Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Four Consecutive Reactions in one Pot: Cascade Formation of an Unprecedented Triphosphatricyclo[3.2.1.02,7]oct-3-ene

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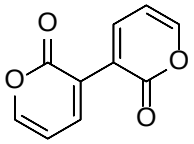
Table of Contents

1. General Remarks

All reactions were performed under argon in oven-dried glassware using modified Schlenk techniques unless otherwise stated. All common solvents and chemicals were commercially available. Trimethylsilylphosphaalkyne[1] and 2-oxo-2*H*-pyran-3-yl trifluoromethanesulfonate[2] were prepared according to literature. All dry or deoxygenated solvents were prepared using standard techniques or were used from a MBraun solvent purification system. Column chromatography was performed with a *Puriflash SX 420* from *Interchim* using spherical high-pressure silica gel with a grain size of 30 µm. The solvent gradient of the performed purifications is given in column volumes (CV) of the respective solvent mixture. The ^{1}H, $^{13}C\{^{1}H\}$ and $^{31}P\{^{1}H\}$ NMR spectra were recorded on a JEOL ECX400 (400 MHz) spectrometer and all chemical shifts are reported relative to the residual resonance in the deuterated solvents. *J* values are given in Hz. The ESI-TOF-Mass spectrometry measurements were performed on an Agilent 6210 ESI-TOF, *Agilent Technologies*, Santa Clara, CA, USA. Elemental analysis was performed on an elemental analysator VARIO EL by *Elementar*, Langenselbold, Germany.

2. Experimental Procedures

2*H*,2'*H*-[3,3'-bipyran]-2,2'-dione (2)



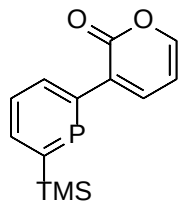
A mixture of 2-oxo-2*H*-pyran-3-yl trifluoromethanesulfonate (0.50 g, 2.05 mmol, 1.0 eq.), bis(pinacolato)diboron (0.29 g, 1.13 mmol, 0.55 eq.), K_3PO_4 (1.31 g, 6.15 mmol, 3.0 eq.) and $PdCl_2$(dppf) (0.07 g, 0.01 mmol, 0.05 eq.) was dissolved in a degassed solution of 40 mL THF and 4 mL dest. H_2O. The resulting mixture was stirred for two hours at room temperature and subsequently treated with 100 mL dest. H_2O. After extracting with EtOAc (3 x 100 mL), the combined organic fractions were dried over $MgSO_4$, filtered and the solvent was evaporated. Column chromatography on silica gel column (100 % *n*-hexane, 5 CV; 100 % *n*-hexane → *n*-hexane/EtOac: 1:4; 35 CV) of the yellow residue yielded **2** (0.14 g, 70%) as a yellow solid.

^{1}H NMR (400 MHz, Methylene Chloride-d_2): δ = 8.12 (1H, dd, *J* = 6.9, 2.2), 7.52 (1H, dd, *J* = 5.1, 2.1), 6.38 (1H, dd, *J* = 6.9, 5.1) ppm. **$^{13}C\{^{1}H\}$ NMR** (101 MHz, Methylene Chloride-d_2): δ = 161.1, 152.0, 142.9, 121.4, 107.1 ppm. **ESI-TOF** (m/z): 213.0149 (calc. 213.0158) [$M+Na^+$]

Cascade reaction of 2*H*,2'*H*-[3,3'-bipyran]-2,2'-dione and trimethylsilyl-phosphaalkyne

Remark: Me_3Si-CP has been reported to be temperature sensitive. A solution of Me_3Si-CP (2.88 mmol, 1.56 eq.) in toluene (80 mL) was added to 2*H*,2'*H*-[3,3'-bipyran]-2,2'-dione (350 mg, 1.84 mmol, 1.0 eq.) in toluene (100 mL). The resulting mixture was refluxed for 12 hours. After 4 hours, a reaction control by $^{31}P\{^1H\}$ NMR spectroscopy indicates, that unreacted Me_3Si-CP is still present in solution, while no decomposition products of the phosphaalkyne can be detected. Subsequently, all volatiles were evaporated in high vacuum. Column chromatography of the brown residue yielded the desired products:

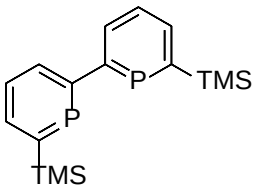
3-(6-(trimethylsilyl)phosphinin-2-yl)-2*H*-pyran-2-one (3)



Column chromatography on silica gel column (100 % *n*-hexane, 4 CV; 100 % *n*-hexane → *n*-hexane/EtOac: 1:4; 20 CV) yielded **3** (74.8 mg, 15%) as a beige solid.

^{1}H NMR (400 MHz, Methylene Chloride-d_2): δ = 8.13 (1H, ddd, *J* = 8.5, 4.8, 0.7), 8.06 (1H, ddd, *J* = 11.1, 7.9, 0.7), 7.60 – 7.52 (3H, m,), 6.37 (1H, ddd, *J* = 6.7, 5.1, 0.4), 0.38 (9H, d, *J* = 0.9) ppm. **^{13}C{^{1}H} NMR** (101 MHz, Methylene Chloride-d_2): δ = 171.4 (d, *J* = 77.4), 164.2 (d, *J* = 61.4), 161.8 (d, *J* = 4.4), 151.8 (d, *J* = 1.5), 140.0 (d, *J* = 15.3), 138.3 (d, *J* = 12.6), 135.2 (d, *J* = 10.9), 131.2 (d, *J* = 23.7), 128.6 (d, *J* = 20.3), 107.4, 0.1 (d, *J* = 6.4) ppm. **^{31}P{^{1}H} NMR** (162 MHz, Methylene Chloride-d_2): δ = 229.9 (s) ppm. **ESI-TOF** (m/z): 285.0470 (calc. 285.0471) [M+Na^+]

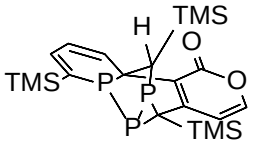
6,6'-bis(trimethylsilyl)-2,2'-biphosphinine (4)



Column chromatography on silica gel column (100 % *n*-hexane, 2 CV) and subsequent vacuum sublimation (50 °C, 5 x 10^{-2} mbar) yielded **4** (70.1 mg, 11%) as a white solid.

^{1}H NMR (400 MHz, Methylene Chloride-d_2): δ = 8.11 – 8.05 (1H, m), 8.04 – 8.00 (1H, m), 7.64 – 7.58 (1H, m), 0.40 (9H, s) ppm. **^{13}C{^{1}H} NMR** (101 MHz, Methylene Chloride-d_2): δ = 173.6 (d, *J* = 38.4), 171.8 (d, *J* = 76.3), 137.6 (t, *J* = 5.5, 5.5), 133.7, 129.4 (t, *J* = 9.9, 9.9), 0.2 (t, *J* = 3.1, 3.1) ppm. **^{31}P{^{1}H} NMR** (162 MHz, Methylene Chloride-d_2): δ = 221.3 (s) ppm. **ESI-TOF** (m/z): 357.0778 (calc. 357.0784) [M+Na^+]

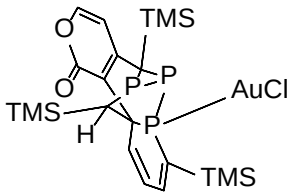
(1*R*,2*R*,7a*R*,11b*S*,12*R*)-4,11b,12-tris(trimethylsilyl)-1,7a-methanodiphosphireno[1',3':1,6]phosphinino[1',2':2,3][1,2]diphosphinino[4,5-*c*]pyran-8(11b*H*)-one (5)



Column chromatography on silica gel column (100 % *n*-hexane, 4 CV; 100 % *n*-hexane → *n*-hexane/EtOac: 1:4; 20 CV) and subsequent vacuum sublimation (110 °C, 5 x 10^{-2} mbar) yielded **5** (367 mg, 40%) as a white solid.

^{1}H NMR (400 MHz, Methylene Chloride-d_2): δ = 8.01 – 7.95 (1H, m), 7.30 (1H, dd, *J* = 5.6, 2.1), 6.55 (1H, ddd, *J* = 15.5, 5.5, 1.4), 6.46 (1H, d, *J* = 5.6), 5.97 (1H, dd, *J* = 10.7, 5.5), 1.70 (1H, d, *J* = 3.3), 0.28 (9H, t, *J* = 1.2, 1.2), 0.26 (9H, s) 0.05 (9H, d, *J* = 1.1) ppm. **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*): δ = 159.7 (d, *J* = 4.0), 152.8 – 152.6 (m), 147.4 (d, *J* = 3.3), 136.7 (t, *J* = 5.5, 5.5), 134.9 – 134.7 (m), 129.1 (d, *J* = 57.0), 123.3 (dd, *J* = 13.4, 2.5), 121.5 (d, *J* = 12.9), 110.3 (d, *J* = 2.9), 45.5 (d, *J* = 29.9), 40.9 (dt, *J* = 61.7, 4.9, 4.9), 23.7 – 22.4 (m), 1.8 (d, *J* = 6.2), 0.3 (t, *J* = 6.4, 6.4), -0.2 (dd, *J* = 5.5, 1.0) ppm. **^{31}P{^{1}H} NMR** (162 MHz, Methylene Chloride-d_2): δ = 20.8 (dd, *J* = 360.7, 10.4), -107.3 (dd, *J* = 214.2, 10.4), -210.8 (dd, *J* = 360.8, 214.2) ppm. **ESI-TOF** (m/z): 533.0835 (calc. 533.0633) [M+K^+] **Elemental analysis** calculated for $C_{21}H_{33}O_2P_3Si_3$: C 50.99 H 6.72; found: C 50.99 H 6.776

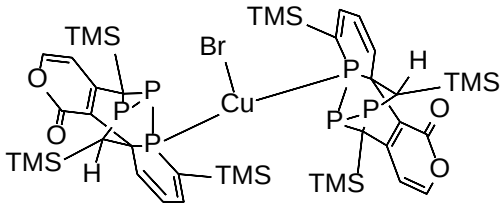
Reaction of 5 with AuCl·SMe_2 (6)



A mixture of **5** (25 mg, 0.05 mmol, 1.0 eq.) and AuCl·SMe_2 (15 mg, 0.05 mmol, 1.0 eq.) was dissolved in DCM (2 ml) and stirred over night at room temperature. The yellow solution was filtrated over Celite and concentrated in high vacuum, yielding **6** (31 mg, 85%) as a yellow solid.

^{1}H NMR (400 MHz, Methylene Chloride-d_2): δ = 8.13 (1H, dd, *J* = 15.2, 10.8), 7.48 (1H, dd, *J* = 5.6, 2.3), 6.81 (1H, dd, *J* = 37.8, 5.8), 6.55 (1H, d, *J* = 5.6), 6.19 (1H, ddd, *J* = 10.7, 5.8, 3.4), 1.64 (1H, d, *J* = 4.8), 0.38 (9H, s), 0.33 (9H, s), 0.09 (9H, s) ppm. **^{13}C{^{1}H} NMR** (101 MHz Methylene Chloride-d_2): δ = 159.2 (d, *J* = 4.7), 152.0 (d, *J* = 12.9), 149.6 (d, *J* = 3.2), 143.6 (dd, *J* = 5.4, 2.2), 136.3, 122.7 (d, *J* = 26.2), 121.7, 120.3, 110.0 (d, *J* = 3.6), 43.3 (d, *J* = 15.6), 38.1 (dd, *J* = 63.7, 3.4), 25.2 (d, *J* = 2.6), 1.3 – 1.1 (m), -0.1 (t, *J* = 6.7, 6.7), -0.2 (dd, *J* = 5.1, 1.5) ppm. **^{31}P{^{1}H} NMR** (162 MHz): δ = 51.4 (d, *J* = 369.6), -105.0 (dd, *J* = 203.9, 6.6), -250.5 (dd, *J* = 369.6, 205.1) ppm. **ESI-TOF** (m/z): 749.0247 (calc. 749.0230) [M+Na^+]

Reaction of 5 with CuBr·SMe_2 (7)



A mixture of **5** (25 mg, 0.05 mmol, 1.0 eq.) and CuBr·SMe_2 (10 mg, 0.05 mmol, 1.0 eq.) was dissolved in DCM (2 mL) and stirred for 15 min at room temperature. The yellow-green reaction mixture was filtrated over Celite and concentrated in high vacuum, yielding **7** (51 mg, 90%) as a yellow solid.

^{1}H NMR (400 MHz, Methylene Chloride-d_2): δ = 8.21 (1H, dd, *J* = 11.6, 11.6), 7.40 – 7.33 (1H, m), 6.64 (1H, dd, *J* = 27.3, 5.5), 6.47 (1H, d, *J* = 5.6), 6.01 (1H, ddd, *J* = 10.6, 5.4, 2.2), 1.76 (1H, d, *J* = 4.1), 0.33 (9H, s), 0.32 (9H, s), 0.05 (9H, s) ppm. **^{13}C{^{1}H} NMR** (101 MHz Methylene Chloride-d_2): δ = 159.8 (d, *J* = 4.4), 153.1 (d, *J* = 6.3), 148.6 , 139.4 (d, *J* = 2.9), 135.3 , 125.1 (d, *J* = 20.9), 123.4 (d, *J* = 21.1), 120.2 (d, *J* = 6.0), 110.5 , 43.9, 39.7 (d, *J* = 51.6), 23.0, 1.4, 0.5 (d, *J* = 5.7), 0.4 (t, *J* = 6.4, 6.4) ppm. **^{31}P{^{1}H} NMR** (162 MHz, Methylene Chloride-d_2): δ = 22.2 (d, *J* = 359.3), -107.3 (d, *J* = 205.1), -229.3 (dd, *J* = 351.3, 206.7) ppm. **ESI-TOF** (m/z): 1153.0329 (calc. 1153.0374) [M+Na^+]

3. NMR Spectra

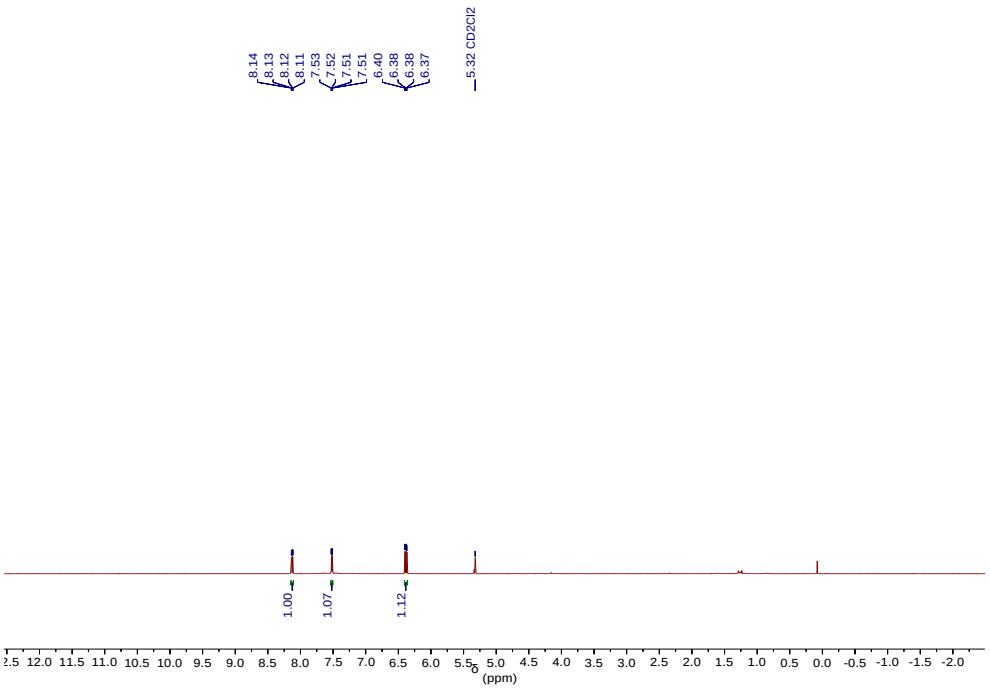


Figure S1. ^{1}H NMR of 2*H*,2'*H*-[3,3'-bipyran]-2,2'-dione **(2)** in Methylene Chloride-d_2

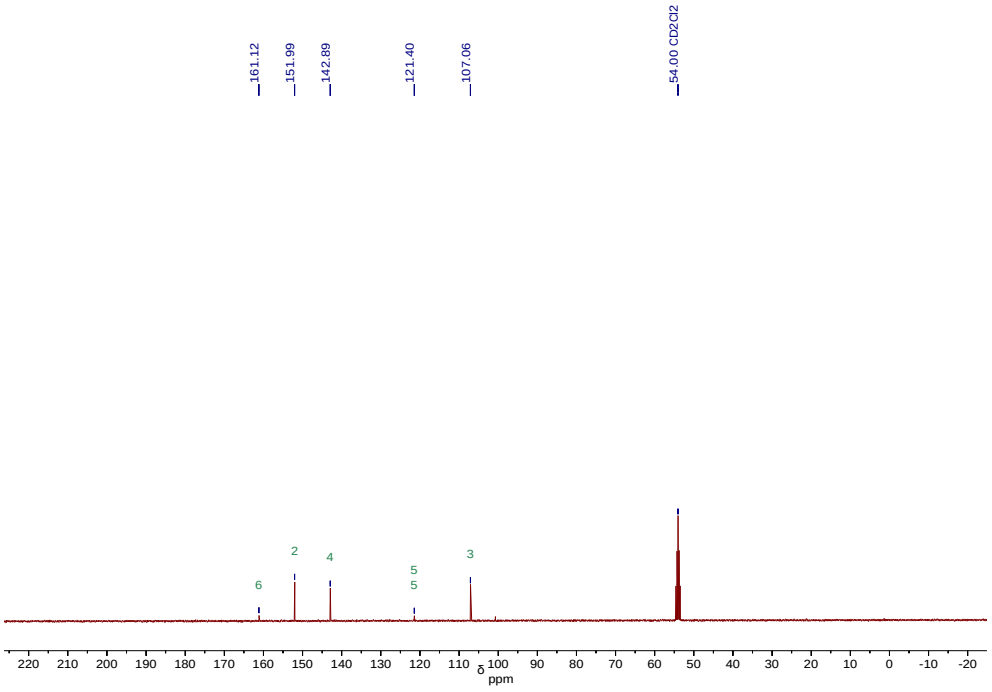


Figure S2. ^{13}C{^{1}H} NMR of 2*H*,2'*H*-[3,3'-bipyran]-2,2'-dione **(2)** in Methylene Chloride-d_2

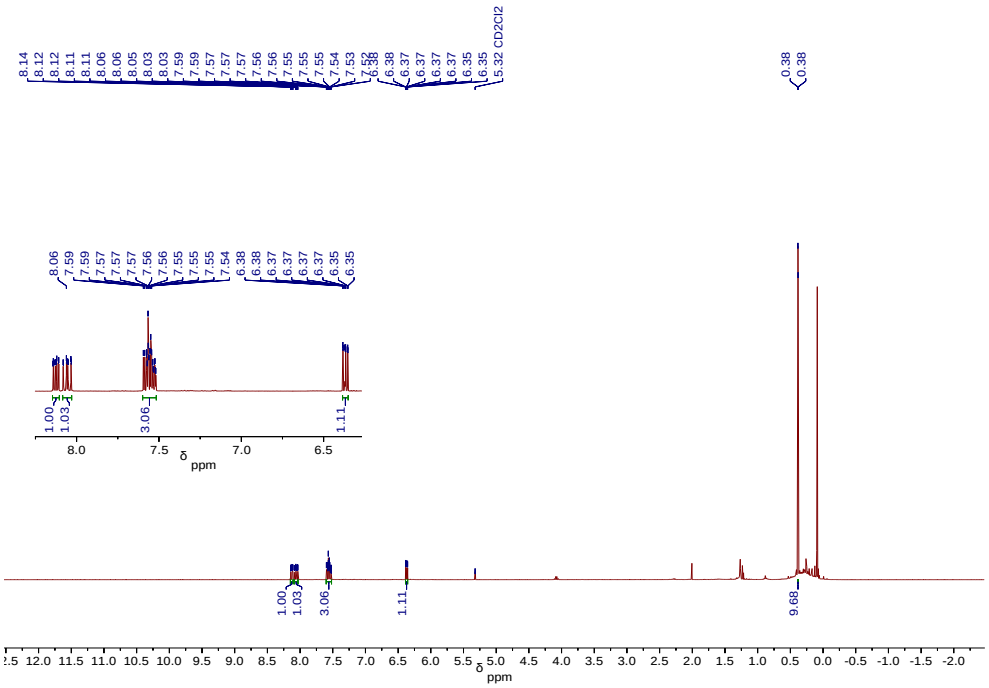


Figure S3. ^{1}H NMR of 6-(6-(trimethylsilyl)phosphinin-2-yl)-2H-pyran-2-one **(3)** in Methylene Chloride-d_2

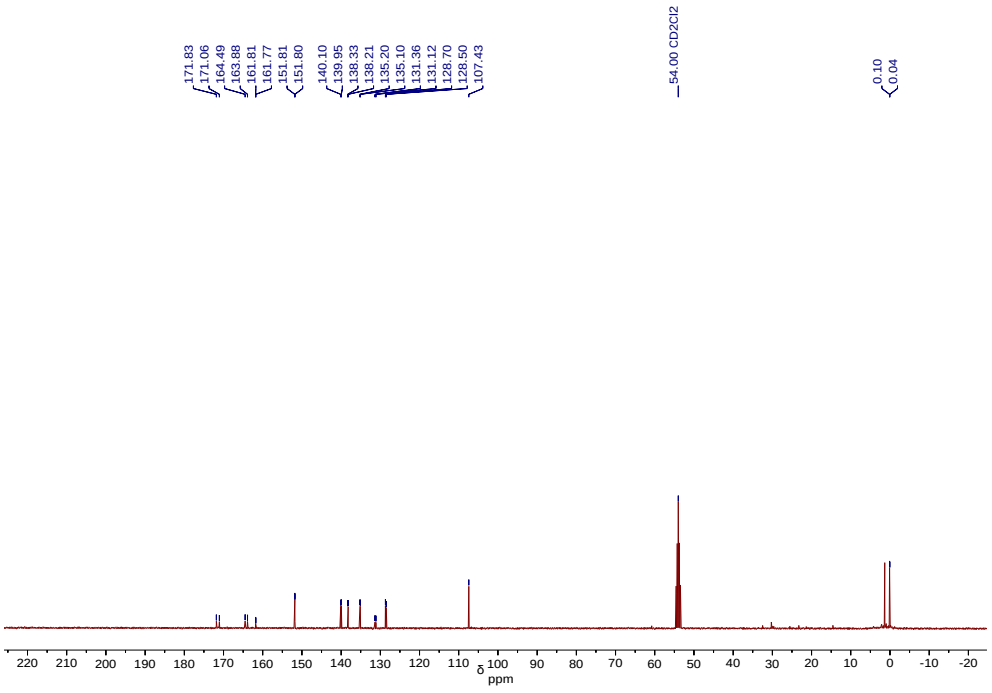


Figure S4. ^{13}C{^{1}H} NMR of 6-(6-(trimethylsilyl)phosphinin-2-yl)-2*H*-pyran-2-one **(3)** in Methylene Chloride-d_2

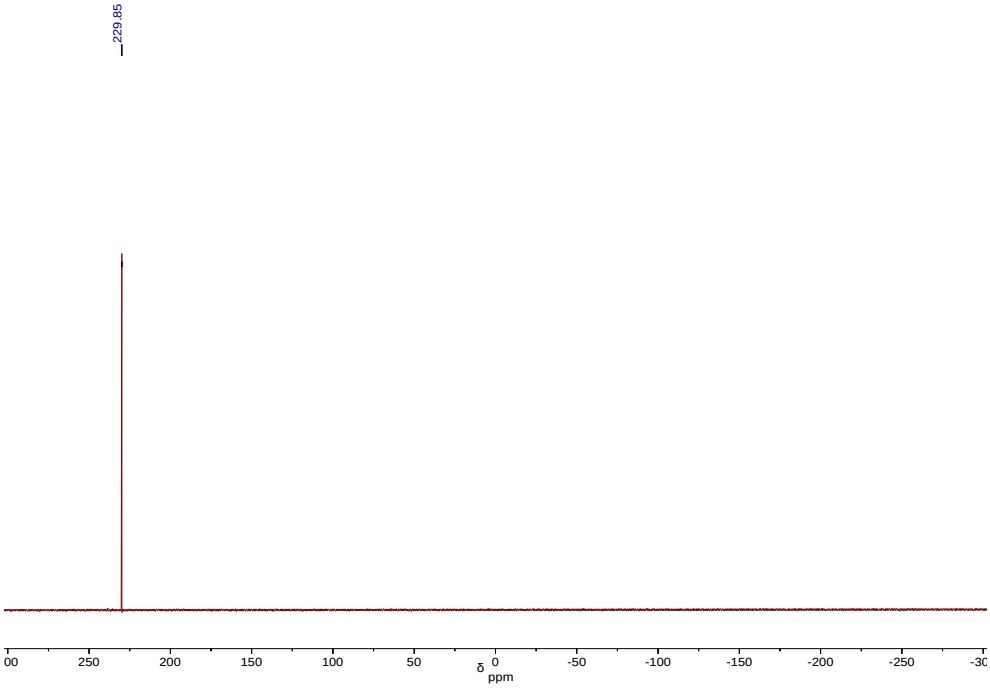


Figure S5. $^{31}P\{^{1}H\}$ NMR of 6-(6-(trimethylsilyl)phosphinin-2-yl)-2*H*-pyran-2-one **(3)** in Methylene Chloride-d_2

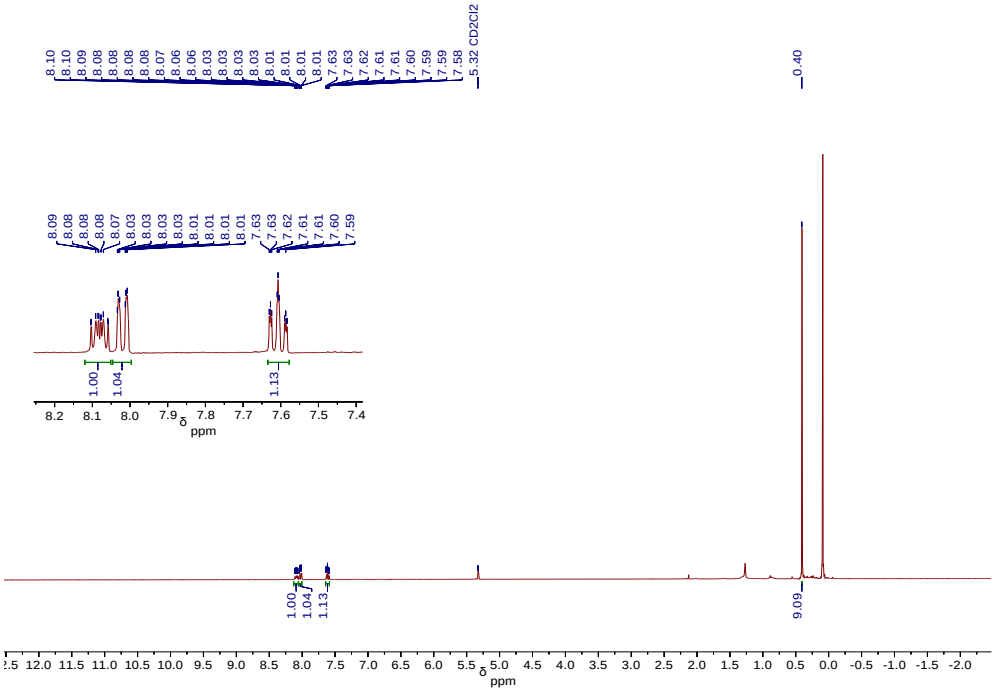


Figure S6. ^{1}H NMR of 6,6'-bis(trimethylsilyl)-2,2'-biphosphinine **(4)** in Methylene Chloride-d_2

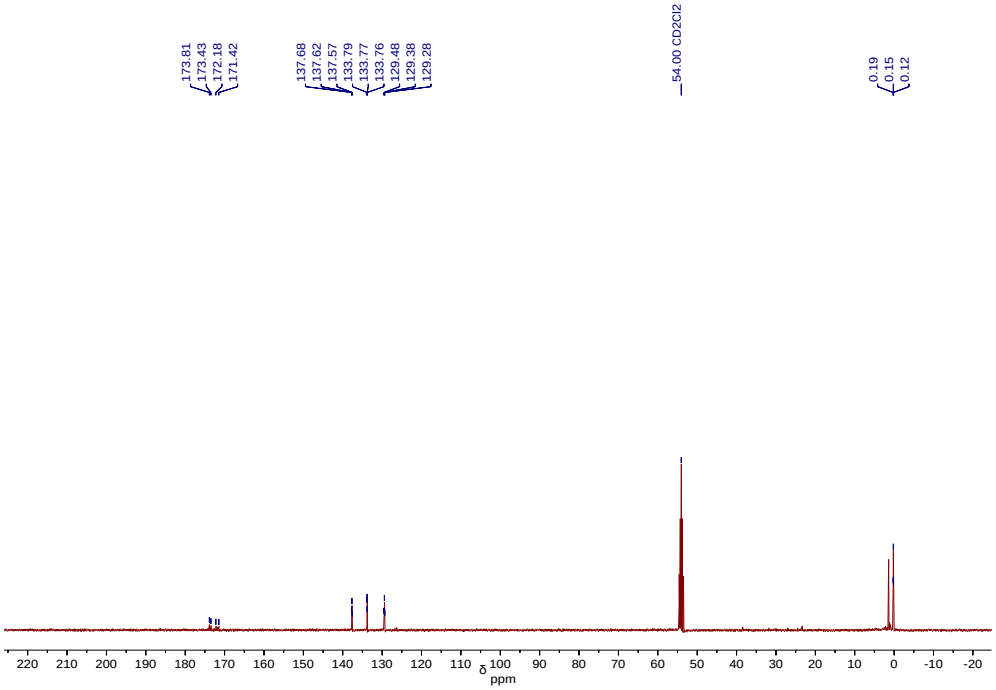


Figure S7. $^{13}C\{^{1}H\}$ NMR of 6,6'-bis(trimethylsilyl)-2,2'-biphosphinine **(4)** in Methylene Chloride-d_2

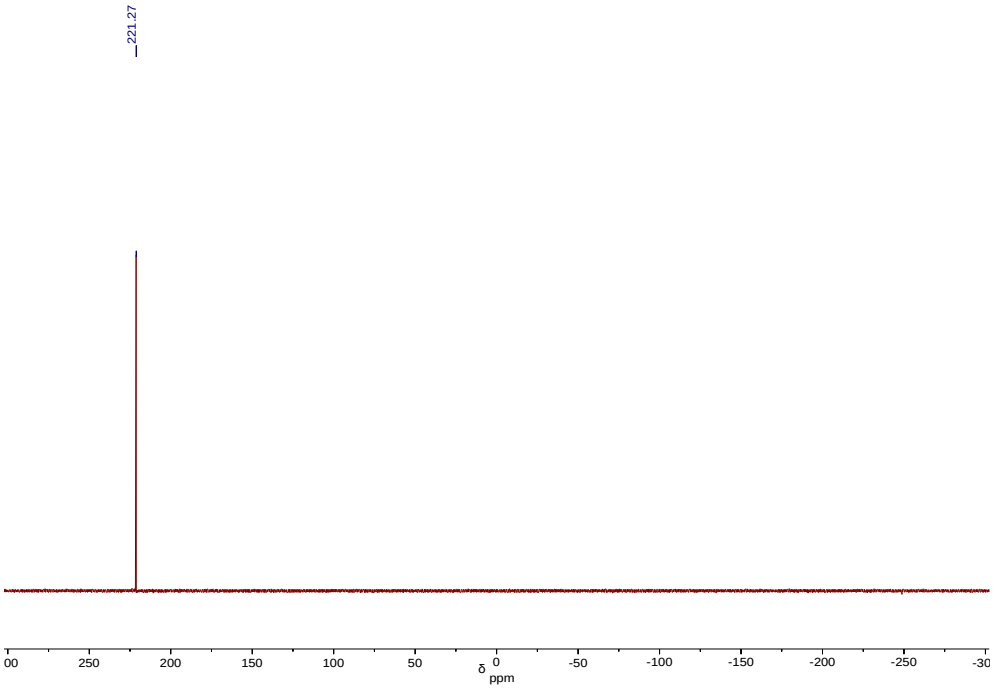


Figure S8. $^{31}P\{^{1}H\}$ NMR of 6,6'-bis(trimethylsilyl)-2,2'-biphosphinine **(4)** in Methylene Chloride-d_2

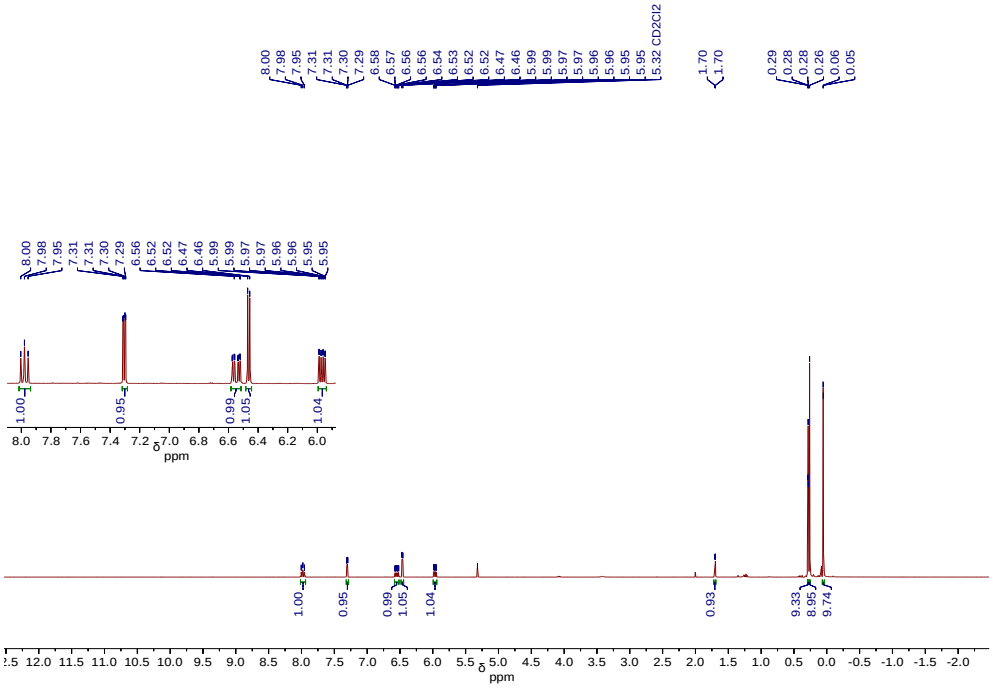


Figure S9. ^{1}H NMR of (1*R*,2*R*,7a*R*,11b*S*,12*R*)-4,11b,12-tris(trimethylsilyl)-1,7a-methanodiphosphireno[1',3':1,6]phosphinino[1',2':2,3][1,2]diphosphinino[4,5-*c*]pyran-8(11b*H*)-one **(5)** in Methylene Chloride-d_2

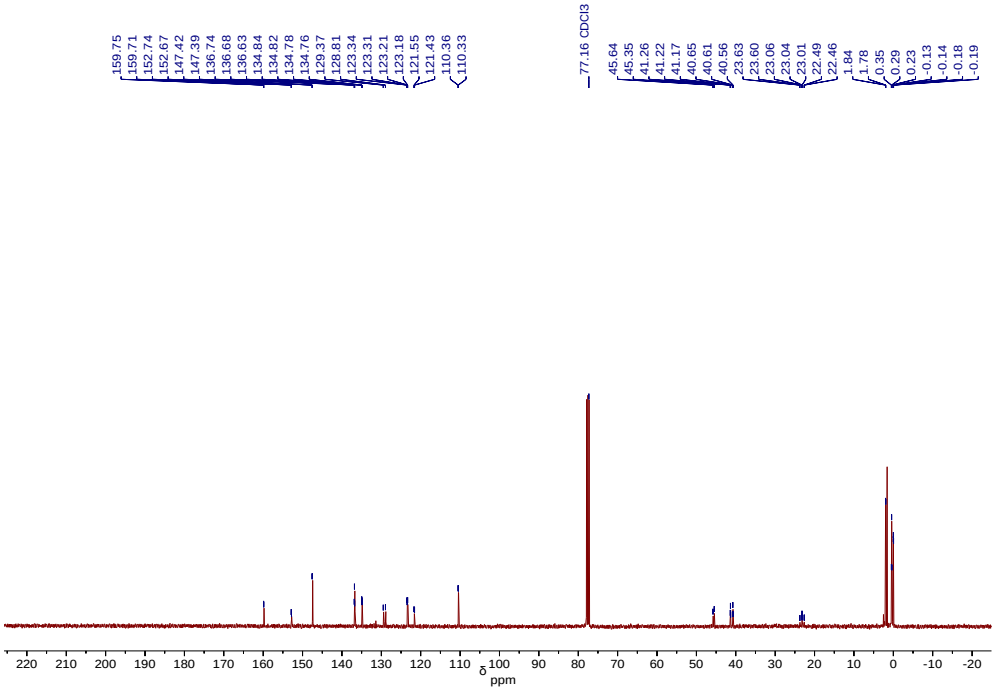


Figure S10. ^{13}C{^{1}H} NMR of (1*R*,2*R*,7a*R*,11b*S*,12*R*)-4,11b,12-tris(trimethylsilyl)-1,7a-methanodiphosphireno[1',3':1,6]phosphinino[1',2':2,3][1,2]diphosphinino[4,5-*c*]pyran-8(11b*H*)-one **(5)** in Chloroform-d

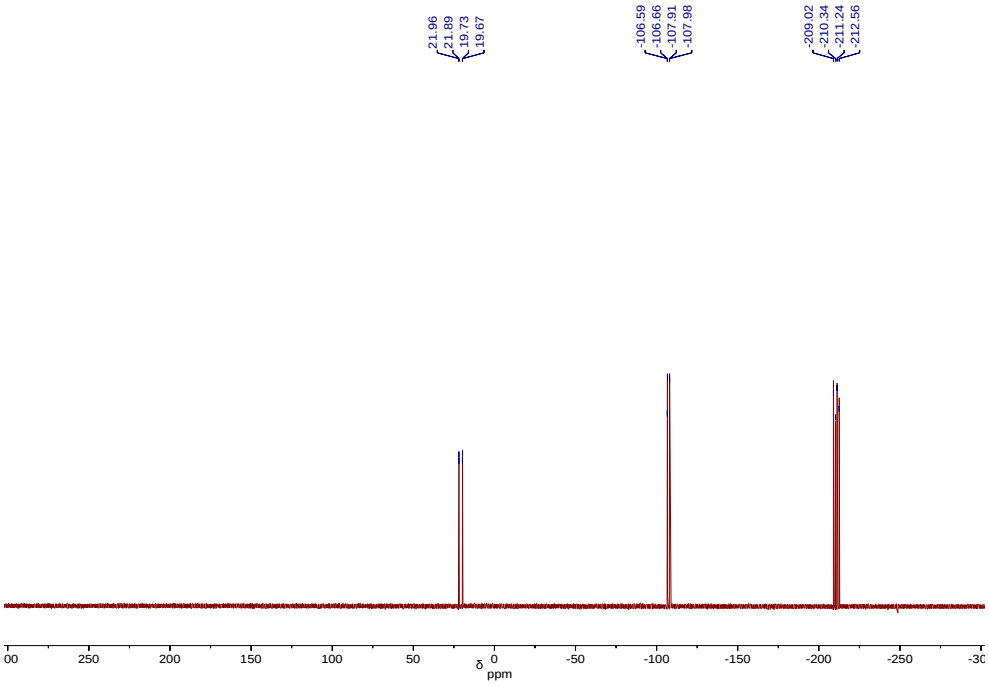


Figure S11. $^{31}P\{^{1}H\}$ NMR of (1*R*,2*R*,7a*R*,11b*S*,12*R*)-4,11b,12-tris(trimethylsilyl)-1,7a-methanodiphosphireno[1',3':1,6]phosphinino[1',2':2,3][1,2]diphosphinino[4,5-*c*]pyran-8(11b*H*)-one **(5)** in Methylene Chloride-d_2

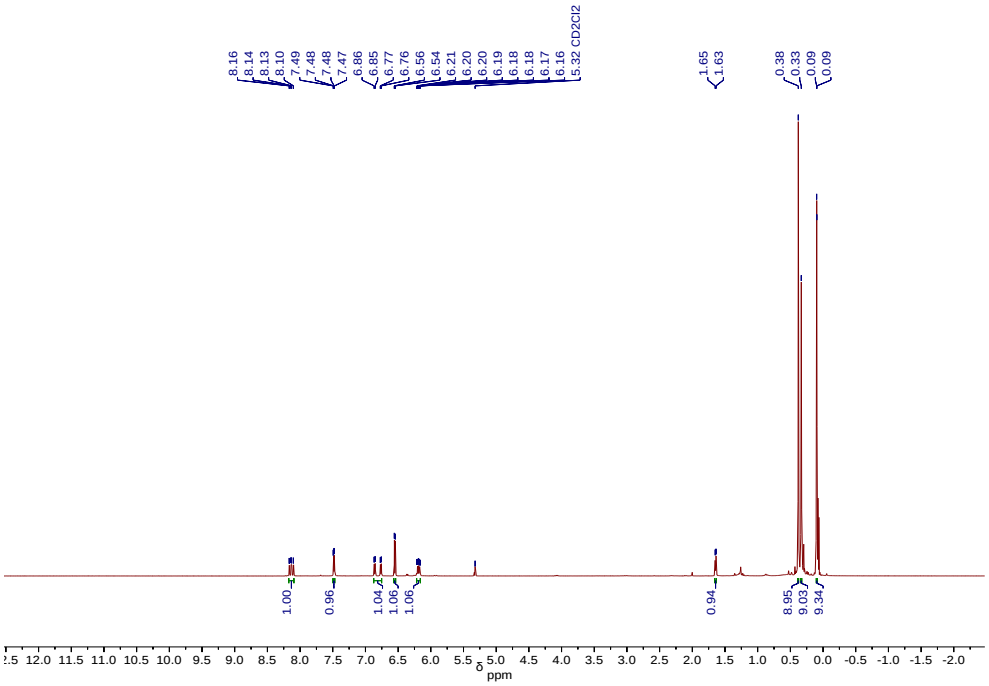


Figure S12. ^{1}H NMR of [(**5**)AuCl] in Methylene Chloride-d_2

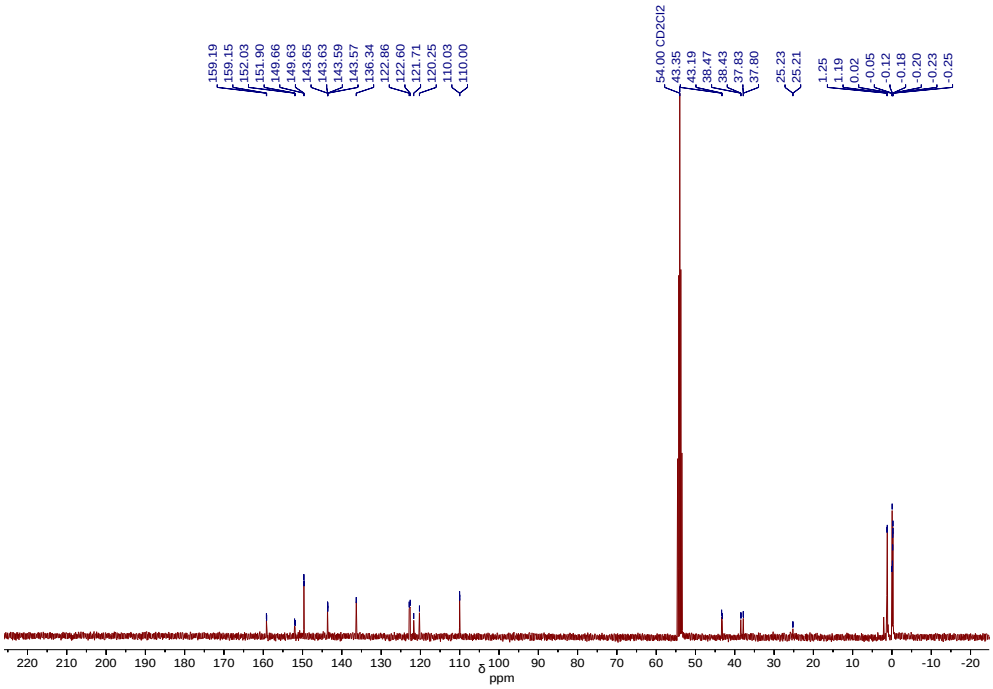


Figure S13. $^{13}C\{^{1}H\}$ NMR of [(**5**)AuCl] in Methylene Chloride-d_2

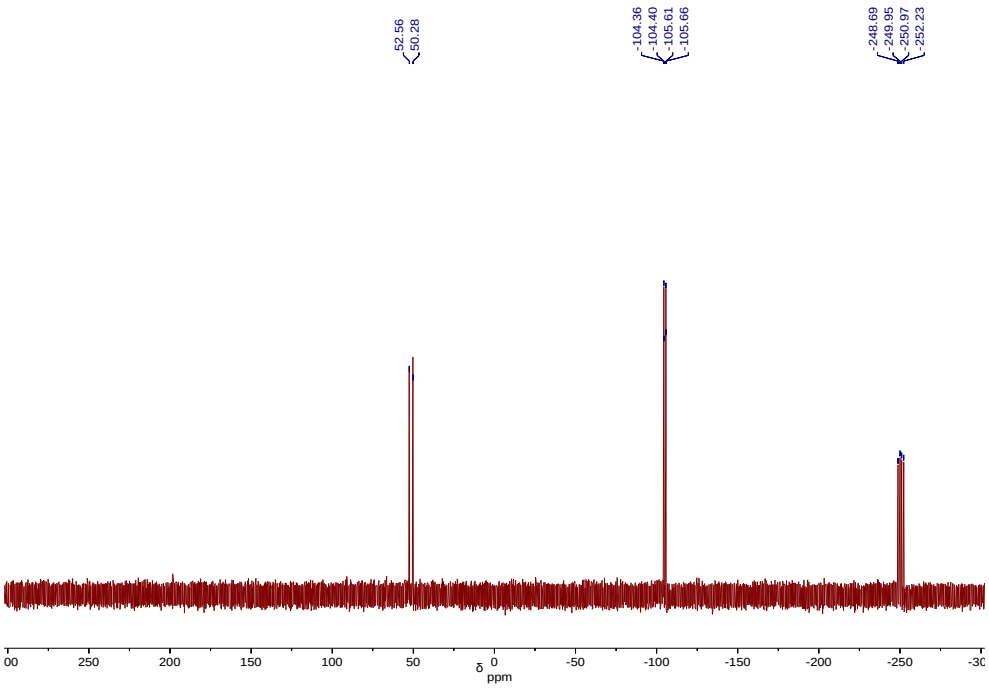


Figure S14. $^{31}P\{^{1}H\}$ NMR of [(**5**)AuCl] in Methylene Chloride

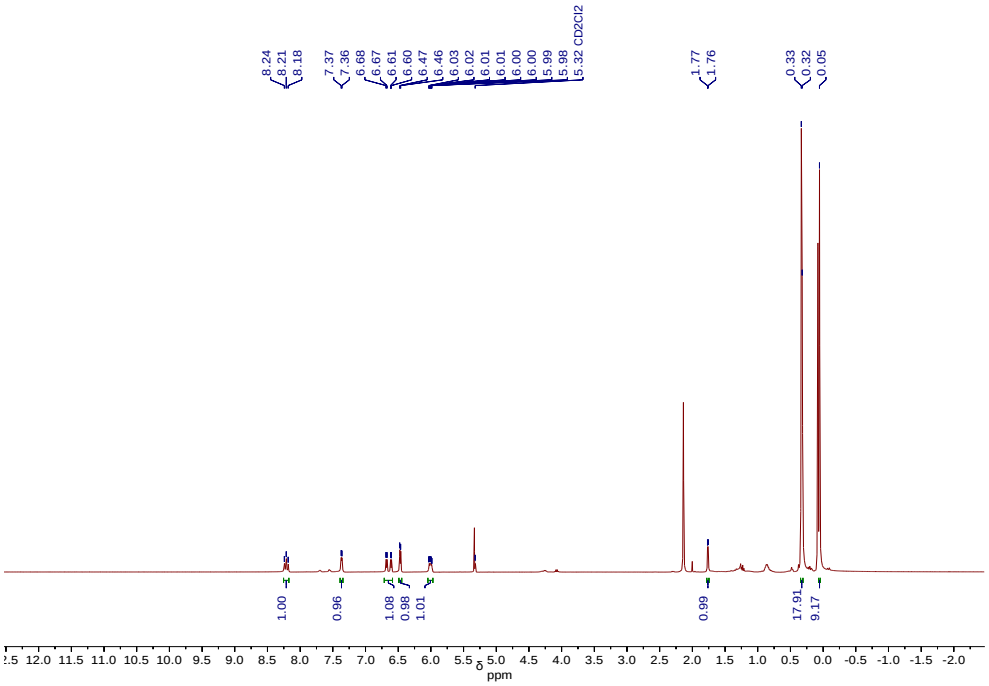


Figure S15. ^{1}H NMR of [(**5**)$_2$CuBr] in Methylene Chloride-d$_2$

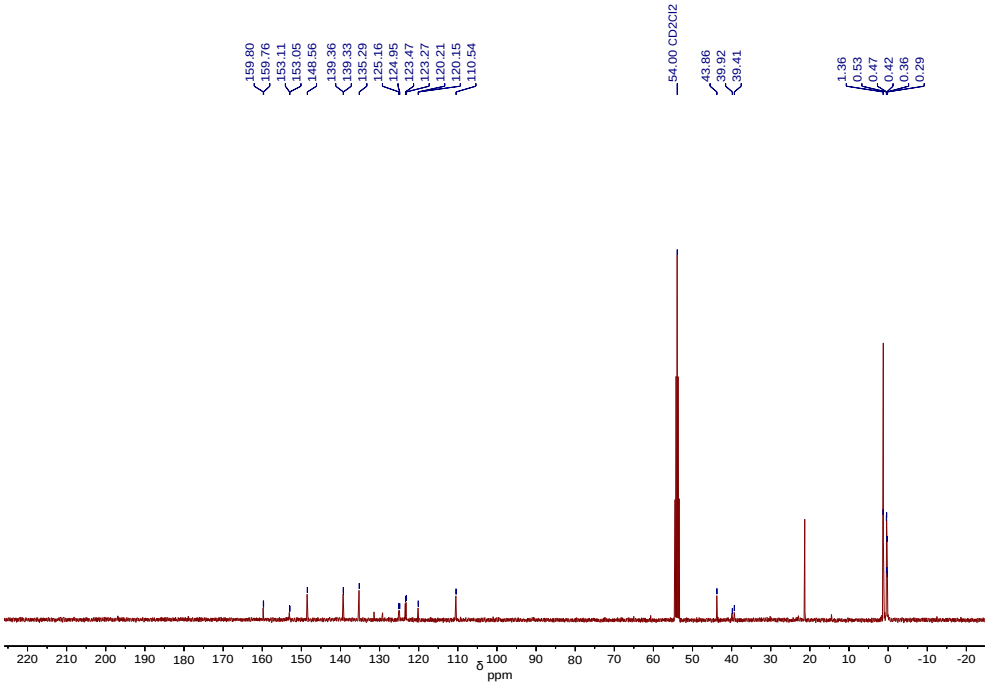


Figure S16. ^{13}C{^{1}H} NMR of [(**5**)$_2$CuBr] in Methylene Chloride-d$_2$

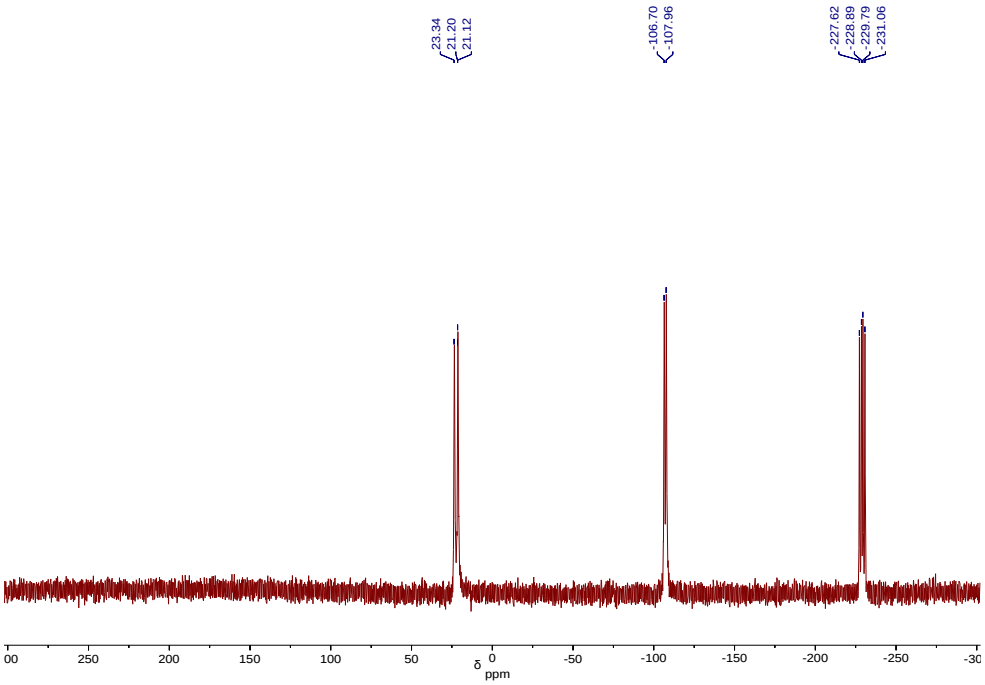


Figure S17. $^{31}P\{^{1}H\}$ NMR of [(**5**)$_2$CuBr] in Methylene Chloride-d$_2$

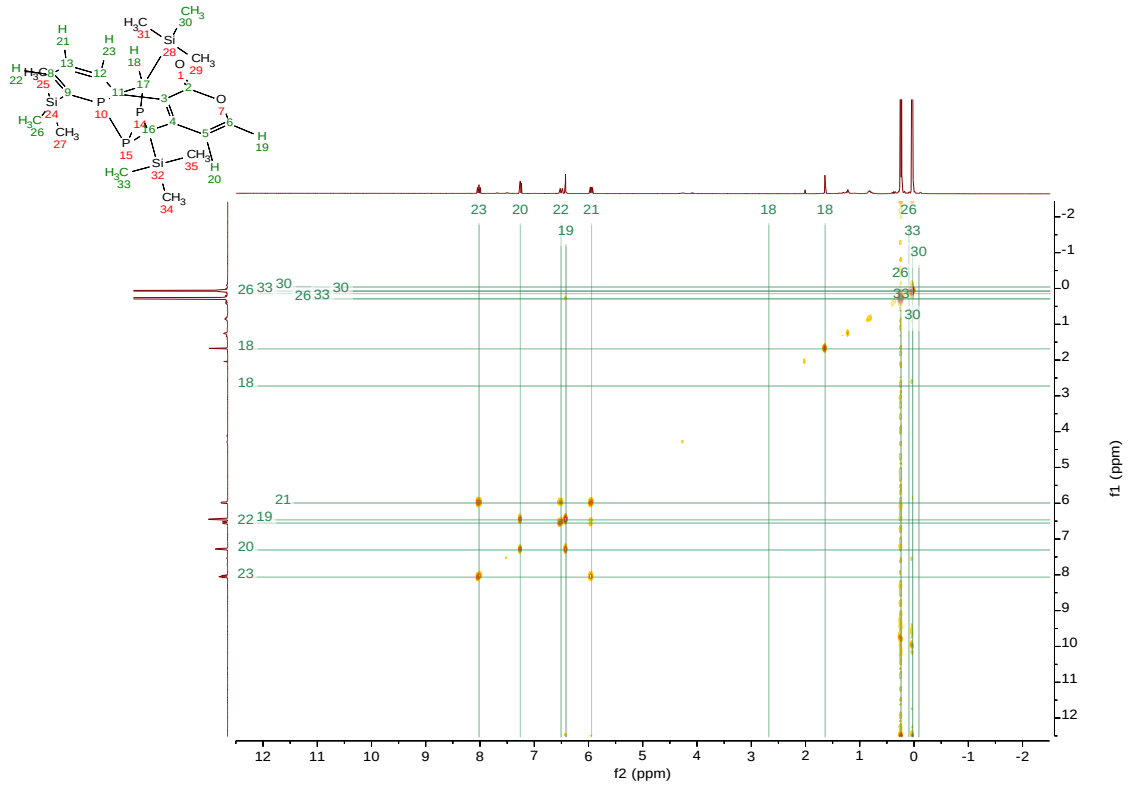


Figure S18. ^{1}H COSY in Methylene Chloride-d$_2$ of **5**

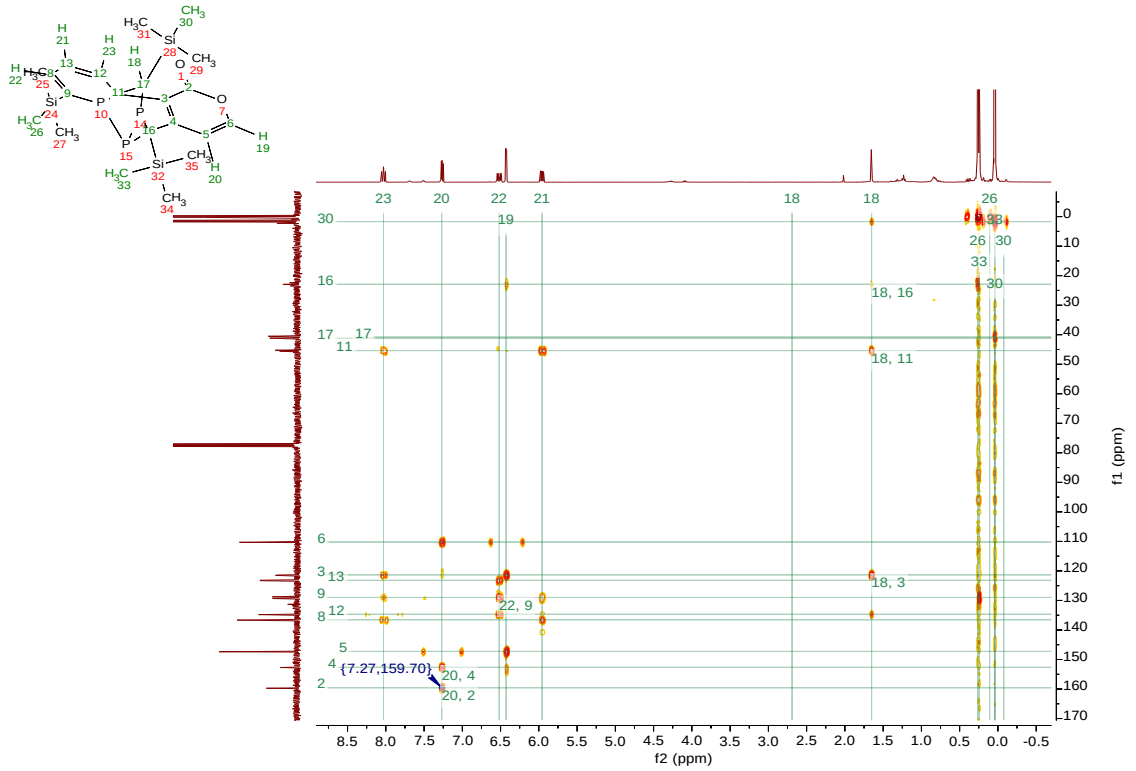


Figure S19. ^{1}H ^{13}C HMBC in Methylene Chloride-d_2 of **5**

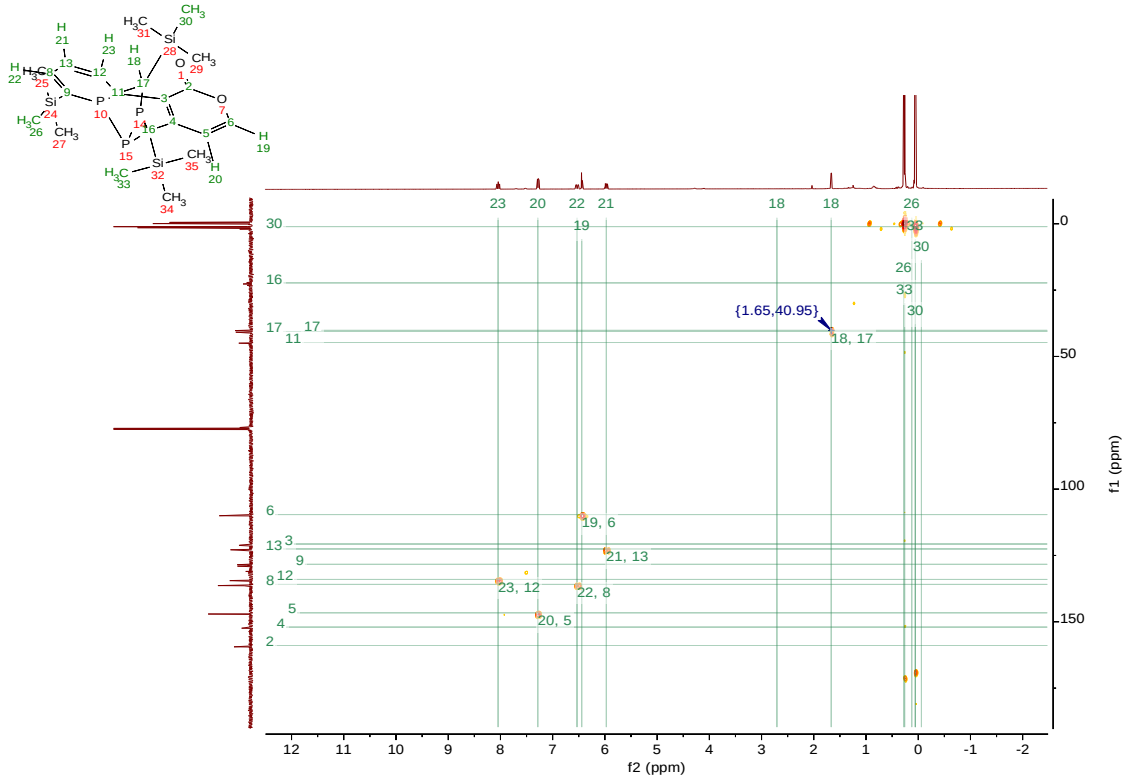


Figure S20. ^{1}H ^{13}C HMQC in Methylene Chloride-d_2 of **5**

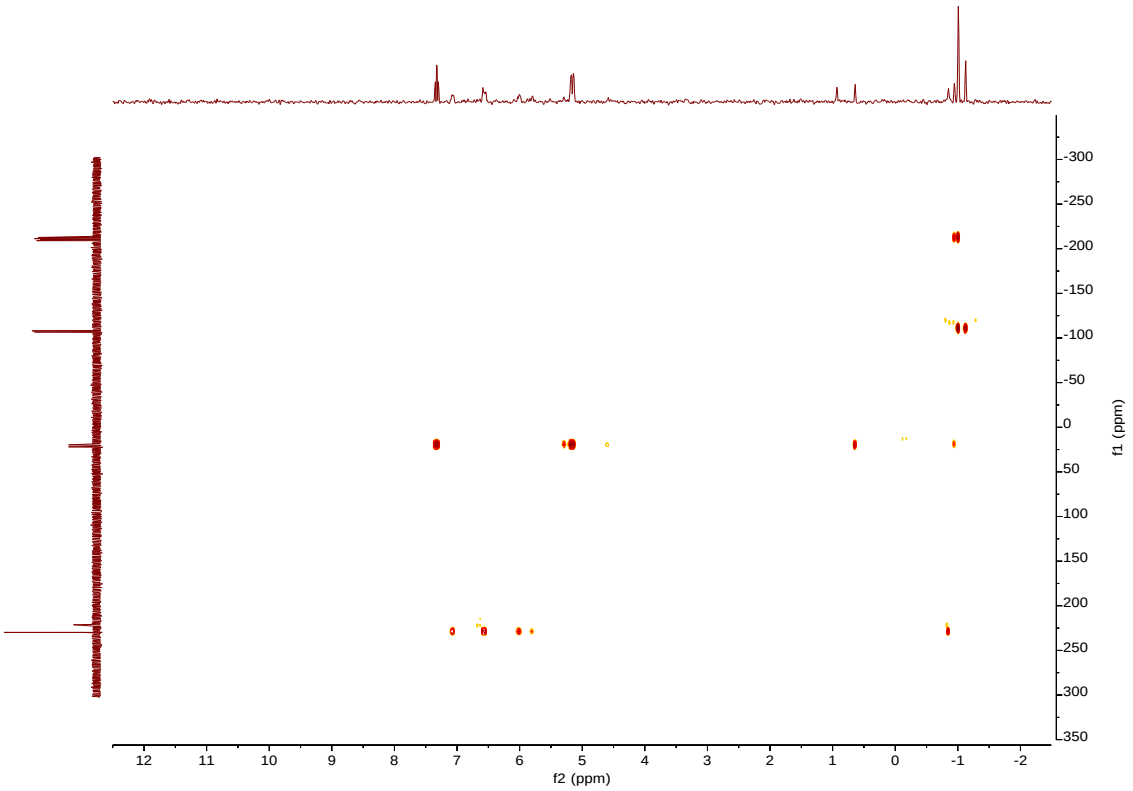


Figure S21. ^{1}H ^{31}P HMBC of crude product **5** in Methylene Chloride-d_2

4. Crystallographic Data

X-ray crystal structure determination of 2

Crystals suitable for X-ray diffraction were obtained by evaporating a saturated solution of **2** DCM. *Crystallographic data* $C_{10}H_6O_4$, *F*w = 190.15 g/mol, 0.460×0.04×0.03 mm^3, colorless plate, orthorhombic, *Fdd2*, *a* = 20.886(2), *b* = 21.280(3), *c* = 3.6073(4), Å, α =90° *β* = 90° γ = 90°, *V* = 1603.2(3) $Å^3$, *Z* = 8, D_x = 1.576 gcm^{-3}, μ = 0.124 mm^{-1}. 3485 reflections were measured by using a Bruker D8-Venture CMOS diffractometer[3] with a rotating anode (MoKα radiation, λ = 0.71073 Å) up to a resolution of $(\sin\theta/\lambda)_{max}$ = 0.58 $Å^{-1}$ at a temperature of 100 K. 454 reflections were unique (R_{int} = 0.0310). The structures were solved with SHELXL-2014[4] by using direct methods and refined with SHELXL-2014[4] on F^2 for all reflections. Non-hydrogen atoms were refined by using anisotropic displacement parameters. The positions of the hydrogen atoms were calculated for idealized positions. 65 parameters were refined with one restraint. R_1 = 0.0279 for 658 reflections with $I>2\sigma(I)$ and wR_2 = 0.0727 for 699 reflections, *S*=1.119, residual electron density was between -0.22and 0.12 $eÅ^{-3}$. Geometry calculations and checks for higher symmetry were performed with the PLATON program.[5]

CCDC-1897251 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

X-ray crystal structure determination of 5

Crystals suitable for X-ray diffraction were obtained by cooling down a saturated solution of **5** in *n*-pentane. *Crystallographic data* $C_{21}H_{33}O_2P_3Si_3$, *F*w = 494.65 g/mol, 0.230×0.110×0.04 mm^3, yellow plate, triclinic, *P-1*, a = 8.941(3), b = 9.608(4), c = 16.384(6), Å, α = 106.210(8)° β = 103.338(15)° γ = 93.876(10)°, V = 1301.8(8) $Å^3$, Z = 2, D_x = 1.262 gcm^{-3}, μ = 0.382 mm^{-1}. 58632 reflections were measured by using a Bruker D8-Venture CMOS diffractometer[3] with a rotating anode (MoKα radiation, λ = 0.71073 Å) up to a resolution of $(\sin\theta/\lambda)_{max}$ = 0.58 $Å^{-1}$ at a temperature of 100 K. 4777 reflections were unique (R_{int} = 0.0502). The structures were solved with SHELXL-2014[4] by using direct methods and refined with SHELXL-2014[4] on F^2 for all reflections. Non-hydrogen atoms were refined by using anisotropic displacement parameters. The positions of the hydrogen atoms were calculated for idealized positions. 286 parameters were refined without restraints. R_1 = 0.0273 for 4195 reflections with $I>2\sigma(I)$ and wR_2 = 0.0647 for 4777 reflections, S=1.039, residual electron density was between -0.27 and 0.34 $eÅ^{-3}$. Geometry calculations and checks for higher symmetry were performed with the PLATON program.[5]

CCDC-1897252 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

X-ray crystal structure determination of 6

Crystals suitable for X-ray diffraction were obtained by evaporating a saturated solution of **6** in THF. *Crystallographic data* $C_{21}H_{33}AuClO_2P_3Si_3$, *F*w = 727.07 g/mol, 0.280×0.280×0.14 mm^3, colorless block, monoclinic, *P21/c*, a = 13.2862(18), b = 11.6119(14), c = 19.290(3), Å, α = 90° β = 98.741(5)° γ = 90 , V = 2941.4(7) $Å^3$, Z = 4, D_x = 1.642 gcm^{-3}, μ = 5.394 mm^{-1}. 91626 reflections were measured by using a Bruker D8-Venture CMOS diffractometer[3] with a rotating anode (MoKα radiation, λ = 0.71073 Å) up to a resolution of $(\sin\theta/\lambda)_{max}$ = 0.58 $Å^{-1}$ at a temperature of 100 K. 6044 reflections were unique (R_{int} = 0.0705). The structures were solved with SHELXL-2014[4] by using direct methods and refined with SHELXL-2014[4] on F^2 for all reflections. Non-hydrogen atoms were refined by using anisotropic displacement parameters. The positions of the hydrogen atoms were calculated for idealized positions. 280 parameters were refined without restraints. R_1 = 0.0169 for 5668 reflections with $I>2\sigma(I)$ and wR_2 = 0.0415 for 6044 reflections, S=1.096, residual electron density was between -1.02 and 0.50 $eÅ^{-3}$. Geometry calculations and checks for higher symmetry were performed with the PLATON program.[5]

CCDC-1897250 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

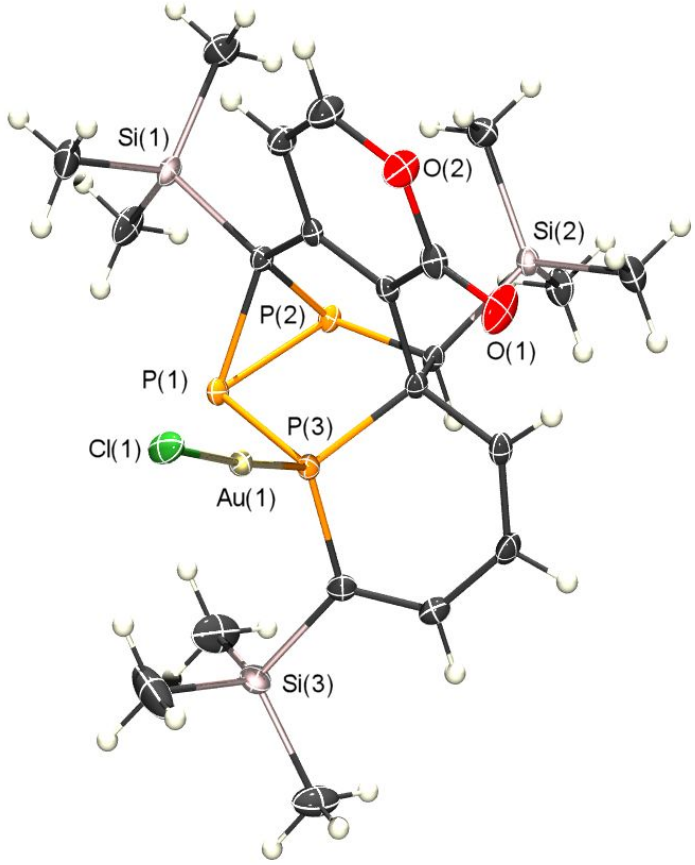


Figure S22. Molecular structure of [(**5**)AuCl] (**6**) in the crystal. Displacement ellipsoids are shown at the 50% probability level. Selected bond lengths (Å) and angles (°): P(1)-P(2): 2.1883(9); P(1)-P(3): 2.1785(8); P(3)-Au(1): 2.2269(6); Au(1)-Cl(1). P(3)-Au(1)-Cl(1): 176.66(2).

X-ray crystal structure determination of 7

Crystals suitable for X-ray diffraction were obtained by evaporating a saturated solution of **7** in THF. *Crystallographic data*: $C_{42}H_{66}BrCuO_4P_6Si_6$, *F*w = 1132.75 g/mol, 0.18×0.07×0.05 mm^3, colorless plate, triclinic, *P-1*, *a* = 12.381(4), *b* = 13.372(4), *c* = 17.518(5), Å, α = 106.111(7)° *β* = 99.386(8)° γ = 99.154(7)° , *V* = 2684.4(14) Å^3, *Z* = 2, D_x = 1.401 gcm^{-3}, μ = 1.502 mm^{-1}. 149326 reflections were measured by using a Bruker D8-Venture CMOS diffractometer[3] with a rotating anode (MoKα radiation, λ = 0.71073 Å) up to a resolution of $(\sin\theta/\lambda)_{max}$ = 0.58 Å^{-1} at a temperature of 100 K. 9906 reflections were unique (R_{int} = 0.0786). The structures were solved with SHELXL-2014[4] by using direct methods and refined with SHELXL-2014[4] on F^2 for all reflections. Non-hydrogen atoms were refined by using anisotropic displacement parameters. The positions of the hydrogen atoms were calculated for idealized positions. 543 parameters were refined without restraints. R_1 = 0.0314 for 8205 reflections with $I>2\sigma(I)$

and wR_2 = 0.0671 for 4389 reflections, S=1.040, residual electron density was between -0.34 and 0.51 eÅ^{-3}. Geometry calculations and checks for higher symmetry were performed with the PLATON program.[5]

CCDC-1897253 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

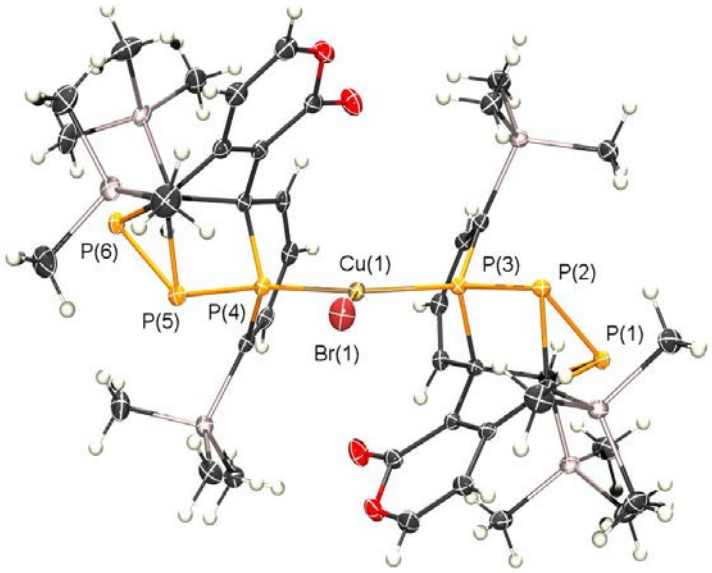


Figure S23. Molecular structure of [(**5**)$_2$CuBr] (**7**) in the crystal. Displacement ellipsoids are shown at the 50% probability level. Selected bond lengths (Å) and angles (°): P(1)-P(2): 2.1852(10); P(2)-P(3): 2.1832(12); P(4)-P(5): 2.1851(9); P(5)-P(6): 2.1837(11); P(3)-Cu(1): 2.2478(8)); P(4)-Cu(1): 2.2515(9); Cu(1)-Br(1): 2.3550(9). P(4)-Cu(1)-P(3): 173.80(12).

5. Computational data of all structures

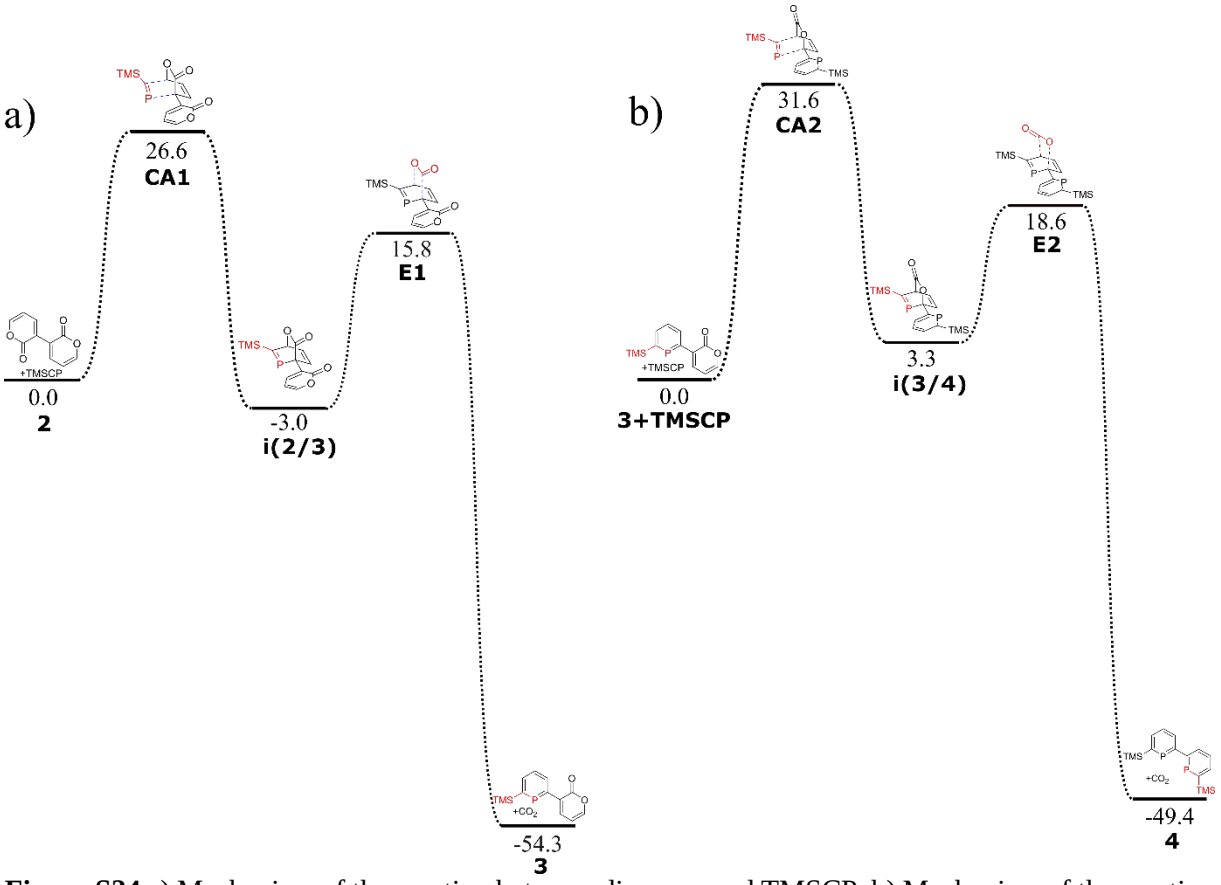


Figure S24 a) Mechanism of the reaction between dipyrone and TMSCP, b) Mechanism of the reaction between compound **3** and TMSCP to yield compound **4**. Gibbs free energies (kcal/mol) were obtained at the ωB97X-D/6-311+G** (PCM=toluene, T=383K, p=atmospheric) level of theory.

Table S1 Gibbs free energies (kcal/mol) of the intermediates and transition states (cycoaddition and elimination steps) depicted in **Figure S24** at different levels of the theory. Unless otherwise stated Gibbs free energies are at 298 K.

	with respect to compound **2**				with respect to compound **3**+TMSCP			
level of calc.	**CA1**	**i(2/3)**	**E1**	**3**	**CA2**	**i(3/4)**	**E2**	**4**
M06-2X/ 6-31+G*	25.2	-2.1	21.2	-44.9	20.0	-6.3	13.7	-51.0
M06-2X/ cc-pVTZ	22.7	-4.0	19.0	-55.5	24.0	-2.1	17.9	-55.4
M06-2X-D3/ cc-pVTZ PCM=toluene	23.0	-3.6	18.8	-54.0	24.6	-1.0	18.3	-53.1
M06-2X-D3/ cc-pVTZ T=383K	26.6	0.3	22.5	-50.5	28.7	3.2	22.5	-49.2

B3LYP/ cc-pVTZ T=383K	29.4	10.0	23.3	-50.3	31.4	14.6	23.8	-48.7
ωB97XD/ 6-311+G**	26.3	-3.6	15.4	-51.4	27.8	-1.0	14.7	-50.8
local-CCSD(T)/ cc-pVTZ[a]	27.4	0.0	21.9	-51.3	28.6	2.2	21.4	-50.3

[a]Geometry and correction to Gibbs free energy is obtained from M06-2X/cc-pVTZ calculation on 383K.

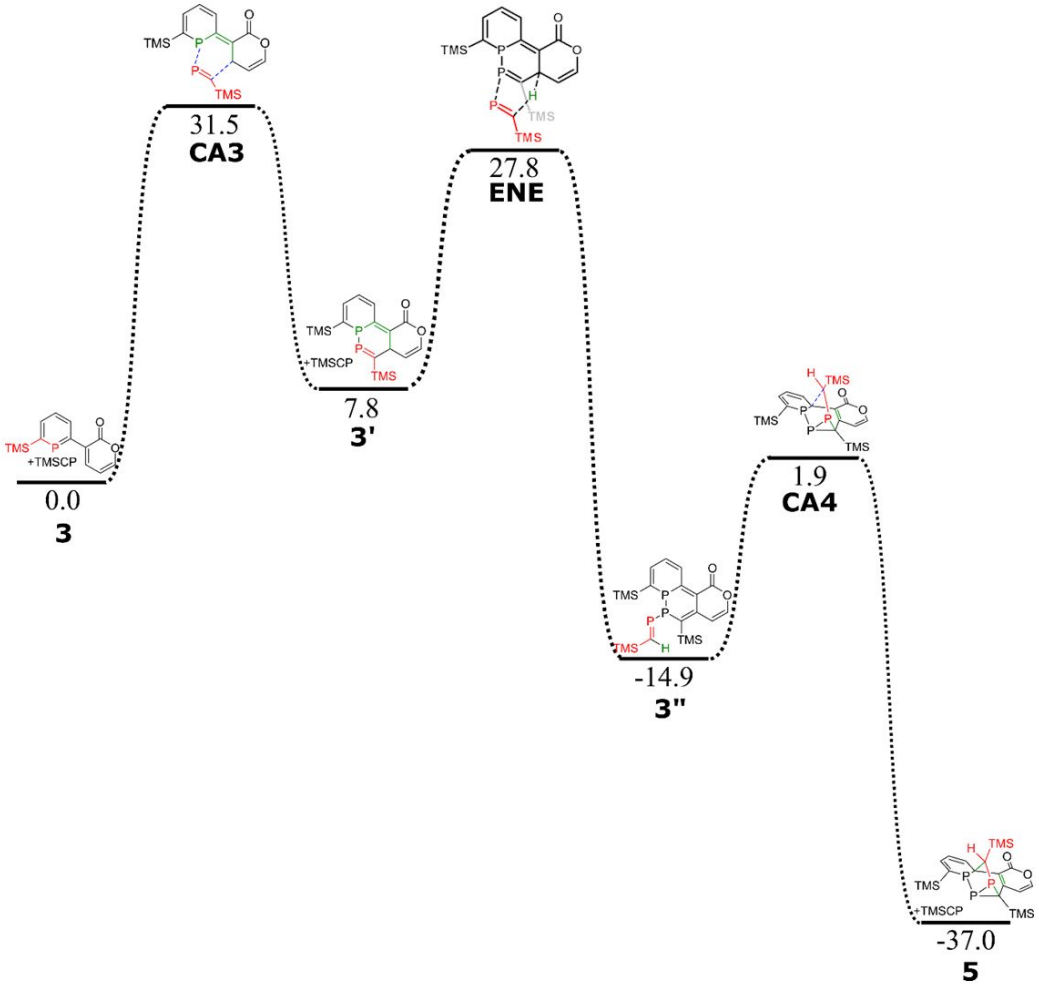


Figure S25 Mechanism of the reaction between compound **3** and two molecules of TMSCP - yielding compound **5**. Gibbs free energies (kcal/mol) were obtained at the ωB97X-D/6-311+G** (PCM=toluene) level of the theory at T=383K.

Table S2 Gibbs free energies (kcal/mol) of the intermediates and transition states depicted in **Figure S25** at different levels of the theory. Unless otherwise stated Gibbs free energies are at 298 K.

level of theory.	**CA3**	**3‘**	**ENE**	**3“**	**CA4**	**5**
M06-2X/ 6-31+G*	22.9	-1.2	14.0	-17.3	-3.9	-44.4
M06-2X/ cc-pVTZ	23.4	1.3	12.5	-18.6	-4.0	-39.5
M06-2X-D3/ cc-pVTZ PCM=toluene	25.0	2.2	13.9	-16.2	-3.2	-41.9
M06-2X-D3/ cc-pVTZ T=383K	29.1	6.7	22.5	-8.3	5.8	-32.4
B3LYP/ cc-pVTZ T=383K	28.6	12.4	26.2	-2.2	13.7	-24.4
ωB97XD/ 6-311+G**	27.5	3.2	18.9	-14.8	0.8	-39.7

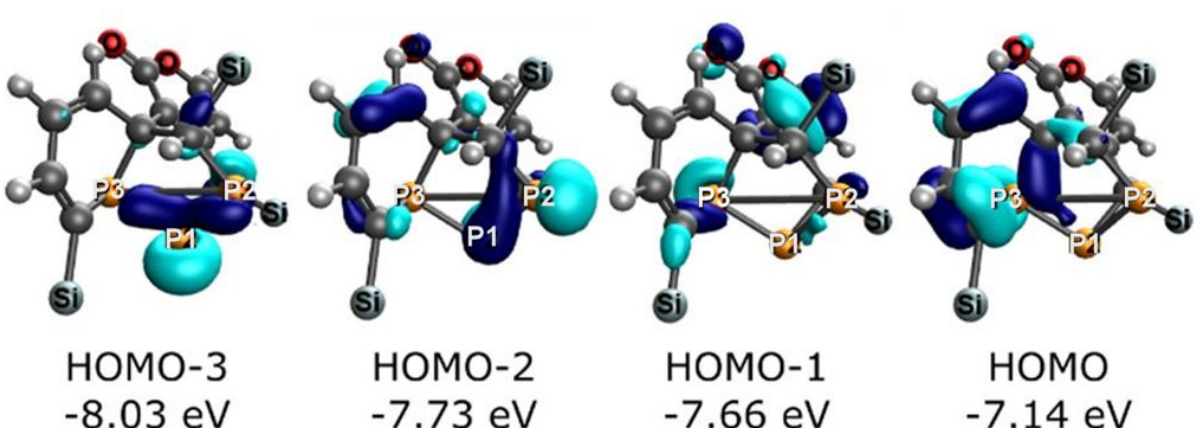


Figure S26. The HOMO-3, HOMO-2, HOMO-1 and HOMO frontier orbitals of **5**. The methyl substituents on the trimethylsilyl groups are omitted for clarity and the carbon and hydrogen atoms are not indexed.

Total energies, thermal corrections and Cartesian coordinates of the investigated compounds

2
E(M06-2X/6-31+G*) = -685.296125702
E+ZPE=-685.152508
E+thermalE=-685.142874
E+thermalH=-685.141930
E+thermalG=-685.187657
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C 0.63049000 3.48226600 -0.00000000
C 1.68104800 2.64236300 -0.00000000
C 1.42349900 1.23755200 -0.00000000
C 0.15033700 0.72578300 -0.00000000
C -0.96929800 1.68749900 0.00000000
H 0.67308700 4.56520900 -0.00000000
H 2.69328400 3.02558100 -0.00000000
H 2.26478400 0.55891200 -0.00000000
C -0.15033700 -0.72578300 -0.00000000
O -2.15408300 1.45279400 0.00000000
C -1.42349900 -1.23755200 -0.00000000
C -1.68104800 -2.64236300 -0.00000000
C -0.63049000 -3.48226600 -0.00000000
O 0.63049000 -3.02968800 -0.00000000
C 0.96929800 -1.68749900 -0.00000000
H -2.26478400 -0.55891200 -0.00000000
H -2.69328400 -3.02558100 -0.00000000
H -0.67308700 -4.56520900 -0.00000000
O 2.15408300 -1.45279400 0.00000000

E(M06-2X/cc-pvtz PCM=toluene T=383 K) =
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E(L-CCSD(T)/cc-pVTZ)=-684.439569223511
E+ZPE=-685.400274
E+thermalE=-685.384814
E+thermalH=-685.383601
E+thermalGa=-685.449208
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C 0.14660000 0.72486900 -0.00000000
C -0.96831300 1.68256800 -0.00000000
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O -2.14990900 1.45340300 -0.00000000
C -1.41259000 -1.23694200 -0.00000000
C -1.67292800 -2.63515800 -0.00000000
C -0.62944400 -3.47160300 -0.00000000
O 0.62944400 -3.01942600 -0.00000000
C 0.96831300 -1.68256800 -0.00000000
H -2.24897900 -0.56016500 -0.00000000
H -2.68064200 -3.01678400 -0.00000000
H -0.67758200 -4.55013100 -0.00000000
O 2.14990900 -1.45340300 -0.00000000

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) =
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E+thermalE=-685.335505
E+thermalH=-685.334292
E+thermalG=-685.401338
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C -0.00026800 0.74213200 0.00000000
C -1.14612300 1.49004800 0.00000000
C -1.12537400 2.91361100 0.00000000
C 0.06464600 3.53110500 0.00000000
O 1.21144400 2.84641000 0.00000000
C 0.00000000 -0.74202900 -0.00000000
C 1.14600100 -1.48970900 -0.00000000
C 1.12556900 -2.91327300 -0.00000000
C -0.06431800 -3.53102100 -0.00000000
O -1.21126200 -2.84657100 -0.00000000
C -1.28329700 -1.46227800 -0.00000000
O -2.39616300 -1.00600500 0.00000000
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H 2.04222300 -3.48522800 -0.00000000
H 2.09946100 -0.98302400 -0.00000000
H -2.09969400 0.98358800 0.00000000
H -2.04190400 3.48576500 0.00000000
H 0.22771200 4.60074900 0.00000000

E(B3LYP/cc-pVTZ PCM=toluene T=383 K) =
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E+thermalH= -685.657628
E+thermalG= -685.723623
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C 1.41486400 1.24384300 0.00000000
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H -0.68652200 -4.56262500 0.00000000
O 2.16238000 -1.46017200 0.00000000

CA1
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E+thermalH=-1473.524361
E+thermalG=-1473.596713
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H 4.86340900 -1.37983500 -2.16857200
C 3.10553300 -1.04435500 -0.88991400
H 2.56507100 -1.92210700 -1.22975900
C 5.02342700 0.36209500 -0.98432300
H 5.99867700 0.70882200 -1.30481500
O 4.48127800 1.18026100 -0.06681100
C 3.24268100 0.96058600 0.50737600
O 2.85108600 1.76855400 1.31186000
C 2.53699200 -0.23993800 0.05325800
C 1.19517500 -0.50640100 0.59800600
P -0.21670800 1.21507300 -0.61509600
O 0.61166000 -1.57186700 -0.04642500
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H 1.37559800 0.46108900 2.50547400

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H -0.96824300 -0.21278300 3.17261100
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O -1.18391700 -2.82818500 -0.40438900
C -1.34224800 -1.09213700 1.23423100
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C -1.59335800 0.53880200 -0.19338900
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C -4.25619700 0.87975400 1.26419700
C -3.89027700 1.95169300 -1.58729500
C -4.00383900 -1.09558500 -1.11823500
H -5.09365200 -1.10527200 -1.23911200
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H -5.33839800 1.00291100 1.13791900
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H -3.41472900 1.80161300 -2.56218300

E(M06-2X/cc-pvtz PCM=toluene T=383 K) =
-1474.18329417
E(L-CCSD(T)/cc-pVTZ)=-1471.944402409651
E+ZPE=-1473.922503
E+thermalE=-1473.890188
E+thermalH=-1473.888975
E+thermalG=-1473.994553
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C 1.72549000 -0.29939300 -0.35872000
P 0.36362100 -0.80026900 -0.98261800
C -1.18703900 0.65027000 0.51129800
C -2.53534600 0.18363100 0.13422300
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E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) =
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E+ZPE=-1473.907575
E+thermalE=-1473.875521
E+thermalH=-1473.874308
E+thermalG=-1473.978627
C 4.40860200 -0.71052800 -1.41634800
H 4.88303500 -1.33815800 -2.15639800
C 3.11845100 -1.01281900 -0.89699300
H 2.59003600 -1.88837000 -1.25207300
C 5.03124000 0.38847100 -0.95955400
H 6.00852400 0.73448400 -1.26733400
O 4.47931500 1.19520800 -0.04227600
C 3.23597800 0.97064000 0.51541100
O 2.84732100 1.77297000 1.32407600
C 2.53660700 -0.21857800 0.04301400
C 1.18937000 -0.50208600 0.57225700
P -0.24466200 1.20126900 -0.61751100
O 0.62533000 -1.57473900 -0.07500900
C 0.74979100 -0.20358500 1.86569500
H 1.35689800 0.42964000 2.49433300
C -0.53198700 -0.57870800 2.20474100
H -0.96727200 -0.28734100 3.15214600
C -0.66443300 -1.94721000 0.18201900
O -1.12732000 -2.87491600 -0.42786600
C -1.32907600 -1.14703100 1.20771600
H -2.34380900 -1.45449400 1.42129400
C -1.60844000 0.50709300 -0.19476900
Si -3.46783800 0.56832200 -0.39499400
C -4.23955200 0.85845100 1.29197200
C -3.88343800 2.00086800 -1.53032700
C -4.05227500 -1.04697900 -1.14116100
H -5.14067000 -1.03415000 -1.25753300
H -3.60668200 -1.19512400 -2.12855200
H -3.78155300 -1.91061300 -0.52916200
H -3.82713200 1.75863300 1.75633000
H -5.31964600 1.00045500 1.18511900
H -4.08215700 0.02169000 1.97740500
H -4.96608600 2.07998700 -1.67110300
H -3.52466900 2.94593400 -1.11333200
H -3.42134700 1.86571600 -2.51199600

E(B3LYP/cc-pVTZ PCM=toluene T=383 K) =
-1474.61986997
E+ZPE= -1474.361701
E+thermalE= -1474.329152
E+thermalH= -1474.327939
E+thermalG= -1474.434411
C 1.34281200 1.29861300 1.01026000
C 1.76829600 -0.24182400 -0.32825800
P 0.44915100 -0.78502600 -1.04443300
C -1.22553300 0.65151100 0.50965900
C -2.56927700 0.17186300 0.13610600
C -3.52975700 0.94357900 -0.45523800
C -4.80450200 0.41269800 -0.79026600
C -5.05330500 -0.88018300 -0.51842400
O -4.13497700 -1.67836700 0.05372400
C -2.86173400 -1.23316100 0.41032100
O 0.63422200 2.13932400 0.19109100
C -0.65224300 1.81588000 -0.17890200
C -0.65609800 0.29213500 1.75060800
C 0.64490200 0.62259100 2.02257800
O -1.18227000 2.52009000 -1.00800500
O -2.12167500 -2.05401200 0.89679900
Si 3.62439100 -0.48222800 -0.27571200
C 4.09037600 -1.95652900 -1.34627800
C 4.44688900 1.08333100 -0.92606400
C 4.12324500 -0.79852200 1.51537400
H -5.56317100 1.02516500 -1.25093900
H -3.31287100 1.97607800 -0.67558800

H -5.97736100 -1.40078100 -0.72039100
H -1.21367900 -0.34308200 2.42022800
H 1.17390800 0.24469300 2.88348600
H 2.33345800 1.69273500 1.17527700
H 5.53262100 0.96642500 -0.91350100
H 4.13869500 1.28041600 -1.95349000
H 4.19921400 1.96173400 -0.32896000
H 3.59640100 -1.66518300 1.91695800
H 5.19526300 -0.99774600 1.57342300
H 3.91032600 0.05510000 2.16021700
H 5.17016800 -2.11845700 -1.32707700
H 3.60311500 -2.86472000 -0.98924900
H 3.78834200 -1.79397300 -2.38165200

i(2/3)
E(M06-2X/6-31+G*) = -1473.85540248
E+ZPE=-1473.590796
E+thermalE=-1473.570447
E+thermalH=-1473.569502
E+thermalG=-1473.640057
C 4.51750300 0.62177600 1.16481400
H 5.13628900 1.26183400 1.78054100
C 5.01171500 -0.53237500 0.67930400
H 6.01284100 -0.91221800 0.84384900
O 4.28512800 -1.36691900 -0.08967200
C 2.97825700 -1.10353700 -0.43720900
O 2.39100700 -1.90975000 -1.11944000
C 3.16260500 0.96860700 0.84310500
H 2.72915400 1.89056200 1.21768500
C 2.41524400 0.14633500 0.06433800
C 0.99096100 0.39666000 -0.31767600
C 0.72418600 0.47348800 -1.79868700
H 1.48526200 0.17387600 -2.51028200
O 0.60075000 1.64253400 0.29838600
C -0.64166400 2.09008000 -0.00211300
C -0.49942400 0.90057700 -2.10725600
H -0.86415300 1.05907900 -3.11618200
O -1.05376300 3.12757200 0.44002100
C -1.40413400 1.13774500 -0.91723800
H -2.35246100 1.60696600 -1.18426200
C -1.58209700 -0.14799200 -0.08110100
Si -3.33570700 -0.68520400 0.34993000
C -4.12220300 0.70842000 1.33837800
H -3.61574900 0.83592100 2.30103100
H -4.06112200 1.66481500 0.80683500
H -5.18008400 0.49932600 1.53469100
C -4.26250200 -0.94010000 -1.27012200
H -4.26461500 -0.03138200 -1.88268100
H -5.30728600 -1.21076600 -1.07888500
H -3.80654900 -1.74316500 -1.85911900
C -3.28575100 -2.27908900 1.34227000
H -4.30340700 -2.60718000 1.58287800
H -2.79709300 -3.08551300 0.78479800
H -2.74607100 -2.14531200 2.28608800
P -0.21108000 -0.95033800 0.42365200

E(M06-2X/cc-pVTZ PCM=toluene T=383 K) = -1474.22938512
E(L-CCSD(T)/cc-pVTZ)=-1471.992439518377
E+ZPE=-1473.966275
E+thermalE=-1473.934555
E+thermalH=-1473.933342
E+thermalG=-1474.036384
C 4.51346700 0.61837400 1.14596300
H 5.13554100 1.25778400 1.75075700
C 4.99933000 -0.53342200 0.66825500
H 5.99719200 -0.91118100 0.82982200
O 4.26438200 -1.36839100 -0.08957200
C 2.96336500 -1.10341100 -0.42758200
O 2.37280000 -1.91192800 -1.09809500
C 3.16335200 0.96581700 0.82993000
H 2.74160200 1.88967400 1.20012700
C 2.40916700 0.14600100 0.06659500
C 0.98927800 0.40168000 -0.31367000
C 0.72448900 0.48431200 -1.79051500
H 1.48760500 0.20050800 -2.49883200
O 0.59183000 1.64256000 0.30557200
C -0.64630800 2.08302800 0.00706600
C -0.49038700 0.91143300 -2.09937600
H -0.84891600 1.08095300 -3.10343700
O -1.06211100 3.11033900 0.45804900
C -1.40022100 1.14107500 -0.91619100
H -2.34423800 1.60541000 -1.18538700
C -1.57843700 -0.14467100 -0.08727400
Si -3.32722400 -0.68793000 0.34577700
C -4.10637300 0.70081900 1.33522100
H -3.59893300 0.82240900 2.29259200
H -4.04377200 1.65052700 0.80181600
H -5.15926900 0.49058600 1.52941800
C -4.25159200 -0.94080400 -1.26767300
H -4.24304700 -0.03641000 -1.87766200
H -5.29307700 -1.20098300 -1.07243000
H -3.80102400 -1.74698100 -1.84741500
C -3.26105900 -2.27573700 1.33322400
H -4.27115600 -2.61002000 1.57445300
H -2.76727900 -3.06974600 0.77182100
H -2.72030200 -2.13285900 2.26939600
P -0.21289500 -0.94441700 0.41417500

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) = -1474.21999482
E+ZPE=-1473.956248
E+thermalE=-1473.924804
E+thermalH=-1473.923592
E+thermalG=-1474.025821
C 4.51514600 0.63894900 1.14482500
H 5.12667000 1.29262200 1.74961100
C 5.02262800 -0.50842000 0.66870100
H 6.02877300 -0.86936000 0.83073300
O 4.30173700 -1.35655100 -0.08532400
C 2.98985800 -1.11684400 -0.42432100
O 2.42012900 -1.94534700 -1.09102000
C 3.16017000 0.96186700 0.82859000
H 2.72220000 1.88064500 1.19766100
C 2.41606500 0.12579000 0.06512800
C 0.98697700 0.37596700 -0.31049700
C 0.71328500 0.45101800 -1.79021300
H 1.47026900 0.16090500 -2.50514300
O 0.60585100 1.63738500 0.29396800
C -0.62556100 2.08899100 -0.00711800
C -0.50475400 0.87955100 -2.09566100
H -0.87010300 1.04147300 -3.10070200
O -1.02027300 3.13803400 0.41894900
C -1.40159400 1.13474200 -0.90498000
H -2.34435000 1.60514400 -1.17628200
C -1.58866300 -0.14252000 -0.06112700
Si -3.34858600 -0.67935400 0.34569800
C -4.16225300 0.73348500 1.27346800
H -3.67424200 0.89643900 2.23836600
H -4.10793600 1.67056100 0.71178300
H -5.21851200 0.51491400 1.45868200
C -4.22071700 -0.97498900 -1.29063500
H -4.19258600 -0.08484100 -1.92630900
H -5.27184400 -1.23080500 -1.12560100

H -3.75284600 -1.79733000 -1.83902700
C -3.32926000 -2.23918700 1.38122300
H -4.35519000 -2.55352000 1.59670200
H -2.82964200 -3.06243300 0.86297500
H -2.82130800 -2.07948100 2.33639400
P -0.22111000 -0.94083700 0.44623300

E(B3LYP/cc-pVTZ PCM=toluene T=383 K) =
-1474.65528149
E+ZPE= -1474.394964
E+thermalE= -1474.362986
E+thermalH= -1474.361773
E+thermalG= -1474.465283
C 4.51531000 0.64590900 1.17382900
H 5.11302500 1.29855800 1.78981200
C 5.03968800 -0.49523100 0.69475600
H 6.04503100 -0.84739900 0.86826000
O 4.33249200 -1.34296200 -0.07841100
C 3.01139100 -1.09932900 -0.43574100
O 2.45639000 -1.92462100 -1.12378400
C 3.16639900 0.96404700 0.84495600
H 2.72540400 1.87648900 1.21747300
C 2.42916500 0.13240300 0.06355600
C 1.00492700 0.37736500 -0.32120800
C 0.72731600 0.44264900 -1.79736000
H 1.48385000 0.14393700 -2.50469400
O 0.59771000 1.64011200 0.28902000
C -0.64439700 2.07727900 -0.02173700
C -0.49297800 0.86128900 -2.10990400
H -0.85469600 1.01227400 -3.11542100
O -1.06053100 3.11968400 0.40600800
C -1.40195100 1.11231200 -0.92784900
H -2.34226100 1.57483800 -1.20879100
C -1.59268700 -0.16531000 -0.07777900
Si -3.36016200 -0.67488900 0.35154400
C -4.11238600 0.72785300 1.36044400
H -3.60632800 0.82595800 2.32176900
H -4.02496700 1.68296200 0.84048900
H -5.17139000 0.54072600 1.54918400
C -4.29360600 -0.88008700 -1.27454600
H -4.26032300 0.03260400 -1.87194700
H -5.34274200 -1.11451900 -1.08404800
H -3.86754600 -1.68929200 -1.86930000
C -3.36088000 -2.28356800 1.32453800
H -4.38622700 -2.57790800 1.55721600
H -2.90006800 -3.09247200 0.75598700
H -2.81994000 -2.17918700 2.26592800
P -0.22192700 -0.96548800 0.44320400

E1
E(M06-2X/6-31+G*) = -1473.81402418
E+ZPE=-1473.552509
E+thermalE=-1473.531939
E+thermalH=-1473.530995
E+thermalG=-1473.602515
C -3.53470800 -0.26859100 -0.83924400
O -4.74865900 0.26967000 -0.42460400
C -4.86860000 1.13022200 0.59376200
C -3.80820700 1.57665300 1.29800400
C -2.52070100 1.08854700 0.92616200
C -2.35996500 0.19388500 -0.09394000
C -1.00757500 -0.30457000 -0.40854900
P 0.28531100 0.99310300 -0.62819900
C 1.61946100 -0.01023700 -0.36232900
Si 3.37910600 0.67927900 -0.23812800
C 4.44103300 -0.24058800 -1.49044200
O -3.57109500 -1.02860300 -1.77156800
C -0.80220400 -1.57106900 -1.06256300
C 0.41006300 -2.14664600 -0.87597200
C 1.41255800 -1.44258400 -0.08391300
C 3.34932600 2.51818300 -0.62514700
C 3.98669300 0.35748200 1.50930300
C 0.65328700 -1.37404500 1.48896600
O 1.34322600 -1.85065900 2.35903900
O -0.47391500 -0.83489500 1.44708800
H -5.90268500 1.40446600 0.76951700
H -3.94330300 2.26906000 2.11832700
H -1.64401200 1.39980600 1.48907500
H -1.63304200 -2.07906700 -1.53563900
H 0.60017900 -3.17231100 -1.17826900
H 2.32045100 -2.01453100 0.10711200
H 5.03468200 0.66159100 1.61385600
H 3.39295100 0.91999700 2.23788500
H 3.90975600 -0.70176800 1.77791000
H 5.47250000 0.12916200 -1.46474500
H 4.46980400 -1.31529500 -1.27952100
H 4.05873500 -0.10591800 -2.50788600
H 4.36571100 2.92608400 -0.58119600
H 2.95471900 2.71539200 -1.62805600
H 2.73717700 3.07292200 0.09419200

E(M06-2X/cc-pVTZ PCM=toluene T=383K) =
-1474.18945822
E(L-CCSD(T)/cc-pVTZ)= -1471.952904675188
E+ZPE=-1473.929653
E+thermalE=-1473.897607
E+thermalH=-1473.896394
E+thermalG=-1474.001050
C -3.52741800 -0.27565600 -0.82911500
O -4.73537200 0.25282300 -0.40641700
C -4.85025600 1.13109500 0.59376000
C -3.79007300 1.59533200 1.27297500
C -2.51120800 1.10608200 0.89952400
C -2.35383900 0.19575700 -0.09977700
C -1.00568400 -0.30445600 -0.40784200
P 0.29047000 0.98575100 -0.62622000
C 1.61618300 -0.01297600 -0.35542800
Si 3.37255400 0.67873400 -0.23860000
C 4.42044400 -0.23032000 -1.49983400
O -3.57057300 -1.03704100 -1.75476400
C -0.79478200 -1.56544800 -1.05878300
C 0.40859600 -2.14091600 -0.86909200
C 1.40708100 -1.44209700 -0.07409700
C 3.32875300 2.51322900 -0.60897400
C 3.98435000 0.34136200 1.49815400
C 0.65220800 -1.36966900 1.47993300
O 1.33204900 -1.83924300 2.35822000
O -0.47193400 -0.83692200 1.44442500
H -5.87901300 1.40321600 0.77870300
H -3.92027800 2.30102500 2.07629800
H -1.63505900 1.43241700 1.44607400
H -1.62034200 -2.07219200 -1.53093000
H 0.59766100 -3.16151100 -1.17225500
H 2.31088300 -2.01145100 0.11484100
H 5.03131800 0.63297000 1.59524700
H 3.40099100 0.90413400 2.22755100
H 3.89656400 -0.71593600 1.75103100
H 5.44940500 0.13113200 -1.46752100
H 4.43631500 -1.30254800 -1.30079400
H 4.03666900 -0.07629600 -2.50870200
H 4.33985800 2.92190800 -0.57872000
H 2.91696900 2.70802700 -1.60013500
H 2.72576500 3.05171600 0.12287000

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) =
-1474.18557843
E+ZPE=-1473.924955
E+thermalE=-1473.893152
E+thermalH=-1473.891939
E+thermalG=-1473.995843
C -3.55197400 -0.32754400 -0.77606500
O -4.75827200 0.21508300 -0.34504100
C -4.85126300 1.16294700 0.58879800
C -3.77104300 1.70029400 1.18511200
C -2.49899200 1.21215000 0.79473200
C -2.35828500 0.23060400 -0.14681900
C -1.01247200 -0.27292000 -0.45188700
P 0.30832100 1.00063400 -0.65229200
C 1.62188600 -0.00249000 -0.34756400
Si 3.39111300 0.66272200 -0.22884000
C 4.44255600 -0.33129800 -1.42344900
O -3.62580000 -1.17097200 -1.62765500
C -0.79059500 -1.54142600 -1.09454500
C 0.40529400 -2.12365500 -0.87728100
C 1.38643800 -1.43393700 -0.03542600
C 3.41581200 2.47905200 -0.68731300
C 3.95479000 0.39875800 1.53785600
C 0.63630900 -1.37769100 1.47694700
O 1.28095000 -1.87585400 2.37427300
O -0.48305700 -0.82268100 1.44726600
H -5.87949900 1.42711100 0.79778200
H -3.88309700 2.46146600 1.94263600
H -1.61218000 1.60180900 1.28242700
H -1.60859200 -2.04155100 -1.59184300
H 0.60052000 -3.14266800 -1.18874200
H 2.29281400 -2.00956800 0.13506900
H 5.01168200 0.65970200 1.64923700
H 3.37407700 1.02058900 2.22476200
H 3.82430400 -0.64175800 1.84751700
H 5.48389500 0.00271900 -1.38213200
H 4.42631000 -1.39794100 -1.18217100
H 4.08939500 -0.21021800 -2.45141100
H 4.43859700 2.86223200 -0.61714800
H 3.06845200 2.64358400 -1.71124700
H 2.79157600 3.07520600 -0.01592300

E(B3LYP/cc-pVTZ PCM=toluene T=383 K) =
-1474.62970075
E+ZPE= -1474.372105
E+thermalE= -1474.339945
E+thermalH= -1474.338732
E+thermalG= -1474.444036
C -3.54944600 -0.33330700 -0.78887200
O -4.77665900 0.22887200 -0.38353200
C -4.88035800 1.17159800 0.55744000
C -3.80413400 1.68642400 1.18630500
C -2.53239700 1.18783300 0.82506200
C -2.37124000 0.20880400 -0.12127400
C -1.01968100 -0.29081200 -0.40587100
P 0.30568100 1.00726200 -0.64370900
C 1.62959100 0.00732600 -0.33720100
Si 3.40699700 0.65969200 -0.23758000
C 4.44895000 -0.36260000 -1.43058900
O -3.61922800 -1.17113400 -1.64894200
C -0.78024000 -1.54693800 -1.08182600
C 0.41873800 -2.12008800 -0.87648200
C 1.38801500 -1.42825500 -0.00991500
C 3.45481400 2.47836500 -0.71690700
C 3.99044000 0.40867500 1.53415100
C 0.63779000 -1.36627700 1.47727100
O 1.26530100 -1.83252000 2.40649400
O -0.50537100 -0.82411400 1.44176900
H -5.90637500 1.45286000 0.74533800
H -3.92382900 2.44159600 1.94590500
H -1.65700200 1.56265100 1.33731100
H -1.58370000 -2.03034700 -1.61132800
H 0.63857200 -3.11990800 -1.22225400
H 2.29254600 -2.00071900 0.16302400
H 5.05506600 0.63462300 1.62134100
H 3.44487200 1.06390600 2.21458500
H 3.82709900 -0.61754300 1.86497200
H 5.48922900 -0.03219900 -1.40267600
H 4.42878100 -1.42175200 -1.16970200
H 4.08806000 -0.25854400 -2.45488900
H 4.48257500 2.84392500 -0.66853000
H 3.09178200 2.63639000 -1.73341900
H 2.85175100 3.08711400 -0.04200600

3
E(M06-2X/6-31+G*) = -1285.38664265
E+ZPE=-1285.137041
E+thermalE=-1285.118839
E+thermalH=-1285.117894
E+thermalG=-1285.184010
O 4.63509800 0.07133800 0.52809500
C 3.38751300 0.67573800 0.46626300
C 2.32095700 -0.11248100 -0.17296400
C 2.62169200 -1.34679200 -0.66679500
C 3.93950300 -1.89829800 -0.56444000
C 4.88723600 -1.15239700 0.03375800
O 3.28866100 1.77872900 0.93869200
C 0.95472800 0.45773400 -0.23332700
P -0.37501200 -0.62815800 0.11023800
C -1.77326600 0.38066900 -0.13236600
Si -3.46772000 -0.42239400 0.14778600
C -3.57158200 -2.00541900 -0.86580000
C 0.77577900 1.80681200 -0.55437500
C -0.47295000 2.40875100 -0.67888900
C -1.67673100 1.72959200 -0.48296900
C -3.65923200 -0.83474900 1.97400400
C -4.81805300 0.77621500 -0.38627600
H -2.59482800 2.30362000 -0.61230800
H -0.50880300 3.46138900 -0.94620200
H 1.65735900 2.41899800 -0.72371800
H -5.79933200 0.30244600 -0.26758500
H -4.81991100 1.68903200 0.21964600
H -4.71443000 1.06470900 -1.43827800
H -4.62944200 -1.30647400 2.16841700
H -2.87585200 -1.52728300 2.30199000
H -3.58930300 0.06655800 2.59258900
H -4.55089200 -2.48227600 -0.74333100
H -3.42251800 -1.80444600 -1.93225700
H -2.80723600 -2.72455900 -0.54997700
H 1.84289800 -1.92197300 -1.16114800
H 4.17939000 -2.87792400 -0.95748700
H 5.92253400 -1.43871300 0.17784000

E(M06-2X/cc-pvtz PCM=toluene T=383 K) =
-1285.68915410
E(L-CCSD(T)/cc-pVTZ)=-1283.718864218276
E+ZPE=-1285.441194
E+thermalE=-1285.412809
E+thermalH=-1285.411596
E+thermalG=-1285.508054
C 3.93443200 -1.87688700 -0.58264900
C 4.87318700 -1.14111600 0.02477300
O 4.61409300 0.07209700 0.53699600
C 3.36978900 0.66709400 0.48326300

C 2.31529300 -0.10955900 -0.17267600
C 2.62048800 -1.32995000 -0.68035100
O 3.26368200 1.75484000 0.98036900
C 0.95213800 0.45780500 -0.23753200
P -0.37290200 -0.62172000 0.11316800
C -1.76848700 0.37913100 -0.13567800
Si -3.45974200 -0.42409600 0.15152100
C -3.64406100 -0.80933300 1.97801300
C 0.76971400 1.79681600 -0.57069300
C -0.47392800 2.39397700 -0.70039700
C -1.67207800 1.71864700 -0.49772100
C -4.80188400 0.76428100 -0.40000600
C -3.55099800 -2.01471600 -0.83975000
H -2.58677600 2.28824500 -0.63289500
H -0.51099900 3.43913700 -0.97825200
H 1.64741800 2.40430300 -0.75020800
H -5.77981100 0.29565900 -0.27900500
H -4.79702400 1.67959600 0.19319200
H -4.68740000 1.03596500 -1.45023000
H -4.60086900 -1.29502300 2.17604800
H -2.84842400 -1.47719100 2.31157300
H -3.59246700 0.10161100 2.57530300
H -4.52037600 -2.49692400 -0.70417600
H -3.41112000 -1.82026100 -1.90365600
H -2.77764300 -2.71461300 -0.51951400
H 1.84775300 -1.89775700 -1.18305900
H 4.17894400 -2.84501900 -0.98791300
H 5.90488900 -1.42720900 0.16348400

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) = -1285.69444998
E+ZPE=-1285.446027
E+thermalE=-1285.417820
E+thermalH=-1285.416607
E+thermalG=-1285.512814
O 4.60113400 0.05523400 0.60646100
C 3.35108400 0.64684300 0.54269600
C 2.32715700 -0.09678300 -0.19308500
C 2.65751600 -1.28562300 -0.76431100
C 3.97315300 -1.82756400 -0.65344700
C 4.88693900 -1.12344600 0.03170600
O 3.22193700 1.70643100 1.09686900
C 0.95662500 0.46323100 -0.26708500
P -0.36018000 -0.61404100 0.11592500
C -1.76770300 0.37099600 -0.14504900
Si -3.46041900 -0.42957100 0.16619800
C -3.56732900 -2.03736800 -0.79791100
C 0.76676700 1.79565000 -0.62936900
C -0.48294500 2.38307700 -0.76375200
C -1.67868400 1.70609700 -0.53863600
C -3.64288100 -0.77769700 2.00187900
C -4.81103400 0.74450100 -0.40263300
H -2.59680200 2.27128200 -0.68178500
H -0.52874000 3.42480500 -1.06262400
H 1.64094900 2.40719300 -0.82683200
H -5.78915100 0.27486500 -0.25961200
H -4.80822900 1.67957300 0.16494800
H -4.71080900 0.98821200 -1.46443300
H -4.61442800 -1.23464200 2.21463400
H -2.86473700 -1.46364300 2.34949600
H -3.56431800 0.14380000 2.58577600
H -4.54420200 -2.50887800 -0.65187300
H -3.43062500 -1.86362100 -1.86917700
H -2.80101500 -2.74663100 -0.47167500
H 1.90735100 -1.83108800 -1.32646800
H 4.23945800 -2.77027100 -1.10888900
H 5.91730900 -1.41114900 0.19022500

E(B3LYP/cc-pVTZ PCM=toluene T=383 K) = -1286.06067037
E+ZPE= -1285.815051
E+thermalE= -1285.786410
E+thermalH= -1285.785197
E+thermalG= -1285.882748
C 3.95307700 -1.87279800 -0.59622500
C 4.89525900 -1.14950400 0.03367300
O 4.63639200 0.06087300 0.55874800
C 3.37605000 0.66827200 0.49257100
C 2.33110100 -0.10226500 -0.18062600
C 2.64587700 -1.32388300 -0.70260800
O 3.27744100 1.75688700 0.99968900
C 0.96616500 0.46025900 -0.25078000
P -0.36986200 -0.62011900 0.12056400
C -1.77674400 0.38407200 -0.12928800
Si -3.47585600 -0.42401200 0.15453600
C -3.59135000 -1.00199400 1.94545000
C 0.77440400 1.80004000 -0.58990300
C -0.47344700 2.39481900 -0.71410900
C -1.67547700 1.72408700 -0.50003200
C -4.83755100 0.83052000 -0.20153800
C -3.64861800 -1.90268300 -1.00353700
H -2.58471000 2.30130800 -0.63031600
H -0.51197500 3.43911400 -0.99627900
H 1.64652000 2.41251600 -0.77505200
H -5.81305000 0.36339100 -0.05263100
H -4.77679900 1.69209600 0.46534200
H -4.79599300 1.19252500 -1.23011000
H -4.55379500 -1.48168400 2.13519100
H -2.80390900 -1.72138300 2.17562400
H -3.48905100 -0.16160000 2.63397000
H -4.61025400 -2.39894600 -0.85756600
H -3.58251800 -1.59061000 -2.04718300
H -2.85999900 -2.63454600 -0.82131800
H 1.88234200 -1.88689300 -1.22239900
H 4.19659700 -2.83701300 -1.01301300
H 5.92338800 -1.44602900 0.17801100

CA2
E(M06-2X/6-31+G*) = -2073.89811057
E+ZPE=-2073.530808
E+thermalE=-2073.502618
E+thermalH=-2073.501674
E+thermalG=-2073.591215
C -3.61827600 0.20693900 -0.23338900
Si -5.18494700 -0.82301300 0.04820400
C -4.82227600 -2.25220700 1.21362000
H -5.72987900 -2.84794900 1.36581900
H -4.04912300 -2.91609400 0.81195600
H -4.48437400 -1.90130900 2.19464300
C -5.77065500 -1.47403500 -1.61940800
H -5.96223800 -0.65724500 -2.32431600
H -6.70095600 -2.04310000 -1.50938000
H -5.02061900 -2.13379800 -2.06865900
C -6.49990200 0.30522900 0.78629300
H -7.43422400 -0.24223600 0.95529500
H -6.72214500 1.14782300 0.12171900
H -6.16918200 0.71577000 1.74645900
C -3.69373100 1.29230000 -1.11701200
H -4.64495600 1.50175500 -1.60970100
C -2.62700400 2.13140300 -1.42140900
H -2.78604800 2.94431500 -2.12452500
C -1.35552700 1.98441400 -0.86468600
H -0.58247100 2.69070400 -1.15466300
P -2.16255600 -0.24102400 0.59460300

C -1.02740800 0.98620400 0.05180000
C 0.35420400 0.93570400 0.58833500
P 1.43268900 -0.96264900 -0.72716100
O 1.17820800 1.87817400 0.02071700
C 0.68965000 0.44094700 1.85564700
H -0.07186600 -0.05226900 2.44951100
C 2.51677400 1.91826400 0.31604200
O 3.20831500 2.74362800 -0.22326600
C 2.01939400 0.47086600 2.23508900
H 2.34995000 0.01782000 3.16434400
C 2.95320900 0.90593300 1.28630000
H 4.00667900 0.96686900 1.53645800
C 2.90583300 -0.63868100 -0.21877500
Si 4.72317800 -1.05894600 -0.39210300
C 4.88186100 -2.43249600 -1.66580800
H 4.49851100 -2.10386800 -2.63754100
H 4.31553200 -3.31897000 -1.36132100
H 5.93050700 -2.72509300 -1.79454500
C 5.35580400 -1.67175900 1.27415000
H 4.73755900 -2.49725000 1.64335100
H 6.38239700 -2.04214500 1.17034800
H 5.36436500 -0.88708900 2.03789300
C 5.65891800 0.46753400 -0.95629900
H 5.27235300 0.82083100 -1.91795500
H 6.72195300 0.22978100 -1.08197300
H 5.57367500 1.30149400 -0.25279600

E(B3LYP/cc-pVTZ PCM=toluene T=383 K) =
-2074.86419068
E+ZPE= -2074.501976
E+thermalE= -2074.457450
E+thermalH= -2074.456237
E+thermalG= -2074.590358
C -2.00297600 0.48127300 -2.23189500
C -2.94887800 0.89710700 -1.27036200
C -2.51327200 1.93544800 -0.33298800
O -1.17619300 1.88881800 -0.01941000
C -0.34636300 0.92864000 -0.57402100
C -0.68671600 0.44854000 -1.85246400
O -3.19795100 2.78713800 0.17428400
C 1.02713100 0.97226600 -0.03672200
C 1.35466700 1.92704200 0.92380100
C 2.61772500 2.05532700 1.49251800
C 3.69379200 1.24129600 1.16743000
C 3.64043700 0.19704300 0.23871700
Si 5.22579800 -0.81088000 -0.05977500
C 5.77949100 -1.52239600 1.59707600
P 2.19254800 -0.21938900 -0.62652300
C 6.54500100 0.36248700 -0.72345700
C 4.92092500 -2.20162400 -1.29126800
C -2.95198800 -0.60886300 0.15989400
P -1.50150100 -0.98791400 0.72987800
Si -4.76035000 -1.06000400 0.38539000
C -5.45615900 -1.61248900 -1.27859500
C -5.66871700 0.45641500 1.02921100
C -4.88024600 -2.47728900 1.61773300
H 5.84400500 -2.76518500 -1.44251400
H 4.15865800 -2.89556800 -0.93454800
H 4.59946900 -1.81884800 -2.26083000
H 5.93269600 -0.73304200 2.33482700
H 6.71958700 -2.06697400 1.48854800
H 5.03170500 -2.21098400 1.99357800
H 7.49041400 -0.16403300 -0.86916000
H 6.72401100 1.18857500 -0.03309100
H 6.24210100 0.78675300 -1.68204400
H 4.63047500 1.43845100 1.68061500
H 2.76439800 2.83640900 2.22726600
H 0.58587600 2.61658700 1.24433600
H 0.07284200 -0.02305100 -2.45653100
H -2.33043900 0.05509600 -3.16879800
H -3.98809700 0.97808300 -1.54709800
H -4.46132600 -2.18826300 2.58229500
H -4.33754900 -3.35343900 1.26031600
H -5.92360600 -2.76205100 1.77006500
H -4.88080500 -2.44779500 -1.68048500
H -6.48899300 -1.94442300 -1.15345200
H -5.45294600 -0.81203900 -2.01893700
H -5.31993100 0.70896700 2.03145900
H -6.74181000 0.26066500 1.08044300
H -5.50269100 1.32904100 0.39814900

E(M06-2X/cc-pvtz PCM=toluene T=383 K) =
-2074.32735547
E(L-CCSD(T)/cc-pVTZ)=-2071.223691132129
E+ZPE=-2073.962944
E+thermalE=-2073.919481
E+thermalH=-2073.918268
E+thermalG=-2074.049981
C -2.02810300 0.57417800 -2.21563200
C -2.95660000 0.95896600 -1.24766500
C -2.52734600 1.92953000 -0.24130900
O -1.19090800 1.90609800 0.03404800
C -0.36173000 0.99330400 -0.57200300
C -0.70226900 0.54436000 -1.84921800
O -3.22335800 2.71711700 0.33870700
C 1.02287400 1.03669800 -0.05455700
C 1.38664400 2.04971000 0.82087500
C 2.66455000 2.18699200 1.35081100
C 3.70402500 1.32067800 1.05842600
C 3.59440700 0.21390000 0.21461300
Si 5.13068500 -0.86199000 -0.04571100
C 5.67292600 -1.51430300 1.62820000
P 2.12218700 -0.22691900 -0.57265300
C 6.47536700 0.22202900 -0.77867600
C 4.73002800 -2.28048800 -1.20131700
C -2.86913600 -0.62785400 0.19195600
P -1.39041900 -0.94932600 0.66972700
Si -4.66916000 -1.10433200 0.37623800
C -5.29248500 -1.70111300 -1.29075200
C -5.63792000 0.37970500 0.97662100
C -4.76997200 -2.49531600 1.62533200
H 5.61850000 -2.89539500 -1.35404700
H 3.94491000 -2.91679800 -0.79137500
H 4.39724000 -1.92000200 -2.17529500
H 5.85321100 -0.69803100 2.32898200
H 6.59611100 -2.08864500 1.53655800
H 4.90803100 -2.16303100 2.05612800
H 7.39673500 -0.34631900 -0.91473200
H 6.69600100 1.06988100 -0.12877900
H 6.16850500 0.61247900 -1.74956200
H 4.66280600 1.52402300 1.52915600
H 2.85097900 3.01492000 2.02186600
H 0.63785900 2.77919700 1.10100100
H 0.05787400 0.08980700 -2.46661700
H -2.36019700 0.16075000 -3.15713000
H -4.00936000 1.00937900 -1.48261200
H -4.39563700 -2.16406900 2.59424600
H -4.17406900 -3.34960400 1.30316100
H -5.80278600 -2.82477700 1.75063800
H -4.69400500 -2.54308100 -1.64046100
H -6.32698300 -2.03661000 -1.19964300
H -5.25993700 -0.92087500 -2.05122400
H -5.24826800 0.72384600 1.93497000
H -6.68558000 0.10439500 1.11096900

H -5.58724100 1.21914700 0.28403600

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) = -2074.36041718
E+ZPE=-2073.994346
E+thermalE=-2073.950328
E+thermalH=-2073.949115
E+thermalG=-2074.082069
C 2.01404000 0.46884000 2.23218500
C 2.94737100 0.92582000 1.29606000
C 2.50175100 1.93792100 0.33963400
O 1.17234500 1.87894900 0.03293800
C 0.35808600 0.91779600 0.58086500
C 0.69289600 0.42474500 1.84697700
O 3.17591800 2.78872300 -0.17904200
C -1.02187300 0.96198900 0.03666800
C -1.33600800 1.91796100 -0.92288400
C -2.59611300 2.04774600 -1.49915500
C -3.67120100 1.23492400 -1.17419400
C -3.61826400 0.19374200 -0.24083300
Si -5.20170700 -0.80662700 0.06139400
C -5.70269400 -1.60188900 -1.56417000
P -2.17940400 -0.21863800 0.62299000
C -6.53523300 0.38900900 0.62626200
C -4.92031300 -2.12206400 1.36731100
C 2.92425800 -0.62132400 -0.21639800
P 1.46164700 -0.95864100 -0.73624600
Si 4.73498700 -1.06235900 -0.38982500
C 5.35835600 -1.67603900 1.27175900
C 5.67969700 0.45475000 -0.94952100
C 4.88469900 -2.42922200 -1.66381700
H -5.85032700 -2.67465600 1.53411800
H -4.15379000 -2.84019900 1.06331100
H -4.61471300 -1.68597800 2.32247100
H -5.83325900 -0.85145000 -2.34952400
H -6.64899600 -2.14093500 -1.45602500
H -4.94320700 -2.31248200 -1.90229700
H -7.48153600 -0.13602500 0.78958100
H -6.71247300 1.17072900 -0.11832800
H -6.25192100 0.87669400 1.56332800
H -4.61068600 1.42994300 -1.68859500
H -2.73913800 2.82800500 -2.23879500
H -0.55921900 2.60541300 -1.23758400
H -0.06052200 -0.08136500 2.43559900
H 2.34428500 0.01735100 3.15902600
H 3.99495900 0.99682100 1.55621900
H 4.48372900 -2.10588600 -2.62822500
H 4.33688200 -3.32199000 -1.34990200
H 5.93414600 -2.70590300 -1.80675900
H 4.75481200 -2.51646100 1.62603000
H 6.39229100 -2.02239000 1.17522700
H 5.34021500 -0.89851000 2.03978400
H 5.30340300 0.80679000 -1.91380800
H 6.74117400 0.21368100 -1.06572900
H 5.59149400 1.28417600 -0.24392300

i(3/4)
E(M06-2X/6-31+G*) = -2073.94358392
E+ZPE=-2073.573378
E+thermalE=-2073.545207
E+thermalH=-2073.544262
E+thermalG=-2073.633226
C 2.04293600 0.77543300 2.18798400
C 3.02433500 0.86604500 1.04023200
C 2.57014800 2.06558200 0.20906400
O 1.26909500 1.99480700 -0.14568600
C 0.52961700 0.84713300 0.33794600
C 0.76239900 0.72244800 1.82202400
C 2.89329900 -0.33940100 0.08913700
Si 4.46495500 -1.27368900 -0.36917600
C 5.20908900 -1.93650700 1.23001600
O 3.26395200 2.98726600 -0.12540300
C -0.91189300 0.97975900 -0.08558400
C -1.30325100 2.01911300 -0.92218800
C -2.61431000 2.18787000 -1.37604000
C -3.65477300 1.32754900 -1.04315700
C -3.51629900 0.20043900 -0.22287800
Si -5.05110100 -0.86293700 0.10109700
C -5.65261200 -1.54272200 -1.54961700
P 1.37947500 -0.68506500 -0.51927900
P -2.00500800 -0.26741000 0.49056700
C 4.04773500 -2.68128100 -1.53995600
C 5.63608200 -0.04086500 -1.17193400
C -4.63178900 -2.27392000 1.26999800
C -6.38070200 0.23740500 0.85518700
H -2.82600600 3.03602200 -2.02161900
H -4.63877800 1.55679400 -1.45685700
H -0.55387500 2.74096500 -1.23435900
H -0.07828000 0.60981500 2.49899900
H 2.39511500 0.75916500 3.21357500
H 4.05093300 1.04461300 1.36416000
H 5.21468300 0.34606200 -2.10571500
H 5.83014700 0.81760200 -0.51898400
H 6.59846400 -0.51296800 -1.40094700
H 5.40405200 -1.13218300 1.94856700
H 6.16192200 -2.44154900 1.03461500
H 4.53510600 -2.65713100 1.70565800
H 4.95222300 -3.24679400 -1.79148000
H 3.33179300 -3.37884100 -1.09174200
H 3.61636000 -2.30839100 -2.47521600
H -7.29630600 -0.33349800 1.04773900
H -6.04247300 0.66549900 1.80503500
H -6.63986200 1.06740800 0.18836200
H -6.57186300 -2.12567600 -1.42080400
H -5.86556900 -0.73499900 -2.25893600
H -4.89785700 -2.19427500 -2.00306700
H -5.52315200 -2.88632900 1.44941300
H -3.85515700 -2.92587400 0.85569100
H -4.27701300 -1.90660700 2.23901300

E(M06-2X/cc-pvtz PCM=toluene T=383 K) = -2074.37120328
E(L-CCSD(T)/cc-pVTZ)=-2071.268858796002
E+ZPE=-2074.003873
E+thermalE=-2073.960104
E+thermalH=-2073.958891
E+thermalG=-2074.090634
C -2.03564600 0.80522400 -2.18130100
C -3.01857800 0.87216600 -1.03751000
C -2.57689100 2.05721100 -0.19012800
O -1.28089900 1.99806700 0.15990500
C -0.52964100 0.86488200 -0.33699200
C -0.76242100 0.75482000 -1.81793800
C -2.87704000 -0.34031200 -0.10278100
Si -4.43588600 -1.28658300 0.36584700
C -5.18167500 -1.96087800 -1.21915800
O -3.27698500 2.96257400 0.16042000
C 0.90703400 0.99527800 0.08596900
C 1.30925800 2.03158800 0.90976800
C 2.61721500 2.19346700 1.35812100
C 3.64640400 1.32808900 1.03062200
C 3.50032200 0.20079100 0.22158700
Si 5.02668600 -0.87102500 -0.10039700
C 5.62246600 -1.54077600 1.54887700

P -1.36496900 -0.68255500 0.49257900
P 1.98949900 -0.25909700 -0.48100800
C -3.99333400 -2.67479100 1.53894400
C -5.60197600 -0.05737200 1.16750000
C 4.58997800 -2.27808000 -1.25725000
C 6.34908800 0.21946300 -0.86442300
H 2.83496000 3.04089300 1.99483300
H 4.62881900 1.55180300 1.43964100
H 0.57114600 2.75928900 1.22027200
H 0.07592400 0.65761800 -2.49240500
H -2.38735600 0.80258500 -3.20195500
H -4.04146400 1.04244600 -1.35954800
H -5.17923700 0.32534200 2.09674200
H -5.79420900 0.79384400 0.51261200
H -6.55813700 -0.53166100 1.39410300
H -5.37445000 -1.16414900 -1.93903800
H -6.12971700 -2.45960200 -1.01230300
H -4.51032800 -2.68391900 -1.68346300
H -4.88553000 -3.24746400 1.79641500
H -3.27257400 -3.35827500 1.08844000
H -3.56377900 -2.28572700 2.46269000
H 7.26446000 -0.34846500 -1.03762000
H 6.01119600 0.62174200 -1.82009900
H 6.59281600 1.05931900 -0.21251600
H 6.54469800 -2.11025600 1.42357500
H 5.81929300 -0.73026600 2.25196500
H 4.87257500 -2.19678000 1.99210900
H 5.47258500 -2.89229600 -1.44287800
H 3.81639400 -2.91751800 -0.83053100
H 4.22844600 -1.90695500 -2.21694600

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) =
-2074.41093848
E+ZPE=-2074.041915
E+thermalE=-2073.998756
E+thermalH=-2073.997543
E+thermalG=-2074.127217
C 3.00893100 0.83695400 1.07887100
C 2.53678300 2.06521200 0.30638600
O 1.25101600 1.98462000 -0.06995800
C 0.52855400 0.78943800 0.34285700
C 0.74528600 0.60477700 1.82188400
C 2.01462800 0.66700900 2.20507900
C -0.90495000 0.91221000 -0.11190500
P -2.04695800 -0.24458600 0.54092400
C -3.52159100 0.17233200 -0.26285300
C -3.60707800 1.21294600 -1.19266700
C -2.53932600 2.01467800 -1.56679600
C -1.25231500 1.86933800 -1.05451900
P 1.42425800 -0.67245800 -0.56540900
C 2.92092700 -0.32637000 0.07414000
Si 4.51087300 -1.22996800 -0.38391500
C 4.14387600 -2.59122500 -1.61655300
O 3.20615500 3.02381500 0.03769700
C 5.68712800 0.03703100 -1.11038200
C 5.21391800 -1.94044700 1.20553200
H -2.70969400 2.79748300 -2.29812700
H -4.56747000 1.41900100 -1.66245800
H -0.48380300 2.54712800 -1.40807700
H -0.09547300 0.44955700 2.48526700
H 2.35407900 0.61519800 3.23074800
H 4.02228400 1.01858500 1.43081300
H 5.28127400 0.46158800 -2.03261600
H 5.87006200 0.86249100 -0.41643100
H 6.65143200 -0.42549700 -1.34257300
H 5.39211800 -1.15877700 1.95004300
H 6.16902100 -2.43938600 1.01486900
H 4.52970300 -2.67358700 1.64187900
H 5.06647400 -3.12341000 -1.86817200
H 3.43610500 -3.32096800 -1.21327000
H 3.72617400 -2.18887900 -2.54366400
Si -5.09756600 -0.80889100 0.12498600
C -4.76149600 -2.12757300 1.41513900
C -6.38756400 0.39900500 0.76059400
C -5.69371000 -1.60130900 -1.46981900
H -7.32819000 -0.11736200 0.97609000
H -6.04796700 0.88394800 1.68024000
H -6.59792300 1.18229500 0.02642700
H -6.63585600 -2.13460000 -1.30939800
H -5.86268900 -0.85048300 -2.24738900
H -4.95810100 -2.31667000 -1.84851900
H -5.68638400 -2.67262900 1.62886500
H -4.01725900 -2.85178400 1.07244900
H -4.40311000 -1.69506300 2.35345000

E(B3LYP/cc-pVTZ PCM=toluene T=383 K) =
-2074.89727569
E+ZPE= -2074.533022
E+thermalE= -2074.490138
E+thermalH= -2074.488925
E+thermalG= -2074.617043
C -2.01779100 0.66986700 -2.21012300
C -3.01582400 0.82290000 -1.08553100
C -2.55606100 2.04947200 -0.29770700
O -1.26349700 1.97891700 0.08009400
C -0.51884600 0.78903200 -0.35332700
C -0.74695100 0.61281000 -1.82885700
C -2.93050000 -0.34981800 -0.08616500
Si -4.54011900 -1.22016900 0.38415800
C -5.33050300 -1.83601800 -1.21392800
O -3.24125000 2.99572400 -0.01555200
C 0.91119300 0.91436600 0.10106000
C 1.26436000 1.87388700 1.04053200
C 2.55295600 2.02541700 1.54781800
C 3.62463500 1.22584300 1.17709300
C 3.54487600 0.17830800 0.25599800
Si 5.12789000 -0.80628700 -0.11739900
C 5.74902800 -1.54034000 1.50563100
P -1.42924400 -0.70431100 0.55826500
P 2.06382300 -0.25027200 -0.55070800
C -4.19117300 -2.65553400 1.54720000
C -5.64437500 0.06668300 1.20507600
C 4.79260100 -2.17985800 -1.36052100
C 6.41217400 0.38970100 -0.80920700
H 2.72181200 2.81207700 2.27191000
H 4.58153500 1.44048600 1.64416800
H 0.50046600 2.55090700 1.39716200
H 0.09072800 0.46208200 -2.49252900
H -2.35665800 0.62297200 -3.23370500
H -4.02588900 1.00274400 -1.43830000
H -5.20322100 0.41072900 2.14143700
H -5.78507800 0.93837200 0.56425900
H -6.62732800 -0.35513200 1.42414300
H -5.49925200 -1.01869000 -1.91705800
H -6.29679900 -2.29965100 -1.00587900
H -4.69717300 -2.57777700 -1.70267600
H -5.12419500 -3.15789500 1.81038100
H -3.53304200 -3.39162900 1.08339500
H -3.72186600 -2.31431000 2.47085300
H 7.35525000 -0.12634200 -1.00047000
H 6.06936400 0.82841800 -1.74765600
H 6.61158900 1.20500000 -0.11164600
H 6.68814800 -2.07609300 1.35332400
H 5.92380600 -0.76116700 2.24938700

H 5.02138300 -2.24060200 1.91887100
H 5.71459600 -2.73289300 -1.55186700
H 4.04833700 -2.88599300 -0.98999300
H 4.43517200 -1.78393400 -2.31205600

E2
E(M06-2X/6-31+G*) = -2073.90763601
E+ZPE=-2073.540407
E+thermalE=-2073.511961
E+thermalH=-2073.511017
E+thermalG=-2073.601360
C -3.60343900 0.20683800 0.31412400
Si -5.37791300 0.19553800 -0.35713300
H -7.09006600 1.99160000 -0.60316700
H -6.02583900 -1.97561200 0.68682200
C -6.40802800 -0.94994100 0.72576800
H -7.45198500 -0.96412100 0.39212600
H -6.39819400 -0.62943200 1.77356200
C -6.05206600 1.95069300 -0.25365000
H -6.03102500 2.32657000 0.77545000
H -5.45896700 2.63405900 -0.87092300
C -5.39378800 -0.40405900 -2.13861200
H -6.42188400 -0.41024300 -2.51857600
H -4.99785400 -1.42145300 -2.22839100
H -4.79956200 0.24445800 -2.79143300
C -3.40240600 0.60065100 1.64231000
H -4.27158300 0.87585700 2.24291900
C -2.15907200 0.66887400 2.26764300
H -2.11261400 0.97997900 3.30741100
C -0.96796500 0.35580500 1.61767800
H -0.03688500 0.41921600 2.17857600
P -2.30808400 -0.27085000 -0.73837400
C -0.90022300 -0.07845000 0.29176400
C 0.44075900 -0.32347300 -0.28059300
O 1.23706000 -1.43712500 1.19037000
C 0.61766100 -1.26243800 -1.35566100
H -0.24867300 -1.67524000 -1.86501200
C 1.86407000 -1.76321300 -1.53052300
H 2.05018500 -2.60370900 -2.19269000
P 1.63942200 1.07045100 -0.14815900
C 3.03670300 0.15411100 -0.41525100
C 2.93390200 -1.29352500 -0.65949100
C 2.37617900 -1.86223600 0.91466000
O 3.19389300 -2.56412800 1.46065700
H 3.88245700 -1.81514000 -0.78700800
Si 4.76522200 0.90239000 -0.21582100
C 4.60806900 2.74336400 0.12518500
H 4.08580500 3.26336000 -0.68542400
H 4.06362000 2.93544600 1.05599800
H 5.60316500 3.19238000 0.22271100
H 5.79724000 -0.46037000 -2.04128500
C 5.70731900 0.60874900 -1.81936500
H 6.72143200 1.01884500 -1.74924500
H 5.20623400 1.08919300 -2.66649300
C 5.59918700 0.00837400 1.21077600
H 5.58754600 -1.07783700 1.06861900
H 5.08402800 0.21600500 2.15483200
H 6.64222000 0.33047200 1.31116900

E(M06-2X/cc-pvtz PCM=toluene T=383 K) =
-2074.33753192
E(L-CCSD(T)/cc-pVTZ)=-2071.235427440195
E+ZPE=-2073.973314
E+thermalE=-2073.929268
E+thermalH=-2073.928055
E+thermalG=-2074.059970
C -6.35531700 -0.96038700 0.77985300
Si -5.37065500 0.15805300 -0.35997500
C -5.37493800 -0.51794600 -2.10626800
C -3.59380900 0.23908900 0.29507600
P -2.30433700 -0.30598000 -0.72092400
C -0.89629300 -0.03240400 0.28207700
C 0.43807800 -0.31884000 -0.27148200
P 1.65088200 1.06332500 -0.21614900
C 3.03364500 0.12373800 -0.41430200
Si 4.76450900 0.87097200 -0.25923800
C 5.59043600 0.04068400 1.20229000
C -3.38898200 0.72801300 1.58404000
C -2.14822500 0.85335500 2.19289300
C -0.96381600 0.50230000 1.56481500
C -6.07674500 1.89569300 -0.32650400
C 0.61508800 -1.31485900 -1.28642500
C 1.84971400 -1.83594300 -1.42211400
C 2.91693500 -1.33248000 -0.57166900
C 2.35445000 -1.79891300 1.00994700
O 3.15460100 -2.47513600 1.60684100
O 1.22337300 -1.35585800 1.26397900
C 4.61312800 2.71916100 -0.00679100
C 5.68927100 0.49412800 -1.84727100
H -7.11394700 1.89698800 -0.66517100
H -5.95807600 -1.97570000 0.76273900
H -7.40104100 -0.99724800 0.47040800
H -6.32171800 -0.60258500 1.80974100
H -6.05161100 2.31052200 0.68205300
H -5.50373900 2.55705400 -0.97724900
H -6.39691000 -0.54912100 -2.48717500
H -4.97002600 -1.52989500 -2.14364100
H -4.78304800 0.10694500 -2.77617600
H -4.25395900 1.03705600 2.16627600
H -2.09921800 1.24206000 3.20108000
H -0.03501400 0.61891600 2.11235300
H -0.24800200 -1.74335000 -1.77800500
H 2.03147500 -2.70891300 -2.03379500
H 3.85705400 -1.86509600 -0.66750700
H 4.09290900 3.19345000 -0.83999400
H 4.06988400 2.95043800 0.90989200
H 5.60589100 3.16572900 0.06786000
H 5.74650700 -0.58013700 -2.02652200
H 6.70854200 0.87952300 -1.79138800
H 5.19688200 0.95708000 -2.70292800
H 5.56585400 -1.04538600 1.10442900
H 5.07823000 0.29930000 2.12955600
H 6.63143200 0.35746900 1.28270100

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) =
-2074.38122536
E+ZPE=-2074.015699
E+thermalE=-2073.971912
E+thermalH=-2073.970699
E+thermalG=-2074.102849
C -6.38047600 -0.82886700 0.92815900
Si -5.39340100 0.11613200 -0.35896400
C -5.43482300 -0.78881500 -2.00030600
C -3.60954900 0.26388900 0.27483700
P -2.31404900 -0.33394100 -0.70311300
C -0.90001000 0.03211400 0.26402400
C 0.43431200 -0.28380000 -0.27455400
P 1.67578600 1.07579500 -0.25825400
C 3.04857900 0.11283700 -0.39893200
Si 4.79593700 0.83510000 -0.29486900
C 5.58944600 0.12727400 1.24752400
C -3.40214000 0.85306500 1.52521800
C -2.15824900 1.03441900 2.11677600
C -0.96956600 0.65222300 1.51122300

C -6.08073500 1.85203600 -0.55343100
C 0.61459600 -1.32888900 -1.24442300
C 1.84402800 -1.87173800 -1.33996000
C 2.90476300 -1.35978300 -0.47024600
C 2.34972600 -1.76873300 1.08368600
O 3.12239100 -2.45512800 1.71718000
O 1.22378100 -1.29834700 1.33828100
C 4.70576100 2.70486100 -0.21956700
C 5.72102100 0.28476400 -1.83245800
H -7.11824100 1.82193200 -0.90037200
H -5.96590800 -1.82960400 1.07913000
H -7.42290100 -0.93720700 0.61310700
H -6.37611100 -0.31502000 1.89390700
H -6.06104900 2.39484900 0.39631500
H -5.49646000 2.42480700 -1.27919200
H -6.47110700 -0.88572400 -2.33905000
H -5.01494700 -1.79531400 -1.91802600
H -4.87890400 -0.25373400 -2.77525900
H -4.26761800 1.19701700 2.08931000
H -2.10964600 1.49543100 3.09682000
H -0.04152200 0.81314000 2.05187300
H -0.24586900 -1.76151000 -1.74128900
H 2.02474600 -2.76664100 -1.92307300
H 3.84347600 -1.89911800 -0.56911500
H 4.21751500 3.12359400 -1.10412000
H 4.16192000 3.04802800 0.66482000
H 5.71719300 3.12008800 -0.16978300
H 5.79666700 -0.80488800 -1.88901900
H 6.73830900 0.68840700 -1.82659900
H 5.22337300 0.63882500 -2.73966500
H 5.50564600 -0.96275000 1.27437500
H 5.10017800 0.51493900 2.14540400
H 6.65022500 0.39206800 1.29456900

E(B3LYP/cc-pVTZ PCM=toluene T=383 K)= -2074.87732096
E+ZPE= -2074.515361
E+thermalE=-2074.471266
E+thermalH=-2074.470053
E+thermalG=-2074.602268
C -6.43407500 -0.93497100 0.74288800
Si -5.40408400 0.19136800 -0.36412200
C -6.06204900 1.95644200 -0.27492700
C -5.44583000 -0.42996900 -2.14008300
C -3.62340000 0.20307000 0.31090100
C -3.42735300 0.59237400 1.63747900
C -2.18928400 0.66313300 2.26721000
C -0.99344900 0.36053300 1.63174000
C -0.90080200 -0.06793200 0.30676400
C 0.43647600 -0.30230200 -0.25795900
C 0.62920300 -1.19094700 -1.37947400
C 1.86422700 -1.69039100 -1.56079700
C 2.92122600 -1.28726900 -0.61939400
C 2.38372000 -1.88112100 0.85540300
O 1.23352900 -1.46964900 1.17202100
P -2.31260400 -0.26428200 -0.73358300
P 1.66258800 1.09587500 -0.10757000
C 3.05361200 0.17616500 -0.37692900
Si 4.80179000 0.89137200 -0.20980700
C 5.72601800 0.49183300 -1.80424800
C 5.60871600 0.02975200 1.25640600
C 4.72065500 2.75251100 0.05111600
O 3.15614000 -2.62105500 1.43095800
H -7.10248700 1.99837900 -0.60323200
H -6.06331700 -1.96050900 0.70809800
H -7.47729900 -0.93976800 0.42079200
H -6.40651600 -0.60352700 1.78218600
H -6.01521800 2.34193700 0.74501600
H -5.47769300 2.62212600 -0.91207300
H -6.47633200 -0.43010400 -2.50119000
H -5.06242400 -1.44813900 -2.21945500
H -4.85787800 0.20412300 -2.80492700
H -4.29354100 0.86102700 2.23552600
H -2.15310600 0.96955100 3.30425600
H -0.07840700 0.42674900 2.20692400
H -0.22508000 -1.53929700 -1.94309000
H 2.06573700 -2.47195300 -2.27921000
H 3.86344900 -1.79598600 -0.79113700
H 4.22841200 3.25416100 -0.78325000
H 4.18265400 3.00598400 0.96538500
H 5.73184900 3.15603000 0.13443800
H 5.76629700 -0.58398400 -1.98136800
H 6.75253800 0.85980900 -1.75007800
H 5.24379700 0.95901100 -2.66426500
H 5.50211200 -1.05321600 1.18432000
H 5.13975700 0.34371000 2.18999900
H 6.67202800 0.27179600 1.30822700

4
E(M06-2X/6-31+G*) = -1885.47858259
E+ZPE=-1885.123151
E+thermalE=-1885.097138
E+thermalH=-1885.096194
E+thermalG=-1885.180665
C -6.26857200 -0.37617600 0.49232800
Si -4.62347600 -1.01240900 -0.17106600
C -4.15884700 -2.61732200 0.69551500
C -3.27422400 0.27785100 0.16110100
C -3.59110700 1.49487500 0.76878100
C -2.66174200 2.49953900 1.04589300
C -1.30763400 2.38568400 0.74473400
C -0.73126300 1.26696400 0.13461300
C 0.73123200 1.26698000 -0.13457300
C 1.30757600 2.38567200 -0.74476800
C 2.66168700 2.49951500 -1.04597100
C 3.59106000 1.49486400 -0.76881300
C 3.27419600 0.27788500 -0.16102300
Si 4.62346000 -1.01239500 0.17104000
C 4.15959300 -2.61678600 -0.69692400
P -1.65779400 -0.13997400 -0.34292900
C -4.74781800 -1.31203400 -2.02508900
P 1.65785100 -0.13992000 0.34308900
C 6.26886400 -0.37547100 -0.49093400
C 4.74685400 -1.31324900 2.02492800
H -4.62628900 1.68695600 1.05235000
H -3.00750700 3.40930900 1.52982000
H -0.65045200 3.20882200 1.02447600
H -7.04924900 -1.12702200 0.32486700
H -6.22481300 -0.18029000 1.56956000
H -6.58394100 0.54516100 -0.01019800
H -4.92336300 -3.38601900 0.53408300
H -3.20656100 -3.00521500 0.31690700
H -4.05166800 -2.46565400 1.77515300
H -5.52274200 -2.05418900 -2.24949700
H -4.99506000 -0.38917400 -2.56076900
H -3.79795200 -1.68621800 -2.42320100
H 4.62623000 1.68693600 -1.05243300
H 3.00745600 3.40924800 -1.52996800
H 7.04962500 -1.12615200 -0.32312300
H 6.22589000 -0.17924600 -1.56813700
H 6.58358200 0.54579200 0.01213400
H 4.92411600 -3.38548700 -0.53554800
H 3.20713100 -3.00505200 -0.31913500
H 4.05303500 -2.46440200 -1.77652100

H 5.52169500 -2.05553100 2.24920700
H 4.99386700 -0.39072700 2.56130000
H 3.79682900 -1.68769500 2.42240200
H 0.65037900 3.20877400 -1.02456500

E(M06-2X/cc-pvtz PCM=toluene T=383 K) =
-1885.83499156
E(L-CCSD(T)/cc-pVTZ)=-1882.999045156336
E+ZPE=-1885.482200
E+thermalE=-1885.442011
E+thermalH=-1885.440798
E+thermalG=-1885.564727
C 6.23719600 -0.39531000 -0.51581100
Si 4.60445500 -1.01954300 0.16812800
C 4.74048200 -1.30656500 2.01697000
C 4.11472800 -2.61802400 -0.68263800
C 3.26280900 0.27766300 -0.15634300
P 1.64757400 -0.13403600 0.33359700
C 0.72955500 1.27602800 -0.13107800
C -0.72955500 1.27602800 0.13107600
P -1.64757600 -0.13403300 -0.33360500
C -3.26281000 0.27766600 0.15633900
Si -4.60445500 -1.01954200 -0.16812700
C -4.74044000 -1.30661800 -2.01696400
C 3.58391400 1.49447700 -0.74800300
C 2.66387800 2.50203800 -1.01601700
C 1.31407400 2.39311700 -0.72264600
C -1.31407300 2.39311600 0.72264700
C -2.66387600 2.50203700 1.01602000
C -3.58391200 1.49447800 0.74800500
C -4.11475800 -2.61800100 0.68269800
C -6.23721000 -0.39528100 0.51575500
H 4.61645200 1.68427300 -1.02551100
H 3.01476300 3.41183700 -1.48554800
H 0.66657400 3.22120400 -0.99265500
H 7.01175900 -1.14780500 -0.36034200
H 6.17215800 -0.19864300 -1.58680600
H 6.55722800 0.52091800 -0.01771800
H 4.86853000 -3.38989400 -0.51949500
H 3.16341100 -2.98596900 -0.29543300
H 4.00500000 -2.46818300 -1.75730700
H 5.50120600 -2.05795500 2.23496300
H 5.00776900 -0.38682600 2.53812400
H 3.78975200 -1.65938600 2.41958800
H -4.61645100 1.68427400 1.02551500
H -3.01476000 3.41183500 1.48555400
H -7.01177800 -1.14776800 0.36026700
H -6.17220400 -0.19860600 1.58675000
H -6.55721300 0.52094700 0.01764200
H -4.86855500 -3.38987500 0.51954900
H -3.16342800 -2.98595800 0.29553400
H -4.00506600 -2.46813400 1.75736700
H -5.50114900 -2.05802500 -2.23494900
H -5.00773100 -0.38689700 -2.53814700
H -3.78969800 -1.65943600 -2.41955500
H -0.66657100 3.22120200 0.99265700

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) =
-1885.88858077
E+ZPE=-1885.534803
E+thermalE=-1885.494974
E+thermalH=-1885.493761
E+thermalG=-1885.616392
C 6.25807200 -0.38578600 -0.55092200
Si 4.64080100 -1.00195900 0.17888300
C 4.81753200 -1.22105200 2.03510500
C 4.16493600 -2.63679900 -0.61202600
C 3.27584200 0.27022800 -0.16891300
P 1.66787100 -0.13212200 0.35958000
C 0.72955400 1.25183000 -0.14329200
C -0.72955400 1.25183000 0.14329000
P -1.66787200 -0.13212000 -0.35958500
C -3.27584200 0.27022900 0.16891000
Si -4.64080200 -1.00195900 -0.17888200
C -4.81751700 -1.22107500 -2.03510300
C 3.57625600 1.47071400 -0.81192800
C 2.64103100 2.45982100 -1.10419600
C 1.29385700 2.35225300 -0.78833800
C -1.29385600 2.35225200 0.78833900
C -2.64103000 2.45982100 1.10419800
C -3.57625600 1.47071400 0.81192900
C -4.16494600 -2.63679000 0.61205200
C -6.25807800 -0.38577300 0.55090100
H 4.60408000 1.66189200 -1.11171100
H 2.97859600 3.35615300 -1.61377800
H 0.63413800 3.16593600 -1.07990100
H 7.04297200 -1.12989900 -0.38384300
H 6.17861300 -0.22410300 -1.62997000
H 6.58468300 0.54973000 -0.08738300
H 4.94344700 -3.38860300 -0.44839600
H 3.23200500 -3.02100800 -0.18913800
H 4.02231700 -2.52330100 -1.69050000
H 5.60531200 -1.94446400 2.26748300
H 5.07040000 -0.27412400 2.52068800
H 3.88529400 -1.58621800 2.47607700
H -4.60407900 1.66189100 1.11171300
H -2.97859500 3.35615100 1.61378100
H -7.04298200 -1.12987800 0.38380700
H -6.17863300 -0.22409500 1.62995100
H -6.58467200 0.54974800 0.08736100
H -4.94346000 -3.38859300 0.44843200
H -3.23201700 -3.02100900 0.18917000
H -4.02232800 -2.52327600 1.69052400
H -5.60529100 -1.94449500 -2.26747800
H -5.07038600 -0.27415500 -2.52070000
H -3.88527300 -1.58624200 -2.47606300
H -0.63413600 3.16593400 1.07990200

(B3LYP/cc-pVTZ PCM=toluene T=383 K)= -
1886.30628687
E+ZPE=-1885.956190
E+thermalE= -1885.915741
E+thermalH=-1885.914528
E+thermalG=-1886.039330
C 6.27085100 -0.42203000 -0.55472400
Si 4.63569800 -1.01465900 0.17495700
C 3.28048300 0.27423000 -0.17341700
C 3.58641200 1.47910200 -0.80391300
C 2.65815700 2.48037000 -1.08164000
C 1.30950000 2.38439900 -0.76640000
C 0.72726100 1.28185900 -0.13902500
C -0.72726100 1.28185900 0.13902300
C -1.30949900 2.38439900 0.76640000
C -2.65815600 2.48037000 1.08164000
C -3.58641200 1.47910300 0.80391300
C -3.28048300 0.27423100 0.17341500
Si -4.63569900 -1.01465900 -0.17495600
C -6.27085400 -0.42202200 0.55471000
C 4.80928000 -1.23193400 2.04021700
C 4.14173700 -2.65558000 -0.61193400
P 1.66151300 -0.12326200 0.35545100
P -1.66151400 -0.12326100 -0.35545400
C -4.80926900 -1.23195000 -2.04021600
C -4.14174400 -2.65557400 0.61195100

H 4.61113200 1.66751300 -1.10630100
H 3.00306900 3.37732600 -1.58021300
H 0.66343900 3.20873300 -1.04893800
H 7.04622500 -1.16879900 -0.37290100
H 6.19945200 -0.27214700 -1.63329900
H 6.59982000 0.51481600 -0.10202000
H 4.89899300 -3.41882100 -0.42090800
H 3.19309600 -3.01222600 -0.20782500
H 4.02793000 -2.55261600 -1.69233900
H 5.57326100 -1.97645500 2.27355600
H 5.09251000 -0.29278500 2.51844900
H 3.86796900 -1.56288000 2.48184300
H -4.61113200 1.66751300 1.10630100
H -3.00306700 3.37732600 1.58021400
H -7.04623100 -1.16878700 0.37288100
H -6.19946400 -0.27214000 1.63328700
H -6.59981500 0.51482600 0.10200400
H -4.89899800 -3.41881600 0.42092700
H -3.19310000 -3.01222300 0.20785100
H -4.02794200 -2.55260100 1.69235600
H -5.57324700 -1.97647600 -2.27355100
H -5.09249900 -0.29280600 -2.51845800
H -3.86795500 -1.56289900 -2.48183300
H -0.66343800 3.20873200 1.04893900

CA3

E(M06-2X/6-31+G*) = -2073.89707517
E+ZPE=-2073.528539
E+thermalE=-2073.500811
E+thermalH=-2073.499867
E+thermalG=-2073.586301
C 3.69710900 1.62238900 1.39349600
O 3.34010000 2.49906600 0.43234200
C 2.06815400 2.53942700 -0.12299100
C 1.08072300 1.58705700 0.41655100
C 1.54014100 0.58779400 1.28884700
C 2.87252700 0.66438200 1.83775400
O 1.90057600 3.37524600 -0.97629300
C -0.29444900 1.60681200 0.00021500
C -0.80994700 2.49426300 -0.98268100
C -2.10807600 2.46593400 -1.44389500
C -3.08459900 1.52925800 -1.03409400
C -2.86926700 0.52288000 -0.11571700
Si -4.23773000 -0.72661600 0.26538000
C -5.85670200 0.19409900 0.53913300
C 1.38914600 -1.30375500 0.03049000
Si 3.11074600 -1.85051300 -0.45959000
C 4.18111100 -2.27413200 1.03815300
P -1.33800600 0.37162800 0.73515900
P -0.12291700 -1.66096800 -0.31673300
C -4.39669700 -1.87807600 -1.21608800
C -3.77894300 -1.71547600 1.79930000
C 2.93181400 -3.40453300 -1.50965800
C 3.87016300 -0.48996600 -1.50983600
H -4.07095700 1.62126200 -1.49308800
H -2.39418800 3.20231600 -2.19034200
H -0.13460100 3.22892500 -1.40286300
H -6.66583000 -0.51100400 0.76185100
H -5.77553400 0.89296000 1.37840900
H -6.15302900 0.76650400 -0.34678700
H -4.57111800 -2.43707600 2.03056000
H -2.84990800 -2.27967000 1.65572400
H -3.64509600 -1.06908900 2.67351800
H -5.18004600 -2.62692600 -1.05243600
H -4.64977300 -1.31694800 -2.12265500
H -3.45587800 -2.40757200 -1.40361500
H 3.19464000 -0.01972600 2.61287300
H 4.70906100 1.79766000 1.74084300
H 4.86976900 -0.78952800 -1.84729600
H 3.25533700 -0.31181400 -2.39890100
H 3.96912700 0.45933300 -0.97563900
H 4.88143200 -3.07165300 0.76386500
H 4.76848300 -1.41937400 1.38535500
H 3.57571000 -2.63988600 1.87467600
H 3.91199400 -3.75646600 -1.85323700
H 2.46166000 -4.21336000 -0.93974500
H 2.31305800 -3.20933600 -2.39211300
H 0.80865200 0.04572400 1.88133800

E(M06-2X/cc-pvtz PCM=toluene T=383 K) =
-2074.32849147
E+ZPE=-2073.962890
E+thermalE=-2073.918706
E+thermalH=-2073.917493
E+thermalG=-2074.049354
C 1.53983800 0.61258700 1.29704800
C 2.86948800 0.68193000 1.83727000
C 3.69624100 1.62208700 1.38229400
O 3.34029300 2.49082300 0.41532300
C 2.07026900 2.53918500 -0.12901300
C 1.08614600 1.59472700 0.41233000
O 1.90631200 3.37254300 -0.98000100
C -0.28462700 1.60892500 -0.00306000
C -0.80709300 2.48496600 -0.98338300
C -2.09956100 2.45180400 -1.44171400
C -3.06855600 1.51682900 -1.03037800
C -2.85097800 0.51883600 -0.11332500
Si -4.22327400 -0.72468600 0.26401300
C -4.53861400 -1.70633000 -1.30373400
P -1.32426900 0.37881200 0.73413700
C -3.66562900 -1.86722600 1.64175800
C -5.76930600 0.21055100 0.76694400
C 1.38297100 -1.30022700 0.06376300
Si 3.08627300 -1.86378100 -0.46072300
C 2.86599900 -3.40942600 -1.50247600
P -0.12659800 -1.65351300 -0.27504300
C 3.83060000 -0.51053000 -1.52108100
C 4.18383800 -2.29399500 1.00282700
H -4.05115600 1.60142000 -1.48919500
H -2.38716100 3.18166900 -2.18730800
H -0.13865600 3.21800000 -1.40558300
H -6.59309100 -0.48092900 0.95043900
H -5.59346600 0.78280600 1.67827100
H -6.08090500 0.90527900 -0.01416700
H -4.44888900 -2.59474500 1.86087500
H -2.76652100 -2.41990400 1.36278300
H -3.45099800 -1.31430800 2.55692700
H -5.33894900 -2.43251200 -1.15406300
H -4.82683700 -1.04741600 -2.12398400
H -3.64025000 -2.24650900 -1.60598700
H 3.18736400 0.00596900 2.61433500
H 4.70769300 1.78747200 1.72247800
H 3.99677100 0.41389400 -0.97005300
H 4.79185100 -0.84233900 -1.91852200
H 3.17369800 -0.29134300 -2.36370400
H 3.62053100 -2.81364900 1.77872300
H 4.97468200 -2.96381400 0.66002400
H 4.65396600 -1.41755700 1.44413700
H 3.83113500 -3.77127100 -1.86211300
H 2.39766300 -4.20469900 -0.92149000
H 2.23371800 -3.20151400 -2.36625800
H 0.80984900 0.06997100 1.88197700

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) =

-2074.36241950
E+ZPE=-2073.995814
E+thermalE=-2073.951930
E+thermalH=-2073.950717
E+thermalG=-2074.082239
C 2.87103100 0.72011900 1.84925900
C 3.70124200 1.65908400 1.39107300
O 3.35155200 2.51769700 0.41233500
C 2.08351500 2.55769500 -0.14261000
C 1.09629800 1.61963800 0.40340000
C 1.54663600 0.63931500 1.29711400
O 1.92491800 3.38303300 -1.00574600
C -0.27600800 1.62782100 -0.01532000
P -1.31004000 0.39109500 0.71885500
C -2.85132400 0.53400300 -0.11307200
Si -4.21328400 -0.72577900 0.26797200
C -3.84977700 -1.57885700 1.89910400
C -0.80347800 2.50820000 -0.99321700
C -2.10014300 2.47419000 -1.44204100
C -3.07229900 1.54028000 -1.02326800
C -5.86429400 0.16277000 0.35164800
C -4.23010400 -1.98510400 -1.12505600
C 1.37872100 -1.29009500 0.05561700
P -0.13882200 -1.62937900 -0.27647300
Si 3.06320100 -1.90917600 -0.46046700
C 3.87182500 -0.57007700 -1.49430900
C 4.11598300 -2.37175100 1.02497100
C 2.82902200 -3.44490500 -1.51768900
H -4.05931500 1.63663500 -1.47239600
H -2.39452700 3.20744400 -2.18537000
H -0.13412000 3.24342900 -1.41752500
H -6.66300000 -0.54782000 0.58604300
H -5.85811500 0.93359400 1.12719500
H -6.11710800 0.64097400 -0.59894400
H -4.63317100 -2.31012200 2.12098700
H -2.89536400 -2.11330100 1.87379000
H -3.81187200 -0.86274800 2.72487000
H -5.00661100 -2.73879500 -0.96125200
H -4.42569300 -1.49955400 -2.08569100
H -3.26865100 -2.50130800 -1.20154400
H 3.18479200 0.05009200 2.63600600
H 4.71062200 1.83236500 1.73858400
H 4.82647100 -0.92956700 -1.89193200
H 3.23338600 -0.30484900 -2.34167000
H 4.06837200 0.33888600 -0.92297500
H 4.94990400 -2.99827700 0.69232800
H 4.53548600 -1.49863500 1.52723000
H 3.53848700 -2.94721200 1.75403800
H 3.79698100 -3.82806100 -1.85753100
H 2.32952400 -4.23881500 -0.95505600
H 2.22361600 -3.22229400 -2.40082400
H 0.81116100 0.10179300 1.88449800

E(B3LYP/cc-pVTZ PCM=toluene T=383 K) =
-2074.87070369
E+ZPE= -2074.507821
E+thermalE= -2074.463503
E+thermalH= -2074.462290
E+thermalG= -2074.594740
C 1.57111400 0.65273100 1.28641500
C 2.89620400 0.73548900 1.82790800
C 3.73372400 1.66335800 1.35639500
O 3.38502700 2.51992000 0.36950800
C 2.09127100 2.58093200 -0.16041400
C 1.11111900 1.64359200 0.39268400
O 1.92833900 3.41993200 -1.01307500
C -0.26097400 1.65958100 -0.00460000
C -0.81812700 2.56002100 -0.94417200
C -2.12497900 2.53201900 -1.36939600
C -3.08693800 1.58015500 -0.96923800
C -2.85356900 0.54180900 -0.09832000
Si -4.20984300 -0.73906000 0.25177700
C -4.31829700 -1.87729000 -1.24823000
P -1.29708700 0.39010600 0.71912200
C -3.77633900 -1.74221400 1.78631400
C -5.84926600 0.15565900 0.50469200
C 1.38652400 -1.26936000 0.08364500
Si 3.04488100 -1.94275600 -0.45924900
C 2.75835700 -3.48171500 -1.51358200
P -0.14766700 -1.61085900 -0.24308000
C 3.88849100 -0.62355700 -1.50665300
C 4.10832000 -2.42829600 1.02108400
H -4.07761400 1.68863600 -1.40129600
H -2.43472300 3.28588100 -2.08190500
H -0.16523800 3.30947600 -1.36173200
H -6.64965200 -0.56537000 0.68304700
H -5.79920700 0.82626400 1.36378900
H -6.12536800 0.74755700 -0.36921300
H -4.56799100 -2.46647100 1.98895000
H -2.84545400 -2.29692000 1.65812100
H -3.66971600 -1.10481600 2.66514500
H -5.09014900 -2.63617100 -1.10493200
H -4.56284400 -1.31077500 -2.14831000
H -3.36924000 -2.38731000 -1.42071800
H 3.21061200 0.07089600 2.61566200
H 4.74637100 1.82422200 1.69422100
H 4.07620000 0.29053100 -0.94648500
H 4.84656000 -0.99725800 -1.87463600
H 3.27128500 -0.37001000 -2.36946800
H 3.54237000 -3.03808600 1.72691600
H 4.95770800 -3.02059000 0.67363300
H 4.49844800 -1.56140600 1.55097700
H 3.71037000 -3.88402500 -1.86770500
H 2.25351000 -4.26059200 -0.94013200
H 2.14263300 -3.24813200 -2.38314600
H 0.83514000 0.14488500 1.89453800

i(3/5)
E(M06-2X/6-31+G*) = -2073.93761347
E+ZPE=-2073.566772
E+thermalE=-2073.538623
E+thermalH=-2073.537679
E+thermalG=-2073.625002
O -3.52086700 2.35575900 -0.22747100
C -2.21773600 2.51147100 0.19476900
C -1.21420400 1.56729300 -0.32575400
C -1.64724800 0.34721400 -1.10878800
C -3.04871200 0.47531200 -1.61536000
C -3.85829700 1.43309500 -1.17847500
O -2.01358600 3.41809600 0.96481500
C 0.12794200 1.71029600 -0.06451000
P 1.19145800 0.41038500 -0.75206200
C 2.78268900 0.61075400 0.04698800
Si 4.09890500 -0.73514800 -0.16249200
C 3.92584500 -1.97470400 1.24304400
C 0.76703700 2.79514700 0.65306000
C 2.08934700 2.82338900 0.96404400
C 3.04863400 1.77425100 0.69861500
C 3.82665200 -1.59485400 -1.81394000
C 5.80086400 0.06334400 -0.09911300
H 4.05570000 1.94435900 1.08122200
H 2.45775500 3.69549300 1.49858100
H 0.13414700 3.61373800 0.97409900
H 6.57440000 -0.69455800 -0.26813100

H 5.91215000 0.83620600 -0.86688800
H 6.00038100 0.52071100 0.87627200
H 4.59887300 -2.35494100 -1.97885800
H 2.85468300 -2.10089400 -1.85274300
H 3.86610800 -0.88498300 -2.64727400
H 4.69986300 -2.74776900 1.16912100
H 4.03196000 -1.48104200 2.21519100
H 2.95059300 -2.47303700 1.22422100
C -1.36436700 -0.94129200 -0.30348500
H -3.40349000 -0.21252400 -2.37511000
H -4.87783100 1.58279000 -1.51558400
P 0.19780900 -1.37992700 0.11445900
Si -2.77730900 -1.96525500 0.45224900
C -2.04478100 -3.44825400 1.35330800
C -3.66021400 -0.85778300 1.69102700
C -3.97944900 -2.61117300 -0.85251200
H -4.51869100 -1.38185600 2.12806200
H -2.98274000 -0.58037800 2.50618600
H -4.02911400 0.06517500 1.23184100
H -4.54441300 -3.45224100 -0.43267100
H -4.69917800 -1.84880300 -1.16434500
H -3.45467100 -2.97658500 -1.74221000
H -2.85764700 -4.03093200 1.80360000
H -1.49548900 -4.11218900 0.67670600
H -1.36630800 -3.15003100 2.15950300
H -0.97677800 0.28116800 -1.98960000

E(M06-2X/cc-pvtz PCM=toluene T=383 K) =
-2074.36819873
E+ZPE=-2074.000366
E+thermalE=-2073.956613
E+thermalH=-2073.955400
E+thermalG=-2074.085151
C -3.03908400 0.48268700 -1.61177400
C -3.84409600 1.43564600 -1.18122800
O -3.50693800 2.35814800 -0.22950700
C -2.21190100 2.50314200 0.20428200
C -1.21234300 1.56547800 -0.31677800
C -1.64292500 0.35267200 -1.10444600
O -2.01615200 3.39705100 0.98526200
C 0.12488600 1.70905400 -0.06077500
P 1.18471800 0.41379400 -0.74390900
P 0.19479700 -1.37601200 0.11031600
C -1.36122500 -0.93533100 -0.30464600
Si -2.76444500 -1.96773500 0.45049600
C -3.65540200 -0.86565800 1.67953800
C 0.77041700 2.79092000 0.64354000
C 2.08755500 2.81948500 0.94725600
C 3.04249400 1.77280700 0.68446900
C 2.77564700 0.61437200 0.03872900
Si 4.08561200 -0.73650000 -0.16213200
C 3.78996900 -1.61695500 -1.79096600
C 5.78079400 0.05964700 -0.12694000
C 3.91459300 -1.94373500 1.26307600
C -3.95526500 -2.61713800 -0.85208000
C -2.01846300 -3.43621500 1.34938000
H 4.04639400 1.94246100 1.06252000
H 2.45781100 3.69219100 1.47038600
H 0.14600100 3.61283800 0.95678100
H 6.54812300 -0.70137900 -0.27742000
H 5.88406500 0.80811100 -0.91280600
H 5.97720300 0.54035500 0.83211800
H 4.54818600 -2.38618100 -1.94512300
H 2.81373000 -2.10519900 -1.80881600
H 3.83346700 -0.92128500 -2.62972100
H 4.66778700 -2.72963700 1.18288500
H 4.05260100 -1.43553000 2.21806400
H 2.93182400 -2.41634300 1.26971000
H -3.39403000 -0.20369100 -2.36582000
H -4.85815100 1.58278300 -1.52194500
H -4.48905500 -1.40546700 2.13257100
H -2.97568700 -0.55930800 2.47563800
H -4.05246000 0.03247300 1.20644200
H -4.53998900 -3.43016600 -0.41716700
H -4.64803700 -1.84920700 -1.19173700
H -3.42364300 -3.01404100 -1.71769100
H -2.82272300 -4.03002100 1.78815100
H -1.45587400 -4.08129900 0.67339900
H -1.35354300 -3.12525000 2.15541400
H -0.97224600 0.28849900 -1.97888300

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) =
-2074.40620427
E+ZPE=-2074.036649
E+thermalE=-2073.993483
E+thermalH=-2073.992270
E+thermalG=-2074.120047
C 3.01256000 0.49730600 1.64214300
C 3.81486800 1.46990700 1.24308000
O 3.49165000 2.38964300 0.28345800
C 2.20906200 2.51170900 -0.19553400
C 1.20718900 1.56474800 0.30105200
C 1.63399600 0.34773900 1.08987000
O 2.02639600 3.40108400 -0.98912300
C -0.13201900 1.69822600 0.03276300
P -1.18197300 0.39059200 0.71454200
P -0.17217600 -1.38411900 -0.15803400
C 1.37986600 -0.93860800 0.27453200
Si 2.80577700 -1.96390600 -0.45072300
C 3.72990000 -0.84800500 -1.64348100
C -0.77623400 2.77378800 -0.68410900
C -2.09557100 2.79613900 -0.98717500
C -3.05148500 1.75294100 -0.70599200
C -2.78450200 0.59241300 -0.05698800
Si -4.11729000 -0.73569100 0.17869100
C -3.89677300 -1.52864500 1.86475500
C -5.80571600 0.07050600 0.04885300
C -3.91948000 -2.02332100 -1.17206000
C 3.95520800 -2.61153400 0.88945000
C 2.10541100 -3.43542800 -1.38411000
H -4.05969500 1.92871300 -1.07403900
H -2.46986300 3.66286100 -1.52247800
H -0.14794700 3.59060100 -1.01186400
H -6.58496700 -0.68102200 0.20931300
H -5.93264600 0.85446500 0.80052200
H -5.97427600 0.51165500 -0.93760900
H -4.66991400 -2.28551300 2.02924600
H -2.92533600 -2.02365500 1.95779200
H -3.97260700 -0.78647200 2.66447500
H -4.69510500 -2.79080500 -1.08439500
H -4.00705500 -1.56473200 -2.16119200
H -2.94726200 -2.52037400 -1.11621600
H 3.35466600 -0.18753300 2.40628000
H 4.81508800 1.63764600 1.61893700
H 4.56357600 -1.38954700 -2.10190100
H 3.06608100 -0.50766600 -2.44320200
H 4.13771100 0.03380900 -1.14376600
H 4.56547700 -3.42160800 0.47713700
H 4.63306500 -1.83925400 1.25820800
H 3.39661000 -3.01592300 1.73840100
H 2.93464700 -4.00895600 -1.81125300
H 1.53978300 -4.10556600 -0.73059400
H 1.45264700 -3.13190900 -2.20685500
H 0.93868500 0.27296600 1.94890600

E(B3LYP/cc-pVTZ PCM=toluene T=383 K) =
-2074.90092207
E+ZPE= -2074.535773
E+thermalE= -2074.491878
E+thermalH= -2074.490665
E+thermalG= -2074.620510
C -3.00770100 0.51150000 -1.65182400
C -3.81762900 1.47547600 -1.24719500
O -3.49980900 2.39072600 -0.27771800
C -2.19992900 2.52589700 0.19231700
C -1.20477100 1.57866500 -0.29816400
C -1.63475200 0.36168800 -1.09007700
O -2.02188100 3.43288100 0.97299000
C 0.14198000 1.70649000 -0.02619500
P 1.19331300 0.38656600 -0.69991700
P 0.16615900 -1.40731100 0.14938200
C -1.39101300 -0.93728600 -0.27618900
Si -2.83152800 -1.95615700 0.44789100
C -3.77219000 -0.83327500 1.63460800
C 0.79064800 2.76598200 0.69155700
C 2.11980600 2.79413500 0.98130800
C 3.07395200 1.76602400 0.68410500
C 2.80686200 0.59681000 0.04003300
Si 4.13521200 -0.74389800 -0.17787300
C 3.82797400 -1.67868500 -1.78440600
C 5.83320800 0.07046400 -0.20939900
C 4.01205000 -1.92149900 1.28888700
C -3.97799600 -2.61454700 -0.90129300
C -2.15439100 -3.43590000 1.40167500
H 4.08472600 1.94930400 1.03378700
H 2.49194500 3.65728900 1.51905600
H 0.16644700 3.57528000 1.03640600
H 6.60367400 -0.68928000 -0.35544900
H 5.91168000 0.79255400 -1.02322400
H 6.05413600 0.58654600 0.72601100
H 4.60070700 -2.43648000 -1.92800400
H 2.86295400 -2.18798800 -1.77774200
H 3.84791300 -1.00790800 -2.64454100
H 4.76463200 -2.70918000 1.21320300
H 4.17272800 -1.38766100 2.22689100
H 3.03080900 -2.39529900 1.33615900
H -3.33963200 -0.17064100 -2.41874400
H -4.81747600 1.63673300 -1.62185000
H -4.62932600 -1.36645300 2.05174300
H -3.12981200 -0.52561500 2.46077300
H -4.14084400 0.06440100 1.14050200
H -4.60835500 -3.39907700 -0.47675400
H -4.62961400 -1.83875500 -1.29912000
H -3.41455400 -3.05034400 -1.72767300
H -2.99495200 -3.99977000 1.81297300
H -1.58387700 -4.11020600 0.76148900
H -1.51630500 -3.13513600 2.23301400
H -0.93439800 0.27916500 -1.94180900

ENE

E(M06-2X/6-31+G*) = -2862.46189581
E+ZPE=-2861.975738
E+thermalE=-2861.937220
E+thermalH=-2861.936276
E+thermalG=-2862.046662
C 2.74487900 -0.81476000 -2.01781400
C 1.47126700 -0.63597100 -1.35115500
C 0.77387700 -1.81341700 -1.03314200
C 1.32721900 -3.12959700 -1.36629200
O 2.56921600 -3.16456500 -1.97592800
C 3.22552700 -2.03914400 -2.28343200
C 1.10317500 0.71920400 -0.92950600
Si 2.26807900 2.19294200 -1.30671000
C 3.91240700 1.98416100 -0.40231200
C -0.54758900 -1.81469800 -0.41591500
P -1.56678500 -0.44838200 -0.69424500
C -3.12129500 -0.64240100 0.00784500
Si -4.45088100 0.70343900 -0.18448900
C -4.53496000 1.16092100 -2.00527500
O 0.81309200 -4.20556800 -1.16446800
P -0.60360100 1.42108300 -0.96930200
C -1.12677600 -2.88059400 0.30080100
C -2.42930200 -2.89525900 0.79080400
C -3.37011300 -1.86812200 0.62515400
C -6.07972200 -0.02875300 0.40323700
C -4.00688100 2.21569600 0.83664000
C 2.51224600 2.47285600 -3.15874200
C 1.50935600 3.78170400 -0.62814300
P -0.50704800 1.61841700 1.74533100
C 0.87532900 0.80674800 1.78332600
Si 2.09584700 -0.10679900 2.84818200
C 3.17150200 -1.19535000 1.74543100
C 3.16720800 1.11488900 3.80125300
C 1.13117300 -1.19848000 4.04130600
H 1.22523100 0.63893700 0.41236600
H -4.36594800 -2.03675900 1.03309600
H -2.74228800 -3.78136900 1.33517200
H -0.50895600 -3.75063800 0.48767300
H -6.88052900 0.70579600 0.26039900
H -6.35111300 -0.92820600 -0.15995700
H -6.05555900 -0.28322000 1.46859300
H -5.28705000 1.94015100 -2.17352800
H -3.57273200 1.54850700 -2.36135900
H -4.79939300 0.29455300 -2.62094100
H -4.83475700 2.93445000 0.80920600
H -3.81375300 1.95735800 1.88291600
H -3.11594300 2.72041000 0.44608200
H 3.34219000 0.03340800 -2.31632300
H 4.17425400 -2.24041100 -2.76789800
H 4.54405300 2.86139200 -0.58856900
H 3.72586900 1.93766400 0.67762900
H 4.48470700 1.09461100 -0.68088100
H 1.53473700 2.58594800 -3.64188700
H 3.06953500 3.40434700 -3.31620800
H 3.04655800 1.67318400 -3.67985700
H 2.23258800 4.59106300 -0.79023600
H 0.57971100 4.07018000 -1.13012400
H 1.31628200 3.72034300 0.44762000
H 3.74336300 1.76132900 3.13056900
H 2.54450000 1.75675500 4.43332200
H 3.87642900 0.58322400 4.44657200
H 0.50799000 -0.59030700 4.70559400
H 0.47088300 -1.87361800 3.48522200
H 1.80248200 -1.80762200 4.65798300
H 3.64237200 -0.61730500 0.94157100
H 2.56631900 -1.98146200 1.27728200
H 3.96721500 -1.68035200 2.32313800

E(M06-2X/cc-pvtz PCM=toluene T=383 K) =
-2863.02450142
E+ZPE=-2862.543067
E+thermalE=-2862.483288
E+thermalH=-2862.482075
E+thermalG=-2862.647618
C -3.16483900 2.39848800 -1.98347700
C -2.71622500 1.14701700 -1.87347300
C -1.44921100 0.85669700 -1.24312500
C -0.72769800 1.96199100 -0.78171800

C -1.23342100 3.31725800 -0.97096500
O -2.47586300 3.45870900 -1.55080400
C -1.10744800 -0.54676000 -1.01938900
P 0.57766200 -1.26334600 -1.15854700
P 1.56479100 0.49993600 -0.55829200
C 3.13271600 0.59844200 0.11185300
C 3.40292500 1.73935100 0.86055200
C 2.48481300 2.74719700 1.15378900
C 1.18595400 2.81024500 0.67253500
C 0.58780600 1.85609200 -0.16243600
O -0.68078700 4.34745000 -0.67526400
Si -2.30177400 -1.92756900 -1.58998700
C -1.58632200 -3.60154000 -1.12225100
C -3.94446000 -1.79586900 -0.68156400
C -2.52927500 -1.95117000 -3.45818200
Si 4.44414500 -0.72292900 -0.26313300
C 3.94743100 -2.36053500 0.49359200
C 4.55714900 -0.88756900 -2.12507700
C 6.05699500 -0.11981400 0.47082000
P 0.48841800 -1.83616800 1.49094900
C -0.89017500 -1.04560200 1.65232500
Si -2.13073200 -0.33253500 2.83266500
C -1.20776200 0.50437200 4.23732800
C -3.16307500 0.94466500 1.91850700
C -3.22826000 -1.69825500 3.50877000
H -1.21890900 -0.66759900 0.32376400
H 4.40221200 1.84813600 1.26827900
H 2.81416500 3.55611900 1.79141400
H 0.58936700 3.66273800 0.95725400
H 6.84441000 -0.84499200 0.26045600
H 6.35981700 0.83751200 0.04531400
H 5.98712700 -0.01020100 1.55380900
H 5.29561300 -1.64298400 -2.39772300
H 3.59633600 -1.19252200 -2.54533500
H 4.84566900 0.05750300 -2.58584200
H 4.74261400 -3.09089200 0.33216900
H 3.77706000 -2.27030200 1.56644000
H 3.03663600 -2.75225200 0.03845500
H -3.33696800 0.36465700 -2.27047600
H -4.10842600 2.67648100 -2.42936300
H -4.57506600 -2.64103400 -0.96491100
H -3.76507400 -1.86401900 0.39325300
H -4.50168300 -0.88019400 -0.87169600
H -1.55765100 -2.09117700 -3.93552600
H -3.16107500 -2.79760700 -3.73477900
H -2.97439600 -1.04815600 -3.87231800
H -2.31801700 -4.36096600 -1.40781400
H -0.65625700 -3.83081300 -1.64262800
H -1.41436300 -3.68702200 -0.04957900
H -3.77111000 -2.21147700 2.71492500
H -2.62749400 -2.43770300 4.03921000
H -3.95945000 -1.28548400 4.20604300
H -0.61963600 -0.22442000 4.79579700
H -0.52715300 1.26109100 3.84487700
H -1.90260000 0.98970400 4.92487600
H -3.60833100 0.52317800 1.01531400
H -2.53819700 1.78861600 1.61879700
H -3.96770000 1.32473600 2.55032900

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) =
-2863.09122944
E+ZPE=-2862.606480
E+thermalE=-2862.548000
E+thermalH=-2862.546787
E+thermalG=-2862.707841
C 2.74166700 -0.70310700 -2.11598500
C 1.49898000 -0.54949800 -1.39980500
C 0.80396200 -1.73334100 -1.11461600
C 1.33665900 -3.03059400 -1.51328500
O 2.55330400 -3.04497100 -2.16761400
C 3.20303100 -1.91201100 -2.45232600
C 1.14460700 0.77557900 -0.88476500
Si 2.34490100 2.24799700 -1.12400700
C 3.97501100 1.87872400 -0.25946100
C -0.50397700 -1.74181100 -0.47453700
P -1.55524000 -0.41078900 -0.79389000
C -3.08332700 -0.60536200 -0.02689600
Si -4.46200100 0.69303200 -0.22864300
C -4.63010400 1.05015600 -2.06127700
O 0.83026900 -4.11271900 -1.33541500
P -0.56065100 1.47491800 -0.91660800
C -1.04340300 -2.79840800 0.27560500
C -2.32965000 -2.82110000 0.79028400
C -3.29210900 -1.81764000 0.61905200
C -6.03961400 -0.04352200 0.46295200
C -4.02077200 2.26203700 0.69226700
C 2.59370300 2.69713400 -2.93600600
C 1.63828900 3.77715800 -0.28842600
P -0.55323300 1.52829800 1.72728900
C 0.80368000 0.68606400 1.80622300
Si 1.97298100 -0.27941100 2.86591800
C 3.04702000 -1.35952600 1.76158500
C 3.05550600 0.89490700 3.85651100
C 0.97347300 -1.38336000 4.01237800
H 1.20896800 0.60079700 0.41365800
H -4.27006200 -1.99875200 1.05611300
H -2.61723800 -3.69494100 1.36417900
H -0.40603900 -3.64894200 0.47432600
H -6.85945300 0.66790200 0.32454300
H -6.31516800 -0.97261000 -0.04365000
H -5.95666000 -0.24486800 1.53482200
H -5.42135300 1.78536800 -2.23680000
H -3.70153200 1.46018000 -2.47127300
H -4.87626400 0.14329400 -2.62050900
H -4.84546000 2.97743700 0.60980600
H -3.84076300 2.06966600 1.75286000
H -3.12686200 2.73749900 0.27923600
H 3.33213100 0.15060800 -2.40313300
H 4.13038000 -2.09301000 -2.97905800
H 4.64336100 2.74122700 -0.34731500
H 3.78951700 1.71100300 0.80571600
H 4.50239400 1.00456400 -0.64713300
H 1.62069500 2.84944600 -3.41303500
H 3.14702200 3.63962700 -3.00268200
H 3.13642100 1.95307800 -3.52311400
H 2.36618100 4.58715600 -0.40663500
H 0.69763400 4.11665600 -0.73043500
H 1.48144700 3.62150600 0.78112200
H 3.64573300 1.54409800 3.20331100
H 2.44328700 1.53240900 4.50032600
H 3.75052000 0.33423100 4.48979400
H 0.34492300 -0.78497100 4.67766500
H 0.31962100 -2.03830900 3.42869000
H 1.62700100 -2.01148400 4.62639900
H 3.54314600 -0.77054600 0.98465200
H 2.43747800 -2.11950500 1.26344500
H 3.81915300 -1.87220700 2.34390600

E(B3LYP/cc-pVTZ PCM=toluene T=383 K) =
-2863.72769710
E+ZPE= -2863.249758
E+thermalE= -2863.189517
E+thermalH= -2863.188304
E+thermalG= -2863.356116

O -2.50335100 3.18598400 -2.03305500
C -3.14138400 2.06489700 -2.39561100
C -2.68036000 0.84085300 -2.11103600
C -1.45616300 0.64601500 -1.38109300
C -0.75309600 1.81788700 -1.02298900
C -1.28792100 3.13544000 -1.34782100
C -1.12533800 -0.70591200 -0.93245600
Si -2.31270500 -2.17332500 -1.31160700
C -2.43988900 -2.51325800 -3.16652800
C 0.55154600 1.79324100 -0.38671000
C 1.11287700 2.81827800 0.39278100
C 2.40704600 2.81928300 0.89198900
C 3.36219800 1.81513900 0.68718500
C 3.14090300 0.61681400 0.01846900
Si 4.49674100 -0.70782000 -0.18854100
C 6.13745800 0.06619700 0.31307800
O -0.79920100 4.21408200 -1.09754900
P 0.58928000 -1.41924200 -0.95895200
P 1.59814300 0.44832700 -0.74228200
C -1.65875800 -3.75428300 -0.51307100
C -4.00935500 -1.87276600 -0.53411900
C 4.11370600 -2.18949800 0.90418700
C 4.53714000 -1.23081400 -1.99643400
P 0.48875400 -1.60287600 1.74166800
C -0.89250200 -0.78064900 1.78251200
Si -2.12586800 0.09958400 2.85529700
C -3.23438200 -1.16364700 3.71521200
C -1.19188900 1.13253400 4.12798800
C -3.17564900 1.24644500 1.78471600
H -1.23078300 -0.61806500 0.39338800
H 4.34458400 1.98454200 1.11231600
H 2.70483700 3.67419700 1.48448000
H 0.48654800 3.66416500 0.62579500
H 6.94209300 -0.65303300 0.14851200
H 6.35826500 0.95698500 -0.27657500
H 6.15241500 0.34131800 1.36874000
H 5.29898200 -1.99769000 -2.14938700
H 3.57908800 -1.64701800 -2.31283400
H 4.77040700 -0.38567000 -2.64560000
H 4.93235900 -2.91016700 0.84664100
H 3.99142400 -1.89368800 1.94639100
H 3.19994600 -2.69320900 0.58932000
H -3.26175800 0.00508800 -2.45211700
H -4.05519000 2.26663700 -2.93474400
H -4.65203300 -2.73236400 -0.73644700
H -3.90576800 -1.78739300 0.54820000
H -4.52042500 -0.98011000 -0.89059700
H -1.44888200 -2.73808300 -3.56477200
H -3.07457300 -3.38565100 -3.33752800
H -2.84670300 -1.68483900 -3.74523000
H -2.38249900 -4.54758100 -0.71573700
H -0.69864000 -4.07702300 -0.91580200
H -1.56294500 -3.65348400 0.56687600
H -3.76537000 -1.78475500 2.99231000
H -2.64298200 -1.82227200 4.35269700
H -3.97833500 -0.66133000 4.33747100
H -0.59212300 0.49676200 4.78056600
H -0.51992600 1.83180100 3.62778300
H -1.88384400 1.70783900 4.74706600
H -3.68454300 0.69909500 0.99095100
H -2.55361000 2.00957600 1.31493800
H -3.93375200 1.75043400 2.38765000

i(5/3)
E(M06-2X/6-31+G*) = -2862.51236208
E+ZPE=-2862.023097
E+thermalE=-2861.983558
E+thermalH=-2861.982614
E+thermalG=-2862.096524
O 2.86177800 -0.19402000 -3.21839700
C 1.75944200 -0.86508700 -2.73353300
C 0.75997300 -0.08452400 -1.96520700
C 1.22703300 1.16259400 -1.31953700
C 2.35750100 1.78642300 -2.01075000
C 3.07491800 1.11164300 -2.91133600
O 1.70249800 -2.04050000 -2.99810600
C -0.53504200 -0.55652600 -1.85771600
C -1.03501200 -1.80475700 -2.40380100
C -2.27306600 -2.30074900 -2.14133500
C -3.26361600 -1.71413300 -1.26150500
C -3.13575900 -0.50825300 -0.65405100
Si -4.45292500 0.15589900 0.53626700
C -4.65941500 1.99892500 0.22959300
C 0.76183000 1.70294300 -0.14489000
P -0.73633900 1.11222700 0.72826200
P -0.16157000 -0.91527500 1.57990800
C 1.47122400 -1.05416700 1.27643400
Si 2.47333400 -2.58873300 1.71358800
C 3.22802300 -3.21691500 0.10957000
P -1.76289900 0.55798800 -1.12930100
C -6.06217400 -0.76601200 0.21571800
C -3.89483700 -0.15049000 2.30712200
Si 1.70112200 3.03041400 0.83746900
C 3.57364500 2.76404400 0.76867900
C 1.25165500 4.74899800 0.20960400
C 1.18587500 2.87268300 2.64399900
C 3.83476000 -2.08711700 2.91610500
C 1.35926300 -3.88825200 2.49116200
H 2.00856500 -0.25767800 0.75048200
H -4.15462600 -2.31454000 -1.07626700
H -2.52868000 -3.25618100 -2.59352500
H -0.36211900 -2.39900500 -3.00847500
H -6.86126100 -0.34100000 0.83408300
H -6.37156400 -0.68833800 -0.83210600
H -5.98253000 -1.82829300 0.47179400
H -5.42864000 2.41378600 0.89102000
H -3.72530600 2.53739300 0.42963600
H -4.95288600 2.20541900 -0.80525700
H -4.70550200 0.09463100 3.00400100
H -3.62184000 -1.20035500 2.46039700
H -3.02953500 0.46596300 2.57369800
H 2.61621000 2.81905400 -1.81116900
H 3.91470700 1.51549900 -3.46450400
H 4.02452100 3.12441000 1.70068300
H 3.82282500 1.70144000 0.66721600
H 4.05535200 3.29652300 -0.05733500
H 1.77167000 5.52214800 0.78730500
H 1.51279500 4.88409400 -0.84588000
H 0.17380900 4.91934700 0.30793000
H 1.79951500 3.55231800 3.24755800
H 0.13616000 3.13092700 2.81301800
H 1.35163300 1.85642900 3.02327600
H 4.47044700 -1.30502900 2.48549400
H 3.41419300 -1.70180100 3.85118500
H 4.47547000 -2.94255000 3.15949500
H 0.90388700 -3.52478500 3.41899600
H 0.55071000 -4.17829000 1.81132200
H 1.93614900 -4.78884600 2.73099100
H 3.89865500 -2.46851300 -0.32894800
H 2.45463900 -3.43641400 -0.63456000
H 3.81171200 -4.12944200 0.27894000

E(M06-2X/cc-pvtz PCM=toluene T=383 K) = -2863.07315679

E+ZPE=-2862.588096
E+thermalE=-2862.527203
E+thermalH=-2862.525990
E+thermalG=-2862.696805
C -3.07670600 1.13359500 2.88952800
O -2.85238800 -0.16472400 3.21459000
C -1.74957100 -0.83185100 2.73976000
C -0.76203800 -0.05827200 1.95988100
C -1.23705500 1.17391500 1.30145400
C -2.37018500 1.79520100 1.98236100
O -1.68825600 -1.99934800 3.01800800
C 0.53395300 -0.51402100 1.86606100
P 1.74989800 0.58437400 1.11258800
P 0.71748300 1.11217300 -0.74178600
P 0.17562300 -0.93664500 -1.53716500
C -1.45649600 -1.07771000 -1.27044800
Si -2.42644700 -2.63173900 -1.69069000
C -1.27536100 -3.93114000 -2.39586000
C -0.77838200 1.70153600 0.12708800
Si -1.73214300 3.00375400 -0.87183900
C -1.20297100 2.82777700 -2.66635600
C 1.05062000 -1.73582500 2.44193900
C 2.28617500 -2.22506400 2.19098000
C 3.26620700 -1.65723800 1.29518500
C 3.12954300 -0.47282600 0.66380000
Si 4.43720400 0.17331700 -0.54331900
C 3.86611100 -0.16504700 -2.29771500
C 4.63146800 2.01578400 -0.26547500
C 6.04026500 -0.74040700 -0.21459200
C -3.21237100 -3.22840700 -0.09609100
C -3.75594500 -2.18333700 -2.93865800
C -3.59219100 2.70244600 -0.80921200
C -1.31591500 4.73052400 -0.26458700
H -2.00711400 -0.27210700 -0.78572500
H 4.15794400 -2.25221600 1.12396000
H 2.55195200 -3.15937100 2.66991500
H 0.39224500 -2.31459100 3.06873200
H 6.82691900 -0.34468900 -0.85886000
H 6.35951800 -0.62537800 0.82149900
H 5.94359200 -1.80533000 -0.42915300
H 5.37716400 2.42646900 -0.94773300
H 3.68834000 2.53470700 -0.44836100
H 4.94564900 2.23115000 0.75627100
H 4.65864100 0.10078900 -2.99997700
H 3.62930300 -1.22087900 -2.43405100
H 2.98145000 0.41863700 -2.55412300
H -2.63750200 2.81803300 1.76998400
H -3.91487000 1.54117000 3.43418900
H -4.04363900 3.07858200 -1.72881300
H -3.81619400 1.63688800 -0.73625800
H -4.07701900 3.20224500 0.02807900
H -1.84011900 5.48070900 -0.85917000
H -1.59268800 4.87278400 0.78064800
H -0.24411900 4.91231000 -0.35457500
H -1.83315600 3.47312100 -3.28124300
H -0.16499800 3.11499200 -2.82920800
H -1.33336400 1.80244900 -3.02028300
H -4.41053600 -1.40463000 -2.54480400
H -3.31312900 -1.81717000 -3.86544800
H -4.37110900 -3.05308100 -3.17516200
H -0.79571200 -3.58002700 -3.31042500
H -0.49307300 -4.18876800 -1.68074000
H -1.83207500 -4.83915500 -2.63237500
H -3.89975900 -2.47979300 0.30181000
H -2.45342400 -3.41711500 0.66422100
H -3.77455200 -4.14913600 -0.26053800

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) =
-2863.14311929
E+ZPE=-2862.655194
E+thermalE=-2862.595172
E+thermalH=-2862.593959
E+thermalG=-2862.763448
C -2.93010100 0.99554000 3.03618300
O -2.71210900 -0.31860800 3.29324300
C -1.62351100 -0.97160000 2.76314500
C -0.65277900 -0.17349900 1.98883800
C -1.13708500 1.09038100 1.39266700
C -2.23775900 1.69382400 2.14220500
O -1.56218200 -2.15117000 2.99751100
C 0.63959200 -0.63688100 1.83227600
P 1.83122200 0.47786500 1.06367200
P 0.73128900 1.06088300 -0.72996000
P 0.06231200 -0.90849000 -1.62983100
C -1.55750000 -0.98894300 -1.27378700
Si -2.71195700 -2.38862500 -1.75850100
C -1.77018600 -3.76861100 -2.60866100
C -0.71257600 1.66091400 0.22011800
Si -1.68469900 3.02375800 -0.68001700
C -1.02471100 3.17719400 -2.43265600
C 1.16646100 -1.88026000 2.35168100
C 2.39765400 -2.36099700 2.05543300
C 3.36199800 -1.76143500 1.16269500
C 3.20928200 -0.56022100 0.55898200
Si 4.50888600 0.12305300 -0.64338300
C 3.91811200 -0.16581300 -2.40067000
C 4.72079400 1.95898700 -0.32492600
C 6.12164100 -0.79167000 -0.35895900
C -3.50897900 -2.99227500 -0.17060100
C -4.01869800 -1.67826000 -2.90759500
C -3.49983600 2.54768900 -0.82702400
C -1.48333800 4.68577200 0.17665700
H -2.01744700 -0.19399800 -0.68364400
H 4.25619400 -2.34789100 0.96670900
H 2.67327400 -3.31426100 2.49540700
H 0.51650200 -2.48408200 2.96756800
H 6.89193000 -0.39279300 -1.02620800
H 6.47366600 -0.67583300 0.66981100
H 6.02645200 -1.86035300 -0.57125000
H 5.47450000 2.37516900 -1.00042400
H 3.78575000 2.50093900 -0.49694200
H 5.04083000 2.15235300 0.70270000
H 4.69475500 0.13562800 -3.11093800
H 3.69251900 -1.22197800 -2.57222900
H 3.01931400 0.41488700 -2.62478700
H -2.50155000 2.72988500 1.98997400
H -3.74906900 1.38543200 3.62483600
H -4.03921000 3.31929500 -1.38588600
H -3.59774400 1.60891700 -1.38150400
H -3.99605100 2.41986100 0.13686400
H -1.94648700 5.47353500 -0.42619200
H -1.93763000 4.71950000 1.17017900
H -0.42214400 4.92610800 0.28807400
H -1.66661700 3.87100200 -2.98574800
H -0.00285300 3.56169900 -2.46811900
H -1.04595700 2.21936400 -2.96234600
H -4.55635100 -0.85518000 -2.42692400
H -3.56587100 -1.29359300 -3.82595800
H -4.75266300 -2.44136000 -3.18493100
H -1.27719600 -3.41530100 -3.51894800
H -1.00422200 -4.18856600 -1.95056500
H -2.45385700 -4.57594000 -2.88886500
H -4.06047600 -2.18291900 0.31794400
H -2.75812200 -3.35338000 0.53754200

H -4.21426900 -3.80540500 -0.36885000

E(B3LYP/cc-pVTZ PCM=toluene T=383 K) = -2863.77640658
E+ZPE= -2863.293929
E+thermalE= -2863.233162
E+thermalH= -2863.231949
E+thermalG= -2863.401468
C -2.27171800 1.75231700 2.09232800
C -2.97685400 1.08385900 3.00192800
O -2.77670700 -0.22933300 3.28420200
C -1.69667900 -0.91515600 2.74406400
C -0.71948900 -0.14463200 1.95710400
C -1.17672900 1.12916100 1.36292000
O -1.66752800 -2.09689400 2.99469400
C 0.56861900 -0.64459900 1.78894300
C 1.05024900 -1.92017900 2.24054900
C 2.29128900 -2.41152000 1.97122500
C 3.30345200 -1.78769300 1.16701800
C 3.19249700 -0.56231200 0.59252900
Si 4.55033400 0.14562200 -0.53532500
C 6.15699800 -0.77822500 -0.19859500
C -0.73552500 1.69565500 0.18466200
Si -1.71362800 3.04054900 -0.74631600
C -1.52056800 4.72546700 0.08762200
P 1.79677700 0.46733100 1.06105400
P 0.72937400 1.12579900 -0.75000300
P 0.08827300 -0.85148400 -1.72317500
C -1.51922200 -1.02233900 -1.30747100
Si -2.60970700 -2.50234800 -1.70987400
C -4.01165000 -1.92558200 -2.83508100
C -1.61522500 -3.86381800 -2.54723500
C -3.30768700 -3.09287200 -0.06141100
C -1.05822900 3.18920800 -2.51061200
C -3.53652700 2.56292700 -0.89576300
C 4.03299000 -0.10960600 -2.32937500
C 4.75182200 1.98282500 -0.17535000
H -1.99716800 -0.26054500 -0.69566500
H 4.20148400 -2.37277300 1.00049500
H 2.52409600 -3.39479700 2.36123900
H 0.36368600 -2.54868000 2.78249500
H 6.95898200 -0.34995800 -0.80312900
H 6.44892900 -0.70458400 0.84982400
H 6.07864200 -1.83490200 -0.45849500
H 5.53110400 2.40774800 -0.81108200
H 3.82651900 2.52624000 -0.37380400
H 5.03019900 2.15659600 0.86498900
H 4.83340300 0.21404200 -2.99828400
H 3.82452700 -1.16085500 -2.53200400
H 3.13990500 0.46562600 -2.57361900
H -2.52633600 2.78305700 1.91385800
H -3.79051800 1.49858800 3.57742100
H -4.06747200 3.32492600 -1.47048700
H -3.63261300 1.61687100 -1.43197400
H -4.03668000 2.45457200 0.06482200
H -2.02508800 5.49179800 -0.50502200
H -1.93507300 4.75761600 1.09534800
H -0.46448700 4.99187700 0.15425000
H -1.70334800 3.88579900 -3.05152700
H -0.03928800 3.57231900 -2.55398900
H -1.08686400 2.23622800 -3.04163100
H -4.57130100 -1.10909800 -2.37493700
H -3.62552500 -1.57291900 -3.79272800
H -4.70909300 -2.74303700 -3.02983600
H -1.17949800 -3.52036200 -3.48678000
H -0.80276500 -4.20722100 -1.90512200
H -2.25626700 -4.71997100 -2.76698400
H -3.93516600 -2.32216500 0.39027100
H -2.51006200 -3.31918500 0.64706500
H -3.91821400 -3.98857400 -0.19306200

CA4
E(M06-2X/6-31+G*) = -2862.49694986
E+ZPE=-2862.007160
E+thermalE=-2861.969259
E+thermalH=-2861.968315
E+thermalG=-2862.075271
C 2.03688600 -1.79654200 -2.03855900
C 1.13439600 -0.76087800 -1.47837100
C 1.68536400 0.51402200 -1.11462200
C 3.05521300 0.76074900 -1.54594500
C 3.77147600 -0.17434700 -2.17534400
O 3.30564700 -1.41799400 -2.41080800
C -0.22605800 -1.09553300 -1.25376900
C -0.82505200 -2.40790300 -1.44447100
C -2.14427200 -2.68276200 -1.25024300
C -3.14486000 -1.74539200 -0.79994900
C -2.94461800 -0.40464500 -0.68699400
Si -4.29713400 0.74118200 -0.02003100
C -5.93822800 -0.17628600 -0.08679900
C 1.09643900 1.47675100 -0.25073700
Si 2.10675800 2.97296600 0.40349000
C 2.32089300 4.20471800 -1.01098500
O 1.77634800 -2.96219600 -2.22337600
P -1.41578300 0.26638000 -1.35849900
P -0.69938700 1.70521100 0.13416800
P 0.35331100 0.48432400 1.65245900
C -0.04364300 -1.13973400 1.32373000
Si 1.13248400 -2.47600200 1.92350200
C 2.89238900 -1.83055900 1.69301200
C 1.14502900 3.86894900 1.75351800
C 3.76316500 2.40708000 1.11823000
C -3.89802400 1.18231100 1.76756200
C -4.36085300 2.29084900 -1.08434500
C 0.84742900 -2.82410100 3.75747600
C 0.88235800 -4.07308500 0.96141600
H -1.06804900 -1.38798600 1.04438700
H -4.11161900 -2.16699300 -0.52321600
H -2.45981200 -3.71426100 -1.38638500
H -0.16923000 -3.22800700 -1.69754500
H -6.74717200 0.49359100 0.22674100
H -6.16659100 -0.52567200 -1.09953600
H -5.95228100 -1.04092700 0.58570600
H -5.14712700 2.96711500 -0.72954700
H -3.41352800 2.84169600 -1.05087400
H -4.57213600 2.04613900 -2.13092600
H -4.76113800 1.66978700 2.23643800
H -3.65974000 0.28508800 2.34969900
H -3.04809900 1.86871000 1.84450900
H 3.51712800 1.72644300 -1.39968700
H 4.77903400 -0.04353700 -2.55096800
H 3.76871500 1.32348600 1.28129900
H 4.60873200 2.65356800 0.46681200
H 3.93794300 2.89038300 2.08582600
H 1.33823800 4.53792200 -1.36416000
H 2.86553800 5.08919500 -0.65935800
H 2.85998600 3.79832700 -1.87249200
H 1.75590900 4.72059700 2.07942000
H 0.18757900 4.26612900 1.40174000
H 0.95857900 3.24134400 2.63063900
H 3.04481100 -1.43319000 0.68107600
H 3.11429900 -1.02474500 2.40299100
H 3.62642600 -2.62844900 1.85386900
H 0.96552200 -1.91016400 4.35043700

H -0.16373300 -3.20842300 3.93275200
H 1.56064900 -3.56814700 4.13198700
H 1.26456000 -3.99470200 -0.06172800
H -0.17845300 -4.34571400 0.91107600
H 1.41488200 -4.89181700 1.46023400

E(M06-2X/cc-pvtz PCM=toluene T=383 K) =
-2863.05774017
E+ZPE=-2862.572264
E+thermalE=-2862.513269
E+thermalH=-2862.512056
E+thermalG=-2862.674242
O 3.26622500 -1.43804900 -2.44016800
C 1.97884900 -1.78881100 -2.12729600
C 1.11942300 -0.77874500 -1.47769000
C 1.68017800 0.48090900 -1.10671900
C 3.05822500 0.70657900 -1.50709700
C 3.76221800 -0.22235200 -2.14356700
O 1.66954700 -2.91014600 -2.44003200
C -0.23704400 -1.11183100 -1.22909100
P -1.42707600 0.23450900 -1.32090100
P -0.69753800 1.70794800 0.12164400
P 0.36914400 0.51013600 1.63268100
C -0.01694800 -1.11859000 1.34654000
Si 1.17269300 -2.42489600 1.96192500
C 1.04712600 -3.99078800 0.93536800
C 1.09571000 1.45251000 -0.25397000
Si 2.10188100 2.96233500 0.37128000
C 3.73272000 2.40695400 1.13568700
C -0.82897800 -2.42460200 -1.36630500
C -2.14106300 -2.70006400 -1.16263000
C -3.14435900 -1.76081600 -0.74620900
C -2.95070800 -0.42313600 -0.65652800
Si -4.30522000 0.73310900 -0.01757000
C -4.32750900 2.27828300 -1.07900200
C -5.94327700 -0.16984500 -0.11979100
C -3.93177000 1.15683700 1.77265500
C 2.34924300 4.13971900 -1.07351300
C 1.12255200 3.90040400 1.66937700
C 2.90989900 -1.71207100 1.83106800
C 0.81260300 -2.85655600 3.75800300
H -1.03878900 -1.37227800 1.08532100
H -4.10919500 -2.17736400 -0.47324600
H -2.44711500 -3.73416600 -1.25851000
H -0.17310400 -3.24642800 -1.59041300
H -6.74914800 0.49632000 0.19207100
H -6.15208100 -0.50129400 -1.13741300
H -5.96250300 -1.04045900 0.53664900
H -5.10247800 2.96270900 -0.73039500
H -3.37343800 2.80656100 -1.03630000
H -4.53387800 2.03215100 -2.12118100
H -4.74053800 1.76083000 2.18799200
H -3.84630600 0.24757000 2.36931800
H -3.00457100 1.72051200 1.87949200
H 3.54624500 1.64564200 -1.31639400
H 4.78099200 -0.10572500 -2.47980200
H 3.73102500 1.32992400 1.30965900
H 4.58805500 2.64596500 0.50292900
H 3.87890100 2.90250600 2.09596400
H 1.37853300 4.47010900 -1.44681200
H 2.89675800 5.02275100 -0.73846200
H 2.89456800 3.69869700 -1.90699300
H 1.74306600 4.74070600 1.99020200
H 0.18915700 4.30570000 1.27988200
H 0.90047600 3.29647100 2.54847200
H 3.08670200 -1.30201400 0.83301100
H 3.06121600 -0.90889900 2.55458800
H 3.66004100 -2.48159900 2.01958200
H 0.87022100 -1.96554200 4.38466800
H -0.18816000 -3.27792700 3.86341400
H 1.52963200 -3.58868100 4.13422900
H 1.43319200 -3.84156400 -0.07347900
H 0.01416100 -4.33371500 0.85818800
H 1.63073900 -4.78240900 1.40938900

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) =
-2863.12283329
E+ZPE=-2862.635495
E+thermalE=-2862.576884
E+thermalH=-2862.575671
E+thermalG=-2862.736674
C 1.99974100 -1.78238300 -2.08278600
C 1.12536400 -0.75735500 -1.47883300
C 1.69339800 0.50180100 -1.11001800
C 3.04378500 0.74979700 -1.58105500
C 3.72810600 -0.16471900 -2.26292300
O 3.24595500 -1.39773200 -2.50949500
C -0.23736000 -1.08052000 -1.23480000
C -0.84776100 -2.38104000 -1.43663200
C -2.16538400 -2.64445300 -1.25664800
C -3.15992100 -1.70487900 -0.81122900
C -2.95268500 -0.37086300 -0.67845700
Si -4.31399800 0.77189800 -0.02023400
C -5.96490100 -0.10018100 -0.19642600
C 1.13305000 1.45602500 -0.21394000
Si 2.14981900 2.95670400 0.42073100
C 2.35591700 4.17828000 -0.99506600
O 1.74065900 -2.94709900 -2.26441600
P -1.41150600 0.28815600 -1.32240500
P -0.66229700 1.70631900 0.16585000
P 0.38523600 0.46728100 1.65575900
C -0.00784400 -1.15254700 1.31618200
Si 1.12630100 -2.51251700 1.92776900
C 2.90575100 -1.95293300 1.67838300
C 1.20950800 3.85497200 1.77776200
C 3.80104500 2.41370700 1.14244400
C -3.96962100 1.11410200 1.79328000
C -4.31541600 2.36583600 -1.00877200
C 0.83204300 -2.82298500 3.76197100
C 0.81340100 -4.10389700 0.98358300
H -1.04242700 -1.38231200 1.07578000
H -4.13156600 -2.12200900 -0.55791300
H -2.48907100 -3.66953000 -1.40447200
H -0.19485300 -3.19988200 -1.69047400
H -6.76574500 0.56322300 0.14451200
H -6.16792600 -0.36448800 -1.23792300
H -6.01580600 -1.01198400 0.40529800
H -5.10816900 3.03018800 -0.65112800
H -3.36767400 2.90405100 -0.91449600
H -4.49072500 2.17192700 -2.07076500
H -4.77757900 1.71306800 2.22524600
H -3.90319500 0.17862500 2.35622700
H -3.03461400 1.66144800 1.93984400
H 3.51556500 1.70620200 -1.43021300
H 4.71696700 -0.02446500 -2.67632600
H 3.69643000 1.44682700 1.64272600
H 4.59658000 2.32298700 0.40003100
H 4.12663400 3.14410900 1.88939100
H 1.37271300 4.50108100 -1.35093400
H 2.89097000 5.06673900 -0.64456600
H 2.90036200 3.77399100 -1.85150600
H 1.82792200 4.70291900 2.09218900
H 0.25049600 4.25403400 1.43897600
H 1.03421000 3.23001400 2.65649600

H 3.10589500 -1.72651700 0.62686000
H 3.12665500 -1.05368500 2.26172100
H 3.60517400 -2.73396000 1.99200100
H 1.01798500 -1.91482300 4.34322300
H -0.20085900 -3.13319200 3.94698400
H 1.49459900 -3.60983000 4.13742200
H 1.18774400 -4.03593100 -0.04071900
H -0.25459200 -4.33803700 0.94120200
H 1.32248800 -4.93825300 1.47669700

E(B3LYP/cc-pVTZ PCM=toluene T=383 K) =
-2863.75509849
E+ZPE= -2863.273338
E+thermalE= -2863.213780
E+thermalH= -2863.212567
E+thermalG= -2863.376029
C 3.60708300 -0.11201500 -2.41385100
O 3.13930500 -1.35205800 -2.65620100
C 1.90465100 -1.76748100 -2.18115400
C 1.06420600 -0.77695400 -1.48925500
C 1.62140800 0.49201300 -1.15139600
C 2.93039900 0.77901900 -1.68725100
O 1.64614300 -2.92884500 -2.40155400
C -0.28484700 -1.14049000 -1.16879000
C -0.84799200 -2.46066700 -1.25504200
C -2.15830600 -2.76218300 -1.03368200
C -3.17879800 -1.83740200 -0.64702200
C -3.02284900 -0.48655900 -0.57567200
Si -4.42232200 0.64533300 0.02779700
C -4.08140000 1.11409400 1.82267000
C 1.07930900 1.43600600 -0.20521200
Si 2.07986600 2.99131900 0.34533700
C 1.13763900 3.97679100 1.65091300
P -1.50343400 0.19542700 -1.24626200
P -0.73409100 1.69737800 0.17197500
P 0.43046100 0.53183800 1.64970800
C 0.13955400 -1.14146500 1.40208800
Si 1.43169800 -2.38896400 1.94117800
C 1.28958200 -2.71115900 3.80052800
C 1.20298000 -4.02446700 1.03154600
C 3.14749100 -1.69046100 1.56881000
C 3.72814500 2.50148000 1.12171100
C 2.28754000 4.15892200 -1.12764700
C -4.48355800 2.18940000 -1.04945500
C -6.05244900 -0.29201700 -0.07940800
H -0.89062600 -1.45589700 1.28717900
H -4.13605300 -2.27198500 -0.37926300
H -2.44016900 -3.80570700 -1.09320000
H -0.17312700 -3.27239800 -1.45347000
H -6.87305100 0.36718100 0.21051300
H -6.24574700 -0.64455600 -1.09341900
H -6.06998000 -1.15249400 0.59095300
H -5.29185500 2.84487000 -0.71910800
H -3.55346100 2.75712800 -0.99346600
H -4.66118600 1.93355200 -2.09499800
H -4.89294700 1.73395600 2.20991400
H -4.00839400 0.22263300 2.44742300
H -3.15309200 1.67593500 1.92885800
H 3.38912800 1.73803300 -1.53903600
H 4.57249600 0.05875400 -2.86487600
H 3.54344900 1.93175500 2.03361400
H 4.36447300 1.89790000 0.47756100
H 4.28050500 3.40243800 1.39750400
H 1.31012800 4.38893800 -1.55569800
H 2.72681700 5.09665400 -0.78044700
H 2.91644800 3.77193200 -1.92787900
H 1.77487100 4.81792300 1.93607500
H 0.19971900 4.38474200 1.27499000
H 0.92704400 3.40046000 2.55075700
H 3.26554300 -1.47391100 0.50648900
H 3.33327900 -0.76654100 2.11869700
H 3.91877900 -2.40899800 1.85306600
H 1.43577100 -1.78941700 4.36622300
H 0.30381500 -3.10621700 4.05349400
H 2.03828200 -3.43606700 4.12875500
H 1.48404000 -3.93988600 -0.01778200
H 0.16788400 -4.36624700 1.08011800
H 1.83146700 -4.79093200 1.49023800

5
E(M06-2X/6-31+G*) = -2862.56556101
E+ZPE=-2862.072560
E+thermalE=-2862.035202
E+thermalH=-2862.034258
E+thermalG=-2862.139846
C -3.57577000 -0.30684600 -2.38549900
O -3.05893400 -1.52332400 -2.59879600
C -1.86655000 -1.93530200 -2.02288800
C -1.17219300 -0.96342800 -1.17625600
C -1.72675900 0.28516900 -0.95435500
C -2.98085400 0.60288100 -1.59854900
C 0.15094800 -1.29362800 -0.52236500
C 0.01562700 -1.07256100 1.01312000
Si -1.36247100 -2.10190600 1.88819800
C -1.40572000 -3.88828500 1.30047800
C -1.10576000 1.31284200 -0.07076300
Si -2.03765400 2.94618900 0.29774900
C -2.34494100 3.90531100 -1.30278700
O -1.53597200 -3.07105800 -2.27274900
C -0.97509500 4.02187400 1.42078100
P 1.37747500 -0.09858300 -1.34509500
C 2.91122800 -0.55886600 -0.45601400
C 3.07512400 -1.88384300 -0.22883100
C 2.07738400 -2.90699800 -0.54679800
C 0.76856400 -2.66846300 -0.74644300
P 0.75306100 1.69234900 -0.22159300
P -0.21181400 0.70282900 1.48013600
Si 4.29548400 0.67169500 -0.10198000
C 4.39961900 1.89119500 -1.53232100
C 5.91801500 -0.26920700 0.06977600
C 3.95948700 1.58773600 1.51146500
H -1.71740000 -3.97306500 0.25320300
H -0.43346200 -4.38004200 1.40987500
H -2.13383500 -4.43885100 1.90933700
H 5.91761000 -0.92769500 0.94548000
H 6.13031700 -0.87792000 -0.81567900
H 6.74396600 0.44053300 0.19564900
H 3.77091400 0.87909200 2.32608500
H 4.83134500 2.19313400 1.78753900
H 3.09569000 2.25717100 1.44192500
H 0.11709000 -3.49232900 -1.00065900
H 4.01990400 -2.24611300 0.17978700
H -3.45464500 1.56605400 -1.47671400
H -4.50975800 -0.16062500 -2.91566900
H 2.42884400 -3.93306200 -0.62546500
H 0.96275200 -1.37251700 1.48501000
H 5.22041500 2.60014100 -1.37365500
H 4.57683500 1.37371000 -2.48150500
H 3.47661800 2.47372300 -1.63558100
C -0.94677700 -2.05854400 3.72667200
C -3.07440200 -1.34829200 1.63069600
H -1.67664400 -2.64573200 4.29619400
H 0.04503400 -2.48339800 3.91957700
H -0.95834200 -1.03698300 4.12288900

H -3.77220500 -1.78441800 2.35605800
H -3.07971800 -0.26236800 1.77979700
H -3.46872800 -1.55019500 0.62839900
C -3.64362500 2.57713600 1.21379100
H -4.21788600 3.50236400 1.34366300
H -4.28527600 1.85041600 0.70480800
H -3.42252600 2.18435500 2.21325700
H -2.25124200 4.97998500 -1.10909300
H -1.60458800 3.64269200 -2.06745300
H -3.34005900 3.73661300 -1.72716100
H -1.56608100 4.90094500 1.70667600
H -0.67758200 3.50938400 2.34157400
H -0.06928300 4.37815400 0.91948600

E(M06-2X/cc-pvtz PCM=toluene T=383 K) =
-2863.12457155
E+ZPE=-2862.635540
E+thermalE=-2862.577182
E+thermalH=-2862.575970
E+thermalG=-2862.735208
C -2.99929900 0.54136200 -1.57640700
C -3.58110000 -0.37652000 -2.35099600
O -3.02845000 -1.56996900 -2.58896900
C -1.80669600 -1.93777200 -2.06013800
C -1.16019100 -0.97971500 -1.17344400
C -1.73345200 0.25446200 -0.95148500
O -1.41003500 -3.02728900 -2.38813300
C 0.15503000 -1.29608600 -0.50790700
C 0.77760300 -2.66694300 -0.70769700
C 2.08164200 -2.89542200 -0.51529000
C 3.07393700 -1.86765800 -0.21409800
C 2.90770700 -0.55201400 -0.44995400
Si 4.27871700 0.68871600 -0.09556400
C 3.92947600 1.58830600 1.51726900
C -1.12370300 1.29507900 -0.08365700
P -0.22434800 0.70892500 1.46497700
P 0.72918600 1.68850300 -0.23821900
P 1.37340400 -0.10728600 -1.32988300
C 0.01191100 -1.06096900 1.02016800
Si -1.35809100 -2.08280800 1.91031100
C -3.06380300 -1.33062500 1.65777300
C -1.40886000 -3.86390900 1.32407800
C -0.92090200 -2.03285100 3.73575900
Si -2.05124700 2.93188200 0.26976200
C -3.67650700 2.57677400 1.14365500
C -2.27039600 3.91675100 -1.31465800
C -1.01737800 3.98507900 1.43013900
C 4.36285100 1.90805800 -1.51897700
C 5.90159500 -0.23736200 0.07165900
H -1.72981700 -3.94232000 0.28417600
H -0.44051500 -4.35391500 1.42398900
H -2.13110400 -4.40666100 1.93781600
H 5.89362200 -0.90558700 0.93374400
H 6.11808800 -0.82814400 -0.81879500
H 6.71622500 0.47460500 0.21387700
H 3.78169200 0.87110300 2.32619800
H 4.77972800 2.22168000 1.77796900
H 3.04319300 2.22033600 1.45912000
H 0.12974800 -3.49543800 -0.93401300
H 4.01767700 -2.22209300 0.19182300
H -3.50273500 1.48146800 -1.43876000
H -4.53031100 -0.25453400 -2.85097800
H 2.43501000 -3.91721300 -0.57475400
H 0.95188500 -1.34849200 1.50142600
H 5.15796000 2.63591600 -1.35054700
H 4.56425600 1.39355600 -2.45931100
H 3.42639700 2.45772000 -1.62915900
H -1.64957400 -2.60199900 4.31506500
H 0.06374500 -2.46862400 3.91181600
H -0.91202700 -1.01063000 4.11628600
H -3.75976200 -1.78401200 2.36656900
H -3.06962200 -0.25302600 1.82923800
H -3.44323200 -1.51467000 0.65182000
H -4.22251400 3.51143200 1.28487000
H -4.32621200 1.87973400 0.61652200
H -3.47245000 2.16288700 2.13312500
H -2.62225900 4.91918400 -1.06351100
H -1.30453500 4.02105200 -1.81264600
H -2.97003100 3.48646300 -2.02861100
H -1.60200300 4.87246300 1.68256000
H -0.77697900 3.46894100 2.35942000
H -0.08739400 4.31753600 0.96946800

E(ωB97X-D/6-311+G** (PCM=toluene, T=383 K)) =
-2863.19328096
E+ZPE=-2862.701115
E+thermalE=-2862.643703
E+thermalH=-2862.642490
E+thermalG=-2862.798730
C -3.56155100 0.39076000 2.39861300
O -2.99755900 1.57825500 2.63581400
C -1.78082500 1.94167400 2.08437800
C -1.15165200 0.98088000 1.18778800
C -1.73883500 -0.24996600 0.96490400
C -2.99681600 -0.52694000 1.60728800
C 0.16696600 1.28697500 0.51121800
C 0.00677900 1.06357500 -1.02307100
Si -1.34101700 2.10796200 -1.92186600
C -1.36653000 3.88994900 -1.33791900
C -1.14514100 -1.29284300 0.07781400
Si -2.10107800 -2.91626200 -0.28229400
C -2.32549300 -3.91074400 1.29716300
O -1.37827800 3.03309300 2.40561000
C -1.10635400 -3.98709500 -1.46254100
P 1.37493000 0.08159800 1.32541400
C 2.92494000 0.52198400 0.46093100
C 3.10150100 1.84219200 0.24216600
C 2.11112700 2.87377400 0.53967900
C 0.80196200 2.65297200 0.71907000
P 0.70792500 -1.70209800 0.22661500
P -0.24781500 -0.70342500 -1.47208900
Si 4.29690500 -0.71909200 0.08950200
C 4.35074400 -2.01026200 1.45210300
C 5.93865300 0.18899900 0.00987300
C 3.96707900 -1.53780000 -1.56994200
H -1.70118700 3.97932400 -0.30088200
H -0.38502000 4.36268200 -1.42302000
H -2.06807400 4.45301000 -1.96272200
H 5.96397200 0.92114800 -0.80230900
H 6.14990800 0.71148500 0.94703200
H 6.74725400 -0.52695200 -0.16767900
H 3.90546800 -0.78611200 -2.36254500
H 4.77779000 -2.22907600 -1.82191800
H 3.03179000 -2.10371600 -1.56991900
H 0.15711300 3.48639200 0.94473800
H 4.05044800 2.19782800 -0.15478500
H -3.51256000 -1.46284400 1.47407300
H -4.50481300 0.27150300 2.91413100
H 2.47104600 3.89544800 0.60873200
H 0.95253100 1.33626400 -1.50617400
H 5.16576900 -2.71765700 1.26998400
H 4.51731300 -1.54532800 2.42807400
H 3.42168800 -2.58543900 1.50699400
C -0.88941200 2.06182600 -3.74500800

C -3.06078600 1.38452000 -1.68415500
H -1.60516300 2.64901000 -4.32866900
H 0.10509500 2.48661300 -3.91255600
H -0.89184300 1.04196700 -4.14036200
H -3.75667600 1.88622200 -2.36448900
H -3.09899100 0.31379100 -1.90161600
H -3.42741700 1.53271400 -0.66519300
C -3.73238100 -2.52265500 -1.12932800
H -4.28594900 -3.45044200 -1.30587400
H -4.37842100 -1.84674100 -0.56549800
H -3.54135400 -2.06432300 -2.10453000
H -2.70947900 -4.90473500 1.04618600
H -1.35678200 -4.04590100 1.78804500
H -3.00733600 -3.46774600 2.02561400
H -1.69635000 -4.88540700 -1.67407100
H -0.90552200 -3.49157300 -2.41549000
H -0.15435200 -4.31046000 -1.03473200

E(B3LYP/cc-pVTZ PCM=toluene T=383 K) =
-2863.80170830
E+ZPE=-2863.316150
E+thermalE=-2863.257370
E+thermalH=-2863.256157
E+thermalG=-2863.416892
C -1.73276400 0.26285900 -0.98977500
C -2.95510300 0.55708800 -1.68407300
C -3.48983800 -0.33840800 -2.52352000
O -2.93129500 -1.53383600 -2.74814100
C -1.74292200 -1.92754400 -2.12043700
C -1.13229100 -0.96969100 -1.21503500
O -1.36805100 -3.04287300 -2.40267200
C 0.17539300 -1.27966900 -0.51785200
C -0.00468200 -1.08616300 1.02329300
Si -1.33957500 -2.17962600 1.90796200
C -0.88108700 -2.16275900 3.73774300
C -1.18254200 1.28973600 -0.06147200
Si -2.17719900 2.89482700 0.31762500
C -1.25801800 3.94699000 1.58563700
C 0.83551300 -2.63043500 -0.73598800
C 2.14839100 -2.83828400 -0.55251200
C 3.13343600 -1.81060900 -0.25315100
C 2.95794200 -0.48423200 -0.45011600
P 1.39794800 -0.02537400 -1.29444300
P 0.68363600 1.73681500 -0.15913900
P -0.30168500 0.67622500 1.50289700
Si 4.33831000 0.75470900 -0.08460200
C 5.99292900 -0.14892000 -0.04756700
C 4.03607200 1.55299000 1.59927100
C 4.36730500 2.07717600 -1.42882300
C -3.07898000 -1.48186700 1.68578900
C -1.34191700 -3.95660600 1.28441200
C -3.84689300 2.44996400 1.07713400
C -2.34687500 3.95017100 -1.23882100
H -1.66703900 -4.02213500 0.24584900
H -0.35889800 -4.41991900 1.36461700
H -2.04139700 -4.53627100 1.89145900
H 6.03423200 -0.88973200 0.75242700
H 6.18844600 -0.65776400 -0.99244200
H 6.79943000 0.56673000 0.12466300
H 4.00461400 0.79416000 2.38301600
H 4.84155300 2.25142700 1.83693200
H 3.09540000 2.10311200 1.62675700
H 0.20301500 -3.46806600 -0.96260200
H 4.08810900 -2.17081600 0.11797800
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H -4.39908800 -0.19229700 -3.08748100
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H 0.93914100 -1.34774200 1.50822500
H 5.18731300 2.77515000 -1.24800700
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H -4.45155700 1.78469600 0.46294800
H -3.69405900 1.96412200 2.04223400
H -2.74030600 4.93191300 -0.96688600
H -1.36492000 4.10033100 -1.69129700
H -3.00167500 3.52965200 -2.00043400
H -1.87649400 4.82428100 1.79064400
H -1.09733200 3.42556400 2.52881400
H -0.29405200 4.29962100 1.21974400

6. References

[1] S.M. Mansell, M. Green, R. J. Kilby, M. Murray, C.A. Russel, *C. R. Chim.* **2010**, *13*, 1073-1081.
[2] F. Frébault, M. T. Oliveira, E. Wöstefeld, N. Maulide, *J. Org. Chem.* **2010**, *75*, 7962-7965.
[3] Bruker (2010). APEX2, SAINT, SADABS and XSHELL. Bruker AXS Inc., Madison, Wisconsin, USA.
[4] G. M. Sheldrick, *Acta Cryst*. **2008**, *A64*, 112.
[5] A. L. Spek, *Acta Cryst*. **2009**, *D65*, 148.