887
H	-1.901471	-2.871945	-0.871482
H	-1.295787	0.862176	-4.845547
H	0.918675	-2.332442	-0.171708
C	-3.539523	-4.249109	-1.119262
H	-5.332723	-5.454710	-1.190170
H	-3.000278	-4.866164	-1.842482
C	1.358630	-1.331016	-0.134472
C	1.081017	1.067725	0.077107
H	0.418202	1.924677	0.228052
H	-6.557035	-4.027754	0.444488
H	0.385982	0.875128	5.887476
H	-1.567309	1.934559	4.760291
C	-0.009740	0.450555	4.961093
C	-1.102970	1.044435	4.327727
H	1.438296	-1.153669	4.892237
C	0.579833	-0.684312	4.403606
C	0.068249	-1.222321	3.223055
H	0.522891	-2.117199	2.786026
C	2.738333	-1.163428	-0.293232
C	2.460623	1.251394	-0.050298
C	3.275497	0.128334	-0.246781
H	4.356525	0.262125	-0.363166
C	3.054282	2.613341	0.045410
C	2.873595	3.537467	-1.009952
C	3.791855	2.976025	1.197921
C	3.465161	4.802955	-0.905112
C	4.354443	4.256800	1.262293
C	4.201961	5.163454	0.218232
H	3.347006	5.518584	-1.724160
H	4.914623	4.551347	2.154783
H	4.653910	6.156775	0.282866
C	2.110146	3.193604	-2.278015
H	1.618649	2.215132	-2.142689
C	1.002857	4.199019	-2.567106
H	1.390670	5.223093	-2.683240
H	0.477622	3.945162	-3.498657
H	0.251354	4.218024	-1.762853
C	3.065150	3.053288	-3.458953
H	3.847187	2.304110	-3.260565
H	2.528710	2.739771	-4.367453
H	3.572972	4.003674	-3.688995
C	3.932771	2.059886	2.402796
H	3.530986	1.069100	2.136124
C	5.385892	1.863540	2.815888
H	5.998802	1.468395	1.991912
H	5.851170	2.804327	3.148334
H	5.462148	1.156861	3.655636
C	3.094286	2.578990	3.566711
H	2.031668	2.665890	3.294075
H	3.162452	1.905176	4.434221
H	3.432686	3.573987	3.897049

H	2.716149	-3.727028	3.677066
H	4.665208	-2.049920	3.772611
H	5.685313	-3.162328	2.839861
H	3.676053	-4.865323	2.725390
C	3.017896	-3.985728	2.651128
C	4.937884	-2.357954	2.751331
H	2.114068	-4.300701	2.108022
H	5.433509	-1.502407	2.268352
C	3.711273	-2.813059	1.967977
H	3.001836	-1.969417	1.962062
H	5.269116	-4.840309	1.085366
C	4.071411	-3.131717	0.527840
C	4.903374	-4.225374	0.257360
H	5.924274	-5.396654	-1.240670
C	5.275808	-4.538181	-1.046642
C	3.617899	-2.338670	-0.549787
C	4.818001	-3.756220	-2.102943
C	3.987867	-2.650683	-1.878156
H	5.104786	-4.011501	-3.127716
C	3.486874	-1.852133	-3.069582
H	3.076512	-3.560289	-4.371322
C	2.555445	-2.692916	-3.936081
H	2.895730	-1.001425	-2.693225
C	4.635024	-1.273407	-3.887552
H	5.295202	-0.641508	-3.274551
H	5.258940	-2.061985	-4.336602
H	4.256439	-0.651661	-4.712600
H	1.700898	-3.078047	-3.359659
H	2.149994	-2.101158	-4.770316

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Scheme_S16_NHC(S)-4a-Cu-Me / electronic energy: -3841.84975758 a.u. / lowest freq: 15.72 cm-1

C	1.511890	0.854342	0.631564
H	1.832400	0.489314	1.618756
C	0.037256	1.320609	0.667854
H	-0.048288	2.347839	0.273855
C	0.233353	-0.544554	-0.795338
C	2.600413	-1.024951	-0.712549
C	2.917886	-1.027550	-2.077372
C	3.399642	-1.752309	0.187410
C	4.028494	-1.719197	-2.551022
H	2.269880	-0.473910	-2.762038
C	4.520429	-2.429948	-0.300920
C	4.843790	-2.410572	-1.655309
H	4.259369	-1.709983	-3.618746
H	5.118128	-3.004572	0.409384
H	5.723217	-2.951390	-2.013365
S	2.970224	-1.989232	1.936792
O	3.799427	-3.134135	2.367739
O	1.512969	-2.273891	1.908825
O	3.318509	-0.719734	2.628852
Cu	-0.204426	-1.977078	-2.004541
C	2.503069	1.885117	0.154027
C	3.671203	2.128126	0.883838
C	2.293428	2.578036	-1.045718
C	4.603208	3.064590	0.432386
H	3.846850	1.558561	1.800949
C	3.222095	3.512395	-1.497115
H	1.392173	2.374910	-1.633518
C	4.379622	3.760747	-0.754936
H	5.512074	3.248438	1.011059
H	3.044603	4.048671	-2.433231
H	5.109224	4.493955	-1.108010
N	1.453908	-0.297654	-0.302205
N	-0.612950	0.378189	-0.287250
C	-2.019665	0.229172	-0.385714
C	-2.873955	1.316872	-0.665795
C	-2.552680	-1.041194	-0.154699
C	-4.253463	1.062825	-0.648985
C	-3.926077	-1.300263	-0.193509
C	-4.774052	-0.210653	-0.427858
H	-5.857312	-0.343862	-0.452126
H	-1.847418	-1.843545	0.080694
H	0.054203	-0.745573	2.463706
H	-1.144334	-0.862162	4.633886
C	-0.544178	0.108235	2.806779
C	-1.210243	0.046236	4.029300
C	-0.619844	1.269340	2.024156
C	-1.953980	1.137068	4.486169
H	-2.474994	1.083182	5.445511
C	-1.357590	2.361537	2.491319
C	-2.021516	2.298327	3.717514
H	-1.407531	3.271939	1.885647
H	-2.592836	3.160058	4.072187

H	-4.936708	1.889249	-0.863850
C	-2.384143	2.665792	-1.021887
C	-1.370240	2.839959	-1.978842
C	-2.956320	3.810858	-0.443681
C	-0.932853	4.115191	-2.331250
H	-0.929567	1.961681	-2.459088
C	-2.516094	5.086083	-0.793832
H	-3.741036	3.692821	0.309519
C	-1.499583	5.243719	-1.736773
H	-1.152392	6.242993	-2.010302
C	-4.414809	-2.729086	0.037624
H	-2.966808	5.963118	-0.322435
H	-0.144359	4.227776	-3.080318
C	-0.567515	-3.371289	-3.323451
H	-0.596689	-4.391301	-2.891637
H	0.204870	-3.410489	-4.117463
H	-1.533113	-3.249370	-3.853331
C	-5.935193	-2.830139	-0.031803
C	-3.951546	-3.204265	1.419894
C	-3.807038	-3.635243	-1.040071
H	-4.143356	-3.342245	-2.046587
H	-4.102633	-4.683697	-0.881107
H	-2.706388	-3.596842	-1.041643
H	-6.427622	-2.217805	0.738506
H	-6.253255	-3.870880	0.128149
H	-6.327453	-2.517050	-1.010939
H	-4.352061	-2.565946	2.222315
H	-2.855551	-3.203205	1.512624
H	-4.293651	-4.233134	1.610401

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Scheme_S16_NHC(S)-4b-Cu-Me / electronic energy: -4151.28099913 a.u. / lowest freq: 14.36 cm-1

C	2.446663	0.493192	0.739120
H	2.529104	0.189538	1.792903
C	1.243546	1.440850	0.527964
H	1.571041	2.365014	0.020537
C	0.891517	-0.560278	-0.711897
C	2.909396	-1.812939	-0.248609
C	3.310349	-2.128500	-1.554144
C	3.333085	-2.620972	0.822071
C	4.139539	-3.217646	-1.803789
H	2.948675	-1.499656	-2.372603
C	4.177750	-3.703003	0.557084
C	4.588192	-4.000210	-0.740120
H	4.438918	-3.448522	-2.828807
H	4.480430	-4.331050	1.397461
H	5.244878	-4.854605	-0.921198
S	2.730002	-2.426655	2.525845
O	3.046524	-3.715092	3.176341
O	1.276414	-2.170564	2.363831
O	3.476472	-1.278148	3.104867
Cu	0.187372	-1.821622	-1.983104
C	3.777468	1.040166	0.286927
C	4.886824	0.994946	1.137351
C	3.931706	1.559391	-1.005462
C	6.123660	1.481805	0.709486
H	4.770730	0.554198	2.131334
C	5.164816	2.044376	-1.433687
H	3.072663	1.577113	-1.684192
C	6.265140	2.009783	-0.573272
H	6.983505	1.443235	1.383147
H	5.270544	2.448747	-2.443964
H	7.234007	2.389349	-0.907505
N	2.061721	-0.690321	-0.070307
N	0.389861	0.655876	-0.410428
C	-0.957548	1.003430	-0.676787
C	-1.307827	2.264963	-1.200762
C	-1.950816	0.080848	-0.326461
C	-2.676836	2.566283	-1.296507
C	-3.307705	0.375434	-0.466353
C	-3.657427	1.648785	-0.941149
H	-4.712907	1.914867	-1.046515
H	-1.640625	-0.879209	0.096085
H	0.436034	-0.188662	2.586657
H	-0.934591	0.453059	4.554652
C	0.112913	0.852570	2.715129
C	-0.653710	1.214075	3.821793
C	0.483225	1.822735	1.772952
C	-1.062494	2.538139	3.999959
H	-1.665268	2.813866	4.869279
C	0.079143	3.148386	1.962047
C	-0.691248	3.507286	3.068807
H	0.376613	3.906527	1.230698
H	-0.998006	4.547594	3.204756

H	-2.970969	3.538665	-1.700936
C	-0.311434	3.244452	-1.684900
C	0.744988	2.850696	-2.523174
C	-0.425489	4.604687	-1.352880
C	1.664844	3.784052	-2.996797
H	0.835641	1.800970	-2.816139
C	0.498783	5.536505	-1.821404
H	-1.240230	4.928234	-0.698385
C	1.551295	5.128996	-2.641962
H	2.277960	5.858062	-3.008414
C	-4.354617	-0.608871	-0.072921
C	-4.606231	-1.744023	-0.886110
C	-5.092600	-0.399125	1.113218
C	-5.628270	-2.622080	-0.508807
C	-6.112810	-1.302011	1.444560
C	-6.385470	-2.400101	0.639516
H	-5.841766	-3.499290	-1.123019
H	-6.693517	-1.143095	2.358276
H	-7.182916	-3.096604	0.911973
C	-3.823444	-1.982922	-2.167774
H	-2.765355	-1.723232	-1.970625
C	-3.839198	-3.430228	-2.633810
H	-4.841258	-3.754261	-2.955205
H	-3.174393	-3.558348	-3.499155
H	-3.499118	-4.124084	-1.850813
C	-4.314723	-1.065799	-3.285571
H	-4.269158	-0.002931	-3.008147
H	-3.709915	-1.194547	-4.195846
H	-5.360619	-1.291846	-3.548342
C	-4.798685	0.744491	2.069039
H	-3.919267	1.293066	1.693884
C	-5.959657	1.729689	2.139526
H	-6.211401	2.140540	1.150612
H	-6.870317	1.253831	2.536678
H	-5.721438	2.577043	2.799978
C	-4.436771	0.221666	3.455162
H	-3.583293	-0.471178	3.417286
H	-4.165343	1.048042	4.128738
H	-5.276011	-0.314496	3.924945
H	0.398863	6.587633	-1.539285
H	2.476832	3.456817	-3.651804
C	-0.261756	-3.072000	-3.413328
H	-0.748281	-3.999310	-3.053112
H	0.654899	-3.408693	-3.939150
H	-0.924016	-2.669147	-4.205043

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Scheme_S16_IPr-Cu-Me / electronic energy: -2840.46968028 a.u. / lowest freq: 29.99 cm-1

C	-0.778703	0.129035	-2.421488
H	-1.349677	-0.583931	-3.033305
C	0.719267	-0.123617	-2.432789
H	1.279304	0.582621	-3.062201
C	-0.012062	0.013884	-0.204721
C	-2.439750	0.123787	-0.517145
C	-2.921605	1.392777	-0.142872
C	-3.251158	-1.029825	-0.465887
C	-4.252802	1.485585	0.285388
C	-2.042033	2.627611	-0.134002
C	-4.574746	-0.884598	-0.040390
C	-5.073201	0.363763	0.328521
H	-4.649332	2.457308	0.592897
H	-5.224960	-1.760962	0.014660
H	-6.110228	0.459001	0.660314
C	2.406946	-0.109040	-0.547868
C	2.885225	-1.380164	-0.176049
C	3.222431	1.041582	-0.496474
C	4.215244	-1.477030	0.254911
C	4.545242	0.892021	-0.070171
C	5.038947	-0.357712	0.300497
H	6.074839	-0.456040	0.634929
C	-2.659496	-2.391444	-0.768834
Cu	0.048146	-0.003738	1.721656
H	-1.042716	1.145824	-2.763717
N	-1.102341	-0.012407	-0.993852
N	1.065533	0.033382	-1.012676
H	5.198153	1.766400	-0.014551
C	2.635106	2.405440	-0.797037
C	2.009674	-2.618221	-0.185474
H	4.608020	-2.450145	0.563231
H	1.860125	2.267555	-1.570887
H	1.047452	-2.353769	-0.654637
C	2.621171	-3.748103	-1.004938
H	3.556315	-4.120889	-0.559547
H	1.931846	-4.603399	-1.063975

H	2.849632	-3.435530	-2.034718
C	1.709588	-3.065595	1.241912
H	1.071757	-3.962003	1.255229
H	2.633538	-3.312054	1.788551
H	1.189732	-2.271267	1.806235
C	3.645741	3.406293	-1.333744
H	4.187018	3.021754	-2.210701
H	3.143261	4.335914	-1.637115
H	4.394976	3.685793	-0.577856
C	1.938789	2.945641	0.451730
H	1.411774	3.888522	0.239662
H	1.206720	2.226569	0.859610
H	2.670122	3.146446	1.250761
H	0.977044	-1.144197	-2.768546
C	0.178661	-0.083472	3.671711
H	-0.374636	-0.943318	4.099530
H	-0.207479	0.808690	4.202646
H	1.222265	-0.205734	4.024733
C	-1.948286	-2.926838	0.473715
H	-1.892729	-2.251344	-1.550568
C	-3.670010	-3.398468	-1.294034
H	-1.209321	-2.207943	0.869001
H	-1.425397	-3.871258	0.258642
H	-2.669658	-3.123883	1.282676
H	-4.410518	-3.680304	-0.530441
H	-3.165592	-4.326055	-1.600302
H	-4.221517	-3.018340	-2.166507
C	-1.693545	3.008172	1.301989
C	-2.670516	3.795495	-0.883202
H	-1.097213	2.379285	-0.645573
H	-3.585482	4.158881	-0.390945
H	-2.936026	3.527798	-1.916753
H	-1.974485	4.645972	-0.930517
H	-2.598460	3.236006	1.887327
H	-1.046811	3.897626	1.336823
H	-1.164944	2.184206	1.814052

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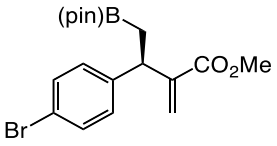
Scheme_S16_SIMes-Cu-Me / electronic energy: -2604.79370496 a.u. / lowest freq: 24.92 cm-1

C	0.757244	-2.544436	0.115632
H	1.314668	-3.166011	-0.597949
C	-0.741269	-2.547801	-0.130619
H	-1.295510	-3.175256	0.580254
C	0.002344	-0.322763	-0.003546
C	2.426089	-0.632672	0.033356
C	2.863446	0.078584	1.170749
C	3.290924	-0.878060	-1.049284
C	4.180414	0.545508	1.189710
C	1.955828	0.339506	2.329902
C	4.604402	-0.398872	-0.973538
C	5.070136	0.317175	0.132348
H	4.526656	1.099477	2.068312
H	5.278116	-0.578748	-1.817394
C	6.477541	0.820023	0.198830
C	-2.419539	-0.643676	-0.038031
C	-2.863086	0.064321	-1.171666
C	-3.279100	-0.888719	1.052277
C	-4.182314	0.533488	-1.182496
C	-4.589869	-0.409020	0.985099
C	-5.062772	0.308446	-0.120249
C	-6.470848	0.812161	-0.155869
C	2.826498	-1.619371	-2.262285
Cu	-0.008128	1.604021	-0.005897
H	1.024417	-2.885175	1.131275
N	1.089743	-1.118654	-0.028104
N	-1.080981	-1.124457	0.018802
H	-5.259202	-0.587118	1.833181
C	-2.804828	-1.629855	2.261675
C	-1.963339	0.324997	-2.336858
H	-4.533624	1.087364	-2.058957
H	-1.006601	-2.885909	-1.147619
C	-0.040987	3.556583	-0.020025
H	0.585789	4.000794	-0.818477
H	0.317238	4.016900	0.921849
H	-1.056389	3.970030	-0.182158
H	7.020698	0.648569	-0.739454
H	7.045491	0.327268	1.003022
H	6.514409	1.897814	0.415327
H	2.525527	0.620056	3.225408
H	1.333717	-0.533061	2.578238
H	1.253411	1.163925	2.111071
H	3.444191	-1.378694	-3.137023
H	1.780078	-1.389528	-2.510301
H	2.885895	-2.711529	-2.127592

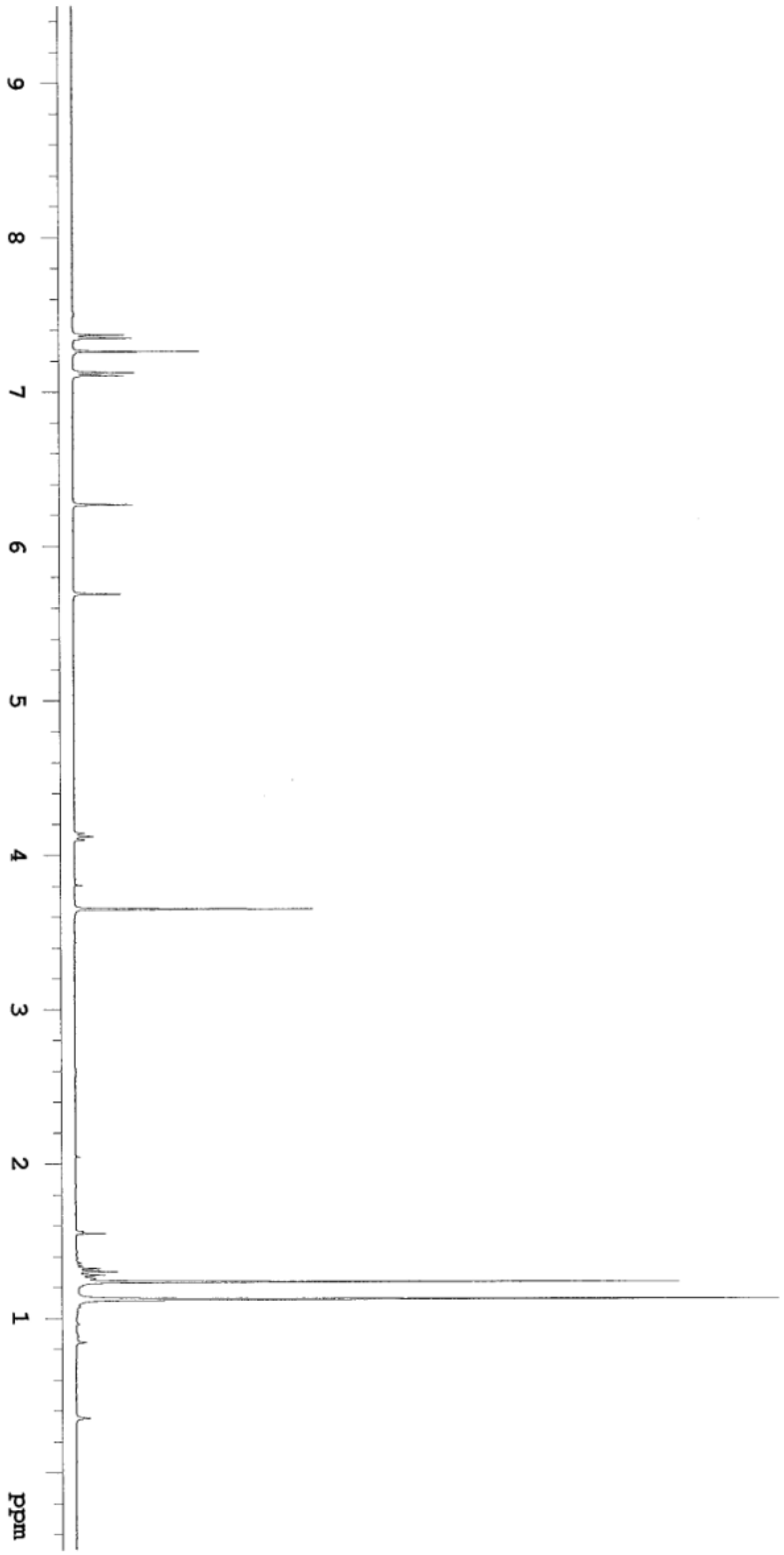
H	**-2.538997**	**0.600195**	**-3.230220**
H	**-1.338359**	**-0.545389**	**-2.585586**
H	**-1.263350**	**1.153285**	**-2.124409**
H	**-1.761224**	**-1.387965**	**2.510215**
H	**-2.849666**	**-2.721948**	**2.121604**
H	**-3.424963**	**-1.401216**	**3.137804**
H	**-6.671545**	**1.407377**	**-1.055754**
H	**-6.699640**	**1.440255**	**0.717892**
H	**-7.198339**	**-0.013845**	**-0.137088**

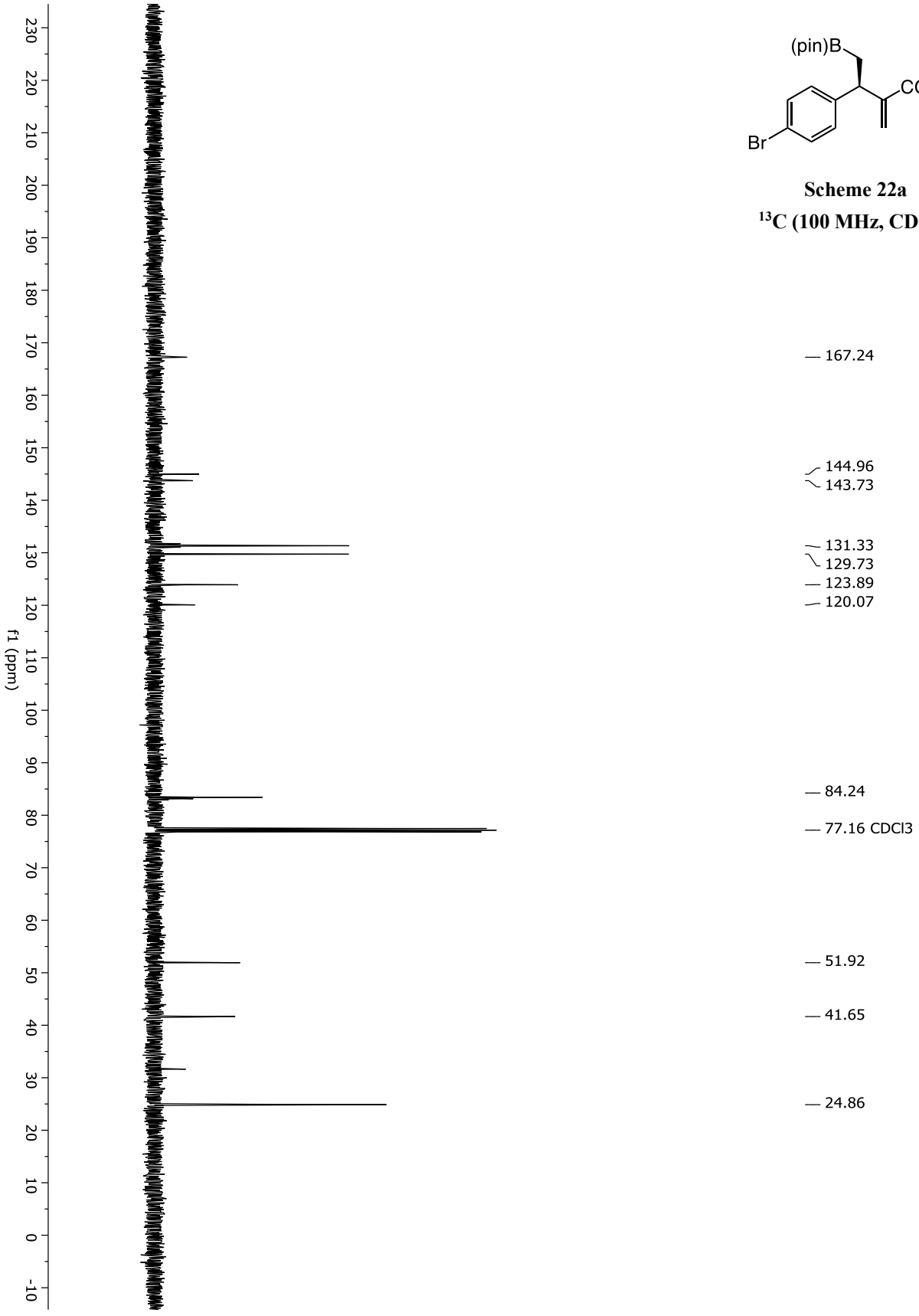
13 NMR Spectra



Scheme 22a

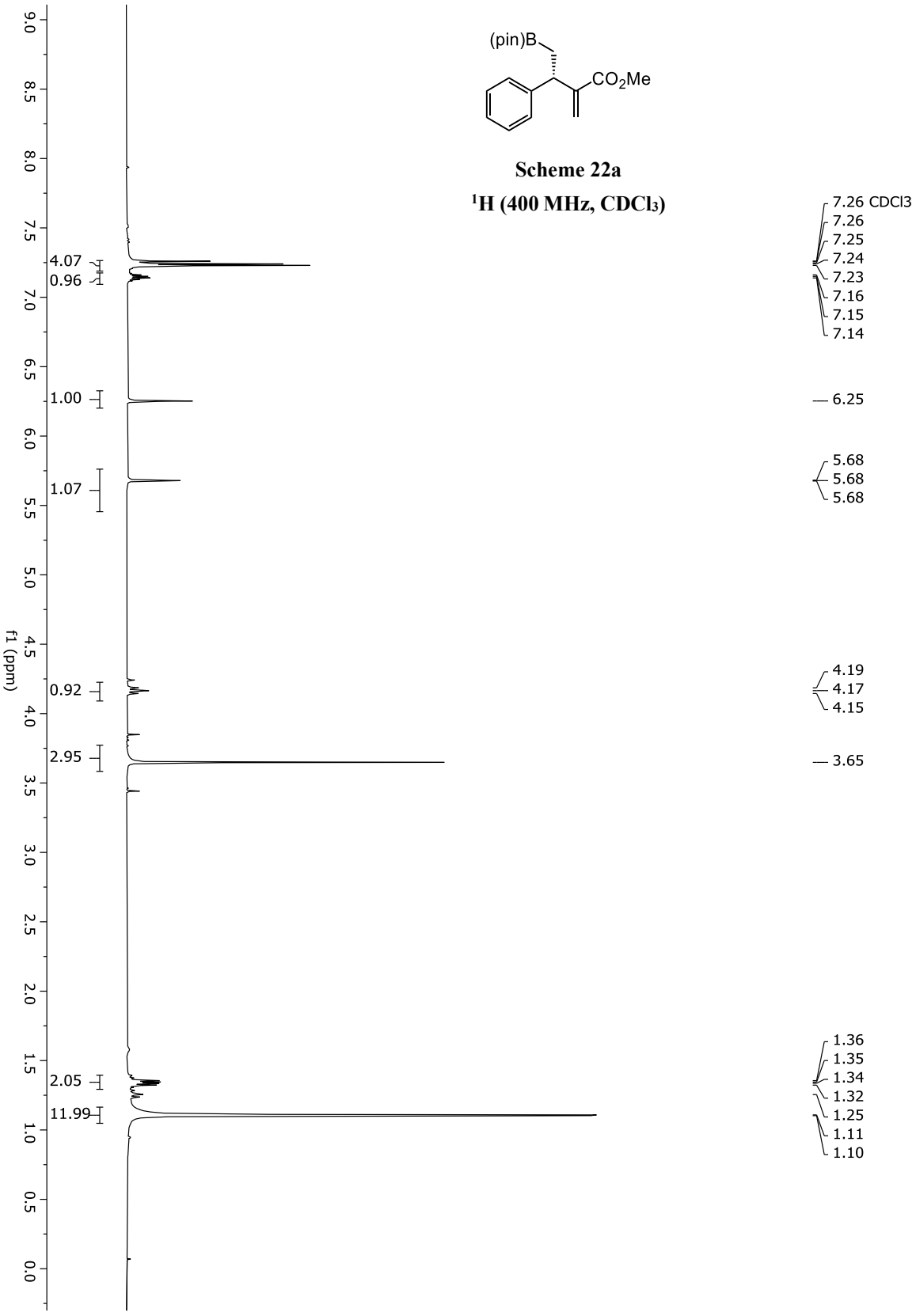
^{1}H (400 MHz, $CDCl_3$)





Scheme 22a

^{13}C (100 MHz, $CDCl_3$)


(pin)B
CO2Me
Scheme 22a
1H (400 MHz, CDCl3)
f1 (ppm)
4.07
0.96
1.00
1.07
0.92
2.95
2.05
11.99
7.26 CDCl3
7.26
7.25
7.24
7.23
7.16
7.15
7.14
6.25
5.68
5.68
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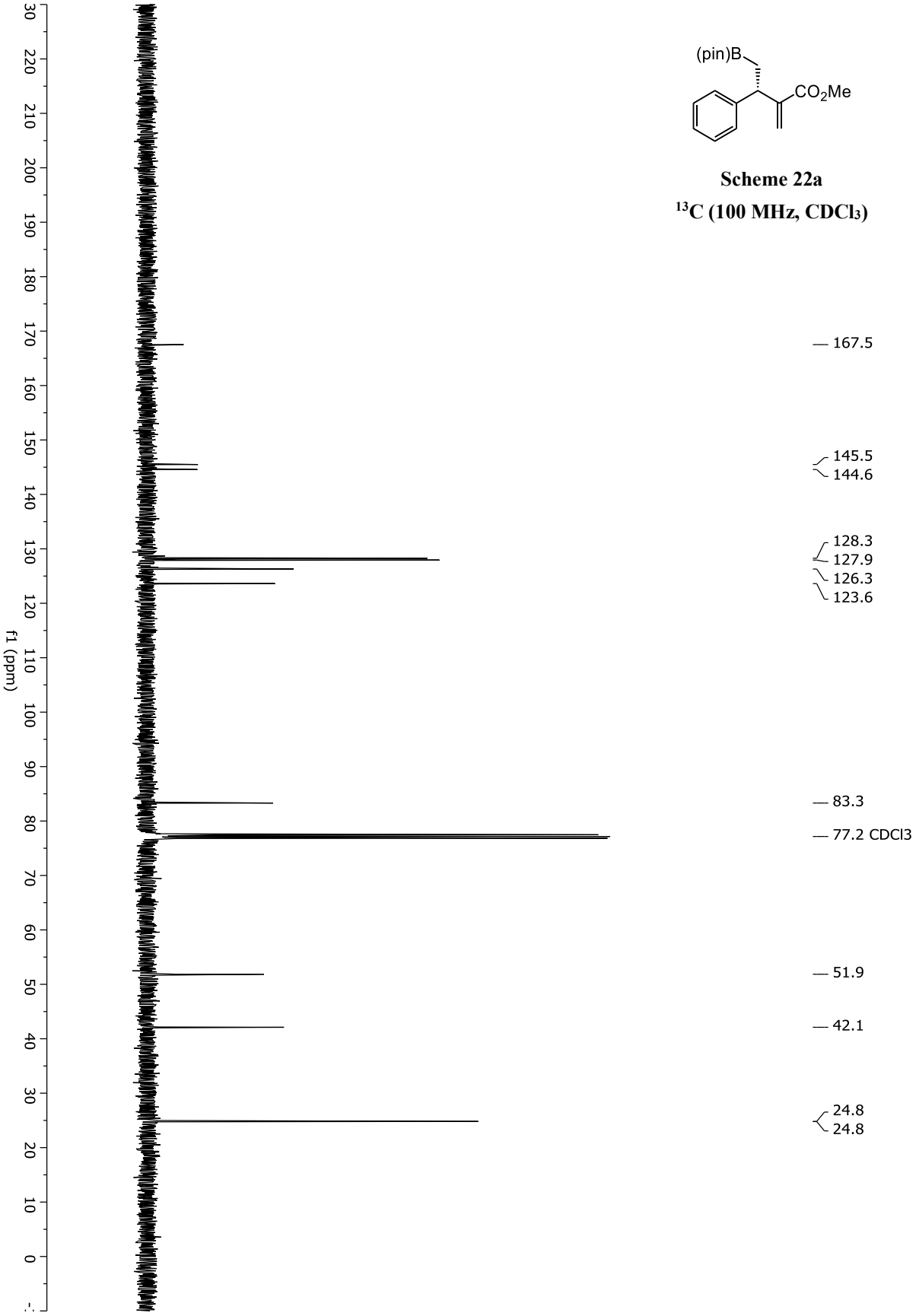
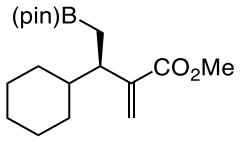
1.35
1.34
1.32
1.25
1.11
1.10



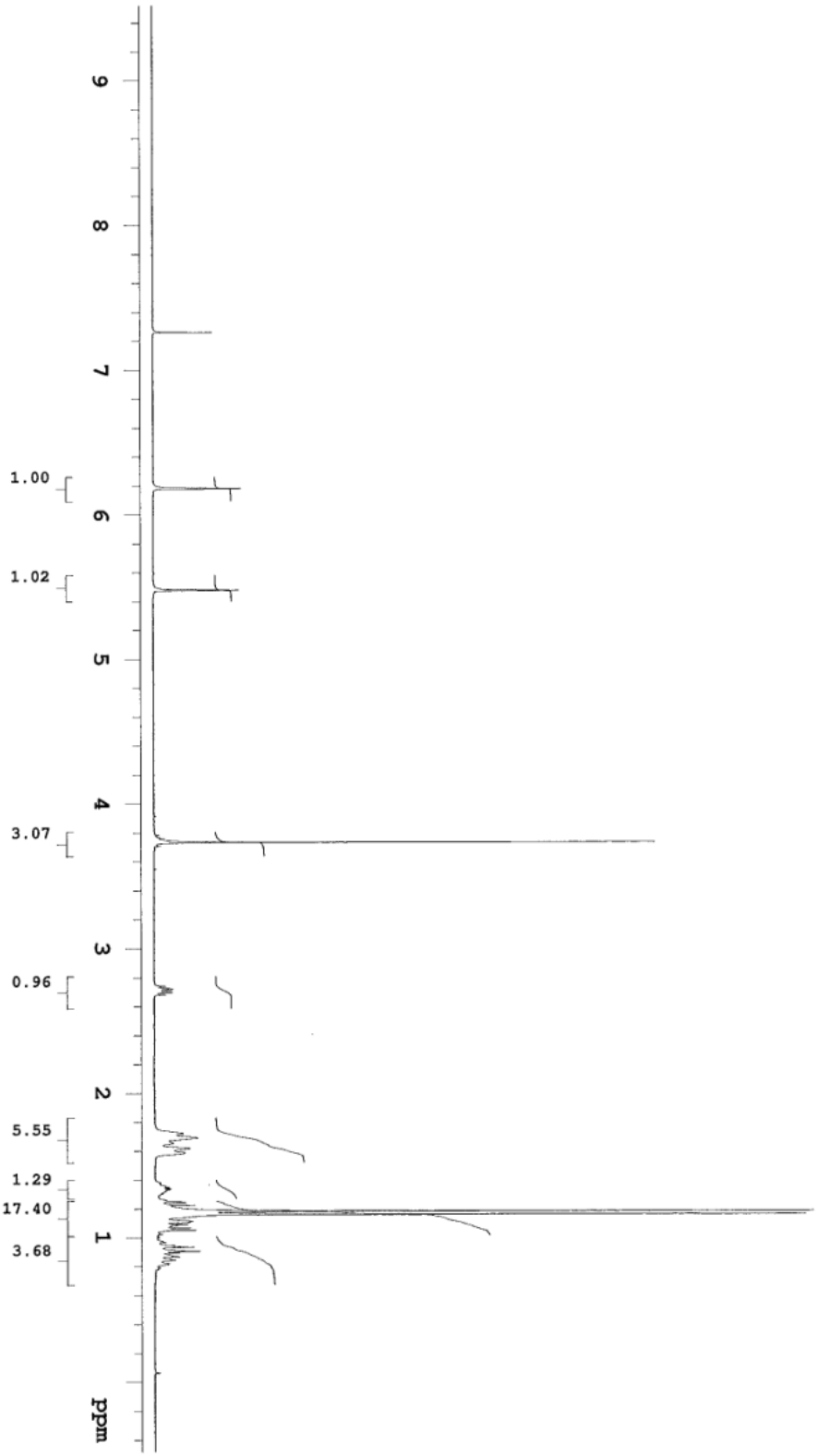
Scheme 22a

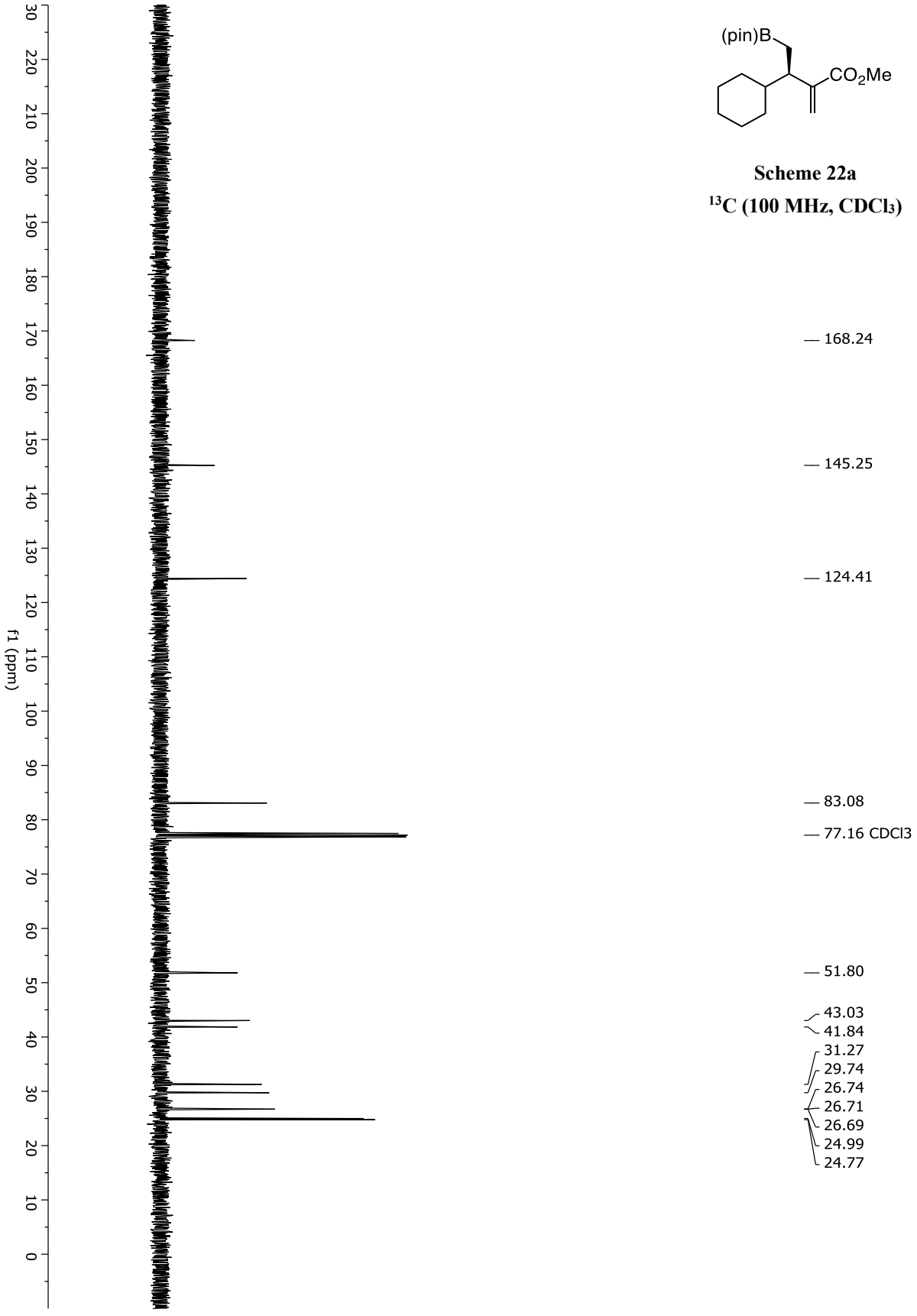
^{13}C (100 MHz, $CDCl_3$)



Scheme 22a

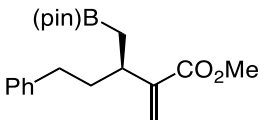
^{1}H (400 MHz, $CDCl_3$)





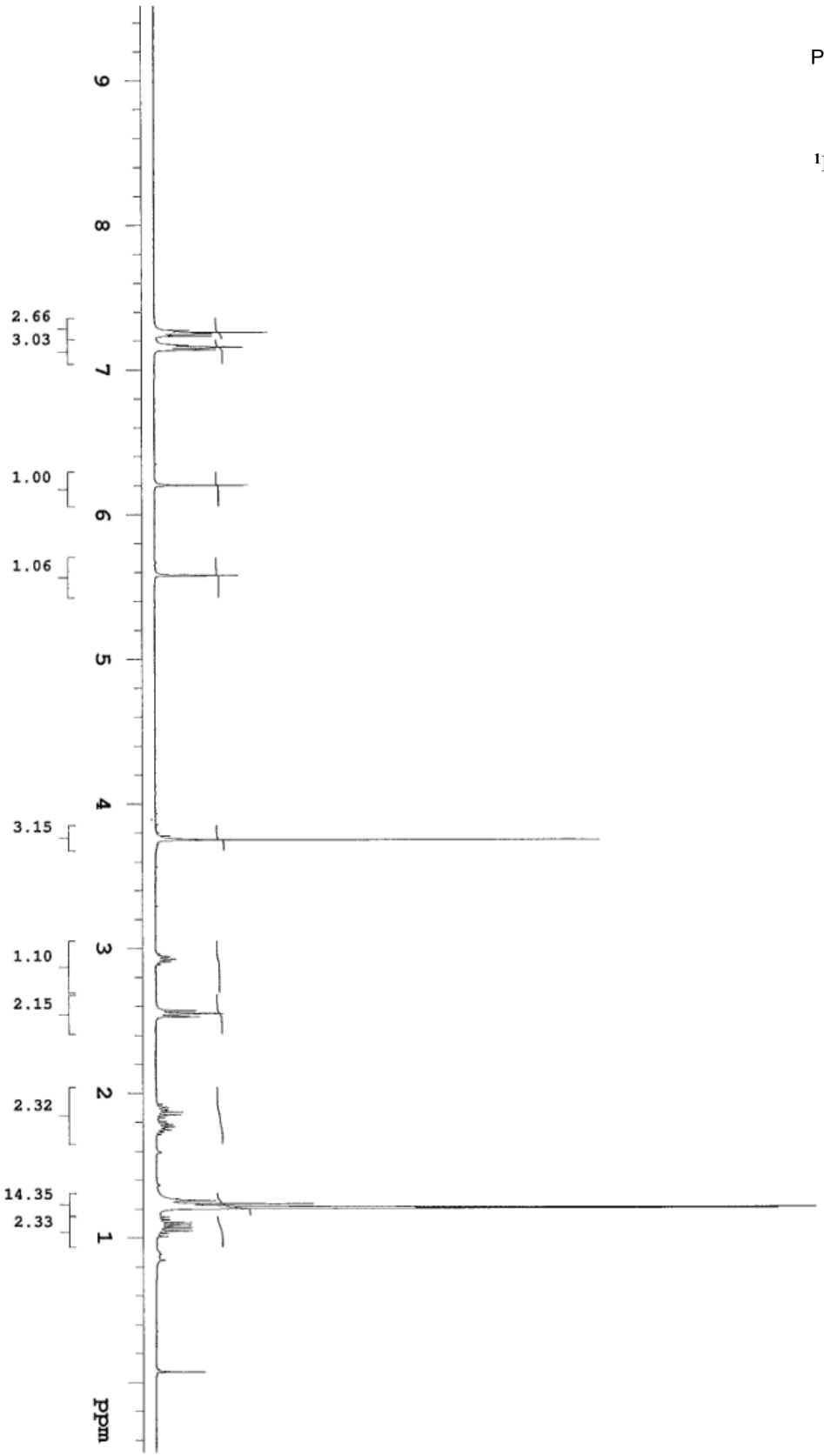
Scheme 22a

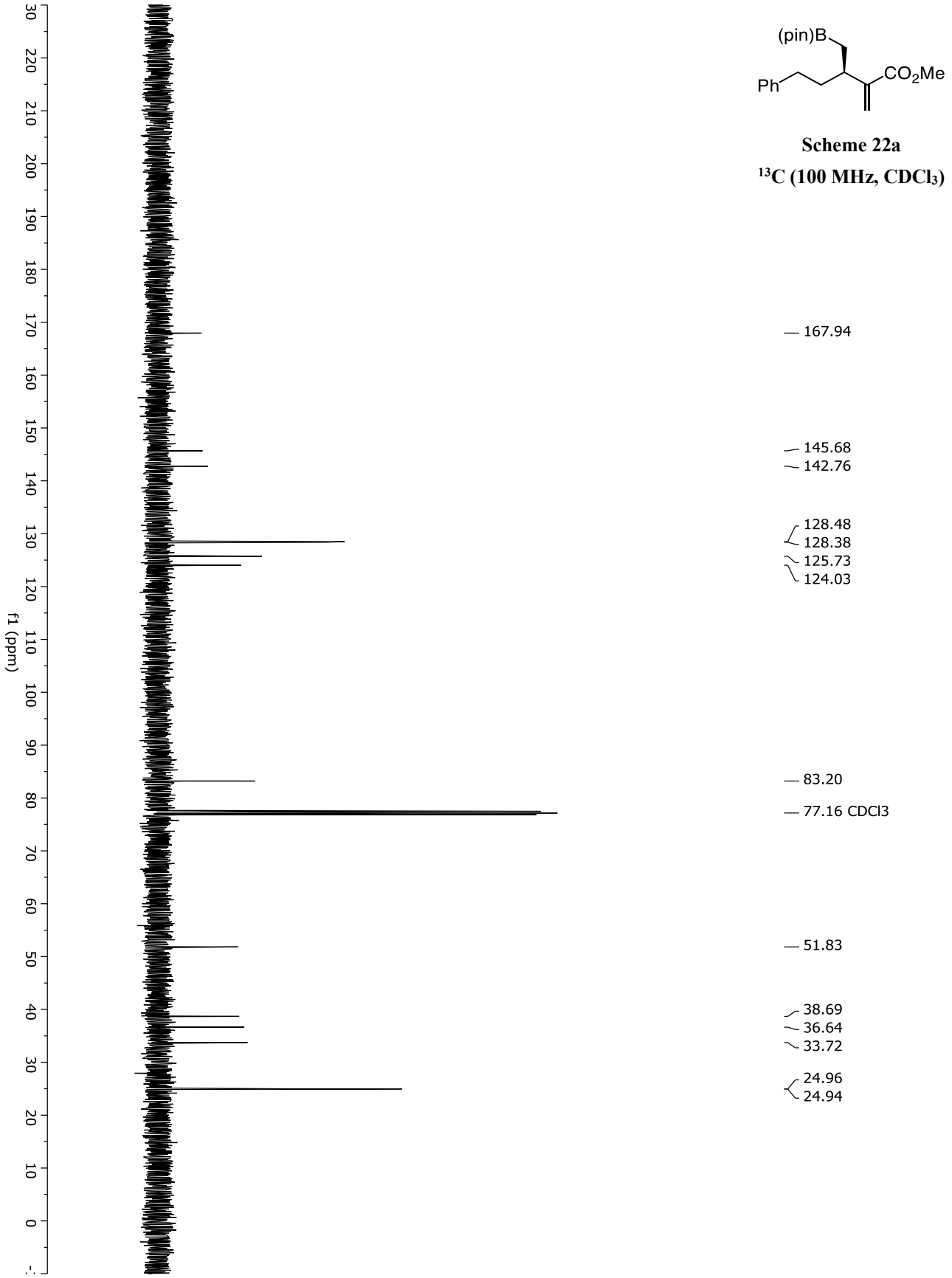
^{13}C (100 MHz, $CDCl_3$)



Scheme 22a

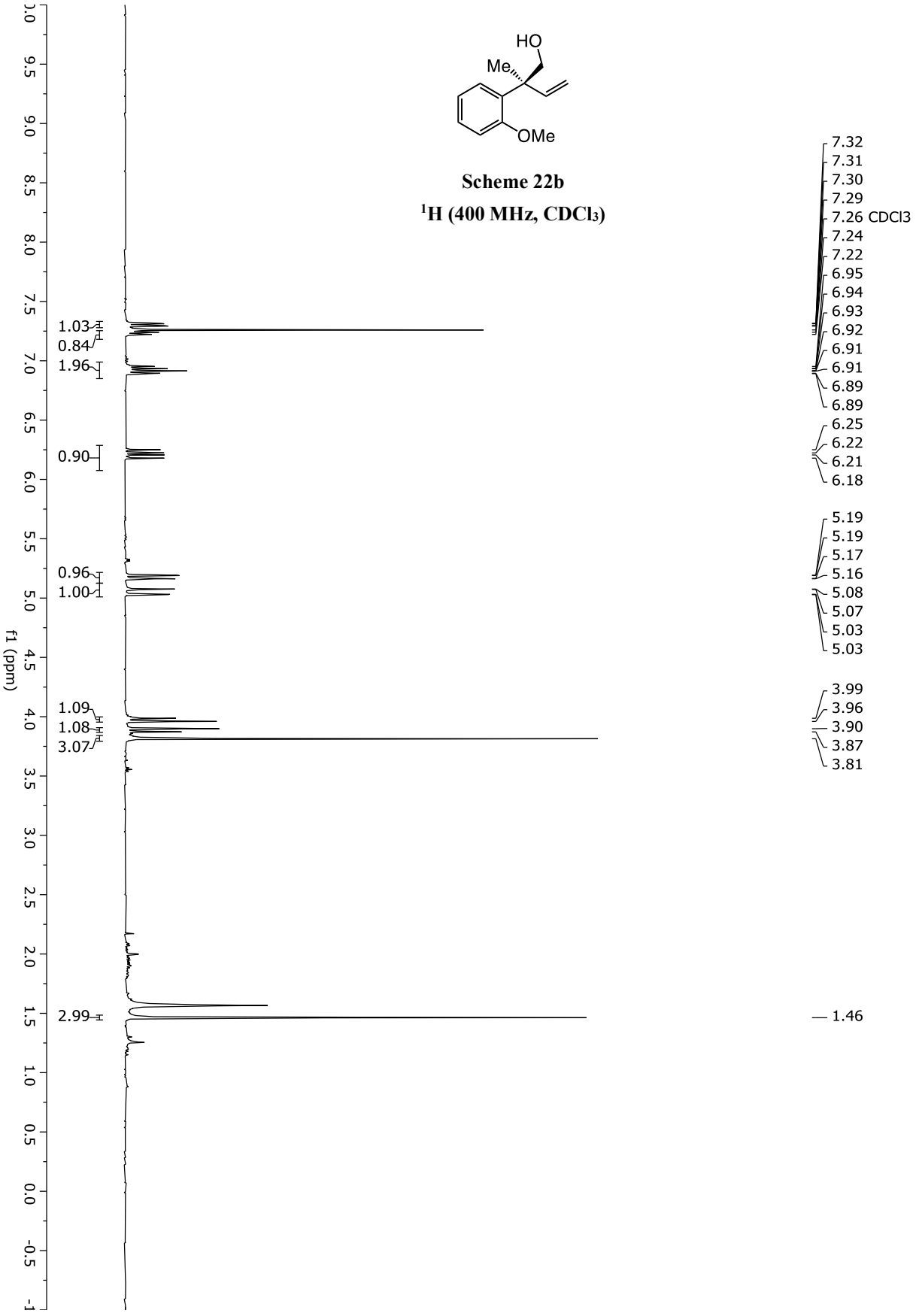
^{1}H (400 MHz, $CDCl_3$)





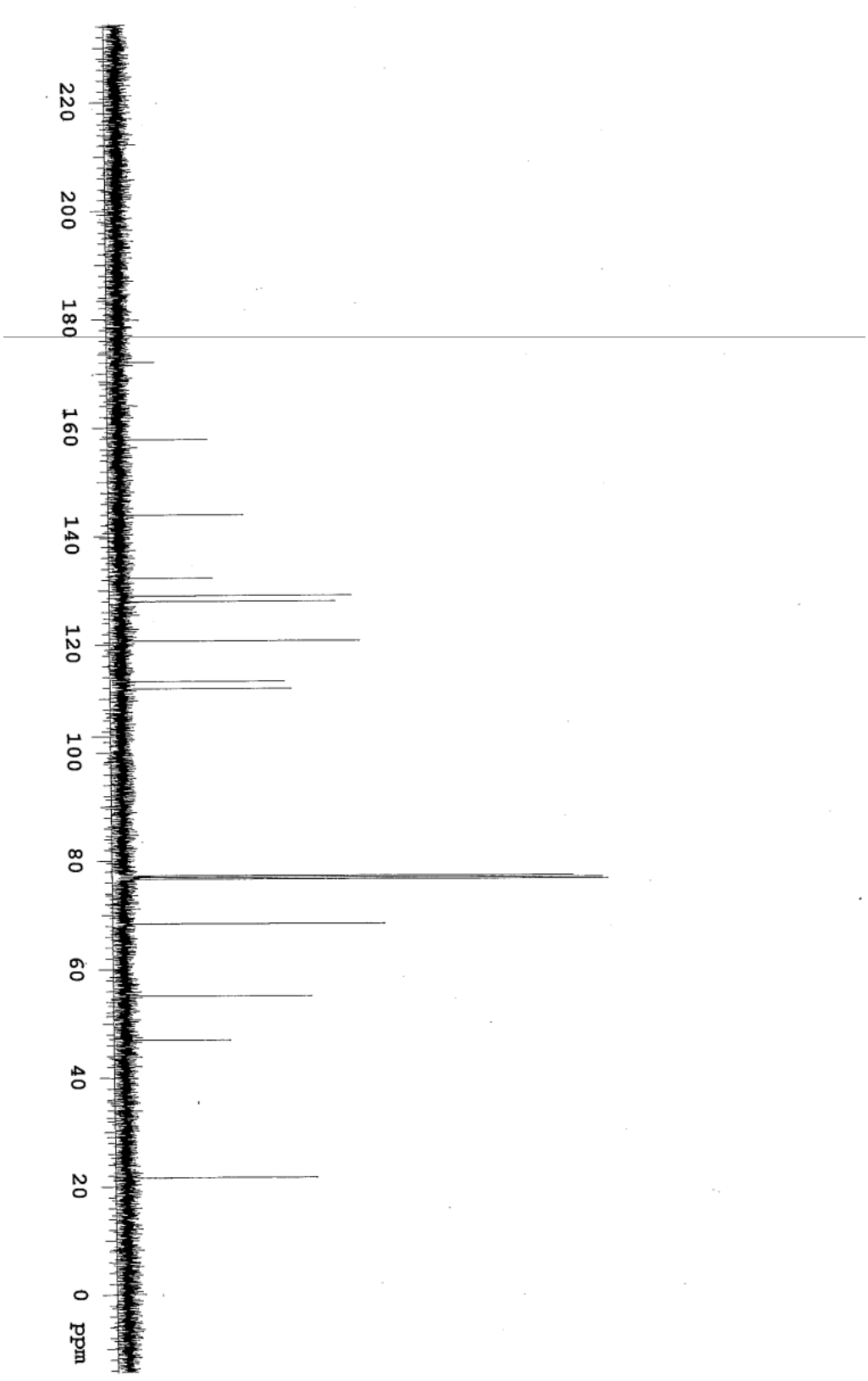
Scheme 22a

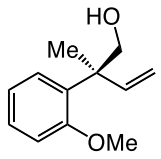
^{13}C (100 MHz, $CDCl_3$)



Scheme 22b

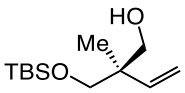
^{1}H (400 MHz, $CDCl_3$)





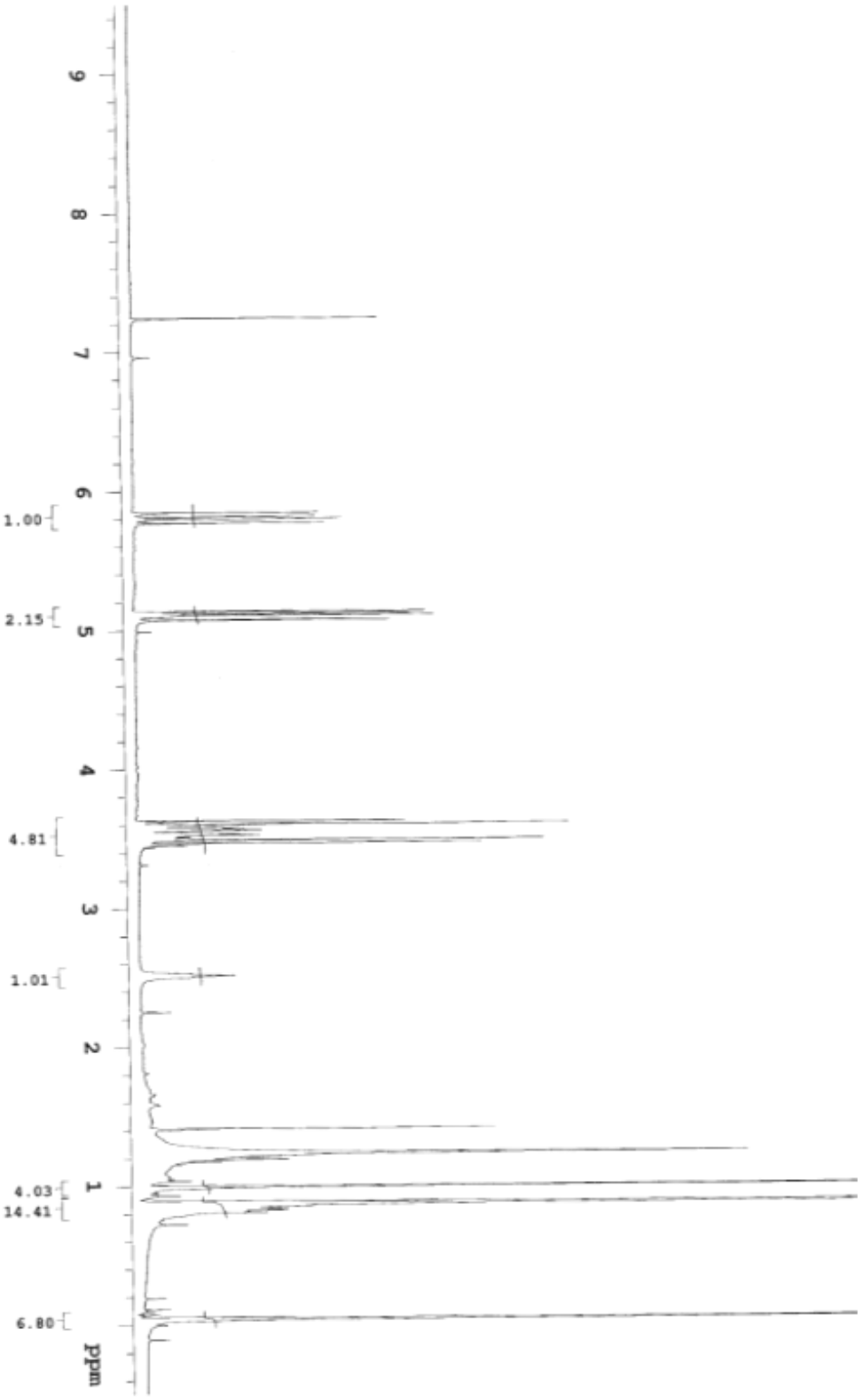
Scheme 22b

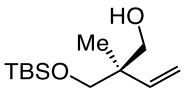
^{13}C (100 MHz, $CDCl_3$)



Scheme 22b

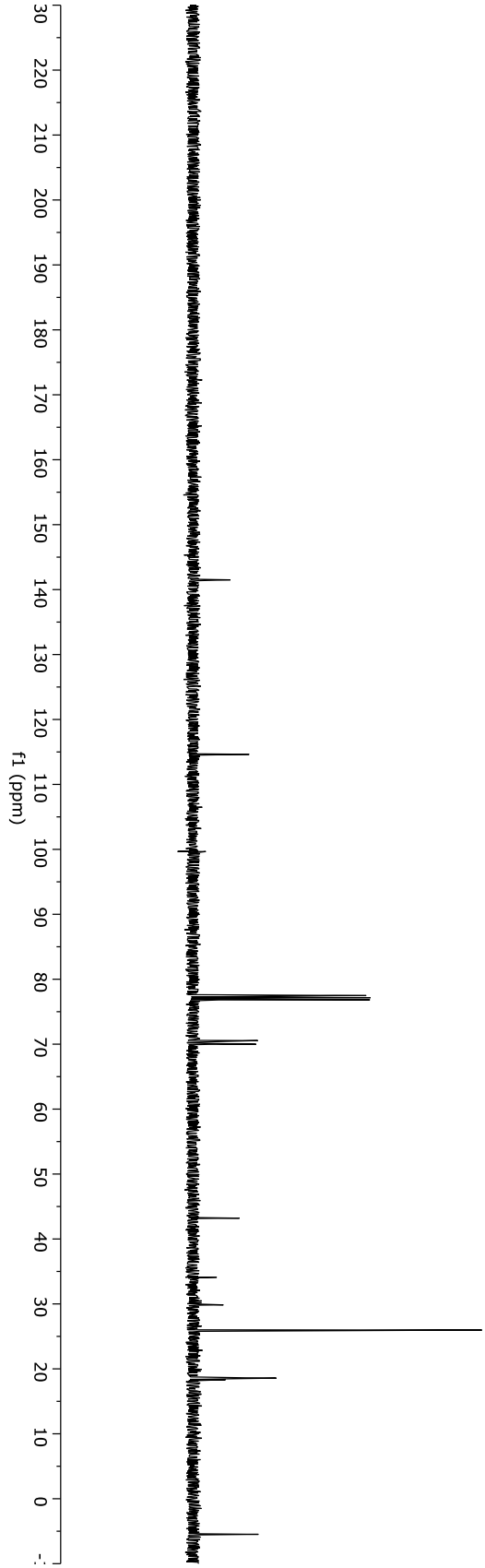
^{1}H (400 MHz, $CDCl_3$)



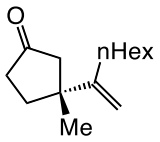


Scheme 22b

^{13}C (100 MHz, CDCl$_3$)

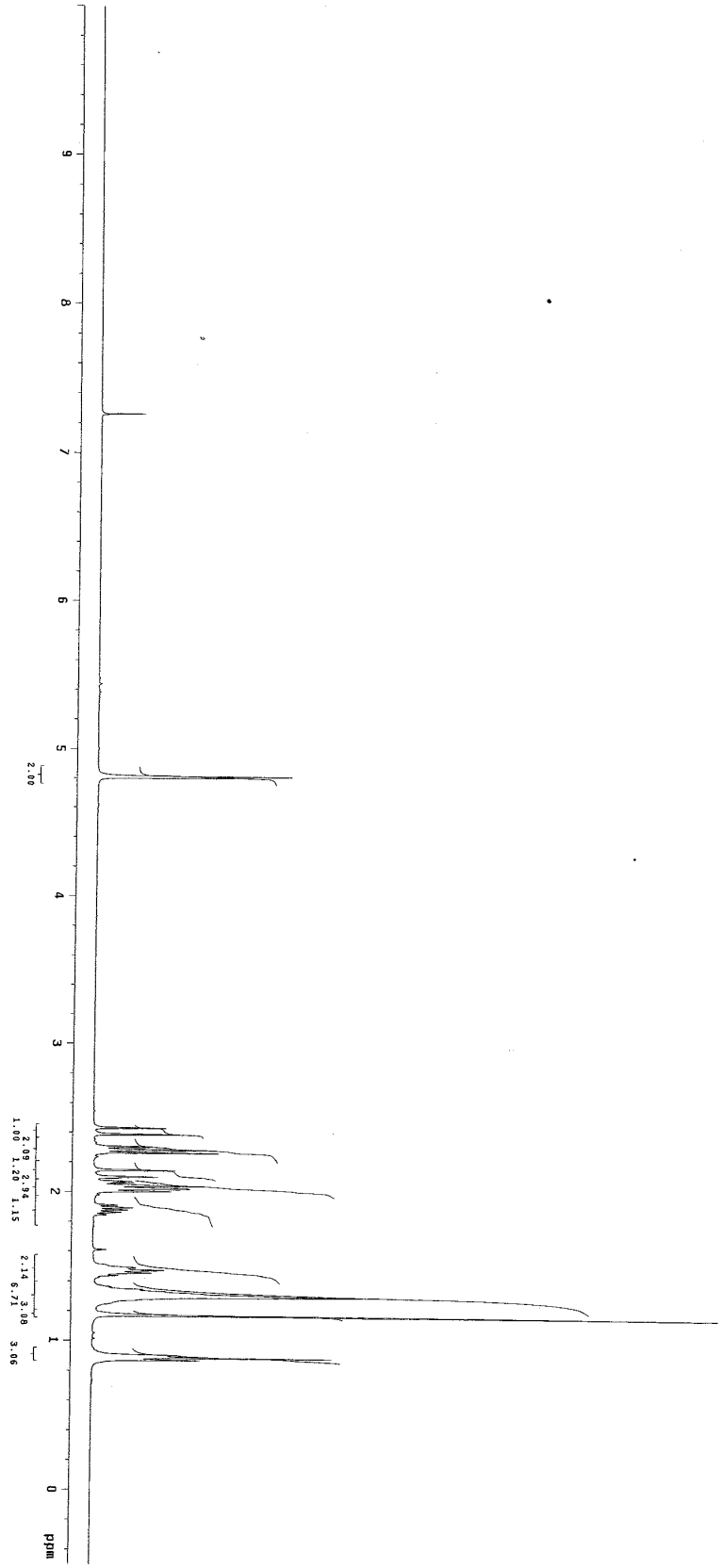


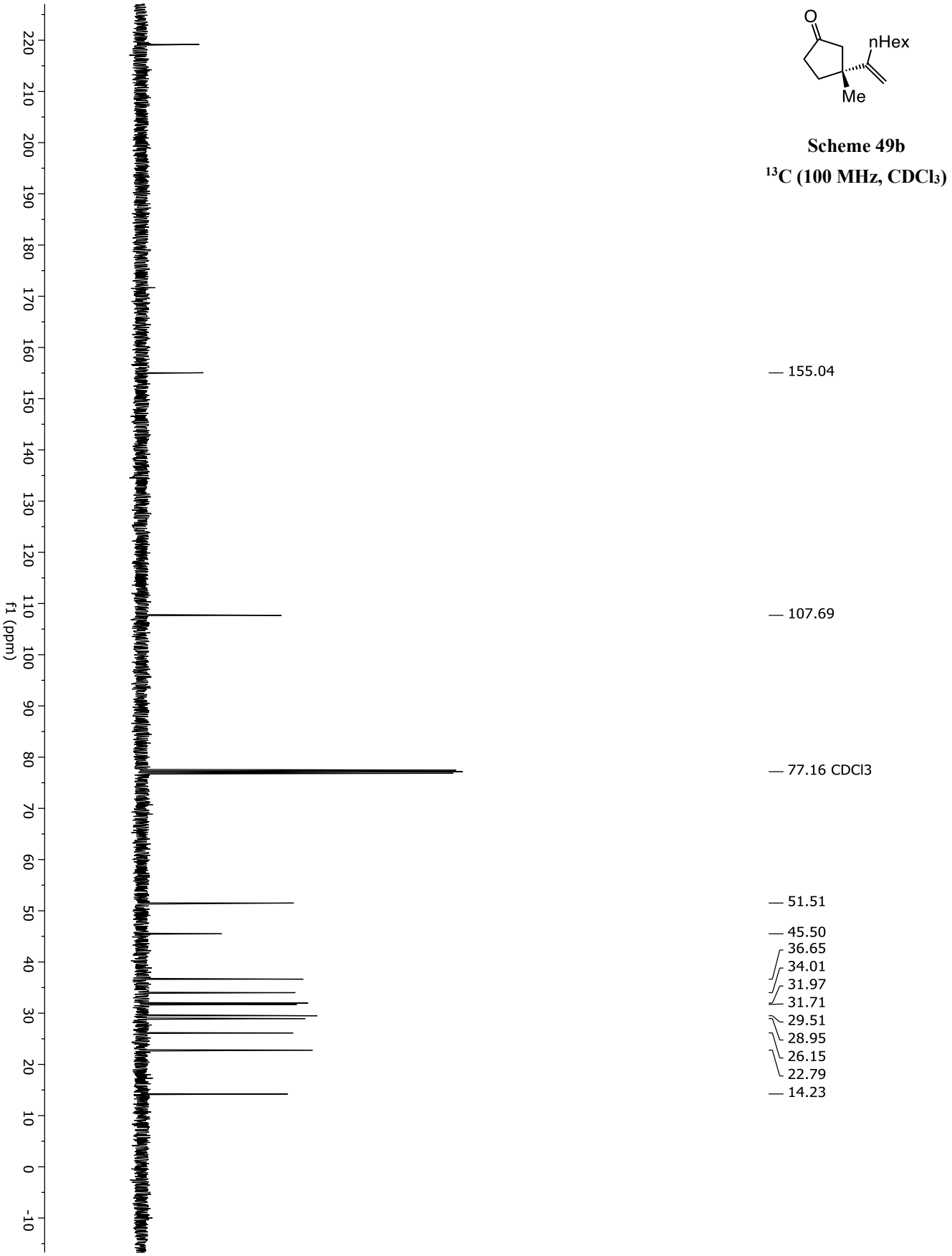
— 77.16 CDCl3



Scheme 49b

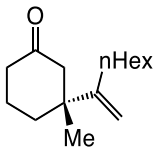
^{1}H (400 MHz, $CDCl_3$)





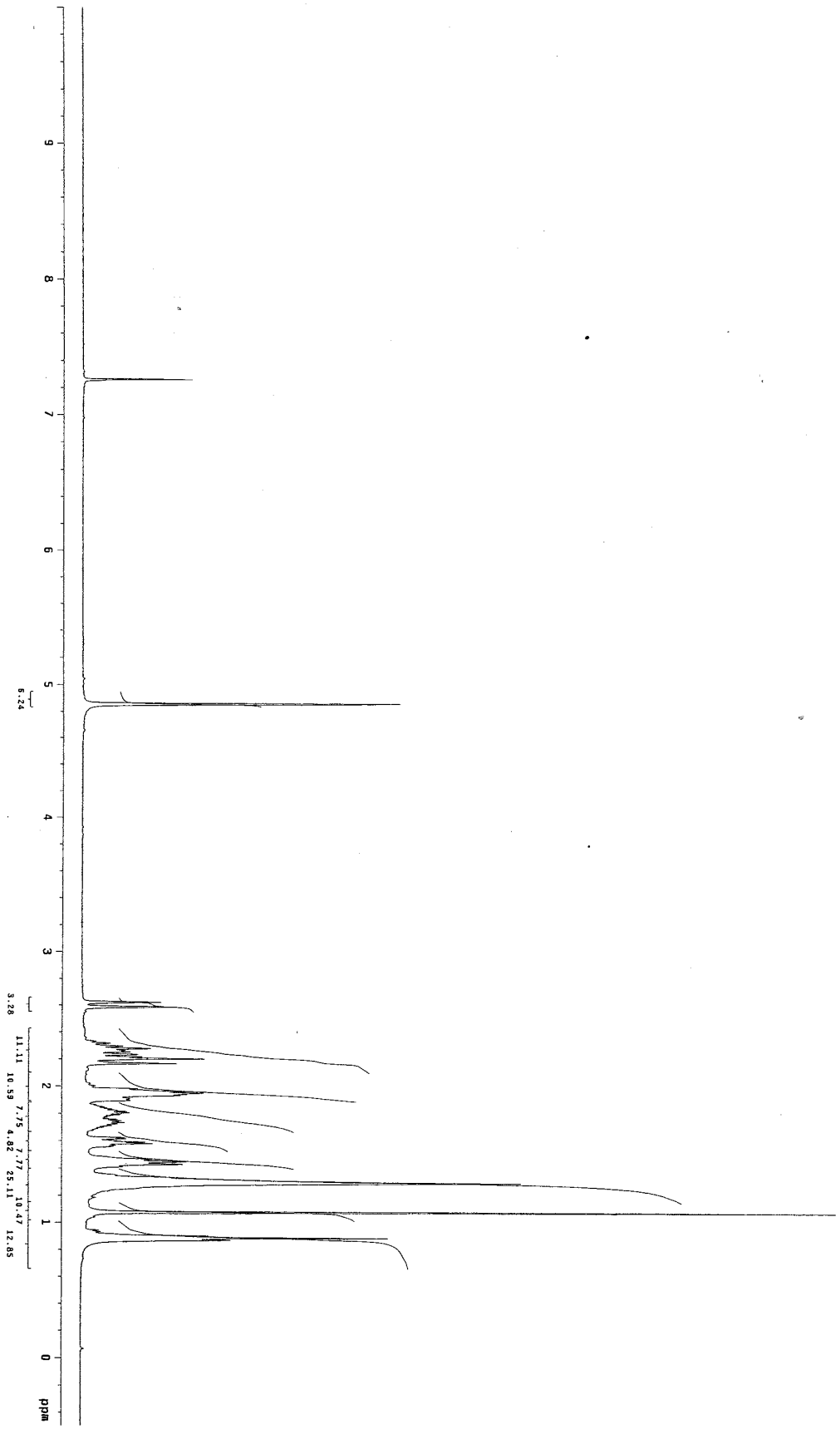
Scheme 49b

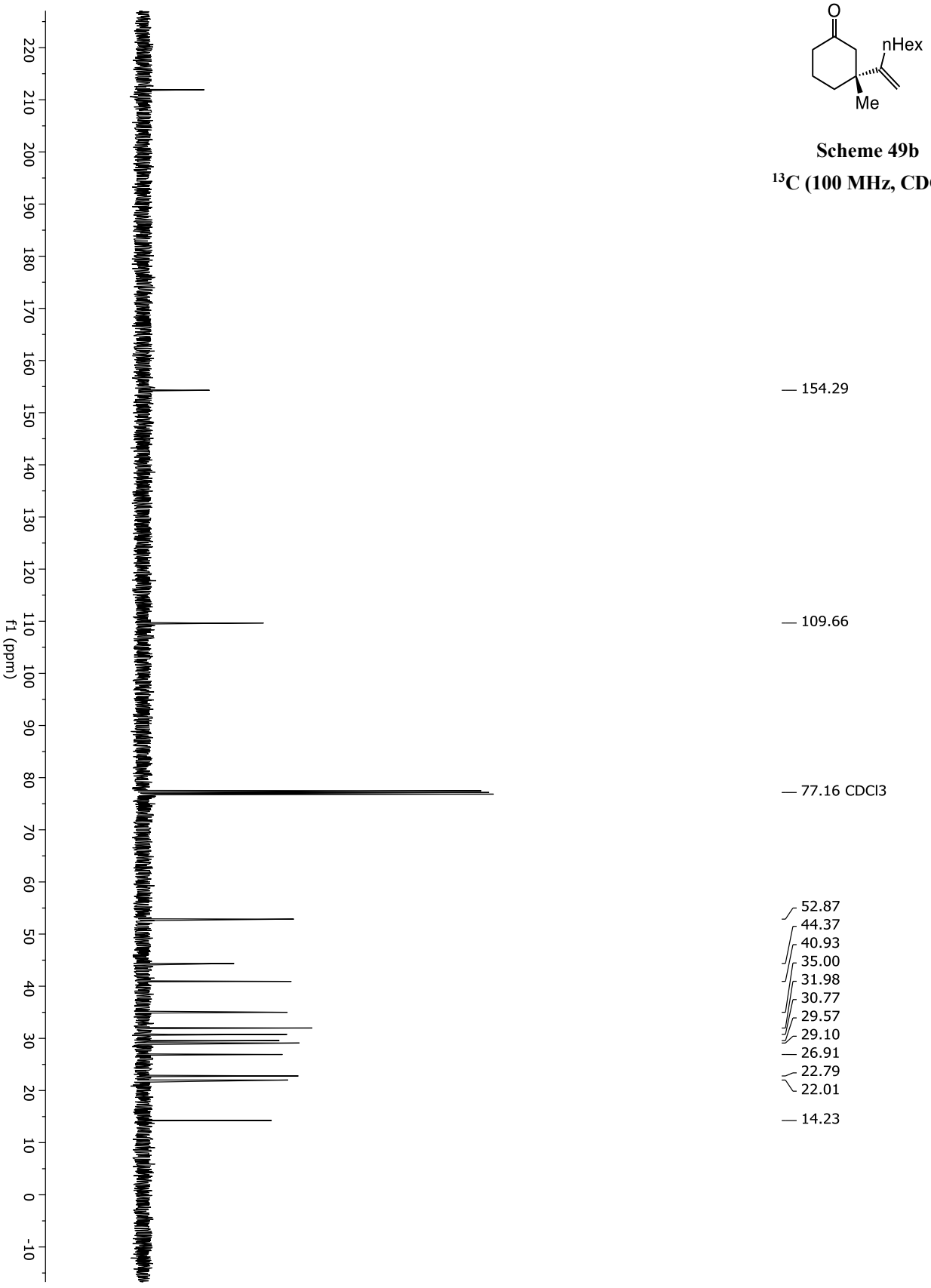
^{13}C (100 MHz, $CDCl_3$)



Scheme 49b

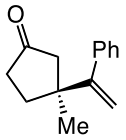
^{1}H (400 MHz, $CDCl_3$)





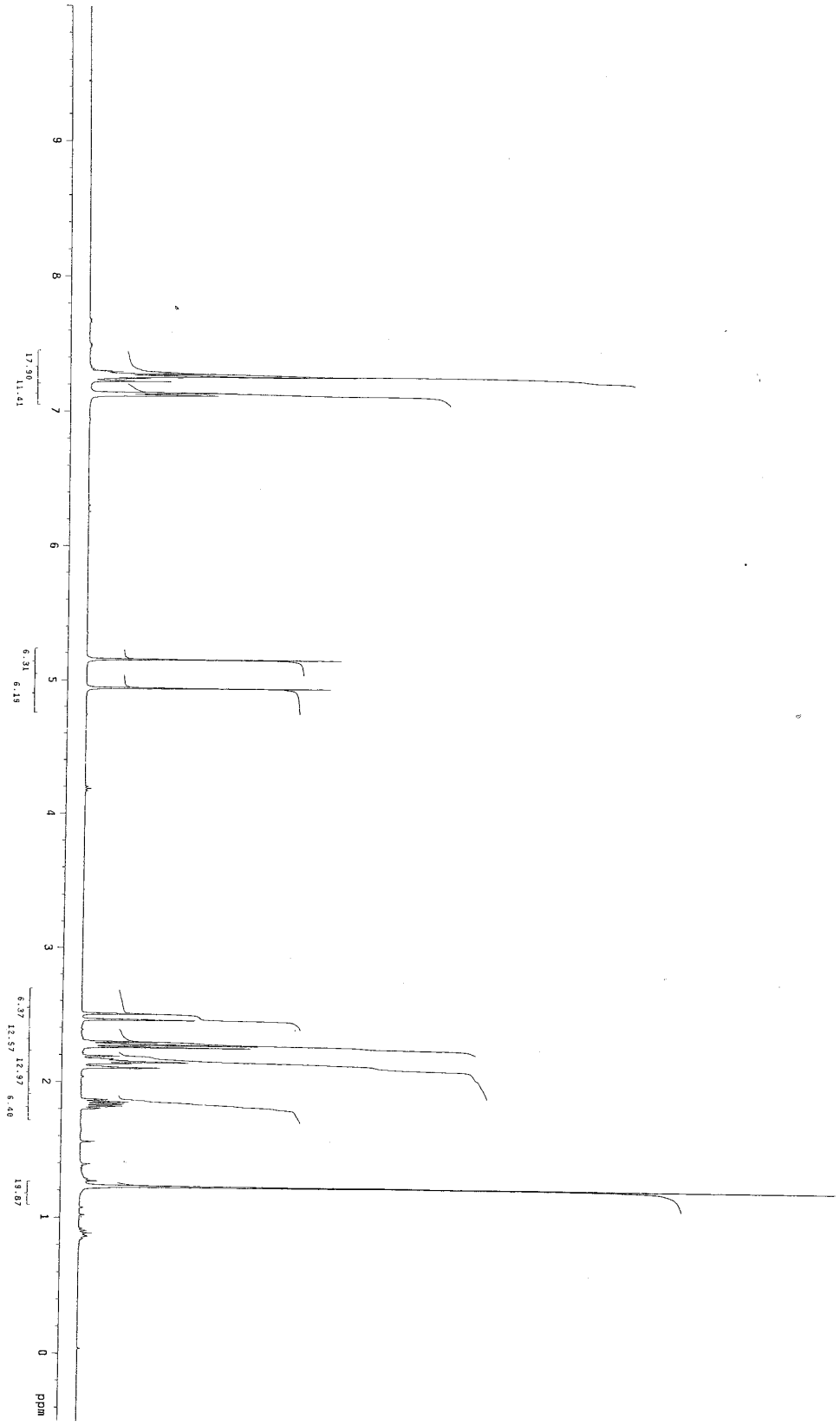
Scheme 49b

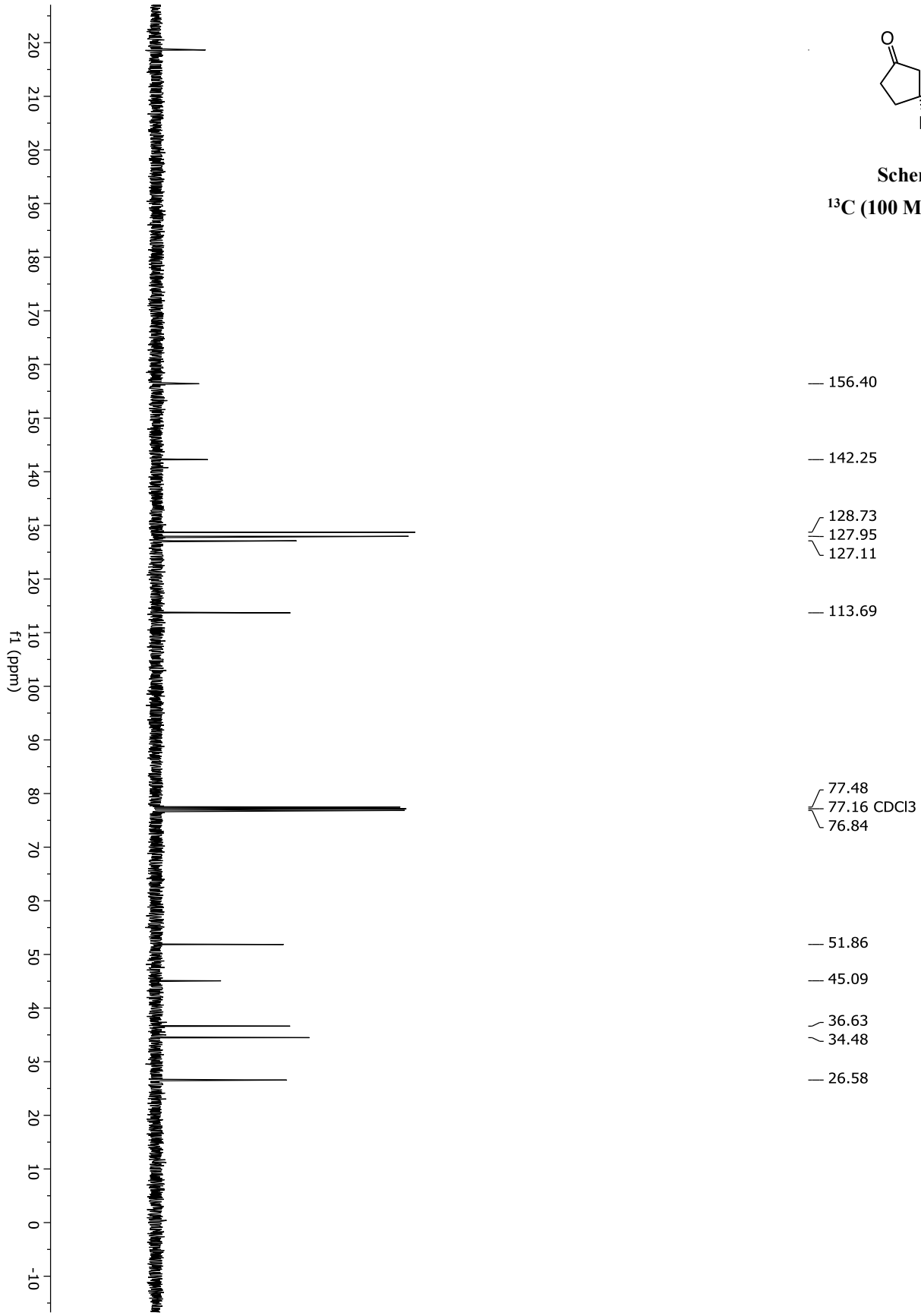
^{13}C (100 MHz, $CDCl_3$)

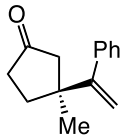


Scheme 50

^{1}H (400 MHz, $CDCl_3$)

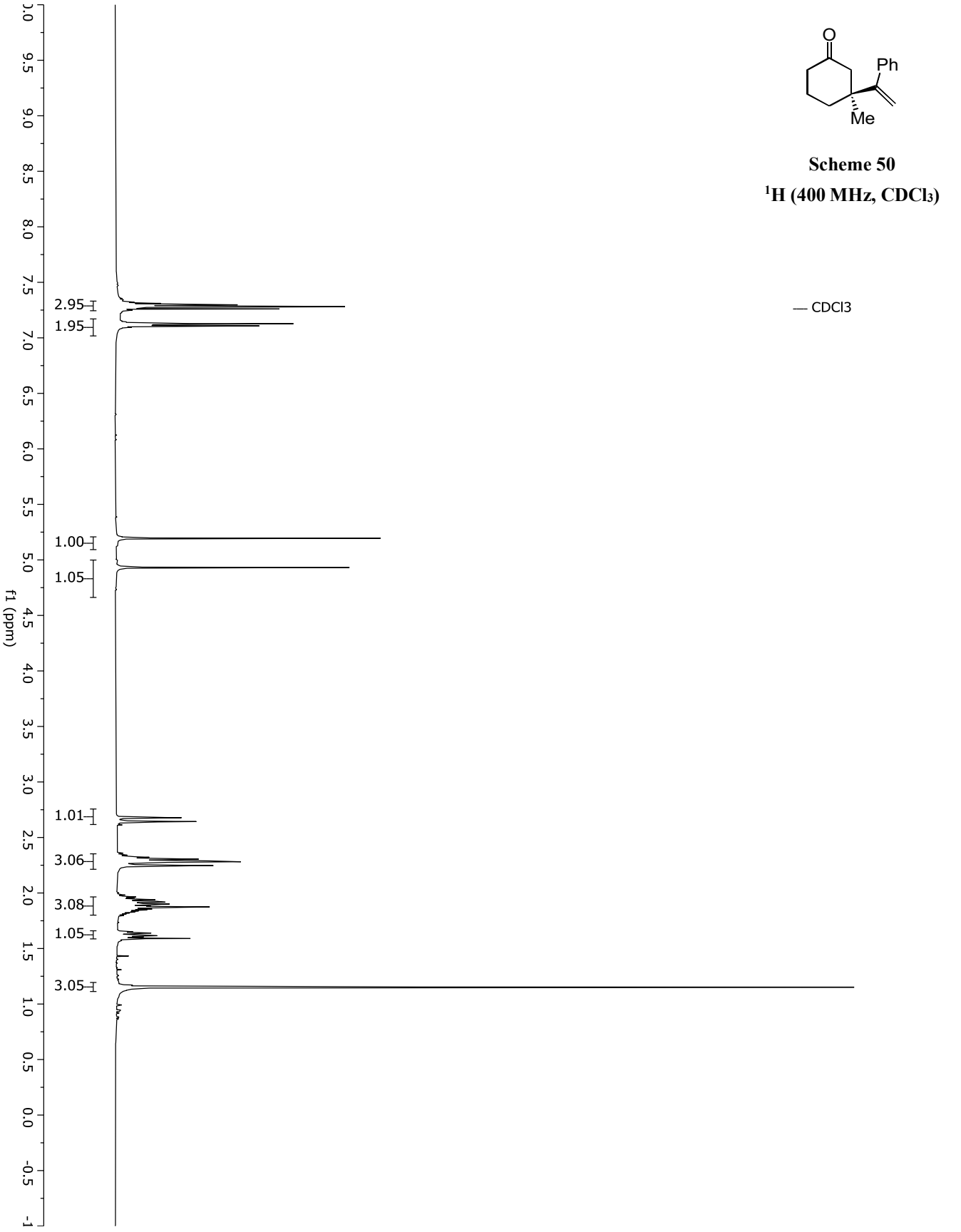






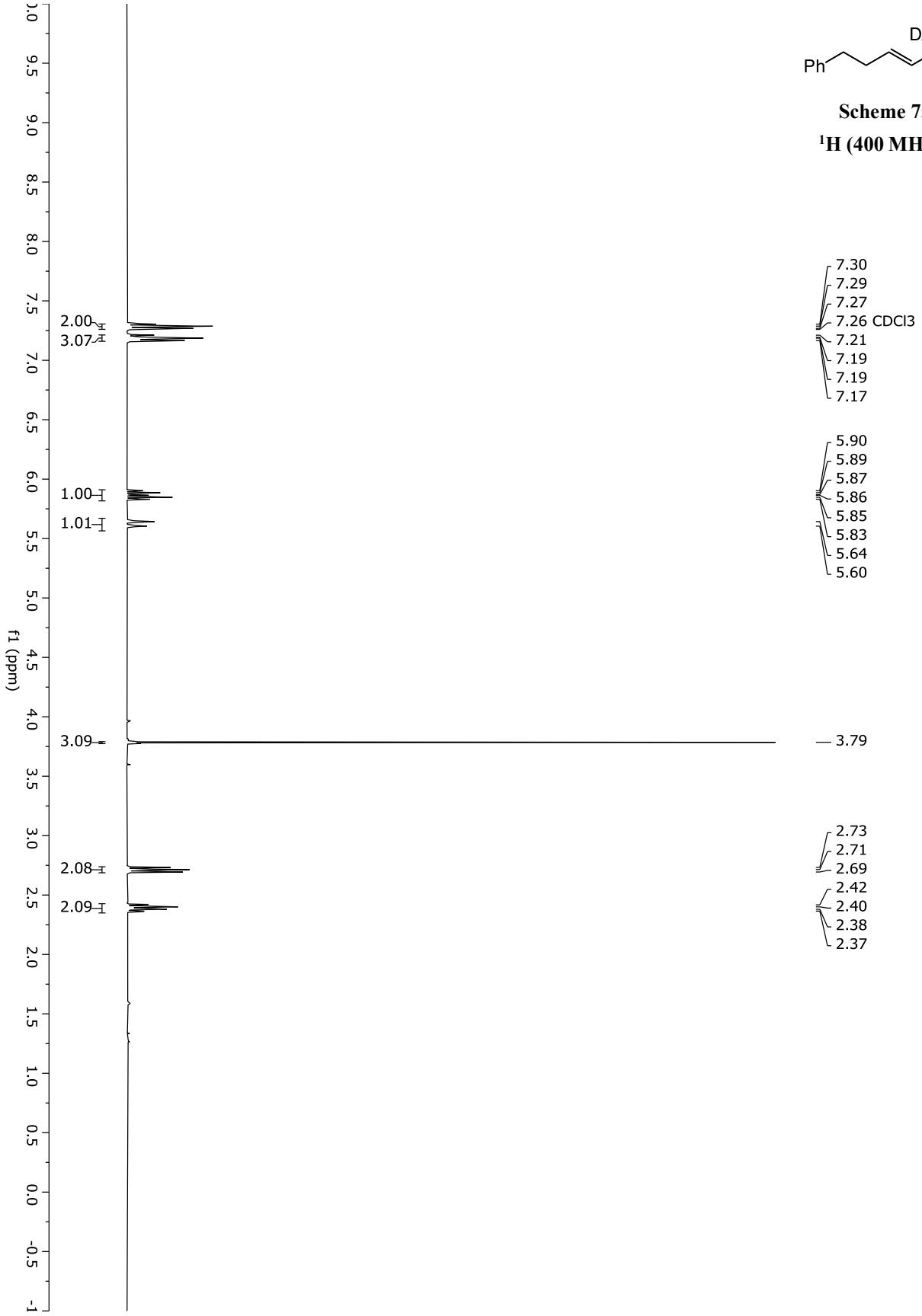
Scheme 50

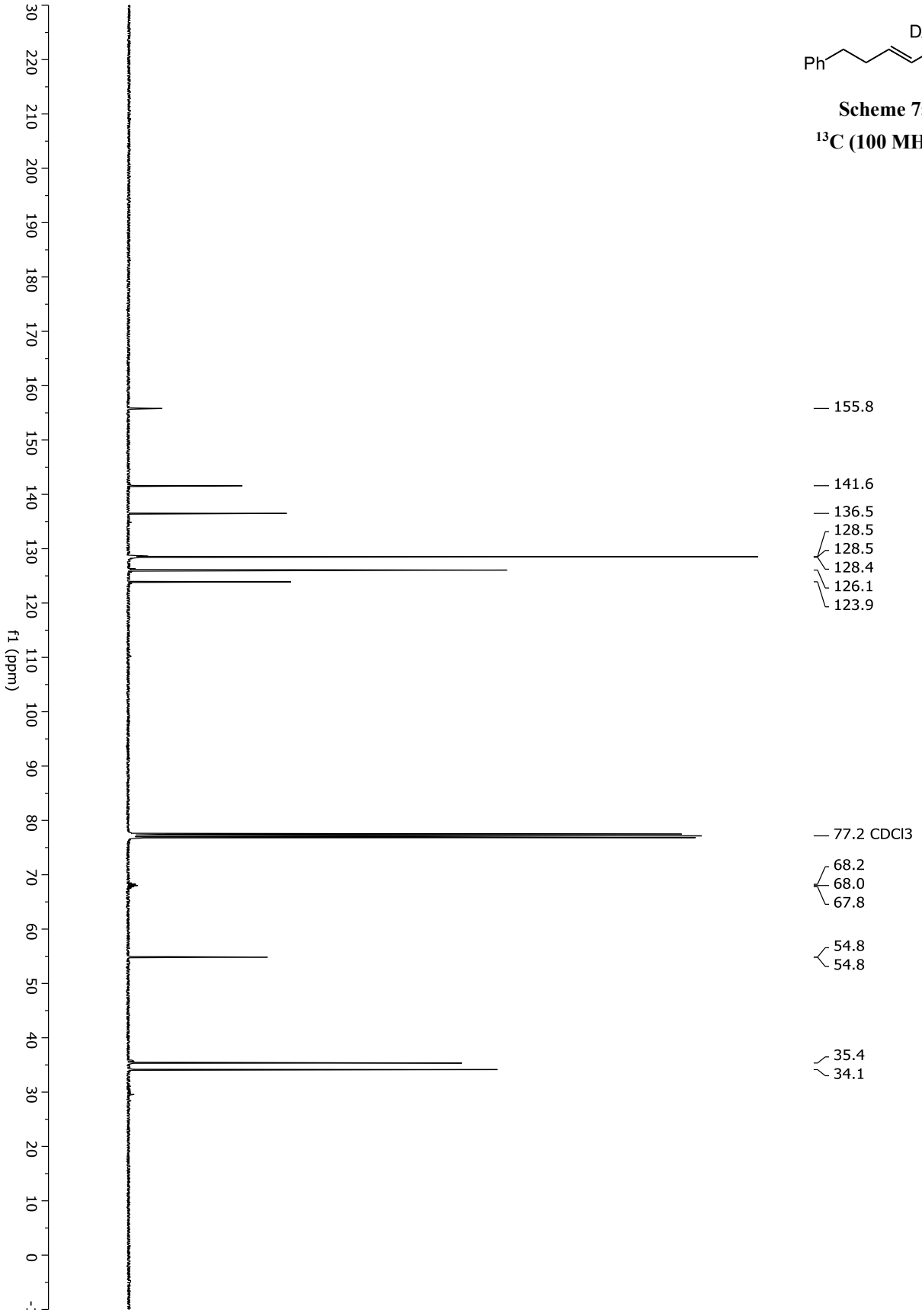
^{13}C (100 MHz, $CDCl_3$)



Scheme 50

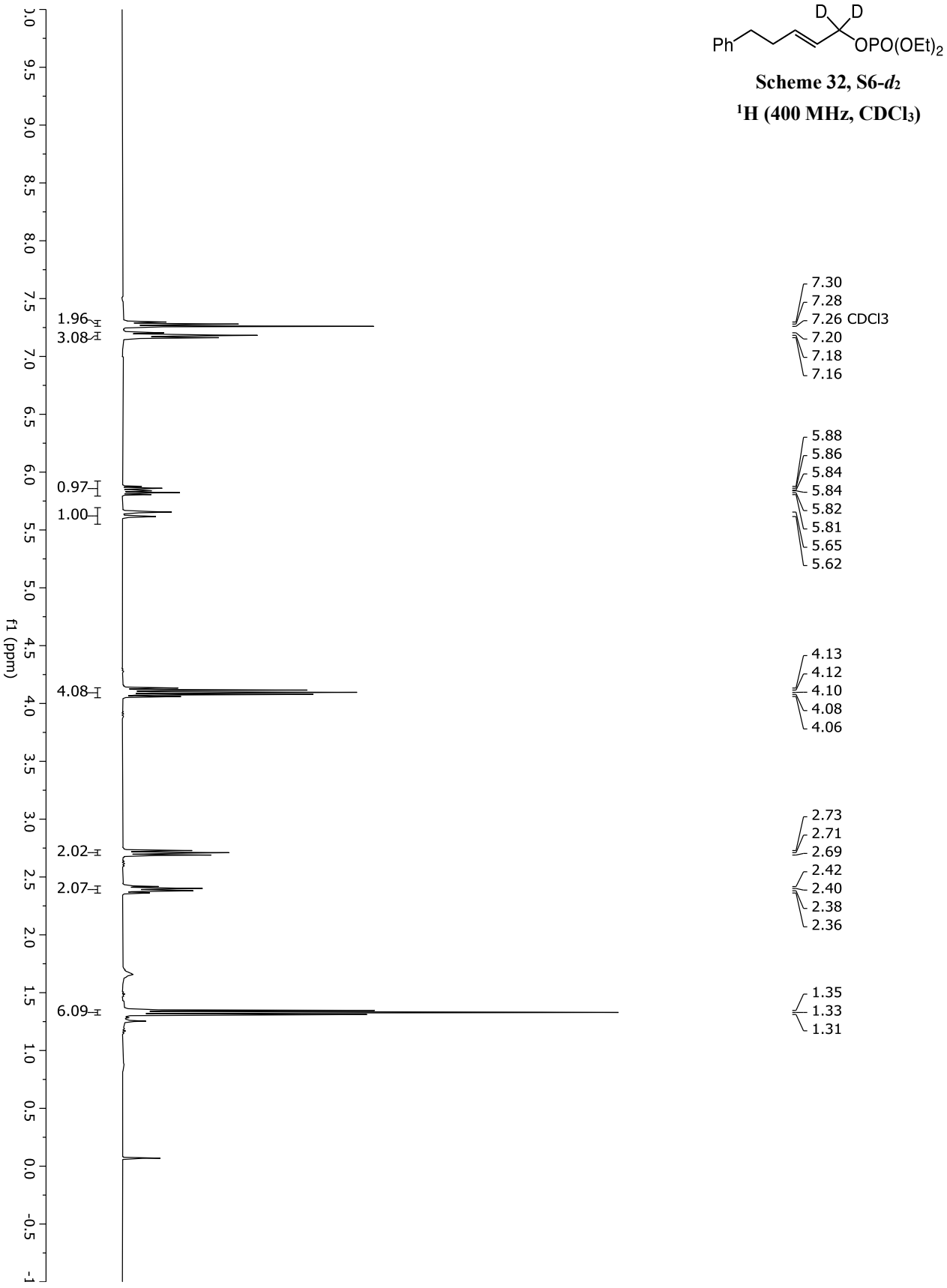
^{1}H (400 MHz, $CDCl_3$)


D
D
Ph
OCO2Me
Scheme 75, S4-d2
1H (400 MHz, CDCl3)
f1 (ppm)
2.00
3.07
1.00
1.01
3.09
2.08
2.09
7.30
7.29
7.27
7.26 CDCl3
7.21
7.19
7.19
7.17
5.90
5.89
5.87
5.86
5.85
5.83
5.64
5.60
3.79
2.73
2.71
2.69
2.42
2.40
2.38
2.37



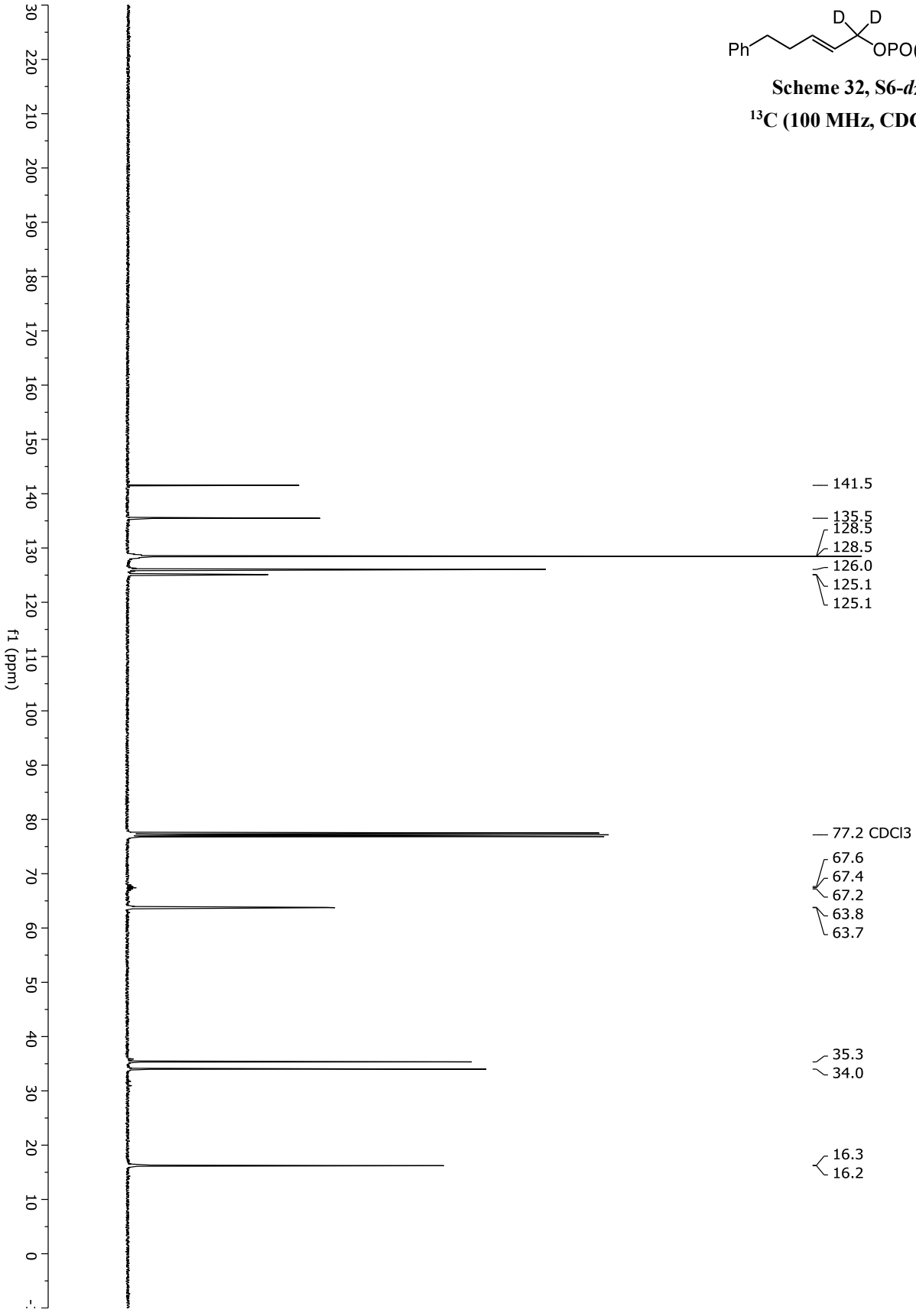
Scheme 75, S4-d_2

^{13}C (100 MHz, $CDCl_3$)



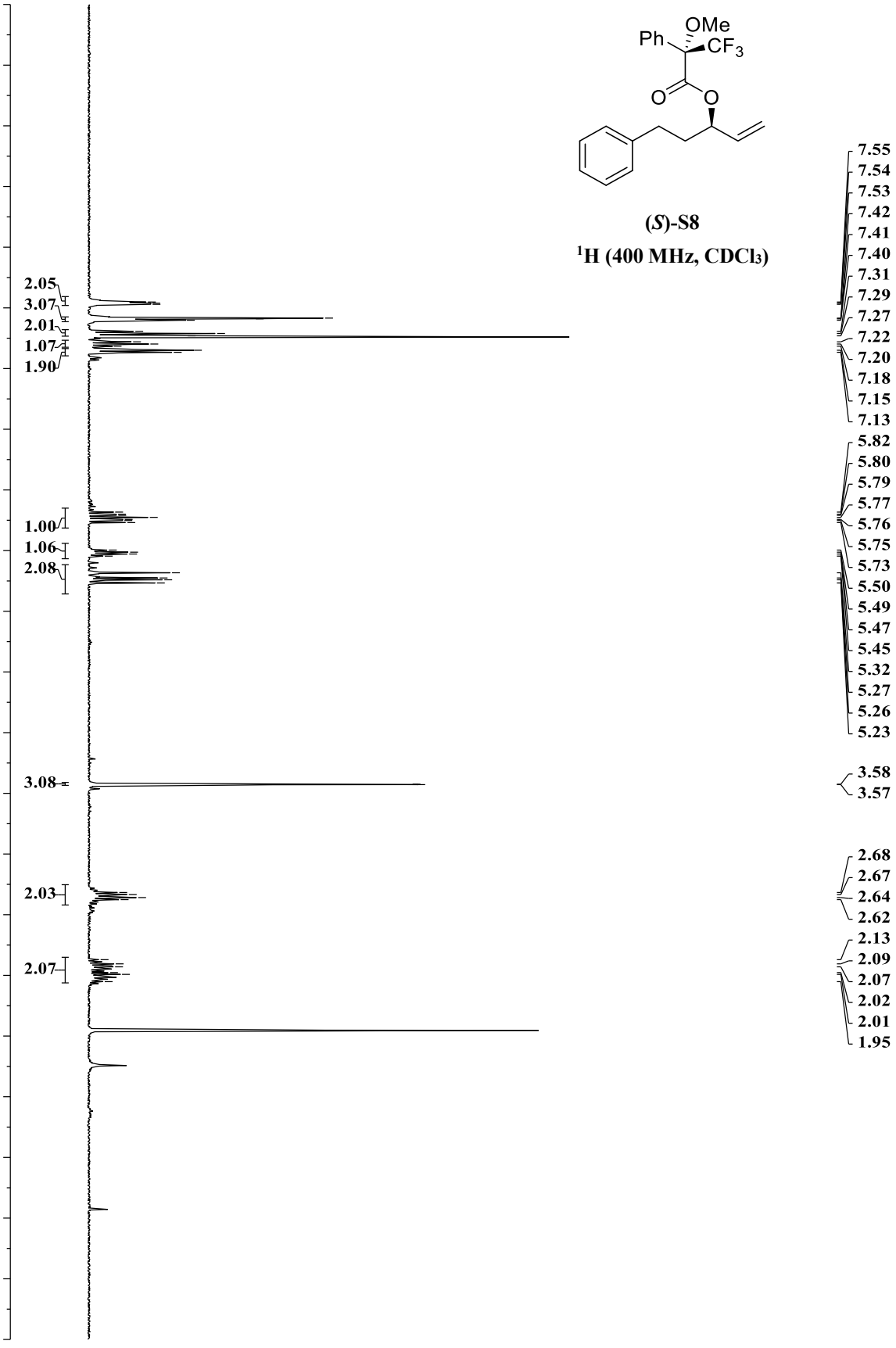
Scheme 32, S6-d_2

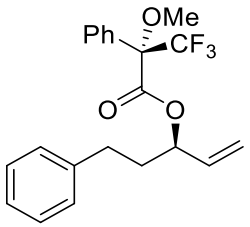
^{1}H (400 MHz, $CDCl_3$)



Scheme 32, S6-d_2

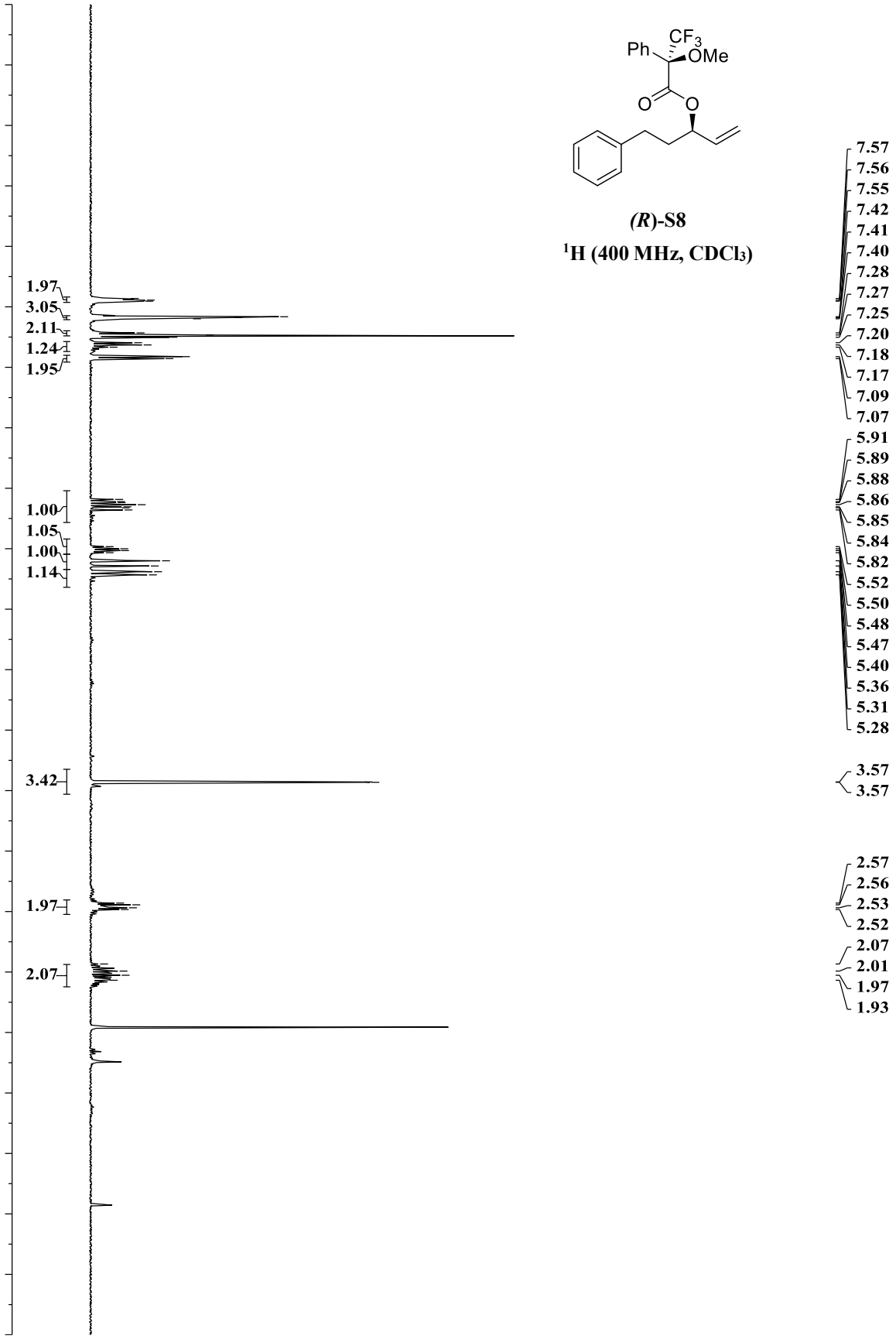
^{13}C (100 MHz, $CDCl_3$)

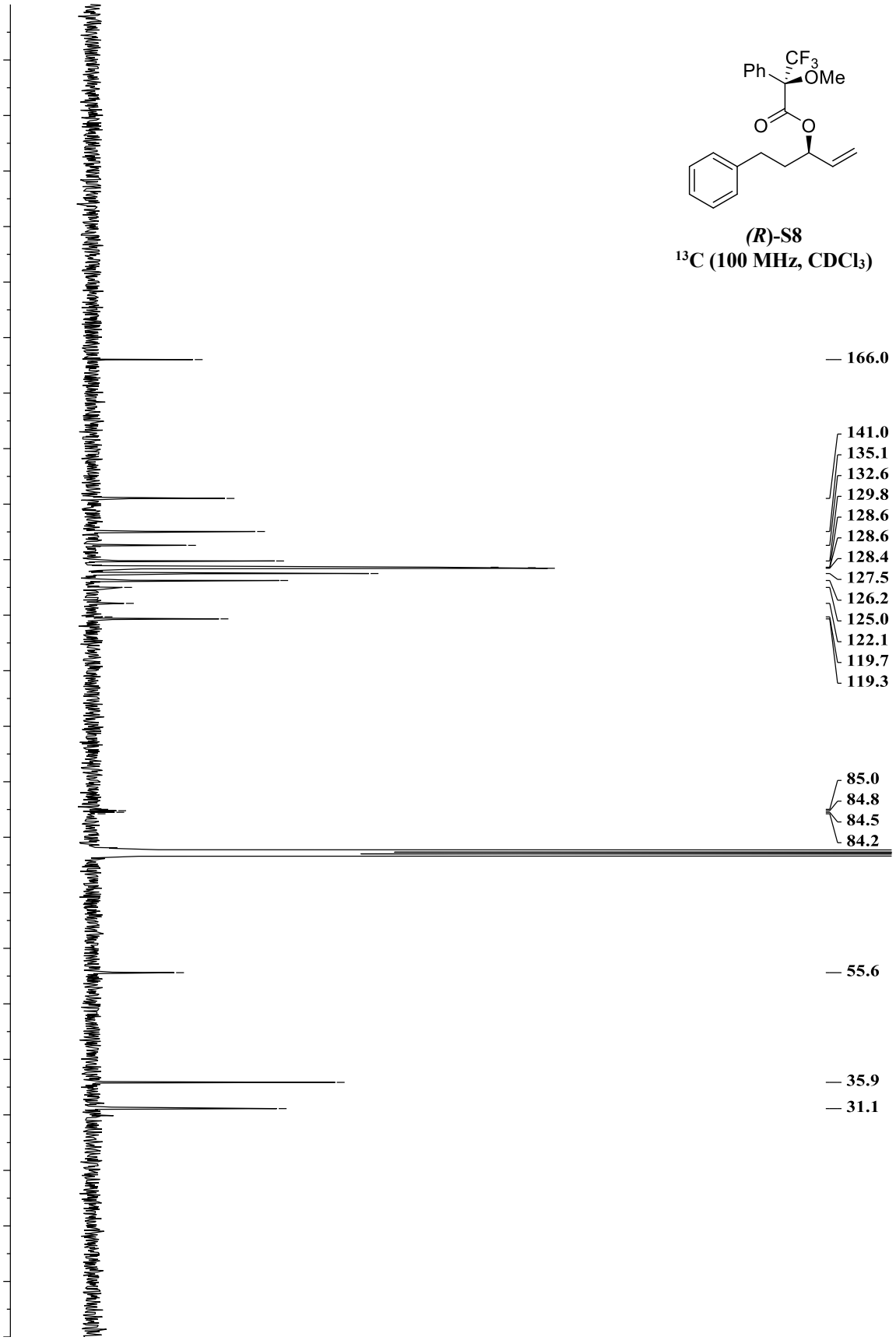

OMe
Ph
CF3
O
O
(S)-S8
1H (400 MHz, CDCl3)
2.05
3.07
2.01
1.07
1.90
1.00
1.06
2.08
3.08
2.03
2.07
7.55
7.54
7.53
7.42
7.41
7.40
7.31
7.29
7.27
7.22
7.20
7.18
7.15
7.13
5.82
5.80
5.79
5.77
5.76
5.75
5.73
5.50
5.49
5.47
5.45
5.32
5.27
5.26
5.23
3.58
3.57
2.68
2.67
2.64
2.62
2.13
2.09
2.07
2.02
2.01
1.95



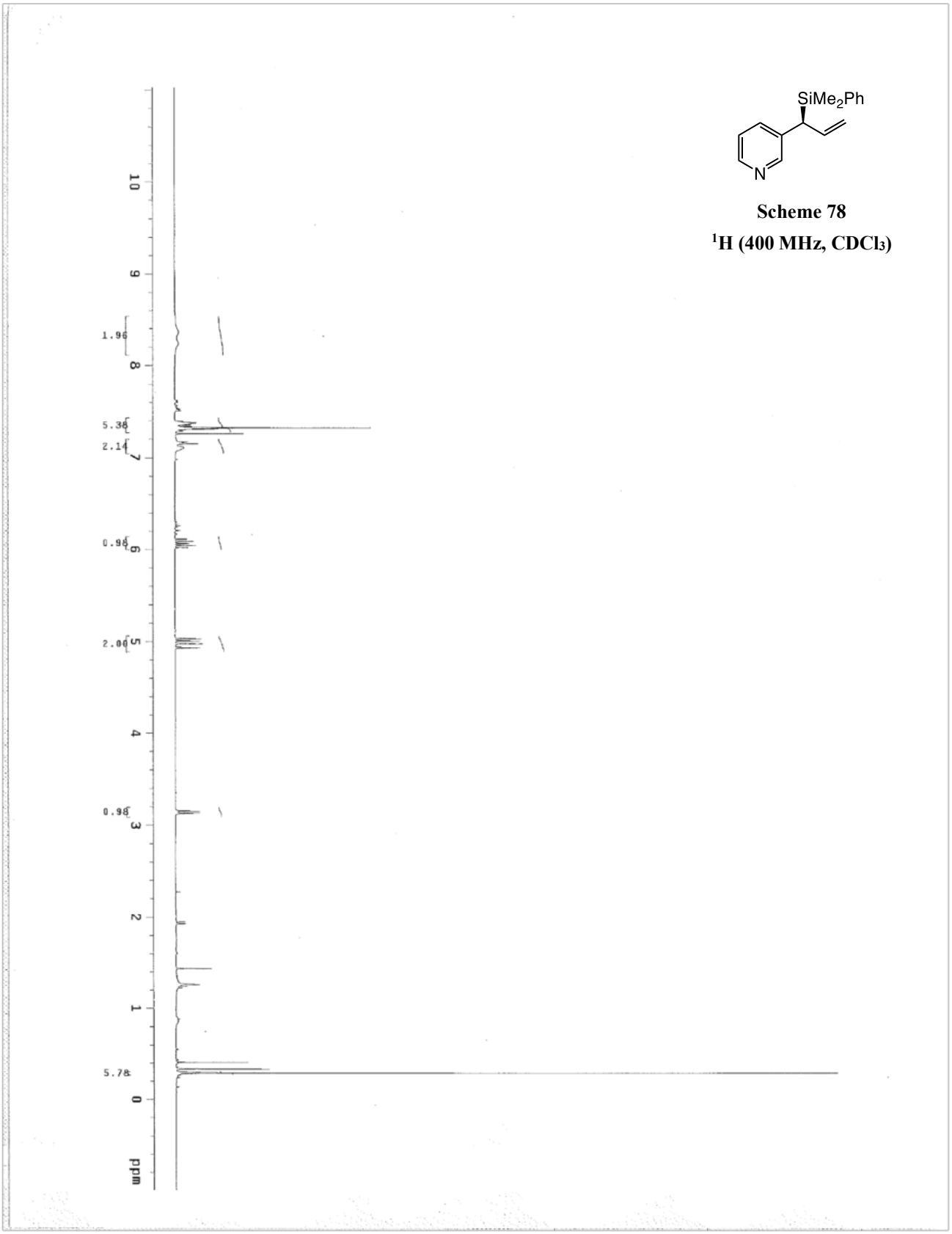
(*S*)-S8

^{13}C (100 MHz, $CDCl_3$)


Ph
CF3
OMe
O
O
(R)-S8
1H (400 MHz, CDCl3)
1.97
3.05
2.11
1.24
1.95
1.00
1.05
1.00
1.14
3.42
1.97
2.07
7.57
7.56
7.55
7.42
7.41
7.40
7.28
7.27
7.25
7.20
7.18
7.17
7.09
7.07
5.91
5.89
5.88
5.86
5.85
5.84
5.82
5.52
5.50
5.48
5.47
5.40
5.36
5.31
5.28
3.57
3.57
2.57
2.56
2.53
2.52
2.07
2.01
1.97
1.93

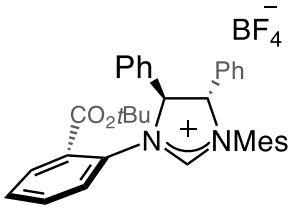


***(R)*-S8**
^{13}C (100 MHz, $CDCl_3$)



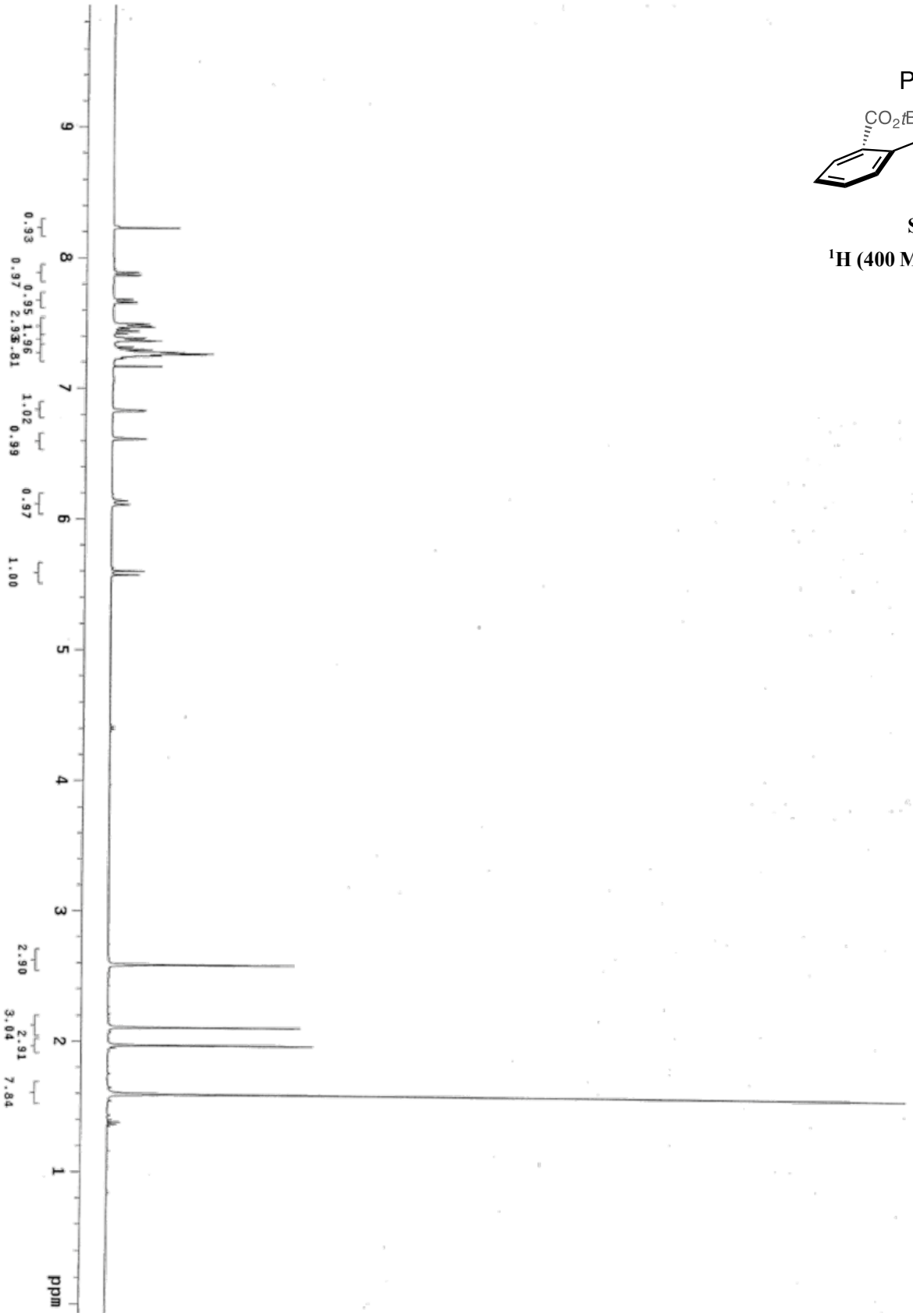
Scheme 78

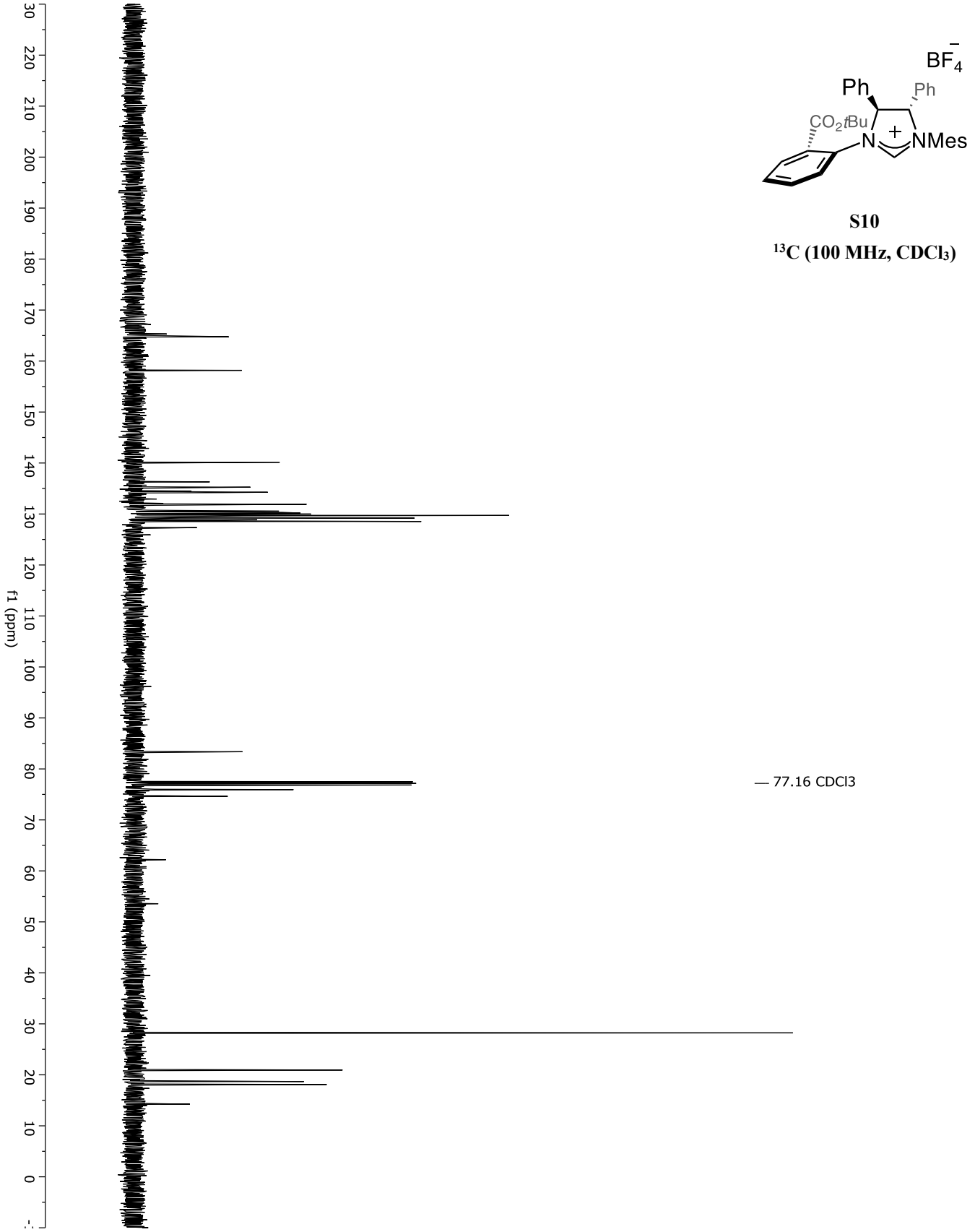
^{1}H (400 MHz, $CDCl_3$)



S10

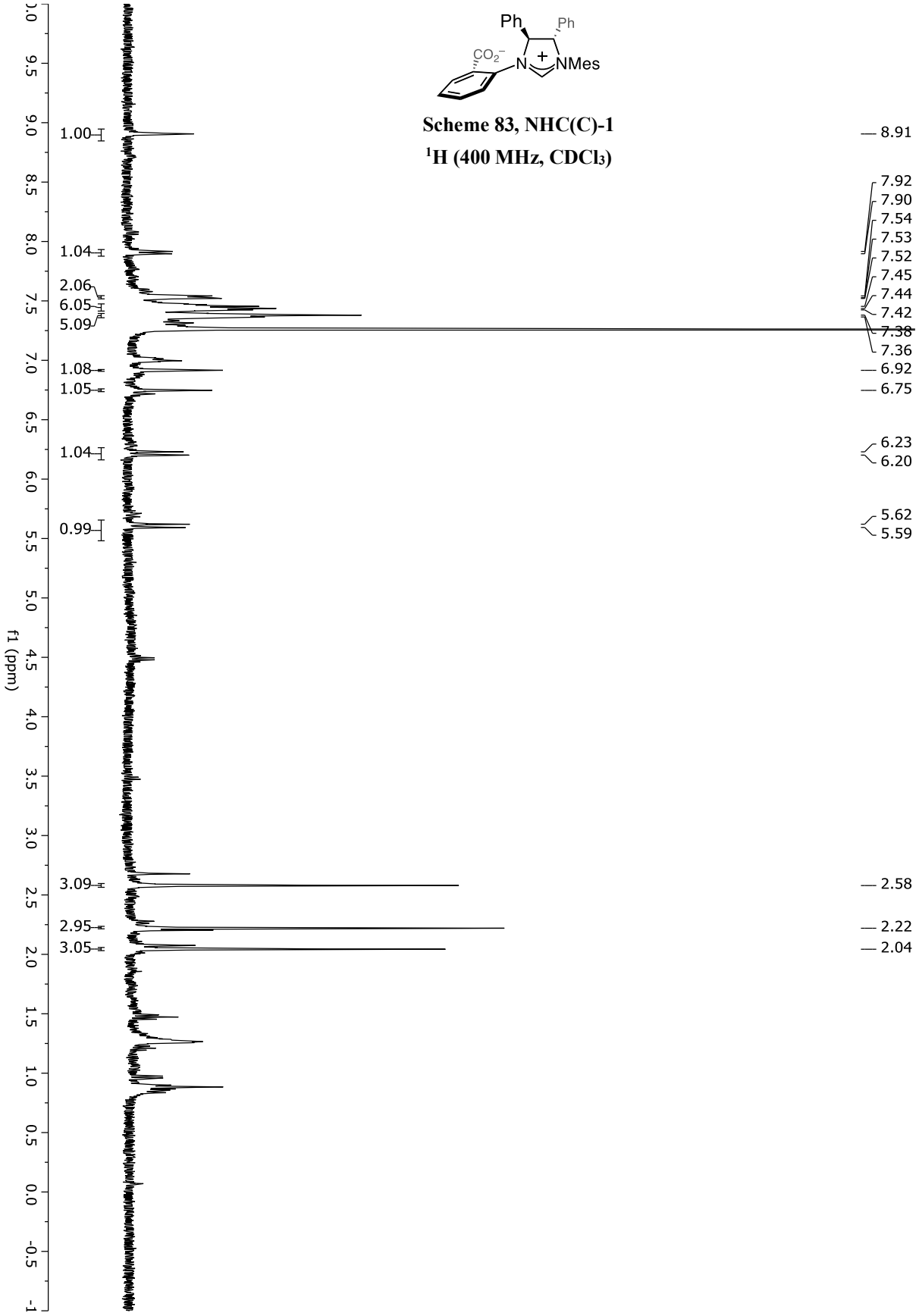
^{1}H (400 MHz, $CDCl_3$)





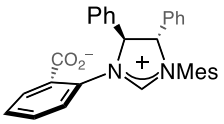
S10

^{13}C (100 MHz, $CDCl_3$)



Scheme 83, NHC(C)-1

^{1}H (400 MHz, $CDCl_3$)



Scheme 83, NHC(C)-1

^{13}C (100 MHz, $CDCl_3$)

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