Supporting information

to the manuscript

Generation and reactivity of an elusive base-stabilized phosphinidene

by

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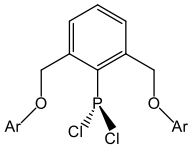
Synthetic Methods

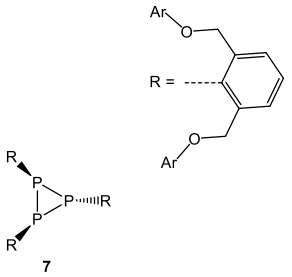
General Methods and Instrumentation. All manipulations were carried out using conventional inert atmosphere glove-box and Schlenk techniques. Solvents were pre-dried by using Grubbs-type purification columns and stored in ampoules equipped with Teflon valve. Deuterated solvents were dried over sodium, potassium, or CaH_2 as appropriate, distilled under reduced pressure and stored in ampoules equioped with Teflon valves. NMR samples were prepared in Wilmad tubes equipped with J. Young Teflon valves. NMR spectra were obtained at room temperature with a Bruker DPX-400 and Bruker DPX-600 instruments (^{1}H: 400 and 600 MHz; ^{13}C: 100.6 and 151 MHz). ^{1}H and ^{13}C spectra were referenced internally to residual protio-solvent (^{1}H) or solvent (^{13}C) resonances and are reported relative to tetramethylsilane (δ = 0 ppm). Elemental analyses were performed in the analytical laboratory of Université de Montreal and University of Toronto.



6

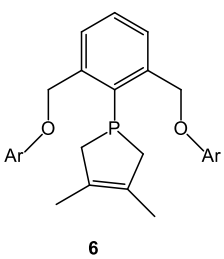
Synthesis of (2,6-(2,6-^{i}Pr$_2$C$_6$H$_3$OCH$_2$)$_2$C$_6$H$_3$)PCl$_2$ (6). 2,6-(2,6-^{i}Pr$_2$C$_6$H$_3$OCH$_2$)C$_6$H$_3$-1-Br (0.955 g, 1.78 mmol) was suspended in 20 mL of hexane. Then, 1.20 mL of hexane solution of *n*BuLi (1.6 M, 1.90 mmol) was added dropwise into the suspension at room temperature. A white precipitate was formed after 10 mins. The mixture was stirred for a day at room temperature. The precipitate was filtered and dissolved in toluene (10 mL). This solution was added dropwise into a solution of PCl_3 (0.16 mL, 1.78) in hexane (5 mL) at 0 ^{o}C. The solution was stirred for one day at room temperature. The LiCl salt was filtered off, and the volatiles were removed under vacuum to give a white oil. The pure solid of **6** was obtained by crystallization from a toluene/hexane mixture at -30 ^{o}C. Yield: 0.750 g, 1.40 mmol, 80%. **^{1}H NMR** (600 MHz, C_6D_6, 22^{o}C): δ (ppm) = 1.22 (d, 24H, $J_{H\text{-}H}$ = 6.9 Hz, ^{i}Pr-CH_3), 3.48 (sept, 4H, $J_{H\text{-}H}$ = 6.9 Hz, $CH(CH_3)_2$), 5.39 (s, 4H, CH_2-O) 7.10-7.11 (m, 6H, Ph-O), 7.23 (t, 1H, $J_{H\text{-}H}$ = 7.5 Hz, p-H Ph-P), 7.78 (m, 2H, m-H Ph-P). **^{13}C{^{1}H} NMR** (151 MHz, C_6D_6, 25^{o}C): δ (ppm) = 24.3 (^{i}Pr-CH_3), 27.2 (-$CH(CH_3)_2$), 74.1 (CH_2-O-), 124.3 - 148.9

(aromatic ring), 153.8 (C-O(CH_2)). **^{31}P{^{1}H} NMR** (243 MHz, C_6D_6, 22^{o}C): 158.5 (s). **Anal. Calcd** for $C_{32}H_{41}Cl_2O_2P$: C, 68.69; H, 7.39. Found: C, 68.91; H, 7.42 %.



7

(2,6-(2,6-^{i}Pr$_2$C$_6$H$_3$OCH$_2$)C$_6$H$_3$)$_3$P$_3$ (7) was prepared by two different methods**: The method 1:** 0.100 g (0.18 mmol) of **6** was dissolved into benzene. 0.050 g (0.37 mmol) of KC_8 was added into this solution and the mixture was stirred for 18 hours at room temperature. The precipitate was filtered off and dried to give a crude solid of **7** (0.064 g). **The method 2**: 0.100 g (0.18 mmol) of **6** was dissolved in benzene. 22 µL (0.22 mmol) of PMe_3 was added to this solution. A white precipitate formed within 5 mins and was filtered off. The volatiles were removed under vacuum, and the obtained solid was dissolved in 2 mL of Et_2O. Pure solid of **7** was formed from the ether solution after 2 days at -30 ^{o}C. Yield: 0.0272 g, 0.06 mmol. **^{1}H NMR** (600 MHz, C_6D_6, 22^{o}C): 1.09 (d, 24H, $J_{H\text{-}H}$ = 6.9 Hz, ^{i}Pr-CH_3), 1.12 (d, 48H, $J_{H\text{-}H}$ = 6.9 Hz, ^{i}Pr-CH_3), 3.24 (sept, 8H, $J_{H\text{-}H}$ = 6.9 Hz, $CH(CH_3)_2$), 3.34 (sept, 4H, $J_{H\text{-}H}$ = 6.9 Hz, $CH(CH_3)_2$), 4.97(s, 4H, CH_2-O), 5.70 (s, 4H, CH_2-O), 5.75 (s, 4H, CH_2-O) 6.99 (m, 6H, Ph-O), 7.00 (m, 12H, Ph-O), 7.14 (t, 2H, $J_{H\text{-}H}$ = 7.5 Hz, p-H Ph-P), 7.24 (t, 1H, $J_{H\text{-}H}$ = 7.5 Hz, p-H Ph-P), 7.55 (d, 4H, $J_{H\text{-}H}$ = 7.5 Hz, m-H Ph-P) 8.00 (d, 2H, $J_{H\text{-}H}$ = 7.5 Hz, m-H Ph-P). **^{13}C{^{1}H} NMR** (151 MHz, C_6D_6, 22^{o}C): 24.2, 24.3 (^{i}Pr-CH_3), 27.1, 27.2 ($CH(CH_3)_2$), 74.9, 75.6 (CH_2-O), 124.4 – 142.1 (aromatic ring), 153.6 (C-O-CH_2). **^{31}P{^{1}H} NMR** (243 MHz, C_6D_6, 22^{o}C): -113.9 (d, $J_{P\text{-}P}$ = 192.7 Hz), -150.2 (t, $J_{P\text{-}P}$ = 192.7 Hz). **Anal. Calcd** for $C_{96}H_{123}O_6P_3$: C, 78.66; H, 8.46. Found: C, 77.96; H, 8.92%.

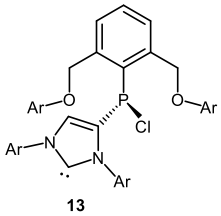


6

Reduction of 6 in the presence of butadiene. 0.100 g (0.18 mmol) of **6** was dissolved into benzene. 20 µL g (0.18 mmol) of 2,3-dimethyl-1,3-butadiene was added into solution of **6**. The solution was stirred for 10 min before adding 0.050 g (0.36 mmol) of KC_8 into the mixture. The suspension was stirred for 3 days. The precipitate was filtered off and the solution was dried to give a crude solid of **8**. **^{1}H NMR** (600 MHz, C_6D_6, 22^{o}C): 1.22 (d, 24H, $J_{H\text{-}H}$ = 6.9 Hz, ^{i}Pr-CH_3), 1.31 (s, 6H, CH_3-butadiene), 2.70 (m, 4H, CH_2-butadiene), 3.49

(sept, 4H, $J_{H\text{-}H}$ = 6.9 Hz, $CH(CH_3)_2$), 5.29 (s, 4H, CH_2-O) 6.95-7.12 (m, 6H, Ph-O), 7.36 (t, 1H, $J_{H\text{-}H}$ = 7.5 Hz, p-H Ph-P), 7.95 (d, 2H, $J_{H\text{-}H}$ = 7.5 Hz, m-H Ph-P).

$^{31}P\{^1H\}$ NMR (243 MHz, C_6D_6, 22°C): 50.0 (s).



13

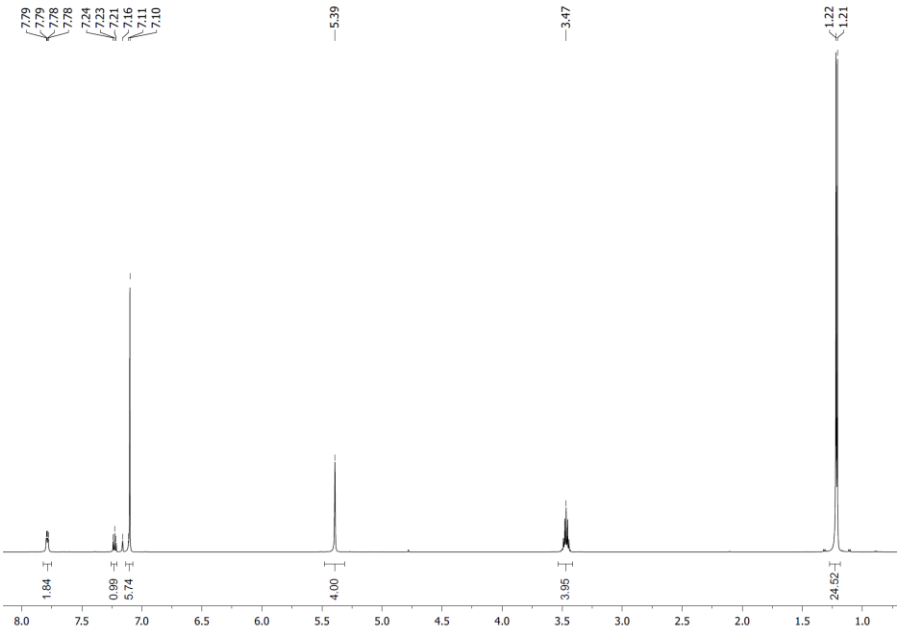
Synthesis of (2,6-(2,6-^{i}Pr$_2$C$_6$H$_3$OCH$_2$)$_2$C$_6$H$_3$)P(Cl)NHC (13). 0.100 g (0.18 mmol) of **6** was dissolved into benzene. 0.140 g (0.36 mmol) of NHC carbene was added into above solution. The whole mixture was stirred for 1 hour at room temperature. The white precipitate was formed and was filtered off. The volatiles were removed under vacuum and the obtained solid was dissolved into 2 mL of hexane for the purification. Pure solid of **13** was formed from the hexane solution after a week at -30°C. Yield: 0.077 g, 0.085 mmol. **^{1}H NMR** (600 MHz, C_6D_6, 22°C): δ (ppm) = 0.69 (d, 3H, $J_{H\text{-}H}$ = 6.9 Hz, ^{i}Pr-CH_3), 0.72 (d, 3H, $J_{H\text{-}H}$ = 6.9 Hz, ^{i}Pr-CH_3), 1.07 (d, 3H, $J_{H\text{-}H}$ = 6.9 Hz, ^{i}Pr-CH_3), 1.15 (d, 3H, $J_{H\text{-}H}$ = 6.9 Hz, ^{i}Pr-CH_3), 1.22 - 1.27 (m, 36H, ^{i}Pr-CH_3), 2.49 (sept, 1H, $J_{H\text{-}H}$ = 6.9 Hz, $CH(CH_3)_2$ of [NHC]), 2.73 (sept, 1H, $J_{H\text{-}H}$ = 6.9 Hz, $CH(CH_3)_2$ of [NHC]), 2.84 (sept, 1H, $J_{H\text{-}H}$ = 6.9 Hz, $CH(CH_3)_2$ of [NHC]), 3.00 (sept, 1H, $J_{H\text{-}H}$ = 6.9 Hz, $CH(CH_3)_2$ of [NHC]), 3.46 (br, 4H, $CH(CH_3)_2$ of [OCO]), 5.27 (s, 2H, CH_2-O) 7.20, (s, 2H, CH_2-O), 6.92 - 7.29 (m, 13H, Ph & 1H, NC(H=C), 8.01 (br, 2H, Ph-O). **$^{13}C\{^1H\}$ NMR** (151 MHz, C_6D_6, 22°C): δ (ppm) = 21.2, 22.1, 23.4, 24.0, 24.2, 24.4, 24.6, 26.1 (^{i}Pr-CH_3), 27.2, 28.7, 28.8, 29.7 ($CH(CH_3)_2$), 73.5 (CH_2-O), 123.4 – 147.3 (aromatic ring & N-C(H)=C(P)-N), 153.0 (-NCN-). **$^{31}P\{^1H\}$ NMR** (243 MHz, C_6D_6, 22°C): δ (ppm) = 51.9 (s). **Anal. Calcd** for $C_{59}H_{76}ClN_2O_2P$: C, 77.73; H, 8.40; N, 3.07. Found: C, 76.56; H, 8.45; N, 2.80%.

NMR study of the reduction of 6 with PMe_3 to form intermediate (OCO)P=PMe_3 (9). 0.010 g (0.018 mmol) of **6** was dissolved into toluene-d_8 and the NMR tube was precooled to -60 °C. 4 equivalents of PMe_3 were added by syringe to the tube, and the sampled was quickly placed into a 600 MHz magnet precooled to -60 °C. NMR spectra showed the formation of (OCO)P=PMe_3. This species is persistent up to 10 °C, at which point $\{(OCO)P\}_3$ starts to form.

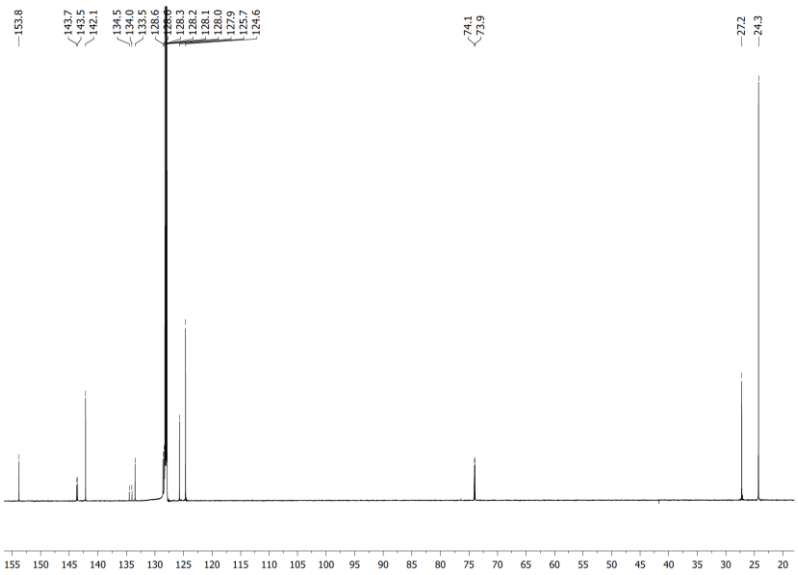
^{1}H NMR (600 MHz, C_6D_6, -40^{o}C): δ (ppm) = 8.30 (b, 2, m-Ph), 7.54 (b, 1H, p-Ph), 7.18 (m-Ar), 5.55 (b, 4, CH_2O), 3.64 (b, 4H, CH), 1.30 (b, 24H, Me), 0.78 (b, free PMe_3), 0.54 (bd, J= 10 Hz, P-PMe_3). **^{13}C{^{1}H} NMR** (151 MHz, C_6D_6, -60^{o}C): δ (ppm) = 153.7 (i-Ar), 149.1 (o-Ar), 147.1 (o-Ph), 131.8 (i-Ph), 124.9 (m-Ph), 124.6 (m-Ar), 127.9 (p-Ph), 76.5 (CH2-O), 26.6 (CH), 24.3 (Me), 15.5 (PMe3). **^{31}P{^{1}H} NMR** (243 MHz, C_6D_6, -40^{o}C): δ (ppm) = 5.87 (d, $J_{P\text{-}P}$= 530.7 Hz, PMe_3), -168.1 (d, $J_{P\text{-}P}$= 530.7 Hz, (COC)P).

NMR Spectra

^{1}H NMR spectrum



$^{13}C\{^{1}H\}$ NMR spectrum



$^{31}P\{^{1}H\}$ NMR spectrum

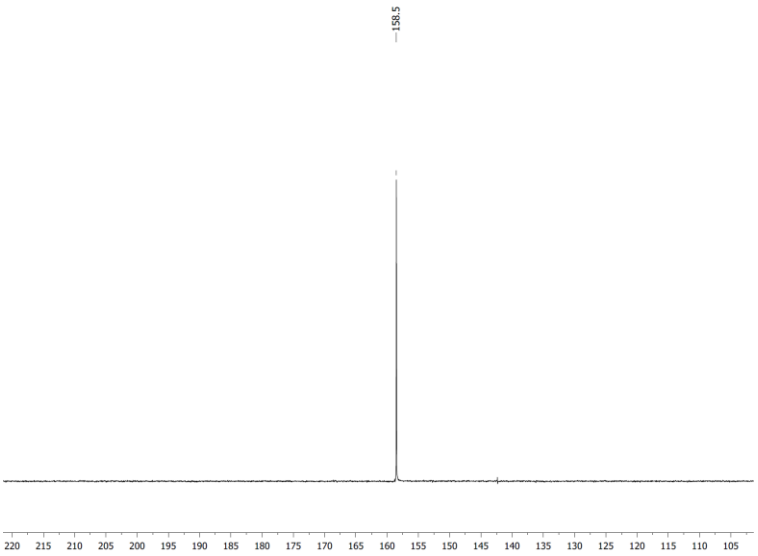
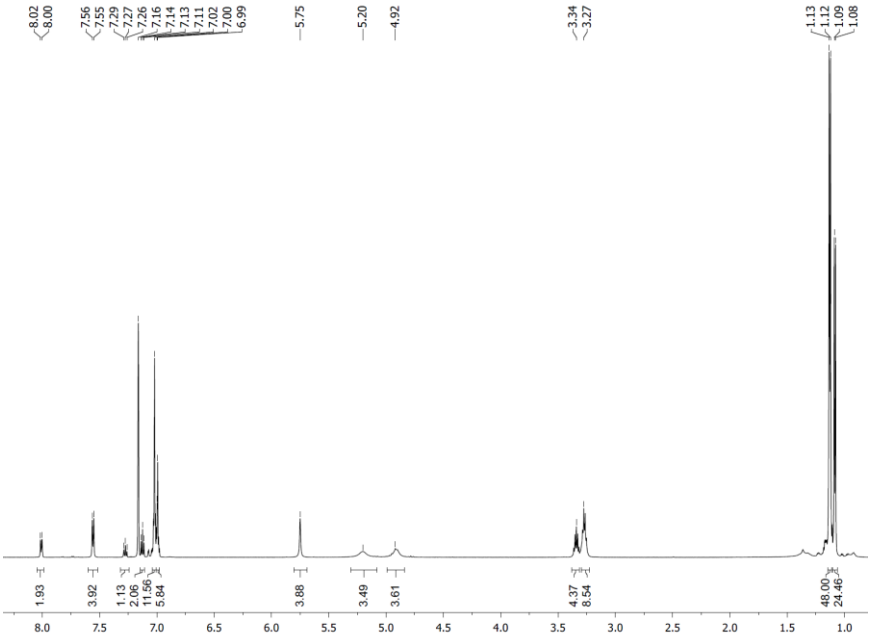
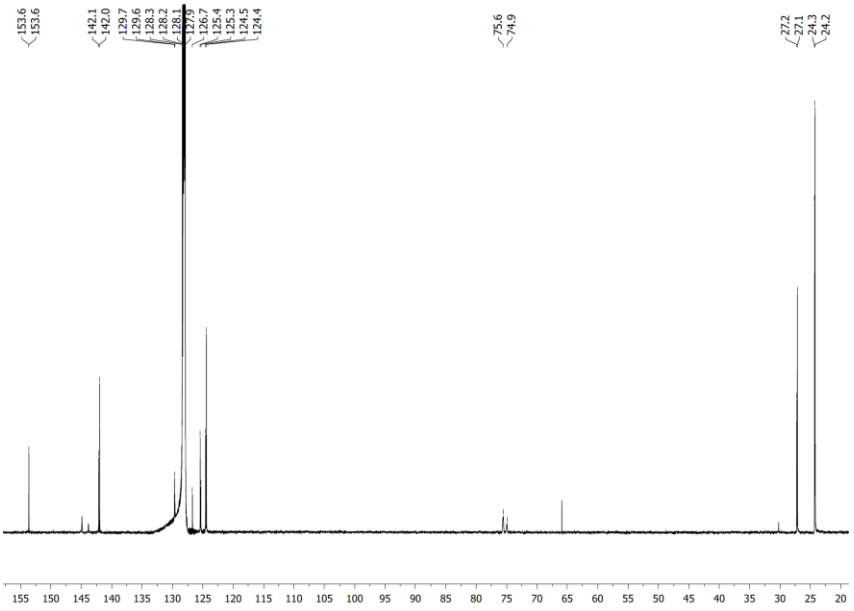


Figure SI1. ^{1}H, $^{13}C\{^{1}H\}$, $^{31}P\{^{1}H\}$ NMR spectra of **6** in C_6D_6

^{1}H NMR spectrum



$^{13}C\{^{1}H\}$ NMR spectrum



$^{31}P\{^{1}H\}$ NMR spectrum

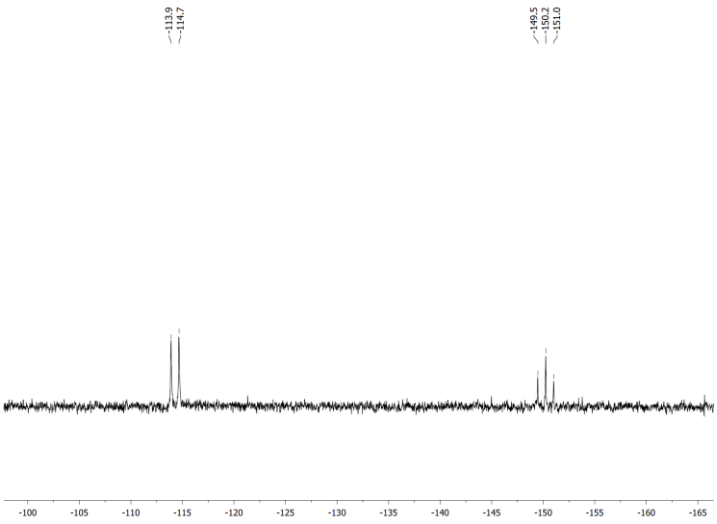


Figure SI2. ^{1}H, $^{13}C\{^{1}H\}$, $^{31}P\{^{1}H\}$ NMR spectra of **7** in C_6D_6

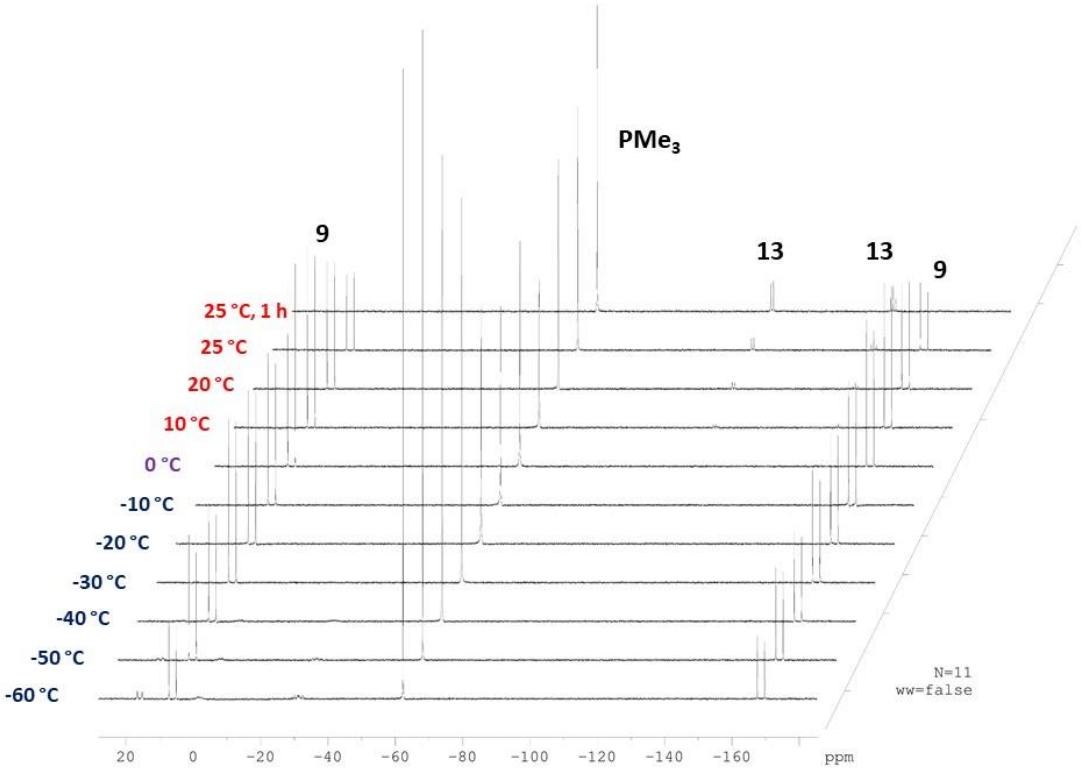
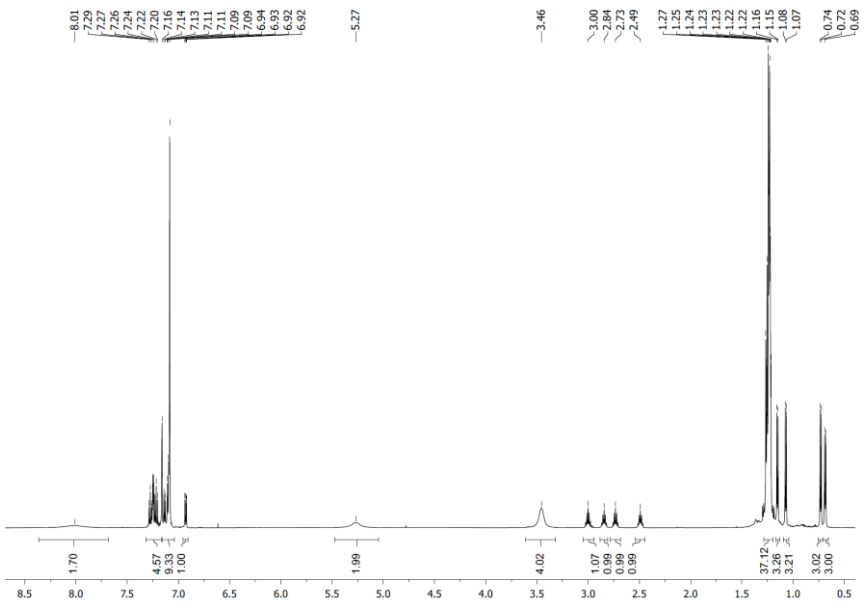
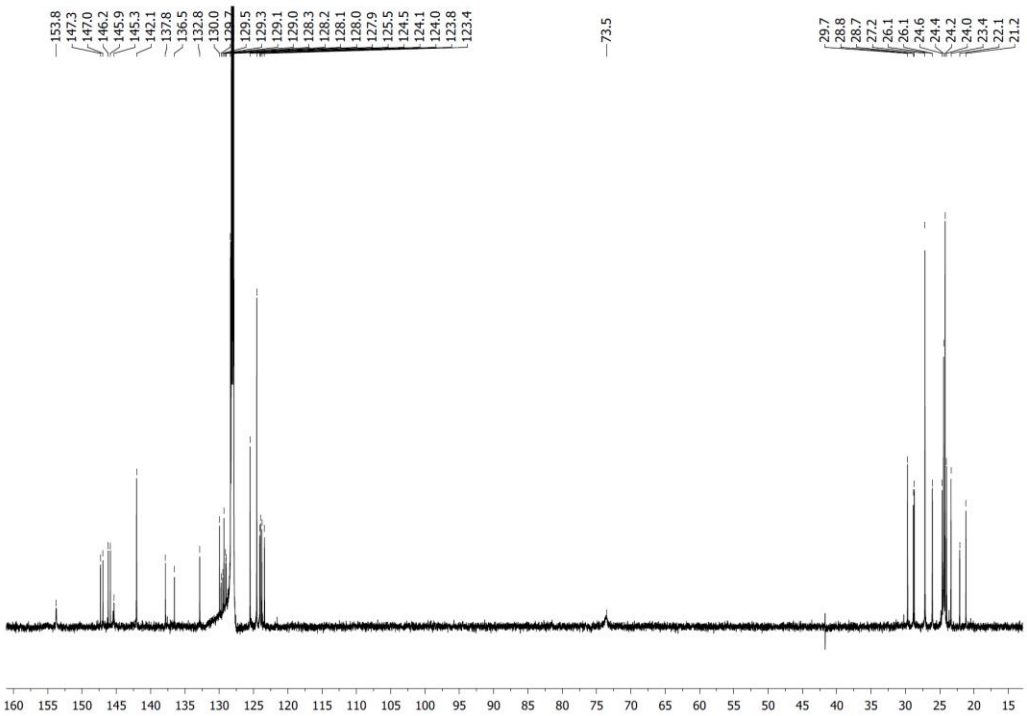


Figure SI3. VT $^{31}P\{^{1}H\}$ NMR spectra for the reaction of **6** with 4 eqvs of PMe_3 in toluene-d_8

^{1}H NMR spectrum



$^{13}C\{^{1}H\}$ NMR spectrum



$^{31}P\{^{1}H\}$ NMR spectrum

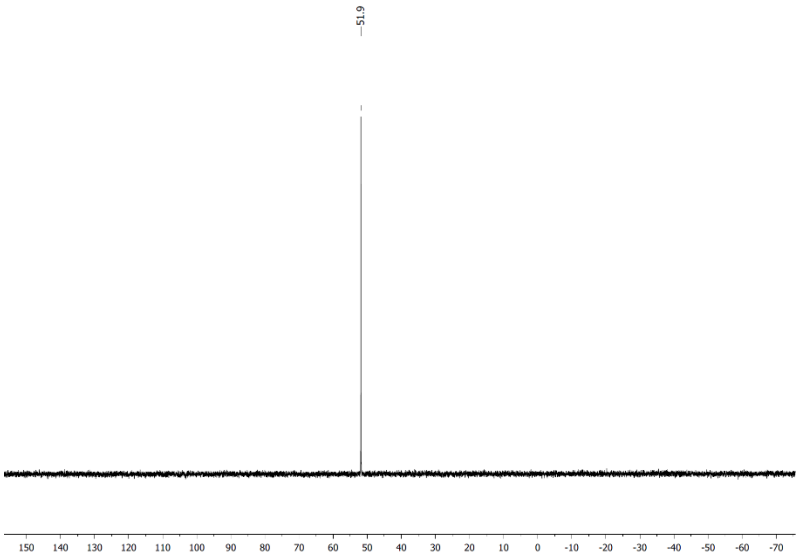


Figure SI4. ^{1}H, $^{13}C\{^{1}H\}$, $^{31}P\{^{1}H\}$ NMR spectra of **13** in C_6D_6

X-ray crystallography

Crystals of **7** and **13** were grown from ether and hexane solutions, respectively, at at -30ºC. The crystals were mounted in a film of perfluoropolyether oil on a glass fiber and transferred to a diffractometer.Single crystal X-ray diffraction data for compounds **7** and **13** were collected using the Canadian Macromolecular Crystallography Facility CMCF-BM beamline at the Canadian Light Source (CLS).[1] The CMCF-BM is a bending magnet beamline equipped with a Si (111) double crystal monochromator, Pilatus 6M detector (or Rayonix MX300HE CCD in case of **7**) and MD2 microdiffractometer equipped with Mini Kappa Goniometer Head. The data for compounds **7** and **13** were collected at 19.0000 keV (0.6526 Å) and 18.0000 keV (0.68883 Å), respectively. The data for both compounds were acquired at 100 K, using Oxford Instruments Cryojet5.

Cell refinement and data reduction were performed using XDS.[2] A semi-empirical absorption correction, based on the multiple measurements of equivalent reflections, and merging of data was performed using SADABS.[3] Data conversion from the XDS file format to the SADABS file format was performed using XDS2SAD.[4] The space group was confirmed by XPREP routine.[5]

The initial model and difference Fourier map for compound **7** was obtained with SHELXL-2018.**Error! Bookmark not defined.** The crystal structure of **7** was solved by a combination of direct-methods and real-space refinement. The real-space refinement was performed using COOT.[6] Direct methods refinement was performed with SHELXL-2018,[7] using a conjugate-gradient refinement (CGLS and BLOC) in the initial stages and then by full-matrix least-squares and difference Fourier techniques at the final stages. The disorders of isopropyl groups were modeled as two-component disorders. The disorder of 2,6-Diisopropylphenyl (Dipp) was model as a three-component disorder using COOT [6] and the site occupancy factors were refined using the SUMP command appropriate for the three-component disorders. The disordered diethyl either molecule located near the three-component disorders of the Dipp fragment

was modeled using COOT[6] and refined as a two-component disorder. All atoms of disordered fragments were restrained using SADI restraints (bonds and angles) whenever possible and DFIX, DANG constraints in special cases. SIMU restraints to U_{ij} components were applied whenever necessary.

The structure of compound **13** was solved by direct-methods and refined by full-matrix least-squares and difference Fourier techniques with SHELXL-2018.[Error! Bookmark not defined.] All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were set in calculated positions and refined as riding atoms with a common thermal parameter. All publication materials were prepared using LinXTL[8] and Mercury[9] programs. CheckCIF routine and structure factor analyses were performed by Platon.[10]

Table SI1. Crystal Data Collection and Refinement Parameters for Compounds 7 and 13

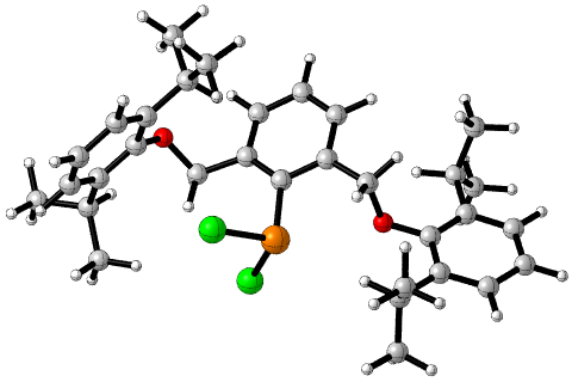
	7	**13**
chemical formula	$C_{98.37}H_{127.93}O_{6.32}P_3$	$C_{59}H_{76}ClN_2O_2P$
crystal colour	colourless	colourless
***Fw*; *F*(000)**	1504.50; 3255	911.63; 1968
***T* (K)**	100	100
wavelength (Å)	0.65254	0.68883
space group	P21/n	P21/c
***a* (Å)**	19.179(4)	19.486(4)
***b* (Å)**	17.115(3)	15.653(3)
***c* (Å)**	27.588(6)	18.087(4)
α (deg)	90	90
β (deg)	94.15(3)	101.44(3)
γ (deg)	90	90
Z	4	4
***V* (Å^3)**	9032(3)	5407(2)
ρ_{calcd} (g·cm^{-3})	1.106	1.120
μ (mm^{-1})	0.096	0.130
θ range (deg); completeness	1.149 − 24.499; 1.000	1.033 − 24.206; 0.989
collected reflections; R_σ	142930; 0.0286	107369; 0.0400
unique reflections; R_{int}	19428; 0.0509	9453; 0.0866
R1[a]; wR2[b] [I > 2σ(I)]	0.0458; 0.1185	0.0683; 0.1975
R1; wR2 [all data]	0.0530; 0.1242	0.0810; 0.2281
GOF	1.062	1.176
largest diff peak and hole	0.307 and -0.517	0.533 and -0.541

Computational Methods

Density Functional Theory (DFT) calculations were performed using Gaussian 16, Revision C. 01 software package.[11] All optimizations were conducted using the B97-D[12] exchange-correlation functional with a 6-31G(d,p) basis set and the IEFPCM solvent model (toluene, e = 2.38)[13] with default frequency scaling. The optimized geometries of all computed structures were verified as minima (zero imaginary frequency) by frequency calculations and the keyword (integral=grid=ultrafine) was used throughout for all calculations The 3D images of all optimized geometries were generated using the program CYLview.[14] GaussView6[15] was used to construct all structures prior to optimization and to visualize the output from the Gaussian16 calculations.

1. Cartesian Coordinates of Optimized Structures

Structure of 6_{DFT}



Zero-point correction =	0.643495 (Hartree/Particle)
Thermal correction to Energy =	0.684351
Thermal correction to Enthalpy =	0.685295
Thermal correction to Gibbs Free Energy =	0.565633
Sum of electronic and zero-point Energies =	-2654.772649
Sum of electronic and thermal Energies =	-2654.731793
Sum of electronic and thermal Enthalpies =	-2654.730848
Sum of electronic and thermal Free Energies =	-2654.850511

Charge = 0 Multiplicity = 1

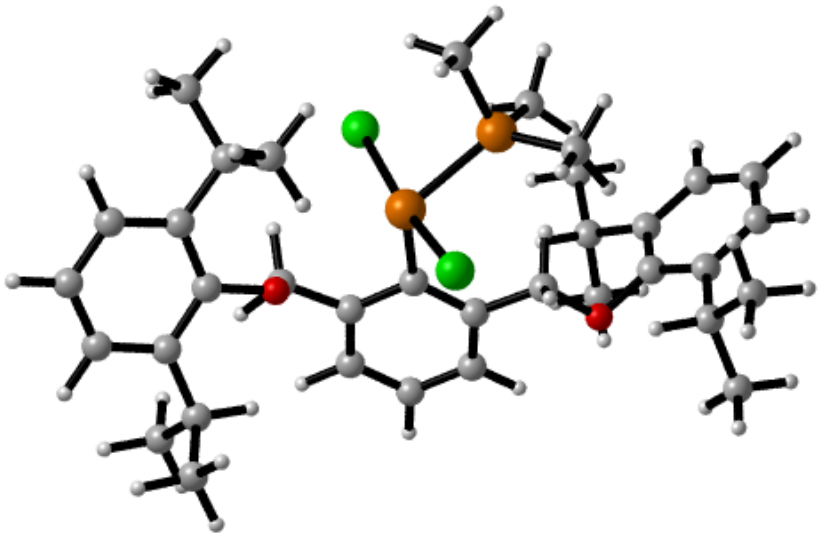
H	0.06560600	4.40929800	-0.80850000
C	0.03844700	3.32705400	-0.67985900
C	-0.03993200	0.51925000	-0.35632200
C	1.10155900	2.66363600	-0.05546100
C	-1.05382400	2.59113600	-1.14410300
C	-1.11993300	1.19292300	-0.98457100
C	1.08028800	1.26995900	0.11223800
H	1.96597900	3.22358400	0.30275200
H	-1.89462100	3.09782200	-1.61697900
C	2.30355000	0.62498400	0.73572600

H	2.05354900	-0.08687900	1.54270700
H	2.94925900	1.40557600	1.16659500
C	-2.38940100	0.53209100	-1.50832400
H	-2.43699000	-0.53721700	-1.29562200
H	-2.43410500	0.66281400	-2.60052000
P	0.12797400	-1.31478500	-0.07610500
Cl	-0.27612800	-2.07291800	-2.02864200
Cl	-1.66400200	-1.75141700	0.99401000
O	3.01390200	-0.07275300	-0.31586000
O	-3.55841900	1.19906500	-0.96816300
C	-4.24983100	0.49425600	0.02068700
C	-5.69014500	-0.84972600	1.99546300
C	-5.07901600	-0.58455700	-0.35528600
C	-4.12670000	0.92334600	1.36401700
C	-4.87122800	0.23642100	2.33856500
C	-5.78872100	-1.25336300	0.66030300
H	-4.79549400	0.54070700	3.38194400
H	-6.42736400	-2.09588900	0.39101000
H	-6.24856100	-1.37740600	2.77006700
C	4.36904800	-0.26499600	-0.02721100
C	7.08298000	-0.64253700	0.48560400
C	4.77798400	-1.44990200	0.62030900
C	5.28147900	0.74147000	-0.41758100
C	6.64550800	0.52797300	-0.14914000
C	6.15391600	-1.62039900	0.86331000
H	7.36820400	1.29064600	-0.44311300

H	6.49261100	-2.53148300	1.35894500
H	8.14516100	-0.79165200	0.68484300
C	-3.22356300	2.10317700	1.70921300
H	-2.31442200	2.00009200	1.10372600
C	-3.89506200	3.43445700	1.29857900
H	-3.21851200	4.28127000	1.49535600
H	-4.81957800	3.58881500	1.87690400
H	-4.14768000	3.42513500	0.23015500
C	-2.79102300	2.14936500	3.18546500
H	-2.05431200	2.95394300	3.32752200
H	-2.33680200	1.19779600	3.49921900
H	-3.64447500	2.35882000	3.84917100
C	-5.21817800	-1.03342100	-1.80646600
H	-4.68108400	-0.31446300	-2.43950300
C	-4.59272600	-2.43075700	-2.01803500
H	-3.53036100	-2.44387200	-1.73620200
H	-4.67888300	-2.73404400	-3.07297600
H	-5.11391500	-3.17935700	-1.40172500
C	-6.69537400	-1.02797800	-2.25937300
H	-6.76669600	-1.30760900	-3.32171500
H	-7.14447000	-0.03297600	-2.12627300
H	-7.28752600	-1.75127400	-1.67855500
C	4.81215100	2.02720800	-1.09022800
H	3.73634800	1.92990500	-1.28807200
C	5.51976300	2.25372000	-2.44374400
H	6.60457400	2.37847000	-2.30516800

H	5.13261700	3.16416800	-2.92633900
H	5.35629400	1.40173300	-3.11919100
C	5.02196100	3.24280800	-0.15904200
H	6.09196200	3.38385000	0.05798700
H	4.50131300	3.10698900	0.80138800
H	4.64433400	4.16110300	-0.63515700
C	3.77682300	-2.51340400	1.05375800
H	2.77796000	-2.18777300	0.73673000
C	3.76395300	-2.66741100	2.59108400
H	3.53283400	-1.71094400	3.08387400
H	4.74475700	-3.00877300	2.95671700
H	3.00842500	-3.40852900	2.89382100
C	4.06442600	-3.86802400	0.37050100
H	5.05539900	-4.25034000	0.66021600
H	4.04182900	-3.76774200	-0.72429400
H	3.31048000	-4.61189800	0.67030200

Structure of INT_1



Zero-point correction=	0.756666 (Hartree/Particle)
Thermal correction to Energy=	0.804880
Thermal correction to Enthalpy=	0.805824
Thermal correction to Gibbs Free Energy=	0.672631
Sum of electronic and zero-point Energies=	-3115.691441
Sum of electronic and thermal Energies=	-3115.643227
Sum of electronic and thermal Enthalpies=	-3115.642283
Sum of electronic and thermal Free Energies=	-3115.775476

Charge = 0 Multiplicity = 1

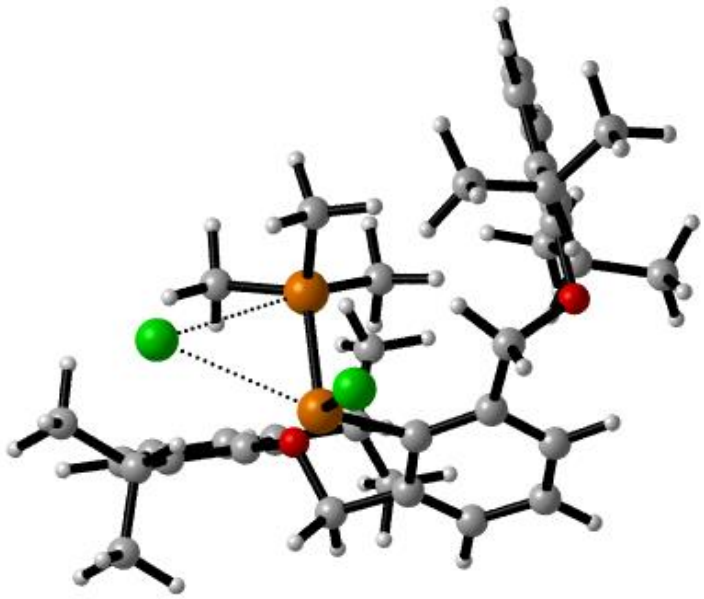
P	0.64722600	1.01245300	-0.17077000
Cl	0.82967700	1.85083600	2.32974100
P	-1.22232100	2.37821100	-0.07612900
Cl	0.33895500	0.51620800	-2.43610500
C	0.28645700	-0.73127400	0.44067100
C	1.41717400	-1.39581900	1.00380100
C	1.28812100	-2.72465800	1.44573300
H	2.16181200	-3.21996100	1.87121900
C	0.07439100	-3.41077000	1.34565300
C	-1.02569300	-2.77743200	0.76156700
H	-1.97390000	-3.29878600	0.65160500
C	-0.92706000	-1.45506700	0.29831600
H	-0.00854700	-4.43809200	1.70132300
C	2.78791100	-0.76438600	1.13985100
H	3.48202300	-1.49429400	1.58334500
H	2.76280000	0.13119200	1.77906200
C	-2.11777200	-0.81638000	-0.37118200
H	-1.90004700	-0.63145200	-1.43536600
H	-2.29919300	0.15321200	0.10540500

O	3.26099000	-0.39510500	-0.18411000
C	4.63869400	-0.17400700	-0.22322300
C	7.38827000	0.25361700	-0.36900100
C	5.49110900	-1.28491300	-0.40544500
C	5.12595700	1.14747300	-0.10235800
C	6.51712400	1.33806000	-0.18832700
C	6.87604700	-1.04483200	-0.47593400
H	6.92303300	2.34605500	-0.10360000
H	7.55263600	-1.88917800	-0.61825200
H	8.46460000	0.42326900	-0.42672500
C	4.15329100	2.31123100	0.05171500
H	3.28052500	1.94982500	0.61092900
C	3.65085400	2.75957500	-1.34026900
H	3.17400200	1.92537300	-1.87122000
H	4.49193500	3.13055400	-1.94755300
H	2.91490200	3.57274800	-1.23494200
C	4.73478900	3.50685000	0.82877200
H	5.53635200	4.00666900	0.26256100
H	5.14296900	3.19247200	1.80052200
H	3.94115600	4.24691600	1.00868400
C	4.94313000	-2.70337600	-0.52273800
H	3.84670000	-2.64420000	-0.51392800
C	5.39162600	-3.57255300	0.67354900
H	4.95949700	-4.58248900	0.59764600
H	5.07777000	-3.12885000	1.63072200
H	6.48821200	-3.66925000	0.69241100

C	5.36291500	-3.35881800	-1.85669100
H	4.93067200	-4.36818000	-1.93715500
H	6.45804900	-3.45120500	-1.92089300
H	5.01834300	-2.75997500	-2.71196900
O	-3.31954900	-1.59688700	-0.25272200
C	-4.44349600	-0.78039200	-0.09823100
C	-6.66626300	0.85650100	0.21900300
C	-5.16716700	-0.39928600	-1.24781600
C	-4.79019500	-0.36021100	1.20708500
C	-5.92220300	0.46542900	1.34168700
C	-6.29467400	0.42401500	-1.06055000
H	-6.22080500	0.80872300	2.33151600
H	-6.87901200	0.73653300	-1.92538800
H	-7.53923800	1.49864500	0.34345100
C	-4.75715500	-0.93148000	-2.61797200
H	-3.66036600	-1.00760600	-2.63383600
C	-5.18010000	-0.02390000	-3.78778600
H	-4.82629500	1.00849300	-3.64638900
H	-6.27490800	0.00044700	-3.89961400
H	-4.75878200	-0.41153100	-4.72634900
C	-5.31203700	-2.36347600	-2.80572400
H	-4.95326100	-3.02286200	-2.00376200
H	-4.98808900	-2.77546700	-3.77378900
H	-6.41283400	-2.34996700	-2.78385200
C	-3.96948100	-0.84225900	2.40127000
H	-2.90688300	-0.80955100	2.11801800

C	-4.30779400	-2.32094600	2.70773800
H	-3.66892300	-2.69555900	3.52185100
H	-4.15096200	-2.94587300	1.81924100
H	-5.35971600	-2.41086600	3.02005000
C	-4.14102900	0.01823000	3.66562600
H	-3.44106300	-0.32466800	4.44046200
H	-5.16056700	-0.07038900	4.07117000
H	-3.94297200	1.08132700	3.46570200
C	-2.34694700	2.37628100	-1.53701000
H	-1.76127500	2.32051400	-2.46089100
H	-3.04187100	1.53036800	-1.48357700
H	-2.91904700	3.31500700	-1.50569400
C	-2.35595200	2.37739600	1.37979800
H	-2.69267800	3.41257000	1.53445300
H	-3.22557000	1.74101800	1.17111000
H	-1.81722100	2.02936100	2.26685400
C	-0.38849700	4.01592900	-0.13296400
H	-1.15368400	4.80445300	-0.12799900
H	0.26572000	4.10418200	0.74206500
H	0.20609700	4.08044900	-1.05398700

Structure of INT_1^I



Zero-point correction=	0.757768 (Hartree/Particle)
Thermal correction to Energy=	0.805971
Thermal correction to Enthalpy=	0.806915
Thermal correction to Gibbs Free Energy=	0.677414
Sum of electronic and zero-point Energies=	-3115.688519
Sum of electronic and thermal Energies=	-3115.640315
Sum of electronic and thermal Enthalpies=	-3115.639371
Sum of electronic and thermal Free Energies=	-3115.768873

Charge = 0 Multiplicity = 1

H	-0.61359500	3.37075400	3.75814000
C	-0.44747800	2.43706600	3.22048900
C	-0.03364000	-0.01676600	1.85442100
C	0.85226900	2.00761200	2.93131600
C	-1.53401800	1.67561800	2.78314900
C	-1.35031800	0.47035300	2.07515500
C	1.06804900	0.79206500	2.26404900
H	1.71185100	2.61476900	3.21801100
H	-2.54951800	2.03215900	2.94649800

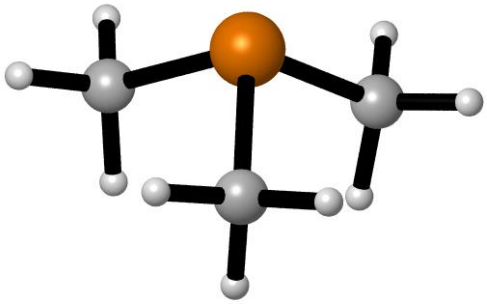
C	2.48705100	0.42537600	1.89233200
H	2.82621600	-0.51477300	2.35782600
H	3.17845400	1.23135800	2.17739700
C	-2.61000100	-0.22125200	1.56762600
H	-3.04849800	-0.85301200	2.35461200
H	-2.39043700	-0.87307500	0.71537300
P	0.52319400	-1.68798500	1.13529400
O	2.50257900	0.25880600	0.44578700
O	-3.60998600	0.75364800	1.17766800
C	-3.93209500	0.73542100	-0.17882100
C	-4.50611300	0.69423000	-2.90658800
C	-3.49428700	1.81674000	-0.98247600
C	-4.69338300	-0.33616700	-0.69711600
C	-4.95279100	-0.34406800	-2.08176400
C	-3.80146500	1.77452600	-2.35400600
H	-5.52868400	-1.16799200	-2.50539100
H	-3.47096400	2.58667500	-3.00067000
H	-4.71884200	0.67287900	-3.97621100
C	3.71142800	0.58327800	-0.18006000
C	6.06293300	1.25472600	-1.49915400
C	4.64635700	-0.44098200	-0.44539200
C	3.90716000	1.92715400	-0.56791700
C	5.10576400	2.24301300	-1.23244500
C	5.82962900	-0.07224100	-1.11344600
H	5.28236100	3.27302700	-1.54559400
H	6.57069600	-0.84061500	-1.33425500

H	6.98760600	1.51714300	-2.01500600
C	-5.28232800	-1.42038900	0.20276600
H	-5.05259800	-1.15753800	1.24385900
C	-6.82231000	-1.45504700	0.06662200
H	-7.24515200	-2.19000900	0.76799200
H	-7.11943200	-1.74674500	-0.95198900
H	-7.25930300	-0.46929500	0.28204900
C	-4.68511400	-2.81456500	-0.08686500
H	-5.18162600	-3.57590600	0.53327200
H	-3.61003100	-2.85015100	0.13525900
H	-4.83073600	-3.08830600	-1.14311000
C	-2.73119500	2.97524000	-0.34487300
H	-2.03807400	2.54313000	0.39053200
C	-1.90113900	3.80494700	-1.34016600
H	-1.21942200	3.17223400	-1.92671000
H	-1.30084300	4.54444000	-0.79030400
H	-2.54741900	4.35523900	-2.04111900
C	-3.70516500	3.88493500	0.44024100
H	-3.15017200	4.68836000	0.94927300
H	-4.25500900	3.30392100	1.19241500
H	-4.43200400	4.34670800	-0.24582700
C	2.85350100	2.99969600	-0.30978300
H	2.03331700	2.54600800	0.26234700
C	2.26420100	3.51805100	-1.64120000
H	3.04499500	3.99907900	-2.24965700
H	1.47225200	4.25743800	-1.44749900

H	1.83564500	2.69369600	-2.23012500
C	3.41847600	4.16603200	0.52889200
H	4.23419700	4.67552500	-0.00595900
H	3.81624700	3.80742700	1.48998700
H	2.62863500	4.90558700	0.73061300
C	4.39215200	-1.87955700	-0.01352300
H	3.31727600	-1.99937000	0.17327900
C	5.13312700	-2.18768700	1.30853900
H	4.84482200	-1.48601300	2.10550000
H	6.22227300	-2.10824500	1.16431800
H	4.89679800	-3.20938700	1.64035700
C	4.78353300	-2.90527400	-1.09644200
H	5.87681200	-2.96519000	-1.21548500
H	4.34563800	-2.64097200	-2.06952400
H	4.40228600	-3.89445600	-0.81049300
P	0.07662000	-1.24385300	-1.05445500
C	1.54728400	-1.52126700	-2.10193700
H	1.87832800	-2.55728800	-1.94519600
H	2.33027700	-0.80447300	-1.83360700
H	1.23046600	-1.35746800	-3.14285400
C	-1.31844200	-2.22662100	-1.70904500
H	-1.34684500	-2.08590900	-2.79919200
H	-2.26486600	-1.87991500	-1.27699300
H	-1.12120300	-3.27940500	-1.46617300
C	-0.33183900	0.53157600	-1.24846600
H	-1.24676800	0.77578100	-0.70450100

H	-0.48168800	0.73978800	-2.31709000
H	0.50498200	1.12152300	-0.85794800
Cl	-1.06674700	-2.94659900	1.74885200
Cl	1.23348600	-4.43903900	-0.51151900

Structure of PMe_3



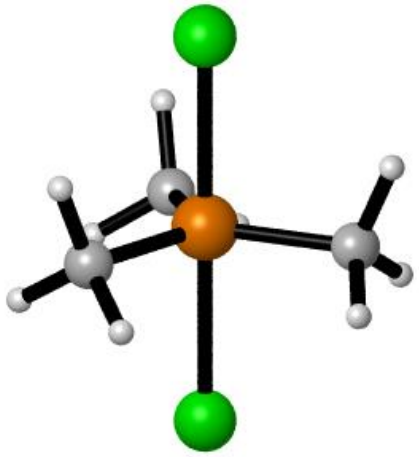
Zero-point correction=	0.109731 (Hartree/Particle)
Thermal correction to Energy=	0.116632
Thermal correction to Enthalpy=	0.117576
Thermal correction to Gibbs Free Energy=	0.080194
Sum of electronic and zero-point Energies=	-460.897852
Sum of electronic and thermal Energies=	-460.890951
Sum of electronic and thermal Enthalpies=	-460.890007
Sum of electronic and thermal Free Energies=	-460.927389

Charge = 0 Multiplicity = 1

P	0.00003400	-0.00000200	-0.61962900
C	1.64854600	-0.02213000	0.28643900
H	2.23886600	0.86097200	0.00025700
H	2.21541200	-0.92023900	-0.00049300
H	1.51042600	-0.02077700	1.37992400

C	-0.84346200	-1.41655700	0.28640300
H	-0.37392300	-2.36939300	0.00024900
H	-1.90467500	-1.45827600	-0.00051300
H	-0.77322000	-1.29762100	1.37988800
C	-0.80512000	1.43869100	0.28641000
H	-0.31040600	2.37862900	0.00000900
H	-0.73787400	1.31803800	1.37989800
H	-1.86490500	1.50867900	-0.00030200

Structure of PMe_3-Cl_2



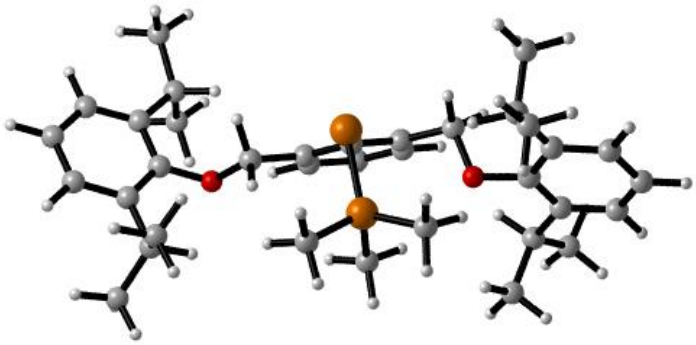
Zero-point correction=	0.114670 (Hartree/Particle)
Thermal correction to Energy=	0.124923
Thermal correction to Enthalpy=	0.125867
Thermal correction to Gibbs Free Energy=	0.079017
Sum of electronic and zero-point Energies=	-1381.356350
Sum of electronic and thermal Energies=	-1381.346096
Sum of electronic and thermal Enthalpies=	-1381.345152
Sum of electronic and thermal Free Energies=	-1381.392003

Charge = 0 Multiplicity = 1

Cl	2.34317700	0.00034000	-0.00024600
Cl	-2.37823000	0.00060100	0.00018500
P	-0.04994600	0.00008600	0.00001500

C	0.03532000	1.84722200	-0.07665700
H	0.60293500	2.10963200	-0.97772700
H	0.60389200	2.18301200	0.79907900
H	-0.96647700	2.28582900	-0.09421900
C	0.03530200	-0.85801700	1.63743400
H	0.60224700	-0.20921800	2.31607900
H	0.60437100	-1.78399500	1.48975600
H	-0.96649600	-1.06288500	2.02565300
C	0.03418400	-0.99091900	-1.56070900
H	0.60149200	-0.40104500	-2.29085600
H	-0.96796800	-1.22626900	-1.93029500
H	0.60226300	-1.90207700	-1.33706700

Structure of INT$_2$



Zero-point correction=	0.753499 (Hartree/Particle)
Thermal correction to Energy=	0.798433
Thermal correction to Enthalpy=	0.799377
Thermal correction to Gibbs Free Energy=	0.673567
Sum of electronic and zero-point Energies=	-2195.214749
Sum of electronic and thermal Energies=	-2195.169815
Sum of electronic and thermal Enthalpies=	-2195.168871
Sum of electronic and thermal Free Energies=	-2195.294681

Charge = 0 Multiplicity = 1

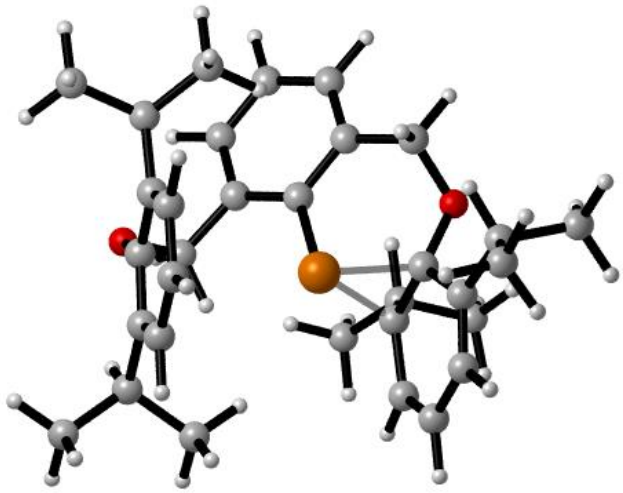
H	-0.47725300	4.15047900	-1.10083200
C	-0.34832100	3.17248200	-0.63477000
C	-0.02103000	0.61918600	0.58039400
C	0.90249500	2.77761900	-0.15165700
C	-1.44024400	2.30395900	-0.51090700
C	-1.28816900	1.03678400	0.08187100
C	1.07265800	1.52041200	0.46019700
H	1.76210900	3.44587600	-0.23607300
H	-2.41969300	2.59758700	-0.88291600
C	2.45043200	1.17012600	0.96074700
H	2.39578100	0.64683900	1.92559300
H	3.06173400	2.08107200	1.06669100
C	-2.49209900	0.11482100	0.19431400
H	-2.79186700	0.01530200	1.25212000
H	-2.23581800	-0.89994100	-0.14998400
P	0.15735600	-1.05953700	1.43704100
O	3.09595300	0.29462700	-0.01526300
O	-3.59671200	0.62782500	-0.58289500
C	-4.83944100	0.19904500	-0.12584800
C	-7.36360900	-0.58739300	0.75521700
C	-5.37019300	-1.02128100	-0.59034400
C	-5.53504000	1.03446400	0.78041700
C	-6.80907000	0.62080800	1.20594600
C	-6.64811400	-1.39790000	-0.13328400
H	-7.37097400	1.24404300	1.90132400

H	-7.07807800	-2.33938600	-0.47889800
H	-8.35220400	-0.89444000	1.09990200
C	4.48675400	0.28871400	0.05973400
C	7.27557200	0.26702600	0.09386900
C	5.14738000	-0.45516700	1.06226300
C	5.18872300	1.02572900	-0.92500400
C	6.59336500	0.99252500	-0.89453900
C	6.55633200	-0.44586600	1.05967800
H	7.15934900	1.54726400	-1.64283900
H	7.08921700	-1.00862300	1.82737800
H	8.36653000	0.25901800	0.10856400
C	-4.90996100	2.35884600	1.20892000
H	-3.82559300	2.19970000	1.30602600
C	-5.11368500	3.41611700	0.09783500
H	-4.60526700	4.35632500	0.36321000
H	-6.18683200	3.62585400	-0.03352100
H	-4.71184300	3.05403500	-0.85823000
C	-5.43170800	2.88605400	2.55776500
H	-4.86394800	3.78154500	2.85020200
H	-5.32848600	2.13089600	3.35097200
H	-6.49285500	3.17232400	2.49147100
C	-4.58599700	-1.92187200	-1.53758900
H	-3.68171300	-1.37730700	-1.84395300
C	-4.15303500	-3.21814000	-0.81603800
H	-3.54640300	-2.99327200	0.07361100
H	-3.56562000	-3.85969000	-1.49194200

H	-5.03592100	-3.78820500	-0.48811200
C	-5.39047700	-2.25213700	-2.81325300
H	-4.78534600	-2.86823600	-3.49622700
H	-5.68844800	-1.33362100	-3.33931400
H	-6.30258000	-2.81702300	-2.56747100
C	4.41030700	1.77003200	-2.00540900
H	3.47183400	2.12199700	-1.55264100
C	4.02693600	0.78936400	-3.13917700
H	4.93464500	0.40846200	-3.63325400
H	3.40574800	1.29502500	-3.89513700
H	3.46650500	-0.06623400	-2.73873900
C	5.15259600	2.99181000	-2.57723400
H	6.04640500	2.68889800	-3.14422000
H	5.47023000	3.67833500	-1.77842300
H	4.49226500	3.53760600	-3.26738400
C	4.38000700	-1.22673700	2.13076200
H	3.32088900	-1.25883400	1.83896100
C	4.47693200	-0.50777400	3.49602600
H	4.10337600	0.52414300	3.42935100
H	5.52386100	-0.46999600	3.83574900
H	3.88508000	-1.04424800	4.25336500
C	4.87403400	-2.68349200	2.26192000
H	5.90968300	-2.72147500	2.63247400
H	4.83923600	-3.20435600	1.29453700
H	4.24089900	-3.22953300	2.97789000
P	0.74848400	-2.13603600	-0.31823000

C	2.43445200	-2.90776100	-0.32350100
H	2.54092100	-3.53749600	0.56962100
H	3.18321400	-2.11034200	-0.29108300
H	2.56714400	-3.52495900	-1.22511600
C	-0.34170000	-3.60436500	-0.62797100
H	0.03948300	-4.20235300	-1.46967000
H	-1.36062800	-3.25915500	-0.84164000
H	-0.36591000	-4.22597300	0.27801100
C	0.68448300	-1.14692500	-1.87015300
H	-0.32485700	-0.73934800	-2.00679200
H	0.95305400	-1.78863500	-2.72160600
H	1.39802600	-0.32065300	-1.77508200

Structure of INT_3



Zero-point correction=	0.640707 (Hartree/Particle)
Thermal correction to Energy=	0.676916
Thermal correction to Enthalpy=	0.677860
Thermal correction to Gibbs Free Energy=	0.574746
Sum of electronic and zero-point Energies=	-1734.277006
Sum of electronic and thermal Energies=	-1734.240796

Sum of electronic and thermal Enthalpies= -1734.239852
Sum of electronic and thermal Free Energies= -1734.342967

Charge = 0 Multiplicity = 1

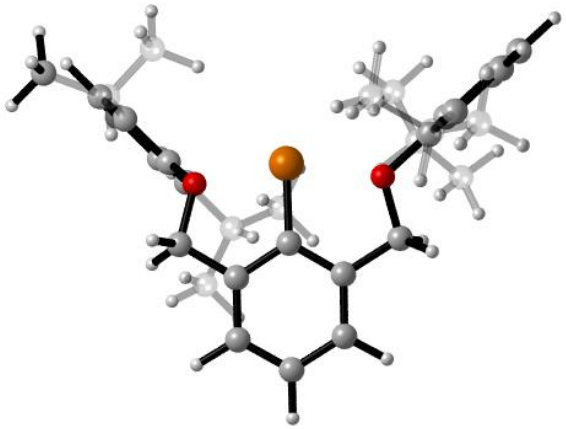
H	1.18610200	-4.90386300	-1.89666200
C	0.87008800	-3.91630900	-1.55899600
C	0.04880900	-1.34471700	-0.69588400
C	1.60358300	-2.77968200	-1.91564700
C	-0.28479000	-3.77164500	-0.77587800
C	-0.69051300	-2.50308700	-0.33890300
C	1.20711700	-1.49273200	-1.50212600
H	2.50068000	-2.87888900	-2.52982900
H	-0.87446000	-4.64707600	-0.49622400
C	2.07777000	-0.32141300	-1.91708200
H	1.49116900	0.60782800	-1.97237600
H	2.52086500	-0.51757700	-2.90287500
C	-1.91170700	-2.35451500	0.53872800
H	-1.60286200	-2.08647100	1.56515800
H	-2.48404500	-3.29049800	0.57806700
P	-0.46873700	0.31328700	-0.03776300
O	3.22060300	-0.12045400	-1.03903200
O	-2.83287200	-1.35979400	0.04133800
C	-2.38438300	-0.01875000	0.12780900
C	-2.91181400	2.78232300	-0.26479000
C	-2.04283600	0.65591300	-1.20123200
C	-3.07674000	0.78567500	1.17619100
C	-3.25566500	2.12571700	0.98151600

C	-2.38346400	2.08595500	-1.30777400
H	-3.71537600	2.72486300	1.76738600
H	-2.22183600	2.56919500	-2.27114400
H	-3.14067800	3.84325900	-0.37639300
C	2.90097700	0.47846100	0.18034200
C	2.29926300	1.67171900	2.63533600
C	2.69096700	1.87708300	0.23146600
C	2.83761900	-0.33181500	1.33802300
C	2.53675300	0.29363700	2.56236700
C	2.38574000	2.45298000	1.47688300
H	2.48780500	-0.31340400	3.46721400
H	2.21355700	3.52891000	1.53185500
H	2.05709100	2.13594600	3.59252200
C	-3.55924300	0.05842600	2.42189000
H	-2.88576600	-0.79645000	2.58955100
C	-3.52339800	0.93034900	3.69261700
H	-3.78336000	0.31830400	4.56902600
H	-4.25556700	1.74988700	3.63286600
H	-2.52667600	1.36783600	3.84836400
C	-4.98305800	-0.50862300	2.19812300
H	-5.30775100	-1.08497400	3.07897500
H	-5.00583100	-1.16018800	1.31560300
H	-5.69283600	0.31881100	2.04366000
C	-2.18962800	-0.16071400	-2.49713700
H	-1.91355400	-1.19716300	-2.27407200
C	-3.67032900	-0.15988600	-2.93320200

H	-4.30207000	-0.57010400	-2.13329600
H	-3.80039600	-0.77497700	-3.83712700
H	-4.01211700	0.86186600	-3.15883400
C	-1.26809800	0.34257900	-3.62026600
H	-1.37818500	-0.29691700	-4.50872700
H	-0.21673400	0.31888100	-3.30436500
H	-1.51569700	1.37213000	-3.92020300
C	3.15853400	-1.82135900	1.29025900
H	3.14966700	-2.13211800	0.23954900
C	2.12289500	-2.67905000	2.04466500
H	2.13023800	-2.45944400	3.12351700
H	2.35915900	-3.74650600	1.91815100
H	1.11160700	-2.49972600	1.65727300
C	4.58049300	-2.06782400	1.84584400
H	4.64073500	-1.75543900	2.90034500
H	5.32824600	-1.49632600	1.27647200
H	4.83672000	-3.13757000	1.78763500
C	2.79560500	2.76092400	-1.00771400
H	3.11160600	2.13122400	-1.85010600
C	3.87484400	3.85135000	-0.82209800
H	4.85298400	3.40226400	-0.59609300
H	3.60936300	4.52765600	0.00464900
H	3.96749200	4.45462400	-1.73846600
C	1.43373300	3.40297000	-1.35843400
H	1.09838900	4.05994800	-0.54135100
H	0.65537500	2.64142000	-1.50780900

H	1.52140700	4.00984800	-2.27326500

Structure of INT_3^I



Zero-point correction=	0.639630 (Hartree/Particle)
Thermal correction to Energy=	0.676718
Thermal correction to Enthalpy=	0.677662
Thermal correction to Gibbs Free Energy=	0.570960
Sum of electronic and zero-point Energies=	-1734.259008
Sum of electronic and thermal Energies=	-1734.221920
Sum of electronic and thermal Enthalpies=	-1734.220976
Sum of electronic and thermal Free Energies=	-1734.327678

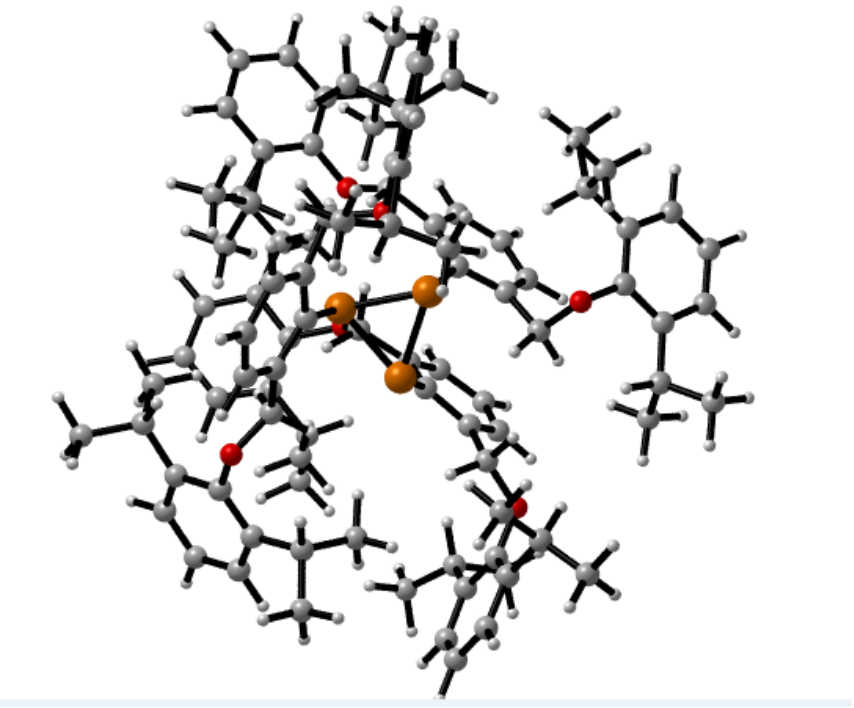
Charge = 0 Multiplicity = 1

H	0.19362200	3.79239400	4.27974400
C	0.15194000	2.98836500	3.54534500
C	0.03632600	0.87777100	1.62656000
C	1.29075500	2.21083800	3.27400800
C	-1.04220100	2.71534100	2.85381200
C	-1.09886400	1.69425900	1.89994600
C	1.23220600	1.16544700	2.34623000
H	2.22806800	2.41079200	3.79858400
H	-1.93374200	3.31691000	3.04631300
C	2.41807000	0.27313900	2.07913800
H	2.55952800	-0.48554900	2.86864000
H	3.35261900	0.83714500	1.95184000
C	-2.33454700	1.46756900	1.06680400
H	-2.41875300	2.20278800	0.24725700
H	-3.26375700	1.49512000	1.65963700
P	-0.00104500	-0.44098700	0.39765400
O	2.14698300	-0.47600800	0.84617700
O	-2.19992800	0.14055300	0.48499200
C	-3.18645600	-0.20907900	-0.45582200
C	-5.16738900	-0.96585400	-2.24258400
C	-3.10827200	0.27160200	-1.77668700
C	-4.21466500	-1.06100700	0.00537800
C	-5.20470000	-1.43349100	-0.92030600
C	-4.13072900	-0.12565900	-2.66159300
H	-6.01493600	-2.08897700	-0.60350900

H	-4.10179000	0.23188000	-3.69155200
H	-5.94777100	-1.26105800	-2.94542300
C	3.13388400	-0.46102800	-0.16537200
C	5.06596800	-0.54683900	-2.15074900
C	3.33952800	0.69627300	-0.94094100
C	3.85564200	-1.66110300	-0.34326000
C	4.82493100	-1.68085500	-1.36198000
C	4.33276100	0.62536700	-1.93766500
H	5.40255300	-2.58853500	-1.53199300
H	4.52222600	1.50608600	-2.55215500
H	5.82718300	-0.57968200	-2.93146300
C	-4.19026700	-1.58029800	1.44050300
H	-3.82943800	-0.76276500	2.08325000
C	-5.57154600	-2.01656400	1.96272000
H	-5.49801800	-2.26924600	3.03039900
H	-5.93220700	-2.91246100	1.43419400
H	-6.32110800	-1.22035100	1.84069400
C	-3.17096900	-2.73884600	1.56275700
H	-3.13517600	-3.10290500	2.60149100
H	-2.16368300	-2.40772500	1.27282800
H	-3.47171000	-3.57526200	0.91234200
C	-1.98572900	1.18196900	-2.26393200
H	-1.24707600	1.28451200	-1.45797800
C	-1.24869800	0.55703200	-3.46791800
H	-0.80109200	-0.40746100	-3.18931200
H	-0.44664400	1.22919800	-3.80727000

H	-1.93457900	0.39338400	-4.31294500
C	-2.52646900	2.58436200	-2.62041500
H	-1.70025500	3.23945300	-2.93636800
H	-3.03140700	3.04993200	-1.76014700
H	-3.25325800	2.52393500	-3.44526000
C	3.54601500	-2.88629000	0.51251400
H	3.26153900	-2.52745500	1.51319300
C	4.74443500	-3.84055200	0.67612700
H	4.99783800	-4.33108800	-0.27621300
H	4.48879100	-4.63085600	1.39681600
H	5.63756200	-3.30984900	1.03810400
C	2.32689100	-3.64186100	-0.06842500
H	2.55042300	-3.99136100	-1.08850900
H	1.44170800	-2.99221100	-0.10403500
H	2.09131600	-4.51814800	0.55530700
C	2.56196900	1.98889900	-0.72676800
H	1.75320100	1.79413000	-0.01772900
C	1.89810600	2.47527100	-2.03249400
H	1.23863600	1.69673900	-2.43816600
H	2.64865100	2.73290600	-2.79557900
H	1.29643900	3.37454600	-1.83036900
C	3.47154900	3.08536300	-0.12943500
H	4.29444200	3.32847800	-0.81956000
H	3.91342200	2.76278900	0.82516000
H	2.88901900	4.00103000	0.05261800

Structure of INT$_4$



Zero-point correction=	1.930953 (Hartree/Particle)
Thermal correction to Energy=	2.043438
Thermal correction to Enthalpy=	2.044382
Thermal correction to Gibbs Free Energy=	1.778564
Sum of electronic and zero-point Energies=	-5203.017335
Sum of electronic and thermal Energies=	-5202.904851
Sum of electronic and thermal Enthalpies=	-5202.903907
Sum of electronic and thermal Free Energies=	-5203.169725

Charge = 0 Multiplicity = 1

H	-2.05861400	2.11328400	-4.76059300
C	-1.92112300	1.95475700	-3.69076700
C	-1.50294900	1.47025900	-0.92719900
C	-2.62537800	0.94516800	-3.03331100
C	-1.05978000	2.77682200	-2.95571200
C	-0.85246400	2.55517600	-1.58679900
C	-2.45018800	0.70474500	-1.65479500
H	-3.31233400	0.31275400	-3.58943300
H	-0.53194300	3.59868800	-3.43771900

C	-3.36244500	-0.31998200	-1.01317000
H	-4.39902200	0.05320000	-1.04498600
H	-3.10780700	-0.47998700	0.04011900
C	-0.00756300	3.57586800	-0.85554100
H	0.79500600	3.92603900	-1.51567600
H	0.44099100	3.17806500	0.05790200
P	-1.03546600	1.18916100	0.87306100
O	-3.28943300	-1.57654800	-1.72518400
O	-0.80526900	4.70518300	-0.39812200
C	-1.16931700	5.57182900	-1.42709800
C	-1.91908000	7.28736500	-3.49367700
C	-0.20225900	6.45073300	-1.96835300
C	-2.51053700	5.54703900	-1.87871200
C	-2.86498500	6.42750900	-2.91682100
C	-0.60284700	7.30036800	-3.01633000
H	-3.88995700	6.43105100	-3.28739400
H	0.12770000	7.98448900	-3.45152600
H	-2.21193200	7.95316700	-4.30699800
C	-4.36300200	-2.44375300	-1.48134900
C	-6.44018500	-4.27092000	-1.12457500
C	-5.51257500	-2.33940700	-2.30064400
C	-4.24694600	-3.41768200	-0.46438700
C	-5.30230100	-4.33620100	-0.31294600
C	-6.54532400	-3.27451600	-2.10334500
H	-5.23434100	-5.10216300	0.45927700
H	-7.44163800	-3.22086500	-2.71974800

H	-7.24966400	-4.98959400	-0.98957100
C	-3.53127500	4.64014900	-1.19850500
H	-3.00415500	3.73425500	-0.87690500
C	-4.06804600	5.33348200	0.07574000
H	-3.24200700	5.57717000	0.75812100
H	-4.77474500	4.67553500	0.60546700
H	-4.59233300	6.26615100	-0.18620300
C	-4.68604400	4.20352800	-2.11738800
H	-5.33295200	5.05273900	-2.38795400
H	-5.31056700	3.46433700	-1.59523600
H	-4.30240500	3.74658600	-3.04068100
C	1.22610300	6.51099000	-1.43155700
H	1.29065300	5.84141600	-0.56340800
C	2.25463000	6.04196500	-2.48622600
H	2.27234100	6.73588100	-3.34097100
H	2.01350900	5.04027400	-2.87136300
H	3.26358700	6.00560200	-2.04772500
C	1.57694500	7.93043100	-0.93286200
H	2.59210400	7.94131300	-0.50672200
H	0.86732500	8.26124000	-0.16081600
H	1.54706800	8.65595900	-1.75988900
C	-3.01604800	-3.47300700	0.42906100
H	-2.63177800	-2.44979500	0.50728200
C	-1.88591200	-4.30290400	-0.21191300
H	-0.99198200	-4.28703100	0.42855800
H	-1.61289900	-3.90170500	-1.19326900

H	-2.19867700	-5.35103300	-0.33868700
C	-3.30855000	-3.96531600	1.85900700
H	-4.15517800	-3.42309400	2.30513600
H	-2.42170400	-3.80782300	2.48910700
H	-3.54507400	-5.04002900	1.87346900
C	-5.59133200	-1.27051000	-3.38752900
H	-5.17784900	-0.34089300	-2.97046000
C	-7.02432800	-0.95009200	-3.85077200
H	-7.00353900	-0.09699000	-4.54434200
H	-7.67453000	-0.69645700	-3.00052100
H	-7.47127700	-1.80251700	-4.38470500
C	-4.71086700	-1.67108600	-4.59309400
H	-5.10322100	-2.58882200	-5.05695600
H	-3.67862000	-1.85733300	-4.27458500
H	-4.71123800	-0.87402900	-5.35349500
H	2.40689600	1.88257400	-4.76711500
C	2.19643900	1.53003900	-3.75673400
C	1.57592700	0.65773000	-1.13017600
C	2.76860300	2.17084000	-2.65666700
C	1.38794100	0.40832300	-3.55810300
C	1.08734900	-0.05456800	-2.26623700
C	2.48929600	1.73735800	-1.34881100
H	3.46267900	2.99517400	-2.79755700
H	0.99618400	-0.14098600	-4.41076100
C	3.18868700	2.45914000	-0.19668300
H	3.45695700	1.74840300	0.59509200

H	2.53013700	3.21793400	0.25530100
C	0.29726300	-1.34845300	-2.15665900
H	-0.76781100	-1.16062800	-1.96313100
H	0.68311100	-1.95000200	-1.32687700
P	1.11576200	0.47220700	0.67766600
O	4.38283400	3.13204200	-0.65527200
O	0.38783500	-2.11556400	-3.37933200
C	0.70210200	-3.45919900	-3.19431300
C	1.26892500	-6.16347600	-2.84846500
C	2.01038600	-3.83315500	-2.80899000
C	-0.32195400	-4.40471400	-3.43925900
C	-0.01036300	-5.76401500	-3.26239400
C	2.26578200	-5.20569400	-2.62917000
H	-0.78126400	-6.51475500	-3.43433600
H	3.26177200	-5.51928100	-2.31493300
H	1.48738200	-7.22208100	-2.70006500
C	5.53810600	2.80129000	0.05375200
C	7.86611200	2.14887100	1.43503100
C	6.44760100	1.89533600	-0.53960200
C	5.75852800	3.38054800	1.32138800
C	6.93780200	3.02739800	2.00545900
C	7.62415000	1.59663200	0.16888800
H	7.12710600	3.45130000	2.99240100
H	8.34517900	0.90008500	-0.25832600
H	8.77627800	1.88896600	1.97728200
C	-1.68838800	-3.92518100	-3.92341900

H	-1.93406200	-3.01440900	-3.35752500
C	-1.59880200	-3.53391000	-5.41870000
H	-0.84482800	-2.74967200	-5.56872400
H	-2.57063100	-3.16349100	-5.77782700
H	-1.31881200	-4.41168900	-6.02223200
C	-2.82567800	-4.93895800	-3.70637600
H	-2.87944100	-5.26699600	-2.66008100
H	-2.69220000	-5.82656900	-4.34492900
H	-3.78627600	-4.47421900	-3.96768300
C	3.11870600	-2.80017200	-2.62353600
H	2.76772400	-1.85436900	-3.05481900
C	3.45261300	-2.55433000	-1.13612600
H	4.23739400	-1.79007800	-1.04926400
H	3.81622500	-3.47263900	-0.65772700
H	2.58006800	-2.20218200	-0.57056100
C	4.40431700	-3.19846700	-3.38194000
H	4.19531600	-3.39289000	-4.44406400
H	4.85856600	-4.10244600	-2.94844000
H	5.14348000	-2.38664800	-3.30938800
C	4.73945500	4.32494200	1.95092200
H	4.04405100	4.63856000	1.15957500
C	5.39644100	5.59978200	2.52148800
H	5.98503600	6.11984800	1.75180700
H	6.06522200	5.36026200	3.36183700
H	4.62086600	6.28519200	2.89518700
C	3.92759900	3.59800700	3.04891000

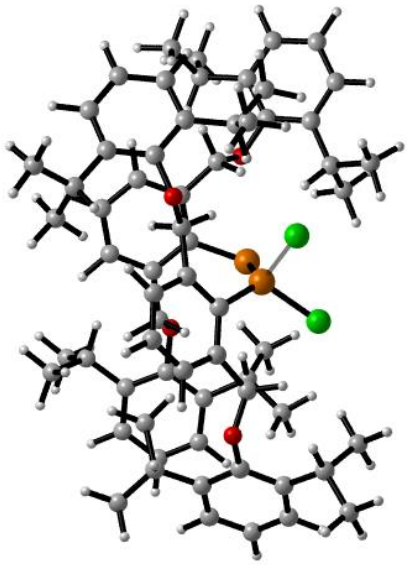
H	4.59889800	3.25010600	3.84939500
H	3.39720500	2.72317400	2.64691900
H	3.18543500	4.27940600	3.49263000
C	6.12261100	1.27972100	-1.89674100
H	5.04367000	1.07063600	-1.90600000
C	6.85474200	-0.04486900	-2.17548800
H	6.49645400	-0.46743000	-3.12559100
H	6.67414400	-0.78261200	-1.37942500
H	7.94171600	0.10527500	-2.26734000
C	6.39546200	2.29858900	-3.02748100
H	7.47009400	2.53450200	-3.07675100
H	5.84293400	3.23067900	-2.84861800
H	6.08532300	1.88387900	-3.99929700
H	-0.31963300	-2.33284500	6.54764600
C	-0.36199400	-2.07510300	5.48897600
C	-0.46024500	-1.37320400	2.74416500
C	0.74806600	-2.29765700	4.66603100
C	-1.53653400	-1.56323300	4.93339800
C	-1.60721900	-1.21604400	3.57160100
C	0.70864000	-1.97415400	3.29845000
H	1.65333300	-2.74228800	5.07315100
H	-2.42633100	-1.43669000	5.55078900
C	1.90259800	-2.30442200	2.42207300
H	2.38509900	-1.38229900	2.05966200
H	1.56919100	-2.86653100	1.53045100
C	-2.95973300	-0.74756100	3.07028700

H	-3.74591400	-1.27553900	3.62949100
H	-3.10403300	-0.98442200	2.00728900
P	-0.54231000	-1.00482000	0.90411700
O	2.86467000	-3.08308700	3.14679700
O	-3.11388500	0.68089600	3.26521300
C	-4.32762100	1.08375100	3.81845700
C	-6.72518900	1.95591900	4.95583300
C	-5.49780700	1.09988000	3.02244000
C	-4.32844700	1.51239600	5.16547200
C	-5.54695600	1.95556000	5.71281600
C	-6.69524400	1.53070000	3.62097200
H	-5.56641700	2.29742000	6.74882200
H	-7.61004300	1.54282000	3.02701700
H	-7.66222200	2.29332500	5.40125600
C	3.85215600	-3.61289900	2.31497300
C	5.83826100	-4.71815100	0.70297400
C	3.65168100	-4.90413700	1.78031200
C	5.01433100	-2.85379700	2.05504100
C	6.00278500	-3.43408800	1.23924300
C	4.66997000	-5.44386400	0.97322700
H	6.90744100	-2.86581400	1.01913000
H	4.53669000	-6.44057700	0.55011100
H	6.61543500	-5.14906900	0.07013600
C	-3.05331300	1.53237900	6.00059900
H	-2.26228800	1.04369700	5.41884300
C	-2.60817000	2.98688200	6.27253200

H	-3.37693900	3.52552200	6.84846300
H	-2.44428200	3.52757300	5.32919300
H	-1.67147800	2.99988700	6.85144900
C	-3.22081800	0.75694200	7.32472100
H	-2.26518400	0.72831900	7.87011300
H	-3.55016500	-0.27747800	7.14323500
H	-3.96822200	1.23747500	7.97461300
C	-5.46464400	0.65902700	1.56343100
H	-4.41071000	0.63983700	1.26109200
C	-6.05206900	-0.76044300	1.39261100
H	-7.11424400	-0.76504100	1.68222400
H	-5.52639100	-1.49073000	2.02314400
H	-5.97567600	-1.09594000	0.34799800
C	-6.18629200	1.65305100	0.62961100
H	-5.76380800	2.66280100	0.72657400
H	-7.26214700	1.70469900	0.85340600
H	-6.08279100	1.33052900	-0.41824400
C	5.17758000	-1.43905500	2.60022600
H	4.38516100	-1.27497900	3.34395500
C	5.00946300	-0.39766700	1.47262100
H	4.02928700	-0.48561200	0.98377100
H	5.78032400	-0.53490600	0.70324300
H	5.12067000	0.62104900	1.86954300
C	6.53600500	-1.23593600	3.30507800
H	6.59706100	-0.21513600	3.71107700
H	7.36985600	-1.36092300	2.59783400

H	6.66945100	-1.95522300	4.12637700
C	2.36560200	-5.68143700	2.03957700
H	1.76429000	-5.10603000	2.75657700
C	2.65263300	-7.06221500	2.66791400
H	3.21178100	-6.95989300	3.60942700
H	3.24523700	-7.68853100	1.98351900
H	1.70785100	-7.58804200	2.87493700
C	1.55025300	-5.83742700	0.73756200
H	1.33941600	-4.86596900	0.26926000
H	0.59257500	-6.34070800	0.94023500
H	2.10341500	-6.43735800	0.00121300

Structure of INT_5



Zero-point correction=	1.289671 (Hartree/Particle)
Thermal correction to Energy=	1.367770
Thermal correction to Enthalpy=	1.368714
Thermal correction to Gibbs Free Energy=	1.174703
Sum of electronic and zero-point Energies=	-4389.092151
Sum of electronic and thermal Energies=	-4389.014052
Sum of electronic and thermal Enthalpies=	-4389.013108
Sum of electronic and thermal Free Energies=	-4389.207119

Charge = 0 Multiplicity = 1

C	0.79158000	-0.29196800	-2.00601300
C	1.61927800	1.63621800	-3.89597800
C	2.16760800	-0.21514600	-2.39194600
C	-0.14367800	0.65150700	-2.53326400
C	0.29161200	1.59765300	-3.47547800
C	2.54479600	0.74715700	-3.34485100
H	-0.43371200	2.30373500	-3.86984100
H	3.58849100	0.79012000	-3.64144500
H	1.94116100	2.36838300	-4.63679900
C	-1.56874500	0.80823500	-2.03621100
H	-1.59095200	1.67621500	-1.36115900
H	-1.90150200	-0.05557300	-1.44753900
C	3.26849600	-1.11533600	-1.83487100
H	3.25935700	-1.09005200	-0.73288700
H	3.10257100	-2.15583200	-2.14490200
O	-2.49329500	1.02994500	-3.11919600
O	4.55164300	-0.68752400	-2.32629700
C	-1.03564900	0.63164300	1.02293900
C	-2.03451500	3.28050600	1.12144500
C	-2.43641900	0.87629800	1.00786000
C	-0.14413400	1.73426600	1.08541700
C	-0.65575000	3.04443200	1.13564500
C	-2.91685000	2.19597500	1.05611500
H	0.04446800	3.87979100	1.17873900
H	-3.99234300	2.36670500	1.00601300

H	-2.41839500	4.29999200	1.14451900
C	1.35233500	1.56019300	1.15220100
H	1.85374800	2.49453000	0.86030600
H	1.70164900	0.76023500	0.48237000
C	-3.45176300	-0.22945400	0.85345900
H	-4.41897300	0.20522500	0.56246900
H	-3.15410500	-0.93624200	0.06183900
O	1.69686700	1.22549400	2.52069800
O	-3.59226200	-0.95275400	2.09966900
P	-0.40584800	-1.12297400	1.14606300
P	0.10709700	-1.55654900	-0.82387900
Cl	1.30472200	-3.25261500	-0.59935100
C	-3.69547500	1.57387600	-2.63600600
C	-6.01347700	2.66669100	-1.53775500
C	-3.83923400	2.97926400	-2.60926200
C	-4.72097900	0.69719100	-2.20440200
C	-5.87954800	1.27548200	-1.65442500
C	-5.00958900	3.50720400	-2.02993600
H	-6.68458600	0.62949500	-1.30785400
H	-5.13636600	4.58898000	-1.98106000
H	-6.91249500	3.09037500	-1.08826300
C	-2.78962900	3.90108700	-3.22570800
H	-2.19151200	3.28669900	-3.91068600
C	-3.42972000	5.02547600	-4.06952200
H	-3.97809500	5.73935000	-3.43657600
H	-4.12996200	4.61558200	-4.81135300

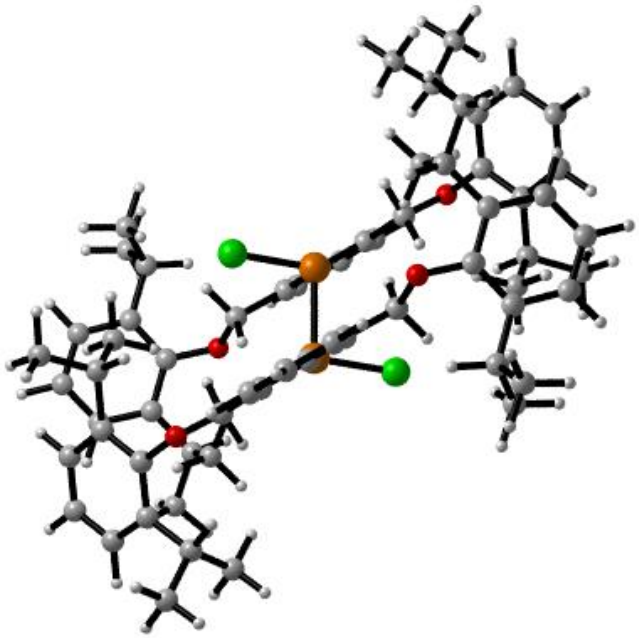
H	-2.64363100	5.58534200	-4.59804200
C	-1.84388200	4.50952500	-2.16707000
H	-2.42040400	5.10313200	-1.44108800
H	-1.11088300	5.17442300	-2.65016200
H	-1.29676500	3.73888700	-1.60948200
C	-4.58508000	-0.80951500	-2.40355900
H	-3.58295100	-1.10640000	-2.07162100
C	-5.60668800	-1.65010500	-1.61719800
H	-6.62744600	-1.48759900	-1.99729900
H	-5.59948800	-1.42621400	-0.54232300
H	-5.37014100	-2.71605800	-1.74136700
C	-4.66575900	-1.15033000	-3.91152200
H	-5.65460700	-0.87519800	-4.31082100
H	-4.51912900	-2.23114100	-4.05922000
H	-3.89198600	-0.61125800	-4.47246100
C	5.62201800	-0.89924600	-1.45478500
C	7.73260900	-1.26400400	0.32694900
C	6.14477900	-2.19821300	-1.27823000
C	6.18716500	0.23885300	-0.82951300
C	7.24156100	0.02534700	0.07510500
C	7.20035300	-2.35944700	-0.36025600
H	7.68483600	0.87757300	0.58719800
H	7.60602100	-3.35808100	-0.19346200
H	8.54467000	-1.40766000	1.04107800
C	5.62098200	-3.39890600	-2.05867800
H	4.89281200	-3.03497900	-2.79578900

C	6.75678200	-4.08911500	-2.84727100
H	7.51587100	-4.49920200	-2.16431500
H	7.25309600	-3.38005500	-3.52559500
H	6.35062700	-4.92102100	-3.44255300
C	4.91870000	-4.41016500	-1.12664900
H	5.63419100	-4.81289100	-0.39338200
H	4.51108300	-5.25144000	-1.70768900
H	4.10074400	-3.93526400	-0.56981100
C	5.66863700	1.63572200	-1.16631900
H	5.44181100	1.63690700	-2.24364800
C	4.35839900	1.94702400	-0.41482400
H	4.54117900	1.97743200	0.66507800
H	3.59221000	1.19262600	-0.61839900
H	3.96322400	2.92517000	-0.73207900
C	6.69416000	2.75240200	-0.89276300
H	6.85969200	2.87567800	0.18851400
H	6.30971000	3.70745500	-1.28010400
H	7.66203400	2.54253400	-1.37138600
C	-4.75141100	-1.73474400	2.08784800
C	-7.07392600	-3.27051500	2.04295600
C	-5.96516400	-1.14209300	2.49726900
C	-4.66649200	-3.07741500	1.65334600
C	-5.85169200	-3.83434400	1.64772300
C	-7.12616400	-1.93742800	2.46642900
H	-5.82048500	-4.87227600	1.31749600
H	-8.07594300	-1.49990400	2.77838500

H	-7.98320600	-3.87316200	2.02168900
C	-6.02973600	0.30852600	2.96376000
H	-5.00682400	0.70852100	2.95906000
C	-6.88857200	1.16753000	2.00968200
H	-6.91480700	2.21300300	2.35523000
H	-7.92352800	0.79302100	1.97647800
H	-6.48792700	1.15107100	0.98650100
C	-6.56407600	0.40349600	4.40994000
H	-7.59507900	0.02244800	4.47148500
H	-6.56760400	1.45172200	4.74658000
H	-5.94025800	-0.18460100	5.09848800
C	-3.31773800	-3.66884900	1.25902800
H	-2.72667900	-2.87476600	0.78226000
C	-3.41704200	-4.83654800	0.26162700
H	-4.00209700	-4.55557000	-0.62636500
H	-3.88765000	-5.71974700	0.72127200
H	-2.40859100	-5.12587700	-0.06646400
C	-2.54000200	-4.09343800	2.52615500
H	-2.41064100	-3.23793500	3.20258200
H	-1.54448100	-4.47534700	2.25149700
H	-3.08462400	-4.88799600	3.06058200
C	3.06438400	1.36304600	2.77142500
C	5.79652300	1.63654700	3.23524200
C	3.88366800	0.21321300	2.69485200
C	3.57463400	2.64020200	3.08528200
C	4.95892100	2.75453200	3.31643000

C	5.25891600	0.37587000	2.93423500
H	5.37641700	3.73410400	3.55435400
H	5.92190400	-0.48340800	2.85447300
H	6.86879000	1.74301100	3.40623900
C	3.25548500	-1.14003300	2.38275500
H	2.51134400	-0.98211800	1.58611400
C	4.26201200	-2.19315600	1.89363600
H	4.95989100	-2.47733400	2.69668700
H	4.85399900	-1.83015400	1.04415400
H	3.72320800	-3.10013900	1.58555300
C	2.47735500	-1.66600100	3.61156700
H	3.16977500	-1.84390500	4.44955100
H	1.97730500	-2.61508200	3.36460000
H	1.71627000	-0.94146400	3.92808800
C	2.67527800	3.86902700	3.15377500
H	1.63835100	3.53478600	3.01415200
C	2.76171600	4.55262200	4.53590500
H	3.78154600	4.91926800	4.72858000
H	2.49280800	3.85036300	5.33797400
H	2.07725300	5.41383800	4.57813000
C	3.02035700	4.87397500	2.03129800
H	2.34011600	5.73930700	2.06706700
H	2.94570400	4.40859900	1.03723400
H	4.05052000	5.24379700	2.14922500
Cl	-1.31749300	-2.57731000	-2.24162300

Structure of INT_6



Zero-point correction=	1.287914 (Hartree/Particle)
Thermal correction to Energy=	1.366879
Thermal correction to Enthalpy=	1.367823
Thermal correction to Gibbs Free Energy=	1.169408
Sum of electronic and zero-point Energies=	-4389.121804
Sum of electronic and thermal Energies=	-4389.042840
Sum of electronic and thermal Enthalpies=	-4389.041895
Sum of electronic and thermal Free Energies=	-4389.240310

Charge = 0 Multiplicity = 1

P	-0.55185100	-0.82008500	-0.60015400
Cl	0.88970900	-1.02958100	-2.16410200
P	0.55186400	0.82007800	0.60014300
Cl	-0.88967900	1.02956800	2.16410700
C	-0.30748700	-2.28146000	0.52589000
C	-1.53753200	-2.84953400	0.98542900
C	-1.51435000	-3.94638800	1.86134000
H	-2.45579100	-4.35963100	2.21412900
C	-0.29762600	-4.50075400	2.27075000

C	0.91002600	-3.96168500	1.81894800
H	1.85800200	-4.38454700	2.14275900
C	0.92735500	-2.85039200	0.95739800
C	0.30748700	2.28145500	-0.52589500
C	-0.92735900	2.85039200	-0.95738300
C	-0.91003900	3.96169300	-1.81892300
H	-1.85801800	4.38455900	-2.14272000
C	0.29760900	4.50076400	-2.27073600
C	1.51433600	3.94639000	-1.86134800
H	2.45577400	4.35963200	-2.21414800
C	1.53752800	2.84952800	-0.98544700
H	-0.29077800	-5.35717900	2.94607100
H	0.29075400	5.35719500	-2.94604900
C	-2.88469700	-2.28569500	0.54374200
H	-2.99764200	-2.37593100	-0.55126400
H	-2.96254300	-1.21309100	0.78859700
C	2.27203100	-2.32844200	0.48340700
H	2.27795000	-1.22887800	0.46745300
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C	-7.69278300	-1.63859000	-0.09929800
C	-5.84699600	-3.23158100	-0.27703200
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C	-7.10518600	-2.76156000	-0.69625700

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C	-5.06101500	-0.67033900	2.52432600
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C	-5.93475700	-0.59390100	3.79551800
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H	-5.38225200	-0.09085000	4.60374000
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H	-4.00684800	0.70864100	1.17898300
H	-4.09719800	1.26011900	2.87018400
C	-5.19600400	-4.42594200	-0.96509100
H	-4.26781100	-4.65931500	-0.42601500
C	-4.82991800	-4.08562100	-2.42762100
H	-4.34372300	-4.94697000	-2.91103700
H	-4.14779400	-3.22485600	-2.47588000
H	-5.73355000	-3.83210800	-3.00325500
C	-6.10325800	-5.67432800	-0.90828800
H	-5.59739500	-6.53313900	-1.37539700
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H	-6.35075700	-5.93487400	0.13110900
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H	2.99766100	2.37591400	0.55121900
H	2.96252800	1.21307400	-0.78864100

O	3.95197800	2.98802600	-1.19722000
C	5.20429400	2.53919200	-0.77203300
C	7.69277700	1.63859600	0.09927200
C	5.84698600	3.23158800	0.27696700
C	5.77709100	1.41258600	-1.40197800
C	7.03130600	0.97405800	-0.94186500
C	7.10517600	2.76157700	0.69620600
H	7.47995600	0.09128400	-1.39664000
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H	8.66390100	1.28145500	0.44514300
C	5.06102400	0.67029400	-2.52434900
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C	5.93478400	0.59381900	-3.79552600
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H	4.09722900	-1.26017600	-2.87019600
H	4.00678600	-0.70864400	-1.17902000
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C	4.82990900	4.08567400	2.42754000
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H	4.34371100	4.94703300	2.91093500
H	5.73354400	3.83218100	3.00317800

C	6.10323900	5.67435000	0.90816400
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H	7.04506800	5.49969600	1.45055900
H	5.59737500	6.53317000	1.37525500
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H	-2.27794600	1.22887200	-0.46743900
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C	-5.56202400	1.95866700	-1.33421700
C	-6.85558300	2.00183700	-0.78588900
C	-6.21010600	3.78206700	0.72584900
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C	-3.89548800	4.82037200	0.70034000
H	-2.97344600	4.72290200	0.11240900
C	-5.19443600	1.00659900	-2.47078700
H	-4.47472200	1.53530600	-3.11325000
C	-6.40083300	0.59412400	-3.33703100
H	-6.96688500	1.46958400	-3.68829700
H	-7.08343700	-0.06003400	-2.77339100
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C	-4.49608000	-0.26067300	-1.93021700

H	-5.17415500	-0.81332400	-1.26944200
H	-3.58659400	-0.01411100	-1.37094400
H	-4.21093800	-0.91926900	-2.76525400
C	-4.41951500	6.25654800	0.47321900
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H	-4.64899000	6.42719700	-0.58867100
H	-3.66317600	6.98974300	0.79272600
C	-3.55006800	4.60120200	2.19061800
H	-4.45054100	4.71936900	2.81264800
H	-2.80296000	5.33758100	2.52385500
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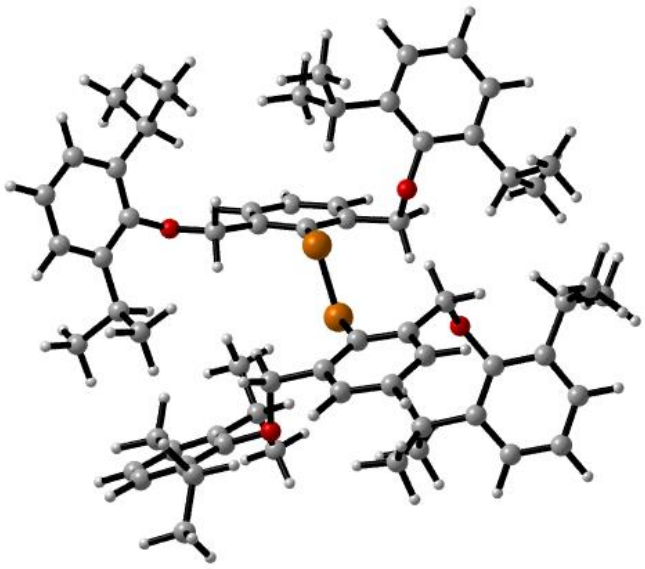
O	3.31376600	-2.79913800	1.35400000
C	4.59113300	-2.83740600	0.79648600
C	7.17836600	-2.89290300	-0.24728900
C	5.56200800	-1.95863800	1.33425800
C	4.90283800	-3.78608800	-0.20400300
C	6.21012600	-3.78206300	-0.72577400
C	6.85557100	-2.00180200	0.78594100
H	6.46676300	-4.49883000	-1.50716900
H	7.61780500	-1.32639400	1.16965700
H	8.18664500	-2.90400000	-0.66389700
C	5.19440000	-1.00655400	2.47080800
H	4.47466800	-1.53524800	3.11326200
C	4.49606500	0.26071700	1.93020600
H	3.58659000	0.01415500	1.37091500
H	5.17415900	0.81335600	1.26944000

H	4.21090800	0.91932400	2.76522900
C	6.40078100	-0.59407700	3.33707300
H	6.96682000	-1.46953700	3.68836000
H	6.04804900	-0.02883400	4.21232500
H	7.08340200	0.06007100	2.77344000
C	3.89551600	-4.82038700	-0.70027300
H	2.97346800	-4.72291600	-0.11235100
C	4.41955100	-6.25655600	-0.47313100
H	3.66322000	-6.98976100	-0.79263600
H	4.64901800	-6.42719100	0.58876300
H	5.33618000	-6.43712700	-1.05449100
C	3.55010600	-4.60123700	-2.19055600
H	2.80300800	-5.33762600	-2.52379100
H	4.45058500	-4.71940300	-2.81257700
H	3.14992700	-3.59253300	-2.36928600

Structure of INT_7



Zero-point correction=	1.284107 (Hartree/Particle)
Thermal correction to Energy=	1.359435
Thermal correction to Enthalpy=	1.360379
Thermal correction to Gibbs Free Energy=	1.170864
Sum of electronic and zero-point Energies=	-3468.651118
Sum of electronic and thermal Energies=	-3468.575790
Sum of electronic and thermal Enthalpies=	-3468.574846
Sum of electronic and thermal Free Energies=	-3468.764361

Charge = 0 Multiplicity = 1

C	0.08419800	2.02051800	0.85034500
C	0.35653200	3.54229900	3.20924300
C	1.36011800	2.47277300	1.26589200
C	-1.06490900	2.37587000	1.60601000
C	-0.91307000	3.13615200	2.77791500
C	1.48795300	3.22139900	2.44839700
H	-1.80190800	3.40995800	3.34887600
H	2.47814700	3.54985900	2.75804300
H	0.46315600	4.12615700	4.12408000
C	-2.45852600	1.96995000	1.16205100

H	-3.21376700	2.40266100	1.83468400
H	-2.58477300	0.87917000	1.16236400
C	2.56554600	2.16322700	0.39802000
H	2.63278500	1.07869400	0.19783900
H	2.43992700	2.66220600	-0.58181800
O	-2.72475700	2.38609800	-0.20767800
O	3.77747500	2.60770800	1.01717700
C	-0.75560700	-1.90582400	-1.22044000
C	-1.38460200	-3.79720000	-3.22867400
C	0.25476100	-2.73602800	-1.76415500
C	-2.09225100	-2.02826300	-1.69457800
C	-2.38686500	-2.98167500	-2.68369200
C	-0.07032500	-3.66494400	-2.77056500
H	-3.41722100	-3.07513000	-3.03095300
H	0.72360100	-4.28876500	-3.18484800
H	-1.62945100	-4.52788000	-3.99986900
C	-3.22539400	-1.17106800	-1.15459900
H	-4.10768400	-1.27793800	-1.80360300
H	-2.94781800	-0.11025800	-1.11324500
C	1.68241300	-2.70974800	-1.26637600
H	2.38332700	-2.85292300	-2.10512100
H	1.93396100	-1.75753900	-0.77393000
O	-3.59010600	-1.50363600	0.21620700
O	1.84601800	-3.79826200	-0.31795700
P	-0.39468500	-0.78065300	0.22657500
P	-0.08249800	1.01294200	-0.72234300
C	-3.35078700	3.63135600	-0.31635600
C	-4.65554200	6.09678600	-0.50275100
C	-2.59712500	4.77700500	-0.65801100
C	-4.75016500	3.68629700	-0.11257600
C	-5.38360700	4.93824400	-0.20285300
C	-3.27940700	6.00637000	-0.74176800

H	-6.46207800	4.99696700	-0.04701600
H	-2.71257700	6.90226700	-0.99920600
H	-5.16102300	7.06157900	-0.56552600
C	-1.10559200	4.72273200	-0.96646800
H	-0.78701100	3.68013400	-0.88309900
C	-0.81995400	5.18287700	-2.41317400
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H	-1.11188800	6.23471600	-2.55640700
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C	-5.57817600	2.42837200	0.13343800
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H	-7.26695400	3.05366000	-1.11344900
H	-7.14194500	1.29074700	-0.88519600
H	-6.02285900	2.13010100	-1.99250100
C	4.81713300	2.77522000	0.10021200
C	6.92998400	3.15048700	-1.67763500
C	4.97278300	4.03828400	-0.51268700
C	5.67354500	1.68696700	-0.17370300
C	6.73510600	1.90212400	-1.07193100
C	6.05222500	4.20662000	-1.39916200
H	7.41012100	1.07576200	-1.29952800
H	6.19744900	5.17652000	-1.87754800
H	7.76067500	3.29837400	-2.36935300

C	4.00672500	5.18721600	-0.24115000
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C	5.43422400	0.31124900	0.43686800
H	4.65527000	0.41468200	1.20435200
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C	6.69484100	-0.25023800	1.12697300
H	7.50735300	-0.40385000	0.40001100
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C	3.10990800	-3.81635800	0.27238200
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C	4.18268000	-4.43790900	-0.40756800
C	3.26863400	-3.23512400	1.55103600
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C	5.43841100	-4.46508100	0.22533500
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C	4.00468200	-5.05298000	-1.79101200
H	2.93539700	-5.01566000	-2.04002500
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H	-1.49724200	-4.77473000	-0.59499700

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