Electronic Supplementary Material

P-Functionalized tetrathiafulvalenes from 1,3-dithiole-2-thiones?

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Experimental

All presented reactions, besides the oxidation with urea-H_2O_2 adduct, where performed using the standard Schlenk technique. tetrahydrofuran and diethylether where distilled over sodium wire/benzophenone. *n*-Pentane was distilled over sodium wire and dichloromethane over calciumhydride. Diphenylchlorophosphane was distilled prior to use and stored under an argon atmosphere. 1,3-Dithiole-2-thione was synthesized following the literature protocol.[1] All other chemicals where used as received. All NMR spectra were recorded on a Bruker Avance DMX-300 spectrometer, with a frequency of 300.1 MHz or ^{1}H, 75.5 MHz for ^{13}C and 121.5 MHz for ^{31}P. 85% H_3PO_4 was used as the external standard for ^{31}P spectra while ^{1}H and ^{13}C spectra were referenced to the residual protons of the deuterated solvents. Melting points were determined in one-side melted off capillaries using a Büchi Type S or a Carl Roth Type MPM-2 apparatus, they are uncorrected. Elemental analyses were carried out on a Vario EL gas chromatograph. Mass spectrometric data were collected on a Kratos MS 50 spectrometer using EI, 70 eV. The infrared spectra were recorded on a Nicolet 80 FT-IR spectrometer, using a diamond ATR. The X-ray analyses were performed on a Nonius Kappa CCD or a Bruker X8-KappaApex TT type diffractometer at 123(2) or 100(2) K, respectively. The structures were solved by the intrinsic phasing method implemented in Sheldrick's XT program system and refined anisotropically by the least-square procedure implemented in the SHELX program system.[2] Hydrogen atoms were included using a riding model on the bound carbon/oxygen atoms.CCDC 2001006 and 2001007 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre viawww.ccdc.cam.ac.uk/structures.

4-Diphenylphosphanyl-dithiole-2-thione (2)

LDA (792.8 mg, 7.40 mmol) was dissolved in 10 mL of dry Et_2O in a Schlenk flask and cooled to -80 °C. A solution of 1,3-dithiole-2-thione **1** (1.0 g, 7.45) in 10 mL dry Et_2O was added dropwise, the reaction mixture was stirred for 3h at this temperature and subsequently warmed to -40 °C. The reaction mixture was cooled again to -90 °C and Ph_2PCl (1.33 mL, 7.41 mmol) was added dropwise, the reaction mixture stirred overnight and warmed to ambient temperature. After removal of all volatiles *in vacuo* (8×10^{-3} mbar) the residue was taken up in dry dichloromethane and filtered over a 3G-frit having a Celite® and silica pad to remove the formed lithium chloride. The filtrate was collected and the solvent was removed *in vacuo* (8×10^{-3} mbar) and then dried. The residue was then re-crystallized from hot toluene, washed with *n*-pentane (10 mL) and dried *in vacuo* (8×10^{-3} mbar).

Yield: 1.24 g (3.89 mmol), 53 %, yellow solid, m.p. 91 °C. ^{1}H NMR (300.1 MHz, $CDCl_3$): δ = 7.17 (d, $^{3}J_{PH}$ = 7.6 Hz, 1H, C^5H), 7.39 – 7.45 (m, 10H, C_6H_5). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$): δ = 129.2 (d, J_{PC} = 7.3 Hz, C_6H_5), 130.1 (s), 133.3 (d, J_{PC} = 20.2 Hz, C_6H_5), 134.3 (d, J_{PC} = 9.4 Hz, C_6H_5), 135.8 (d, $^{2}J_{PC}$ = 32.8 Hz, C^5H), 145.3 (d, $^{1}J_{PC}$ = 44.7 Hz, C^4), 215.9 (b, C=S). $^{31}P\{^{1}H\}$ NMR (121.5 MHz, $CDCl_3$): δ = -12.1. MS (EI, 70 eV): m/z (%) =318 (100) [M]+, 242 (18) $[M\text{-}C_6H_4]^+$, 209 (16) $[C_9H_6PS_2]^+$, 132.9 (18) $[C_3S_3H]^+$; HR-MS: found = 317.9763, calc. = 317.9760; IR (ATR, $\tilde{\nu}$ {cm^{-1}}): $\tilde{\nu}$ = 3054 (w, v(C-H)), 1582 (m, v(C=C)), 1476 (m), 1436 (m), 1430 (m), 1196 (m), 1092 (m), 1054 (s, v(C=S)), 1021 (s), 912 (m), 876 (m), 807 (m), 700 (s), 694 (s). Elemental analysis for $C_{15}H_{11}PS_3$: found: C 56.86, H 3.58, S 30.18.Calc.: C 56.58, H 3.48, S 30.21.

4,5-Bis(diphenylphosphanyl)-dithiole-2-thione (3)

LDA (480 mg, 4.48 mmol) was dissolved in 6 mL of dry Et_2O in a Schlenk flask and cooled to -80 °C. A solution of 1,3-dithiole-2-thione **1** (300 mg, 2.24 mmol) in 5 mL dry Et_2O was added dropwise, the reaction mixture was stirred for 3 h at this temperature and subsequently warmed to -40 °C. The reaction mixture was cooled again to -90 °C and the phosphine (Ph_2PCl) (0.8 mL, 4.48 mmol) was added dropwise, the reaction mixture was stirred overnight and warmed to ambient temperature. After removal of all volatiles *in vacuo* (8×10^{-3} mbar) the residue was taken up in dry dichloromethane and filtered over a 3G-frit having a Celite® and silica pad to remove the formed lithium chloride. The filtrate was collected and the solvent was removed *in vacuo* (8×10^{-3} mbar) and then dried. The residue was recrystallized from hot toluene, washed with *n*-pentane (10 mL) and dried *in vacuo* (8×10^{-3} mbar).

Yield: 448 mg (0.89 mmol), 40 %, yellow crystals, m.p. 193 °C. ^{1}H NMR (300.1 MHz, $CDCl_3$): δ = 7.27 - 7.43 (m, C_6H_5). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ = 129.0 (d, J_{PC} = 3.7 Hz, C_6H_5), 129.0 (d, J_{PC} = 3.8 Hz, C_6H_5), 129.9 (s), 133.4 (d, J_{PC} = 10.5 Hz, C_6H_5), 133.5 (d, J_{PC} = 10.4 Hz, C_6H_5), 134.5 (d, J_{PC}= 3.1 Hz, ipso-C_6H_5), 134.5 (d, J_{PC} = 3.0 Hz, ipso-C_6H_5), 152.1 (dd, $^2J_{PC}$ = 4.2 Hz, $^1J_{PC}$ = 7.5 Hz, C^4), 216.7 (t, $^3J_{PC}$ = 2.9 Hz, C=S).$^{31}P\{^1H\}$ NMR (121.5 MHz, $CDCl_3$): δ = -18.6. MS (EI, 70 eV): m/z (%) = 502 (17) $[M]^+$, 426 (100) $[M\text{-}C_6H_4]^+$, 318 (18) $[C_{15}H_{11}PS_3]$; HR-MS: found = 502.0201, calc. = 502.0202; IR (ATR, $\tilde{\nu}$ {cm^{-1}}): $\tilde{\nu}$ = 3046 (w, ν(C-H)), 1580 (m, ν(C=C)), 1478 (m), 1445 (m), 1432 (m), 1058 (s, ν(C=S)), 1038 (m), 1025 (m), 798 (w), 750 (w), 736 (s), 689 (s). Elemental analysis for $C_{27}H_{20}P_2S_3$: found: C 64.38, H 4.15, S 18.90. Calc.: C 64.53, H 4.01, S 19.14.

Single crystals of compound **3**, suitable for an X-ray diffraction study, were obtained from a solution in CH_2Cl_2 via slow solvent evaporation at room temperature (Figure 4). Data were collected with a Bruker D8-Venture diffractometer equipped with a low-temperature device at 123 K by using graphite-monochromated Cu Kα radiation (λ = 1.54178 Å). The structure was solved by Patterson methods (SHELXS-97) and refined by full-matrix least squares on F2 (SHELXL-97): $C_{27}H_{20}P_2S_3$, Mr = 502.55, crystal dimension 0.24 × 0.18 × 0.14 mm^3, triclinic, Space group $P\bar{1}$, Z = 2, a = 10.7418(4) Å, b = 11.1986(4) Å, c = 11.7876(5) Å, α = 62.450(2)°, β = 75.279(2)°, γ = 88.851(2)°, V = 1208.03(8) $Å^3$, ρ_{calc} = 1.382 g/cm^3, μ = 4.157 mm^{-1}, transmission factors (min/max) 0.3748/0.7536, R_{int} = 0.0740, R_1 (for I >2σ(I)) = 0.0408, wR_2 (for all data) = 0.1142, final R_1 = 0.0452, goodness of fit 1.035, ΔF (max/min) = 0.39/-0.51 e $Å^{-3}$.

4-Diphenylphosphanoyl-dithiole-2-thione (6)

4-Diphenylphosphanyl-dithiole-2-thione **2** (500 mg, 1.57mmol) was dissolved in 10 mL CH_2Cl_2 in a Schlenk flask, then H_2O_2-urea (148 mg, 1.57 mmol) was added at ambient temperature and the reaction mixture was stirred for 5 h. Then the reaction mixture was filtered to remove unreacted urea. The solvent was removed *in vacuo* (8×10^{-3} mbar) and the obtained product was washed with *n*-pentane (5 mL) and dried *in vacuo* (8×10^{-3} mbar). A white yellow powder was obtained.

Yield: 430 mg (1.29mmol), 82 %, yellow powder, m.p. 157 °C. ^{1}H NMR (300.1 MHz, $CDCl_3$): δ = 7.48 - 7.80 (m, C_6H_5, C^5H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ = 129.2 (d, J_{PC} = 13.0 Hz, C_6H_5), 130.1 (d, $^1J_{PC}$ = 111.0 Hz, C_6H_5), 131.8 (d, J_{PC} = 10.7 Hz, C_6H_5), 133.4 (d, J_{PC} = 2.9 Hz, C_6H_5), 139.5 (d, $^2J_{PC}$ = 7.2 Hz, C^5H), 140.0 (d, $^1J_{PC}$ = 89.3 Hz, C^4), 213.2 (d, $^3J_{PC}$ = 6.4 Hz, C=S). $^{31}P\{^1H\}$ NMR (121.5 MHz, $CDCl_3$): δ = 18.1.MS (EI, 70 eV): m/z (%) = 334 (32) $[M]^+$, 258 (100) $[M\text{-}CS_2]^+$; HR-MS: found = 333.9707, calc. = 333.9710. IR (ATR, $\tilde{\nu}$ {cm^{-1}}): $\tilde{\nu}$ = 3050 (w, ν(C-H), 1588 (w, ν(C=C)), 1193 (m,

ν(P=O)), 1064 (s, ν(C=S)), 1025 (w), 962 (m), 748 (s), 727 (s), 703 (s), 693 (s), 662 (m). Elemental analysis for $C_{15}H_{11}OPS_3$: found: C 53.57 , H 3.31, S 28.30.Calc.: C 53.88, H 3.32, S 28.76.

Single crystals of compound **6**, suitable for an X-ray diffraction study, were obtained from a solution in CH_2Cl_2 via slow solvent evaporation at room temperature (Figure 5). Data were collected with a STOE IPDS-2T diffractometer equipped with a low-temperature device at 123 K by using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structure was solved by Patterson methods (SHELXS-97) and refined by full-matrix least squares on F2 (SHELXL-97): $C_{15}H_{11}OPS_3$, M_r = 334.39, crystal dimension 0.3 × 0.25 × 0.2 mm^3, monoclinic, Space group $P2_1/c$, Z = 4, a = 8.9993(5) Å, b = 21.0026(9) Å, c = 9.2456(5) Å, α = 90°, β = 118.641(4)°, γ = 90°, V = 1533.67(15)$Å^3$, ρ_{calc} = 1.448 g/cm^3, μ = 0.578 mm^{-1}, transmission factors (min/max) 0.8079/0.9306, R_{int} = 0.0261, R_1 (for I >2σ(I)) = 0.0267, wR_2 (for all data) = 0.0677, final R_1 = 0.0381, goodness of fit 0.940, ΔF (max/min) = 0.37/-0.39 e $Å^{-3}$.

4,5-Bis(diphenylphosphanoyl)-dithiole-2-thione (7)

In a Schlenk flask 4,5-bis(diphenylphosphanyl)-dithiole-2-thione **3** (500 mg, 0.99 mmol) was dissolved in 10 mL CH_2Cl_2, then H_2O_2-urea (187 mg, 1.98 mmol) was added at ambient temperature and the reaction mixture was stirred for 48 h. Then the reaction mixture was filtered to remove unreacted urea. The solvent was removed *in vacuo* (8 × 10^{-3} mbar) and the obtained product was washed with *n*-pentane (5 mL) and dried *in vacuo* (8 × 10^{-3} mbar). A yellow powder was obtained (still containing some residual grease and solvents).

Yield: 463 mg (0.87 mmol), 87 %, yellow powder, m.p. 128 °C. ^{1}H NMR (300.1 MHz, $CDCl_3$): δ = 7.32 - 7.73 (m, C_6H_5). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ = 128.6 - 128.8 (m, C_6H_5), 130.4 (d, $^1J_{PC}$ = 112.2 Hz, C_6H_5), 131.9 - 132.1 (m, C_6H_5), 133.2 (s, C_6H_5), 149.6 (dd, $^2J_{PC}$ = 5.3 Hz, $^1J_{PC}$= 83.2 Hz, C^4), 211.1 (t, $^3J_{PC}$ = 7.0 Hz, C=S). $^{31}P\{^1H\}$ NMR (121.5 MHz, $CDCl_3$): δ = 19.8. MS (EI, 70 eV): m/z (%) = 534 (32) $[M]^+$, 457 (40) $[M-C_6H_5]^+$, 76.1 (100) $[CS_2]^+$; HR-MS: found = 534.0100, calc. = 534.0101. IR (ATR, $\tilde{\nu}$ {cm^{-1}}): $\tilde{\nu}$ = 3052 (w, (ν(C-H)), 1588 (w, ν(C=C)), 1210 (m, ν(P=O)), 1098(w), 1061 (s, ν(C=S)), 1027 (m), 995 (m), 982 (m), 723 (s), 686 (s). Elemental analysis for $C_{27}H_{20}O_2P_2S_3$: found: C 59.78, H 3.77, S 17.76. Calc.: C 60.66, H 3.77, S 17.99.

4-Diphenylthiophosphanoyl-dithiole-2-thione (8)

In a Schlenk flask 4-diphenylphosphanyl-dithiole-2-thione **2** (500 mg, 1.57mmol) was dissolved in 10 mL toluene, then sulfur (50.3 mg, 1.57 mmol) was added and the reaction mixture was heated at 110 °C for 5 h. The solvent was removed *in vacuo* (8 ×10^{-3} mbar), the product was washed with *n*-pentane (5 mL) and dried *in vacuo* (8 × 10^{-3} mbar); a yellow powder was thus obtained.

Yield: 468 mg (1.34 mmol), 85 %, yellow powder. ^{1}H NMR (300.1 MHz, $CDCl_3$): δ = 7.47 - 7.86 (m, C_6H_5), 7.65 (d, $^3J_{PH}$ = 12.7 Hz, 1H, C^5H),. $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ = 129.2 (d, J_{PC} = 13.3 Hz, C_6H_5), 130.9 (d, $^1J_{PC}$= 90.1 Hz, ipso-C_6H_5),131.9 (d, J_{PC} = 11.5, C_6H_5), 132.9 (d, J_{PC} = 3.1 Hz, C_6H_5), 139.9 (d, $^2J_{PC}$ = 8.9 Hz, C^5H), 140.4 (d, $^1J_{PC}$ = 69.8 Hz, C^4), 213.6 (d, $^3J_{PC}$ = 5.8 Hz, C=S). $^{31}P\{^1H\}$ NMR (121.5 MHz, $CDCl_3$): δ = 32.9. MS (APCI): m/z (%) = 351 (100) $[M]^+$; HR-MS: found = 350.9561, calc. = 350.9554. IR (ATR, $\tilde{\nu}$ {cm^{-1}}): $\tilde{\nu}$ = 3049 (w, ν(C-H)), 1493 (w, ν(C=C)), 1097 (m), 1055 (s,

ν(C=S)), 1025 (m), 800 (m), 745 (m), 713 (s), 686 (s, ν(P=S)), 669 (m). Elemental analysis for $C_{15}H_{11}PS_4$: found: C 51.23, H 3.02, S 36.39.Calc.: C 51.41, H 3.16, S 36.59.

4,5-Bis(diphenylthiophosphanoyl)-dithiole-2-thione (9)

In a Schlenk flask 4,5-bis(diphenylphosphanyl)-dithiole-2-thione **3** (500 mg, 0.99 mmol) was dissolved in 10 mL toluene, then sulfur (63.8 mg, 1.99 mmol) was added and the reaction mixture was heated at 110 °C for 48 h. The solvent was removed *in vacuo* (8×10^{-3} mbar), the product was washed with *n*-pentane (5 mL) and dried *in vacuo* (8×10^{-3} mbar); a yellow powder was thus obtained (still containing some residual grease and solvents).

Yield: 467 mg (0.82 mmol), 83 %, yellow powder, m.p. 161 °C – 165 °C. ^{1}H NMR (300.1 MHz, $CDCl_3$): δ = 7.13 - 7.83 (m, C_6H_5). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$): δ = 128.6-128.9 (m, C_6H_5), 132.2-132.4 (m, C_6H_5), 132.3 (dd, $^{1}J_{PC}$ = 91.3 Hz, $^{4}J_{PC}$ = 1.3 Hz, ipso-C_6H_5), 132.8 (dd, $^{4}J_{PC}$ = 1.3 Hz, para-C_6H_5), 147.5 (dd, $^{1}J_{PC}$ = 62.7 Hz, $^{2}J_{PC}$ = 3.5 Hz, $C^{4/5}$), 209.0 (t, $^{3}J_{PC}$ = 7.1 Hz, C=S). $^{31}P\{^{1}H\}$ NMR (121.5 MHz, $CDCl_3$): δ = 33.0. MS (APCI): m/z (%) = 567 (100) $[M]^+$, 489 (90) $[M\text{-}C_6H_5]^+$, 457 (35) [M-C_6H_5-S]+; HR-MS: found = 566.9727, calc. = 566.9717. IR (ATR, $\tilde{\nu}$ {cm^{-1}}): $\tilde{\nu}$ = 3054 (w, ν(C-H)), 1478 (w, ν(C=C)), 1074 (s, ν(C=S)), 740 (m), 728 (s), 707 (m), 686 (s, ν(P=S)), 657 (m), 651 (m). Elemental analysis for $C_{27}H_{20}P_2S_5$: found: C 58.28, H 3.80, S 27.17.Calc.: C 57.23, H 3.56, S 28.29.

Tetrakis(diphenylphosphanyl)tetrathiofulvalene (II)

In a Schlenk tube 4,5-bis(diphenylphosphanyl)-dithiole-2-thione **3** (400 mg, 0.8 mmol) where desolved in 2mL THF and $P(OEt)_3$ (0,275 mL, 1.6 mmol) was added dropwise. The reaction mixture was heated at 60 °C for two weeks, while an orange precipitate was formed. The reaction mixture was cooled to 0 °C and the orange precipitate was filtered off. The filter residue was washed with 3 mL *n*-pentane and dried in vacuo. The product was thus obtained as orange powder.

Yield: 200 mg (0.21 mmol), 53 %, orange powder, m.p. 250 °C. ^{1}H NMR (300.1 MHz, $CDCl_3$): δ = 7.23 – 7.41 (m, C_6H_5). $^{13}C\{^{1}H\}$ NMR (75.5 MHz, $CDCl_3$): δ= 110.5 (t, $^{3}J_{PC}$ = 1.3 Hz, C^{2}), 128.6 (d, J_{PC} = 3.6 Hz, C_6H_5), 128.6 (d, J_{PC} = 3.6 Hz, C_6H_5), 129.3 (s, C_6H_5), 133.4 (d, J_{PC} = 10.3 Hz, C_6H_5), 133.5 (d, J_{PC} = 10.3 Hz, C_6H_5), 135.3 (d, J_{PC} = 2.8 Hz, C_6H_5), 135.3 (d, J_{PC} = 2.9 Hz, C_6H_5), 142.9 (dd, $^{1}J_{PC}$ = 3.8 Hz, $^{2}J_{PC}$ = 0.9 Hz, C^{4}). $^{31}P\{^{1}H\}$ NMR (121.5 MHz, $CDCl_3$): δ = -18.8 (s).

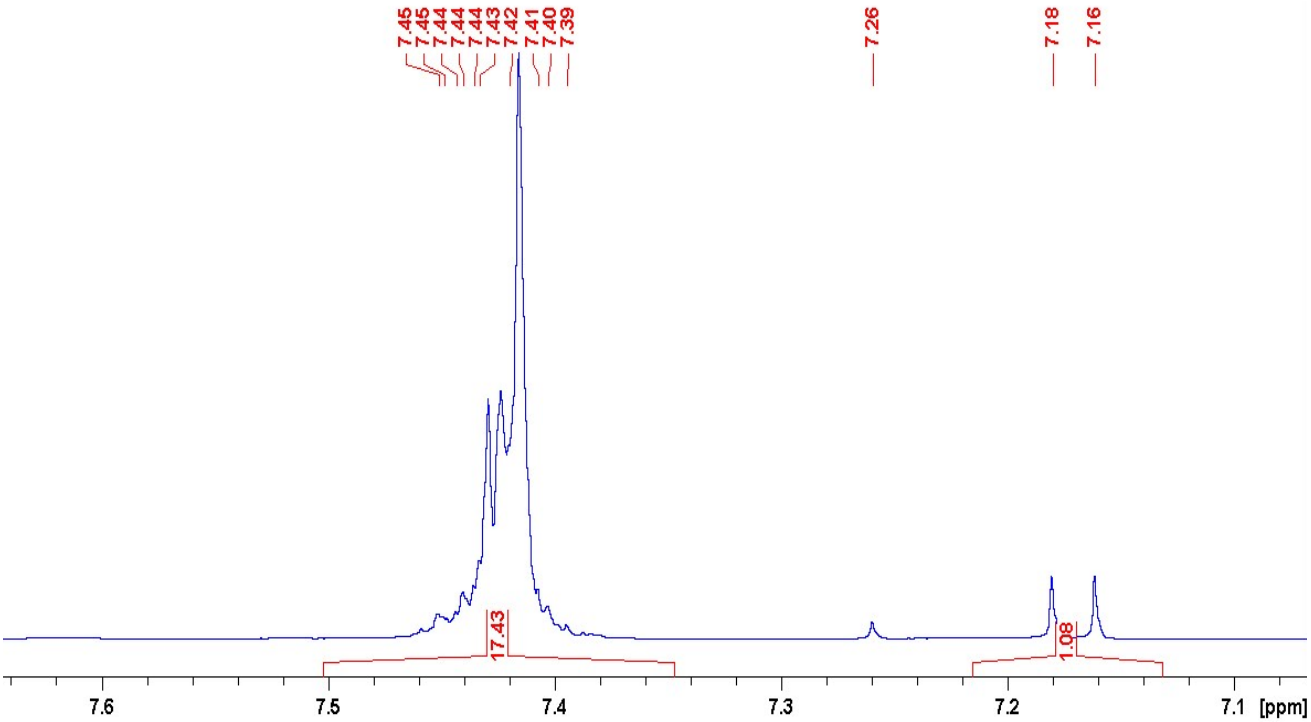


Figure S1: ^{1}H NMR Spectrum of **2** in $CDCl_3$ at 300.1 MHz.

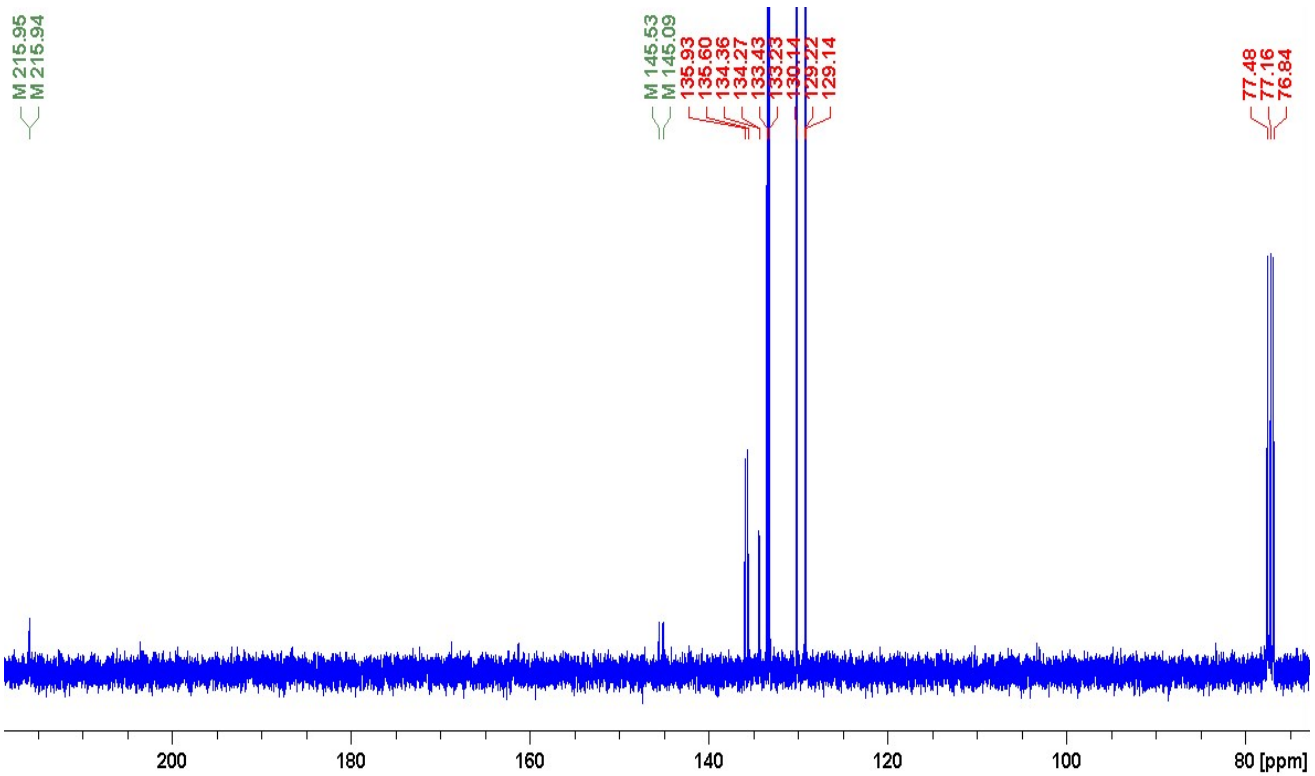


Figure S2: $^{13}C\{^{1}H\}$ NMR Spectrum of **2** in $CDCl_3$ at 75.5 MHz.

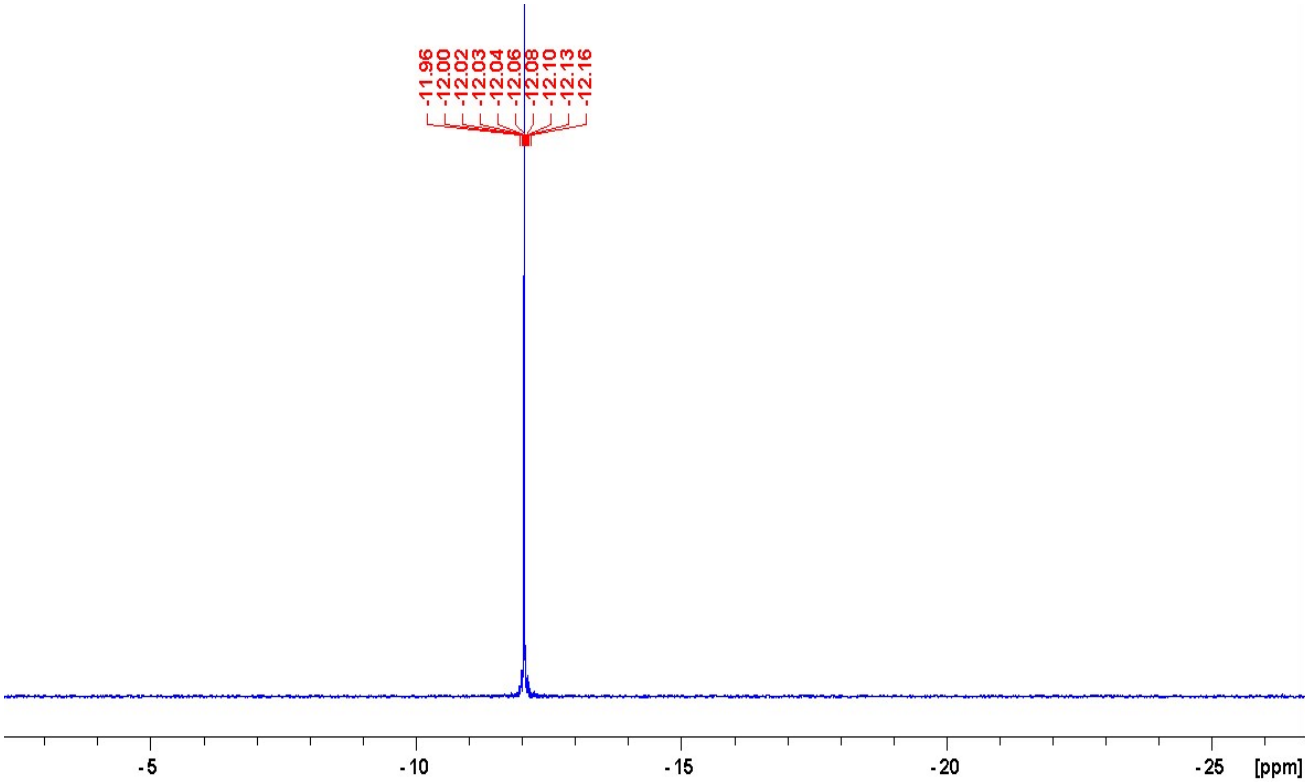


Figure S3: $^{31}P\{^{1}H\}$ NMR Spectrum of **2** in $CDCl_3$ at 121.5 MHz.

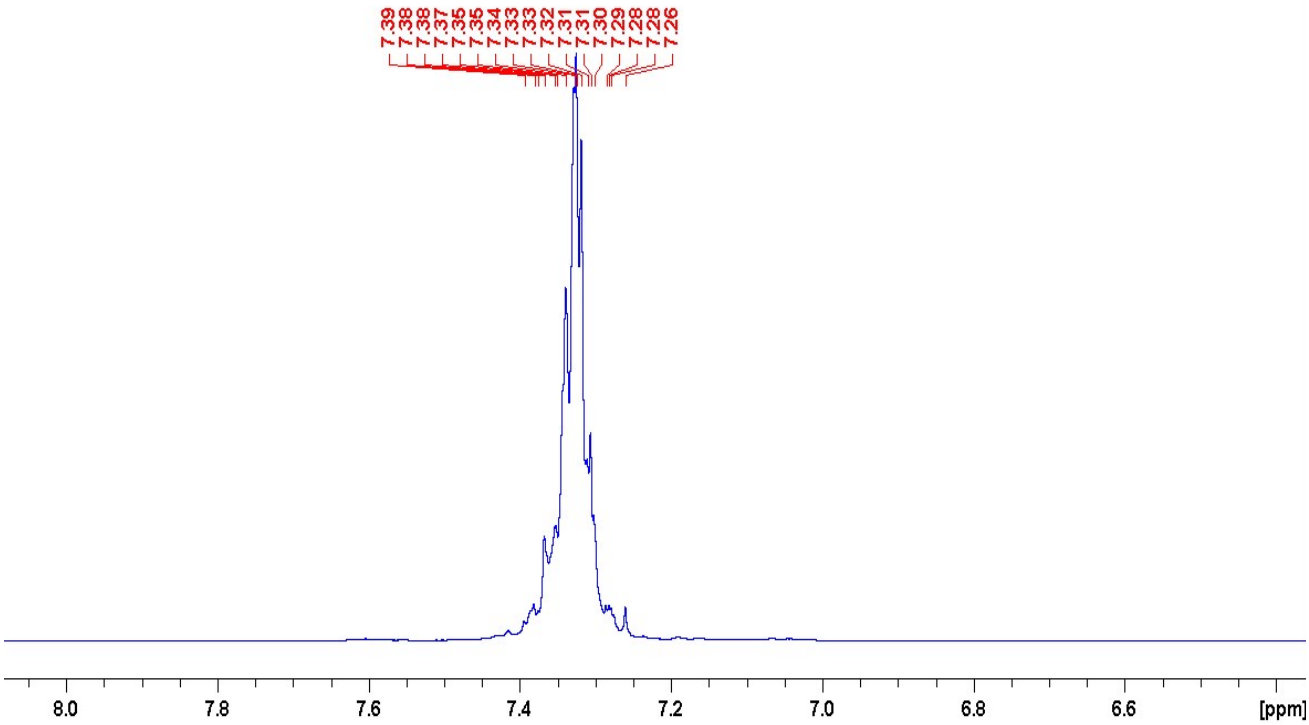


Figure S4:^{1}H NMR Spectrum of **3** in $CDCl_3$ at 300.1 MHz.

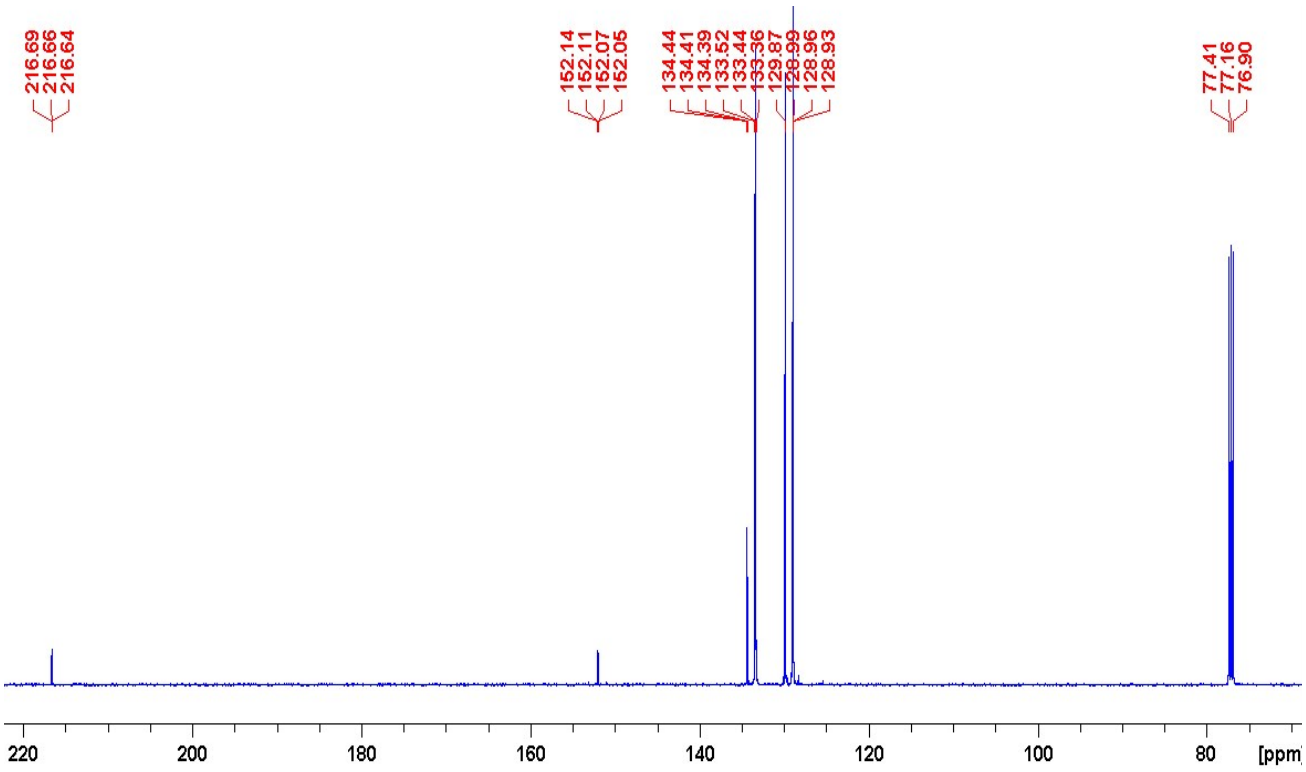


Figure S5: $^{13}C\{^{1}H\}$ NMR Spectrum of **3** in $CDCl_3$ at 75.5 MHz.

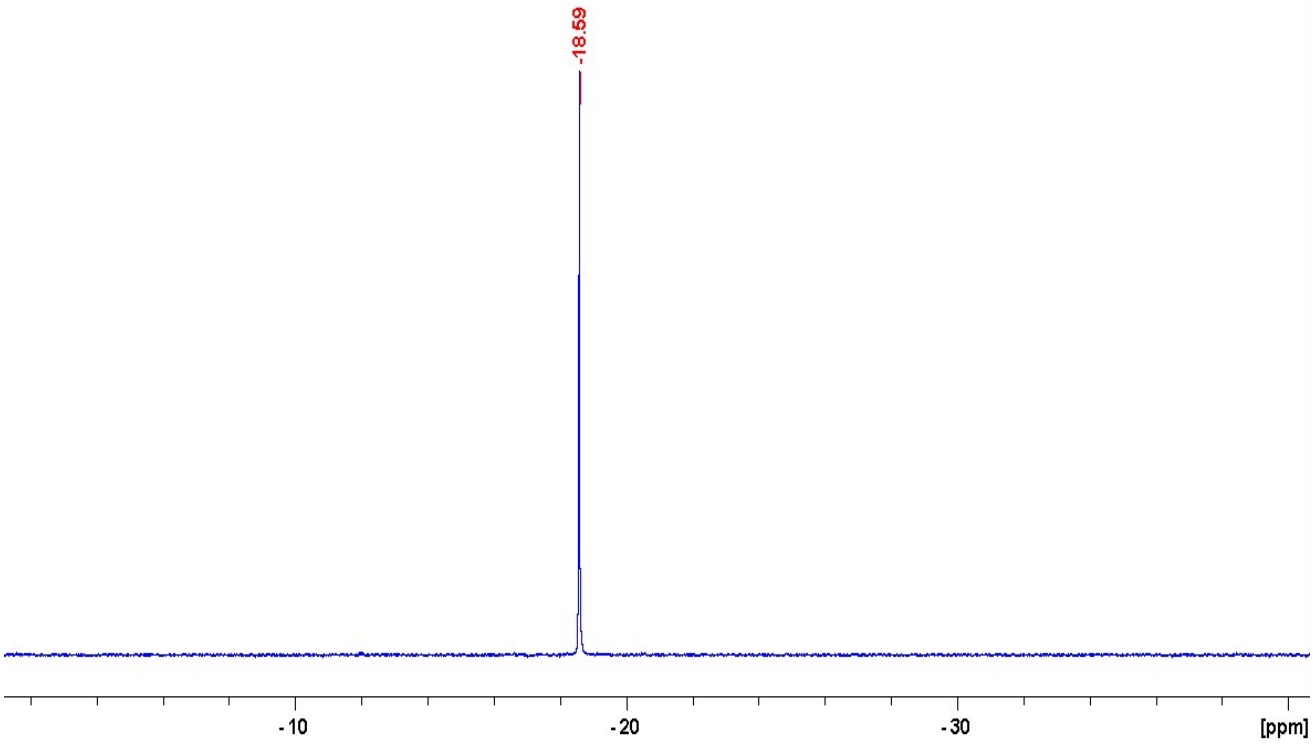


Figure S6: $^{31}P\{^{1}H\}$ NMR Spectrum of **3** in $CDCl_3$ at 121.5 MHz.

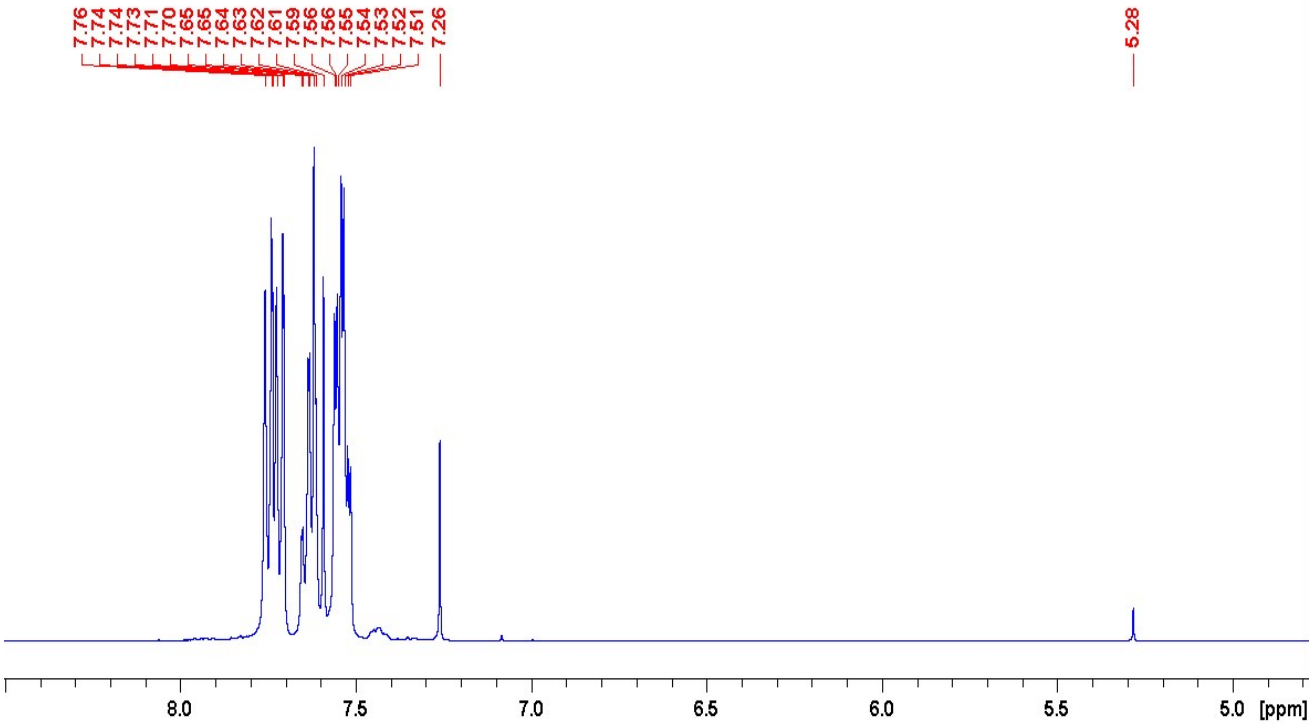


Figure S7: ^{1}H NMR Spectrum of **6** in $CDCl_3$ at 300.1 MHz.

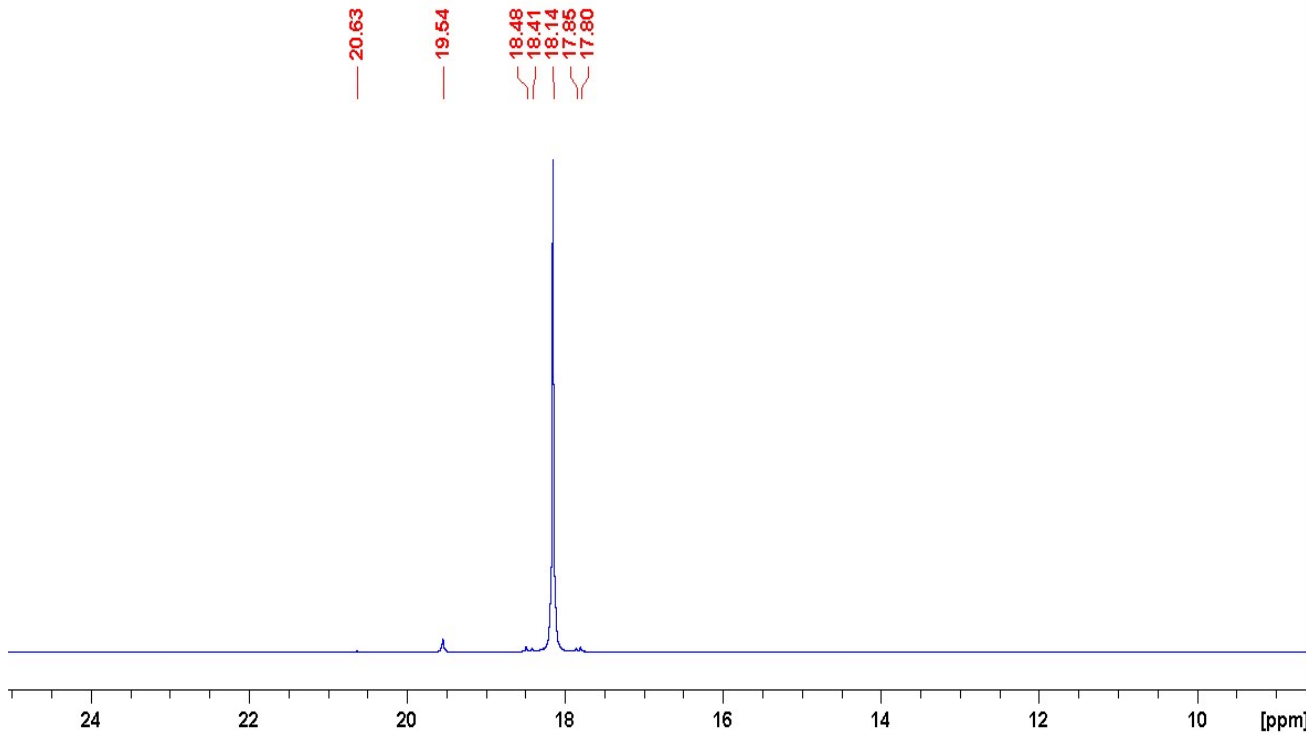


Figure S8: $^{31}P\{^{1}H\}$ NMR Spectrum of **6** in $CDCl_3$ at 121.5 MHz.

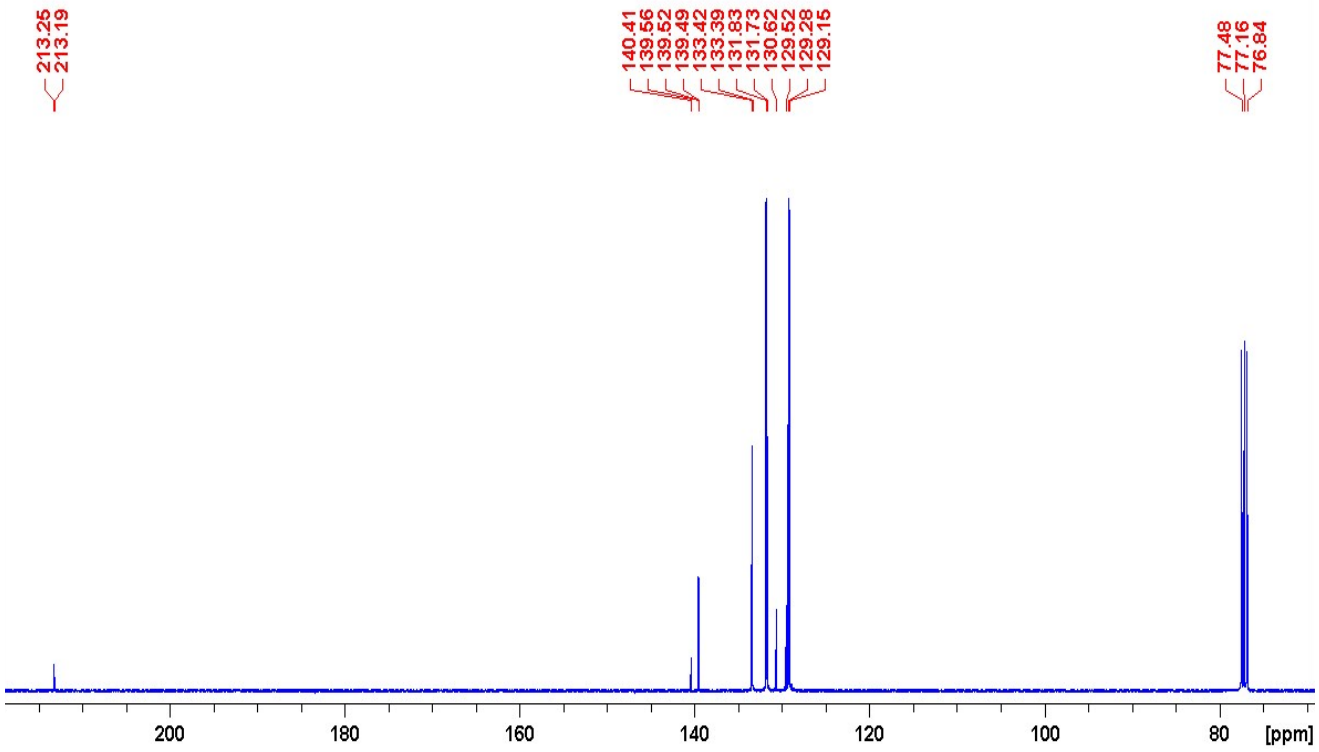


Figure S9: $^{13}C\{^{1}H\}$ NMR Spectrum of **6** in $CDCl_3$ at 75.5 MHz.

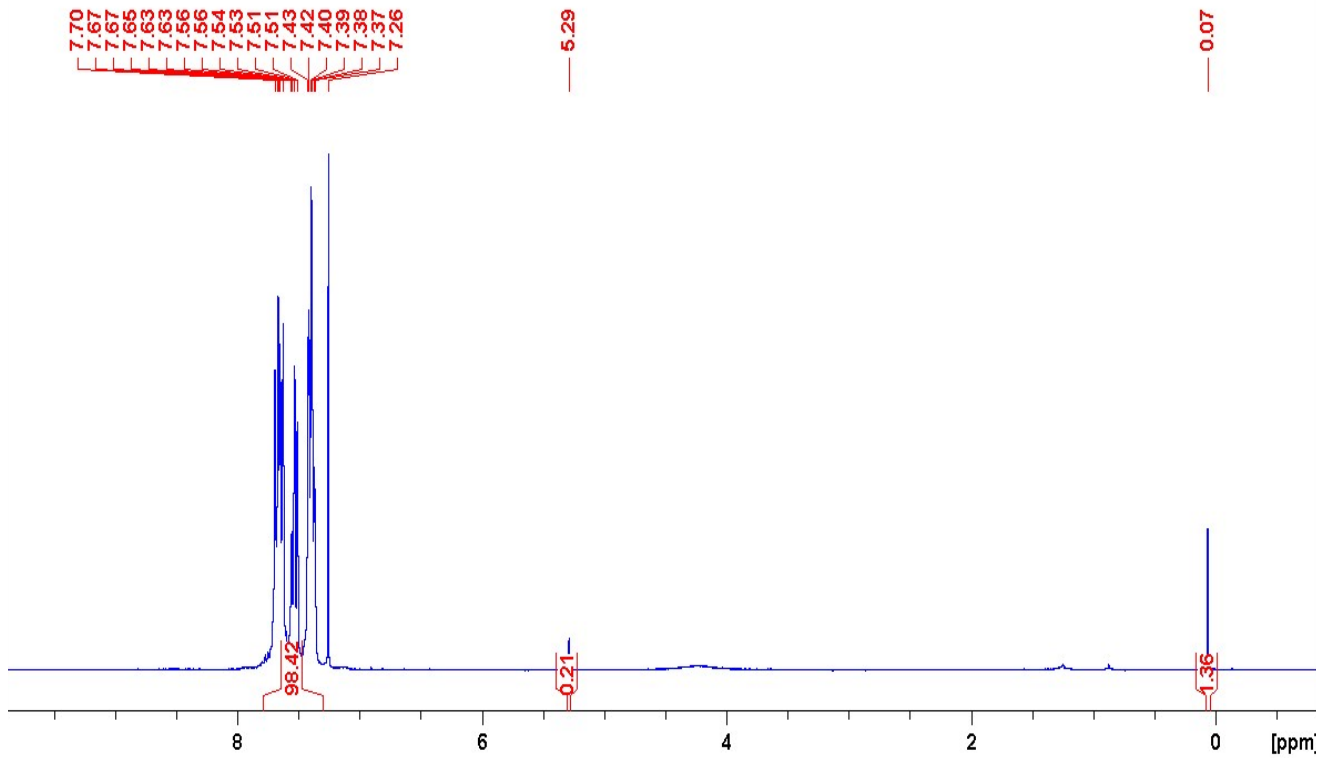


Figure S10: ^{1}H NMR Spectrum of **7** in $CDCl_3$ at 300.1 MHz.

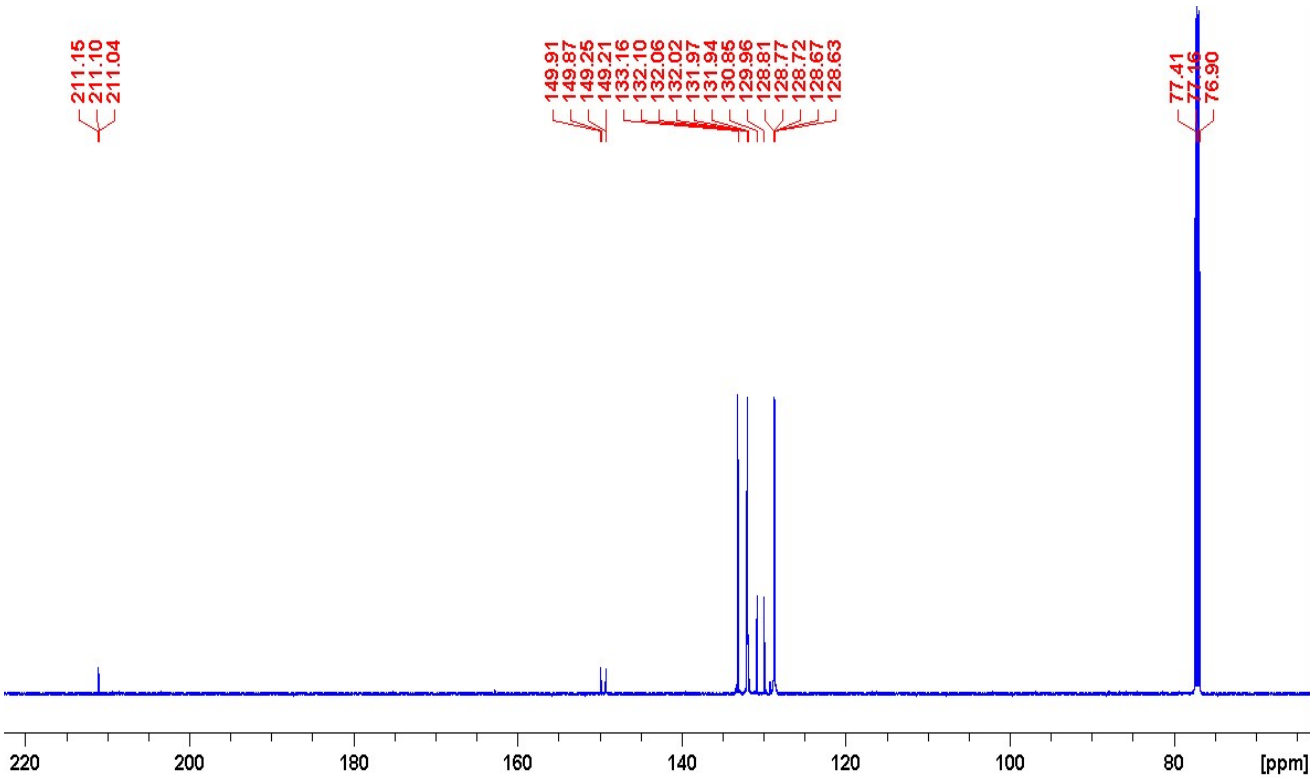


Figure S11: $^{13}C\{^{1}H\}$ NMR Spectrum of **7** in $CDCl_3$ at 75.5 MHz.

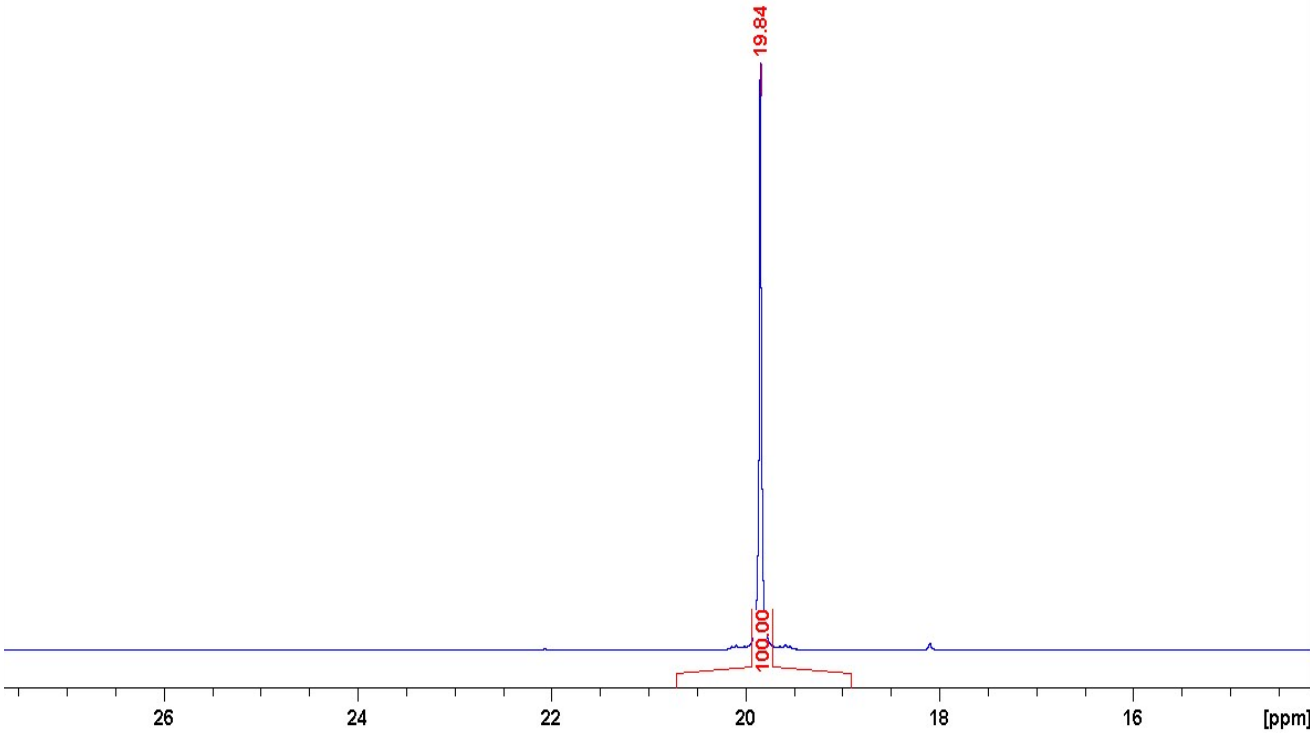


Figure S12: $^{31}P\{^{1}H\}$ NMR Spectrum of **7** in $CDCl_3$ at 121.5 MHz.

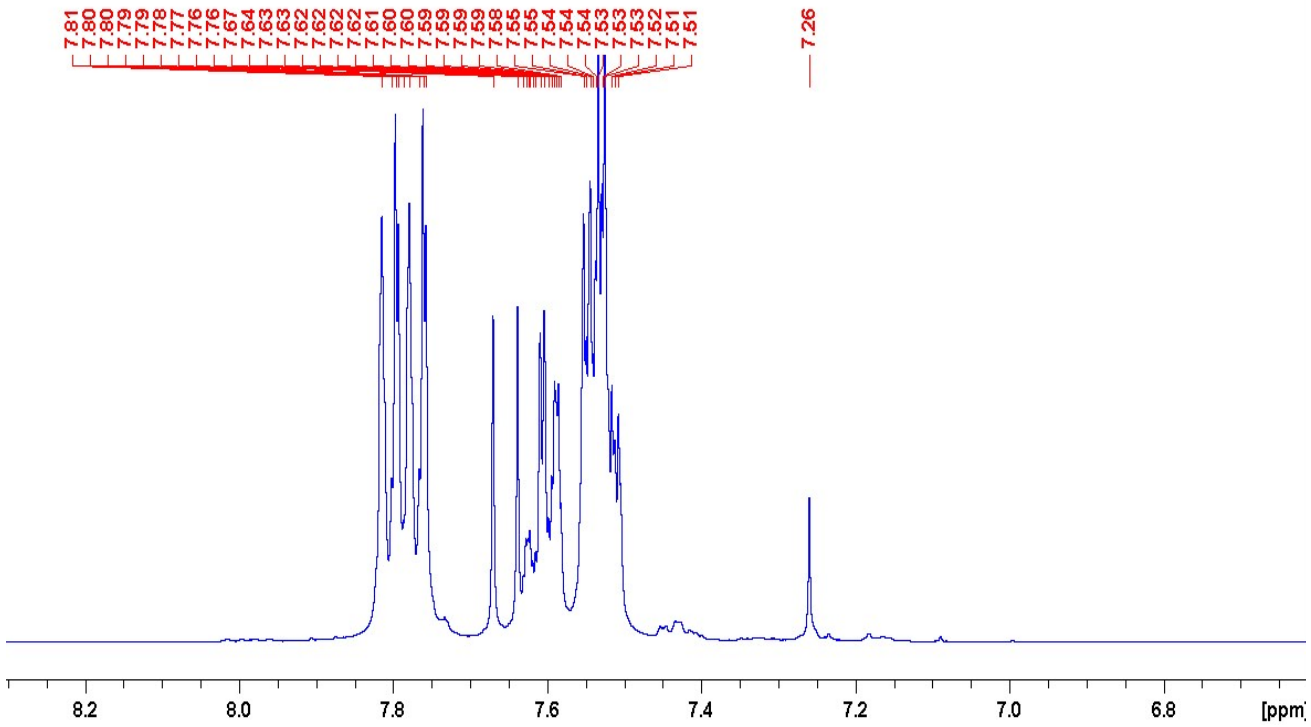


Figure S13: ^{1}H NMR Spectrum of **8** in $CDCl_3$ at 300.1 MHz.

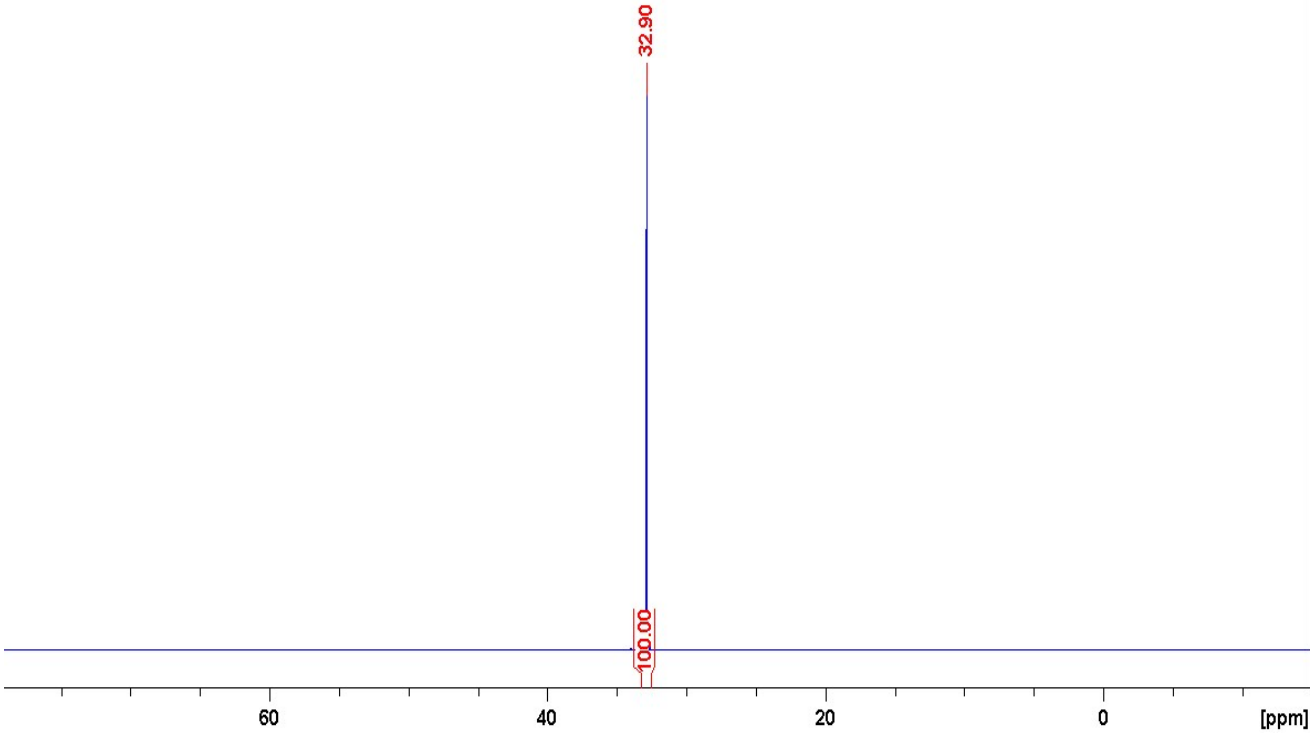


Figure S14: $^{31}P\{^{1}H\}$ NMR Spectrum of **8** in $CDCl_3$ at 121.5 MHz.

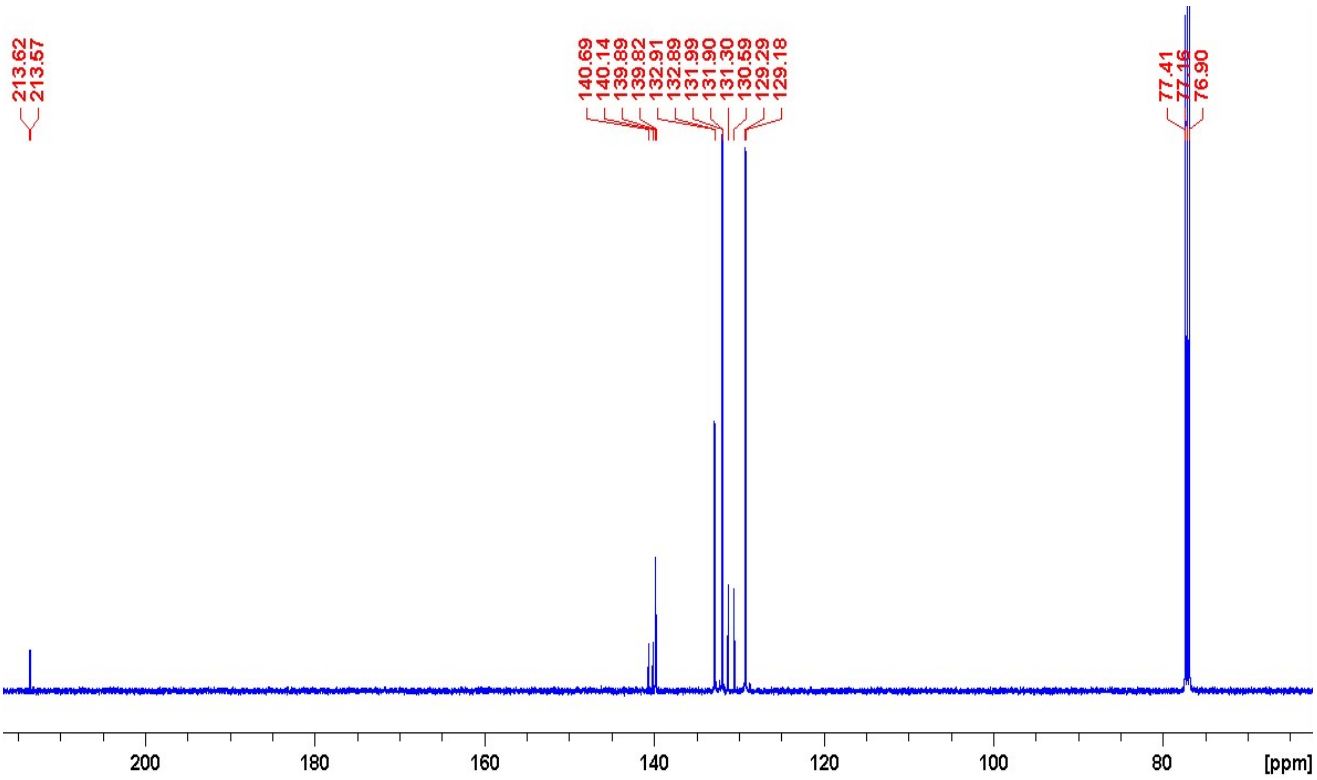


Figure S15: $^{13}C\{^{1}H\}$ NMR Spectrum of **8** in $CDCl_3$ at 75.5 MHz.

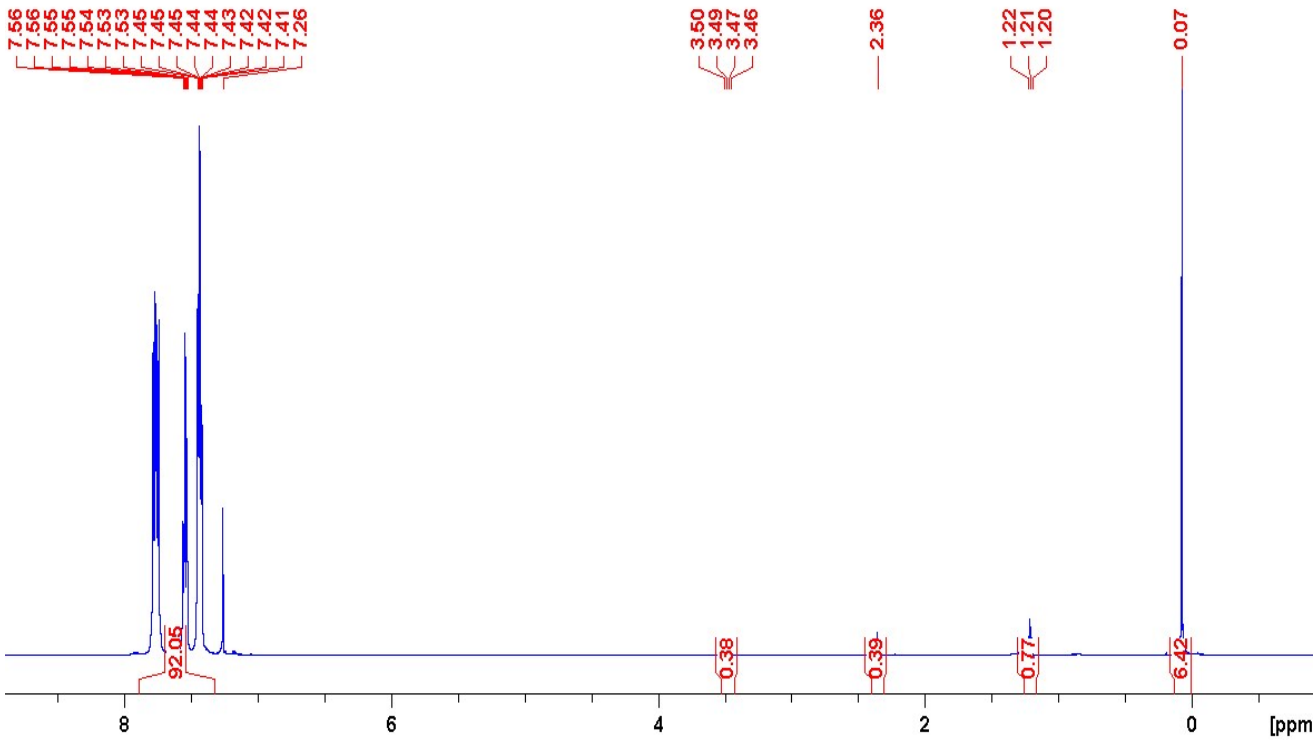


Figure S16: ^{1}H NMR Spectrum of **9** in $CDCl_3$ at 300.1 MHz.

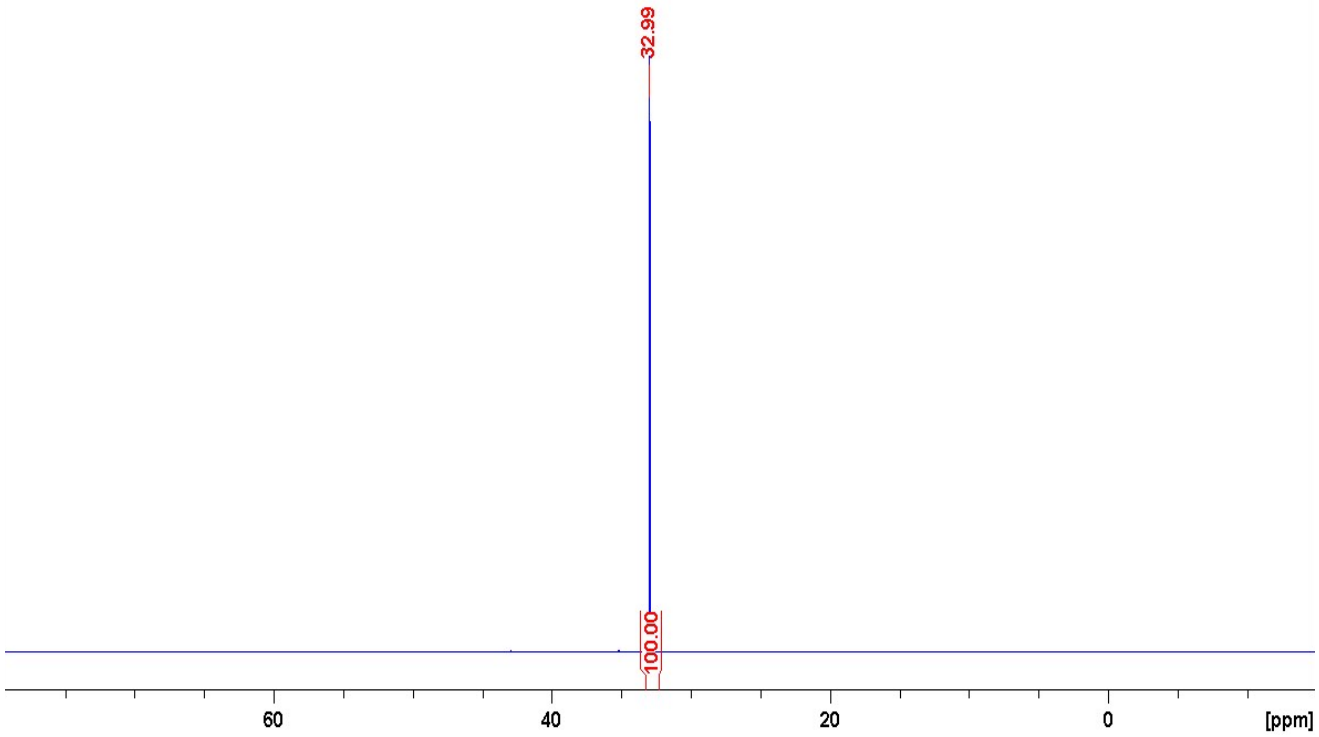


Figure S17: $^{31}P\{^{1}H\}$ NMR Spectrum of **9** in $CDCl_3$ at 121.5 MHz.

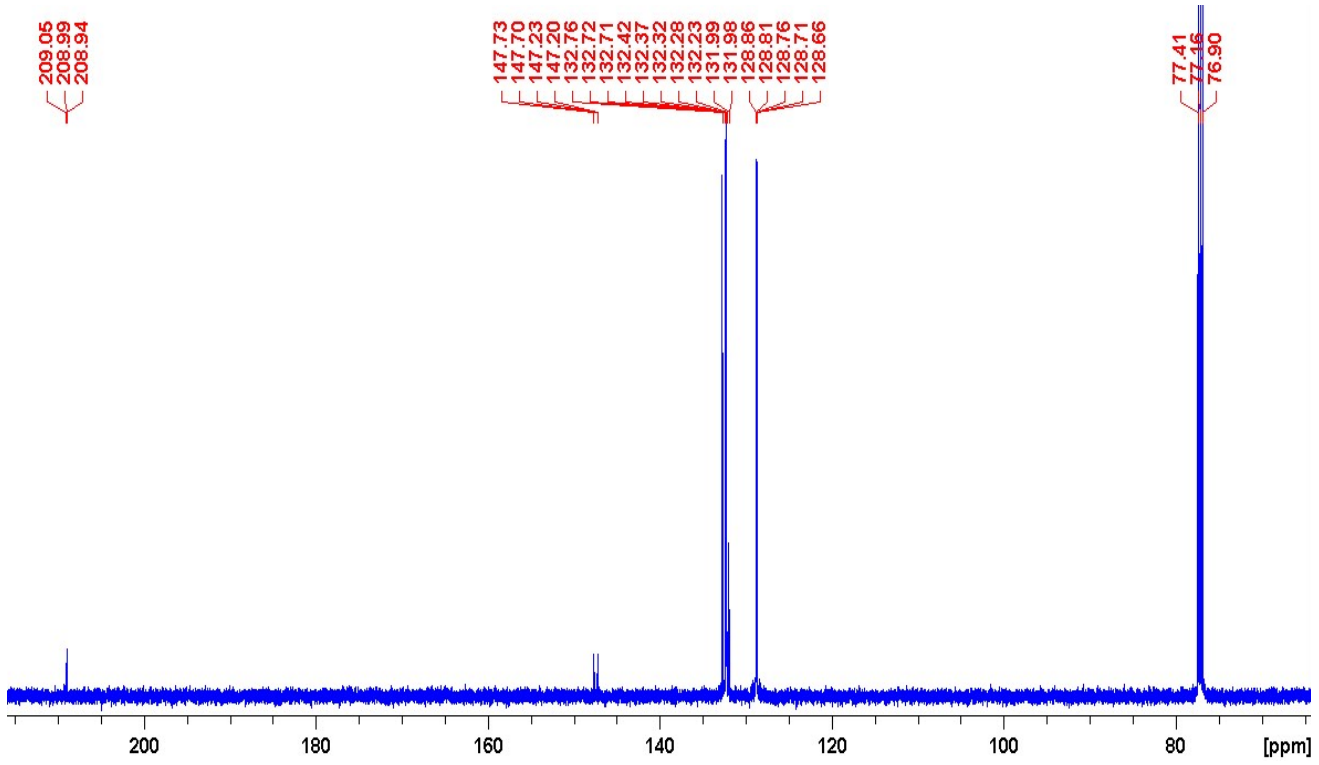


Figure S18: $^{13}C\{^{1}H\}$ NMR Spectrum of **9** in $CDCl_3$ at 75.5 MHz.

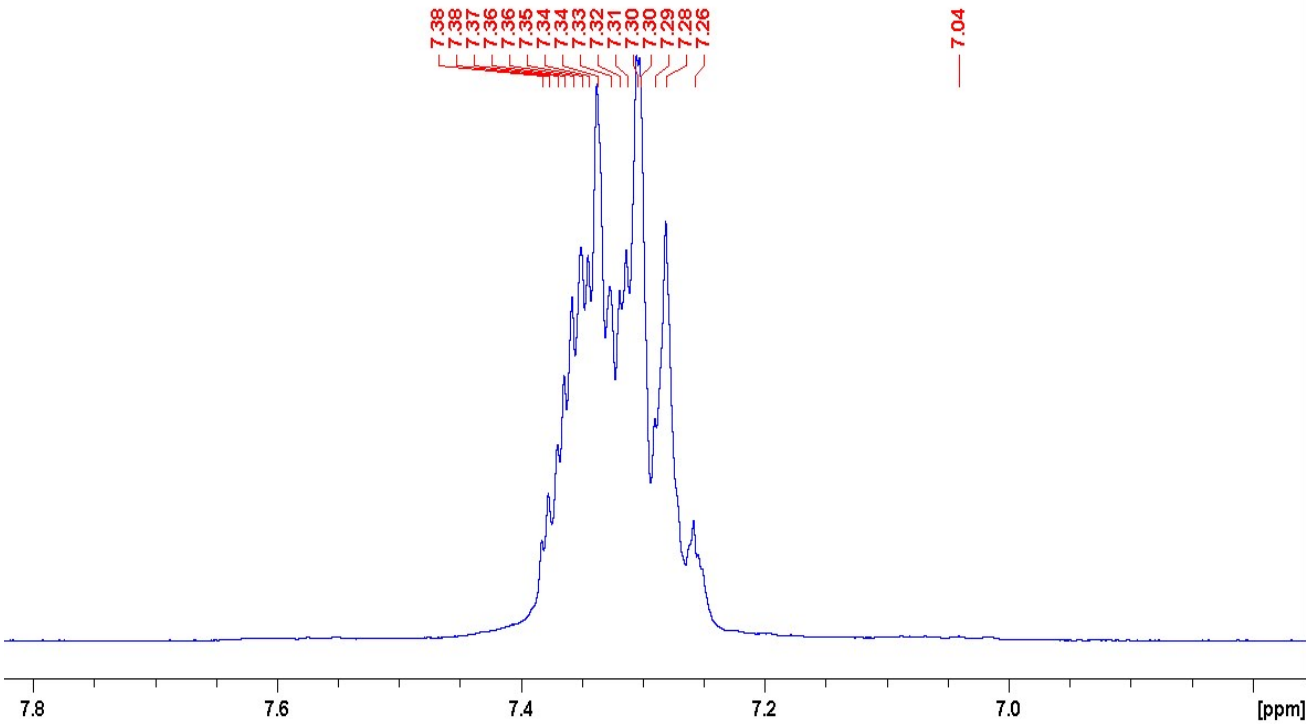


Figure S19: ^{1}H NMR Spectrum of **II** in $CDCl_3$ at 300.1 MHz.

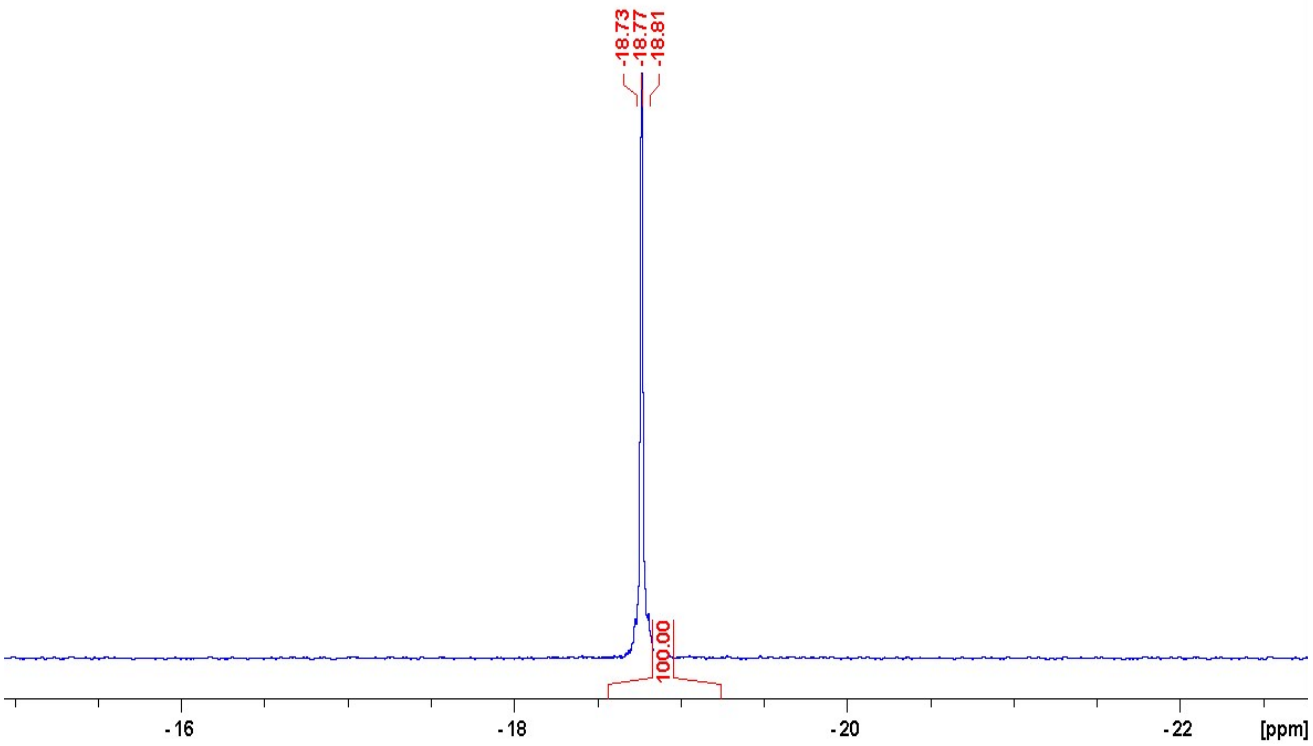


Figure S20: $^{31}P\{^{1}H\}$ NMR Spectrum of **II** in $CDCl_3$ at 121.5 MHz.

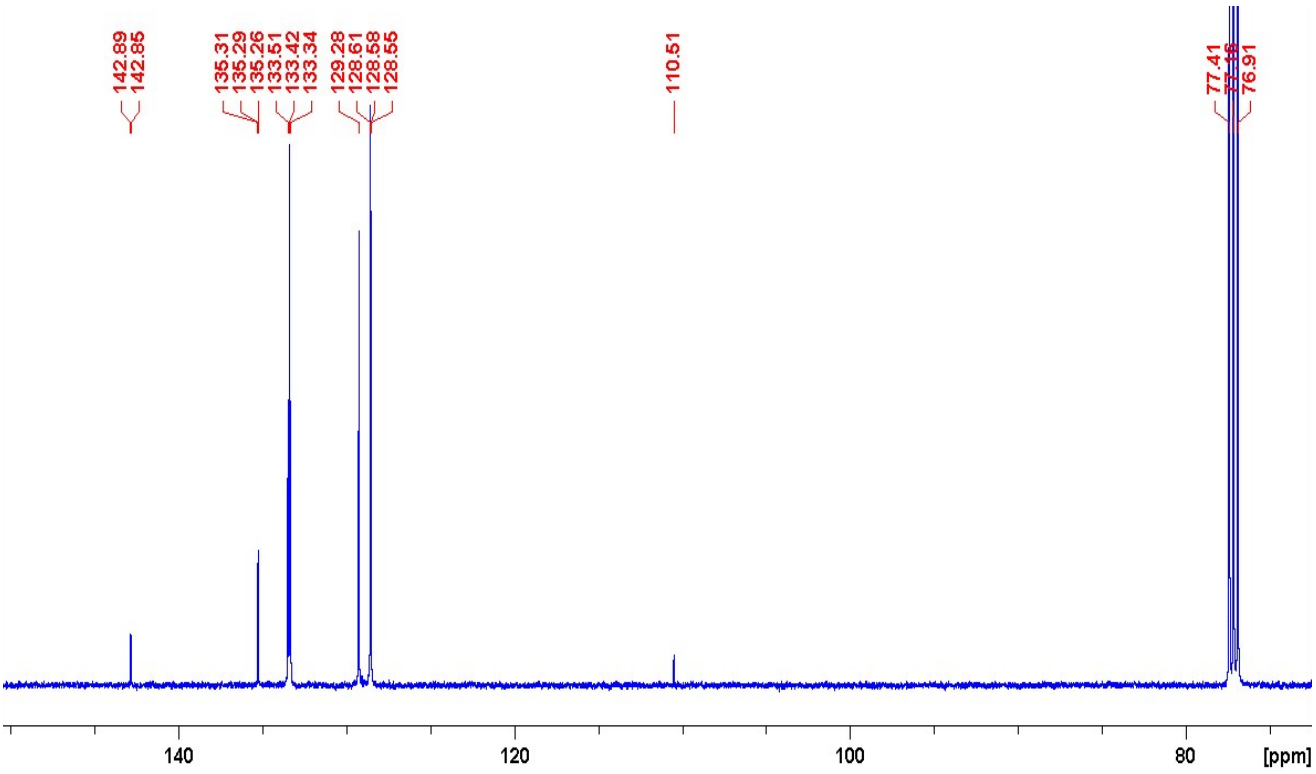


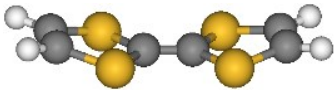
Figure S21: $^{13}C\{^{1}H\}$ NMR Spectrum of **II** in $CDCl_3$ at 75.5 MHz.

Computational Details.

DFT calculations were performed with the ORCA program.[3]All geometry optimizations were run in redundant internal coordinates with tight convergence criteria, using the B3LYP functional[4]together with the def2-TZVP basis set.[5]The 2010 Grimme's semiempirical atom-pair-wise London dispersion correction (DFT-D3) was included in all calculations.[6] Where indicated, additional alternative optimizations and zero-point-energy (ZPE) evaluations at the dispersion-corrected composite PBEh-3c level were performed.[7]Harmonic frequency calculations verified the nature of ground states or transition states (TS) having all positive frequencies or only one imaginary frequency, respectively. From these optimized geometries all reported data were obtained by means of single-point (SP) calculations using the more polarized def2-TZVPP basis set.[8]Reported energies were corrected for the zero-point vibrational term at the optimization level. Final energies were obtained by means of the recently developed near linear scaling domain-based local pair natural orbital (DLPNO) method[9]to achieve coupled cluster theory with single-double and perturbative triple excitations (CCSD(T)).[10]NICS calculations were performed with the GIAO (Gauge-Independent Atomic Orbital) method[11]at the standard B3LYP/6-311+G** level, for comparative purposes. Solvent (THF) effects were taken into account with the COSMO solvation model,[12]except for ASE (and ISE) evaluation and NICS calculation that were computed in the gas-phase. Kohn-Sham isosurfaces for **16** (Figures 4a and 4b) were drawn with VMD.[13]AIM-derived parameters were obtained, and BCP and bond paths (Figure 4c) represented by means of Aimall.[14]

Calculated structures

Cartesian coordinates (in Å),G correction (G-E) and ZPE (in hartrees) for minima and transition states were computed at $COSMO_{THF}$/B3LYP-D3/def2-TZVP. Imaginary frequencies are obtained upon frequency calculation at the optimization level. Electronic energies (in hartrees) are quoted at both the optimization level and at the $COSMO_{THF}$/DLPNO-CCSD(T)/def2-TZVPP level. In some cases, where explicitly indicated, geometries and ZPE were obtained at the $CPCM_{THF}$/PBEh-3c(ecp) level.



I:

E = -1823.61317922566au (opt)
E = -1821.49387292819 au
ZPE = 0.08177485au
G_{corr} = 0.04580523 au

C	1.716041	-0.326734	0.146860	C	1.614934	-0.010121	-1.157066
S	1.529272	0.858094	1.446194	S	1.798315	-1.195089	-2.456883
C	2.107648	-0.213506	2.705072	C	1.863795	-0.000062	-3.735657
C	2.339562	-1.484134	2.378952	C	1.632077	1.270433	-3.408888
S	2.044917	-1.966626	0.721275	S	1.282869	1.629448	-1.730560
H	2.221742	0.201771	3.695615	H	2.061623	-0.355243	-4.736337
H	2.669033	-2.249035	3.066708	H	1.614647	2.095326	-4.105943

I:

E = -1821.49586099329 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.08508058au
G_{corr} = 0.04933742 au

C	1.647859	-0.338476	0.146571	C	1.546925	-0.023203	-1.152267
S	1.470088	0.844359	1.436717	S	1.738423	-1.203562	-2.442692
C	2.128994	-0.202578	2.671557	C	1.889997	-0.002262	-3.703231
C	2.360579	-1.470469	2.345703	C	1.658441	1.265677	-3.377563
S	1.983788	-1.969696	0.713530	S	1.224665	1.610560	-1.719851
H	2.289237	0.219088	3.653115	H	2.133967	-0.347120	-4.697477
H	2.735039	-2.221571	3.025847	H	1.688474	2.093774	-4.070617

***Z*-I^{PMe2}:**

E = -2661.49323300291 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.22150586au
G_{corr} = 0.17415349 au

C	0.565105	-0.020050	0.300768	C	1.084656	-1.328815	2.446440
S	1.009214	1.142576	1.539623	S	0.261172	-1.629715	0.931813
C	1.437400	-0.075037	2.739442	C	0.469761	0.292517	-0.998553

S	0.027429	-0.866472	-2.240639	H	3.792339	3.498828	-4.687120
C	0.645971	0.112817	-3.552678	H	3.383486	3.245091	-2.993243
C	0.997616	1.374086	-3.292308	H	1.233866	-2.182045	3.092826
S	0.777627	1.903481	-1.625868	P	2.155445	0.562617	4.290569
H	0.677179	-0.350304	-4.528754	C	2.480150	-1.008230	5.187765
P	1.523925	2.665079	-4.469107	H	3.059366	-1.720135	4.598544
C	1.670169	1.678567	-6.012909	H	3.042899	-0.769041	6.089998
H	2.113552	2.315447	-6.778198	H	1.543674	-1.471051	5.496870
H	2.298352	0.795358	-5.891553	C	3.855336	0.978358	3.703104
H	0.684917	1.376119	-6.365693	H	4.454108	1.290981	4.558725
C	3.300697	2.818044	-3.992012	H	4.341182	0.131221	3.219118
H	3.814543	1.857051	-4.011620	H	3.814757	1.811948	3.002944

***E*-I^{PMe2}:** E = -2661.49335891401 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.22148486au
G_{corr} = 0.17414768 au

C	0.894945	-0.464692	0.171525	H	1.982465	2.477614	-6.769097
S	0.701458	0.741567	1.432164	H	2.697795	1.148044	-5.846452
C	1.461547	-0.240738	2.664936	H	1.038335	1.022977	-6.475440
C	1.710450	-1.523402	2.391084	C	2.599778	3.359963	-3.895134
S	1.220143	-2.075541	0.790990	H	3.464795	2.698299	-3.851858
H	1.659370	0.240056	3.612472	H	2.825538	4.198595	-4.553976
C	0.803791	-0.184306	-1.135449	H	2.408732	3.760667	-2.900284
S	0.996063	-1.390660	-2.396120	C	2.756690	-1.806027	4.993337
C	1.271644	-0.211124	-3.659107	H	3.276290	-2.448575	5.704017
C	1.047410	1.076251	-3.385939	H	3.400995	-0.957738	4.759380
S	0.480259	1.426894	-1.754803	H	1.847931	-1.447832	5.475512
H	1.577317	-0.596087	-4.621653	C	4.022619	-3.064712	2.789771
P	1.096195	2.497192	-4.529526	H	4.577577	-2.130059	2.710205
P	2.343068	-2.814946	3.513899	H	4.578003	-3.755766	3.424057
C	1.774702	1.696235	-6.038205	H	3.939779	-3.514161	1.800882

***Z*-I^{POMe2}:** E = -2811.86621839731 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.22992313au
G_{corr} = 0.18294876 au

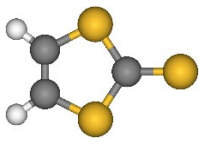
C	0.912811	-0.238022	0.224065	S	0.722800	-1.141129	-2.344466
S	1.013728	0.967484	1.498050	C	1.146551	-0.026262	-3.614907
C	1.626069	-0.167446	2.691962	C	1.185483	1.273067	-3.317901
C	1.584147	-1.461618	2.373626	S	0.778771	1.726286	-1.669234
S	0.952750	-1.896592	0.808810	H	1.328799	-0.446241	-4.594906
C	0.817350	0.073291	-1.075386	C	0.981701	2.159957	-6.045688

H	1.229100	2.940688	-6.765031	H	2.180043	-0.222428	6.481115
H	1.454299	1.233703	-6.370275	H	0.730494	-0.735490	5.599764
H	-0.098660	2.025252	-6.030638	C	3.991557	0.639266	4.098271
C	3.359718	2.720777	-4.502346	H	4.413716	1.067229	5.007842
H	3.763389	1.778795	-4.871069	H	4.399505	-0.360292	3.954287
H	3.665215	3.524635	-5.172504	H	4.276802	1.263566	3.252353
H	3.767647	2.917459	-3.511541	P	1.556435	2.667157	-4.412716
H	1.884263	-2.272329	3.023779	P	2.191115	0.595131	4.234458
C	1.808748	-0.601533	5.528952	O	0.927139	3.911070	-3.861955
H	2.278275	-1.565823	5.338116	O	1.548127	1.940870	4.385959

***E*-I^{POMe2}:**

E = -2811.86618865821 au (optimized with CPCM$_{THF}$/PBEh-3c)
ZPE = 0.2298841 au
G_{corr} = 0.18283995 au

C	1.062185	-0.440973	0.164652	C	3.090372	2.956168	-4.483533
S	0.886178	0.765144	1.432775	H	3.669942	2.109838	-4.849656
C	1.623102	-0.232850	2.656087	H	3.258714	3.811405	-5.138407
C	1.861651	-1.511020	2.360454	H	3.430734	3.211052	-3.480584
S	1.377731	-2.062460	0.763464	C	2.051284	-2.400099	5.089801
H	1.825218	0.232296	3.611485	H	2.500463	-3.113829	5.780499
C	0.966560	-0.142809	-1.137863	H	2.360388	-1.397968	5.384789
S	1.172870	-1.343312	-2.406744	H	0.967375	-2.475875	5.160592
C	1.420979	-0.158229	-3.659581	C	4.362948	-2.498760	3.359080
C	1.190049	1.121485	-3.364401	H	4.604508	-1.495731	3.708169
S	0.629410	1.474350	-1.736511	H	4.870966	-3.226719	3.992059
H	1.724391	-0.527154	-4.630118	H	4.720578	-2.613669	2.336555
C	0.897351	1.981854	-6.092985	P	1.326326	2.569929	-4.442546
H	1.017190	2.801001	-6.802134	P	2.582347	-2.797049	3.412113
H	1.539320	1.159953	-6.407686	O	0.464177	3.671013	-3.902580
H	-0.140220	1.652011	-6.108171	O	2.164172	-4.143345	2.902448



1:

E = -1309.98029708939au (opt)
E = -1308.48697211683 au
ZPE = 0.041708765au
G_{corr} = 0.01226604 au

C	0.020755	-0.000035	0.014207	C	1.733971	0.000019	1.987439
S	0.016519	0.000010	1.753778	C	2.486695	0.000031	0.879053

S	1.636202	-0.000019	-0.631219	H	2.113432	0.000072	2.998883
S	-1.346819	-0.000105	-0.914874	H	3.566780	0.000027	0.858978

1: E = -1308.48828268327 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.04345104au
G_{corr} = 0.01308202 au

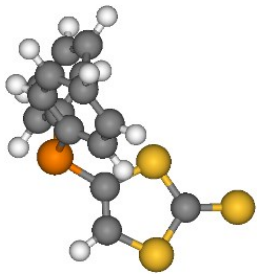
C	0.026427	-0.000041	0.018008	S	1.631722	-0.000154	-0.630631
S	0.015356	-0.000115	1.749359	S	-1.329571	0.000025	-0.903102
C	1.729567	0.000033	1.982242	H	2.113148	0.000126	2.992321
C	2.480268	0.000024	0.876972	H	3.560616	0.000102	0.861076

1^{PMe2}: E = -1728.48476825323 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.11145725au
G_{corr} = 0.075732 au

C	0.062772	0.001582	0.076933	C	4.851563	-1.420556	1.684827
S	0.151346	0.002149	1.806859	H	5.938176	-1.487741	1.743165
C	1.874552	0.000748	1.939874	H	4.455740	-1.319128	2.695463
C	2.582867	-0.000303	0.801280	H	4.480954	-2.347223	1.249031
S	1.630284	-0.000116	-0.652608	C	4.853706	1.419443	1.680162
S	-1.344765	0.002506	-0.763401	H	4.458314	1.321592	2.691335
H	2.298515	0.000784	2.935489	H	5.940423	1.485642	1.737681
P	4.411867	-0.002027	0.594251	H	4.483863	2.345140	1.241657

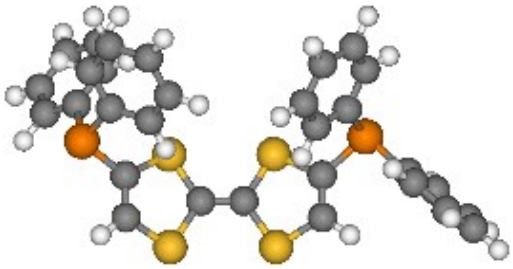
1^{POMe2}: E = -1803.67142938019 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.11577053au
G_{corr} = 0.07905062 au

C	1.142114	-1.213356	-0.556492	H	0.768378	0.262044	4.373225
S	0.732562	0.263717	0.247498	H	2.524803	0.047836	4.502010
C	1.915198	0.158989	1.514987	C	3.583587	2.212693	2.631318
C	2.706238	-0.921786	1.493885	H	3.675293	3.020336	3.357782
S	2.446327	-2.055385	0.218723	H	4.326198	1.449636	2.862210
S	0.384677	-1.761080	-1.900415	H	3.779583	2.609584	1.636341
H	3.490112	-1.137733	2.208103	P	1.910126	1.542985	2.696252
C	1.730152	0.769421	4.315369	O	0.819939	2.494832	2.310343
H	1.770330	1.539001	5.086442				



2: E = -2113.94465021243au (opt)
E = -2111.23120546016 au
ZPE = 0.21462121au
G_{corr} = 0.17117616 au

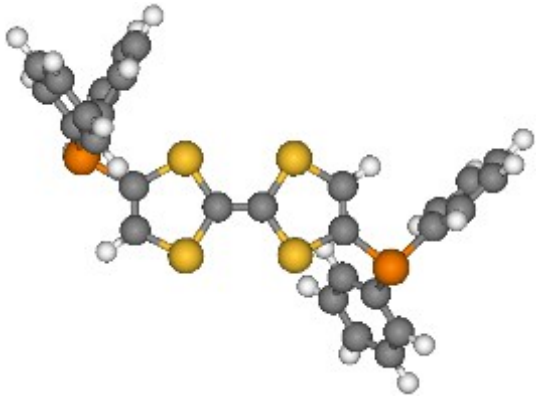
C	1.338186	2.549042	1.062923	H	5.878104	-1.628068	6.471798
S	1.537118	1.836739	2.635643	H	7.396994	-0.084259	5.262620
C	1.809682	0.184249	2.128994	H	6.615701	1.033175	3.192722
C	1.768739	-0.009689	0.797426	H	4.349072	0.627089	2.346086
S	1.479631	1.366196	-0.209194	C	1.045714	-0.678417	4.694299
S	1.040111	4.151214	0.798807	C	-0.222079	-1.263956	4.741739
H	1.907811	-0.968112	0.316486	C	-1.131177	-0.901100	5.729337
P	2.141321	-1.175281	3.305128	C	-0.776307	0.042701	6.687527
C	3.806980	-0.728083	3.930553	C	0.488827	0.622599	6.654286
C	4.262537	-1.367555	5.089513	C	1.395065	0.265428	5.663538
C	5.543957	-1.132931	5.568734	H	-0.498896	-2.005683	4.001907
C	6.397340	-0.266586	4.889471	H	-2.111471	-1.359852	5.754043
C	5.959012	0.359577	3.728785	H	-1.480822	0.322726	7.460371
C	4.672106	0.130136	3.250780	H	0.769496	1.356610	7.399068
H	3.609331	-2.045329	5.626245	H	2.375532	0.722052	5.647836



***Z*-8:** E = -3431.54431408376au (opt)
E = -3426.98451994790 au
ZPE = 0.42767495au
G_{corr} = 0.37275085 au

C	0.881777	-0.632513	0.931879	C	0.082030	-1.700554	1.093612
S	2.090298	-0.525994	-0.346784	S	0.165638	-3.127055	0.064024
C	2.161494	1.242331	-0.319730	C	-1.489167	-3.651708	0.426951
C	1.578753	1.834174	0.729214	C	-2.072078	-3.047039	1.470744
S	0.802476	0.820283	1.929498	S	-1.191342	-1.795716	2.314716

H	1.569149	2.899327	0.905533
H	-3.058165	-3.291019	1.840351
P	3.080411	2.015276	-1.690714
C	2.953173	3.779206	-1.202551
C	3.981671	4.298993	-0.410441
C	3.942038	5.619170	0.021551
C	2.881760	6.441091	-0.349595
C	1.861864	5.935744	-1.149606
C	1.894474	4.610803	-1.571582
H	4.815064	3.665817	-0.129430
H	4.741555	6.007984	0.639448
H	2.853749	7.472312	-0.021029
H	1.036860	6.572234	-1.444186
H	1.093817	4.226740	-2.188902
C	1.852799	1.863503	-3.046853
C	2.326245	1.995160	-4.355372
C	1.455534	1.903751	-5.435298
C	0.102439	1.660999	-5.219451
C	-0.375473	1.516268	-3.920643
C	0.492905	1.619742	-2.840498
H	3.381871	2.168196	-4.529634
H	1.834629	2.011997	-6.443652
H	-0.575338	1.579695	-6.059768
H	-1.427607	1.328694	-3.747255
H	0.110202	1.511588	-1.834523
P	-2.340004	-4.907001	-0.575560
C	-2.510000	-4.036276	-2.184014
C	-2.833407	-4.794570	-3.314844
C	-3.044084	-4.180899	-4.542537
C	-2.948305	-2.796249	-4.658047
C	-2.644294	-2.033826	-3.536354
C	-2.427639	-2.648413	-2.307035
H	-2.910895	-5.872819	-3.238775
H	-3.284562	-4.783301	-5.409586
H	-3.112135	-2.317569	-5.615114
H	-2.567979	-0.956861	-3.615225
H	-2.187201	-2.039962	-1.446139
C	-0.945516	-6.061561	-0.902710
C	-0.827318	-7.169982	-0.059981
C	0.231254	-8.059699	-0.204858
C	1.178567	-7.855933	-1.203073
C	1.063471	-6.760059	-2.053495
C	0.008819	-5.867462	-1.904607
H	-1.567308	-7.336061	0.714088
H	0.312033	-8.913490	0.456027
H	2.000887	-8.550235	-1.321083
H	1.798096	-6.597618	-2.832221
H	-0.069911	-5.019064	-2.570865



***E*-8:** E = -3431.54349929210au (opt)
E = -3426.98375855788 au
ZPE = 0.42779456au
G_{corr} = 0.37049554 au

C	0.668544	-1.116441	-0.786586
S	2.244856	-0.615813	-1.403883
C	2.284046	0.909153	-0.509359
C	1.332035	1.067410	0.417693
S	0.161532	-0.211658	0.642848
C	-0.074054	-2.090369	-1.342117
S	-1.647853	-2.585319	-0.713566
C	-2.081618	-3.573983	-2.112962

C	-1.122071	-3.734657	-3.034618	H	0.503262	3.311981	-4.494478
S	0.432118	-2.990369	-2.776225	H	1.081054	2.223748	-2.362855
H	1.249229	1.925317	1.067938	P	-3.697429	-4.398965	-2.264008
H	-1.236737	-4.330930	-3.928960	C	-3.650497	-5.578720	-0.858140
P	3.692666	2.010936	-0.866721	C	-4.856258	-6.112750	-0.389952
C	3.376059	3.337196	0.361543	C	-4.861813	-7.085291	0.601305
C	4.003587	3.221993	1.605613	C	-3.661456	-7.549143	1.133526
C	3.789114	4.173730	2.595453	C	-2.458188	-7.034567	0.664001
C	2.957675	5.261732	2.346022	C	-2.451787	-6.057418	-0.326436
C	2.340225	5.390960	1.105883	H	-5.797460	-5.761250	-0.795246
C	2.545274	4.432597	0.119119	H	-5.804003	-7.482327	0.957991
H	4.660448	2.382221	1.799633	H	-3.665625	-8.306826	1.906735
H	4.276653	4.070637	3.556648	H	-1.519503	-7.389019	1.071248
H	2.796023	6.008315	3.113263	H	-1.507326	-5.664733	-0.678529
H	1.695308	6.237499	0.905926	C	-4.824341	-3.085758	-1.644425
H	2.057025	4.539755	-0.839990	C	-5.487894	-2.314255	-2.601233
C	3.158338	2.778121	-2.444429	C	-6.316102	-1.265327	-2.215139
C	4.135429	3.443516	-3.190868	C	-6.497631	-0.984465	-0.865350
C	3.805681	4.073383	-4.384979	C	-5.847862	-1.754506	0.095934
C	2.497435	4.027306	-4.857787	C	-5.016293	-2.797710	-0.290592
C	1.521712	3.354113	-4.129104	H	-5.354695	-2.535024	-3.653704
C	1.848738	2.736209	-2.927243	H	-6.823076	-0.674041	-2.967206
H	5.158745	3.469333	-2.834523	H	-7.145640	-0.171877	-0.562050
H	4.570384	4.591033	-4.950276	H	-5.986556	-1.539785	1.148133
H	2.240960	4.509323	-5.792701	H	-4.518264	-3.390021	0.465359

$(MeO)_3P$**:** E = -686.75926971363au (opt)
E = -685.85468067818 au
ZPE = 0.12742508au
G_{corr} = 0.09131810 au

P	0.000229	0.003337	0.000312	H	-0.842362	-3.042434	-1.523632
O	1.633053	-0.010428	-0.010368	H	-0.817213	-1.403444	-2.216039
C	2.321056	1.249989	-0.003625	H	0.711145	-2.275001	-1.934342
H	3.316289	1.075401	-0.407105	O	-0.215709	0.053328	1.618109
H	1.802450	1.984985	-0.624739	C	-1.551535	0.222655	2.117061
H	2.401015	1.630706	1.015811	H	-1.469828	0.620090	3.126561
O	-0.241860	-1.597709	-0.211179	H	-2.117714	0.922674	1.497070
C	-0.297061	-2.101463	-1.554841	H	-2.069298	-0.737493	2.142480

$(MeO)_3P$**:** E = -685.855767151784 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.13153835au

G_{corr} = 0.09598413 au

P	0.014649	-0.020879	0.017530	H	-0.814509	-3.054831	-1.531785
O	1.651233	-0.014578	0.029139	H	-0.860242	-1.414331	-2.191573
C	2.310102	1.243563	-0.002726	H	0.691733	-2.245438	-1.990310
H	3.318841	1.083652	-0.378831	O	-0.220866	0.006241	1.636921
H	1.807290	1.957706	-0.661363	C	-1.541342	0.226917	2.112016
H	2.375777	1.682977	0.994319	H	-1.471902	0.599139	3.132398
O	-0.201662	-1.626542	-0.213589	H	-2.078737	0.967272	1.512336
C	-0.296280	-2.097940	-1.550322	H	-2.121428	-0.697733	2.117376

$(MeO)_3P=S$**:**

E = -1084.97756727925au (opt)
E = -1083.64317828589 au
ZPE = 0.13147754au
G_{corr} = 0.09409607 au

P	0.024760	-0.028661	-0.014707	H	-1.541800	-2.231889	-0.999508
O	0.008038	-0.025911	1.570151	H	-2.122259	-1.957280	0.668178
C	1.229703	0.011956	2.339577	O	0.212591	1.511095	-0.340321
H	0.933474	-0.098054	3.378798	C	0.422372	1.978082	-1.690885
H	1.882829	-0.807199	2.042092	H	0.613495	3.044532	-1.613427
H	1.732467	0.967244	2.191866	H	1.278634	1.469775	-2.131941
O	-1.507269	-0.248654	-0.356262	H	-0.470662	1.799576	-2.289072
C	-2.103548	-1.564172	-0.347834	S	1.273847	-1.242989	-0.856466
H	-3.116624	-1.437020	-0.718447				

$(MeO)_3P=S$**:**

E = -1083.64467557733 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.13532609au
G_{corr} = 0.09824316 au

P	0.008022	-0.011958	-0.004794	H	-1.546340	-2.212623	-1.028395
O	0.004397	0.010140	1.588559	H	-2.099636	-2.002196	0.648626
C	1.224986	0.007311	2.332576	O	0.177864	1.534733	-0.348680
H	0.951585	-0.078455	3.380488	C	0.425020	1.974093	-1.686314
H	1.853011	-0.838096	2.051701	H	0.604538	3.044310	-1.635224
H	1.778738	0.933961	2.181538	H	1.301217	1.479550	-2.105542
O	-1.534326	-0.247564	-0.328444	H	-0.436669	1.785429	-2.326658
C	-2.096093	-1.561843	-0.348472	S	1.253598	-1.217950	-0.842246
H	-3.119864	-1.458409	-0.696927				

TS(**1→10**)**:**

E = -1996.70248963458 au (opt)
E = -1994.29998151287 au

ZPE = 0.16983219au
G_{corr} = 0.12482521au
ν = -156.50 cm^{-1}

C	0.212180	-0.762559	-0.087759	H	-2.851049	2.375392	-2.446604
S	-0.390236	-0.976259	1.570021	H	-3.324601	3.389280	-1.053233
C	0.908349	-0.057290	2.340015	O	0.893552	2.806008	-0.582376
C	2.006572	0.131569	1.604098	C	1.773631	2.783462	-1.731285
S	1.978543	-0.575498	-0.016767	H	2.734504	3.143653	-1.377015
S	-0.693856	0.137067	-1.219154	H	1.869829	1.763785	-2.099198
H	0.776981	0.283162	3.357592	H	1.386040	3.441593	-2.507578
H	2.896221	0.648065	1.935936	O	-1.092939	2.396977	0.822109
P	-0.598644	2.289946	-0.667715	C	-0.643748	3.408184	1.762243
O	-1.292444	3.441424	-1.537465	H	-1.310655	3.334958	2.615858
C	-2.683257	3.320332	-1.930793	H	0.379474	3.187568	2.057004
H	-2.878457	4.149881	-2.603491	H	-0.709206	4.399092	1.315878

TS(**1→10**)**:** E = -1994.30109246173 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.17561098au
G_{corr} = 0.13357134au
ν = -182.12 cm^{-1}

C	0.242446	-0.725277	-0.076666	H	-2.855228	2.388140	-2.417962
S	-0.353333	-0.961304	1.570681	H	-3.343231	3.433179	-1.064781
C	0.940712	-0.037289	2.330863	O	0.901765	2.796192	-0.587337
C	2.032453	0.155669	1.591113	C	1.766201	2.746028	-1.728806
S	2.002454	-0.550755	-0.024138	H	2.777611	2.891425	-1.361750
S	-0.668837	0.102900	-1.216306	H	1.706080	1.777308	-2.224691
H	0.818826	0.307006	3.348540	H	1.516736	3.538193	-2.433542
H	2.918731	0.677164	1.924718	O	-1.093794	2.365141	0.833803
P	-0.603671	2.288301	-0.670320	C	-0.694233	3.390671	1.757960
O	-1.303820	3.467513	-1.511053	H	-1.392018	3.344434	2.588846
C	-2.672825	3.340590	-1.918505	H	0.313356	3.194425	2.119114
H	-2.869335	4.148187	-2.617562	H	-0.740263	4.381952	1.308102

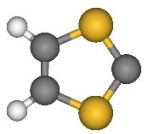
TS(**1^{PMe2}→10^{PMe2}**)**:** E = -2414.3016532224 au(optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.2439406au
G_{corr} = 0.19632099au
ν = -181.01 cm^{-1}

C	0.242446	-0.725277	-0.076666	C	2.032453	0.155669	1.591113
S	-0.353333	-0.961304	1.570681	S	2.002454	-0.550755	-0.024138
C	0.940712	-0.037289	2.330863	S	-0.668837	0.102900	-1.216306

H	0.818826	0.307006	3.348540	C	1.766201	2.746028	-1.728806
H	2.918731	0.677164	1.924718	H	2.777611	2.891425	-1.361750
P	-0.603671	2.288301	-0.670320	H	1.706080	1.777308	-2.224691
O	-1.303820	3.467513	-1.511053	H	1.516736	3.538193	-2.433542
C	-2.672825	3.340590	-1.918505	O	-1.093794	2.365141	0.833803
H	-2.869335	4.148187	-2.617562	C	-0.694233	3.390671	1.757960
H	-2.855228	2.388140	-2.417962	H	-1.392018	3.344434	2.588846
H	-3.343231	3.433179	-1.064781	H	0.313356	3.194425	2.119114
O	0.901765	2.796192	-0.587337	H	-0.740263	4.381952	1.308102

TS($\mathbf{1^{POMe2}}$→$\mathbf{10^{POMe2}}$): E = -2489.49057320876 au(optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.24845513au
G_{corr} = 0.19969166au
ν = -178.41 cm^{-1}

C	0.361438	-1.013101	-0.359027	H	1.470515	3.395084	-2.467914
S	-0.288895	-1.538512	1.193819	O	-0.656760	1.886163	1.017379
C	0.995757	-0.791064	2.157442	C	-0.198963	2.768340	2.056102
C	2.112619	-0.497363	1.481684	H	-0.636892	2.400256	2.977198
S	2.121805	-0.885684	-0.228879	H	0.886165	2.730132	2.136081
S	-0.493986	-0.019409	-1.387775	H	-0.518083	3.793786	1.872508
H	3.007656	-0.070000	1.913644	C	2.219462	0.254103	4.539991
P	-0.370026	2.091865	-0.523780	H	2.123817	0.369892	5.619744
O	-1.191983	3.372166	-1.046509	H	3.116275	-0.328263	4.334396
C	-2.610638	3.278905	-1.233807	H	2.324198	1.243715	4.096676
H	-2.909569	4.143309	-1.819459	C	0.769054	-2.237439	4.598773
H	-2.886279	2.372581	-1.775117	H	0.672247	-2.195880	5.683831
H	-3.129137	3.295354	-0.275917	H	-0.062853	-2.818496	4.201146
O	1.127298	2.638017	-0.552650	H	1.700970	-2.740331	4.343933
C	1.883153	2.668377	-1.768862	P	0.724495	-0.557865	3.923155
H	2.893467	2.962463	-1.500595	O	-0.547215	0.171167	4.245529
H	1.909118	1.683267	-2.234501				



10: E = -911.76418584835au (opt)
E = -910.70696246463 au
ZPE = 0.03909768au
G_{corr} = 0.01213345 au

C	1.623076	-1.868539	0.256323	C	0.564538	-0.208463	2.015859
S	0.326021	-1.785723	1.310156	C	1.644390	0.437552	1.542331

S	2.531760	-0.466200	0.342903	H	1.978298	1.421357	1.838959
H	-0.124174	0.164014	2.760380				

10: E = -910.708129743686 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.04066483au
G_{corr} = 0.01271652 au

C	1.620952	-1.860383	0.262641	S	2.531338	-0.465911	0.343472
S	0.326183	-1.785011	1.310384	H	-0.119130	0.165475	2.757472
C	0.566855	-0.210851	2.012549	H	1.973975	1.417322	1.840081
C	1.643735	0.433356	1.540313				

10^{PMe2}: E = -1330.70567406425 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.10892077au
G_{corr} = 0.07390656 au

C	-0.042668	0.033983	0.253126	H	4.363109	4.658608	0.625062
S	1.605462	0.123681	0.033083	H	2.716904	4.531831	-0.018928
C	1.944077	1.759161	0.576839	H	3.016885	4.431607	1.731508
C	0.833069	2.396188	0.990217	C	4.119070	2.178250	-1.143983
S	-0.632463	1.459334	0.878924	H	3.398768	2.665107	-1.801080
H	0.783817	3.406547	1.370798	H	5.099029	2.630896	-1.295952
P	3.672177	2.347904	0.638512	H	4.198086	1.126358	-1.416781
C	3.399590	4.163655	0.747434				

10^{POMe2}: E = -1405.89173204505 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.11310419au
G_{corr} = 0.07832524 au

C	0.027410	0.079953	1.340423	H	2.878332	4.620951	0.571062
S	1.674722	0.233454	1.490094	H	3.307185	3.994078	2.174023
C	1.942868	1.721256	0.607134	C	3.966057	2.458537	-1.287039
C	0.815044	2.254064	0.109156	H	3.242439	3.113188	-1.771348
S	-0.622956	1.338934	0.463227	H	4.965448	2.864902	-1.443589
H	0.737784	3.165967	-0.467742	H	3.912466	1.471229	-1.743599
C	3.592286	4.010765	1.123071	P	3.650958	2.323475	0.485045
H	4.580553	4.462172	1.033572	O	4.562405	1.393448	1.224617

TS(**10→I**): E = -1823.51655838558 au (opt)
E = -1821.39347948504 au
ZPE = 0.07803001au

G_{corr} = 0.04453874au
ν = -329.40 cm^{-1}

C	1.280563	-0.447392	0.310835	C	2.504509	0.193696	-1.336026
S	1.293784	0.689463	1.572433	S	2.489217	-0.940863	-2.599600
C	2.022982	-0.260184	2.847956	C	1.761241	0.012205	-3.873275
C	2.252880	-1.539951	2.520691	C	1.533471	1.291768	-3.543718
S	1.770852	-1.965239	0.893762	S	2.016307	1.713304	-1.916076
H	2.234796	0.198152	3.803337	H	1.548396	-0.444125	-4.829385
H	2.682091	-2.292681	3.166342	H	1.105384	2.046368	-4.187936

TS(**10→I**): E = -1821.3971892229 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.08132402au
G_{corr} = 0.04426303au
ν = -297.6 cm^{-1}

C	1.252190	-0.453062	0.320734	C	2.533221	0.202510	-1.345414
S	1.287266	0.686533	1.566783	S	2.497474	-0.936430	-2.592035
C	2.021322	-0.259076	2.834532	C	1.763559	0.010113	-3.859173
C	2.250041	-1.535899	2.507081	C	1.535394	1.286856	-3.531027
S	1.761005	-1.960212	0.888082	S	2.024895	1.710154	-1.911905
H	2.241333	0.196439	3.789281	H	1.543182	-0.444844	-4.814106
H	2.685966	-2.284438	3.152948	H	1.099624	2.035878	-4.176442

TS(**10^{PMe2}→*Z*-I^{PMe2}**): E = -2661.39378932977 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.21772824au
G_{corr} = 0.17187891au
ν = -288.74 cm^{-1}

C	0.366202	0.119202	0.548621	H	1.990240	1.043183	-6.330271
S	1.094488	1.098928	1.712018	H	0.272532	1.499669	-6.278843
C	1.292723	-0.041554	3.036957	C	3.332298	3.012688	-4.575662
C	0.743394	-1.238541	2.775649	H	3.912178	2.126034	-4.831308
S	-0.015737	-1.385015	1.210183	H	3.523390	3.786881	-5.318942
C	1.729184	-0.141797	-1.169064	H	3.668351	3.393981	-3.611775
S	1.016663	-1.110776	-2.349267	H	0.726689	-2.088514	3.443170
C	0.945600	0.016930	-3.678941	P	2.065172	0.542398	4.583425
C	1.496285	1.218975	-3.442615	C	2.275691	-1.050416	5.478428
S	2.160269	1.351730	-1.820093	H	2.780942	-1.807192	4.877402
H	0.482232	-0.297298	-4.603725	H	2.871446	-0.860429	6.371323
P	1.517046	2.678995	-4.538684	H	1.309208	-1.433476	5.804012
C	1.292803	1.866592	-6.174083	C	3.787156	0.823854	3.980915
H	1.453323	2.615126	-6.950228	H	4.417814	1.069837	4.835407

H	4.196425	-0.051933	3.477658	H	3.811887	1.671226	3.296627

TS(**10**^{POMe2}→***Z***-**I**^{POMe2})**:** E = -2811.76634651928 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.22612567au
G_{corr} = 0.17968339au
ν = -285.8 cm^{-1}

C	1.212318	-0.200681	0.266424	H	2.662470	1.392764	-6.580227
S	1.277534	0.915547	1.522681	H	2.694380	3.132353	-6.902960
C	1.664352	-0.146666	2.862783	H	3.958836	2.396235	-5.902501
C	1.704996	-1.444558	2.528848	H	1.910046	-2.269502	3.198188
S	1.369869	-1.775834	0.852741	C	0.939848	-0.356033	5.632193
C	2.789778	0.188220	-1.231593	H	1.220249	-1.408435	5.606131
S	2.711267	-0.986088	-2.442468	H	1.091365	0.018668	6.644599
C	2.314236	0.014293	-3.811453	H	-0.114640	-0.263092	5.376527
C	2.271661	1.328847	-3.551542	C	3.657465	0.276766	4.881310
S	2.632577	1.731098	-1.883260	H	3.883589	0.665821	5.874339
H	2.140404	-0.452303	-4.771972	H	3.860069	-0.793469	4.868243
C	0.190104	2.474872	-5.156998	H	4.304035	0.768550	4.155808
H	-0.089296	3.243720	-5.877709	P	1.916455	2.704035	-4.678398
H	0.030504	1.495832	-5.607211	P	1.930451	0.622638	4.483147
H	-0.447770	2.568472	-4.279091	O	2.213546	4.004559	-3.997035
C	2.899758	2.366986	-6.154350	O	1.577431	2.076865	4.415650

TS(**10**^{PMe2}→***E***-**I**^{PMe2})**:** E = -2661.39385128496 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.21770485 au
G_{corr} = 0.17184788 au
ν = -287.89 cm^{-1}

C	0.761369	-0.552418	0.368989	C	1.483618	1.720609	-6.238278
S	0.674670	0.573199	1.622703	H	1.296413	2.460896	-7.016332
C	1.307924	-0.380075	2.941571	H	2.544309	1.468371	-6.240354
C	1.576889	-1.661801	2.645334	H	0.901500	0.833279	-6.483831
S	1.205548	-2.063213	0.973142	C	2.185381	3.760331	-4.401383
H	1.439281	0.088736	3.906672	H	3.206013	3.395976	-4.516750
C	2.242994	0.102977	-1.132418	H	2.000272	4.535659	-5.144991
S	2.391627	-1.049727	-2.352251	H	2.077872	4.217947	-3.418296
C	1.876939	-0.113454	-3.731753	C	2.639728	-2.012963	5.230871
C	1.597350	1.175820	-3.479001	H	3.135536	-2.684395	5.932033
S	1.824802	1.597924	-1.787550	H	3.325898	-1.204051	4.977891
H	1.816034	-0.597997	-4.696229	H	1.765164	-1.600713	5.732772
P	0.931007	2.425678	-4.631143	C	3.777468	-3.360747	3.011117
P	2.131038	-2.994713	3.761380	H	4.388931	-2.465161	2.902468

H	4.299823	-4.072354	3.650736	H	3.650286	-3.825630	2.034068

TS(**10**^{POMe2}→***E*-I**^{POMe2}**):** E = -2811.76646361847 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.22611635au
G_{corr} = 0.18116645au
ν = -288.6 cm^{-1}

C	1.280565	-0.522421	0.157467	C	2.756927	2.798375	-5.966155
S	0.969608	0.560785	1.414251	H	2.837771	1.830108	-6.458769
C	1.505113	-0.388307	2.772544	H	2.422202	3.533883	-6.697845
C	1.900179	-1.632557	2.466974	H	3.738337	3.091440	-5.596141
S	1.777652	-2.012577	0.759797	C	1.337335	-2.988508	4.935289
H	1.483491	0.049462	3.761782	H	1.673497	-3.721954	5.668388
C	2.808708	0.323459	-1.192956	H	1.255057	-2.019355	5.425912
S	3.118891	-0.757793	-2.451529	H	0.356288	-3.283939	4.566186
C	2.585246	0.194449	-3.808341	C	4.054838	-2.293252	4.241229
C	2.191295	1.438532	-3.500625	H	3.897663	-1.341764	4.747834
S	2.313185	1.815140	-1.792678	H	4.463197	-3.008714	4.955309
H	2.607047	-0.241447	-4.798402	H	4.774754	-2.150704	3.436427
C	0.038197	2.105772	-5.274322	P	1.583094	2.749330	-4.595578
H	-0.368769	2.823072	-5.987355	P	2.510651	-2.940356	3.564231
H	0.194150	1.154903	-5.782461	O	1.449215	4.027110	-3.825045
H	-0.682281	1.962940	-4.470074	O	2.646156	-4.219465	2.796178

TS(**1**+$(MeO)_3P$→**11**)**:** E = -1996.71430044456 au (opt)
E = -1994.30891854400 au
ZPE = 0.17032567au
G_{corr} = 0.12563661au
ν = -310.97 cm^{-1}

C	-0.569869	0.335319	0.319224	H	-1.700395	1.316510	-2.539211
S	0.331783	0.166816	1.871306	H	-2.778287	2.530662	-1.808587
C	1.919824	0.151015	1.139058	O	0.821569	3.588998	0.175172
C	1.976290	-0.082399	-0.176916	C	2.082526	3.481133	-0.518457
S	0.453633	-0.341800	-0.999816	H	2.701894	4.291223	-0.143798
S	-2.249194	0.050042	0.290084	H	2.553357	2.523651	-0.302982
H	2.782362	0.306878	1.771338	H	1.928971	3.593512	-1.590951
H	2.890594	-0.146875	-0.749524	O	-1.570611	3.339604	0.690680
P	-0.405905	2.589183	-0.094381	C	-1.789537	3.158328	2.110385
O	-0.737899	2.923194	-1.614924	H	-2.539076	3.892637	2.392029
C	-1.852499	2.377691	-2.359214	H	-2.159666	2.152148	2.296523
H	-1.874468	2.922188	-3.299630	H	-0.868611	3.340135	2.662912

TS(**1**+$(MeO)_3P$→**11**): E = -1994.31370911713 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.17618599au
G_{corr} = 0.13284133au
ν = -325.3 cm^{-1}

C	-0.620568	0.322258	0.324207	H	-1.616316	1.257122	-2.530445
S	0.280973	0.146718	1.854919	H	-2.751424	2.431156	-1.840778
C	1.852947	0.177482	1.101009	O	0.823607	3.627128	0.168979
C	1.891486	-0.053840	-0.214462	C	2.087030	3.523380	-0.484028
S	0.363263	-0.357041	-1.000202	H	2.712167	4.319471	-0.087877
S	-2.290615	0.100674	0.309474	H	2.567610	2.566002	-0.282102
H	2.725060	0.358948	1.713381	H	1.987371	3.654190	-1.561613
H	2.798702	-0.088716	-0.801226	O	-1.558538	3.324700	0.701034
P	-0.377902	2.577421	-0.089410	C	-1.741381	3.148817	2.109712
O	-0.732415	2.916391	-1.616573	H	-2.482291	3.880337	2.422146
C	-1.799030	2.315904	-2.356007	H	-2.112841	2.148454	2.328946
H	-1.841144	2.833652	-3.311117	H	-0.818967	3.329186	2.662353

TS(**1**^{PMe2}+$(MeO)_3P$→**11**^{PMe2}): E = -2414.31411233686 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.24434151au
G_{corr} = 0.19668347au
ν = -318.59 cm^{-1}

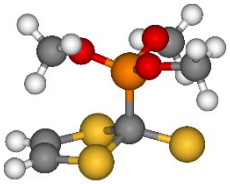
C	-0.180739	-1.056227	0.181411	H	0.599103	3.300130	-1.428697
S	0.189876	-0.725756	1.896550	H	0.474374	4.135544	0.130500
C	1.619009	0.238787	1.569819	O	-2.618763	0.939291	-0.096261
C	2.148727	0.068945	0.347984	C	-3.071815	0.656345	1.231476
S	1.352121	-1.053252	-0.726529	H	-4.139161	0.862025	1.247730
S	-1.384710	-2.159358	-0.216286	H	-2.905878	-0.390940	1.481041
H	3.038734	0.568068	-0.011328	H	-2.582933	1.292599	1.969741
P	-1.054840	0.988648	-0.457864	P	2.140816	1.448758	2.832032
O	-1.091094	1.133865	-2.055797	C	2.326117	0.322280	4.282292
C	-1.387675	0.059700	-2.952223	H	2.772158	0.888581	5.099900
H	-1.417799	0.489929	-3.950215	H	1.350727	-0.025909	4.622195
H	-0.620134	-0.711552	-2.918606	H	2.956971	-0.538717	4.062809
H	-2.353008	-0.390178	-2.724558	C	3.902907	1.685400	2.358785
O	-0.731913	2.514098	-0.031905	H	4.392222	2.253659	3.149919
C	0.495503	3.162193	-0.352485	H	4.430862	0.740836	2.225810
H	1.356719	2.606571	0.019963	H	3.979630	2.272165	1.443756

TS(**1**^{POMe2}+$(MeO)_3P$→**11**^{POMe2}): E = -2489.4999946607 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.24890577au

G_{corr} = 0.20051129au

ν = -323.58 cm^{-1}

C	-0.251552	-1.005104	0.231338	H	0.377530	4.172926	-0.385865
S	0.091847	-0.657438	1.947094	O	-2.703386	0.958452	-0.235714
C	1.578794	0.217481	1.640642	C	-3.207508	0.771155	1.091178
C	2.120985	0.035106	0.428445	H	-4.278502	0.951535	1.048203
S	1.291983	-1.030643	-0.666851	H	-3.031197	-0.248976	1.430786
S	-1.459458	-2.100840	-0.168131	H	-2.763457	1.476016	1.794941
H	3.047773	0.482063	0.093726	C	2.630167	0.095556	4.285513
P	-1.121830	1.019952	-0.504970	H	3.116211	0.627266	5.103692
O	-1.065127	1.089334	-2.107813	H	1.712662	-0.352218	4.667063
C	-1.377033	-0.002058	-2.977501	H	3.290982	-0.695963	3.934799
H	-1.374454	0.398358	-3.988355	C	3.841528	1.842861	2.333490
H	-0.634097	-0.794646	-2.906083	H	4.316859	2.433929	3.116423
H	-2.359620	-0.416719	-2.757111	H	4.502591	1.017456	2.074101
O	-0.843181	2.565932	-0.140883	H	3.702467	2.483119	1.463081
C	0.469121	3.127121	-0.101606	P	2.250245	1.265068	2.962050
H	0.869987	3.065295	0.908366	O	1.300799	2.353389	3.361401
H	1.153759	2.640903	-0.797931				



11:

E = -1996.73363289985au (opt)

E =-1994.33659290658 au

ZPE = 0.17212108au

G_{corr} = 0.12889009 au

C	-0.214497	-0.565821	0.060987	H	-1.689394	-0.805229	-3.110574
S	0.042647	-0.348366	1.897629	H	-3.033001	0.209321	-2.524335
C	1.652071	0.351226	1.786969	O	-0.287529	2.229373	-0.212094
C	2.305845	0.229308	0.633598	C	0.721563	2.912830	-0.996372
S	1.495251	-0.604264	-0.687320	H	0.743330	3.933004	-0.625103
S	-1.250005	-1.933894	-0.416942	H	1.682350	2.430261	-0.840609
H	2.065348	0.806986	2.676213	H	0.447824	2.896303	-2.048118
H	3.319598	0.568581	0.470283	O	-2.482128	1.116968	-0.034198
P	-1.042950	0.908684	-0.581230	C	-3.144262	0.563597	1.133775
O	-1.114485	0.933688	-2.136021	H	-4.194045	0.812461	1.011773
C	-2.047617	0.210935	-2.983577	H	-3.000256	-0.514117	1.147090
H	-2.062193	0.753352	-3.924626	H	-2.738665	1.030553	2.027136

11: E = -1994.34124790742 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.17818548au
G_{corr} = 0.13521538 au

C	-0.261334	-0.574936	0.080741	H	-1.349816	-0.800166	-3.201490
S	0.017035	-0.370743	1.889391	H	-2.858103	-0.098593	-2.588398
C	1.602899	0.368323	1.738482	O	-0.296156	2.223788	-0.160938
C	2.234265	0.230085	0.577502	C	0.668227	2.918143	-0.967313
S	1.409109	-0.666352	-0.690416	H	1.177748	3.610125	-0.303961
S	-1.337385	-1.904324	-0.375884	H	1.395513	2.234374	-1.400312
H	2.021414	0.867686	2.601456	H	0.166056	3.472365	-1.757601
H	3.231194	0.599957	0.380692	O	-2.526016	1.122150	-0.032342
P	-1.067551	0.908177	-0.559298	C	-3.139883	0.635203	1.173826
O	-1.109884	0.955697	-2.123935	H	-4.192877	0.888259	1.094317
C	-1.882077	0.126449	-3.010736	H	-3.021869	-0.444187	1.245536
H	-1.997429	0.697680	-3.927441	H	-2.708280	1.126579	2.042457

11^{PMe2}: E = -2414.34143498369 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.24644886au
G_{corr} = 0.19757612 au

C	-0.153269	-0.588277	0.031998	H	1.280646	2.350786	-1.356829
S	0.205558	-0.452475	1.829367	H	0.078965	3.658928	-1.470096
C	1.717171	0.447913	1.649728	O	-2.505036	0.983492	0.073266
C	2.297901	0.361345	0.451213	C	-3.028968	0.447238	1.300860
S	1.488476	-0.582854	-0.794208	H	-4.093835	0.659255	1.286793
S	-1.186441	-1.947103	-0.431563	H	-2.864599	-0.627743	1.338625
H	3.238060	0.829716	0.190957	H	-2.568117	0.935353	2.156305
P	-1.051232	0.887096	-0.498844	P	2.248581	1.485249	3.049124
O	-1.142168	1.023284	-2.056056	C	2.287461	0.214632	4.388870
C	-1.839094	0.167024	-2.979103	H	2.724568	0.667308	5.278961
H	-2.004146	0.764499	-3.871068	H	1.275925	-0.099389	4.646530
H	-1.228516	-0.700814	-3.208718	H	2.873592	-0.662123	4.113982
H	-2.791009	-0.159389	-2.568351	C	4.046960	1.646137	2.691195
O	-0.351335	2.221417	-0.039970	H	4.527274	2.103160	3.556499
C	0.601923	2.986952	-0.792651	H	4.519930	0.683820	2.493588
H	1.170815	3.564571	-0.070332	H	4.210072	2.307522	1.840886

11^{POMe2}: E = -2489.52816004088 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.25105771au
G_{corr} = 0.20299422 au

C	-0.191321	-0.628592	-0.002603	S	0.224636	-0.532333	1.788394

C	1.724231	0.373537	1.568506	O	-2.588236	0.861072	0.081652
C	2.272519	0.310624	0.352977	C	-3.061884	0.348320	1.340189
S	1.428094	-0.597995	-0.880437	H	-4.131040	0.536486	1.354584
S	-1.214315	-1.989190	-0.471492	H	-2.872458	-0.721664	1.398029
H	3.209705	0.778399	0.078598	H	-2.587443	0.867878	2.169801
P	-1.119372	0.861316	-0.457186	C	2.165813	0.370085	4.388101
O	-1.181891	1.085346	-2.004345	H	2.614726	0.878274	5.241588
C	-1.734463	0.206965	-3.002807	H	1.110075	0.209578	4.607052
H	-1.874508	0.818941	-3.888851	H	2.653096	-0.595493	4.257046
H	-1.042563	-0.604612	-3.208258	C	4.128751	1.528776	2.625151
H	-2.686657	-0.202894	-2.676845	H	4.577125	2.068545	3.459363
O	-0.493088	2.182786	0.112860	H	4.591555	0.545976	2.552429
C	0.544303	2.992006	-0.464612	H	4.331699	2.090075	1.713812
H	1.169572	3.325383	0.357730	P	2.349066	1.405437	2.918126
H	1.147482	2.439248	-1.181948	O	1.646593	2.727434	3.009389
H	0.086084	3.845956	-0.958477				

TS(**11→12**)**:** E = -1996.71754048685 au (opt)
E = -1994.32376366527 au
ZPE = 0.17212911 au
G_{corr} = 0.12986405 au
ν = -50.53 cm^{-1}

C	0.582215	-0.384034	0.569642	H	-2.040135	-0.832423	-2.800498
S	1.939013	0.752827	0.964373	H	-2.084326	0.943759	-2.815562
C	3.118227	-0.519208	1.225690	O	-0.875828	1.843024	0.207195
C	2.825852	-1.729599	0.746804	C	-1.089772	2.833892	-0.817519
S	1.302208	-1.900593	-0.105151	H	-0.937495	3.796643	-0.337722
S	-0.753857	-0.585927	1.875563	H	-0.374867	2.705839	-1.629075
H	4.025730	-0.267269	1.755961	H	-2.109057	2.771652	-1.199797
H	3.461060	-2.599764	0.831631	O	-2.517427	-0.035743	-0.382829
P	-0.952632	0.278239	-0.116203	C	-3.511206	0.084258	0.638102
O	-0.555923	0.082529	-1.668133	H	-4.469949	-0.044023	0.140909
C	-1.433667	0.070991	-2.805514	H	-3.379240	-0.695552	1.389114
H	-0.788375	0.080980	-3.681572	H	-3.465106	1.064903	1.112130

TS(**11→12**)**:** E = -1994.3276057047 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.17825457 au
G_{corr} = 0.13692238 au
ν = -44.54 cm^{-1}

C	0.501364	-0.320720	0.537533	C	3.022605	-0.348852	1.179256
S	1.800371	0.873322	0.898764	C	2.772415	-1.572180	0.717901

S	1.262618	-1.798209	-0.140809	O	-1.081380	1.837845	0.165659
S	-0.777511	-0.544178	1.857287	C	-0.661922	2.792964	-0.813943
H	3.920499	-0.063082	1.708973	H	-0.592523	3.747333	-0.298614
H	3.439736	-2.416133	0.820513	H	0.314235	2.548827	-1.232579
P	-1.077969	0.256130	-0.122240	H	-1.389878	2.882656	-1.620375
O	-0.704554	0.035930	-1.684589	O	-2.633615	-0.151978	-0.338851
C	-1.591414	0.090277	-2.797495	C	-3.595812	-0.110961	0.700175
H	-0.967997	0.149754	-3.687624	H	-4.558226	-0.324403	0.240309
H	-2.204516	-0.807961	-2.856786	H	-3.395534	-0.871392	1.457617
H	-2.245149	0.962446	-2.771411	H	-3.640400	0.867967	1.178868

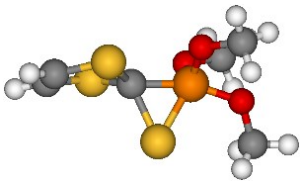
TS(**11^{PMe2}→12^{PMe2}**)**:** E = -2414.32890593638 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.24667978 au
G_{corr} = 0.19984356 au
ν = -50.69 cm^{-1}

C	0.891464	-0.327943	0.120895	H	-2.501656	2.545300	0.324760
S	2.126359	0.850767	0.666170	H	-1.482310	1.990696	1.679038
C	3.334487	-0.389297	1.006664	O	-2.272328	-0.058948	-0.781081
C	3.144723	-1.557752	0.384507	C	-3.214717	-0.455140	0.198743
S	1.745727	-1.689291	-0.664247	H	-4.171888	-0.542039	-0.311470
S	-0.425803	-0.763796	1.354416	H	-2.958375	-1.425741	0.626377
H	3.798687	-2.415312	0.461571	H	-3.314287	0.271678	1.005537
P	-0.695821	0.255885	-0.516338	P	4.720958	0.124857	2.068432
O	-0.295076	0.137109	-2.076614	C	5.707623	-1.425489	2.135379
C	-1.150669	0.416024	-3.180345	H	6.517870	-1.283067	2.850315
H	-0.512124	0.474063	-4.059622	H	5.117758	-2.287366	2.450021
H	-1.883349	-0.375902	-3.328902	H	6.155967	-1.631225	1.164043
H	-1.670547	1.367659	-3.064394	C	3.891125	0.075398	3.717026
O	-0.618602	1.830724	-0.212115	H	3.439814	-0.896417	3.917291
C	-1.482463	2.489315	0.708201	H	4.625747	0.294391	4.492065
H	-1.098466	3.498538	0.833051	H	3.117092	0.840479	3.762061

TS(**11^{POMe2}→12^{POMe2}**)**:** E = -2489.51695520336 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.25089708 au
G_{corr} = 0.20408374 au
ν = -51.75 cm^{-1}

C	0.830970	-0.332681	0.207294	S	-0.523052	-0.679353	1.421955
S	2.088474	0.836058	0.725824	H	3.683947	-2.482007	0.662097
C	3.249524	-0.427750	1.119030	P	-0.719931	0.272769	-0.497487
C	3.045783	-1.616463	0.543721	O	-0.281266	0.078862	-2.038790
S	1.654111	-1.760411	-0.499985	C	-1.097636	0.343297	-3.176020

H	-0.433985	0.348762	-4.038290	H	-3.366417	0.423283	0.959188
H	-1.850973	-0.430564	-3.315518	C	5.887139	-1.152863	2.009154
H	-1.589257	1.314352	-3.108824	H	6.695257	-0.932926	2.706858
O	-0.601128	1.853793	-0.251470	H	5.543353	-2.169904	2.193308
C	-1.463774	2.575509	0.622490	H	6.273799	-1.082535	0.993549
H	-1.051896	3.577218	0.713297	C	3.893293	-0.254723	3.899271
H	-2.472512	2.644570	0.214596	H	3.614190	-1.300552	4.019726
H	-1.497948	2.118038	1.612686	H	4.636839	0.004574	4.653265
O	-2.295705	-0.011641	-0.787985	H	3.010684	0.365785	4.051420
C	-3.273627	-0.337615	0.183746	P	4.568357	0.056062	2.250786
H	-4.220997	-0.412424	-0.346090	O	4.959382	1.485308	2.016476
H	-3.059810	-1.298753	0.653754				



12: E = -1996.72133928763au (opt)
E =-1994.32791747147 au
ZPE = 0.17221589au
G_{corr} = 0.13028034 au

C	0.757200	-0.314143	0.317811	H	-2.150146	-1.272462	-2.532474
S	1.820072	0.688138	1.349156	H	-2.052513	0.381863	-3.181710
C	3.022751	-0.570295	1.573172	O	-0.445398	1.856776	-0.132560
C	2.994128	-1.586211	0.706638	C	-1.310753	2.979277	-0.375868
S	1.758017	-1.523769	-0.537966	H	-0.685641	3.861845	-0.260891
S	-0.816466	-1.030255	1.214012	H	-1.718694	2.943343	-1.384043
H	3.740555	-0.457972	2.373238	H	-2.121610	3.010558	0.349513
H	3.685416	-2.416843	0.701977	O	-2.441361	0.505239	-0.634527
P	-0.826895	0.314265	-0.378724	C	-3.403936	0.471860	0.413791
O	-0.513716	-0.156218	-1.876550	H	-4.360847	0.733740	-0.034330
C	-1.478111	-0.494605	-2.889411	H	-3.470310	-0.530161	0.843011
H	-0.898006	-0.861818	-3.733016	H	-3.168295	1.183253	1.207290

12: E = -1994.33173339296 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.17866825au
G_{corr} = 0.13661165 au

C	0.748160	-0.301741	0.312462	S	1.708487	-1.554012	-0.514660
S	1.845541	0.742165	1.251335	S	-0.765299	-0.935062	1.256100
C	3.005585	-0.540557	1.541822	H	3.729947	-0.417203	2.334573
C	2.942137	-1.596158	0.730940	H	3.607818	-2.446539	0.775527

P	-0.821943	0.324859	-0.394168	H	-0.662926	3.875757	-0.224075
O	-0.517952	-0.224742	-1.874492	H	-1.753622	3.020236	-1.323974
C	-1.468485	-0.503338	-2.900258	H	-2.057447	3.009486	0.427091
H	-0.900107	-0.918251	-3.729743	O	-2.439794	0.518861	-0.632426
H	-2.207872	-1.235494	-2.579637	C	-3.394061	0.427569	0.405213
H	-1.976913	0.398791	-3.237031	H	-4.364370	0.658941	-0.030676
O	-0.412976	1.873229	-0.196373	H	-3.439667	-0.582285	0.821711
C	-1.285188	2.991358	-0.341387	H	-3.203611	1.129535	1.219665

12^{PMe2}: E = -2414.33135632539 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.24692344au
G_{corr} = 0.19918918 au

C	1.046946	-0.096079	0.066734	H	-2.121661	2.936016	-0.773459
S	2.032896	0.945754	1.119366	H	-2.277093	2.561362	0.957106
C	3.398894	-0.173210	1.153081	O	-2.306580	0.263316	-0.518524
C	3.436449	-1.048614	0.141829	C	-3.129589	-0.177017	0.542147
S	2.138741	-0.968310	-1.035441	H	-4.161536	-0.066393	0.213770
S	-0.234753	-1.161749	0.953751	H	-2.956855	-1.231480	0.773811
H	4.215821	-1.781711	-0.014405	H	-2.991602	0.405442	1.455323
P	-0.665295	0.340359	-0.415581	P	4.620594	0.095122	2.474118
O	-0.406757	0.132277	-1.988840	C	5.827357	-1.246259	2.118721
C	-1.383026	-0.138950	-2.992247	H	6.558527	-1.271117	2.926575
H	-0.829220	-0.277354	-3.918181	H	5.356997	-2.227907	2.048779
H	-1.942180	-1.048296	-2.777642	H	6.363776	-1.037937	1.193649
H	-2.077508	0.690395	-3.116805	C	3.706979	-0.635195	3.902796
O	-0.516184	1.876969	0.053923	H	3.393068	-1.660131	3.704887
C	-1.577915	2.822063	0.163137	H	4.351485	-0.622633	4.781867
H	-1.110736	3.771714	0.414213	H	2.826879	-0.032290	4.122979

12^{POMe2}: E = -2489.51948351281 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.25116475au
G_{corr} = 0.20346862 au

C	0.991004	-0.138477	0.114735	C	-1.402490	-0.221420	-2.973499
S	2.010129	0.918499	1.121113	H	-0.844170	-0.429277	-3.883478
C	3.328426	-0.248921	1.198046	H	-2.007406	-1.091854	-2.724792
C	3.344785	-1.174488	0.233294	H	-2.053887	0.633766	-3.146077
S	2.049374	-1.117400	-0.936534	O	-0.482458	1.895730	-0.014195
S	-0.339445	-1.104303	1.031763	C	-1.502239	2.891025	0.043528
H	4.106001	-1.934182	0.114951	H	-0.994396	3.829667	0.252942
P	-0.695576	0.348006	-0.412741	H	-2.036018	2.983789	-0.900968
O	-0.426476	0.049853	-1.968995	H	-2.215290	2.698495	0.844473

O	-2.335822	0.334629	-0.531095	H	6.416897	-0.459745	1.164143
C	-3.188147	-0.025534	0.537299	C	3.791575	-0.948362	3.931967
H	-4.210705	0.115969	0.192263	H	3.659112	-1.998460	3.675366
H	-3.063663	-1.076016	0.813396	H	4.450315	-0.873535	4.797454
H	-3.033844	0.587648	1.427392	H	2.822626	-0.523845	4.193018
C	5.991952	-0.912461	2.058794	P	4.499694	-0.022092	2.549490
H	6.721858	-0.843703	2.865406	O	4.692686	1.437827	2.836838
H	5.790784	-1.965751	1.867734				

TS(**12→13**)**:** E = -1996.72008658910 au (opt)
E = -1994.32364803450 au
ZPE = 0.17176371 au
G_{corr} = 0.13031720 au
ν = -183.67 cm^{-1}

C	0.849271	0.182493	0.189686	H	-2.102167	-0.966686	-2.460900
S	1.836582	1.101961	1.294829	H	-2.059420	0.633578	-3.237016
C	3.086029	-0.106923	1.467761	O	-0.407889	2.281754	-0.170617
C	3.056781	-1.115941	0.590441	C	-1.274829	3.420514	-0.284168
S	1.773678	-1.071452	-0.594362	H	-0.627897	4.291349	-0.200731
S	-0.973581	-0.586882	1.143839	H	-1.786496	3.428321	-1.243938
H	3.826511	0.026432	2.243104	H	-2.005754	3.435351	0.523002
H	3.769911	-1.926236	0.545200	O	-2.425459	1.018772	-0.754193
P	-0.830213	0.739236	-0.413201	C	-3.464668	0.982284	0.215251
O	-0.495168	0.246532	-1.910518	H	-4.361454	1.361752	-0.273614
C	-1.455418	-0.198652	-2.882120	H	-3.641876	-0.040538	0.553257
H	-0.871770	-0.615479	-3.700502	H	-3.239906	1.604198	1.083844

TS(**12→13**)**:** E = -1994.32658481823 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.17808984 au
G_{corr} = 0.13638415 au
ν = -195.92 cm^{-1}

C	0.877468	0.214426	0.154250	C	-1.453908	-0.275185	-2.834046
S	1.855636	1.136452	1.221603	H	-0.883793	-0.781079	-3.611209
C	3.115074	-0.050681	1.394344	H	-2.166839	-0.982971	-2.411167
C	3.052583	-1.095281	0.564563	H	-1.997800	0.555897	-3.280308
S	1.722175	-1.100304	-0.555721	O	-0.361882	2.286782	-0.193802
S	-1.054131	-0.492133	1.194811	C	-1.211575	3.426539	-0.176498
H	3.888417	0.114374	2.130589	H	-0.563945	4.282274	0.005402
H	3.767743	-1.904214	0.526755	H	-1.725067	3.571326	-1.125655
P	-0.845031	0.744188	-0.394746	H	-1.948076	3.380869	0.626298
O	-0.502087	0.166385	-1.873432	O	-2.422513	1.091275	-0.776512

C	-3.508687	0.978083	0.114060	H	-3.714349	-0.062892	0.373888
H	-4.383743	1.386517	-0.391626	H	-3.360871	1.535089	1.042494

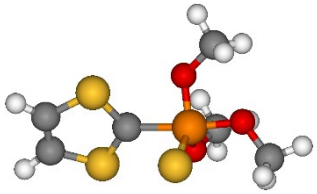
TS(**12^{PMe2}→13^{PMe2}**): E = -2414.32522597997 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.24623917 au
G_{corr} = 0.19875646 au
ν = -179.35 cm^{-1}

C	0.051746	0.050532	0.523206	H	-0.488788	-4.225402	1.542627
S	1.756846	0.067789	0.665063	H	0.501534	-4.179622	0.068843
C	1.952234	1.808278	0.658298	O	-1.862080	-2.849787	-0.181976
C	0.805376	2.492842	0.781439	C	-1.870287	-3.464622	-1.449712
S	-0.656884	1.559458	0.909420	H	-2.456345	-4.379458	-1.360229
S	-0.607415	-0.681563	-1.589115	H	-2.334977	-2.828708	-2.206694
H	0.719563	3.569296	0.828702	H	-0.871403	-3.733221	-1.802167
P	-0.955355	-1.517836	0.219024	P	3.662527	2.447118	0.615780
O	-2.087749	-0.919384	1.219450	C	3.343967	4.256761	0.581359
C	-3.471457	-1.248022	1.191911	H	4.295955	4.762882	0.421788
H	-3.966137	-0.520832	1.833401	H	2.659568	4.550538	-0.215331
H	-3.892780	-1.168409	0.189634	H	2.949465	4.591675	1.539966
H	-3.660937	-2.247465	1.580258	C	4.062592	2.134407	-1.158705
O	0.216603	-2.329747	1.008997	H	3.323554	2.571611	-1.829841
C	0.358707	-3.743368	1.057931	H	5.040340	2.564186	-1.376982
H	1.254191	-3.935560	1.646183	H	4.121774	1.062626	-1.344670

TS(**12^{POMe2}→13^{POMe2}**): E = -2489.51136686424 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.25043437 au
G_{corr} = 0.20310655 au
ν = -147.25 cm^{-1}

C	0.043538	0.021788	0.354782	O	0.139849	-2.273312	1.142820
S	1.733176	0.037205	0.591907	C	0.291525	-3.672625	1.343481
C	1.939439	1.758449	0.388725	H	1.158271	-3.791622	1.990987
C	0.805440	2.470192	0.335263	H	-0.575247	-4.114162	1.832471
S	-0.671432	1.572326	0.459711	H	0.487637	-4.204446	0.411818
S	-0.521632	-1.007849	-1.699863	O	-1.885878	-2.935254	-0.063849
H	0.741013	3.546238	0.244647	C	-1.876328	-3.711095	-1.239992
P	-0.976501	-1.569275	0.185854	H	-2.481116	-4.597013	-1.045471
O	-2.147188	-0.818763	1.029978	H	-2.311555	-3.173723	-2.085510
C	-3.532611	-1.138180	0.981670	H	-0.874654	-4.038864	-1.528227
H	-4.047034	-0.320884	1.484098	C	3.658940	3.919337	1.186428
H	-3.904063	-1.204047	-0.041113	H	4.658928	4.350117	1.134546
H	-3.754749	-2.068004	1.502744	H	2.958503	4.624384	0.740212

H	3.395327	3.765898	2.231721	H	3.848995	1.800440	-2.012526
C	3.947300	2.711283	-1.423279	P	3.656531	2.338153	0.319083
H	3.236323	3.449685	-1.791697	O	4.553286	1.282738	0.891753
H	4.958002	3.101146	-1.545984				



13: E = -1996.72310589691au (opt)
E =-1994.32482085479 au
ZPE = 0.17236047au
G_{corr} = 0.12808551 au

C	-0.003314	-0.008093	-0.004073	H	-4.019340	-1.349786	0.075650
S	1.685560	-0.010426	-0.002759	H	-3.520301	-2.275283	1.508557
C	1.926344	1.703570	0.014658	O	0.176374	-2.472592	0.361527
C	0.804476	2.440506	0.089272	C	0.028965	-3.150140	1.614406
S	-0.669215	1.535384	0.155809	H	0.958041	-3.689085	1.787232
S	-0.942527	-1.180420	-2.237831	H	-0.130308	-2.430926	2.421025
H	2.934322	2.090376	-0.019142	H	-0.805567	-3.850553	1.582789
H	0.758976	3.519076	0.126651	O	-2.079109	-2.998917	-0.369326
P	-1.085818	-1.657393	-0.295076	C	-1.751538	-4.117247	-1.177503
O	-2.090501	-0.946659	0.767094	H	-2.508937	-4.878831	-0.990313
C	-3.458885	-1.311905	1.007979	H	-1.757326	-3.846692	-2.235525
H	-3.858135	-0.527918	1.649491	H	-0.766979	-4.519574	-0.923644

13: E = -1994.3295933313 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.17835445au
G_{corr} = 0.13580016 au

C	-0.023801	-0.046757	-0.003215	H	-3.864049	-0.532987	1.626070
S	1.655883	-0.075126	0.014389	H	-4.056591	-1.394979	0.093010
C	1.910597	1.632537	0.061939	H	-3.529881	-2.270518	1.544483
C	0.797739	2.377580	0.132548	O	0.178800	-2.505119	0.305596
S	-0.682612	1.488492	0.166444	C	0.104836	-3.009193	1.630345
S	-0.943784	-1.189909	-2.249158	H	1.014331	-3.579398	1.808577
H	2.920325	2.016352	0.047458	H	0.052591	-2.203490	2.367552
H	0.767827	3.456251	0.184050	H	-0.753044	-3.669477	1.770091
P	-1.102298	-1.683163	-0.329353	O	-2.090282	-3.028709	-0.404048
O	-2.110490	-0.964039	0.735628	C	-1.789659	-4.124725	-1.232997
C	-3.460088	-1.328986	1.002353	H	-2.584382	-4.861038	-1.107875

H	-1.746092	-3.836371	-2.286460	H	-0.840616	-4.600755	-0.970478

13^{PMe2}: E = -2414.32733999946 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.24639741au
G_{corr} = 0.19757946 au

C	0.000367	0.053096	0.319679	H	0.253764	-2.520114	2.182909
S	1.677022	0.048621	0.222571	H	-0.595695	-3.852331	1.370777
C	1.954528	1.729607	0.580294	O	-2.081509	-2.810290	-0.559390
C	0.832861	2.410553	0.882837	C	-1.832132	-3.704561	-1.616269
S	-0.641697	1.507646	0.854535	H	-2.618470	-4.460102	-1.602027
S	-1.058301	-0.608995	-2.045251	H	-1.851879	-3.201331	-2.586428
H	0.783035	3.456202	1.151877	H	-0.869325	-4.213477	-1.515907
P	-1.091693	-1.496801	-0.265629	P	3.685672	2.323046	0.625127
O	-2.027133	-1.032888	0.989952	C	3.403177	4.130835	0.794231
C	-3.352634	-1.470998	1.266886	H	4.366064	4.630080	0.686446
H	-3.713053	-0.832319	2.071866	H	2.722405	4.525489	0.039275
H	-4.013017	-1.354528	0.408181	H	3.022024	4.366255	1.787196
H	-3.379954	-2.506959	1.600489	C	4.089879	2.203916	-1.171289
O	0.229058	-2.414497	0.097832	H	3.358993	2.717487	-1.795314
C	0.250950	-3.166739	1.301315	H	5.071135	2.650568	-1.332260
H	1.170059	-3.749184	1.299776	H	4.149448	1.159706	-1.476427

13^{POMe2}: E = -2489.51237498243 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.25049228au
G_{corr} = 0.20179833 au

C	0.014332	0.004592	0.052107	H	1.017185	-3.575585	1.850001
S	1.692065	-0.021933	0.117262	H	0.001592	-2.249304	2.433178
C	1.940897	1.695661	0.146474	H	-0.745142	-3.704584	1.740643
C	0.817121	2.431042	0.189313	O	-2.043774	-2.968632	-0.401881
S	-0.660026	1.539293	0.205638	C	-1.726483	-4.053057	-1.240943
S	-0.855466	-1.103767	-2.194821	H	-2.525422	-4.788925	-1.145025
H	0.769304	3.511014	0.230800	H	-1.658508	-3.748274	-2.288418
P	-1.056199	-1.628851	-0.285594	H	-0.784455	-4.534802	-0.964256
O	-2.080150	-0.919119	0.769089	C	3.789722	3.426833	1.498032
C	-3.431734	-1.290892	1.017784	H	4.795096	3.847538	1.521552
H	-3.842980	-0.505525	1.649992	H	3.075490	4.240800	1.378746
H	-4.019122	-1.343834	0.101737	H	3.597758	2.919141	2.441970
H	-3.504256	-2.240915	1.544313	C	3.849537	3.194579	-1.383487
O	0.211738	-2.452894	0.366528	H	3.135124	4.016124	-1.421389
C	0.100800	-3.019380	1.663853	H	4.858439	3.603999	-1.438223

H	3.686922	2.542544	-2.240433	O	4.557796	1.041349	0.252311
P	3.674836	2.246027	0.140336				

TS(**13**→**10**+$(MeO)_3PS$)**:** E = -1996.71759482398 au (opt)
E = -1994.31957417465 au
ZPE = 0.17152429 au
G_{corr} = 0.12904365 au
ν = -120.61 cm^{-1}

C	0.946483	0.480134	0.256418	H	-2.436718	-0.750329	-2.250473
S	1.921889	1.157302	1.445553	H	-2.586495	0.995470	-2.578418
C	3.280727	0.081884	1.338485	O	-0.866499	2.401146	0.362814
C	3.171263	-0.863892	0.388821	C	-0.250423	3.200165	-0.654011
S	1.698773	-0.798240	-0.529749	H	0.026799	4.138962	-0.180380
S	-1.370801	-0.419980	1.573917	H	0.641242	2.706823	-1.043805
H	4.119215	0.214969	2.006576	H	-0.950501	3.390019	-1.468732
H	3.907110	-1.622684	0.165408	O	-2.865606	1.283294	-0.180622
P	-1.290485	0.872695	0.078078	C	-3.975846	0.413144	0.031487
O	-0.923305	0.433971	-1.436036	H	-4.834519	0.890485	-0.440235
C	-1.890565	0.167788	-2.466024	H	-3.821690	-0.570782	-0.413507
H	-1.313639	0.037854	-3.379048	H	-4.161605	0.285540	1.097819

TS(**13**→**10**+$(MeO)_3PS$)**:** E = -1994.3245986887 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.17746726 au
G_{corr} = 0.13611816 au
ν = -119.57 cm^{-1}

C	0.958990	0.528034	0.251939	H	-2.434807	-0.775671	-2.151739
S	1.905881	1.111006	1.502124	H	-2.497868	0.894372	-2.758225
C	3.266870	0.051130	1.332664	O	-0.913521	2.411871	0.362670
C	3.171052	-0.819980	0.317214	C	-0.242968	3.224113	-0.589041
S	1.711783	-0.690018	-0.609940	H	-0.017987	4.165981	-0.093973
S	-1.392726	-0.431684	1.495163	H	0.693872	2.771610	-0.920964
H	4.099556	0.131585	2.016432	H	-0.868980	3.425818	-1.459802
H	3.915092	-1.557027	0.051680	O	-2.901859	1.276656	-0.252175
P	-1.329037	0.885144	0.042387	C	-4.007983	0.452720	0.056514
O	-0.898788	0.474099	-1.469423	H	-4.886621	0.928649	-0.377925
C	-1.836475	0.079904	-2.467786	H	-3.922097	-0.554315	-0.356917
H	-1.245252	-0.219805	-3.330468	H	-4.151322	0.361549	1.133928

TS($\mathbf{13^{PMe2}}$→$\mathbf{10^{PMe2}}$+$(MeO)_3PS$)**:** E = -2414.32618511771 au (optimized with $CPCM_{THF}$/PBEh-3c)
ZPE = 0.24561768 au

G_{corr} = 0.19665983 au

ν = -118.79 cm^{-1}

C	0.167813	-0.013755	0.557500	H	0.406929	-2.320666	2.150940
S	1.810006	0.091118	0.277213	H	-0.557568	-3.749845	1.710492
C	2.078486	1.771479	0.677838	O	-2.170674	-3.010445	-0.615236
C	0.960421	2.393961	1.098300	C	-1.965987	-3.841954	-1.739278
S	-0.469471	1.410215	1.146411	H	-2.742893	-4.605142	-1.723665
S	-1.052972	-0.718709	-1.955835	H	-2.041192	-3.280270	-2.672449
H	0.890092	3.428703	1.402650	H	-0.993426	-4.339125	-1.710848
P	-1.168108	-1.745226	-0.293327	P	3.780308	2.435451	0.596924
O	-2.014116	-1.251364	0.991674	C	3.437699	4.235758	0.743239
C	-3.425218	-1.431762	1.115854	H	4.367580	4.771047	0.550916
H	-3.737921	-0.773572	1.923754	H	2.684777	4.580475	0.033755
H	-3.956135	-1.144125	0.208145	H	3.121826	4.482539	1.756171
H	-3.681943	-2.457892	1.372442	C	4.075079	2.290340	-1.219077
O	0.143699	-2.606928	0.104835	H	3.282227	2.753930	-1.805586
C	0.288740	-3.124417	1.420744	H	5.021419	2.777917	-1.453620
H	1.189519	-3.733670	1.422279	H	4.164952	1.242929	-1.505293

TS(**13^{POMe2}→10^{POMe2}**+$(MeO)_3PS$)**:**E = -2489.51185801544 au (optimized with $CPCM_{THF}$/PBEh-3c)

ZPE = 0.24982237 au

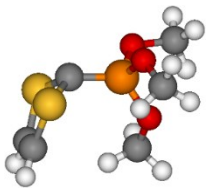
G_{corr} = 0.20156181 au

ν = -117.9 cm^{-1}

C	0.122024	-0.013258	0.280577	H	-0.774149	-3.468046	2.095668
S	1.785811	0.015139	0.178227	O	-2.140935	-3.186076	-0.439761
C	2.033334	1.738901	0.227555	C	-1.842490	-4.237059	-1.336340
C	0.901165	2.451988	0.358112	H	-2.632823	-4.980078	-1.239095
S	-0.548707	1.507967	0.452333	H	-1.812828	-3.886031	-2.369746
S	-0.868106	-1.220633	-2.117080	H	-0.888128	-4.715755	-1.104624
H	0.834012	3.530371	0.413564	C	3.950296	3.471361	1.478830
P	-1.152197	-1.879333	-0.294808	H	4.947520	3.909654	1.436689
O	-2.104283	-1.129791	0.774781	H	3.215268	4.274445	1.438528
C	-3.518394	-1.318853	0.840942	H	3.840577	2.935202	2.420296
H	-3.895161	-0.511623	1.465529	C	3.784800	3.317815	-1.403951
H	-3.987626	-1.247401	-0.140302	H	3.053189	4.123891	-1.363286
H	-3.779551	-2.272522	1.295827	H	4.777923	3.750634	-1.525706
O	0.106273	-2.634898	0.390349	H	3.568896	2.686029	-2.264390
C	0.105682	-2.900508	1.787218	P	3.749342	2.323735	0.101530
H	0.993677	-3.492577	1.995445	O	4.670993	1.143108	0.108284
H	0.156632	-1.975537	2.365995				

TS(**10**+$(MeO)_3P$→**14**): E = -1598.51219248647 au (opt)
E = -1596.54238168945 au
ZPE = 0.16690045 au
G_{corr} = 0.12359805 au
ν = -246.74cm^{-1}

C	0.536485	-0.392974	-0.717973	P	-1.474222	0.359948	-1.160386
S	0.519396	-1.780948	0.292879	O	-2.975502	0.995311	-0.822765
C	1.243845	-1.099414	1.742368	O	-2.003370	-0.897114	-2.033145
C	1.746904	0.130257	1.585285	C	-3.042673	2.036036	0.158795
S	1.566634	0.796746	-0.030970	C	-2.886246	-1.859206	-1.432633
H	1.285224	-1.690287	2.646219	H	-4.069993	2.081324	0.515417
H	2.263755	0.703074	2.342044	H	-2.377284	1.826222	1.000609
H	-2.633968	2.410219	-2.933802	H	-2.769181	2.998440	-0.280069
C	-1.798774	1.850113	-3.353345	H	-2.890779	-2.728556	-2.086226
O	-0.942084	1.352137	-2.310221	H	-2.532197	-2.154876	-0.443094
H	-1.184923	2.504596	-3.967502	H	-3.892181	-1.448662	-1.351010
H	-2.178080	1.024823	-3.955552				



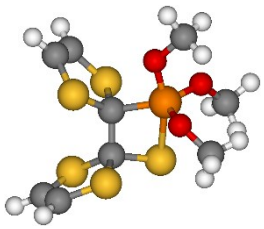
14: E = -1598.54610894151au (opt)
E =-1596.58220119679 au
ZPE = 0.17052754au
G_{corr} = 0.12768362 au

C	0.354695	-0.330324	-0.839997	P	-1.151391	0.106970	-1.472740
S	0.340590	-1.714369	0.273088	O	-2.364062	0.683276	-0.600763
C	0.525298	-0.699225	1.730061	O	-1.859942	-1.115009	-2.168217
C	1.023921	0.520120	1.525221	C	-2.152345	1.712118	0.391669
S	1.400401	0.936869	-0.168022	C	-2.920786	-1.904345	-1.577964
H	0.310367	-1.127482	2.699186	H	-3.136284	1.969862	0.773129
H	1.268705	1.228247	2.304812	H	-1.523395	1.329197	1.192726
H	-2.530982	2.453690	-2.578790	H	-1.686806	2.588543	-0.058969
C	-1.945475	1.862295	-3.280538	H	-3.109657	-2.712723	-2.278338
O	-0.870341	1.181311	-2.593193	H	-2.596825	-2.305644	-0.619836
H	-1.469687	2.509952	-4.010675	H	-3.811419	-1.293083	-1.453400
H	-2.583793	1.136966	-3.783525				

TS(**14**+**1**→**15**): E = -2908.51284991663 au (opt)
E = -2905.04766544769 au

ZPE = 0.21229415 au
G_{corr} = 0.16300416 au
ν = -234.64 cm^{-1}

S	0.383213	1.495015	-0.439153	C	4.750944	-1.630809	-3.411131
C	3.271202	0.395209	-0.165111	O	4.548409	-0.816224	-2.225318
S	3.960200	2.040504	-0.413388	H	5.819946	-1.621269	-3.598295
C	5.567778	1.666791	0.204966	H	4.407279	-2.644949	-3.217803
C	5.731095	0.500631	0.822610	P	3.113625	-0.465941	-1.691594
S	4.324159	-0.549360	0.959522	O	2.306781	0.240324	-2.822913
H	6.331135	2.424849	0.100163	O	2.384060	-1.835165	-1.512942
H	6.647671	0.174030	1.293851	C	2.484531	1.565214	-3.382441
C	1.345979	0.757614	0.780605	C	0.970370	-2.068307	-1.777365
S	1.907736	1.772379	2.147970	H	1.955522	1.553023	-4.330887
C	1.944944	0.528044	3.367942	H	2.038507	2.286707	-2.703271
C	1.477092	-0.674896	3.030516	H	3.541349	1.769534	-3.535805
S	0.855420	-0.853714	1.411916	H	0.681327	-2.895320	-1.137318
H	2.349338	0.782850	4.337381	H	0.390054	-1.177961	-1.544092
H	1.446868	-1.534874	3.684458	H	0.859745	-2.334561	-2.825810
H	4.216209	-1.201409	-4.256881				

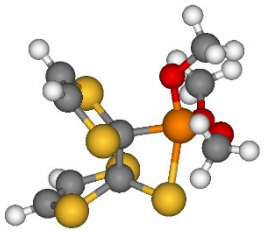


15:

E = -2908.54416391233au (opt)
E =-2905.08921701006 au
ZPE = 0.21392731au
G_{corr} = 0.16451824 au

S	2.674941	0.570051	-2.886145	H	-2.028591	-1.142979	-1.452745
C	2.428616	-0.259045	-0.482579	H	-0.730805	-3.278884	-2.010124
S	2.314364	1.434937	0.257755	H	6.758996	-0.043243	0.456646
C	2.021077	0.910825	1.902567	C	6.201411	-0.979383	0.438081
C	1.872474	-0.389046	2.134568	O	4.810095	-0.727023	0.229222
S	1.967415	-1.494549	0.780524	H	6.285239	-1.478835	1.401297
H	1.956772	1.685360	2.654023	H	6.599322	-1.628858	-0.343035
H	1.674876	-0.819699	3.106414	P	4.193062	-0.300184	-1.196399
C	1.593130	-0.362808	-1.782979	O	5.257457	0.872244	-1.431795
S	-0.102781	0.339161	-1.628824	O	4.573485	-1.627246	-1.997072
C	-0.968072	-1.181386	-1.659429	C	5.354885	1.805960	-2.514205
C	-0.294941	-2.291444	-1.950085	C	4.956916	-1.721561	-3.379176
S	1.409583	-2.136258	-2.312591	H	6.338618	2.260082	-2.416341

H	5.279500	1.309123	-3.479839	H	4.177779	-1.315410	-4.020511
H	4.582365	2.566316	-2.424545	H	5.895569	-1.191443	-3.539429
H	5.094371	-2.781174	-3.577355				



15^{sp}:

E = -2908.53797243782au (opt)
E =-2905.08345846636 au
ZPE = 0.21380761 au
G_{corr} = 0.16495226 au

S	0.307368	-1.266824	0.227733	C	3.313854	-0.242860	-3.612030
C	2.638160	-0.251246	0.266631	O	3.152733	-0.159062	-2.192465
S	3.801772	1.136010	0.493788	H	4.208341	0.327611	-3.855489
C	5.266380	0.176871	0.566355	H	3.447712	-1.279596	-3.919376
C	5.154423	-1.146983	0.568278	P	1.752959	-0.455021	-1.418112
S	3.552395	-1.847260	0.486802	O	0.837438	0.792609	-1.783930
H	6.202598	0.713508	0.632711	O	1.218661	-1.594356	-2.439370
H	5.982814	-1.837650	0.642676	C	1.322387	2.069414	-2.256546
C	1.389517	-0.186574	1.191062	C	1.598633	-2.975151	-2.343440
S	0.715949	1.541657	1.284927	H	1.010368	2.188503	-3.292595
C	1.212628	1.868286	2.931080	H	0.860585	2.832511	-1.634978
C	1.636264	0.840132	3.661488	H	2.403966	2.133564	-2.177257
S	1.703643	-0.742707	2.916987	H	1.095174	-3.484420	-3.161327
H	1.117650	2.882876	3.291737	H	2.678751	-3.088355	-2.441238
H	1.930485	0.903689	4.699854	H	1.272785	-3.391732	-1.389997
H	2.458570	0.177993	-4.140760				

TS(**15**→**I**+$(MeO)_3PS$)**:**

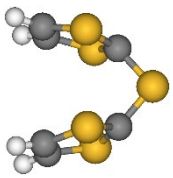
E = -2908.52377445964 au (opt)
E = -2905.06434040452 au
ZPE = 0.21393194 au
G_{corr} = 0.16547655 au
ν = -154.98 cm^{-1}

S	0.995151	-1.587833	0.057783	H	6.535489	1.309352	1.186643
C	3.257082	-0.102969	0.181446	H	6.401655	-1.170446	1.819181
S	4.427946	1.300339	-0.070009	C	2.277219	0.211983	1.299341
C	5.725680	0.647844	0.911231	S	1.251411	1.608153	1.231053
C	5.655526	-0.640639	1.243152	C	0.833272	1.622700	2.908128
S	4.268188	-1.558776	0.688523	C	1.472133	0.744105	3.692442

S	2.629517	-0.283558	2.916056	O	1.101722	-0.873460	-2.654538
H	0.089745	2.334589	3.236211	C	0.800255	1.685202	-2.215660
H	1.330746	0.633917	4.757470	C	0.670748	-2.191068	-2.963996
H	3.331088	-0.173061	-3.978436	H	-0.157873	1.279299	-1.895474
C	3.647722	-1.107376	-3.516617	H	0.861317	2.740734	-1.956244
O	3.451400	-1.073576	-2.100526	H	0.909581	1.555971	-3.289776
H	4.718679	-1.240407	-3.661914	H	0.394252	-2.200650	-4.019222
H	3.114220	-1.937191	-3.977186	H	1.455380	-2.933521	-2.796863
P	2.111207	-0.549732	-1.354903	H	-0.195152	-2.464923	-2.358416
O	1.879658	1.050436	-1.515687				

TS(**10**+**I**→**16**): E = -2221.73587806411 au (opt)
E = -2219.17436705452 au
ZPE = 0.08124498 au
G_{corr} = 0.04425927 au
ν = -197.26 cm^{-1}

S	-0.258843	0.062301	0.217709	C	-0.121191	-0.584482	-1.723205
C	1.367681	0.185391	0.576013	S	0.684063	-2.110367	-1.825687
S	2.325794	1.561911	0.105948	C	2.098856	-1.619275	-2.725525
C	3.865107	0.783725	0.229278	C	2.095397	-0.348790	-3.149817
C	3.868089	-0.490898	0.654061	S	0.676904	0.577678	-2.723072
S	2.332161	-1.194000	1.024259	H	2.888152	-2.335988	-2.901421
H	4.748714	1.352198	-0.021946	H	2.881448	0.122267	-3.722394
H	4.754401	-1.092743	0.792866				

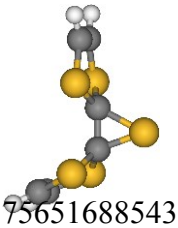


16: E = -2221.73777517207au (opt)
E = -2219.17774344428 au
ZPE = 0.08187249au
G_{corr} = 0.04430934 au

S	-0.308497	0.018285	0.093853	C	0.195254	-0.517458	-1.503905
C	1.285050	0.262960	0.798804	S	0.893929	-2.101496	-1.685040
S	2.244603	1.616413	0.271704	C	2.139633	-1.653230	-2.808686
C	3.766080	0.781745	0.207297	C	2.131906	-0.381574	-3.237104
C	3.771197	-0.489844	0.635760	S	0.877444	0.641546	-2.608971
S	2.255750	-1.126381	1.195818	H	2.846467	-2.407321	-3.123471
H	4.633200	1.316287	-0.152894	H	2.831767	0.036192	-3.946367
H	4.642952	-1.127195	0.670272				

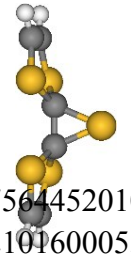
TS(**16→17**)**:** E = -2221.72773959120 au (opt)
E = -2219.17592775287 au
ZPE = 0.08209078 au
G_{corr} = 0.04552257 au
ν = -330.21 cm^{-1}

S	-0.310259	0.021339	0.106669	C	0.512237	-0.463537	-1.335326
C	1.377122	0.153320	0.462032	S	0.882971	-2.136642	-1.706056
S	2.275696	1.648169	0.282868	C	1.993130	-1.724521	-2.995853
C	3.834144	0.862605	0.422627	C	1.985498	-0.458303	-3.425685
C	3.842581	-0.403150	0.853848	S	0.865659	0.641666	-2.649777
S	2.294037	-1.129336	1.228897	H	2.609791	-2.511009	-3.406025
H	4.716485	1.439351	0.186200	H	2.594869	-0.077419	-4.232317
H	4.732773	-0.993606	1.014967				



17: E = -2221.75651688543au (opt)
E = -2219.21069147853 au
ZPE = 0.08261933au
G_{corr} = 0.04563956 au

S	-0.138660	-0.094452	-0.242686	C	1.409544	-0.447095	-1.307163
C	1.628469	0.027187	0.082728	S	1.758874	-2.149353	-1.744995
S	2.349273	1.679219	0.330823	C	1.554910	-1.884587	-3.463318
C	3.844651	1.061114	1.015127	C	1.546837	-0.622333	-3.893095
C	3.852265	-0.200684	1.444097	S	1.741164	0.638177	-2.694105
S	2.366004	-1.123596	1.283751	H	1.468171	-2.756385	-4.095585
H	4.679039	1.743006	1.096214	H	1.452494	-0.318525	-4.925613
H	4.693701	-0.682766	1.920888				



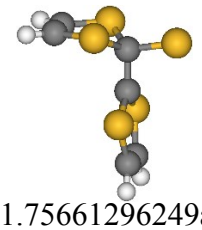
17$^{out\text{-}out}$**:** E = -2221.75644520105 au (opt)
E = -2219.21016000557 au
ZPE = 0.08258995au
G_{corr} = 0.04559928 au

S	0.316144	-0.069960	-0.177583	C	2.180199	-0.067821	-0.205067

S	3.041154	1.519006	-0.129731	S	1.732650	-2.232612	-1.986736
C	3.816744	1.193385	1.403220	C	1.240988	-1.946318	-3.640093
C	3.824516	-0.068776	1.832418	C	1.233550	-0.684226	-4.069442
S	3.058469	-1.269969	0.818590	S	1.716095	0.556108	-2.935472
H	4.259685	2.028628	1.925952	H	0.973751	-2.806034	-4.237180
H	4.274783	-0.407357	2.754203	H	0.959493	-0.369843	-5.065975
C	1.578513	-0.505284	-1.480033				

TS(**17→18**)**:** E = -2221.75519665006 au (opt)
E = -2219.20585723807 au
ZPE = 0.08239776 au
G_{corr} = 0.04610969 au
ν = -155.77 cm^{-1}

S	0.297073	0.067112	0.140802	C	1.574508	-0.447732	-1.002932
C	2.479581	0.023596	0.065909	S	1.678361	-2.233583	-1.394868
S	3.253047	1.585458	0.002139	C	2.696266	-1.986572	-2.807392
C	4.142021	1.377926	1.484872	C	2.701594	-0.767587	-3.350146
C	4.136686	0.157077	2.027428	S	1.690319	0.454951	-2.591933
S	3.241507	-1.076026	1.184932	H	3.241324	-2.834004	-3.198445
H	4.669558	2.235451	1.876007	H	3.251682	-0.495016	-4.239687
H	4.659184	-0.131195	2.927719				



18: E = -2221.75661296249au (opt)
E =-2219.20466150205 au
ZPE = 0.08310620au
G_{corr} = 0.04606648 au

S	0.016044	0.008928	0.006594	C	1.459941	-0.424549	-0.952036
C	2.526027	-0.002892	0.006842	S	1.619826	-2.218472	-1.374014
S	3.208632	1.560342	-0.008659	C	2.742568	-1.939513	-2.699212
C	4.178788	1.345654	1.405633	C	2.748179	-0.719315	-3.242663
C	4.173708	0.119426	1.950142	S	1.632437	0.460942	-2.566938
S	3.198171	-1.067244	1.157975	H	3.349771	-2.764457	-3.044927
H	4.753926	2.189501	1.757057	H	3.360549	-0.428871	-4.084917
H	4.744143	-0.189624	2.813529				

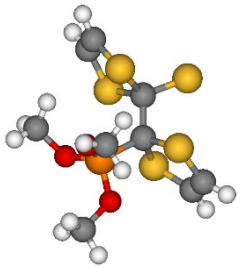
TS(**18**+$(MeO)_3P$→**I**+$(MeO)_3PS$)**:**E = -2908.50688049673 au (opt)

E = -2905.04100028260 au
ZPE = 0.21078745 au
G_{corr} = 0.15957718 au
ν = -263.18 cm^{-1}

S	-0.238562	-0.099499	-0.351135	O	-2.421591	0.766389	2.156075
C	1.551597	-0.974356	-0.128704	C	-1.308113	0.231909	2.892749
S	2.475586	-0.245637	1.259729	H	-1.416080	0.588086	3.915550
C	1.937935	-1.449615	2.407636	H	-1.323296	-0.858552	2.879792
C	1.438931	-2.585993	1.918400	H	-0.367074	0.577686	2.468161
S	1.377060	-2.757746	0.180235	O	-3.334765	-1.045648	0.599584
H	2.040132	-1.222403	3.458784	C	-4.501054	-1.330908	1.400088
H	1.079975	-3.409875	2.517828	H	-5.381332	-0.867632	0.956329
C	1.928510	-0.573925	-1.442504	H	-4.613270	-2.412560	1.407857
S	1.725168	-1.593534	-2.829695	H	-4.365936	-0.964685	2.417443
C	2.332370	-0.441411	-3.979909	O	-3.943746	1.336371	0.332671
C	2.830174	0.698108	-3.489249	C	-3.752636	2.754081	0.208306
S	2.808779	0.884786	-1.761689	H	-4.658313	3.159578	-0.237254
H	2.285363	-0.705037	-5.025984	H	-3.591692	3.201992	1.189850
H	3.249567	1.502110	-4.075428	H	-2.899421	2.977302	-0.437297
P	-2.625719	0.400147	0.576765				

TS(**18**+$(MeO)_3P$→**19**): E = -2908.50333146057 au (opt)
E = -2905.03522072016 au
ZPE = 0.21155302 au
G_{corr} = 0.16171552 au
ν = -203.15 cm^{-1}

S	-0.606967	0.562368	-0.555824	C	6.276981	-0.966472	0.334602
C	2.000075	0.182195	-0.033638	O	4.882424	-0.597218	0.248729
S	2.412562	1.873712	0.161648	H	6.637412	-0.576659	1.282673
C	2.890175	1.767021	1.826705	H	6.372336	-2.050443	0.312308
C	2.675469	0.601541	2.443204	P	4.027034	-0.709048	-1.093766
S	1.967386	-0.665261	1.491725	O	4.885833	0.081906	-2.208223
H	3.318895	2.647606	2.281792	O	4.360305	-2.213202	-1.536249
H	2.901819	0.386938	3.476946	C	4.900804	1.514849	-2.339014
C	0.921045	-0.185907	-1.047986	C	4.036845	-2.721505	-2.847434
S	0.824195	-2.070890	-1.149878	H	5.650181	1.742388	-3.092925
C	0.406936	-2.107603	-2.840611	H	3.928421	1.876032	-2.669641
C	0.704128	-1.033574	-3.579196	H	5.172365	1.985009	-1.394147
S	1.485026	0.300214	-2.776230	H	4.374067	-3.754462	-2.860701
H	-0.095410	-2.987389	-3.217024	H	2.963160	-2.678768	-3.015631
H	0.473774	-0.928274	-4.629584	H	4.561372	-2.146052	-3.608568
H	6.838479	-0.525450	-0.488168				



19:

E = -2908.52074049673au (opt)
E =-2905.06220476684 au
ZPE = 0.21347372au
G_{corr} = 0.16325581 au

S	-0.296345	0.565330	-0.389953	C	6.411045	-0.812613	0.201237
C	2.413459	-0.031188	-0.231486	O	5.025557	-0.374067	0.259495
S	2.708724	1.761025	0.131009	H	6.881341	-0.408274	1.091279
C	2.755258	1.615859	1.873383	H	6.444301	-1.899470	0.208884
C	2.541535	0.424762	2.419370	P	4.034497	-0.590724	-0.923683
S	2.236335	-0.942042	1.375128	O	4.574998	0.129699	-2.194860
H	2.927870	2.527605	2.427405	O	4.107010	-2.099902	-1.279399
H	2.518335	0.232389	3.482836	C	4.868798	1.534101	-2.408250
C	1.099385	-0.236770	-1.082833	C	3.913055	-2.681497	-2.602814
S	0.848918	-2.115895	-1.244770	H	5.559113	1.560932	-3.245660
C	0.391701	-2.101990	-2.922063	H	3.947990	2.053585	-2.659512
C	0.670806	-1.015584	-3.649379	H	5.320625	1.961480	-1.517233
S	1.480609	0.307959	-2.856050	H	3.496207	-3.667980	-2.433622
H	-0.135469	-2.965871	-3.302645	H	3.227279	-2.077354	-3.187819
H	0.396300	-0.887184	-4.686869	H	4.886479	-2.743257	-3.082323
H	6.891410	-0.419462	-0.692907				

TS(**19**→**14**+**1**):

E = -2908.51175033426 au (opt)
E = -2905.05042330424 au
ZPE = 0.21248728 au
G_{corr} = 0.16358955 au
ν = -363.40 cm^{-1}

S	-0.539679	0.745488	0.075765	C	0.513810	-0.020043	-1.033052
C	2.318708	0.019698	-0.115590	S	0.215545	-1.778017	-1.372059
S	2.623663	1.772046	0.248956	C	1.014723	-1.798397	-2.928275
C	2.768751	1.585436	1.987967	C	1.289254	-0.619449	-3.494084
C	2.529433	0.386600	2.508785	S	0.806444	0.818923	-2.619501
S	2.099870	-0.922496	1.422575	H	1.223923	-2.754647	-3.386556
H	2.996723	2.474078	2.559330	H	1.756793	-0.502032	-4.461490
H	2.537357	0.162454	3.566256	H	6.606035	-0.731851	-1.294567

C	6.317408	-0.919495	-0.261085	C	4.132654	-2.896320	-2.278356
O	5.010254	-0.350115	0.012955	H	5.046511	1.306735	-3.546998
H	7.006765	-0.422100	0.413565	H	3.653936	1.996491	-2.664927
H	6.295342	-1.988037	-0.055564	H	5.195140	1.697056	-1.808965
P	3.767905	-0.605893	-0.914444	H	3.622808	-3.853540	-2.244040
O	4.082300	-0.001455	-2.321324	H	3.916753	-2.381212	-3.209603
O	3.606864	-2.134379	-1.161661	H	5.204240	-3.034895	-2.153296
C	4.526894	1.352969	-2.594823				

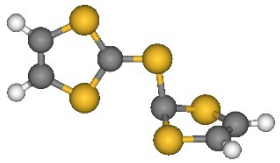
TS(**19→15**)**:** E = -2908.50993038448 au (opt)
E = -2905.05108756349 au
ZPE = 0.21331523 au
G_{corr} = 0.16563930 au
ν = -44.45 cm^{-1}

S	0.401940	1.558006	-1.587874	C	6.400649	-0.631926	0.260628
C	2.409540	0.021526	-0.328040	O	5.018691	-0.189846	0.236261
S	2.618047	1.709061	0.410626	H	6.826557	-0.207093	1.163598
C	2.992440	1.157826	2.032773	H	6.432582	-1.718447	0.296848
C	2.736226	-0.105143	2.349329	P	4.070273	-0.466381	-0.969365
S	2.124775	-1.161649	1.084255	O	4.580846	0.321104	-2.214922
H	3.314830	1.914658	2.734792	O	4.255041	-1.974304	-1.279665
H	2.812644	-0.532320	3.339420	C	4.536250	1.763889	-2.426683
C	1.227618	0.018016	-1.425615	C	4.320028	-2.690039	-2.541341
S	0.056075	-1.424497	-0.980076	H	5.066314	1.930648	-3.358554
C	-0.285684	-1.900674	-2.616370	H	3.500116	2.083516	-2.511993
C	0.562112	-1.519146	-3.574484	H	5.030946	2.267865	-1.600601
S	1.916521	-0.533663	-3.107459	H	3.339755	-3.105199	-2.749573
H	-1.179327	-2.483535	-2.792283	H	4.627920	-2.018873	-3.336987
H	0.450046	-1.744930	-4.625574	H	5.055757	-3.474526	-2.388603
H	6.927596	-0.260320	-0.616572				

TS(**10**+**1→20**)**:** E = -2221.72273468025 au (opt)
E = -2219.16522933298 au
ZPE = 0.08082502 au
G_{corr} = 0.04432814 au
ν = -211.10 cm^{-1}

C	0.164089	-0.071797	0.008550	H	2.946522	2.350615	0.184275
S	1.903797	0.095277	0.098828	H	0.769575	3.518638	-0.608312
C	2.008733	1.856725	-0.028156	S	-0.587096	-0.161476	1.919711
C	0.887929	2.458087	-0.435787	C	-1.174472	-1.713877	1.692489
S	-0.466485	1.366933	-0.761622	S	-0.984035	-2.587666	0.208326

C	-1.830557	-4.006514	0.776542	H	-1.927872	-4.829728	0.082967
C	-2.310758	-3.999936	2.023886	H	-2.853142	-4.796095	2.511747
S	-2.012667	-2.548544	2.928762				



20: E = -2221.72387794219au (opt)
E =-2219.16800259482 au
ZPE = 0.08159338au
G_{corr} = 0.04501082 au

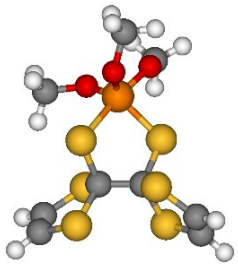
C	-0.231611	0.132317	-0.128853	C	-1.284852	-1.629836	1.553553
S	1.527538	-0.095125	-0.152778	S	-0.925358	-2.606027	0.179142
C	1.963471	1.618966	0.003565	C	-1.643842	-4.048733	0.844776
C	0.988639	2.484041	-0.282490	C	-2.157774	-3.978180	2.077363
S	-0.559577	1.751765	-0.758575	S	-2.021580	-2.439640	2.869267
H	2.978239	1.885431	0.264435	H	-1.630600	-4.936688	0.229372
H	1.090177	3.560326	-0.294691	H	-2.624031	-4.783826	2.624775
S	-0.935278	0.015851	1.573346				

TS(**20**→**16**)**:** E = -2221.71567875539 au (opt)
E = -2219.15839436705 au
ZPE = 0.08210943 au
G_{corr} = 0.04610532 au
ν = -28.34 cm^{-1}

C	0.580947	0.238334	1.142314	C	-1.025287	-1.728124	1.747124
S	2.184468	0.935521	1.184222	S	-0.680095	-2.559008	0.242196
C	1.832250	2.087962	-0.086660	C	-1.725441	-3.912131	0.641313
C	0.696326	1.914834	-0.768157	C	-2.521909	-3.793281	1.707244
S	-0.341168	0.576695	-0.307504	S	-2.461290	-2.276947	2.583865
H	2.580819	2.833546	-0.311469	H	-1.724078	-4.755929	-0.033687
H	0.399772	2.499611	-1.627000	H	-3.250540	-4.527467	2.018650
S	-0.011210	-0.602975	2.469757				

TS(**18**+$(MeO)_3PS$→**21**)**:** E = -3306.70842899841 au (opt)
E = -3302.81490812094 au
ZPE = 0.21477284 au
G_{corr} = 0.16364737 au
ν = -119.15 cm^{-1}

S	0.496193	0.861477	-0.265592	P	-0.428745	-2.185812	-1.158076
C	2.173049	0.365131	0.046104	O	-1.415959	-1.855517	0.006634
S	3.359235	1.829257	-0.020309	C	-1.092911	-1.678226	1.413475
C	3.479272	2.035260	1.706129	H	-0.534598	-0.752973	1.523689
C	3.082017	1.033338	2.492969	H	-2.051828	-1.632389	1.920412
S	2.468762	-0.415174	1.732480	H	-0.513694	-2.527388	1.768394
H	3.869134	2.976944	2.067620	O	-0.805051	-1.384433	-2.427981
H	3.102755	1.058735	3.573441	C	-1.603580	-0.177475	-2.535335
C	2.628641	-0.634669	-1.021238	H	-2.180849	-0.026403	-1.627879
S	4.297844	-1.291148	-0.870951	H	-0.927308	0.655238	-2.695208
C	4.520203	-1.527457	-2.590794	H	-2.258305	-0.334260	-3.388276
C	3.641628	-0.940617	-3.404057	O	-0.833024	-3.641383	-1.637973
S	2.346877	-0.015722	-2.672828	C	-0.783012	-4.781780	-0.748876
H	5.371210	-2.112662	-2.909125	H	-1.199685	-5.613237	-1.308844
H	3.676283	-0.983240	-4.483421	H	0.247586	-4.999301	-0.471268
S	1.553236	-2.361509	-0.727490	H	-1.386330	-4.591587	0.137954



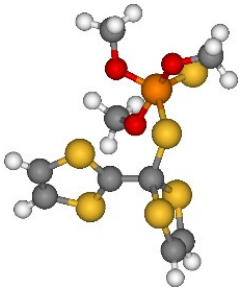
21: E = -3306.72340805320au (opt)
E =-3302.83599826700 au
ZPE = 0.21645727au
G_{corr} = 0.16528486 au

S	0.672295	0.509333	-0.516397	S	1.677660	-2.270977	-1.531121
C	2.380637	-0.011318	-0.155436	P	-0.242852	-1.534402	-0.917161
S	3.397836	1.516275	0.033542	O	-0.786645	-1.780975	0.570331
C	3.342584	1.514492	1.784951	C	-1.069291	-0.827273	1.604460
C	2.974616	0.394403	2.403844	H	-0.148208	-0.456156	2.044626
S	2.556497	-0.988017	1.413634	H	-1.657743	0.001915	1.216213
H	3.638763	2.424176	2.288315	H	-1.647069	-1.375818	2.346050
H	2.923121	0.271384	3.476407	O	-1.238428	-0.711470	-1.866011
C	2.845720	-0.859423	-1.343383	C	-2.453665	-1.237407	-2.443349
S	4.525707	-1.577635	-1.100115	H	-2.218880	-1.950920	-3.228970
C	5.047446	-1.346716	-2.757009	H	-3.068414	-1.712596	-1.681772
C	4.319334	-0.556040	-3.542069	H	-2.969663	-0.373561	-2.856078
S	2.877964	0.178544	-2.874971	O	-0.788084	-3.015053	-1.424430
H	5.959485	-1.843095	-3.057339	C	-0.776660	-4.193794	-0.616802
H	4.555734	-0.327712	-4.571891	H	-0.923221	-5.034382	-1.293118

H	0.175464	-4.314204	-0.096730	H	-1.582994	-4.160561	0.115560

TS(**18**+$(MeO)_3PS$→**22**)**:** E = -3306.69160748536 au (opt)
E = -3302.79927922910 au
ZPE = 0.21559207 au
G_{corr} = 0.16604536 au
ν = -76.33 cm^{-1}

S	-0.280547	0.963942	-2.157811	P	-2.116471	-0.277088	-1.256857
C	1.712539	-0.220708	-0.703439	O	-2.980278	-0.295067	0.141493
S	1.570871	1.027816	0.424164	C	-4.388720	-0.064874	0.142016
C	2.506927	0.268007	1.648821	H	-4.769368	-0.481691	1.074418
C	2.970074	-0.965990	1.368315	H	-4.609677	1.000794	0.094977
S	2.566292	-1.578954	-0.187379	H	-4.863164	-0.571349	-0.701028
H	2.647391	0.793104	2.582328	O	-0.844272	-0.969764	-0.404077
H	3.540865	-1.595219	2.035002	C	-1.060410	-2.151792	0.369497
C	1.188166	-0.086814	-2.102897	H	-1.718967	-2.843007	-0.158201
S	0.993156	-1.757136	-2.887829	H	-0.083123	-2.619446	0.497481
C	2.628045	-1.814951	-3.529707	H	-1.483306	-1.906118	1.342692
C	3.330626	-0.684149	-3.591729	O	-2.846031	1.183219	-1.661611
S	2.543328	0.780183	-3.040920	C	-3.223145	1.507927	-2.999558
H	2.986958	-2.774131	-3.877362	H	-3.277273	2.595454	-3.056183
H	4.335694	-0.599297	-3.979701	H	-2.499676	1.141335	-3.726864
S	-2.719175	-1.633030	-2.573067	H	-4.197647	1.071764	-3.225060



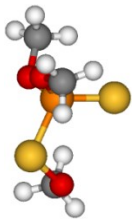
22: E = -3306.69421219985au (opt)
E =-3302.80188059520 au
ZPE = 0.21555660au
G_{corr} = 0.16473650 au

S	-0.487924	1.111793	-0.970524	H	1.880371	1.033982	4.088366
C	1.436972	0.061037	0.688346	H	3.102134	-1.213144	3.574105
S	1.044678	1.247382	1.825044	C	1.076486	0.191767	-0.761240
C	1.908362	0.536803	3.129827	S	1.123372	-1.455791	-1.599225
C	2.540306	-0.622897	2.865505	C	2.745756	-1.277147	-2.241248
S	2.390575	-1.208349	1.254745	C	3.327921	-0.081039	-2.193170

S	2.398631	1.249939	-1.531296	O	-0.879257	-1.038342	0.534885
H	3.207145	-2.159830	-2.662868	C	-1.133686	-2.138301	1.390422
H	4.322058	0.140961	-2.554133	H	-1.850493	-2.822703	0.932795
S	-3.218715	-1.422688	-1.005299	H	-0.183690	-2.657342	1.533718
P	-2.137885	-0.036115	-0.060229	H	-1.515048	-1.800023	2.355877
O	-2.495405	0.350821	1.478961	O	-2.933336	1.404767	-0.599687
C	-3.764303	0.885734	1.861384	C	-3.534815	1.543165	-1.875035
H	-3.865715	0.691002	2.928962	H	-3.786155	2.599686	-1.990509
H	-3.808564	1.956791	1.671513	H	-2.856360	1.251219	-2.681847
H	-4.574070	0.390337	1.324221	H	-4.438135	0.936385	-1.950467

TS(**22**→**1**+**23**): E = -3306.67653333635 au (opt)
E = -3302.77463681106 au
ZPE = 0.21394950 au
G_{corr} = 0.16252065 au
ν = -167.69 cm^{-1}

S	-0.380317	0.592304	-2.033071	P	-1.751028	-0.723376	-1.160066
C	1.737083	-0.332724	-0.343858	O	-2.426409	-0.100569	0.156928
S	1.429682	1.000042	0.662900	C	-3.760251	0.428941	0.179740
C	2.020491	0.282188	2.111428	H	-4.092215	0.362330	1.214513
C	2.454759	-0.986499	2.012183	H	-3.751550	1.460695	-0.161280
S	2.407662	-1.681103	0.437655	H	-4.413027	-0.163592	-0.460828
H	1.986011	0.867107	3.018584	O	-0.674920	-1.663362	-0.380658
H	2.819622	-1.593476	2.827419	C	-1.097900	-2.805323	0.369010
C	1.423760	-0.294852	-1.762643	H	-1.604439	-3.517567	-0.282159
S	1.559480	-1.925031	-2.575948	H	-0.197904	-3.256540	0.783313
C	2.201010	-1.301703	-4.079649	H	-1.764796	-2.505118	1.178152
C	2.605962	-0.035376	-4.121444	O	-2.336681	1.247001	-2.101552
S	2.511818	0.905303	-2.646142	C	-2.808034	1.357614	-3.416191
H	2.222938	-1.980197	-4.920535	H	-2.155603	2.004310	-4.019853
H	2.999426	0.459842	-4.997765	H	-2.876591	0.380710	-3.910383
S	-2.916826	-1.840787	-2.270829	H	-3.811531	1.801781	-3.407048



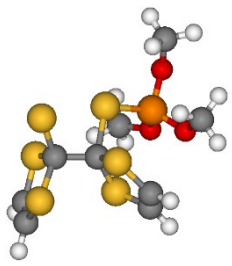
23: E = -1483.09733761429au (opt)
E =-1481.32504741797 au
ZPE = 0.13212489au

G_{corr} = 0.09361371 au

S	1.081036	1.899717	1.174033	C	1.167391	-2.279653	2.332693
S	1.264981	0.563154	4.315863	H	0.743131	-2.279165	3.335520
P	1.667987	0.313920	2.446841	H	0.611076	-2.951886	1.686125
O	3.203331	0.152066	2.035088	H	2.216696	-2.569976	2.365362
C	4.227019	0.989308	2.620769	O	-0.176309	2.578032	2.004096
H	5.164061	0.669523	2.174286	C	-1.448165	1.915868	1.852537
H	4.035499	2.035715	2.385004	H	-1.697669	1.801455	0.796852
H	4.248873	0.845889	3.699522	H	-1.427520	0.941378	2.342154
O	1.035530	-0.963385	1.740749	H	-2.173021	2.561755	2.344519

TS(**18**+$(MeO)_3PS$→**24**)**:** E = -3306.71103994066 au (opt)
E = -3302.81743488993 au
ZPE = 0.21447103 au
G_{corr} = 0.16300513 au
ν = -88.65 cm^{-1}

S	1.431441	2.753468	-1.190003	P	-2.108010	-0.678207	-0.857469
C	1.882268	1.082222	-0.750331	O	-2.140146	-1.590594	-2.129874
S	3.636238	0.669989	-1.223060	C	-2.499009	-1.068323	-3.436602
C	4.042834	-0.276825	0.187364	H	-3.574701	-0.907834	-3.475881
C	3.203560	-0.255170	1.222779	H	-1.957913	-0.145172	-3.634835
S	1.760245	0.728277	1.085563	H	-2.205330	-1.831731	-4.148649
H	4.975524	-0.824128	0.170433	O	-1.898239	-1.767579	0.240654
H	3.367323	-0.777482	2.155377	C	-1.577367	-1.413980	1.614970
C	0.934950	0.110281	-1.511363	H	-1.477347	-2.358799	2.138728
S	1.115422	-1.628409	-1.090592	H	-0.641034	-0.860302	1.640275
C	0.967485	-2.246533	-2.717508	H	-2.387892	-0.826346	2.041706
C	0.946037	-1.358656	-3.709505	O	-3.542717	-0.097008	-0.581648
S	1.053077	0.335765	-3.298394	C	-4.057275	1.193131	-1.012536
H	0.894005	-3.318163	-2.835297	H	-5.129221	1.145412	-0.848841
H	0.857616	-1.607781	-4.757635	H	-3.612737	1.978874	-0.406917
S	-0.856716	0.925518	-0.915576	H	-3.842689	1.359055	-2.065409

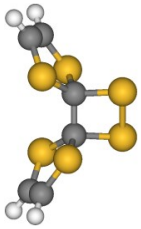


24: E = -3306.71086093197au (opt)
E = -3302.81772283537 au

ZPE = 0.21492558au

G_{corr} = 0.16233091 au

S	1.427903	2.759214	-1.046484	P	-2.111104	-0.661954	-0.807527
C	1.881956	1.068246	-0.684402	O	-2.162007	-1.548286	-2.094869
S	3.605253	0.638351	-1.240389	C	-2.480507	-1.005896	-3.405649
C	4.071732	-0.312781	0.148657	H	-3.555807	-0.858763	-3.479214
C	3.271682	-0.311472	1.214295	H	-1.943954	-0.073622	-3.568751
S	1.817609	0.662009	1.143973	H	-2.150800	-1.752869	-4.119095
H	5.010517	-0.846949	0.092510	O	-1.957762	-1.758855	0.288513
H	3.476252	-0.840105	2.135167	C	-1.570798	-1.441860	1.655854
C	0.871717	0.149573	-1.436527	H	-1.518287	-2.397347	2.166824
S	1.049262	-1.618969	-1.057838	H	-0.599248	-0.952268	1.656277
C	0.960491	-2.193328	-2.707169	H	-2.326524	-0.805828	2.111829
C	0.941480	-1.285430	-3.679278	O	-3.509214	-0.012986	-0.512311
S	0.994846	0.405861	-3.240191	C	-4.116233	1.120172	-1.193995
H	0.922287	-3.263455	-2.853459	H	-4.505226	1.775768	-0.420976
H	0.889234	-1.516597	-4.734149	H	-3.382661	1.650059	-1.796845
S	-0.819660	0.934580	-0.820015	H	-4.922749	0.738757	-1.814844



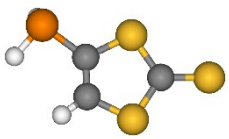
25: E = -2619.92695971898au (opt)

E = -2616.94890315441 au

ZPE = 0.08454276au

G_{corr} = 0.04690330 au

S	1.711698	2.492574	-0.570230	C	1.221146	0.123052	-1.302371
C	2.394408	0.743754	-0.487648	S	0.867944	-1.621025	-0.961851
S	4.044503	0.532275	-1.205301	C	0.512073	-2.073888	-2.617195
C	4.881142	0.251229	0.308889	C	0.796221	-1.198127	-3.577361
C	4.145831	0.055400	1.399970	S	1.470131	0.344421	-3.114692
S	2.408083	0.124767	1.248197	H	0.093779	-3.057107	-2.777978
H	5.961010	0.231923	0.276480	H	0.639771	-1.366102	-4.633588
H	4.542732	-0.144168	2.385340	S	-0.058463	1.334496	-0.648360



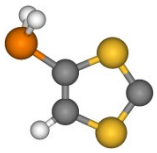
2': E = -1651.90241493476au (opt)

E = -1649.98516761162 au
ZPE = 0.04952190au
G_{corr} = 0.01662455 au

C	0.055960	-0.249600	-0.614889	S	-0.671471	-1.706062	-0.890770
S	1.675015	-0.072791	-0.001121	P	3.250189	2.470623	0.703750
C	1.754982	1.672542	0.003034	H	4.112674	2.237070	-0.396668
C	0.635516	2.288896	-0.416832	H	2.899621	3.781292	0.305119
S	-0.696919	1.290557	-0.898103	H	0.503400	3.360000	-0.474347

TS(**2'**+$(MeO)_3P$→**10^{PH2}**+$(MeO)_3PS$)**:** E = -2338.63166169785 au (opt)
E = -2335.80169431373 au
ZPE = 0.17845479au
G_{corr} = 0.13184888 au
ν = -154.27 cm^{-1}

C	-0.311001	-0.390366	-0.469135	H	-1.427160	-3.736295	4.795438
S	1.448433	-0.333923	-0.681073	H	-1.304900	-3.827486	3.020290
C	1.676307	1.235349	0.125144	H	0.167134	-3.599615	4.007719
C	0.560136	1.975463	0.225860	O	-1.076119	0.377913	3.035994
S	-0.916287	1.283864	-0.432063	C	-2.477840	0.733383	2.975291
S	-1.028702	-1.569430	0.518096	H	-2.525781	1.795121	3.196309
P	3.292627	1.822792	0.705316	H	-2.863097	0.542964	1.975259
H	4.043759	1.537826	-0.465820	H	-3.035192	0.166238	3.719290
H	3.724417	0.641460	1.362091	O	0.996582	-0.928797	2.756141
H	0.522668	2.967030	0.656479	C	1.671696	-0.106217	3.744006
P	-0.568420	-1.072102	2.657899	H	2.718604	-0.389576	3.700032
O	-1.094032	-1.936574	3.898981	H	1.547398	0.941355	3.479455
C	-0.894723	-3.373292	3.921681	H	1.270696	-0.297915	4.737878

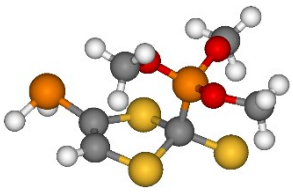


10^{PH2}: E = -1253.68809014994au (opt)
E = -1252.20713787346 au
ZPE = 0.04688362au
G_{corr} = 0.01728504 au

C	-0.240545	-0.364925	-0.989077	P	3.199522	1.799324	0.801931
S	1.392906	-0.369991	-0.649998	H	3.981550	1.493340	-0.339207
C	1.598972	1.179311	0.159344	H	3.583335	0.622906	1.492277
C	0.437699	1.860175	0.253281	H	0.316337	2.833133	0.708681
S	-0.944477	1.051180	-0.435367				

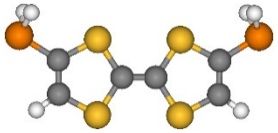
TS(**2'**+$(MeO)_3P$→**11^{PH2}**): E = -2338.63898859954 au (opt)
E = -2335.80898743644 au
ZPE = 0.17821431au
G_{corr} = 0.13049889 au
ν = -303.38 cm^{-1}

C	0.005340	-0.234976	-0.341831	H	-4.068790	-0.155740	1.850078
S	1.795756	-0.016160	-0.281555	H	-3.123236	-0.145105	0.336592
C	1.749608	1.728799	-0.053051	H	-3.033066	-1.549259	1.428661
C	0.587337	2.319291	-0.378118	O	0.115774	0.799365	3.058736
S	-0.705562	1.296830	-0.964633	C	-0.051503	2.230061	3.126727
S	-0.640882	-1.721091	-0.846156	H	0.544640	2.564001	3.971011
P	3.179089	2.529879	0.755987	H	0.306186	2.701204	2.212922
H	4.171976	2.067153	-0.144114	H	-1.100921	2.472829	3.287210
H	3.033508	3.793375	0.133637	O	-0.344957	-1.556192	2.525467
H	0.404276	3.383174	-0.313795	C	0.888661	-2.304541	2.405809
P	-0.529058	-0.103917	1.898524	H	0.779353	-3.165232	3.059764
O	-2.081248	0.175091	2.118819	H	1.020030	-2.628751	1.375522
C	-3.142927	-0.468091	1.374419	H	1.733718	-1.698995	2.730666



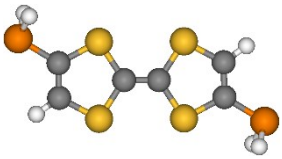
11^{PH2}: E = -2338.65866864151au (opt)
E = -2335.83683468904 au
ZPE = 0.18020268au
G_{corr} = 0.13257485 au

C	0.002164	0.013440	-0.048856	H	-3.990369	-0.435524	2.147579
S	1.866023	0.031550	-0.080209	H	-3.332449	-0.830297	0.522409
C	2.051558	1.789818	0.037903	H	-2.821272	-1.774270	1.945870
C	0.976436	2.515670	-0.282711	O	0.097063	1.092925	2.534234
S	-0.495970	1.668555	-0.744630	C	-0.502189	2.374356	2.850852
S	-0.766400	-1.378230	-0.845170	H	0.272737	2.943298	3.354649
P	3.612897	2.422461	0.737846	H	-0.810896	2.878164	1.938629
H	4.492781	1.796013	-0.182294	H	-1.352992	2.220198	3.510229
H	3.609274	3.669956	0.066601	O	-0.171960	-1.364617	2.407824
H	0.952388	3.597464	-0.284178	C	0.832478	-2.369624	2.106348
P	-0.544083	-0.047032	1.674477	H	0.614763	-3.199214	2.772026
O	-2.076510	0.172572	1.835717	H	0.732450	-2.669847	1.066158
C	-3.131887	-0.795815	1.588116	H	1.818335	-1.960254	2.308851



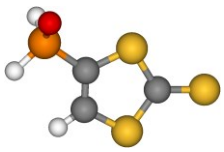
***Z*-8':** E = -2507.46533166116au (opt)
E = -2504.49842679752 au
ZPE = 0.09793221au
G_{corr} = 0.05765117au

C	-0.015551	-0.047637	-0.000684	C	-0.783804	-1.150500	-0.002746
S	1.754084	-0.095887	0.000008	S	-0.124881	-2.793510	-0.004989
C	1.984762	1.650326	0.004332	C	-1.682706	-3.615503	-0.004869
C	0.870287	2.392356	0.005006	C	-2.765196	-2.827518	-0.004171
S	-0.677450	1.594502	0.001646	S	-2.553660	-1.099137	-0.003386
P	3.651569	2.386749	0.007559	P	-1.795454	-5.434239	-0.005902
H	4.212465	1.594220	-1.026461	H	-0.855341	-5.684397	1.026316
H	4.210531	1.589625	1.039097	H	-0.856222	-5.683178	-1.039224
H	0.860612	3.473346	0.007485	H	-3.782465	-3.193322	-0.004179



***E*-8':** E = -2507.46533255336 au (opt)
E = -2504.49854962187 au
ZPE = 0.09789782au
G_{corr} = 0.05764971 au

C	-0.023034	-0.042505	0.022639	C	-0.799942	-1.139168	0.022325
S	1.746955	-0.094610	0.022345	S	-2.569932	-1.087061	0.022138
C	1.981466	1.650484	0.003406	C	-2.804443	-2.832142	0.002081
C	0.868657	2.395171	0.004238	C	-1.691636	-3.576832	0.002426
S	-0.680453	1.600743	0.023132	S	-0.142522	-2.782419	0.021801
P	3.650470	2.381943	-0.013745	P	-4.473451	-3.563585	-0.015559
H	4.201389	1.575950	-1.042673	H	-5.024336	-2.756961	-1.044010
H	4.214256	1.594781	1.022803	H	-5.037259	-2.777051	1.021453
H	0.861287	3.476123	-0.004959	H	-1.684268	-4.657778	-0.007468



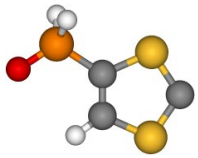
4': E = -1727.16368535315au (opt)

E = -1725.14907390406 au
ZPE = 0.05537240au
G_{corr} = 0.02086591 au

C	0.120770	-0.243177	-0.570700	P	3.238443	2.560888	0.653365
S	1.718034	-0.056705	0.100328	H	4.219838	2.261560	-0.307858
C	1.780772	1.685235	0.062435	H	2.878632	3.889017	0.360678
C	0.680541	2.300260	-0.411061	O	3.636313	2.265355	2.055154
S	-0.624004	1.296294	-0.926247	H	0.557114	3.371811	-0.489274
S	-0.603169	-1.696957	-0.833446				

TS(**4'**+$(MeO)_3P$→**10**^{PH2O}+$(MeO)_3PS$)**:** E = -2413.89608294953 au (opt)
E = -2410.96775014212 au
ZPE = 0.18379825au
G_{corr} = 0.13800214 au
ν = -154.51 cm^{-1}

C	-0.347049	-0.344829	-0.520366	H	-1.246440	-3.661646	4.836550
S	1.398720	-0.320448	-0.833867	H	-1.061082	-3.790623	3.069159
C	1.664578	1.224665	0.012242	H	0.357391	-3.425653	4.092547
C	0.574459	1.993843	0.159801	O	-1.125519	0.425795	2.984546
S	-0.928122	1.339738	-0.460568	C	-2.541227	0.721287	2.937404
S	-1.051933	-1.526214	0.441312	H	-2.628285	1.792402	3.090636
P	3.261773	1.648730	0.672702	H	-2.944297	0.450761	1.962771
H	4.131182	1.593656	-0.435508	H	-3.056793	0.181929	3.730551
H	3.641674	0.493018	1.384231	O	0.998878	-0.791029	2.687289
O	3.321514	2.916915	1.455331	C	1.647485	0.051316	3.679566
H	0.576221	2.966888	0.631349	H	2.692783	-0.241584	3.682049
P	-0.561820	-1.009827	2.623843	H	1.541791	1.093081	3.384620
O	-1.018083	-1.865803	3.899378	H	1.210530	-0.110270	4.663259
C	-0.715187	-3.282505	3.968959				



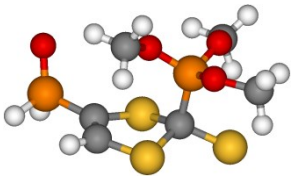
10^{PH2O}**:** E = -1328.94839334829au (opt)
E = -1327.36991450313 au
ZPE = 0.05287981au
G_{corr} = 0.02063503 au

C	-0.332876	-0.379804	-1.081768	C	0.362344	1.769855	0.271674
S	1.301641	-0.428118	-0.757890	S	-1.026301	1.007171	-0.453892
C	1.510062	1.077808	0.130628	P	3.088400	1.642549	0.788717

H	3.944527	1.586481	-0.326155	O	3.024772	2.953022	1.489459
H	3.524587	0.554882	1.567124	H	0.263058	2.718007	0.781219

TS(**4'**+$(MeO)_3P$→**11^{PH2O}**)**:** E = -2413.90256024201 au (opt)
E = -2410.97425914668 au
ZPE = 0.18414804au
G_{corr} = 0.13699841 au
ν = -302.33 cm^{-1}

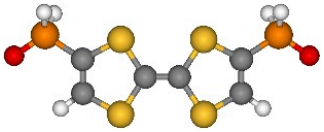
C	0.051202	-0.250528	-0.340721	H	-4.094445	-0.100347	1.741718
S	1.842196	-0.062374	-0.228853	H	-3.100577	-0.074851	0.261039
C	1.809729	1.683553	-0.025271	H	-3.078677	-1.507857	1.319152
C	0.664882	2.299058	-0.375946	O	0.084283	0.681251	3.114871
S	-0.633469	1.305306	-0.959368	C	0.179823	2.125312	3.124421
S	-0.605915	-1.713251	-0.876585	H	1.219717	2.402281	2.968885
P	3.224566	2.560569	0.638383	H	-0.450739	2.567999	2.354665
H	4.281250	2.162538	-0.200462	H	-0.161226	2.453892	4.103249
H	2.947165	3.877092	0.226359	O	-0.451845	-1.630459	2.482179
O	3.493114	2.379225	2.092277	C	0.786294	-2.380118	2.434485
H	0.513792	3.369458	-0.331665	H	0.637439	-3.244662	3.075265
P	-0.558478	-0.148959	1.908702	H	0.979358	-2.698705	1.412052
O	-2.109344	0.175136	2.084753	H	1.610889	-1.777516	2.813332
C	-3.160684	-0.423245	1.289281				



11^{PH2O}: E = -2413.92296422323au (opt)
E = -2411.00305562469 au
ZPE = 0.18604283au
G_{corr} = 0.13844309 au

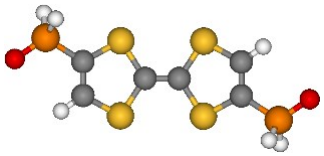
C	-0.002603	-0.060248	-0.062416	H	0.973633	3.521200	-0.325353
S	1.866830	-0.055057	-0.095284	P	-0.537014	-0.104117	1.669124
C	2.047111	1.700463	0.019586	O	-2.052905	0.194194	1.839563
C	0.977684	2.438640	-0.312077	C	-3.164880	-0.696550	1.542669
S	-0.490437	1.609542	-0.760415	H	-4.009306	-0.294319	2.094391
S	-0.781377	-1.435590	-0.862263	H	-3.344625	-0.688854	0.472674
P	3.565791	2.425307	0.623137	H	-2.925527	-1.701884	1.879320
H	4.557648	1.861499	-0.201204	O	0.181957	0.987132	2.522039
H	3.451460	3.745144	0.146404	C	-0.308532	2.307691	2.864828
O	3.836377	2.288848	2.081679	H	0.561989	2.865100	3.195575

H	-0.755713	2.782590	1.995453	H	0.599467	-3.252347	2.797505
H	-1.036212	2.217031	3.667626	H	0.772509	-2.739571	1.092326
O	-0.241364	-1.455039	2.372299	H	1.775926	-1.974841	2.372110
C	0.815691	-2.422946	2.131537				



***Z*-9':** E = -2657.98632030528au (opt)
E = -2654.82437615976 au
ZPE = 0.10930139au
G_{corr} = 0.06609680 au

C	-0.085465	0.001029	-0.424728	C	-0.853840	-1.102398	-0.425876
S	1.669293	-0.048297	-0.626837	S	-0.199060	-2.731159	-0.628701
C	1.910980	1.612576	-0.082380	C	-1.672807	-3.533495	-0.082680
C	0.814816	2.362425	0.081889	C	-2.756407	-2.765500	0.080695
S	-0.732414	1.634188	-0.231257	S	-2.610255	-1.062117	-0.235062
P	3.561036	2.262719	0.188420	P	-1.710104	-5.305955	0.192548
H	4.270970	1.840155	-0.952401	H	-0.746583	-5.515186	1.196903
H	4.092252	1.436282	1.196170	H	-1.072153	-5.828728	-0.949355
O	3.598130	3.722659	0.473561	H	-3.727088	-3.143509	0.369335
H	0.832673	3.404192	0.369712	O	-3.065871	-5.845451	0.484509



***E*-9':** E = -2657.98631193913 au (opt)
E = -2654.82452540092 au
ZPE = 0.10928459au
G_{corr} = 0.06613015 au

C	-0.037818	-0.032058	-0.520612	C	-0.784852	-1.149855	-0.521240
S	1.729063	-0.051840	-0.540616	S	-2.551709	-1.129949	-0.542096
C	1.883241	1.643940	-0.078324	C	-2.706150	-2.825826	-0.080157
C	0.763750	2.377038	-0.080085	C	-1.586753	-3.559065	-0.081983
S	-0.728967	1.594173	-0.508093	S	-0.093898	-2.776182	-0.509649
P	3.483625	2.346004	0.327628	P	-4.306736	-3.527376	0.325850
H	4.320283	1.870587	-0.701027	H	-5.143413	-3.050817	-0.702270
H	3.914275	1.594043	1.436624	H	-4.736631	-2.775807	1.435413
O	3.466687	3.821057	0.523125	H	-1.556776	-4.616751	0.138910
H	0.733621	3.434670	0.141026	O	-4.290613	-5.002529	0.520493

$(HS)_2C=S$**:** E = -1233.780514535322 au (opt)

C	-0.042427	0.000355	-0.038712
S	0.039590	0.000938	1.599562
S	1.430550	-0.000315	-0.978189
H	0.895879	-0.000164	-2.216170
S	-1.509410	0.000224	-0.991103
H	-2.358222	0.000930	0.051600

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