**SUPPORTING INFORMATION**

# A Cyclic Divalent N(I) Species Isoelectronic to Carbodiphosphoranes

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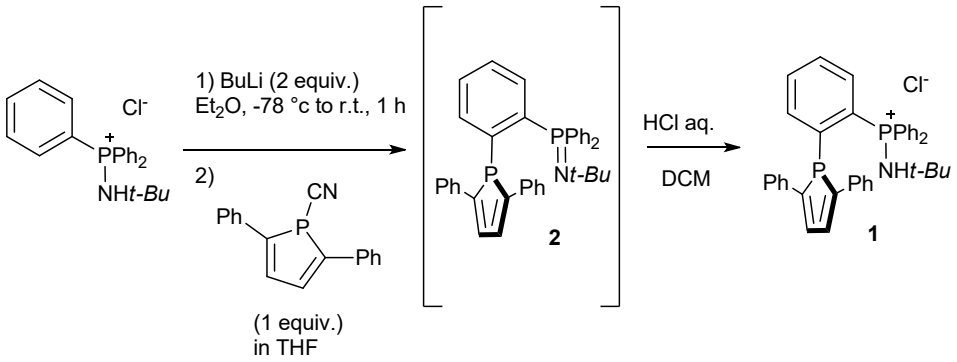
**Experimental procedures.**

**General comments.**

All air and moisture sensitive reactions were performed under inert atmosphere using a vacuum line and a glove box (Ar, <0.1 ppm $H_2O$, <0.1 ppm $O_2$) with oven-dried glassware. 1-Cyano-2,5-diphenylphosphole[1] and *tert*-butylaminotriphenylphosphonium bromide[2] were synthesized following reported procedures. All other reagents were used as received from suppliers unless otherwise stated. Diethyl ether, dichloromethane, pentane, ether and toluene were taken from solvent purification system (MBraun-SPS). THF was distilled over sodium/benzophenone. NMR spectra were recorded on a Bruker AC-300 SY spectrometer at 300 MHz for $^1$H, 120 MHz for $^{31}$P and 75 MHz for $^{13}$C. Solvent peaks were used as internal references for $^1$H and $^{13}$C chemical shifts (ppm). $^{31}$P{$^1$H} NMR spectra are relative to an 85% $H_3PO_4$ external reference. Unless otherwise mentioned, NMR spectra were recorded at 300 K. The abbreviations used to indicate the multiplicity of signals are: s (singlet), d (doublet), t (triplet), m (multiple) or a combination of the above. The coupling constants *J* were expressed in hertz (Hz). The spectra were analyzed with MestReNova software. Mass spectrometry experiments were performed on a Tims-TOF mass spectrometer (Bruker, France). Electrospray source has been used in positive modes. Samples were prepared in acetonitrile with 0.1 % formic acid at µM concentration. 2 to 10 µL were introduced without separation with Elute UHPLC module (Bruker) at a 100 µL min$^{-1}$ flow rate into the interface of the instrument. Capillary and end plate voltages were set at 4.5 kV and 0.5 kV for ESI experiments. Nitrogen was used as the nebulizer and drying gas at 2 bar and 8 L min$^{-1}$, respectively, with a drying temperature of 220 °C for ESI source. Tuning mix (Agilent, France) was used for calibration. The elemental compositions of all ions were determined with the instrument software Data Analysis, the precision of mass measurement was less than 3 ppm. X-ray crystallography data were collected at 150 K on a Bruker Kappa APEX II diffractometer using a Mo-κ (λ=0.71069Å) X-ray source and a graphite monochromator. The crystal structures were solved using Shelxt[3] or olex[4] and refined using Shelxl-97 or Shelxl-2014.[3] ORTEP drawings were made using ORTEP III[5] for Windows or Mercury. Details of crystal data and structure refinements are summarized in Table S1.




**Procedure for the synthesis of 1.**

BuLi (4.56 mL, 1.6 M in hexane, 7.30 mmol, 2,0 equiv.) was added dropwise to a solution of *tert*-butylaminotriphenylphosphonium bromide (1.51 g, 3.65 mmol, 1.0 equiv.) in $Et_2O$ (80 mL) at -78 °C. After 1 h of stirring at room temperature, the *in situ* $^{31}$P{$^1$H} NMR of the reaction mixture ascertained the formation of the lithium species ($\delta_P$ = 12.4 ppm). The reaction mixture was cooled back to -78 °C and a

solution of 1-cyano-2,5-diphenylphosphole (0.953 g, 3.65 mmol, 1.0 equiv.) in THF (30 mL) was added. The cooling bath was removed and stirring was pursued 1 h at room temperature. The formation of **2** was controlled by i*n situ* $^{31}P\{^{1}H\}$ NMR ($\delta_P$ -5.8 and -8.8 ppm ($J_{P,P}$ = 8.0 Hz)). The solvents were removed under vacuum, the crude product was dissolved in $CH_2Cl_2$ (30 mL) and the solution was washed with an aqueous solution of HCl (30 mL; 0.1 M), the aqueous phase was extracted with $CH_2Cl_2$ (3 x 30 mL). The combined organic extracts were dried over anhydrous $MgSO_4$, filtered and concentrated under vacuum. The crude product **1** was washed with $Et_2O$ (3 x 15 mL) to give a yellow solid after drying under vacuum (1.54 g, 2.54 mmol, 70%).

$^{13}P\{^{1}H\}$ (121 MHz, $CD_2Cl_2$): 35.3 (d, $J_{P,P}$ = 11.0 Hz, $P^{V}$), -7.2 (d, $J_{P,P}$ = 11.0 Hz, $P^{III}$);

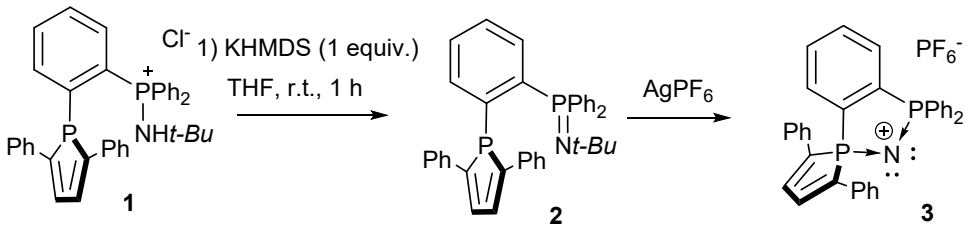
$^{1}H$ ($CD_2Cl_2$, 300 MHz): 1.01 (s, 9H, C(C$H_3$)$_3$), 5.90 (t, $J_{H,H}$ = 5.0 Hz, 1 H, NH), 6.70 (d, $J_{H,H}$ = 7.5 Hz, 4 H, CH-$PPh_2$), 7.04-7.15 (m, 8 H), 7.41-7.65 (m, 7 H), 7.68 (t, $J_{H,H}$ = 7.5 Hz, 2 H), 7.92 (dd, $J_{H,H}$ = 7.5 Hz, $J_{P,H}$ = 13.5 Hz, 4 H, CH-$PPh_2$) 8.07 (ddd, $J_{H,H}$ = 8.0 Hz, $J_{P,H}$ = 13.5 and 4.0 Hz , 1 H, CH-Ar$P_2$);

$^{13}C\{^{1}H\}$ ($CD_2Cl_2$, 75 MHz): 31.6 (d, $J_{P,C}$ = 3.5 Hz, C(*C*$H_3$)$_3$), 57.5 (d, $J_{P,C}$ = 4.5 Hz, *C*(CH$_3$)$_3$), 122.7 (d, $J_{P,C}$ = 100 Hz, $C^{IV}$), 125.6 (d, $J_{P,C}$ = 3.5 Hz, CH), 126.4 (d, $J_{P,C}$ = 5.5 Hz, CH), 126.8 (d, $J_{P,C}$ = 3.0 Hz, CH), 127.4 (*J* not seen, CH), 128.3 (*J* not seen, CH), 128.5 (d, $J_{P,C}$ = 35.0 Hz CH), 129.4 (d, $J_{P,C}$ = 18.5 Hz, CH), 130.2 (d, $J_{P,C}$ = 13.5 Hz, CH), 131.0 (*J* not seen, CH), 133.9, 134.2, 134.3, 134.4, 134.6 (*J* not seen, CH and $C^{IV}$), 134.8 (d, $J_{P,C}$ = 15.0 Hz, CH), 135.3 (d, $J_{P,C}$ = 4.0 Hz, CH), 135.7 (*J* not seen, CH), 135.9 (d, $J_{P,C}$ = 16.5 Hz, CH), 151.8 (br. s, $C^{IV}$).

"*J* not seen" means that the carbon was observed in $^{13}C\{^{1}H\}\{^{31}P\}$ experiment but could not be seen in the non $^{31}P$-decoupled spectrum, therefore we could not have access to the C,P coupling constant.

HRMS-ESI: *m/z* calculated for $C_{38}H_{36}NP_2$ $[M]^+$: 568.2318, found: 568.2309.

**Procedure for the synthesis of 3.**



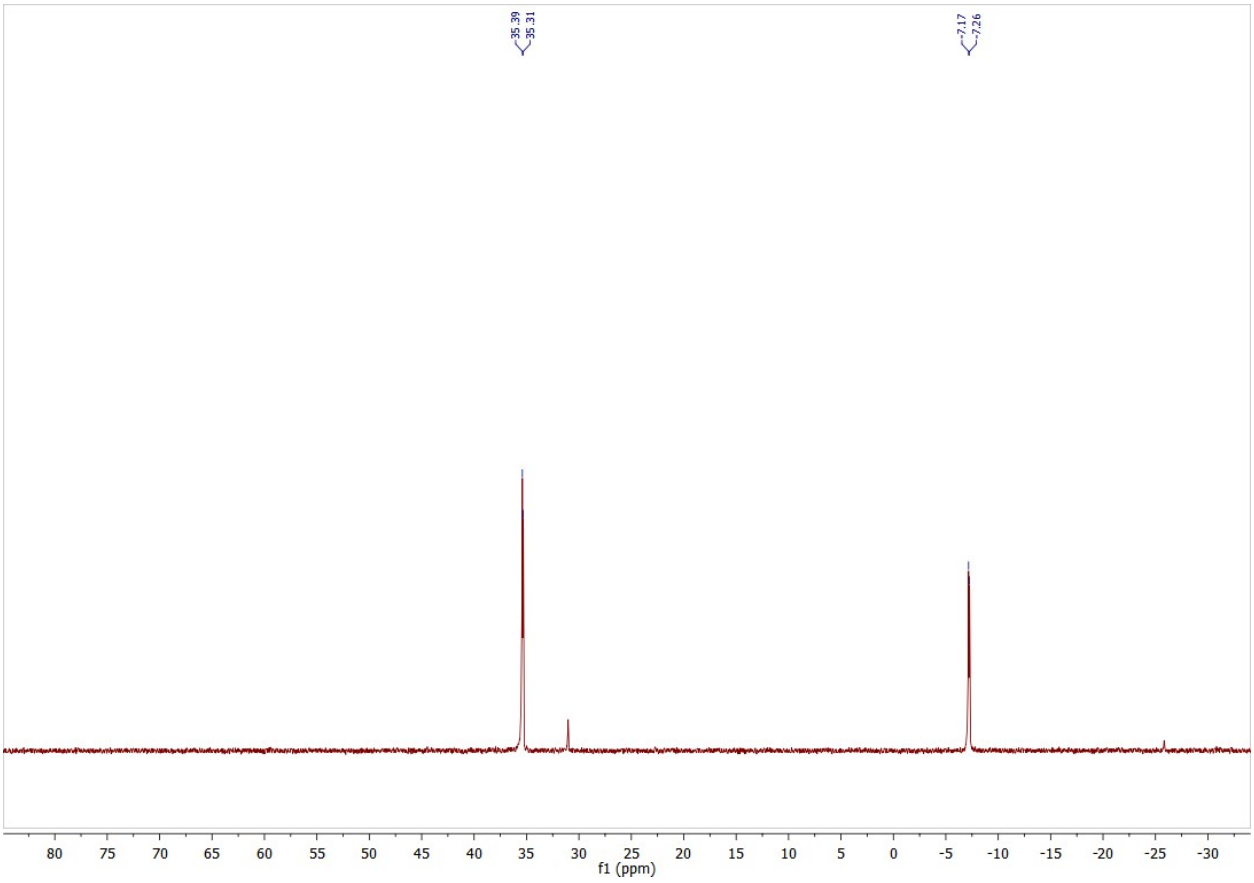

KHMDS (62.0 mg, 0,31 mmol, 1.0 equiv) was added to a suspension of **1** (187.8 mg, 0.31 mmol, 1.0 equiv) in THF (3.0 mL) inside the glovebox. The reaction mixture was stirred at room temperature for 1 h. The precipitated potassium salts were removed by centrifugation and $AgPF_6$ (78.6 mg, 0.31 mmol, 1.0 equiv) was added to the reaction mixture. Stirring was pursued at room temperature overnight and the formed precipitate was isolated and washed with THF (3 x 5 mL). The obtained solid was dissolved in dichloromethane (5.0 mL) and the insoluble impurities were discarded. **3** was isolated as a light yellow solid (132 mg, 65%) after removing the solvents.

$^{13}P\{^{1}H\}$ (121 MHz, $CD_2Cl_2$): 58.7 (d, $J_{P,P}$ = 7.5 Hz), 55.9 (d, $J_{P,P}$ = 7.5 Hz);

$^{1}H$ ($CD_2Cl_2$, 300 MHz): 7.10 (d, $J_{H,H}$ = 5.0 Hz, 8H, CH-$PPh_2$), 7.28-7.36 (m, 2 H), 7.60 (td, $J_{H,H}$ = 7.5 Hz and $J_{P,C}$ = 4.0 Hz, 4 H, CH-$PPh_2$), 7.64-7.75 (m, 6 H), 7.82 (t, $J_{H,H}$ = 7.0 Hz, 2 H), 8.02 (dd, $J_{P,H}$ = 8.0 Hz, 2 H, H-phosphole) 8.10 (m, 1 H, CH-$ArP_2$), 8.35 (t, $J_{H,H}$ = $J_{P,H}$ = 7.5 Hz, 1 H);

$^{13}C\{^{1}H\}$ ($CD_2Cl_2$, 75 MHz): 124.8 (dd, $J_{P,C}$ = 107.0 and 4.0 Hz, $C^{IV}$), 126.9 (d, $J_{P,C}$ = 6.0 Hz, CH), 129.1 (s, CH), 129.7 (d, $J_{P,C}$ = 13.5 Hz, CH), 130.1 (s, CH), 130.2 (d, $J_{P,C}$ = 12.0 Hz, $C^{IV}$), 132.1 (d, $J_{P,C}$ = 9.5 Hz, CH), 132.2 (d, $J_{P,C}$ = 11.5 Hz, CH), 133.5 (dd, $J_{P,C}$ = 3.5 Hz, $C^{IV}$), 134.9 (d, $J_{P,C}$ = 3.0 Hz, CH), 135.2 (dd, $J_{P,C}$ = 9.5 and 2.5 Hz, CH), 135.4 (dd, $J_{P,C}$ = 10.5 and 2.5 Hz, CH), 140.3 (d, $J_{P,C}$ = 33.0 Hz, CH), 1 $C^{IV}$ not observed.

HRMS-ESI: *m/z* calculated for $C_{34}H_{26}NP_2$ $[M]^+$: 510.1540, found: 510.1513.




**NMR spectra**

**Figure S1**: $^{31}P\{^{1}H\}$ NMR spectrum of **1** in $CD_2Cl_2$

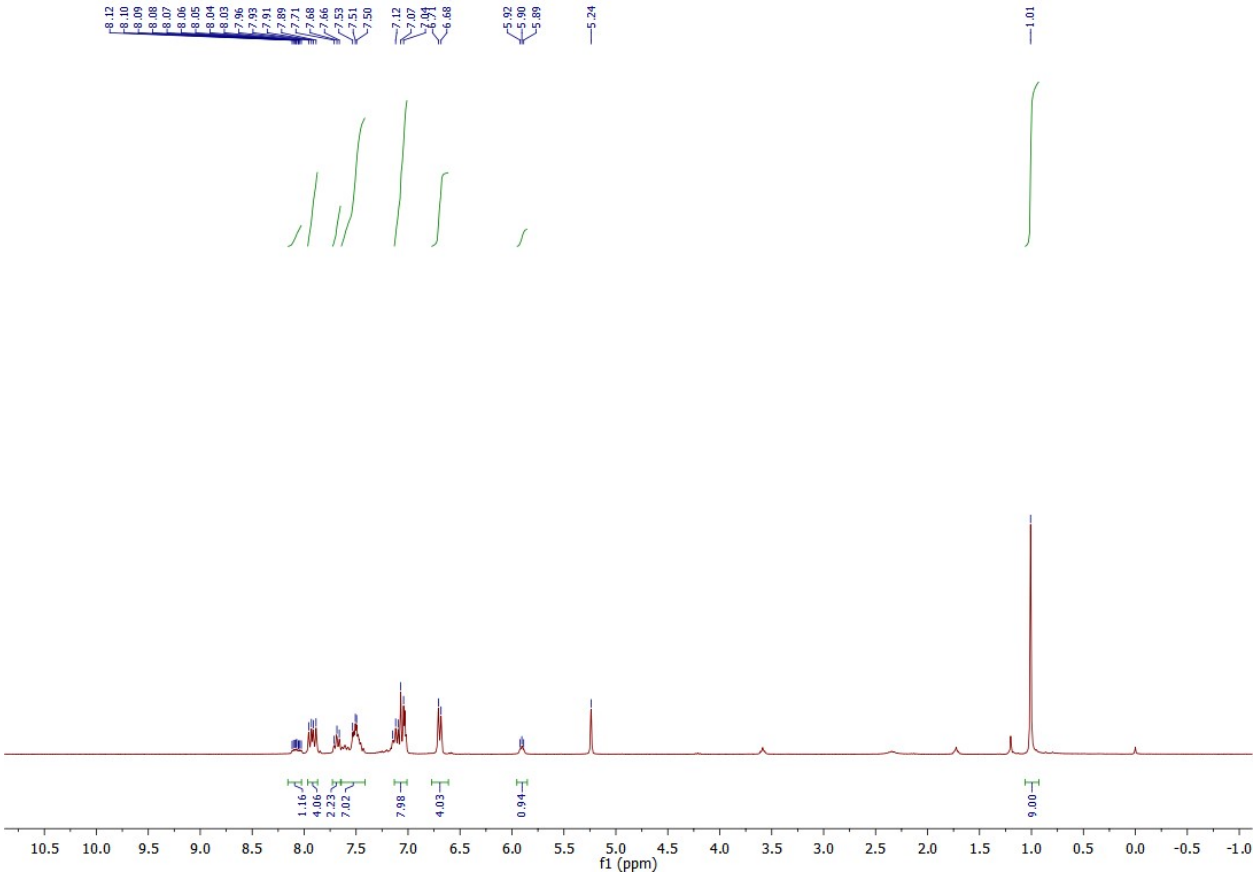



**Figure S2**: $^{1}H$ NMR spectrum of **1** in $CD_2Cl_2$

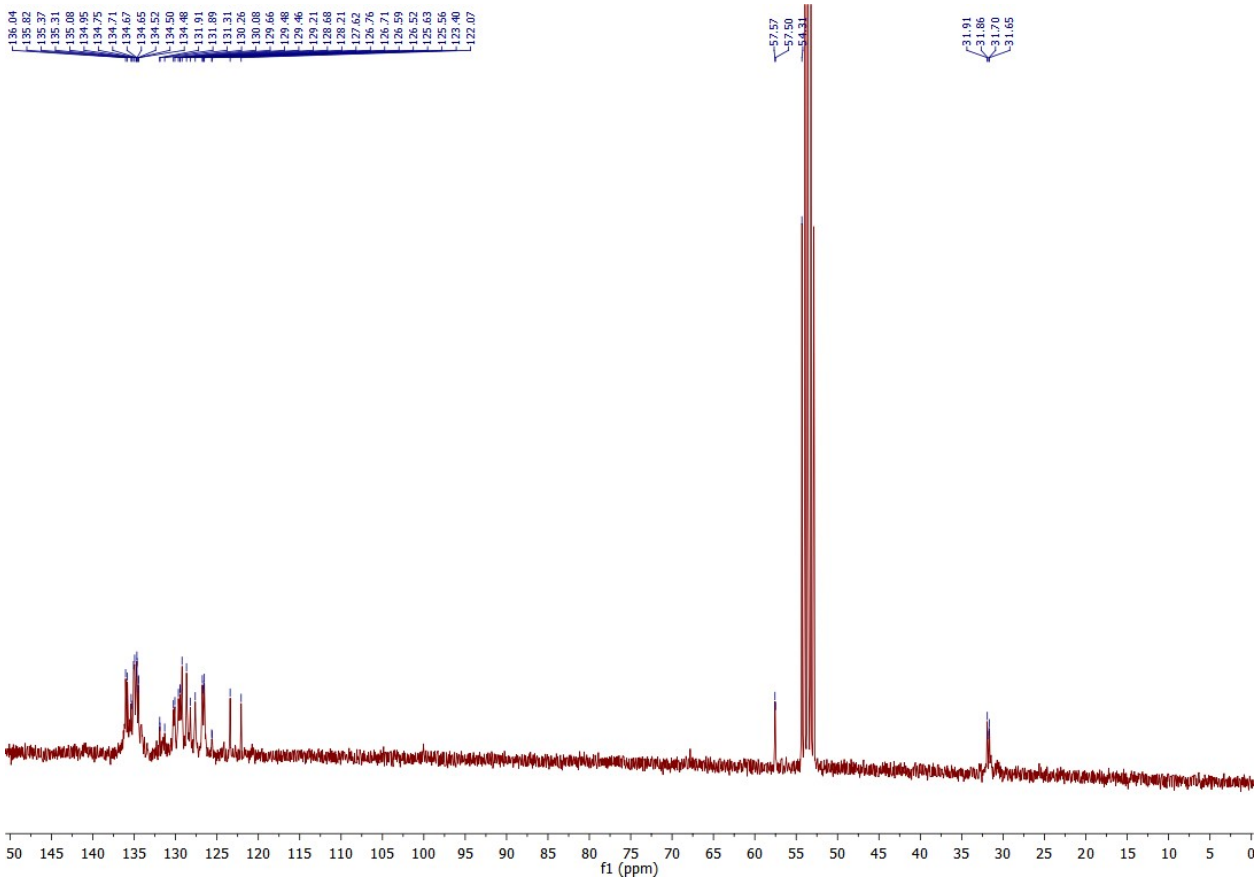


**Figure S3**: $^{13}C\{^{1}H\}$ NMR spectrum of **1** in $CD_2Cl_2$

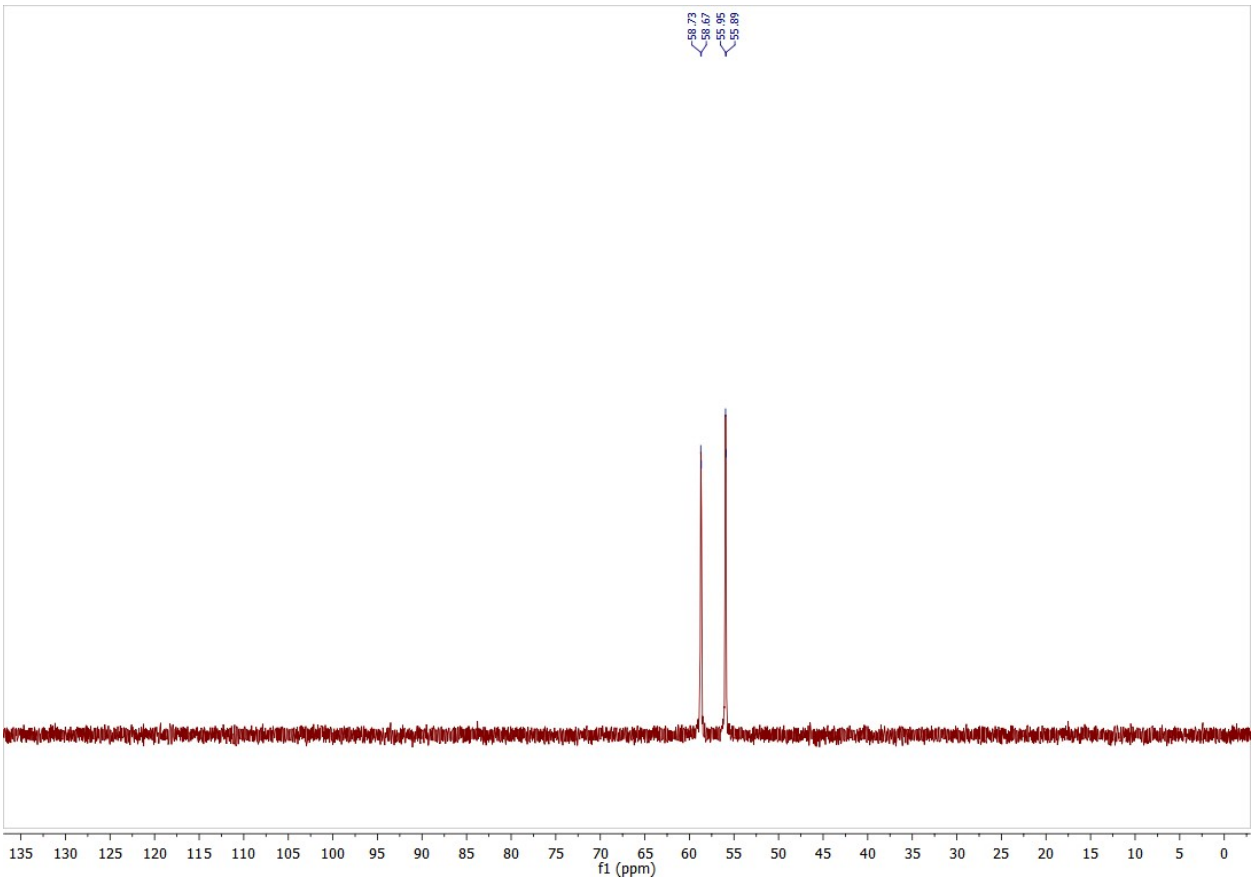



**Figure S4**: $^{31}P\{^{1}H\}$ NMR spectrum of **3** in $CD_2Cl_2$

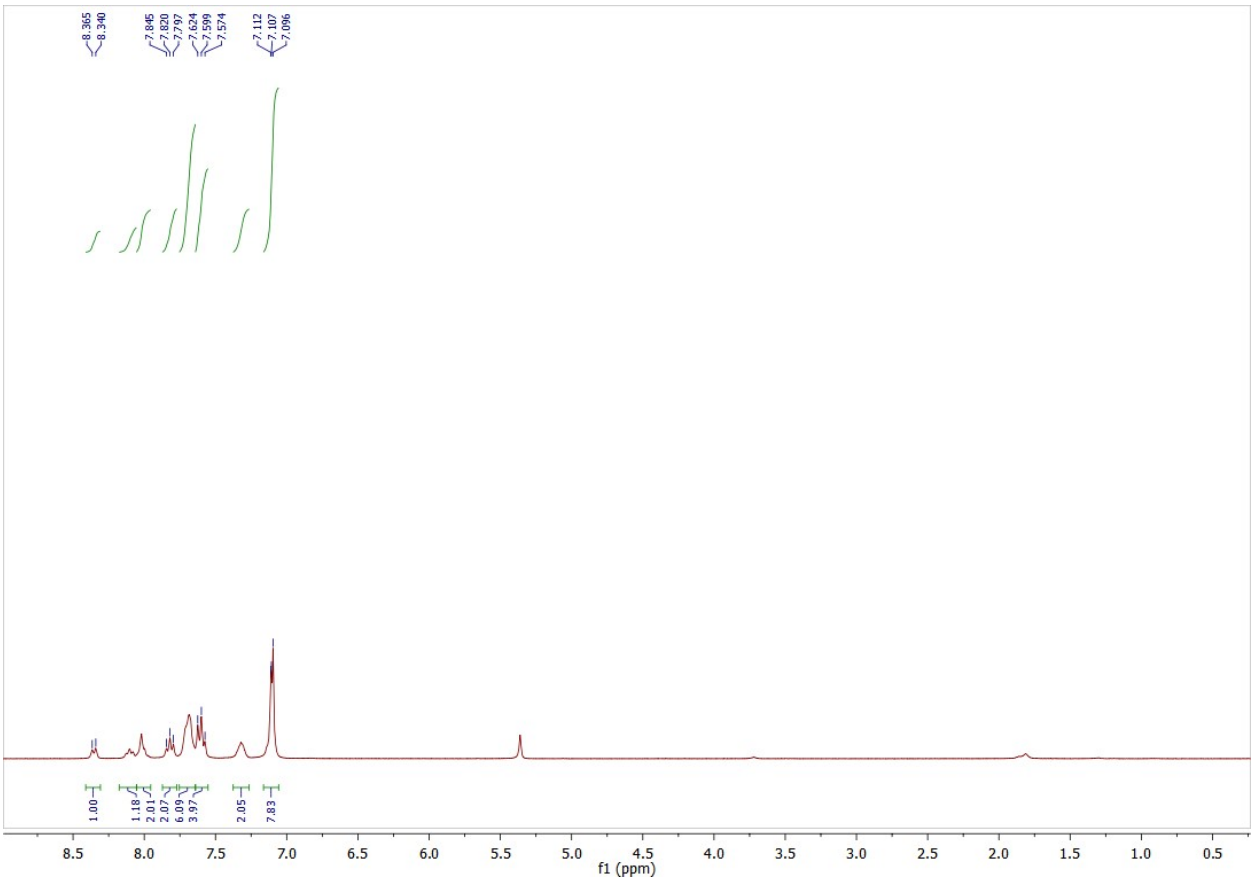



**Figure S5**: $^{1}H$ NMR spectrum of **3** in $CD_2Cl_2$

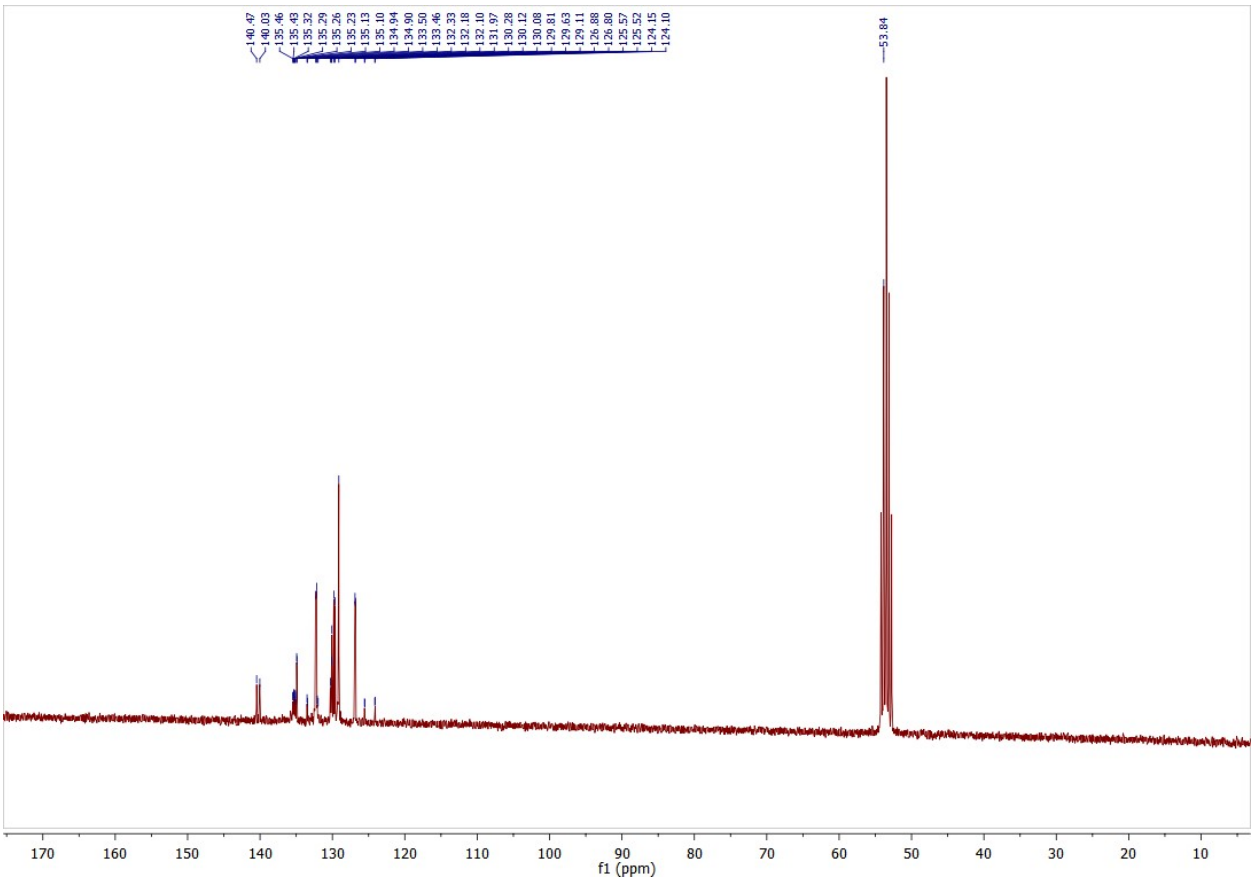



**Figure S6**: $^{13}C\{1H\}$ NMR spectrum of **3** in $CD_2Cl_2$

## X-ray details

**Table S1**: X-ray data for compound **3**.

| Compound | **3** |
|---|---|
| Molecular formula | $C_{34}H_{26}NP_2$, $F_6P$ |
| Molecular weight | 655.47 |
| Space group | P1 |
| V(Å$^3$) | 2156.07(17) |
| a(Å) | 8.2282(7) |
| b(Å) | 9.5081(8) |
| c(Å) | 10.7126(8) |
| α(°) | 101.997(2) |
| β(°) | 91.033(2) |
| γ(°) | 111.831(2) |
| Z | 1 |
| d (g-cm$^{-3}$) | 1.438 |
| F(000) | 336 |
| $\Theta_{max}$ | 26.984 |
| Rflns measd | 19925 |
| Unique data | 6488 |
| Rint | 0.0498 |
| wR2 | 0.0774 |
| R1 | 0.0312 |
| GoF | 1.008 |
| CCDC number | 2156179 |

**Table S2.** Atomic Coordinates (Å x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **3**

| atom | x | y | z | U(eq) |
|---|---|---|---|---|
| P(1) | 6987(1) | 4969(1) | 2736(1) | 19(1) |
| P(2) | 6781(1) | 4742(1) | 5182(1) | 18(1) |
| N(1) | 7871(3) | 4676(3) | 3948(2) | 21(1) |
| C(1) | 5039(3) | 5217(3) | 3313(3) | 19(1) |
| C(2) | 4947(3) | 5129(3) | 4598(3) | 17(1) |
| C(3) | 3582(3) | 5364(3) | 5253(3) | 23(1) |
| C(4) | 2331(4) | 5663(4) | 4596(3) | 26(1) |
| C(5) | 2412(4) | 5715(4) | 3308(3) | 29(1) |
| C(6) | 3772(4) | 5507(4) | 2660(3) | 25(1) |
| C(7) | 8218(4) | 6601(4) | 2067(3) | 23(1) |
| C(8) | 8150(4) | 6016(4) | 805(3) | 29(1) |
| C(9) | 7270(4) | 4326(4) | 360(3) | 29(1) |
| C(10) | 6568(4) | 3536(4) | 1248(3) | 22(1) |
| C(11) | 8973(4) | 8237(4) | 2778(3) | 26(1) |
| C(12) | 9739(4) | 8649(4) | 4044(3) | 34(1) |
| C(13) | 10505(5) | 10192(5) | 4680(4) | 49(1) |
| C(14) | 10498(5) | 11339(4) | 4077(5) | 54(1) |
| C(15) | 9744(5) | 10951(5) | 2828(5) | 52(1) |
| C(16) | 8979(4) | 9415(4) | 2188(4) | 37(1) |
| C(17) | 5689(4) | 1843(4) | 1097(3) | 24(1) |
| C(18) | 4387(4) | 1208(4) | 1855(3) | 33(1) |
| C(19) | 3554(5) | -383(4) | 1693(4) | 41(1) |
| C(20) | 4030(5) | -1361(4) | 772(3) | 39(1) |
| C(21) | 5308(5) | -762(4) | 6(4) | 39(1) |
| C(22) | 6159(4) | 834(4) | 166(3) | 31(1) |
| C(23) | 8004(4) | 6288(3) | 6526(3) | 20(1) |
| C(24) | 9332(4) | 6124(4) | 7228(3) | 26(1) |
| C(25) | 10445(4) | 7383(4) | 8164(3) | 31(1) |
| C(26) | 10216(4) | 8781(4) | 8410(3) | 33(1) |
| C(27) | 8885(4) | 8935(4) | 7722(3) | 34(1) |
| C(28) | 7786(4) | 7699(4) | 6778(3) | 30(1) |
| C(29) | 6104(4) | 2937(3) | 5675(3) | 21(1) |
| C(30) | 6332(5) | 1668(4) | 4902(3) | 34(1) |
| C(31) | 5755(6) | 259(4) | 5249(4) | 46(1) |
| C(32) | 4959(5) | 110(4) | 6367(4) | 41(1) |
| C(33) | 4734(4) | 1358(4) | 7142(4) | 33(1) |
| C(34) | 5306(4) | 2782(4) | 6798(3) | 25(1) |
| P(3) | 1490(1) | 3635(1) | 8929(1) | 25(1) |
| F(1) | 1229(2) | 4944(2) | 10007(2) | 39(1) |
| F(2) | 2154(3) | 4837(3) | 8031(2) | 51(1) |
| F(3) | 3471(3) | 4177(3) | 9523(2) | 54(1) |
| F(4) | 817(3) | 2445(3) | 9830(2) | 56(1) |
| F(5) | -487(2) | 3103(3) | 8315(2) | 45(1) |
| F(6) | 1741(3) | 2322(3) | 7853(2) | 51(1) |

U(eq) is defined as 1/3 the trace of the Uij tensor.

**Table S3.** Bond lengths (Å) for **3**

| Atoms | Bond lengths | Atoms | Bond lengths |
|---|---|---|---|
| P(1)-N(1) | 1.600(2) | P(1)-C(10) | 1.801(3) |
| P(1)-C(1) | 1.807(3) | P(1)-C(7) | 1.808(3) |
| P(1)-P(2) | 2.678(1) | P(2)-N(1) | 1.614(2) |
| P(2)-C(29) | 1.791(3) | P(2)-C(23) | 1.792(3) |
| P(2)-C(2) | 1.811(3) | C(1)-C(6) | 1.386(4) |
| C(1)-C(2) | 1.398(4) | C(2)-C(3) | 1.398(4) |
| C(3)-C(4) | 1.382(4) | C(3)-H(3) | 0.9500 |
| C(4)-C(5) | 1.393(5) | C(4)-H(4) | 0.9500 |
| C(5)-C(6) | 1.382(4) | C(5)-H(5) | 0.9500 |
| C(6)-H(6) | 0.9500 | C(7)-C(8) | 1.342(4) |
| C(7)-C(11) | 1.469(4) | C(8)-C(9) | 1.462(4) |
| C(8)-H(8) | 0.9500 | C(9)-C(10) | 1.341(4) |
| C(9)-H(9) | 0.9500 | C(10)-C(17) | 1.470(4) |
| C(11)-C(16) | 1.394(5) | C(11)-C(12) | 1.398(5) |
| C(12)-C(13) | 1.377(5) | C(12)-H(12) | 0.9500 |
| C(13)-C(14) | 1.379(6) | C(13)-H(13) | 0.9500 |
| C(14)-C(15) | 1.380(6) | C(14)-H(14) | 0.9500 |
| C(15)-C(16) | 1.373(5) | C(15)-H(15) | 0.9500 |
| C(16)-H(16) | 0.9500 | C(17)-C(18) | 1.387(4) |
| C(17)-C(22) | 1.399(4) | C(18)-C(19) | 1.380(5) |
| C(18)-H(18) | 0.9500 | C(19)-C(20) | 1.376(5) |
| C(19)-H(19) | 0.9500 | C(20)-C(21) | 1.373(5) |
| C(20)-H(20) | 0.9500 | C(21)-C(22) | 1.386(5) |
| C(21)-H(21) | 0.9500 | C(22)-H(22) | 0.9500 |
| C(23)-C(24) | 1.389(4) | C(23)-C(28) | 1.392(4) |
| C(24)-C(25) | 1.389(4) | C(24)-H(24) | 0.9500 |
| C(25)-C(26) | 1.384(5) | C(25)-H(25) | 0.9500 |
| C(26)-C(27) | 1.378(5) | C(26)-H(26) | 0.9500 |
| C(27)-C(28) | 1.380(5) | C(27)-H(27) | 0.9500 |
| C(28)-H(28) | 0.9500 | C(29)-C(34) | 1.389(4) |
| C(29)-C(30) | 1.391(4) | C(30)-C(31) | 1.378(5) |
| C(30)-H(30) | 0.9500 | C(31)-C(32) | 1.382(6) |
| C(31)-H(31) | 0.9500 | C(32)-C(33) | 1.375(5) |
| C(32)-H(32) | 0.9500 | C(33)-C(34) | 1.389(4) |
| C(33)-H(33) | 0.9500 | C(34)-H(34) | 0.9500 |
| P(3)-F(4) | 1.590(2) | P(3)-F(3) | 1.590(2) |
| P(3)-F(6) | 1.591(2) | P(3)-F(1) | 1.594(2) |
| P(3)-F(2) | 1.594(2) | P(3)-F(5) | 1.595(2) |

**Table S4.** Angles (deg) for **3**

| Atoms | Bond angles | Atoms | Bond angles |
|---|---|---|---|
| N(1)-P(1)-C(10) | 116.9(1) | N(1)-P(1)-C(1) | 103.1(1) |
| C(10)-P(1)-C(1) | 114.0(1) | N(1)-P(1)-C(7) | 119.3(1) |
| C(10)-P(1)-C(7) | 94.8(1) | C(1)-P(1)-C(7) | 108.9(1) |
| N(1)-P(1)-P(2) | 33.75(8) | C(10)-P(1)-P(2) | 132.5(1) |
| C(1)-P(1)-P(2) | 69.3(1) | C(7)-P(1)-P(2) | 130.4(1) |
| N(1)-P(2)-C(29) | 110.6(1) | N(1)-P(2)-C(23) | 113.1(1) |
| C(29)-P(2)-C(23) | 108.5(1) | N(1)-P(2)-C(2) | 102.6(1) |
| C(29)-P(2)-C(2) | 112.9(1) | C(23)-P(2)-C(2) | 109.0(1) |
| N(1)-P(2)-P(1) | 33.42(8) | C(29)-P(2)-P(1) | 124.0(1) |

| | | | |
|---|---|---|---|
| C(23)-P(2)-P(1) | 123.9(1) | C(2)-P(2)-P(1) | 69.2(1) |
| P(1)-N(1)-P(2) | 112.8(1) | C(6)-C(1)-C(2) | 121.0(3) |
| C(6)-C(1)-P(1) | 128.2(2) | C(2)-C(1)-P(1) | 110.7(2) |
| C(3)-C(2)-C(1) | 120.1(3) | C(3)-C(2)-P(2) | 129.2(2) |
| C(1)-C(2)-P(2) | 110.7(2) | C(4)-C(3)-C(2) | 118.4(3) |
| C(4)-C(3)-H(3) | 120.8 | C(2)-C(3)-H(3) | 120.8 |
| C(3)-C(4)-C(5) | 121.1(3) | C(3)-C(4)-H(4) | 119.5 |
| C(5)-C(4)-H(4) | 119.5 | C(6)-C(5)-C(4) | 120.8(3) |
| C(6)-C(5)-H(5) | 119.6 | C(4)-C(5)-H(5) | 119.6 |
| C(5)-C(6)-C(1) | 118.6(3) | C(5)-C(6)-H(6) | 120.7 |
| C(1)-C(6)-H(6) | 120.7 | C(8)-C(7)-C(11) | 128.6(3) |
| C(8)-C(7)-P(1) | 106.0(2) | C(11)-C(7)-P(1) | 125.3(2) |
| C(7)-C(8)-C(9) | 116.4(3) | C(7)-C(8)-H(8) | 121.8 |
| C(9)-C(8)-H(8) | 121.8 | C(10)-C(9)-C(8) | 116.5(3) |
| C(10)-C(9)-H(9) | 121.7 | C(8)-C(9)-H(9) | 121.7 |
| C(9)-C(10)-C(17) | 128.6(3) | C(9)-C(10)-P(1) | 106.2(2) |
| C(17)-C(10)-P(1) | 125.3(2) | C(16)-C(11)-C(12) | 118.7(3) |
| C(16)-C(11)-C(7) | 120.4(3) | C(12)-C(11)-C(7) | 120.9(3) |
| C(13)-C(12)-C(11) | 120.2(4) | C(13)-C(12)-H(12) | 119.9 |
| C(11)-C(12)-H(12) | 119.9 | C(12)-C(13)-C(14) | 120.2(4) |
| C(12)-C(13)-H(13) | 119.9 | C(14)-C(13)-H(13) | 119.9 |
| C(13)-C(14)-C(15) | 120.4(4) | C(13)-C(14)-H(14) | 119.8 |
| C(15)-C(14)-H(14) | 119.8 | C(16)-C(15)-C(14) | 119.8(4) |
| C(16)-C(15)-H(15) | 120.1 | C(14)-C(15)-H(15) | 120.1 |
| C(15)-C(16)-C(11) | 120.8(4) | C(15)-C(16)-H(16) | 119.6 |
| C(11)-C(16)-H(16) | 119.6 | C(18)-C(17)-C(22) | 118.6(3) |
| C(18)-C(17)-C(10) | 121.6(3) | C(22)-C(17)-C(10) | 119.8(3) |
| C(19)-C(18)-C(17) | 121.2(3) | C(19)-C(18)-H(18) | 119.4 |
| C(17)-C(18)-H(18) | 119.4 | C(20)-C(19)-C(18) | 119.6(3) |
| C(20)-C(19)-H(19) | 120.2 | C(18)-C(19)-H(19) | 120.2 |
| C(21)-C(20)-C(19) | 120.4(3) | C(21)-C(20)-H(20) | 119.8 |
| C(19)-C(20)-H(20) | 119.8 | C(20)-C(21)-C(22) | 120.5(3) |
| C(20)-C(21)-H(21) | 119.8 | C(22)-C(21)-H(21) | 119.8 |
| C(21)-C(22)-C(17) | 119.8(3) | C(21)-C(22)-H(22) | 120.1 |
| C(17)-C(22)-H(22) | 120.1 | C(24)-C(23)-C(28) | 119.8(3) |
| C(24)-C(23)-P(2) | 118.5(2) | C(28)-C(23)-P(2) | 121.2(2) |
| C(23)-C(24)-C(25) | 119.5(3) | C(23)-C(24)-H(24) | 120.3 |
| C(25)-C(24)-H(24) | 120.3 | C(26)-C(25)-C(24) | 120.3(3) |
| C(26)-C(25)-H(25) | 119.9 | C(24)-C(25)-H(25) | 119.9 |
| C(27)-C(26)-C(25) | 120.2(3) | C(27)-C(26)-H(26) | 119.9 |
| C(25)-C(26)-H(26) | 119.9 | C(26)-C(27)-C(28) | 120.1(3) |
| C(26)-C(27)-H(27) | 120.0 | C(28)-C(27)-H(27) | 120.0 |
| C(27)-C(28)-C(23) | 120.2(3) | C(27)-C(28)-H(28) | 119.9 |
| C(23)-C(28)-H(28) | 119.9 | C(34)-C(29)-C(30) | 119.9(3) |
| C(34)-C(29)-P(2) | 120.7(2) | C(30)-C(29)-P(2) | 119.4(2) |
| C(31)-C(30)-C(29) | 119.8(3) | C(31)-C(30)-H(30) | 120.1 |
| C(29)-C(30)-H(30) | 120.1 | C(30)-C(31)-C(32) | 120.1(3) |
| C(30)-C(31)-H(31) | 120.0 | C(32)-C(31)-H(31) | 120.0 |
| C(33)-C(32)-C(31) | 120.6(3) | C(33)-C(32)-H(32) | 119.7 |
| C(31)-C(32)-H(32) | 119.7 | C(32)-C(33)-C(34) | 119.8(3) |
| C(32)-C(33)-H(33) | 120.1 | C(34)-C(33)-H(33) | 120.1 |
| C(33)-C(34)-C(29) | 119.8(3) | C(33)-C(34)-H(34) | 120.1 |
| C(29)-C(34)-H(34) | 120.1 | F(4)-P(3)-F(3) | 91.2(1) |
| F(4)-P(3)-F(6) | 90.4(1) | F(3)-P(3)-F(6) | 90.1(1) |
| F(4)-P(3)-F(1) | 89.3(1) | F(3)-P(3)-F(1) | 90.2(1) |
| F(6)-P(3)-F(1) | 179.7(1) | F(4)-P(3)-F(2) | 179.4(1) |

| | | | |
|---|---|---|---|
| F(3)-P(3)-F(2) | 89.0(1) | F(6)-P(3)-F(2) | 90.0(1) |
| F(1)-P(3)-F(2) | 90.2(1) | F(4)-P(3)-F(5) | 89.6(1) |
| F(3)-P(3)-F(5) | 179.2(2) | F(6)-P(3)-F(5) | 89.7(1) |
| F(1)-P(3)-F(5) | 90.1(1) | F(2)-P(3)-F(5) | 90.2(1) |

**Theoretical details**

The computations were performed using the Gaussian 16 software package.[6] The geometry optimizations and frequency calculations were performed using the M06-2X[7] functional, the LANL2DZ basis set for Au and the 6-311G(d,p)[8] basis set for all other atoms. Minima were characterized by the absence of imaginary frequency. The π- and σ-orbital at the central carbon of the compounds discussed in the manuscript are shown in Figure S7.

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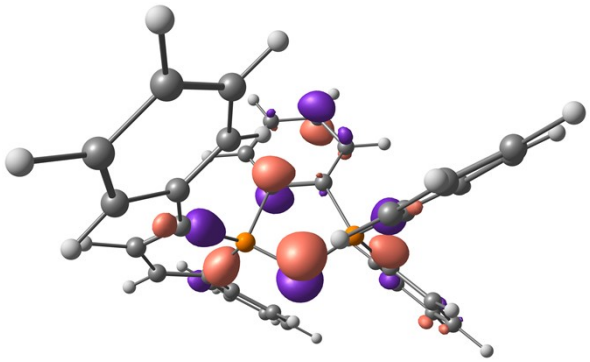
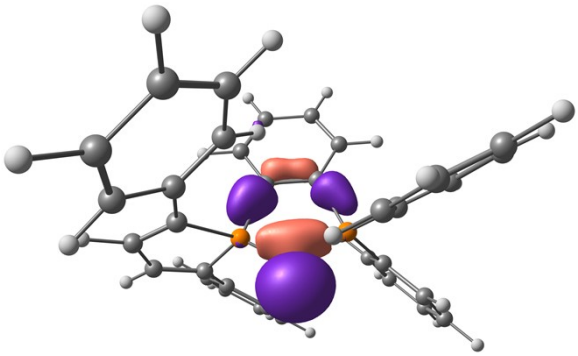
**A**$N^+$



HOMO-9



HOMO-12

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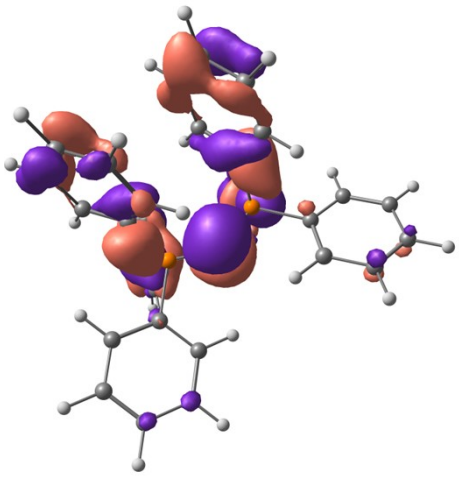
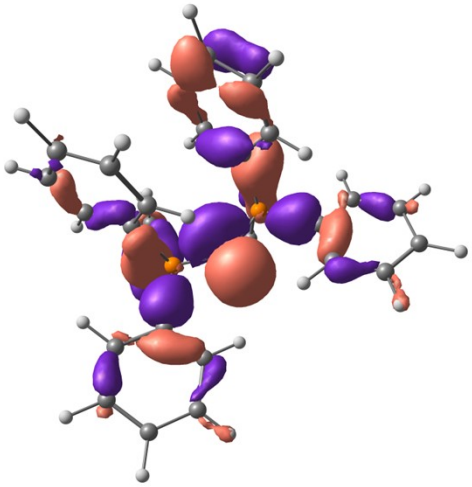
$(Ph_3P)_2N^+$



HOMO-12



HOMO-13

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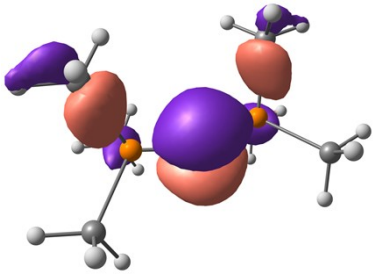
$(Me_3P)_2N^+$



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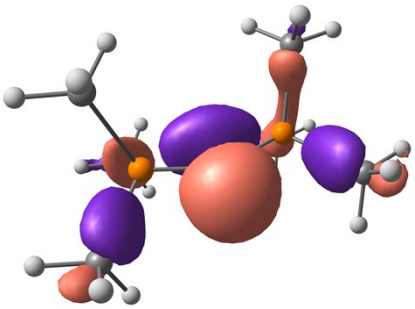
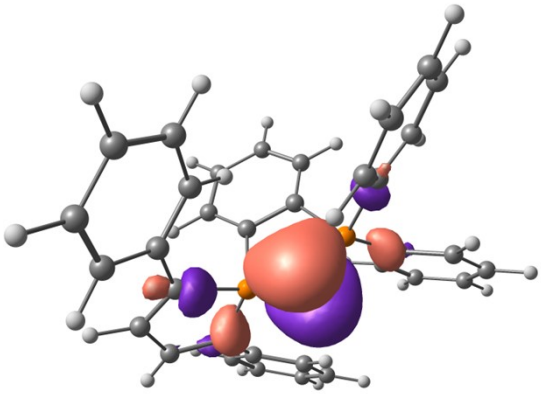


HOMO-1

**AC**



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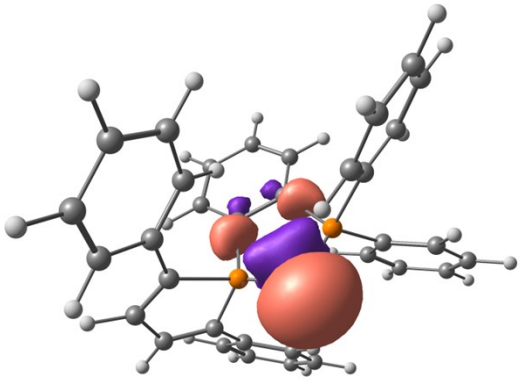
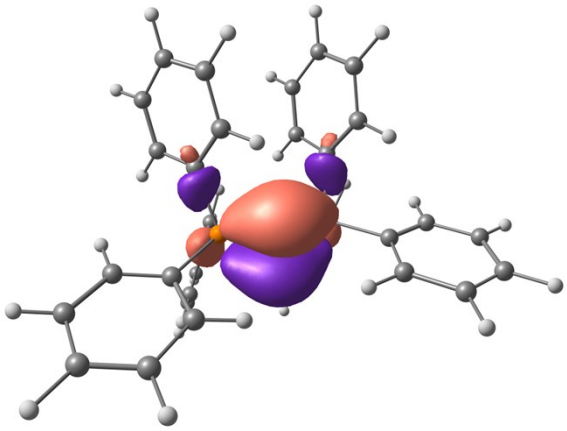
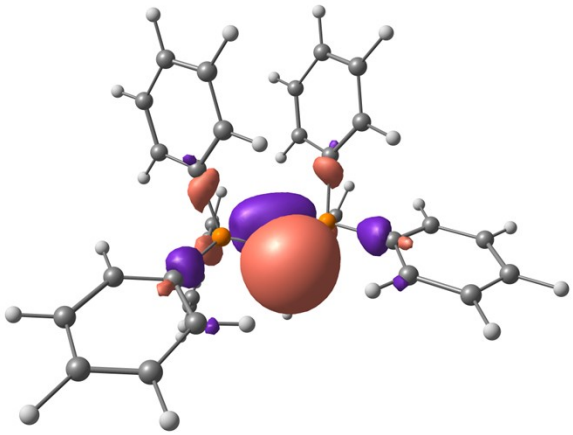


HOMO-1

$(Ph_3P)_2C$

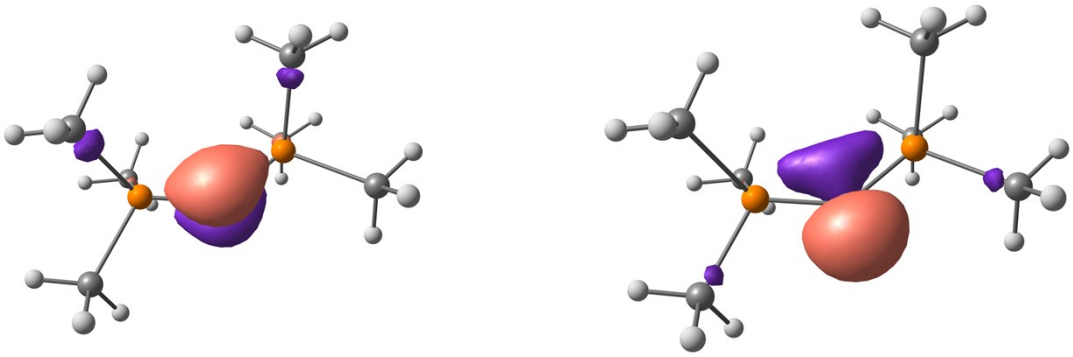


HOMO



HOMO-1

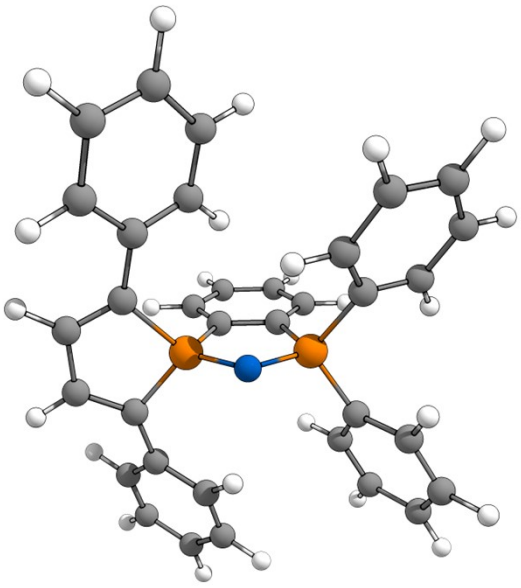
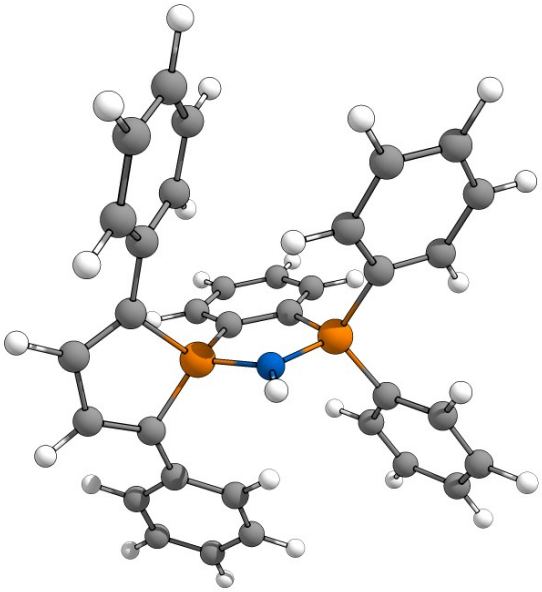
$(Me_3P)_2C$



HOMO HOMO-1

**Figure S7.** π (left) and σ (right) orbitals at the central atom of the computed species

## Energies and Cartesian coordinates for all computed compounds

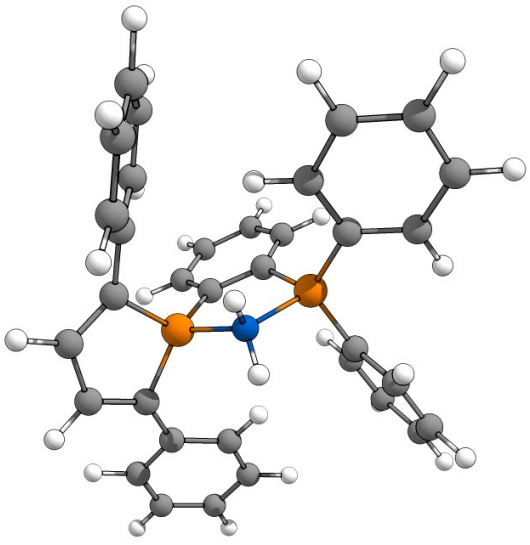
| $AN^+$ | $ANH^{2+}$ |
|---|---|
|  |  |
| Zero-point correction= 0.502608 (Hartree/Particle) | Zero-point correction= 0.514292 (Hartree/Particle) |
| Thermal correction to Energy= 0.532937 | Thermal correction to Energy= 0.545003 |
| Thermal correction to Enthalpy= 0.533882 | Thermal correction to Enthalpy= 0.545948 |
| Thermal correction to Gibbs Free Energy= 0.438001 | Thermal correction to Gibbs Free Energy= 0.450314 |
| Sum of electronic and zero-point Energies= -2047.763989 | Sum of electronic and zero-point Energies= -2048.029660 |
| Sum of electronic and thermal Energies= -2047.733659 | Sum of electronic and thermal Energies= -2047.998948 |

| Sum of electronic and thermal Enthalpies= -2047.732715 | | | | Sum of electronic and thermal Enthalpies= -2047.998004 | | | |
|---|---|---|---|---|---|---|---|
| Sum of electronic and thermal Free Energies= -2047.828595 | | | | Sum of electronic and thermal Free Energies= -2048.093638 | | | |
| P | 0.022328 | -1.401887 | -0.304102 | P | -0.315774 | -1.472945 | -0.239416 |
| P | 0.02238 | 1.28964 | -0.10964 | P | 0.321232 | 1.348644 | -0.028895 |
| N | 0.129224 | -0.00154 | -1.081307 | N | 0.107179 | -0.0332 | -0.991985 |
| C | -0.1345 | -0.880153 | 1.435084 | C | -0.386649 | -0.824846 | 1.429101 |
| C | -0.12438 | 0.512566 | 1.535932 | C | -0.027432 | 0.523234 | 1.536564 |
| C | -0.212072 | 1.127921 | 2.780226 | C | 0.01623 | 1.140835 | 2.780707 |
| H | -0.207213 | 2.208593 | 2.869002 | H | 0.294826 | 2.184841 | 2.875721 |
| C | -0.309386 | 0.328712 | 3.914631 | C | -0.307242 | 0.392206 | 3.909842 |
| H | -0.377173 | 0.791634 | 4.891431 | H | -0.274213 | 0.85948 | 4.886429 |
| C | -0.322108 | -1.062146 | 3.809159 | C | -0.675702 | -0.947423 | 3.797501 |
| H | -0.397882 | -1.666127 | 4.704911 | H | -0.931474 | -1.510757 | 4.686406 |
| C | -0.236026 | -1.680294 | 2.566431 | C | -0.716849 | -1.571414 | 2.554279 |
| H | -0.243928 | -2.761425 | 2.481262 | H | -0.999651 | -2.615067 | 2.46843 |
| C | -1.305029 | -2.577613 | -0.682038 | C | -1.791258 | -2.347141 | -0.793281 |
| C | -0.713568 | -3.772325 | -0.852885 | C | -1.345342 | -3.568012 | -1.151707 |
| H | -1.268505 | -4.684604 | -1.04149 | H | -2.012157 | -4.356908 | -1.482258 |
| C | 0.765887 | -3.784085 | -0.788401 | C | 0.121654 | -3.800386 | -1.074326 |
| H | 1.320383 | -4.702242 | -0.946998 | H | 0.553759 | -4.738655 | -1.405569 |
| C | 1.358425 | -2.605085 | -0.528793 | C | 0.858895 | -2.79215 | -0.576225 |
| C | -2.728191 | -2.231926 | -0.617269 | C | -3.152937 | -1.829769 | -0.645455 |
| C | -3.176623 | -1.00931 | -1.130978 | C | -3.425072 | -0.476346 | -0.881526 |
| H | -2.472306 | -0.333596 | -1.605071 | H | -2.635143 | 0.192825 | -1.208806 |
| C | -4.526662 | -0.685024 | -1.076679 | C | -4.72119 | 0.004986 | -0.76232 |
| H | -4.867513 | 0.257056 | -1.489768 | H | -4.930343 | 1.047384 | -0.970679 |
| C | -5.436409 | -1.5713 | -0.51003 | C | -5.753103 | -0.856474 | -0.401704 |
| H | -6.489207 | -1.3191 | -0.472848 | H | -6.765148 | -0.481558 | -0.31271 |
| C | -4.995052 | -2.787056 | 0.006262 | C | -5.487578 | -2.201684 | -0.159301 |
| H | -5.702103 | -3.476473 | 0.451115 | H | -6.290387 | -2.869841 | 0.125904 |
| C | -3.648256 | -3.115514 | -0.041682 | C | -4.193819 | -2.688692 | -0.274943 |
| H | -3.299643 | -4.051346 | 0.38073 | H | -3.986249 | -3.731474 | -0.062793 |
| C | 2.783029 | -2.265537 | -0.476589 | C | 2.309334 | -2.604924 | -0.446985 |
| C | 3.249143 | -1.263127 | 0.381665 | C | 2.85488 | -2.105215 | 0.742902 |
| H | 2.560995 | -0.737987 | 1.036852 | H | 2.215521 | -1.906512 | 1.597365 |
| C | 4.601412 | -0.949205 | 0.427525 | C | 4.225389 | -1.911465 | 0.85126 |
| H | 4.949986 | -0.175507 | 1.100892 | H | 4.646192 | -1.546703 | 1.780166 |
| C | 5.502826 | -1.630366 | -0.382536 | C | 5.057852 | -2.203448 | -0.226376 |
| H | 6.557684 | -1.387269 | -0.345858 | H | 6.128148 | -2.061222 | -0.136854 |
| C | 5.047373 | -2.625981 | -1.243127 | C | 4.519994 | -2.695724 | -1.412565 |
| H | 5.745405 | -3.151801 | -1.882702 | H | 5.168308 | -2.931746 | -2.247412 |
| C | 3.697227 | -2.938899 | -1.29529 | C | 3.149776 | -2.897133 | -1.526589 |
| H | 3.340311 | -3.690196 | -1.990452 | H | 2.728706 | -3.273988 | -2.452053 |
| C | -1.413475 | 2.337636 | -0.380041 | C | -0.886216 | 2.613814 | -0.357383 |

| | | | |
|---|---|---|---|
| C | -1.346305 | 3.360369 | -1.331184 |
| H | -0.415417 | 3.568397 | -1.847474 |
| C | -2.479712 | 4.11202 | -1.609663 |
| H | -2.431724 | 4.905076 | -2.34527 |
| C | -3.671969 | 3.847435 | -0.94168 |
| H | -4.552429 | 4.440174 | -1.15893 |
| C | -3.739168 | 2.828795 | 0.003681 |
| H | -4.667929 | 2.626097 | 0.522655 |
| C | -2.612161 | 2.066793 | 0.285741 |
| H | -2.669321 | 1.266142 | 1.015735 |
| C | 1.491862 | 2.315713 | -0.21557 |
| C | 2.606922 | 1.834227 | -0.900779 |
| H | 2.55364 | 0.880688 | -1.413712 |
| C | 3.771386 | 2.594911 | -0.922899 |
| H | 4.639813 | 2.229528 | -1.457059 |
| C | 3.816054 | 3.819586 | -0.266867 |
| H | 4.724569 | 4.409414 | -0.287165 |
| C | 2.696614 | 4.301834 | 0.408514 |
| H | 2.734388 | 5.262089 | 0.907403 |
| C | 1.528224 | 3.55431 | 0.433492 |
| H | 0.647939 | 3.939987 | 0.937926 |

| | | | |
|---|---|---|---|
| C | -0.629845 | 3.569985 | -1.351164 |
| H | 0.32072 | 3.58888 | -1.873372 |
| C | -1.606037 | 4.507232 | -1.655949 |
| H | -1.417871 | 5.252164 | -2.418779 |
| C | -2.821444 | 4.493869 | -0.975679 |
| H | -3.57492 | 5.236422 | -1.209922 |
| C | -3.075258 | 3.540863 | 0.008308 |
| H | -4.018836 | 3.54419 | 0.539611 |
| C | -2.113281 | 2.59171 | 0.32045 |
| H | -2.31439 | 1.849535 | 1.085518 |
| C | 1.982995 | 1.955172 | -0.215007 |
| C | 2.996075 | 1.113624 | -0.69025 |
| H | 2.779734 | 0.103986 | -1.021484 |
| C | 4.298171 | 1.591454 | -0.743345 |
| H | 5.084544 | 0.951396 | -1.122995 |
| C | 4.588139 | 2.88254 | -0.312271 |
| H | 5.606793 | 3.248394 | -0.357293 |
| C | 3.579229 | 3.712839 | 0.170576 |
| H | 3.8116 | 4.717471 | 0.500357 |
| C | 2.27008 | 3.257675 | 0.22022 |
| H | 1.484703 | 3.912877 | 0.581642 |
| H | 0.22049 | 0.012737 | -2.000169 |

**$ANH_2^{3+}$**



Zero-point correction= 0.525396 (Hartree/Particle)

Thermal correction to Energy= 0.556538

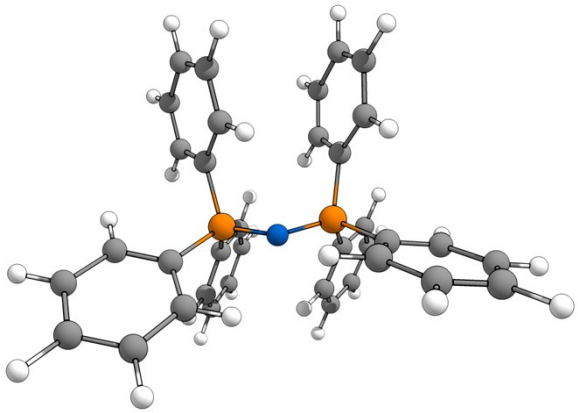
Thermal correction to Enthalpy= 0.557482

Thermal correction to Gibbs Free Energy= 0.461507

Sum of electronic and zero-point Energies= -2048.114932

Sum of electronic and thermal Energies= -2048.083791

**$(Ph_3P)_2N^+$**



Zero-point correction= 0.560214 (Hartree/Particle)

Thermal correction to Energy= 0.593355

Thermal correction to Enthalpy= 0.594299

Thermal correction to Gibbs Free Energy= 0.492529

Sum of electronic and zero-point Energies= -2126.356344

Sum of electronic and thermal Energies= -2126.323203

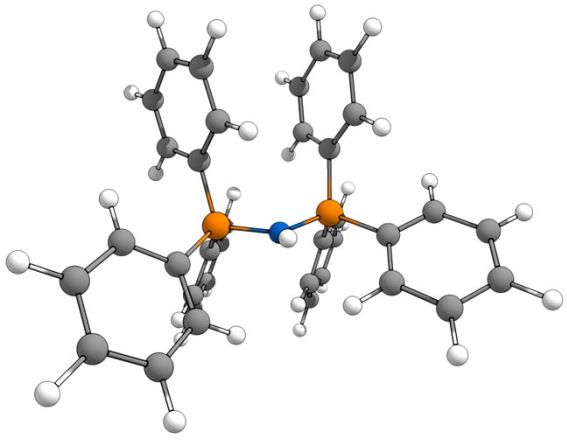
Sum of electronic and thermal Enthalpies= -2126.322259

Sum of electronic and thermal Free Energies= -2126.424029

| Sum of electronic and thermal Enthalpies= | -2048.082846 | | | | | | |
|---|---|---|---|---|---|---|---|
| Sum of electronic and thermal Free Energies= | -2048.178821 | | | | | | |
| P | -0.473854 | -1.51778 | -0.158091 | P | 1.477406 | -0.070995 | 0.274387 |
| P | 0.508172 | 1.395109 | 0.113637 | P | -1.477399 | 0.071024 | 0.274381 |
| N | 0.2041 | -0.070436 | -1.039783 | N | -0.000004 | -0.000038 | 0.88422 |
| C | -0.378774 | -0.820514 | 1.477632 | C | -1.405026 | -1.398612 | -2.098616 |
| C | 0.254703 | 0.429432 | 1.599799 | C | -1.869195 | -1.351239 | -0.780112 |
| C | 0.543561 | 0.948352 | 2.858017 | C | -2.477861 | -2.474185 | -0.216674 |
| H | 1.036999 | 1.9092 | 2.967268 | H | -2.845591 | -2.442259 | 0.80314 |
| C | 0.181161 | 0.213748 | 3.98851 | C | -2.615 | -3.636393 | -0.968151 |
| H | 0.405218 | 0.607928 | 4.973109 | H | -3.092866 | -4.504741 | -0.531584 |
| C | -0.471197 | -1.010512 | 3.86459 | C | -2.147228 | -3.680456 | -2.276698 |
| H | -0.756523 | -1.562805 | 4.75247 | H | -2.257054 | -4.587359 | -2.859145 |
| C | -0.745694 | -1.547344 | 2.606761 | C | -1.546529 | -2.560092 | -2.844518 |
| H | -1.226783 | -2.516489 | 2.518921 | H | -1.187885 | -2.593186 | -3.865866 |
| C | -1.988878 | -2.188096 | -0.853437 | C | -1.762199 | 1.58469 | -0.676148 |
| C | -1.576238 | -3.361379 | -1.393503 | C | -1.105758 | 2.742264 | -0.247466 |
| H | -2.271052 | -4.055553 | -1.855278 | H | -0.444873 | 2.703274 | 0.611562 |
| C | -0.125672 | -3.679082 | -1.335397 | C | -1.291767 | 3.934583 | -0.931752 |
| H | 0.27071 | -4.560335 | -1.831146 | H | -0.778413 | 4.829684 | -0.602573 |
| C | 0.653726 | -2.816202 | -0.655059 | C | -2.132564 | 3.976286 | -2.041008 |
| C | -3.315676 | -1.621476 | -0.644125 | H | -2.274885 | 4.907903 | -2.575242 |
| C | -3.473133 | -0.239473 | -0.472672 | C | -2.797373 | 2.8296 | -2.460587 |
| H | -2.610291 | 0.424629 | -0.478986 | H | -3.457444 | 2.865899 | -3.318397 |
| C | -4.736607 | 0.309657 | -0.326395 | C | -2.61738 | 1.630317 | -1.778978 |
| H | -4.856238 | 1.379334 | -0.207089 | H | -3.137699 | 0.738208 | -2.10973 |
| C | -5.856438 | -0.519205 | -0.346936 | C | -2.619171 | 0.041158 | 1.666724 |
| H | -6.84593 | -0.09327 | -0.233344 | C | -2.173333 | -0.399229 | 2.912478 |
| C | -5.70857 | -1.895394 | -0.508301 | H | -1.133709 | -0.678669 | 3.03883 |
| H | -6.580859 | -2.537042 | -0.513555 | C | -3.06934 | -0.467412 | 3.973472 |
| C | -4.446262 | -2.450114 | -0.652156 | H | -2.729956 | -0.807026 | 4.944199 |
| H | -4.340184 | -3.524155 | -0.753168 | C | -4.397277 | -0.098429 | 3.788527 |
| C | 2.107322 | -2.658337 | -0.510192 | H | -5.092054 | -0.151227 | 4.617919 |
| C | 2.680434 | -2.53171 | 0.764768 | C | -4.838245 | 0.344357 | 2.544175 |
| H | 2.058906 | -2.594768 | 1.652328 | H | -5.871014 | 0.638766 | 2.406214 |
| C | 4.05733 | -2.403966 | 0.891363 | C | -3.950797 | 0.416392 | 1.479198 |
| H | 4.50682 | -2.351438 | 1.875615 | H | -4.291919 | 0.772688 | 0.512594 |
| C | 4.864311 | -2.380241 | -0.247175 | H | -0.944221 | -0.525422 | -2.546414 |
| H | 5.940639 | -2.306019 | -0.142137 | C | 2.619153 | -0.041278 | 1.666749 |
| C | 4.297884 | -2.486318 | -1.515165 | C | 3.950725 | -0.416703 | 1.479272 |
| H | 4.928746 | -2.487425 | -2.395813 | C | 2.173318 | 0.399148 | 2.912495 |
| C | 2.920864 | -2.628293 | -1.652362 | C | 4.838133 | -0.344848 | 2.544299 |
| H | 2.480477 | -2.748314 | -2.637277 | C | 3.069286 | 0.467163 | 3.97353 |
| C | -0.793921 | 2.532551 | -0.209135 | C | 4.397174 | 0.097962 | 3.788643 |

| | | | |
|---|---|---|---|
| C | -0.810148 | 3.234391 | -1.431926 |
| H | -0.031075 | 3.093145 | -2.175676 |
| C | -1.836449 | 4.131208 | -1.675502 |
| H | -1.864257 | 4.677656 | -2.610262 |
| C | -2.82236 | 4.343263 | -0.708431 |
| H | -3.610717 | 5.062484 | -0.899816 |
| C | -2.800884 | 3.650434 | 0.500863 |
| H | -3.564705 | 3.832289 | 1.247236 |
| C | -1.7939 | 2.732194 | 0.759033 |
| H | -1.784076 | 2.189261 | 1.697637 |
| C | 2.135482 | 1.944503 | -0.23844 |
| C | 3.199857 | 1.019521 | -0.222763 |
| H | 3.039403 | -0.036783 | -0.018582 |
| C | 4.482942 | 1.478641 | -0.45283 |
| H | 5.310991 | 0.780871 | -0.450242 |
| C | 4.711685 | 2.840371 | -0.674264 |
| H | 5.722839 | 3.191148 | -0.847008 |
| C | 3.661051 | 3.75415 | -0.664639 |
| H | 3.853552 | 4.808211 | -0.821792 |
| C | 2.362175 | 3.318181 | -0.449271 |
| H | 1.548272 | 4.033131 | -0.425079 |
| H | -0.416582 | 0.215603 | -1.81163 |
| H | 1.110095 | -0.355026 | -1.45896 |
| H | 4.291849 | -0.772994 | 0.512666 |
| H | 1.133736 | 0.678759 | 3.038804 |
| H | 5.870859 | -0.639421 | 2.40638 |
| H | 2.729911 | 0.806827 | 4.944242 |
| H | 5.091916 | 0.150619 | 4.618071 |
| C | 1.869256 | 1.35131 | -0.780011 |
| C | 2.477969 | 2.474182 | -0.216447 |
| C | 1.405133 | 1.398814 | -2.098509 |
| C | 2.615186 | 3.636435 | -0.967816 |
| C | 1.546728 | 2.560358 | -2.844318 |
| C | 2.147457 | 3.680634 | -2.276384 |
| H | 2.845658 | 2.442144 | 0.803378 |
| H | 0.944289 | 0.525698 | -2.54641 |
| H | 3.093078 | 4.504726 | -0.531167 |
| H | 1.188118 | 2.593533 | -3.865675 |
| H | 2.25736 | 4.587587 | -2.85874 |
| C | 1.762187 | -1.584592 | -0.676271 |
| C | 2.617276 | -1.630128 | -1.779174 |
| C | 1.105773 | -2.742201 | -0.247632 |
| C | 2.797178 | -2.829354 | -2.460919 |
| C | 1.291711 | -3.934455 | -0.932036 |
| C | 2.132394 | -3.976065 | -2.041386 |
| H | 3.137593 | -0.738007 | -2.109892 |
| H | 0.444972 | -2.703272 | 0.611463 |
| H | 3.457163 | -2.865577 | -3.318798 |
| H | 0.77839 | -4.829586 | -0.602885 |
| H | 2.274644 | -4.907641 | -2.575709 |

**$(Ph_3P)_2NH^{2+}$**



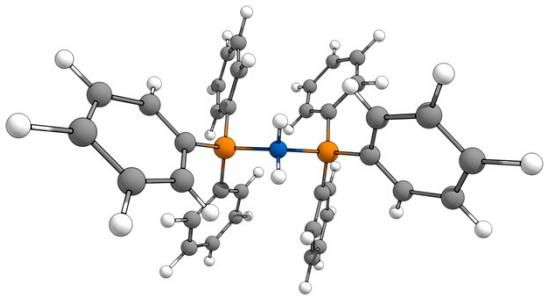
Zero-point correction= 0.572089 (Hartree/Particle)

Thermal correction to Energy= 0.605335

Thermal correction to Enthalpy= 0.606280

Thermal correction to Gibbs Free Energy= 0.505935

**$(Ph_3P)_2NH_2^{3+}$**



Zero-point correction= 0.583728 (Hartree/Particle)

Thermal correction to Energy= 0.617723

Thermal correction to Enthalpy= 0.618667

Thermal correction to Gibbs Free Energy= 0.515237

Sum of electronic and zero-point Energies= -2126.724193

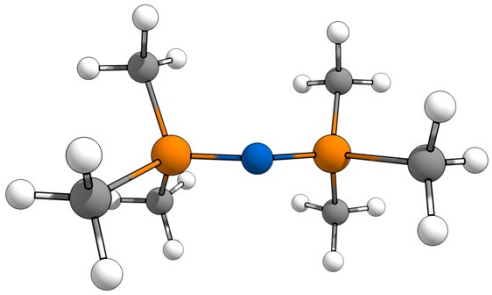
Sum of electronic and thermal Energies= -2126.690198

Sum of electronic and thermal Enthalpies= -2126.689254

| Sum of electronic and zero-point Energies= -2126.621863<br>Sum of electronic and thermal Energies= -2126.588617<br>Sum of electronic and thermal Enthalpies= -2126.587672<br>Sum of electronic and thermal Free Energies= -2126.688017 | | | | Sum of electronic and thermal Free Energies= -2126.792684 | | | |
|---|---|---|---|---|---|---|---|
| P | 1.547546 | 0.058228 | 0.228021 | P | 1.727565 | -0.079966 | 0.161451 |
| P | -1.551818 | -0.11881 | 0.23531 | P | -1.727858 | 0.080009 | 0.159849 |
| N | 0.012202 | -0.182426 | 0.920329 | N | -0.000553 | 0.000096 | 0.929484 |
| C | -1.170713 | -0.979777 | -2.366707 | C | -1.327241 | -1.613545 | -1.992474 |
| C | -1.675552 | -1.303345 | -1.100291 | C | -1.970946 | -1.411329 | -0.757009 |
| C | -2.219622 | -2.568379 | -0.856695 | C | -2.893517 | -2.35328 | -0.269656 |
| H | -2.647159 | -2.812567 | 0.108578 | H | -3.433679 | -2.182184 | 0.6533 |
| C | -2.236526 | -3.511133 | -1.877754 | C | -3.146815 | -3.500698 | -1.009106 |
| H | -2.671391 | -4.486796 | -1.699784 | H | -3.866053 | -4.223634 | -0.644592 |
| C | -1.716879 | -3.195162 | -3.128396 | C | -2.500583 | -3.704317 | -2.223786 |
| H | -1.740788 | -3.932092 | -3.922434 | H | -2.717537 | -4.594152 | -2.803538 |
| C | -1.18792 | -1.929668 | -3.375563 | C | -1.594908 | -2.760764 | -2.716856 |
| H | -0.802456 | -1.682238 | -4.356745 | H | -1.11409 | -2.917523 | -3.674759 |
| C | -1.910039 | 1.533574 | -0.3493 | C | -1.712428 | 1.577478 | -0.782469 |
| C | -1.442044 | 2.625543 | 0.391707 | C | -1.272947 | 2.767947 | -0.176637 |
| H | -0.820494 | 2.478319 | 1.268408 | H | -0.910912 | 2.787469 | 0.847676 |
| C | -1.777564 | 3.911826 | -0.001068 | C | -1.338733 | 3.953937 | -0.886876 |
| H | -1.418908 | 4.759977 | 0.568849 | H | -1.01078 | 4.878273 | -0.427335 |
| C | -2.581198 | 4.109878 | -1.122587 | C | -1.850382 | 3.958932 | -2.186989 |
| H | -2.844055 | 5.11662 | -1.424587 | H | -1.914525 | 4.893487 | -2.732638 |
| C | -3.061897 | 3.024712 | -1.847219 | C | -2.302813 | 2.783557 | -2.778448 |
| H | -3.699636 | 3.183653 | -2.707703 | H | -2.72396 | 2.802448 | -3.776201 |
| C | -2.73391 | 1.729563 | -1.462795 | C | -2.241153 | 1.58273 | -2.080702 |
| H | -3.123523 | 0.886165 | -2.021135 | H | -2.62528 | 0.675419 | -2.532303 |
| C | -2.576692 | -0.550489 | 1.637802 | C | -2.664752 | 0.189982 | 1.663353 |
| C | -2.211345 | -1.631974 | 2.452868 | C | -2.520114 | -0.792906 | 2.662334 |
| H | -1.306808 | -2.197513 | 2.25119 | H | -1.840205 | -1.633615 | 2.544419 |
| C | -3.025155 | -1.985995 | 3.517807 | C | -3.291865 | -0.715269 | 3.807854 |
| H | -2.752476 | -2.820375 | 4.151695 | H | -3.188042 | -1.466349 | 4.581153 |
| C | -4.194516 | -1.269356 | 3.767709 | C | -4.21443 | 0.323466 | 3.956909 |
| H | -4.826483 | -1.549026 | 4.601815 | H | -4.822533 | 0.372955 | 4.852647 |
| C | -4.554475 | -0.198456 | 2.957457 | C | -4.365494 | 1.287281 | 2.965732 |
| H | -5.462007 | 0.355832 | 3.160394 | H | -5.090567 | 2.082596 | 3.085942 |
| C | -3.74796 | 0.169394 | 1.886204 | C | -3.590862 | 1.232563 | 1.812543 |
| H | -4.024125 | 1.010917 | 1.260665 | H | -3.717509 | 1.98184 | 1.039412 |
| H | -0.779193 | 0.01073 | -2.565139 | H | -0.636555 | -0.88106 | -2.391997 |
| C | 2.684683 | -0.193477 | 1.59117 | C | 2.662785 | -0.193795 | 1.66559 |
| C | 3.98327 | 0.31251 | 1.456557 | C | 3.587111 | -1.238046 | 1.814376 |
| C | 2.343085 | -0.989324 | 2.689402 | C | 2.518279 | 0.787733 | 2.665962 |
| C | 4.923435 | 0.048642 | 2.442141 | C | 4.359906 | -1.295879 | 2.968621 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 3.291914 | -1.238758 | 3.672427 | C | 3.288199 | 0.706983 | 3.812486 |
| C | 4.576386 | -0.718909 | 3.550548 | C | 4.208838 | -0.333492 | 3.961206 |
| H | 4.261825 | 0.910057 | 0.594903 | H | 3.7138 | -1.986193 | 1.040166 |
| H | 1.356138 | -1.428629 | 2.784903 | H | 1.839806 | 1.629656 | 2.548422 |
| H | 5.926974 | 0.443032 | 2.344726 | H | 5.083618 | -2.092469 | 3.088581 |
| H | 3.029727 | -1.84514 | 4.530196 | H | 3.184483 | 1.457023 | 4.586808 |
| H | 5.313064 | -0.91732 | 4.319446 | H | 4.815509 | -0.38542 | 4.85778 |
| C | 1.6862 | 1.72981 | -0.408217 | C | 1.972547 | 1.413195 | -0.752043 |
| C | 2.061207 | 2.754593 | 0.470422 | C | 2.896927 | 2.352656 | -0.263333 |
| C | 1.255927 | 2.03903 | -1.704385 | C | 1.328789 | 1.618615 | -1.98689 |
| C | 2.027669 | 4.074496 | 0.039724 | C | 3.151965 | 3.500887 | -1.000954 |
| C | 1.221733 | 3.362028 | -2.122886 | C | 1.598062 | 2.766654 | -2.70939 |
| C | 1.610271 | 4.376958 | -1.253084 | C | 2.505601 | 3.707741 | -2.215023 |
| H | 2.387663 | 2.528352 | 1.479431 | H | 3.437001 | 2.179004 | 0.659212 |
| H | 0.96721 | 1.255375 | -2.393466 | H | 0.636894 | 0.887854 | -2.387474 |
| H | 2.337051 | 4.865625 | 0.711423 | H | 3.872566 | 4.221982 | -0.635492 |
| H | 0.902726 | 3.599854 | -3.129932 | H | 1.117073 | 2.925902 | -3.66679 |
| H | 1.595853 | 5.407556 | -1.587266 | H | 2.723855 | 4.59821 | -2.793304 |
| C | 1.778245 | -1.185702 | -1.038115 | C | 1.712307 | -1.575147 | -0.784575 |
| C | 2.559583 | -0.916262 | -2.16523 | C | 2.243109 | -1.577036 | -2.081949 |
| C | 1.304361 | -2.479637 | -0.790427 | C | 1.271299 | -2.767083 | -0.182744 |
| C | 2.819351 | -1.937967 | -3.071792 | C | 2.305707 | -2.775975 | -2.782866 |
| C | 1.570668 | -3.488856 | -1.701486 | C | 1.337953 | -3.951143 | -0.896154 |
| C | 2.320089 | -3.215463 | -2.844903 | C | 1.851946 | -3.952805 | -2.19535 |
| H | 2.976074 | 0.06976 | -2.33476 | H | 2.628177 | -0.668568 | -2.530414 |
| H | 0.729764 | -2.695904 | 0.103619 | H | 0.907256 | -2.789248 | 0.840784 |
| H | 3.42249 | -1.735354 | -3.94791 | H | 2.728525 | -2.792201 | -3.779958 |
| H | 1.202496 | -4.490673 | -1.518263 | H | 1.008727 | -4.876604 | -0.439787 |
| H | 2.529885 | -4.008449 | -3.552676 | H | 1.916673 | -4.885903 | -2.743417 |
| H | -0.00518 | 0.019169 | 1.919004 | H | -0.029513 | -0.806003 | 1.57017 |
| | | | | H | 0.027948 | 0.806732 | 1.569508 |

**$(Me_3P)_2N^+$**

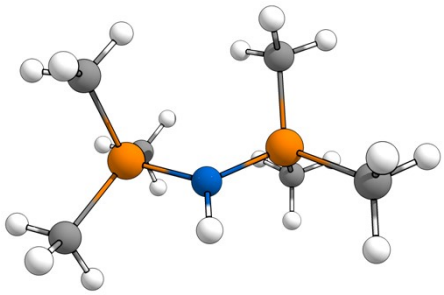


Zero-point correction= 0.236059 (Hartree/Particle)

Thermal correction to Energy= 0.250779

Thermal correction to Enthalpy= 0.251724

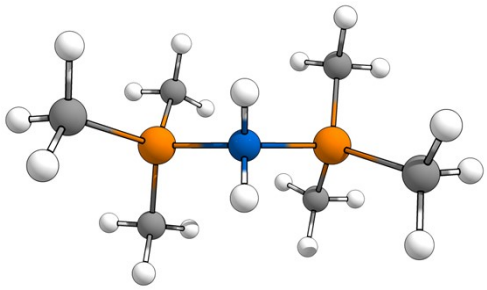
**$(Me_3P)_2NH^{2+}$**



Zero-point correction= 0.245854 (Hartree/Particle)

Thermal correction to Energy= 0.261241

Thermal correction to Enthalpy= 0.262186

| | |
|---|---|
| Thermal correction to Gibbs Free Energy= 0.195297<br>Sum of electronic and zero-point Energies= -976.445983<br>Sum of electronic and thermal Energies= -976.431262<br>Sum of electronic and thermal Enthalpies= -976.430318<br>Sum of electronic and thermal Free Energies= -976.486744 | Thermal correction to Gibbs Free Energy= 0.204241<br>Sum of electronic and zero-point Energies= -976.664377<br>Sum of electronic and thermal Energies= -976.648990<br>Sum of electronic and thermal Enthalpies= -976.648045<br>Sum of electronic and thermal Free Energies= -976.705990 |
| P -1.520892 0.001044 0.070219<br>P 1.521137 0.003365 0.069434<br>N 0.000166 0.021546 0.515209<br>C 2.067756 -1.620858 -0.509563<br>H 1.890444 -2.358075 0.274711<br>H 1.504644 -1.904978 -1.400253<br>H 3.131762 -1.602569 -0.752824<br>C 2.550622 0.438162 1.481376<br>H 3.606212 0.420299 1.205658<br>H 2.277805 1.435428 1.827711<br>H 2.369251 -0.276884 2.284485<br>C 1.904434 1.174964 -1.257456<br>H 1.361064 0.89735 -2.162806<br>H 1.605284 2.178755 -0.951766<br>H 2.974157 1.170964 -1.474486<br>C -2.559277 -0.006478 1.541261<br>H -2.336599 0.880243 2.135722<br>H -3.614915 -0.009139 1.265295<br>H -2.331535 -0.893997 2.132569<br>C -1.969472 -1.453001 -0.911378<br>H -1.717504 -2.356133 -0.353563<br>H -3.038909 -1.452057 -1.129886<br>H -1.416805 -1.446715 -1.852815<br>C -1.994817 1.445712 -0.912741<br>H -1.432314 1.458234 -1.84793<br>H -3.061792 1.419122 -1.141398<br>H -1.770557 2.352179 -0.348668 | P -1.55372 -0.007662 0.060112<br>P 1.553485 0.006266 0.06034<br>N -0.000151 -0.01058 0.7472<br>C 1.987026 -1.616275 -0.573056<br>H 1.895139 -2.360792 0.220378<br>H 1.350314 -1.892216 -1.415432<br>H 3.02503 -1.590965 -0.917653<br>C 2.652091 0.470325 1.397869<br>H 3.673932 0.503975 1.010534<br>H 2.384867 1.456164 1.78342<br>H 2.609699 -0.27349 2.197282<br>C 1.600108 1.217531 -1.264101<br>H 0.936529 0.934335 -2.084416<br>H 1.335178 2.205214 -0.881928<br>H 2.619815 1.252156 -1.659034<br>C -2.651773 -0.522569 1.37933<br>H -2.611885 0.191386 2.205575<br>H -3.6733 -0.544458 0.990299<br>H -2.382462 -1.521206 1.728699<br>C -1.594994 -1.171385 -1.30658<br>H -1.329198 -2.17149 -0.958962<br>H -2.613485 -1.19362 -1.705444<br>H -0.929491 -0.858026 -2.11434<br>C -1.992109 1.634753 -0.515931<br>H -1.349595 1.94552 -1.341609<br>H -3.026953 1.616157 -0.870277<br>H -1.911612 2.349686 0.30544<br>H -0.000035 -0.027611 1.765095 |
| **$(Me_3P)_2NH_2^{3+}$**<br>  <br>Zero-point correction= 0.255625 (Hartree/Particle) | **AC** |

Thermal correction to Energy= 0.271404

Thermal correction to Enthalpy= 0.272348

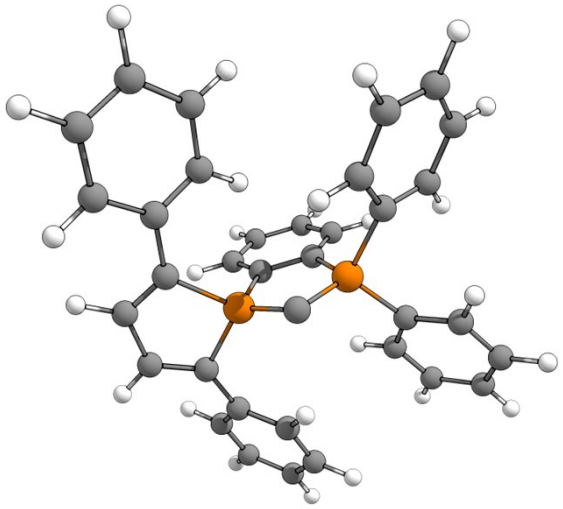
Thermal correction to Gibbs Free Energy= 0.213321

Sum of electronic and zero-point Energies= -976.665726

Sum of electronic and thermal Energies= -976.649948

Sum of electronic and thermal Enthalpies= -976.649003

Sum of electronic and thermal Free Energies= -976.708031



Zero-point correction= 0.501418 (Hartree/Particle)

Thermal correction to Energy= 0.531802

Thermal correction to Enthalpy= 0.532747

Thermal correction to Gibbs Free Energy= 0.437556

Sum of electronic and zero-point Energies= -2031.215922

Sum of electronic and thermal Energies= -2031.185537

Sum of electronic and thermal Enthalpies= -2031.184593

Sum of electronic and thermal Free Energies= -2031.279783

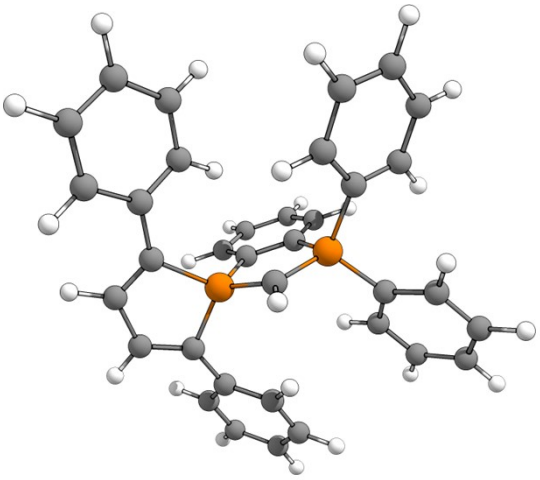
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| P | 1.696876 | 0.000422 | -0.018715 | P | 0.133169 | -1.362795 | -0.442422 |
| P | -1.696922 | -0.000425 | -0.018701 | P | -0.063315 | 1.266751 | -0.275403 |
| N | 0 | 0.00031 | -0.843499 | C | 0.134078 | 0.016786 | -1.359861 |
| C | -2.780594 | -0.452632 | -1.366255 | C | -0.016185 | -0.861856 | 1.337718 |
| H | -2.7295 | 0.270215 | -2.186717 | C | -0.114909 | 0.525442 | 1.425663 |
| H | -2.585164 | -1.469222 | -1.721572 | C | -0.226902 | 1.141349 | 2.667497 |
| H | -3.802711 | -0.427427 | -0.959571 | H | -0.309726 | 2.220057 | 2.746319 |
| C | -1.950288 | 1.670631 | 0.558984 | C | -0.237094 | 0.351372 | 3.81448 |
| H | -2.978769 | 1.69774 | 0.950014 | H | -0.323785 | 0.818673 | 4.788415 |
| H | -1.277745 | 1.93754 | 1.37651 | C | -0.138809 | -1.035983 | 3.721186 |
| H | -1.893242 | 2.394347 | -0.260076 | H | -0.147937 | -1.636347 | 4.623342 |
| C | -1.633661 | -1.224494 | 1.280705 | C | -0.028758 | -1.653789 | 2.478561 |
| H | -1.377205 | -2.215095 | 0.89398 | H | 0.048655 | -2.733616 | 2.398613 |
| H | -0.979947 | -0.922644 | 2.102451 | C | -1.121 | -2.70231 | -0.602071 |
| H | -2.657089 | -1.283612 | 1.681979 | C | -0.486893 | -3.885119 | -0.63187 |
| C | 2.780754 | 0.450862 | -1.366708 | H | -1.00047 | -4.838496 | -0.704724 |
| H | 2.584983 | 1.466765 | -1.723806 | C | 0.986453 | -3.817725 | -0.575299 |
| H | 3.802774 | 0.426841 | -0.95973 | H | 1.585879 | -4.722501 | -0.588083 |
| H | 2.730163 | -0.273384 | -2.185968 | C | 1.512443 | -2.583681 | -0.496612 |
| C | 1.949284 | -1.670321 | 0.560342 | C | -2.562657 | -2.435499 | -0.572958 |
| H | 1.88899 | -2.395102 | -0.257533 | C | -3.087551 | -1.323668 | -1.244559 |
| H | 2.978803 | -1.698394 | 0.948566 | H | -2.417558 | -0.67563 | -1.800311 |

| | | | |
|---|---|---|---|
| H | 1.278615 | -1.935071 | 1.3801 |
| C | 1.634544 | 1.225618 | 1.279666 |
| H | 0.980324 | 0.925165 | 2.101515 |
| H | 2.657936 | 1.284008 | 1.68115 |
| H | 1.379226 | 2.21616 | 0.892029 |
| H | -0.003422 | 0.813417 | -1.483714 |
| H | 0.003433 | -0.81236 | -1.484275 |

**$ACH^+$**

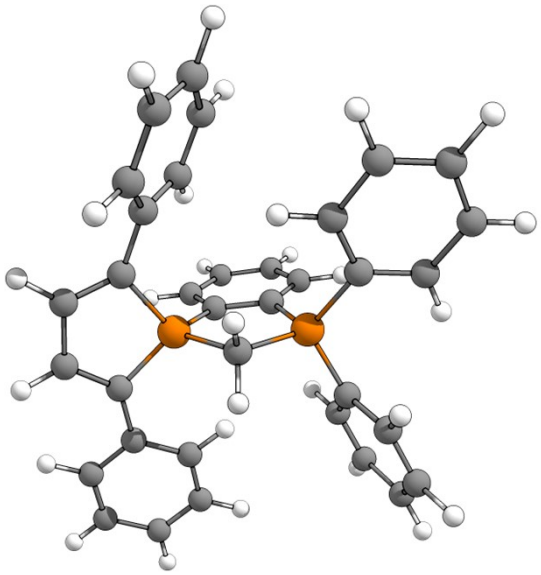
| | | | |
|---|---|---|---|
| C | -4.453313 | -1.06636 | -1.205152 |
| H | -4.847255 | -0.203921 | -1.730449 |
| C | -5.308242 | -1.906965 | -0.500541 |
| H | -6.372309 | -1.70372 | -0.473731 |
| C | -4.792541 | -3.010873 | 0.173539 |
| H | -5.45251 | -3.663249 | 0.733183 |
| C | -3.429719 | -3.27013 | 0.142867 |
| H | -3.021962 | -4.111948 | 0.691707 |
| C | 2.925776 | -2.197599 | -0.46555 |
| C | 3.334737 | -1.042366 | 0.21232 |
| H | 2.605245 | -0.432831 | 0.734071 |
| C | 4.674006 | -0.674099 | 0.238611 |
| H | 4.968515 | 0.224543 | 0.768123 |
| C | 5.626594 | -1.451253 | -0.410597 |
| H | 6.670862 | -1.162511 | -0.391963 |
| C | 5.231023 | -2.598918 | -1.092248 |
| H | 5.966387 | -3.201763 | -1.61175 |
| C | 3.893268 | -2.965205 | -1.125403 |
| H | 3.584932 | -3.838043 | -1.689842 |
| C | -1.582293 | 2.284174 | -0.391344 |
| C | -1.620925 | 3.426527 | -1.192432 |
| H | -0.714776 | 3.781476 | -1.671714 |
| C | -2.818763 | 4.107428 | -1.379261 |
| H | -2.842539 | 4.993538 | -2.002474 |
| C | -3.983054 | 3.649201 | -0.771841 |
| H | -4.916038 | 4.180515 | -0.918598 |
| C | -3.951302 | 2.505236 | 0.019949 |
| H | -4.857806 | 2.13953 | 0.487906 |
| C | -2.755842 | 1.822062 | 0.208038 |
| H | -2.739262 | 0.921083 | 0.813445 |
| C | 1.294325 | 2.49467 | -0.256684 |
| C | 2.453022 | 2.173642 | -0.960935 |
| H | 2.471171 | 1.25325 | -1.536948 |
| C | 3.548748 | 3.030478 | -0.919544 |
| H | 4.447873 | 2.77949 | -1.470034 |
| C | 3.486215 | 4.205756 | -0.179267 |
| H | 4.339409 | 4.873466 | -0.149367 |
| C | 2.325808 | 4.532287 | 0.518952 |
| H | 2.276163 | 5.452397 | 1.089113 |
| C | 1.229111 | 3.680416 | 0.479222 |
| H | 0.317893 | 3.946666 | 1.005675 |

**$ACH_2^{2+}$**



Zero-point correction= 0.512861 (Hartree/Particle)
Thermal correction to Energy= 0.543593
Thermal correction to Enthalpy= 0.544538
Thermal correction to Gibbs Free Energy= 0.448091
Sum of electronic and zero-point Energies= -2031.674448
Sum of electronic and thermal Energies= -2031.643716
Sum of electronic and thermal Enthalpies= -2031.642772
Sum of electronic and thermal Free Energies= -2031.739218

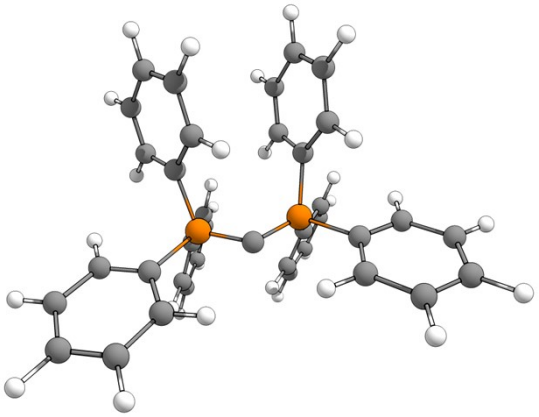
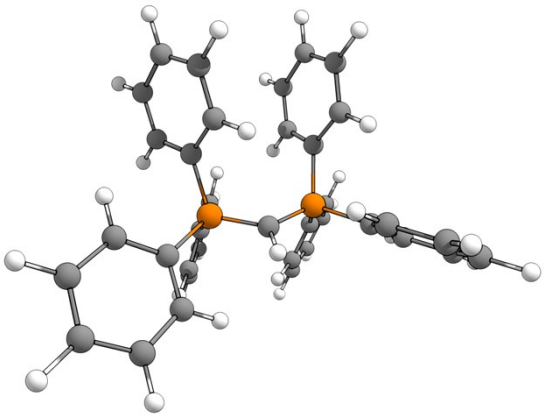
| | | | |
|---|---|---|---|
| P | 0.050522 | -1.456227 | -0.383897 |
| P | 0.017111 | 1.387166 | -0.212744 |
| C | 0.152815 | 0.014384 | -1.236845 |
| C | -0.111642 | -0.837065 | 1.312576 |
| C | -0.136322 | 0.555721 | 1.396012 |
| C | -0.249288 | 1.182404 | 2.631099 |
| H | -0.268332 | 2.264138 | 2.704247 |
| C | -0.341435 | 0.396689 | 3.776374 |
| H | -0.431072 | 0.871726 | 4.74548 |
| C | -0.320268 | -0.993429 | 3.688499 |
| H | -0.391775 | -1.589565 | 4.589737 |
| C | -0.205999 | -1.623269 | 2.45294 |
| H | -0.188331 | -2.705496 | 2.379958 |
| C | -1.277516 | -2.683392 | -0.633922 |
| C | -0.683651 | -3.883569 | -0.745891 |
| H | -1.237785 | -4.808215 | -0.863984 |
| C | 0.793828 | -3.886323 | -0.698851 |
| H | 1.350142 | -4.811801 | -0.798457 |
| C | 1.384376 | -2.692325 | -0.515449 |
| C | -2.70452 | -2.359325 | -0.530721 |



Zero-point correction= 0.524960 (Hartree/Particle)
Thermal correction to Energy= 0.555795
Thermal correction to Enthalpy= 0.556739
Thermal correction to Gibbs Free Energy= 0.460122
Sum of electronic and zero-point Energies= -2031.958233
Sum of electronic and thermal Energies= -2031.927399
Sum of electronic and thermal Enthalpies= -2031.926454
Sum of electronic and thermal Free Energies= -2032.023072

| | | | |
|---|---|---|---|
| P | -0.488116 | -1.493821 | -0.176268 |
| P | 0.446041 | 1.322851 | -0.112144 |
| C | 0.010822 | -0.078722 | -1.227368 |
| C | -0.365812 | -0.759654 | 1.459012 |
| C | 0.198916 | 0.521089 | 1.489485 |
| C | 0.486361 | 1.131582 | 2.707335 |
| H | 0.935017 | 2.119053 | 2.740725 |
| C | 0.184202 | 0.455404 | 3.885292 |
| H | 0.402857 | 0.919937 | 4.839109 |
| C | -0.403292 | -0.809445 | 3.851306 |
| H | -0.641332 | -1.316961 | 4.77806 |
| C | -0.675551 | -1.432779 | 2.638218 |
| H | -1.112505 | -2.425363 | 2.613184 |
| C | -2.019897 | -2.337073 | -0.62733 |
| C | -1.62631 | -3.574991 | -1.000852 |
| H | -2.322452 | -4.333651 | -1.338988 |
| C | -0.176551 | -3.867662 | -0.941726 |
| H | 0.212008 | -4.828451 | -1.262483 |
| C | 0.613603 | -2.882696 | -0.478309 |
| C | -3.344638 | -1.724518 | -0.543915 |

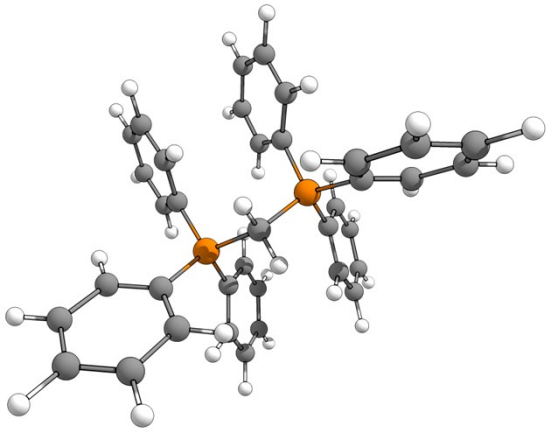
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -3.216513 | -1.189584 | -1.104493 | C | -3.477943 | -0.352102 | -0.298699 |
| H | -2.557015 | -0.522779 | -1.648534 | H | -2.603467 | 0.275587 | -0.146825 |
| C | -4.571719 | -0.898147 | -1.00564 | C | -4.731171 | 0.240361 | -0.247572 |
| H | -4.959767 | 0.002317 | -1.467099 | H | -4.817826 | 1.304329 | -0.06403 |
| C | -5.426522 | -1.763611 | -0.331778 | C | -5.870031 | -0.533786 | -0.437891 |
| H | -6.48329 | -1.537359 | -0.259478 | H | -6.850634 | -0.076115 | -0.398523 |
| C | -4.922748 | -2.924398 | 0.248811 | C | -5.749768 | -1.901621 | -0.675535 |
| H | -5.584567 | -3.596721 | 0.780739 | H | -6.636708 | -2.50615 | -0.817725 |
| C | -3.570585 | -3.219386 | 0.154972 | C | -4.499573 | -2.495864 | -0.727047 |
| H | -3.174681 | -4.111578 | 0.62686 | H | -4.424257 | -3.562355 | -0.901693 |
| C | 2.810467 | -2.356712 | -0.479667 | C | 2.075171 | -2.749152 | -0.382909 |
| C | 3.275757 | -1.294267 | 0.303848 | C | 2.673814 | -2.343173 | 0.817424 |
| H | 2.58373 | -0.713129 | 0.905382 | H | 2.067304 | -2.182143 | 1.702211 |
| C | 4.630937 | -0.991786 | 0.3463 | C | 4.052547 | -2.193745 | 0.89046 |
| H | 4.977439 | -0.173288 | 0.965937 | H | 4.514616 | -1.906073 | 1.826738 |
| C | 5.537192 | -1.743226 | -0.393708 | C | 4.840859 | -2.43411 | -0.232398 |
| H | 6.594198 | -1.509565 | -0.358563 | H | 5.917471 | -2.32957 | -0.169455 |
| C | 5.082657 | -2.797069 | -1.181833 | C | 4.250825 | -2.830997 | -1.42909 |
| H | 5.783629 | -3.378794 | -1.767614 | H | 4.864382 | -3.030841 | -2.299022 |
| C | 3.729831 | -3.099445 | -1.229911 | C | 2.871561 | -2.989829 | -1.508016 |
| H | 3.377091 | -3.901161 | -1.868521 | H | 2.40953 | -3.30117 | -2.438472 |
| C | -1.434807 | 2.442328 | -0.45197 | C | -0.739117 | 2.651054 | -0.313224 |
| C | -1.364426 | 3.561878 | -1.284982 | C | -0.670327 | 3.443862 | -1.467155 |
| H | -0.418382 | 3.865535 | -1.720037 | H | 0.118411 | 3.297155 | -2.198573 |
| C | -2.51603 | 4.29268 | -1.551642 | C | -1.619454 | 4.436623 | -1.663405 |
| H | -2.464729 | 5.161481 | -2.195971 | H | -1.573737 | 5.056371 | -2.550103 |
| C | -3.730045 | 3.9097 | -0.991432 | C | -2.624864 | 4.63815 | -0.719238 |
| H | -4.624186 | 4.484825 | -1.199416 | H | -3.358816 | 5.41941 | -0.875723 |
| C | -3.800941 | 2.791663 | -0.165311 | C | -2.689727 | 3.849038 | 0.424375 |
| H | -4.746273 | 2.494933 | 0.272508 | H | -3.466886 | 4.016846 | 1.159719 |
| C | -2.656883 | 2.051842 | 0.10323 | C | -1.749497 | 2.847215 | 0.633864 |
| H | -2.718744 | 1.174602 | 0.739145 | H | -1.804558 | 2.234788 | 1.526928 |
| C | 1.470215 | 2.464568 | -0.19618 | C | 2.125306 | 1.867278 | -0.383149 |
| C | 2.65805 | 2.001939 | -0.762983 | C | 3.121819 | 0.928107 | -0.680174 |
| H | 2.680122 | 1.03935 | -1.261921 | H | 2.896521 | -0.126324 | -0.80815 |
| C | 3.806257 | 2.782252 | -0.68013 | C | 4.434598 | 1.355112 | -0.807168 |
| H | 4.728011 | 2.427451 | -1.124878 | H | 5.208274 | 0.635285 | -1.043431 |
| C | 3.767927 | 4.01149 | -0.03232 | C | 4.752777 | 2.700248 | -0.633065 |
| H | 4.663809 | 4.617567 | 0.028305 | H | 5.779978 | 3.027862 | -0.737672 |
| C | 2.581154 | 4.472995 | 0.532632 | C | 3.761984 | 3.62777 | -0.327506 |
| H | 2.553578 | 5.433824 | 1.031276 | H | 4.015045 | 4.671822 | -0.193414 |
| C | 1.428383 | 3.704519 | 0.450475 | C | 2.440892 | 3.219205 | -0.198763 |
| H | 0.500312 | 4.075242 | 0.873133 | H | 1.668816 | 3.94486 | 0.031223 |
| H | 0.234441 | 0.078027 | -2.311281 | H | 0.870608 | -0.370377 | -1.836093 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | | H | -0.81176 | 0.215714 | -1.882939 |
| **$(Ph_3P)_2C$** | | | | **$(Ph_3P)_2CH^+$** | | | |
|  | | | |  | | | |
| Zero-point correction= | | 0.558129 (Hartree/Particle) | | Zero-point correction= | | 0.571384 (Hartree/Particle) | |
| Thermal correction to Energy= | | 0.591387 | | Thermal correction to Energy= | | 0.604658 | |
| Thermal correction to Enthalpy= | | 0.592331 | | Thermal correction to Enthalpy= | | 0.605602 | |
| Thermal correction to Gibbs Free Energy= | | 0.490863 | | Thermal correction to Gibbs Free Energy= | | 0.505418 | |
| Sum of electronic and zero-point Energies= | | -2109.798507 | | Sum of electronic and zero-point Energies= | | -2110.249327 | |
| Sum of electronic and thermal Energies= | | -2109.765249 | | Sum of electronic and thermal Energies= | | -2110.216053 | |
| Sum of electronic and thermal Enthalpies= | | -2109.764305 | | Sum of electronic and thermal Enthalpies= | | -2110.215109 | |
| Sum of electronic and thermal Free Energies= | | -2109.865772 | | Sum of electronic and thermal Free Energies= | | -2110.315293 | |
| P | 1.463639 | -0.057737 | 0.414625 | P | 1.540552 | 0.044134 | 0.360386 |
| P | -1.463649 | 0.057719 | 0.414611 | P | -1.540551 | -0.044189 | 0.360375 |
| C | -0.000009 | -0.000022 | 1.178699 | C | -0.000001 | -0.000066 | 1.124895 |
| C | -1.407319 | -1.36551 | -2.020679 | C | -1.275663 | -1.343769 | -2.107708 |
| C | -1.870981 | -1.351098 | -0.702775 | C | -1.729542 | -1.447564 | -0.790758 |
| C | -2.426179 | -2.514852 | -0.167572 | C | -2.17651 | -2.68031 | -0.310073 |
| H | -2.779738 | -2.519531 | 0.858349 | H | -2.551131 | -2.771329 | 0.703016 |
| C | -2.518069 | -3.669074 | -0.938635 | C | -2.153764 | -3.797295 | -1.137079 |
| H | -2.952841 | -4.56631 | -0.513605 | H | -2.514899 | -4.747981 | -0.763813 |
| C | -2.052309 | -3.67363 | -2.249251 | C | -1.679143 | -3.69369 | -2.440651 |
| H | -2.117859 | -4.575549 | -2.846603 | H | -1.661313 | -4.567305 | -3.081094 |
| C | -1.49873 | -2.51811 | -2.790861 | C | -1.245163 | -2.465521 | -2.927501 |
| H | -1.129392 | -2.517073 | -3.809576 | H | -0.889772 | -2.377987 | -3.94686 |
| C | -1.803096 | 1.56105 | -0.601154 | C | -1.941252 | 1.447953 | -0.596289 |
| C | -1.1215 | 2.723913 | -0.236259 | C | -1.339159 | 2.649785 | -0.221831 |
| H | -0.444459 | 2.690642 | 0.610792 | H | -0.627721 | 2.659603 | 0.596485 |
| C | -1.290485 | 3.894615 | -0.963781 | C | -1.645855 | 3.820066 | -0.904496 |
| H | -0.743136 | 4.786244 | -0.680795 | H | -1.17184 | 4.750399 | -0.616523 |
| C | -2.14352 | 3.914903 | -2.062795 | C | -2.554025 | 3.792527 | -1.957804 |
| H | -2.269683 | 4.826139 | -2.635839 | H | -2.790679 | 4.70475 | -2.492154 |
| C | -2.835134 | 2.764102 | -2.42507 | C | -3.165422 | 2.597511 | -2.325362 |
| H | -3.502385 | 2.777173 | -3.279028 | H | -3.877305 | 2.579066 | -3.141311 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.668799 | 1.590163 | -1.696301 | C | -2.86299 | 1.422808 | -1.647009 |
| H | -3.202751 | 0.694422 | -1.995247 | H | -3.341204 | 0.49337 | -1.936821 |
| C | -2.82144 | 0.030698 | 1.641256 | C | -2.774506 | -0.22385 | 1.676256 |
| C | -2.499021 | -0.059591 | 2.991755 | C | -2.513242 | -1.071147 | 2.757714 |
| H | -1.450132 | -0.109554 | 3.266148 | H | -1.568393 | -1.599521 | 2.822403 |
| C | -3.511492 | -0.083598 | 3.946342 | C | -3.468948 | -1.236191 | 3.751419 |
| H | -3.260504 | -0.153509 | 4.998262 | H | -3.265581 | -1.892136 | 4.588785 |
| C | -4.842568 | -0.017383 | 3.551935 | C | -4.681628 | -0.558033 | 3.671406 |
| H | -5.630707 | -0.036504 | 4.295695 | H | -5.424601 | -0.6867 | 4.449078 |
| C | -5.166421 | 0.075692 | 2.200494 | C | -4.939602 | 0.287291 | 2.599105 |
| H | -6.203912 | 0.130096 | 1.892568 | H | -5.879805 | 0.821337 | 2.541266 |
| C | -4.157929 | 0.101701 | 1.246073 | C | -3.98959 | 0.457175 | 1.597906 |
| H | -4.411545 | 0.176505 | 0.193301 | H | -4.191548 | 1.128246 | 0.771317 |
| H | -0.975318 | -0.467211 | -2.447706 | H | -0.968849 | -0.382423 | -2.501107 |
| C | 2.821418 | -0.030855 | 1.641288 | C | 2.774499 | 0.223702 | 1.676286 |
| C | 4.157908 | -0.101863 | 1.246111 | C | 3.989607 | -0.457273 | 1.597871 |
| C | 2.498989 | 0.059342 | 2.991791 | C | 2.513206 | 1.070889 | 2.757822 |
| C | 5.166392 | -0.075952 | 2.200544 | C | 4.939613 | -0.287447 | 2.599086 |
| C | 3.511452 | 0.08325 | 3.946389 | C | 3.468906 | 1.235875 | 3.751542 |
| C | 4.84253 | 0.01703 | 3.551989 | C | 4.68161 | 0.557768 | 3.671465 |
| H | 4.411531 | -0.176593 | 0.193337 | H | 4.19159 | -1.128261 | 0.77122 |
| H | 1.450099 | 0.109312 | 3.266179 | H | 1.568337 | 1.599221 | 2.82256 |
| H | 6.203885 | -0.130361 | 1.892622 | H | 5.879836 | -0.821455 | 2.541197 |
| H | 3.260457 | 0.15309 | 4.998312 | H | 3.265514 | 1.891734 | 4.58897 |
| H | 5.630663 | 0.036074 | 4.295757 | H | 5.42458 | 0.686391 | 4.449148 |
| C | 1.871022 | 1.351172 | -0.702623 | C | 1.729517 | 1.447615 | -0.790624 |
| C | 2.426186 | 2.514882 | -0.16729 | C | 2.176456 | 2.680331 | -0.309833 |
| C | 1.407445 | 1.365688 | -2.020556 | C | 1.275639 | 1.343922 | -2.107581 |
| C | 2.518118 | 3.669168 | -0.93825 | C | 2.153683 | 3.797385 | -1.136745 |
| C | 1.498903 | 2.518352 | -2.790638 | C | 1.245105 | 2.465744 | -2.927277 |
| C | 2.052443 | 3.67383 | -2.248897 | C | 1.679058 | 3.693881 | -2.440323 |
| H | 2.779684 | 2.519476 | 0.858652 | H | 2.55107 | 2.771274 | 0.703266 |
| H | 0.975475 | 0.467422 | -2.447683 | H | 0.968851 | 0.3826 | -2.501059 |
| H | 2.952863 | 4.566369 | -0.51312 | H | 2.514798 | 4.748049 | -0.7634 |
| H | 1.129631 | 2.517398 | -3.809377 | H | 0.889712 | 2.378289 | -3.946642 |
| H | 2.118032 | 4.575797 | -2.846171 | H | 1.661205 | 4.567551 | -3.080691 |
| C | 1.803065 | -1.560982 | -0.601272 | C | 1.94129 | -1.447912 | -0.596414 |
| C | 2.668711 | -1.589998 | -1.696466 | C | 2.863058 | -1.42265 | -1.647104 |
| C | 1.121502 | -2.723883 | -0.236435 | C | 1.339192 | -2.649786 | -0.2221 |
| C | 2.835024 | -2.763878 | -2.425334 | C | 3.16552 | -2.59728 | -2.325569 |
| C | 1.290465 | -3.894525 | -0.964055 | C | 1.64592 | -3.819995 | -0.904874 |
| C | 2.143445 | -3.914717 | -2.063114 | C | 2.554122 | -3.79234 | -1.958152 |
| H | 3.202633 | -0.694226 | -1.995374 | H | 3.341273 | -0.493178 | -1.936804 |
| H | 0.444507 | -2.690689 | 0.610657 | H | 0.627728 | -2.659694 | 0.596193 |

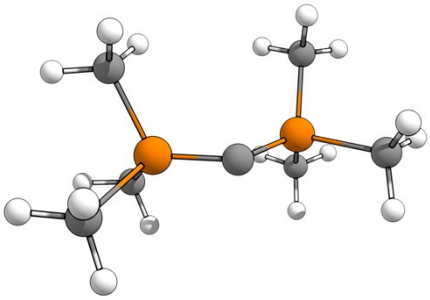
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 3.50223 | -2.776874 | -3.279328 | H | 3.87743 | -2.578745 | -3.141493 |
| H | 0.743139 | -4.786183 | -0.681111 | H | 1.171904 | -4.750361 | -0.617012 |
| H | 2.269589 | -4.825906 | -2.636236 | H | 2.790803 | -4.704506 | -2.492587 |
| | | | | H | -0.000002 | -0.000157 | 2.205359 |

**$(Ph_3P)_2CH_2^{2+}$**



Zero-point correction= 0.582987 (Hartree/Particle)
Thermal correction to Energy= 0.616444
Thermal correction to Enthalpy= 0.617388
Thermal correction to Gibbs Free Energy= 0.516757
Sum of electronic and zero-point Energies= -2110.546866
Sum of electronic and thermal Energies= -2110.513409
Sum of electronic and thermal Enthalpies= -2110.512465
Sum of electronic and thermal Free Energies= -2110.613096

**$(Me_3P)_2C$**



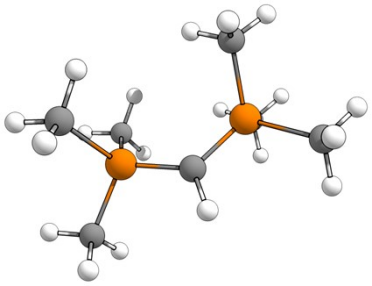
Zero-point correction= 0.233501 (Hartree/Particle)
Thermal correction to Energy= 0.248760
Thermal correction to Enthalpy= 0.249704
Thermal correction to Gibbs Free Energy= 0.190569
Sum of electronic and zero-point Energies= -959.893863
Sum of electronic and thermal Energies= -959.878604
Sum of electronic and thermal Enthalpies= -959.877660
Sum of electronic and thermal Free Energies= -959.936795

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| P | 1.615748 | 0.081135 | 0.296449 | P | 1.508403 | 0.001283 | 0.129108 |
| P | -1.615683 | -0.081157 | 0.296492 | P | -1.507596 | 0.000175 | 0.12913 |
| C | 0.000057 | 0.000029 | 1.176947 | C | 0.000415 | 0.00269 | 0.76911 |
| C | -1.143969 | -1.676374 | -1.948734 | C | -2.091103 | 1.530992 | -0.715097 |
| C | -1.710207 | -1.596282 | -0.669693 | H | -1.985584 | 2.366624 | -0.02199 |
| C | -2.311766 | -2.719583 | -0.093905 | H | -1.455927 | 1.718805 | -1.583038 |
| H | -2.784254 | -2.6579 | 0.879698 | H | -3.131422 | 1.450879 | -1.03935 |
| C | -2.330326 | -3.921549 | -0.793092 | C | -2.784737 | -0.246045 | 1.412127 |
| H | -2.804583 | -4.7895 | -0.352509 | H | -3.793212 | -0.195877 | 0.996545 |
| C | -1.765983 | -3.99953 | -2.060706 | H | -2.621823 | -1.218313 | 1.878284 |
| H | -1.796901 | -4.934088 | -2.607993 | H | -2.655421 | 0.525508 | 2.171673 |
| C | -1.176936 | -2.877136 | -2.640109 | C | -1.94566 | -1.285411 | -1.119841 |
| H | -0.749061 | -2.937993 | -3.633155 | H | -1.357311 | -1.11364 | -2.023864 |
| C | -1.821012 | 1.391879 | -0.70972 | H | -1.686435 | -2.264864 | -0.715254 |
| C | -1.450302 | 2.626586 | -0.162203 | H | -3.007829 | -1.263486 | -1.375188 |
| H | -1.007601 | 2.694386 | 0.825774 | C | 2.790236 | 0.040591 | 1.42983 |
| C | -1.660654 | 3.788436 | -0.887372 | H | 2.632451 | -0.814165 | 2.088094 |
| H | -1.373668 | 4.744227 | -0.466915 | H | 3.797526 | 0.009281 | 1.009912 |
| C | -2.250374 | 3.724541 | -2.148755 | H | 2.657093 | 0.9529 | 2.012179 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -2.420671 | 4.635598 | -2.709927 | C | 2.011819 | 1.401943 | -0.960174 |
| C | -2.642361 | 2.501569 | -2.680781 | H | 1.808362 | 2.33657 | -0.435672 |
| H | -3.123858 | 2.457358 | -3.649804 | H | 3.069968 | 1.354825 | -1.228809 |
| C | -2.43677 | 1.328089 | -1.962154 | H | 1.409989 | 1.376242 | -1.871225 |
| H | -2.771276 | 0.381495 | -2.370012 | C | 2.018463 | -1.446723 | -0.891184 |
| C | -2.848973 | -0.073027 | 1.607676 | H | 1.396116 | -1.484237 | -1.787709 |
| C | -2.646213 | -0.761561 | 2.810364 | H | 3.069366 | -1.392822 | -1.185499 |
| H | -1.725308 | -1.297421 | 3.010942 | H | 1.845399 | -2.354305 | -0.311295 |
| C | -3.646965 | -0.768009 | 3.771662 | | | | |
| H | -3.492137 | -1.294358 | 4.70505 | | | | |
| C | -4.845373 | -0.099293 | 3.535747 | | | | |
| H | -5.623059 | -0.107551 | 4.289745 | | | | |
| C | -5.047853 | 0.580102 | 2.33978 | | | | |
| H | -5.980008 | 1.100511 | 2.159875 | | | | |
| C | -4.052368 | 0.599469 | 1.371201 | | | | |
| H | -4.212426 | 1.140559 | 0.44557 | | | | |
| H | -0.687272 | -0.810238 | -2.410699 | | | | |
| C | 2.849081 | 0.073296 | 1.607605 | | | | |
| C | 4.052582 | -0.599018 | 1.371172 | | | | |
| C | 2.646172 | 0.761769 | 2.810301 | | | | |
| C | 5.048031 | -0.57951 | 2.339789 | | | | |
| C | 3.646887 | 0.76836 | 3.771637 | | | | |
| C | 4.845409 | 0.099833 | 3.535761 | | | | |
| H | 4.212772 | -1.140081 | 0.445548 | | | | |
| H | 1.725175 | 1.297471 | 3.010871 | | | | |
| H | 5.98027 | -1.099772 | 2.159898 | | | | |
| H | 3.491929 | 1.29467 | 4.705024 | | | | |
| H | 5.623061 | 0.108205 | 4.289791 | | | | |
| C | 1.710062 | 1.596169 | -0.669913 | | | | |
| C | 2.311229 | 2.719669 | -0.094106 | | | | |
| C | 1.14406 | 1.675993 | -1.949068 | | | | |
| C | 2.329618 | 3.921581 | -0.793393 | | | | |
| C | 1.176883 | 2.8767 | -2.64055 | | | | |
| C | 1.765537 | 3.999293 | -2.061138 | | | | |
| H | 2.783569 | 2.658195 | 0.879583 | | | | |
| H | 0.687584 | 0.809732 | -2.411014 | | | | |
| H | 2.803554 | 4.789695 | -0.352786 | | | | |
| H | 0.749195 | 2.937364 | -3.633687 | | | | |
| H | 1.796336 | 4.933798 | -2.608522 | | | | |
| C | 1.821172 | -1.392018 | -0.70954 | | | | |
| C | 2.437132 | -1.328411 | -1.961886 | | | | |
| C | 1.450308 | -2.626634 | -0.161936 | | | | |
| C | 2.642759 | -2.501985 | -2.680347 | | | | |
| C | 1.660713 | -3.788586 | -0.88693 | | | | |

| | | | |
|---|---|---|---|
| C | 2.250624 | -3.724875 | -2.148233 |
| H | 2.771757 | -0.381887 | -2.369812 |
| H | 1.0074 | -2.694283 | 0.825957 |
| H | 3.124394 | -2.457916 | -3.649308 |
| H | 1.373605 | -4.744309 | -0.466404 |
| H | 2.420946 | -4.636003 | -2.709281 |
| H | -0.049054 | 0.875301 | 1.830797 |
| H | 0.049166 | -0.874829 | 1.831325 |

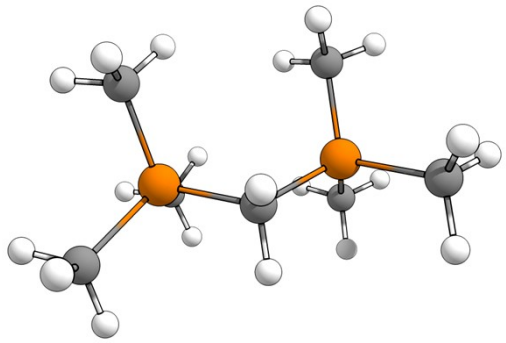
**$(Me_3P)_2CH^+$**



Zero-point correction= 0.245728 (Hartree/Particle)
Thermal correction to Energy= 0.261028
Thermal correction to Enthalpy= 0.261973
Thermal correction to Gibbs Free Energy= 0.202953
Sum of electronic and zero-point Energies= -960.342144
Sum of electronic and thermal Energies= -960.326843
Sum of electronic and thermal Enthalpies= -960.325899
Sum of electronic and thermal Free Energies= -960.384919

| | | | |
|---|---|---|---|
| P | -1.536352 | 0.091473 | 0.034751 |
| P | 1.546918 | 0.116801 | 0.011701 |
| C | 0.000649 | 0.847145 | 0.113719 |
| C | 2.222762 | -0.539358 | 1.568838 |
| H | 2.29057 | 0.271937 | 2.295189 |
| H | 1.548803 | -1.301878 | 1.963194 |
| H | 3.212363 | -0.975259 | 1.417298 |
| C | 2.74868 | 1.332633 | -0.577871 |
| H | 3.748361 | 0.896382 | -0.598091 |
| H | 2.465588 | 1.662986 | -1.57708 |
| H | 2.748655 | 2.192014 | 0.094602 |
| C | 1.566156 | -1.287646 | -1.1368 |
| H | 0.883092 | -2.067925 | -0.793788 |
| H | 1.267685 | -0.951847 | -2.130272 |
| H | 2.570772 | -1.711467 | -1.182599 |
| C | -2.783299 | 1.324238 | 0.471183 |
| H | -2.716241 | 2.163333 | -0.222304 |

**$(Me_3P)_2CH_2^{2+}$**



Zero-point correction= 0.257835 (Hartree/Particle)
Thermal correction to Energy= 0.273142
Thermal correction to Enthalpy= 0.274086
Thermal correction to Gibbs Free Energy= 0.216834
Sum of electronic and zero-point Energies= -960.591863
Sum of electronic and thermal Energies= -960.576557
Sum of electronic and thermal Enthalpies= -960.575612
Sum of electronic and thermal Free Energies= -960.632865

| | | | |
|---|---|---|---|
| P | 1.617408 | 0.002487 | 0.063682 |
| P | -1.617319 | -0.002543 | 0.063763 |
| C | 0.000075 | -0.000008 | 0.938777 |
| C | -1.928857 | 1.61803 | -0.659826 |
| H | -1.860615 | 2.391542 | 0.10817 |
| H | -1.231361 | 1.834322 | -1.469408 |
| H | -2.943538 | 1.620938 | -1.06729 |
| C | -2.853087 | -0.346702 | 1.327383 |
| H | -3.844805 | -0.296846 | 0.870544 |
| H | -2.703507 | -1.344453 | 1.744903 |
| H | -2.792676 | 0.39812 | 2.123915 |
| C | -1.667967 | -1.276757 | -1.209702 |
| H | -1.023688 | -1.017212 | -2.051871 |
| H | -1.381731 | -2.245852 | -0.795414 |
| H | -2.694845 | -1.347441 | -1.579114 |
| C | 2.853377 | 0.346255 | 1.327208 |
| H | 2.793256 | -0.398909 | 2.123439 |

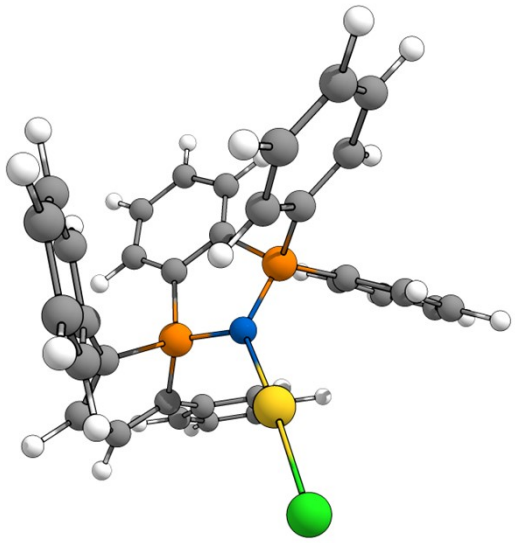
| | | | |
|---|---|---|---|
| H | -3.778322 | 0.882169 | 0.406951 |
| H | -2.606026 | 1.678879 | 1.486759 |
| C | -1.754769 | -1.317943 | 1.163475 |
| H | -1.599636 | -0.979519 | 2.188617 |
| H | -2.756213 | -1.740587 | 1.062268 |
| H | -1.026317 | -2.099035 | 0.933973 |
| C | -1.999484 | -0.548318 | -1.602891 |
| H | -1.316736 | -1.343729 | -1.905394 |
| H | -3.016121 | -0.945943 | -1.584091 |
| H | -1.935934 | 0.26475 | -2.327007 |
| H | -0.01097 | 1.902298 | 0.359285 |

| | | | |
|---|---|---|---|
| H | 3.844993 | 0.296747 | 0.870105 |
| H | 2.703759 | 1.343817 | 1.745166 |
| C | 1.667727 | 1.277189 | -1.20932 |
| H | 1.380498 | 2.245861 | -0.79472 |
| H | 2.694654 | 1.3489 | -1.578368 |
| H | 1.023923 | 1.017458 | -2.051801 |
| C | 1.928658 | -1.617964 | -0.660285 |
| H | 1.23085 | -1.834124 | -1.469629 |
| H | 2.943196 | -1.620905 | -1.068101 |
| H | 1.860622 | -2.391548 | 0.107661 |
| H | 0.007583 | -0.877012 | 1.597482 |
| H | -0.00745 | 0.877184 | 1.59724 |

**AuCl**

Zero-point correction= 0.000715 (Hartree/Particle)
Thermal correction to Energy= 0.003479
Thermal correction to Enthalpy= 0.004423
Thermal correction to Gibbs Free Energy= -0.024378
Sum of electronic and zero-point Energies= -595.515523
Sum of electronic and thermal Energies= -595.512759
Sum of electronic and thermal Enthalpies= -595.511815
Sum of electronic and thermal Free Energies= -595.540615

**$[AN{\cdot}AuCl]^{+}$**

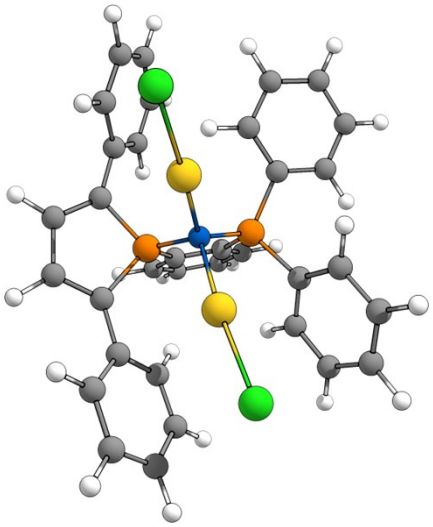
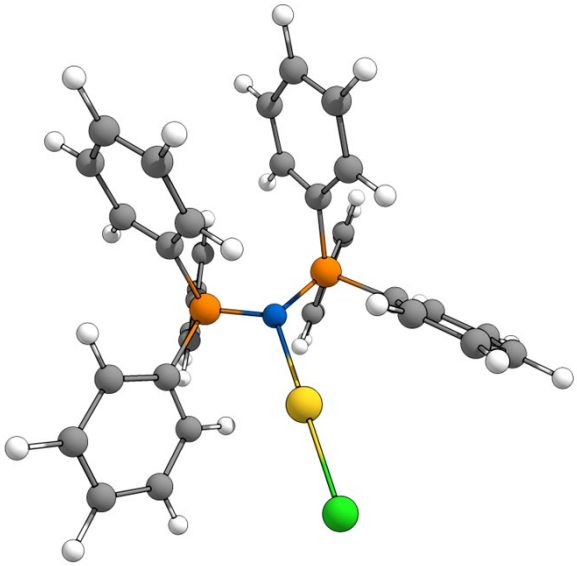


Zero-point correction= 0.504912 (Hartree/Particle)
Thermal correction to Energy= 0.539270
Thermal correction to Enthalpy= 0.540214
Thermal correction to Gibbs Free Energy= 0.434564
Sum of electronic and zero-point Energies= -2643.340926
Sum of electronic and thermal Energies= -2643.306568
Sum of electronic and thermal Enthalpies= -2643.305624
Sum of electronic and thermal Free Energies= -2643.411274

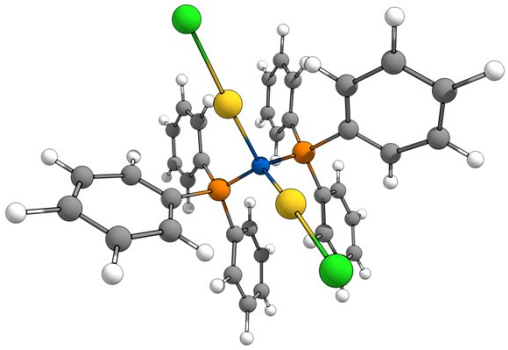
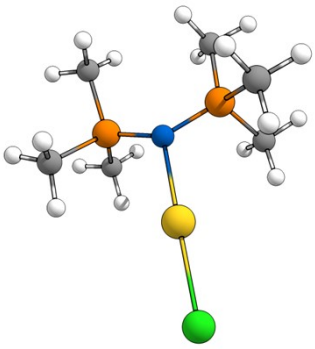
| | | | |
|---|---|---|---|
| Au | 0 | 0 | 0.409885 |
| Cl | 0 | 0 | -1.904759 |

| | | | |
|---|---|---|---|
| P | 0.635104 | 1.236028 | 0.868704 |
| P | 0.224177 | -1.482023 | 0.505236 |
| N | 0.073163 | 0.041643 | -0.089799 |
| C | 1.1953 | 0.272754 | 2.292664 |
| C | 0.981087 | -1.097785 | 2.111941 |
| C | 1.327877 | -2.000738 | 3.110083 |
| H | 1.159398 | -3.064147 | 2.979948 |
| C | 1.895322 | -1.513303 | 4.283574 |

| | | | | |
|---|---|---|---|---|
| | H | 2.169267 | -2.203606 | 5.071694 |
| | C | 2.115798 | -0.147446 | 4.456746 |
| | H | 2.560539 | 0.211488 | 5.376593 |
| | C | 1.768213 | 0.759725 | 3.461301 |
| | H | 1.937886 | 1.822519 | 3.59457 |
| | C | 1.901658 | 2.366452 | 0.248832 |
| | C | 1.369199 | 3.597668 | 0.34435 |
| | H | 1.914643 | 4.494598 | 0.072953 |
| | C | -0.040927 | 3.674878 | 0.81073 |
| | H | -0.57742 | 4.61703 | 0.814804 |
| | C | -0.600613 | 2.512888 | 1.179083 |
| | C | 3.2551 | 1.939742 | -0.118347 |
| | C | 3.438518 | 0.764027 | -0.855683 |
| | H | 2.577436 | 0.191147 | -1.187022 |
| | C | 4.7179 | 0.363317 | -1.217971 |
| | H | 4.850556 | -0.535662 | -1.80789 |
| | C | 5.820289 | 1.125958 | -0.844829 |
| | H | 6.817044 | 0.814845 | -1.132232 |
| | C | 5.64314 | 2.293331 | -0.107899 |
| | H | 6.501271 | 2.885934 | 0.18436 |
| | C | 4.367624 | 2.699099 | 0.258351 |
| | H | 4.229168 | 3.598125 | 0.848413 |
| | C | -1.987519 | 2.148518 | 1.504517 |
| | C | -2.276235 | 1.438939 | 2.675361 |
| | H | -1.485131 | 1.22674 | 3.387748 |
| | C | -3.577406 | 1.029627 | 2.936518 |
| | H | -3.801677 | 0.495037 | 3.851335 |
| | C | -4.590645 | 1.307138 | 2.0222 |
| | H | -5.605356 | 0.986603 | 2.226786 |
| | C | -4.304697 | 1.99754 | 0.847972 |
| | H | -5.087439 | 2.20194 | 0.12784 |
| | C | -3.006816 | 2.422512 | 0.586776 |
| | H | -2.776272 | 2.9345 | -0.341476 |
| | C | 1.314792 | -2.507348 | -0.478389 |
| | C | 0.802685 | -3.087199 | -1.645011 |
| | H | -0.250022 | -2.993368 | -1.892252 |
| | C | 1.655967 | -3.782634 | -2.489827 |
| | H | 1.267433 | -4.22863 | -3.396542 |
| | C | 3.005801 | -3.903155 | -2.170351 |
| | H | 3.665875 | -4.454041 | -2.82947 |
| | C | 3.513451 | -3.32229 | -1.012143 |
| | H | 4.564146 | -3.4204 | -0.768682 |
| | C | 2.672237 | -2.61414 | -0.162945 |
| | H | 3.071787 | -2.148494 | 0.731464 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | | C | -1.367423 | -2.286873 | 0.660998 |
| | | | | C | -2.534185 | -1.518209 | 0.694225 |
| | | | | H | -2.496785 | -0.440015 | 0.579275 |
| | | | | C | -3.758289 | -2.155078 | 0.853794 |
| | | | | H | -4.665827 | -1.564568 | 0.859891 |
| | | | | C | -3.815126 | -3.53771 | 0.990577 |
| | | | | H | -4.773942 | -4.027844 | 1.108946 |
| | | | | C | -2.649534 | -4.299719 | 0.96524 |
| | | | | H | -2.700024 | -5.376716 | 1.063897 |
| | | | | C | -1.420231 | -3.679521 | 0.795065 |
| | | | | H | -0.514745 | -4.275342 | 0.747357 |
| | | | | Au | -1.080417 | 0.587395 | -1.798932 |
| | | | | Cl | -2.44671 | 1.275337 | -3.53307 |
| **$[AN\cdot(AuCl)_2]^+$** | | | | **$[(Ph_3P)_2N\cdot AuCl]^+$** | | | |
|  | | | |  | | | |
| Zero-point correction= | 0.505703 (Hartree/Particle) | | | Zero-point correction= | 0.563910 (Hartree/Particle) | | |
| Thermal correction to Energy= | 0.544418 | | | Thermal correction to Energy= | 0.600614 | | |
| Thermal correction to Enthalpy= | 0.545362 | | | Thermal correction to Enthalpy= | 0.601558 | | |
| Thermal correction to Gibbs Free Energy= | 0.429165 | | | Thermal correction to Gibbs Free Energy= | 0.491381 | | |
| Sum of electronic and zero-point Energies= | -3238.900499 | | | Sum of electronic and zero-point Energies= | -2721.913678 | | |
| Sum of electronic and thermal Energies= | -3238.861784 | | | Sum of electronic and thermal Energies= | -2721.876975 | | |
| Sum of electronic and thermal Enthalpies= | -3238.860840 | | | Sum of electronic and thermal Enthalpies= | -2721.876031 | | |
| Sum of electronic and thermal Free Energies= | -3238.977037 | | | Sum of electronic and thermal Free Energies= | -2721.986207 | | |
| P | -0.322776 | -0.022969 | 1.835999 | P | -0.611041 | -1.490834 | -0.057681 |
| P | -0.441148 | -1.691204 | -0.421082 | P | -0.611093 | 1.49135 | 0.057513 |
| N | -0.175724 | -0.137854 | 0.18027 | N | 0.108596 | 0.000286 | -0.000718 |
| C | -0.479819 | -1.765746 | 2.273175 | C | -3.07061 | 1.214115 | 1.34811 |
| C | -0.571487 | -2.587815 | 1.148303 | C | -1.759034 | 1.688411 | 1.452342 |
| C | -0.763655 | -3.958069 | 1.291316 | C | -1.321084 | 2.224601 | 2.666809 |

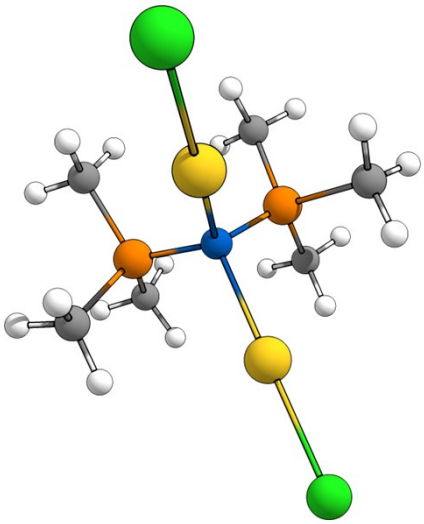
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -0.843416 | -4.600657 | 0.421243 | H | -0.331893 | 2.651678 | 2.761183 |
| C | -0.849098 | -4.488378 | 2.574281 | C | -2.17081 | 2.239859 | 3.767056 |
| H | -0.995426 | -5.553596 | 2.703955 | H | -1.824769 | 2.664197 | 4.701556 |
| C | -0.749426 | -3.664907 | 3.696535 | C | -3.458967 | 1.728079 | 3.666151 |
| H | -0.817553 | -4.097769 | 4.686924 | H | -4.11642 | 1.741236 | 4.527006 |
| C | -0.56835 | -2.293408 | 3.557554 | C | -3.913665 | 1.226919 | 2.450281 |
| H | -0.499117 | -1.651016 | 4.42883 | H | -4.927355 | 0.857526 | 2.356524 |
| C | 0.976568 | 0.934429 | 2.650601 | C | -1.515715 | 1.818922 | -1.468558 |
| C | 0.339392 | 1.936558 | 3.283379 | C | -1.040386 | 1.239248 | -2.648126 |
| H | 0.865735 | 2.690413 | 3.857754 | H | -0.169696 | 0.59315 | -2.623048 |
| C | -1.139443 | 1.977681 | 3.147464 | C | -1.688716 | 1.492789 | -3.848679 |
| H | -1.721498 | 2.767025 | 3.610122 | H | -1.325704 | 1.038618 | -4.762432 |
| C | -1.694876 | 0.996979 | 2.419045 | C | -2.801223 | 2.32955 | -3.874861 |
| C | 2.40706 | 0.683805 | 2.463163 | H | -3.306709 | 2.524473 | -4.813042 |
| C | 2.90335 | -0.622195 | 2.358243 | C | -3.258438 | 2.928531 | -2.705552 |
| H | 2.240375 | -1.470008 | 2.503163 | H | -4.114056 | 3.591679 | -2.731675 |
| C | 4.249461 | -0.835601 | 2.096729 | C | -2.616006 | 2.679235 | -1.498173 |
| H | 4.631055 | -1.846325 | 2.019446 | H | -2.969255 | 3.153119 | -0.58926 |
| C | 5.107188 | 0.246083 | 1.930381 | C | 0.709332 | 2.707749 | 0.218545 |
| H | 6.150606 | 0.078208 | 1.695831 | C | 1.641287 | 2.605028 | 1.261634 |
| C | 4.622348 | 1.545452 | 2.040357 | H | 1.570955 | 1.807897 | 1.994428 |
| H | 5.284891 | 2.386401 | 1.881341 | C | 2.691046 | 3.505809 | 1.341684 |
| C | 3.280024 | 1.767359 | 2.304547 | H | 3.426765 | 3.402257 | 2.128843 |
| H | 2.892193 | 2.779193 | 2.333142 | C | 2.812095 | 4.516771 | 0.391712 |
| C | -3.082861 | 0.787503 | 1.979776 | H | 3.64186 | 5.210362 | 0.448026 |
| C | -3.728684 | -0.436551 | 2.19159 | C | 1.883205 | 4.629586 | -0.63437 |
| H | -3.233986 | -1.224154 | 2.750322 | H | 1.983959 | 5.411744 | -1.376121 |
| C | -5.015593 | -0.634463 | 1.708215 | C | 0.829702 | 3.726009 | -0.72831 |
| H | -5.518933 | -1.576649 | 1.886641 | H | 0.121196 | 3.80855 | -1.543593 |
| C | -5.657086 | 0.377565 | 0.998164 | H | -3.445116 | 0.868169 | 0.394677 |
| H | -6.660196 | 0.219877 | 0.619876 | C | 0.709304 | -2.707145 | -0.220515 |
| C | -5.015402 | 1.592973 | 0.778406 | C | 0.830489 | -3.725693 | 0.725922 |
| H | -5.50486 | 2.380124 | 0.218037 | C | 1.640343 | -2.604147 | -1.2644 |
| C | -3.732641 | 1.803738 | 1.271012 | C | 1.883831 | -4.629321 | 0.630769 |
| H | -3.220659 | 2.738977 | 1.07135 | C | 2.689939 | -3.505019 | -1.345682 |
| C | 0.976675 | -2.231214 | -1.357874 | C | 2.811784 | -4.516278 | -0.396125 |
| C | 1.102794 | -1.794656 | -2.684633 | H | 0.122774 | -3.808412 | 1.541865 |
| H | 0.278396 | -1.296635 | -3.185075 | H | 1.569404 | -1.806744 | -1.996841 |
| C | 2.309805 | -1.97074 | -3.344053 | H | 1.985205 | -5.411683 | 1.372218 |
| H | 2.425023 | -1.610819 | -4.358108 | H | 3.42494 | -3.401333 | -2.133493 |
| C | 3.379422 | -2.573525 | -2.688295 | H | 3.641434 | -5.209927 | -0.453421 |
| H | 4.328081 | -2.682647 | -3.198876 | C | -1.761009 | -1.688182 | -1.450808 |
| C | 3.246445 | -3.02364 | -1.378237 | C | -1.32443 | -2.224027 | -2.665926 |
| H | 4.083306 | -3.494532 | -0.87839 | C | -3.072746 | -1.214709 | -1.344731 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 2.048198 | -2.847744 | -0.701825 | C | -2.175704 | -2.239908 | -3.764957 |
| H | 1.952907 | -3.17473 | 0.327875 | C | -3.917363 | -1.22815 | -2.445701 |
| C | -1.926576 | -1.853903 | -1.407854 | C | -3.464084 | -1.729052 | -3.662202 |
| C | -3.039641 | -1.034548 | -1.195346 | H | -0.335084 | -2.650431 | -2.761688 |
| H | -3.022347 | -0.230625 | -0.468807 | H | -3.446251 | -0.869066 | -0.390794 |
| C | -4.189494 | -1.243926 | -1.944567 | H | -1.830722 | -2.664052 | -4.699936 |
| H | -5.041343 | -0.592737 | -1.795385 | H | -4.931169 | -0.859447 | -2.350508 |
| C | -4.238211 | -2.270781 | -2.881144 | H | -4.122791 | -1.742751 | -4.522085 |
| H | -5.137249 | -2.424874 | -3.46545 | C | -1.513215 | -1.818621 | 1.469802 |
| C | -3.136911 | -3.098502 | -3.0779 | C | -2.613102 | -2.679389 | 1.501044 |
| H | -3.176755 | -3.895246 | -3.80984 | C | -1.036147 | -1.239053 | 2.648719 |
| C | -1.975496 | -2.894012 | -2.34692 | C | -3.253468 | -2.929202 | 2.709417 |
| H | -1.111897 | -3.526125 | -2.520098 | C | -1.682506 | -1.493001 | 3.850252 |
| Au | 1.946824 | 0.630441 | -0.66104 | C | -2.794617 | -2.330231 | 3.878089 |
| Cl | 4.086192 | 0.992483 | -1.509386 | H | -2.967618 | -3.153255 | 0.59262 |
| Au | -0.975397 | 1.648636 | -0.850821 | H | -0.165659 | -0.592735 | 2.622427 |
| Cl | -2.030016 | 3.500727 | -1.743907 | H | -4.10872 | -3.59277 | 2.73681 |
| | | | | H | -1.318184 | -1.038872 | 4.763504 |
| | | | | H | -3.298496 | -2.525522 | 4.81706 |
| | | | | Au | 2.355511 | -0.000071 | -0.000756 |
| | | | | Cl | 4.68222 | -0.000136 | -0.00044 |
| **$[(Ph_3P)_2N{\cdot}(AuCl)_2]^+$** | | | | **$[(Me_3P)_2N{\cdot}AuCl]^+$** | | | |
|  | | | |  | | | |
| | | | | Zero-point correction= 0.239923 (Hartree/Particle) | | | |
| | | | | Thermal correction to Energy= 0.262154 | | | |
| | | | | Thermal correction to Enthalpy= 0.263098 | | | |
| | | | | Thermal correction to Gibbs Free Energy= 0.185425 | | | |
| | | | | Sum of electronic and zero-point Energies= -2167.554638 | | | |
| | | | | Sum of electronic and thermal Energies= -2167.532408 | | | |
| | | | | Sum of electronic and thermal Enthalpies= -2167.531463 | | | |
| | | | | Sum of electronic and thermal Free Energies= -2167.609136 | | | |
| P | -1.223481 | 0.047439 | 1.232914 | P | 1.631192 | -1.496605 | 0.004278 |
| P | -0.188154 | -1.06468 | -1.378849 | P | 1.549968 | 1.536255 | -0.00413 |
| N | -0.074822 | -0.041451 | -0.026143 | N | 0.99795 | 0.002849 | -0.152441 |
| C | -2.889241 | -1.206184 | -2.110345 | C | 0.924885 | 2.301922 | 1.503437 |

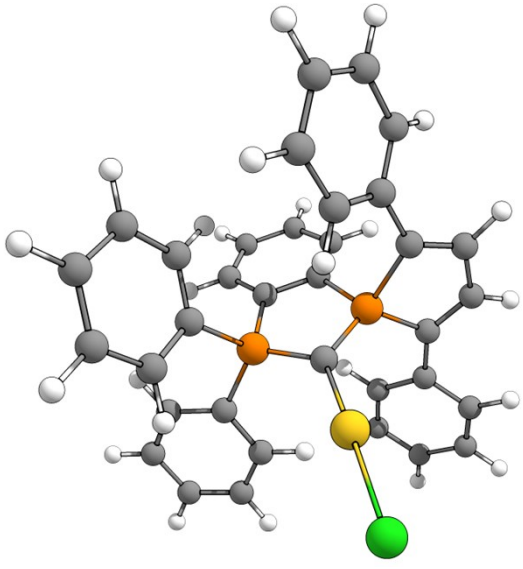
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -1.628098 | -0.664797 | -2.39587 | H | -0.166082 | 2.340299 | 1.467416 |
| C | -1.493254 | 0.270727 | -3.428505 | H | 1.22966 | 1.710587 | 2.368774 |
| H | -0.527368 | 0.674244 | -3.686448 | H | 1.32097 | 3.315352 | 1.59618 |
| C | -2.611346 | 0.674621 | -4.148934 | C | 0.978686 | 2.50427 | -1.408545 |
| H | -2.498602 | 1.397543 | -4.947409 | H | 1.322705 | 3.535717 | -1.30921 |
| C | -3.859664 | 0.13983 | -3.853841 | H | 1.369141 | 2.072408 | -2.331032 |
| H | -4.727684 | 0.451645 | -4.423521 | H | -0.112787 | 2.487299 | -1.440561 |
| C | -3.997822 | -0.805486 | -2.84079 | C | 3.352665 | 1.661153 | 0.046666 |
| H | -4.970124 | -1.229699 | -2.619312 | H | 3.75089 | 1.174498 | 0.938421 |
| C | -0.284533 | -2.791261 | -0.855072 | H | 3.798557 | 1.23171 | -0.850552 |
| C | 0.448832 | -3.17505 | 0.271533 | H | 3.614625 | 2.720742 | 0.091379 |
| H | 0.985632 | -2.443925 | 0.863375 | C | 0.696939 | -2.622934 | -1.042691 |
| C | 0.508036 | -4.501997 | 0.649884 | H | 0.662021 | -2.224146 | -2.057639 |
| H | 1.080627 | -4.777583 | 1.526835 | H | 1.182926 | -3.600871 | -1.045694 |
| C | -0.156029 | -5.465914 | -0.097118 | H | -0.322775 | -2.725752 | -0.666323 |
| H | -0.105997 | -6.507283 | 0.198611 | C | 1.524939 | -2.087525 | 1.704334 |
| C | -0.867143 | -5.10019 | -1.236766 | H | 0.483315 | -2.042683 | 2.030102 |
| H | -1.363791 | -5.856429 | -1.831863 | H | 1.880431 | -3.11809 | 1.767046 |
| C | -0.929856 | -3.763979 | -1.629855 | H | 2.132971 | -1.457391 | 2.356436 |
| H | -1.459971 | -3.495004 | -2.536143 | C | 3.36063 | -1.608785 | -0.509814 |
| C | 1.356509 | -0.886767 | -2.310061 | H | 4.013851 | -1.04989 | 0.158906 |
| C | 1.813222 | 0.332107 | -2.843383 | H | 3.656126 | -2.659881 | -0.478545 |
| H | 1.23551 | 1.245662 | -2.772635 | H | 3.471058 | -1.246019 | -1.532838 |
| C | 3.053668 | 0.395638 | -3.459021 | Au | -1.188263 | -0.019457 | -0.045162 |
| H | 3.403436 | 1.343852 | -3.848578 | Cl | -3.47943 | -0.025297 | 0.106473 |
| C | 3.846259 | -0.742036 | -3.562475 | | | | |
| H | 4.82054 | -0.67817 | -4.031645 | | | | |
| C | 3.389952 | -1.953729 | -3.061104 | | | | |
| H | 4.002551 | -2.843327 | -3.13733 | | | | |
| C | 2.152594 | -2.030922 | -2.437314 | | | | |
| H | 1.825365 | -2.980855 | -2.037201 | | | | |
| H | -3.00583 | -1.946133 | -1.329518 | | | | |
| C | -0.642856 | 1.328542 | 2.379426 | | | | |
| C | -1.441452 | 2.466385 | 2.549095 | | | | |
| C | 0.594374 | 1.253065 | 3.04178 | | | | |
| C | -0.996472 | 3.513202 | 3.345304 | | | | |
| C | 1.028993 | 2.306274 | 3.82963 | | | | |
| C | 0.239427 | 3.440613 | 3.977971 | | | | |
| H | -2.398853 | 2.556154 | 2.054218 | | | | |
| H | 1.247931 | 0.394999 | 2.941898 | | | | |
| H | -1.615527 | 4.395542 | 3.454952 | | | | |
| H | 1.994147 | 2.236456 | 4.315095 | | | | |
| H | 0.589244 | 4.268398 | 4.581796 | | | | |
| C | -1.421078 | -1.56288 | 2.04263 | | | | |

| | | | |
|---|---|---|---|
| C | -0.638968 | -1.956973 | 3.134374 |
| C | -2.340977 | -2.462514 | 1.49367 |
| C | -0.772019 | -3.24625 | 3.646704 |
| C | -2.475941 | -3.736618 | 2.010475 |
| C | -1.685823 | -4.135193 | 3.084982 |
| H | 0.056101 | -1.273972 | 3.602627 |
| H | -2.971447 | -2.159782 | 0.668548 |
| H | -0.169557 | -3.548954 | 4.493904 |
| H | -3.197121 | -4.418639 | 1.577736 |
| H | -1.792591 | -5.133825 | 3.491623 |
| C | -2.872649 | 0.554127 | 0.671958 |
| C | -3.943834 | 0.108412 | 1.448181 |
| C | -3.097279 | 1.475205 | -0.359636 |
| C | -5.23171 | 0.536759 | 1.175636 |
| C | -4.395504 | 1.903673 | -0.623187 |
| C | -5.461689 | 1.428242 | 0.137989 |
| H | -3.776889 | -0.564812 | 2.279684 |
| H | -2.282375 | 1.871664 | -0.953801 |
| H | -6.052776 | 0.181159 | 1.784989 |
| H | -4.567395 | 2.615157 | -1.421416 |
| H | -6.469626 | 1.766085 | -0.068268 |
| Au | 2.087878 | -0.275705 | 0.677704 |
| Cl | 4.199765 | -0.700783 | 1.519538 |
| Au | 0.41089 | 2.132124 | -0.517349 |
| Cl | 0.696015 | 4.33134 | -1.185094 |

**$[(Me_3P)_2N{\cdot}(AuCl)_2]^+$**



**[AC·AuCl]**



Zero-point correction= 0.504066 (Hartree/Particle)

Thermal correction to Energy= 0.538690

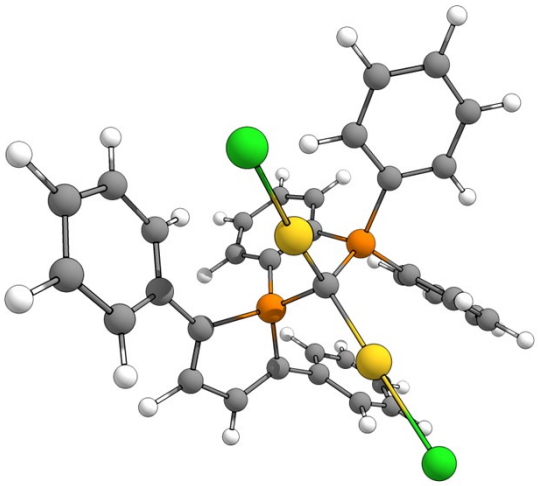
| | | | |
|---|---|---|---|
| P | -0.092119 | 1.68052 | -1.499126 |
| P | 0.091647 | 1.680509 | 1.499163 |
| N | -0.000006 | 0.912412 | 0.000023 |
| C | 1.693925 | 2.468463 | 1.758637 |
| H | 2.485237 | 1.718993 | 1.681558 |
| H | 1.870728 | 3.264341 | 1.036045 |
| H | 1.70446 | 2.899169 | 2.763142 |
| C | -0.130262 | 0.44397 | 2.785483 |
| H | 0.044757 | 0.929634 | 3.749153 |
| H | -1.145511 | 0.043034 | 2.758094 |
| H | 0.589565 | -0.367643 | 2.656301 |
| C | -1.198659 | 2.927843 | 1.689183 |
| H | -1.000426 | 3.800266 | 1.064165 |
| H | -2.171079 | 2.493928 | 1.445118 |
| H | -1.20906 | 3.25236 | 2.732693 |
| C | 0.130861 | 0.444283 | -2.785532 |
| H | -0.588352 | -0.367885 | -2.65642 |
| H | -0.044572 | 0.929921 | -3.749146 |
| H | 1.146415 | 0.044125 | -2.758239 |
| C | 1.196979 | 2.929154 | -1.688796 |
| H | 2.169817 | 2.496256 | -1.444619 |
| H | 1.207187 | 3.253951 | -2.732213 |
| H | 0.997633 | 3.80119 | -1.063583 |
| C | -1.69506 | 2.467137 | -1.758669 |
| H | -1.872755 | 3.262419 | -1.035636 |
| H | -1.705664 | 2.898473 | -2.762908 |
| H | -2.485746 | 1.716945 | -1.682251 |
| Au | -1.664818 | -0.600732 | 0.03651 |
| Cl | -3.473542 | -2.002179 | 0.046139 |
| Au | 1.665061 | -0.600454 | -0.036599 |
| Cl | 3.474047 | -2.00154 | -0.045948 |

| | |
|---|---|
| Thermal correction to Enthalpy= | 0.539634 |
| Thermal correction to Gibbs Free Energy= | 0.431803 |
| Sum of electronic and zero-point Energies= | -2626.850654 |
| Sum of electronic and thermal Energies= | -2626.816031 |
| Sum of electronic and thermal Enthalpies= | -2626.815087 |
| Sum of electronic and thermal Free Energies= | -2626.922917 |

| | | | |
|---|---|---|---|
| P | 0.01314 | 1.611616 | 0.093431 |
| P | 0.244522 | -0.939109 | 1.106279 |
| C | -0.173536 | -0.019504 | -0.253726 |
| C | 0.42575 | 1.622297 | 1.877216 |
| C | 0.538795 | 0.329475 | 2.391349 |
| C | 0.824533 | 0.13299 | 3.736853 |
| H | 0.909765 | -0.869315 | 4.14257 |
| C | 1.000319 | 1.244292 | 4.55746 |
| H | 1.221264 | 1.104541 | 5.608665 |
| C | 0.892622 | 2.532926 | 4.039511 |
| H | 1.031505 | 3.386647 | 4.691558 |
| C | 0.603763 | 2.731505 | 2.691978 |
| H | 0.513841 | 3.732328 | 2.2826 |
| C | 1.264989 | 2.700847 | -0.688059 |
| C | 0.645535 | 3.827272 | -1.074908 |
| H | 1.158111 | 4.654088 | -1.554971 |
| C | -0.810927 | 3.875 | -0.828567 |
| H | -1.397152 | 4.738184 | -1.12542 |
| C | -1.343076 | 2.796887 | -0.227871 |
| C | 2.692095 | 2.365728 | -0.720127 |
| C | 3.106132 | 1.060304 | -1.013759 |
| H | 2.366741 | 0.300916 | -1.245377 |
| C | 4.460324 | 0.747518 | -1.037826 |
| H | 4.766165 | -0.264447 | -1.276243 |
| C | 5.411784 | 1.724769 | -0.767922 |
| H | 6.466823 | 1.478669 | -0.791183 |
| C | 5.006721 | 3.023532 | -0.470166 |
| H | 5.744983 | 3.786774 | -0.254489 |
| C | 3.656629 | 3.341647 | -0.440952 |
| H | 3.337628 | 4.345528 | -0.18311 |
| C | -2.745439 | 2.50757 | 0.081417 |
| C | -3.08268 | 1.713251 | 1.18393 |
| H | -2.304183 | 1.319605 | 1.828762 |
| C | -4.412836 | 1.435061 | 1.471814 |
| H | -4.657558 | 0.820227 | 2.330094 |
| C | -5.423412 | 1.940961 | 0.662102 |
| H | -6.46056 | 1.718752 | 0.882869 |
| C | -5.097828 | 2.72449 | -0.441506 |

| | | | |
|---|---|---|---|
| H | -5.879848 | 3.10544 | -1.08696 |
| C | -3.770142 | 3.001466 | -0.733508 |
| H | -3.517212 | 3.576288 | -1.617034 |
| C | 1.742731 | -1.963895 | 0.990277 |
| C | 1.667251 | -3.194669 | 0.332537 |
| H | 0.709912 | -3.56899 | -0.016109 |
| C | 2.824666 | -3.927857 | 0.106907 |
| H | 2.765609 | -4.876704 | -0.411772 |
| C | 4.055361 | -3.438018 | 0.535219 |
| H | 4.956393 | -4.012983 | 0.357425 |
| C | 4.132697 | -2.207949 | 1.179195 |
| H | 5.091345 | -1.819766 | 1.502206 |
| C | 2.979062 | -1.464205 | 1.400962 |
| H | 3.047772 | -0.492426 | 1.87839 |
| C | -1.063591 | -2.057959 | 1.688352 |
| C | -2.358076 | -1.859089 | 1.209546 |
| H | -2.536026 | -1.093972 | 0.460511 |
| C | -3.39384 | -2.658156 | 1.681241 |
| H | -4.397054 | -2.515158 | 1.298374 |
| C | -3.137669 | -3.645744 | 2.625928 |
| H | -3.945762 | -4.271023 | 2.98669 |
| C | -1.843886 | -3.846395 | 3.10004 |
| H | -1.646492 | -4.625051 | 3.826842 |
| C | -0.802528 | -3.057049 | 2.629352 |
| H | 0.211024 | -3.231105 | 2.976558 |
| Au | -0.571926 | -0.864749 | -2.068655 |
| Cl | -1.004328 | -1.907957 | -4.171123 |

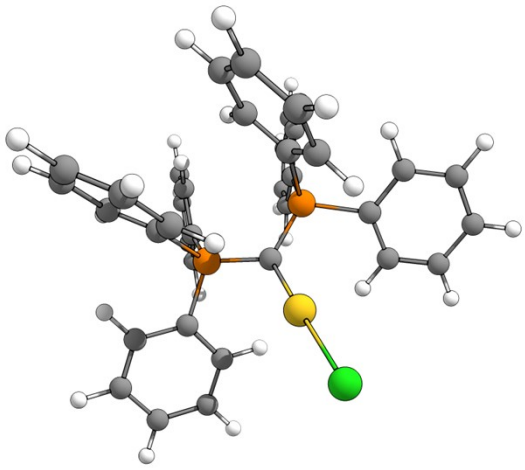
**[AC·(AuCl)$_2$]**



Zero-point correction= 0.505264 (Hartree/Particle)

Thermal correction to Energy= 0.543938

**[(Ph$_3$P)$_2$C·(AuCl)]**



Zero-point correction= 0.560994 (Hartree/Particle)

Thermal correction to Energy= 0.598135

Thermal correction to Enthalpy= 0.599080

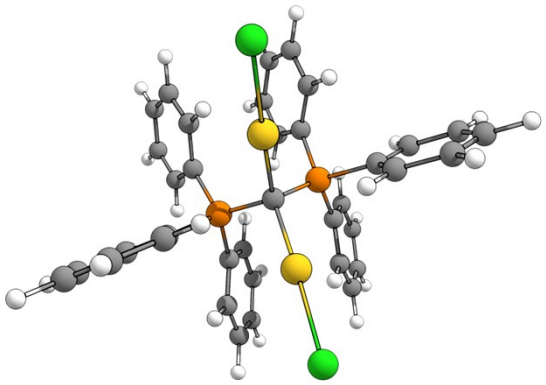
| Thermal correction to Enthalpy= 0.544882 | | | | Thermal correction to Gibbs Free Energy= 0.487332 | | | |
|---|---|---|---|---|---|---|---|
| Thermal correction to Gibbs Free Energy= 0.427491 | | | | Sum of electronic and zero-point Energies= -2705.423446 | | | |
| Sum of electronic and zero-point Energies= -3222.454003 | | | | Sum of electronic and thermal Energies= -2705.386305 | | | |
| Sum of electronic and thermal Energies= -3222.415329 | | | | Sum of electronic and thermal Enthalpies= -2705.385360 | | | |
| Sum of electronic and thermal Enthalpies= -3222.414385 | | | | Sum of electronic and thermal Free Energies= -2705.497107 | | | |
| Sum of electronic and thermal Free Energies= -3222.531776 | | | | | | | |
| P | 0.007211 | 1.102682 | 1.25892 | P | -0.64689 | -1.429722 | -0.049613 |
| P | 0.694867 | -1.452422 | 0.402048 | P | 1.394867 | 0.719818 | -0.136037 |
| C | -0.1055 | 0.032752 | -0.118616 | C | -0.128068 | 0.101802 | -0.587237 |
| C | 0.221392 | -0.045793 | 2.656877 | C | 3.213605 | -1.40027 | 0.272859 |
| C | 0.570542 | -1.324521 | 2.222064 | C | 2.811717 | -0.36052 | -0.569292 |
| C | 0.760335 | -2.35201 | 3.141442 | C | 3.416936 | -0.220162 | -1.81886 |
| H | 1.007034 | -3.35257 | 2.802021 | H | 3.119329 | 0.588457 | -2.477129 |
| C | 0.61211 | -2.075976 | 4.496659 | C | 4.403724 | -1.113274 | -2.222305 |
| H | 0.747502 | -2.867556 | 5.223503 | H | 4.872223 | -0.992713 | -3.191949 |
| C | 0.27826 | -0.792449 | 4.928916 | C | 4.789843 | -2.152586 | -1.383725 |
| H | 0.158312 | -0.597049 | 5.987579 | H | 5.556413 | -2.849636 | -1.701453 |
| C | 0.081098 | 0.234185 | 4.011727 | C | 4.194756 | -2.294723 | -0.133912 |
| H | -0.195704 | 1.230437 | 4.340789 | H | 4.491565 | -3.104149 | 0.52211 |
| C | 1.371639 | 2.309195 | 1.365918 | C | 1.656854 | 1.120022 | 1.64271 |
| C | 0.81927 | 3.519233 | 1.51723 | C | 0.547631 | 1.467094 | 2.417137 |
| H | 1.402939 | 4.429699 | 1.592331 | H | -0.44027 | 1.499374 | 1.970375 |
| C | -0.659715 | 3.544963 | 1.582995 | C | 0.702042 | 1.770075 | 3.764258 |
| H | -1.201292 | 4.47725 | 1.699362 | H | -0.169122 | 2.033523 | 4.35211 |
| C | -1.2856 | 2.358699 | 1.498115 | C | 1.961706 | 1.730242 | 4.350635 |
| C | 2.797945 | 1.92888 | 1.307274 | H | 2.080222 | 1.964181 | 5.402105 |
| C | 3.502738 | 1.998259 | 0.102079 | C | 3.073056 | 1.395326 | 3.583767 |
| H | 3.00498 | 2.332359 | -0.802567 | H | 4.058541 | 1.369786 | 4.03348 |
| C | 4.846647 | 1.643004 | 0.067321 | C | 2.923621 | 1.091967 | 2.234897 |
| H | 5.383598 | 1.69735 | -0.87216 | H | 3.796548 | 0.829412 | 1.647288 |
| C | 5.495006 | 1.231166 | 1.226559 | C | 1.721534 | 2.269428 | -1.038949 |
| H | 6.545639 | 0.965728 | 1.19465 | C | 1.055978 | 2.520235 | -2.238739 |
| C | 4.795117 | 1.154599 | 2.426035 | H | 0.307331 | 1.818334 | -2.587918 |
| H | 5.298463 | 0.838248 | 3.332264 | C | 1.346227 | 3.671754 | -2.961327 |
| C | 3.44769 | 1.492344 | 2.466107 | H | 0.817817 | 3.872533 | -3.88516 |
| H | 2.897763 | 1.441516 | 3.400094 | C | 2.299111 | 4.569189 | -2.491711 |
| C | -2.72411 | 2.074099 | 1.457462 | H | 2.517403 | 5.470077 | -3.052735 |
| C | -3.262386 | 1.003596 | 2.180201 | C | 2.963417 | 4.318608 | -1.295917 |
| H | -2.617169 | 0.394078 | 2.805517 | H | 3.697034 | 5.022651 | -0.922263 |
| C | -4.615415 | 0.713135 | 2.092372 | C | 2.676348 | 3.170493 | -0.567876 |
| H | -5.023151 | -0.129277 | 2.636991 | H | 3.183358 | 2.989714 | 0.372797 |
| C | -5.439731 | 1.475845 | 1.272874 | H | 2.761692 | -1.507729 | 1.252241 |
| H | -6.486311 | 1.218923 | 1.169964 | C | -2.250914 | -1.886046 | -0.783474 |
| C | -4.912452 | 2.540872 | 0.553001 | C | -3.002354 | -2.910408 | -0.204783 |

| | | | |
|---|---|---|---|
| H | -5.547154 | 3.116178 | -0.109251 |
| C | -3.560444 | 2.841349 | 0.642162 |
| H | -3.133529 | 3.635436 | 0.040251 |
| C | 2.456755 | -1.59268 | -0.029709 |
| C | 2.825442 | -1.506557 | -1.37729 |
| H | 2.080269 | -1.330797 | -2.146118 |
| C | 4.157989 | -1.638888 | -1.739037 |
| H | 4.435483 | -1.556065 | -2.782488 |
| C | 5.126245 | -1.86435 | -0.76436 |
| H | 6.166728 | -1.965379 | -1.049583 |
| C | 4.763061 | -1.942553 | 0.573235 |
| H | 5.517485 | -2.093154 | 1.336048 |
| C | 3.430112 | -1.802251 | 0.946515 |
| H | 3.162835 | -1.836526 | 1.996034 |
| C | -0.082226 | -3.018485 | -0.080041 |
| C | -1.412216 | -3.248499 | 0.290091 |
| H | -1.970939 | -2.499802 | 0.841275 |
| C | -2.035061 | -4.43168 | -0.074335 |
| H | -3.073665 | -4.588897 | 0.187372 |
| C | -1.332925 | -5.394882 | -0.793995 |
| H | -1.82637 | -6.313497 | -1.087897 |
| C | -0.004989 | -5.180825 | -1.138661 |
| H | 0.542262 | -5.931648 | -1.694893 |
| C | 0.627402 | -3.993656 | -0.78249 |
| H | 1.662196 | -3.833355 | -1.05745 |
| Au | 0.673581 | 0.996755 | -1.810094 |
| Cl | 1.822906 | 2.077654 | -3.596193 |
| Au | -2.132327 | -0.270877 | -0.716106 |
| Cl | -4.384822 | -0.802396 | -1.291365 |

**$[(Ph_3P)_2C\cdot(AuCl)_2]$**

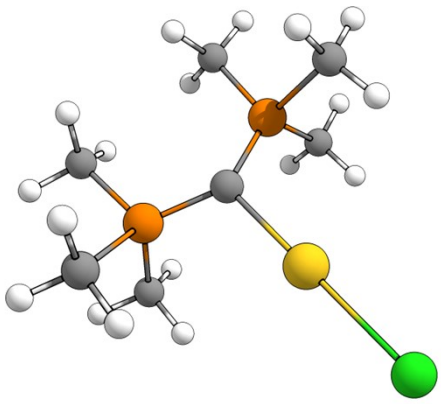
| | | | |
|---|---|---|---|
| C | -2.680085 | -1.287299 | -1.965987 |
| C | -4.192643 | -3.314135 | -0.794685 |
| C | -3.872349 | -1.696899 | -2.552465 |
| C | -4.629404 | -2.704553 | -1.966804 |
| H | -2.668363 | -3.381525 | 0.713936 |
| H | -2.088836 | -0.495909 | -2.412112 |
| H | -4.781461 | -4.099357 | -0.336245 |
| H | -4.213574 | -1.218216 | -3.462013 |
| H | -5.56281 | -3.01437 | -2.421544 |
| C | -0.904999 | -1.532939 | 1.763678 |
| C | -2.071778 | -0.969204 | 2.289864 |
| C | 0.128093 | -1.897629 | 2.629949 |
| C | -2.203218 | -0.790909 | 3.661734 |
| C | -0.00698 | -1.718246 | 4.001814 |
| C | -1.172578 | -1.165226 | 4.518806 |
| H | -2.868787 | -0.647801 | 1.62606 |
| H | 1.045653 | -2.320358 | 2.238029 |
| H | -3.11047 | -0.350653 | 4.057547 |
| H | 0.803553 | -2.000623 | 4.66286 |
| H | -1.275979 | -1.018691 | 5.587567 |
| C | 0.43233 | -2.823985 | -0.54131 |
| C | 0.562196 | -3.994412 | 0.206578 |
| C | 1.067875 | -2.721648 | -1.781206 |
| C | 1.361867 | -5.032536 | -0.26201 |
| C | 1.860484 | -3.761324 | -2.246076 |
| C | 2.017089 | -4.913801 | -1.482137 |
| H | 0.042088 | -4.10398 | 1.151058 |
| H | 0.946639 | -1.816691 | -2.366304 |
| H | 1.465048 | -5.937249 | 0.325252 |
| H | 2.36198 | -3.667056 | -3.201931 |
| H | 2.640612 | -5.723594 | -1.842461 |
| Au | -1.673339 | 1.517349 | -0.412282 |
| Cl | -3.461606 | 3.080545 | -0.199176 |

**$[(Me_3P)_2C\cdot(AuCl)]$**



Zero-point correction= 0.564248 (Hartree/Particle)
Thermal correction to Energy= 0.605113
Thermal correction to Enthalpy= 0.606057
Thermal correction to Gibbs Free Energy= 0.486555
Sum of electronic and zero-point Energies= -3301.033342
Sum of electronic and thermal Energies= -3300.992478
Sum of electronic and thermal Enthalpies= -3300.991533
Sum of electronic and thermal Free Energies= -3301.111035

| | | | |
|---|---|---|---|
| P | 0.752289 | 1.306335 | 0.675798 |
| P | -0.753093 | -1.306224 | 0.676635 |
| C | 0.000193 | -0.000571 | -0.247304 |
| C | -1.960959 | -0.192221 | 2.981267 |
| C | -2.14492 | -0.68044 | 1.685077 |
| C | -3.390202 | -0.534107 | 1.066996 |
| H | -3.546325 | -0.890845 | 0.054211 |
| C | -4.433268 | 0.088987 | 1.741745 |
| H | -5.389358 | 0.2079 | 1.247211 |
| C | -4.24576 | 0.560817 | 3.036157 |
| H | -5.061386 | 1.046746 | 3.558803 |
| C | -3.009447 | 0.418833 | 3.656811 |
| H | -2.852779 | 0.798766 | 4.659044 |
| C | 0.335996 | -2.282181 | 1.788528 |
| C | 1.617707 | -2.641894 | 1.35996 |
| H | 2.000686 | -2.307161 | 0.402416 |
| C | 2.425708 | -3.437997 | 2.160458 |
| H | 3.416665 | -3.702228 | 1.81194 |
| C | 1.967939 | -3.887275 | 3.394096 |
| H | 2.602304 | -4.505592 | 4.018459 |
| C | 0.685362 | -3.557735 | 3.814503 |
| H | 0.310427 | -3.923796 | 4.762899 |
| C | -0.13331 | -2.768984 | 3.012975 |
| H | -1.138547 | -2.548198 | 3.348371 |
| C | -1.48819 | -2.574537 | -0.409051 |



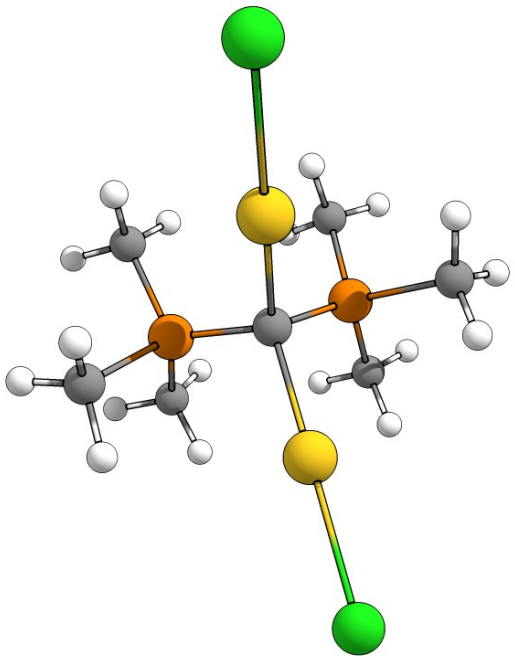
Zero-point correction= 0.237740 (Hartree/Particle)
Thermal correction to Energy= 0.256252
Thermal correction to Enthalpy= 0.257196
Thermal correction to Gibbs Free Energy= 0.189147
Sum of electronic and zero-point Energies= -1555.526045
Sum of electronic and thermal Energies= -1555.507533
Sum of electronic and thermal Enthalpies= -1555.506589
Sum of electronic and thermal Free Energies= -1555.574639

| | | | |
|---|---|---|---|
| P | 1.576113 | -1.531199 | -0.006942 |
| P | 1.576281 | 1.531091 | -0.006959 |
| C | 0.901026 | -0.000005 | -0.186772 |
| C | 1.278599 | 2.346097 | 1.601553 |
| H | 0.201379 | 2.361874 | 1.776795 |
| H | 1.747469 | 1.754969 | 2.389912 |
| H | 1.671529 | 3.364968 | 1.617766 |
| C | 0.890014 | 2.70895 | -1.211958 |
| H | 1.322883 | 3.70256 | -1.080155 |
| H | 1.093292 | 2.337065 | -2.216509 |
| H | -0.191558 | 2.753902 | -1.073398 |
| C | 3.386562 | 1.66788 | -0.22605 |
| H | 3.910937 | 1.149365 | 0.576656 |
| H | 3.679438 | 1.244787 | -1.187002 |
| H | 3.669723 | 2.721766 | -0.201051 |
| C | 0.889698 | -2.70916 | -1.211735 |
| H | 1.093875 | -2.338066 | -2.216395 |
| H | 1.321878 | -3.702967 | -1.079093 |
| H | -0.191976 | -2.753376 | -1.07378 |
| C | 1.278406 | -2.345912 | 1.601717 |
| H | 0.201082 | -2.36307 | 1.776222 |
| H | 1.672725 | -3.364227 | 1.618808 |
| H | 1.745813 | -1.753641 | 2.390086 |
| C | 3.386336 | -1.668232 | -0.226274 |
| H | 3.910913 | -1.148828 | 0.575721 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -1.3482 | -2.591506 | -1.794617 | H | 3.669521 | -2.722084 | -0.200226 |
| H | -0.794401 | -1.817776 | -2.310166 | H | 3.678955 | -1.246149 | -1.187753 |
| C | -1.930104 | -3.616561 | -2.534386 | Au | -1.178173 | 0.000062 | -0.04859 |
| H | -1.817146 | -3.620497 | -3.611033 | Cl | -3.55776 | 0.000009 | 0.117508 |
| C | -2.649919 | -4.618596 | -1.89899 | | | | |
| H | -3.103547 | -5.412345 | -2.480268 | | | | |
| C | -2.790145 | -4.604307 | -0.513827 | | | | |
| H | -3.350188 | -5.384333 | -0.012903 | | | | |
| C | -2.209351 | -3.588806 | 0.230245 | | | | |
| H | -2.323504 | -3.584571 | 1.309283 | | | | |
| H | -0.999107 | -0.279886 | 3.469926 | | | | |
| C | 1.488516 | 2.573487 | -0.410552 | | | | |
| C | 2.209518 | 3.588137 | 0.228325 | | | | |
| C | 1.349884 | 2.589097 | -1.796267 | | | | |
| C | 2.791591 | 4.60251 | -0.516265 | | | | |
| C | 1.933095 | 3.613016 | -2.536587 | | | | |
| C | 2.652849 | 4.615344 | -1.901599 | | | | |
| H | 2.322609 | 3.585072 | 1.30748 | | | | |
| H | 0.796034 | 1.815275 | -2.311634 | | | | |
| H | 3.351515 | 5.382785 | -0.015593 | | | | |
| H | 1.821208 | 3.615794 | -3.613347 | | | | |
| H | 3.107513 | 5.408192 | -2.483287 | | | | |
| C | 2.143266 | 0.6821 | 1.686402 | | | | |
| C | 3.389287 | 0.535626 | 1.069833 | | | | |
| C | 1.958115 | 0.195288 | 2.98295 | | | | |
| C | 4.431902 | -0.086142 | 1.746483 | | | | |
| C | 3.006159 | -0.41444 | 3.660379 | | | | |
| C | 4.243232 | -0.556521 | 3.04124 | | | | |
| H | 3.546342 | 0.891234 | 0.056794 | | | | |
| H | 0.995692 | 0.283109 | 3.470464 | | | | |
| H | 5.388627 | -0.205169 | 1.253199 | | | | |
| H | 2.848596 | -0.79316 | 4.662925 | | | | |
| H | 5.058551 | -1.041411 | 3.565327 | | | | |
| C | -0.337884 | 2.283793 | 1.785325 | | | | |
| C | 0.130632 | 2.772066 | 3.009495 | | | | |
| C | -1.619106 | 2.643503 | 1.355242 | | | | |
| C | -0.688325 | 3.562268 | 3.809319 | | | | |
| C | -2.427362 | 3.441032 | 2.154043 | | | | |
| C | -1.970398 | 3.891809 | 3.387457 | | | | |
| H | 1.135464 | 2.551266 | 3.346066 | | | | |
| H | -2.001555 | 2.307647 | 0.397872 | | | | |
| H | -0.313946 | 3.929339 | 4.757547 | | | | |
| H | -3.417937 | 3.705192 | 1.804377 | | | | |
| H | -2.60501 | 4.511255 | 4.010445 | | | | |

| | | | | |
|---|---|---|---|---|
| Au | -1.545428 | 0.734189 | -1.502435 | |
| Cl | -3.375285 | 1.508486 | -2.799718 | |
| Au | 1.54662 | -0.73598 | -1.50105 | |
| Cl | 3.376802 | -1.509667 | -2.798116 | |

**$[(Me_3P)_2C\cdot(AuCl)_2]$**



Zero-point correction= 0.239654 (Hartree/Particle)

Thermal correction to Energy= 0.262104

Thermal correction to Enthalpy= 0.263048

Thermal correction to Gibbs Free Energy= 0.185091

Sum of electronic and zero-point Energies= -2151.140624

Sum of electronic and thermal Energies= -2151.118174

Sum of electronic and thermal Enthalpies= -2151.117230

Sum of electronic and thermal Free Energies= -2151.195186

| | | | | |
|---|---|---|---|---|
| P | 0.029434 | 1.533395 | 1.518332 | |
| P | -0.02942 | 1.533183 | -1.518509 | |
| C | -0.000008 | 0.654192 | -0.000029 | |
| C | -1.57002 | 2.439548 | -1.866067 | |
| H | -2.397777 | 1.728861 | -1.892638 | |
| H | -1.766123 | 3.179514 | -1.090085 | |
| H | -1.486507 | 2.946963 | -2.829435 | |
| C | 0.16025 | 0.373697 | -2.894774 | |
| H | 0.014284 | 0.902209 | -3.838765 | |
| H | 1.157074 | -0.068194 | -2.860432 | |
| H | -0.583534 | -0.4183 | -2.792588 | |
| C | 1.296242 | 2.766609 | -1.720672 | |
| H | 1.106532 | 3.633278 | -1.084646 | |

| | | | | |
|---|---|---|---|---|
| H | 2.250735 | 2.311001 | -1.450832 | |
| H | 1.33236 | 3.10075 | -2.759295 | |
| C | -0.15879 | 0.373951 | 2.894836 | |
| H | 0.586689 | -0.416559 | 2.793477 | |
| H | -0.014681 | 0.903067 | 3.838769 | |
| H | -1.154672 | -0.070019 | 2.85986 | |
| C | -1.29707 | 2.765827 | 1.720934 | |
| H | -2.251459 | 2.309122 | 1.452585 | |
| H | -1.332298 | 3.100904 | 2.759284 | |
| H | -1.108893 | 3.632076 | 1.083886 | |
| C | 1.569457 | 2.44103 | 1.865196 | |
| H | 1.763522 | 3.182638 | 1.090265 | |
| H | 1.486589 | 2.946719 | 2.82953 | |
| H | 2.398133 | 1.731339 | 1.889519 | |
| Au | -1.730076 | -0.564131 | 0.011168 | |
| Cl | -3.721585 | -1.835018 | 0.021477 | |
| Au | 1.730088 | -0.564101 | -0.011113 | |
| Cl | 3.721496 | -1.835146 | -0.021286 | |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