Supporting Information for:

# Reactivity of a Cl-boratabenzene Pt(II) complex with Lewis bases: generation of the kinetically favoured Cl-boratabenzene anion

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# 1. Synthetic procedure

## a. General experimental

Unless otherwise specified, manipulations were carried out under an atmosphere of dinitrogen, using standard glovebox and Schlenk techniques. Dry, deoxygenated, distilled solvents were used for all manipulations. Toluene and benzene were distilled from Sodium/benzophenone. Pyridine was dried over $CaH_2$. Deuterated solvents were dried over NaK, degassed using freeze-pump-thaw cycles, and purified by vacuum transfer. The synthesis of **1** and **4-Py** was previously reported. [S1]

NMR spectra were recorded on a Varian Inova NMR AS400 spectrometer, at 400.0 MHz ($^{1}$H), 100.580 MHz ($^{13}$C), 161.923 MHz ($^{31}$P), Bruker Avance NMR 400 MHz spectrometer at 128.336 MHz ($^{11}$B), or on a Bruker NMR AC-300 at 300MHz ($^{1}$H), 75.435 MHz ($^{13}$C), 121.442 MHz ($^{31}$P). $^{1}$H NMR (7.15 ppm) and $^{13}$C{$^{1}$H} (128.02 ppm) NMR chemical shifts are referenced to residual protons in deuterated solvent. Multiplicities are reported as singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), or overlapping (ov). Chemical shifts are reported in ppm. Coupling constants are reported in Hz. The probe temperature was calibrated ay looking at the difference in chemical shift in ethylene glycol to give the equation $T_{real} = (T_{observed} \times 0.9994) - 0.8879$.

HPLC-MS analyses were performed on a Dionex Ultimate 3000 Liquid Chromatograph and an Applied Biosystem API2000 triple quadrupole mass spectrometer (LC-MSdelay 0.27 min), using a reversed-phase gradient column (RSLC PA2 2.2 μm 120 Å, 2.1 x

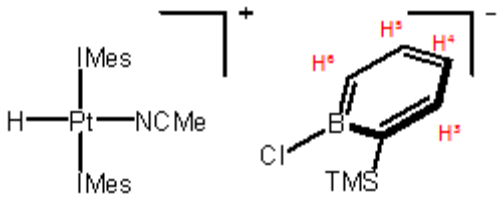
150mm). The analysis employed the mass spectrometry (Q1MS) with electrospray ionization (ESI-MS) in positive mode.

HRMS characterization was possible using an Agilent Technologies 6210 LC Time of Flight Mass Spectrometer. Products in toluene solutions were introduced to the nebulizer by direct injection. Neutral borabenzene adducts were characterized using APPI ionization in positive mode. Ionic species were ionized by electrospray (ESI-MS) in both positive and negative modes.

**b. Reactions of 1 with Lewis Bases; Preparation of 2-L**

An equivalent of **L** (L=$PMe_3$, Pyridine, Acetonitrile, *tert*-butylisocyanide) was added, *via* microsyringe, to a J-Young tube containing a $C_6D_6$ solution of freshly prepared $(IMes)_2Pt(H)(ClBC_5H_4SiMe_3)$ (**1**). Total conversion of **1** was observed within 5 minutes by NMR.

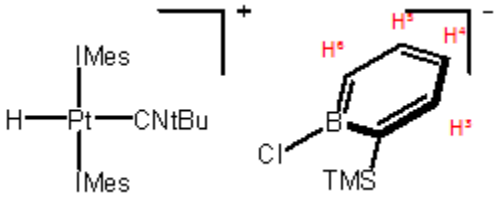
**2-MeCN**




**1** in $C_6D_6$ (5.9 mg, 0.006 mmol), MeCN (0.3 mg, 0.006 mmol); $\delta_H$ ($C_6D_6$) 8.02 (dd, $J_{H\text{-}H}$ = 7.2 and 1.5 Hz, 1H, $H^3$), 7.75 (ddd, $J_{H\text{-}H}$ = 10.5, 6.8 and 1.5 Hz, 1H, $H^5$), 6.95 (dd, $J_{H\text{-}H}$ = 10.3 and 1.0, Hz, 1H, $H^6$), 6.82 (td, $J_{H\text{-}H}$ = 6.8 and 1.2 Hz, 1H, $H^4$), 6.74 (s, 8H, $H^{meta}$Mes), 5.95 (s, 4H, $H^{imid}$), 2.28 (s, 12H, $Me^{para}$Mes), 1.64 (s, 24H, $Me^{ortho}$Mes), 1.38 (s, 3H, *Me*CN), 0.84 (s, 9H, $SiMe_3$), -19.13 (s, $^1J_{Pt\text{-}H}$ = 1520 Hz, H-Pt); $\delta_B$ ($C_6D_6$) 38.7 (br); $\delta_C$ ($C_6D_6$) 171.8 (carbene), 139.5 ($C^3$), 138.5 ($C^{para}$Mes), 136.5 ($C^{ipso}$Mes), 135.8

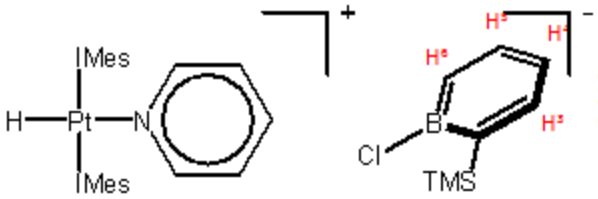
($C^5$), 135.1 ($C^{ortho}$Mes), 129.2 ($C^{meta}$Mes), 128.6 (Me*CN*), 127.4 (br, $C^6$), 121.8 ($C^{imid}$), 111.6 ($C^4$), 21.2 ($Me^{para}$Mes), 17.8 ($Me^{ortho}$Mes), 2.0 ($SiMe_3$), 1.7 (*Me*CN), $C^2$ was not detected.

**2-CN*t*Bu**



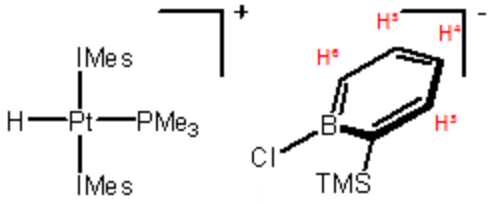

**1** in $C_6D_6$ (5.9 mg, 0.006 mmol), CN*t*Bu (0.5 mg, 0.006 mmol); $\delta_H$ ($C_6D_6$) 7.97 (dd, $J_{H\text{-}H}$ = 7.0 and 1.3 Hz, 1H, $H^3$), 7.75 (ddd, $J_{H\text{-}H}$ = 10.6, 6.8 and 1.6 Hz, 1H, $H^5$), 6.96 (dd, $J_{H\text{-}H}$ = 10.3 and 1.0 Hz, 1H, $H^6$), 6.76 (td, $J_{H\text{-}H}$ = 7.0 and 1.2 Hz, 1H, $H^4$), 6.65 (s, 8H, $H^{meta}$Mes), 6.10 (s, 4H, $H^{imid}$), 2.27 (s, 12H, $Me^{para}$Mes), 1.65 (s, 24H, $Me^{ortho}$Mes), 1.03 (s, 9H, CNtBu), 0.83 (s, 9H, $SiMe_3$), -7.79 (s, $^1J_{Pt\text{-}H}$ = 1101 Hz, H-Pt); $\delta_B$ ($C_6D_6$) 38.5 (br); $\delta_C$ ($C_6D_6$) 167.3 (carbene), 156.2 ($C$NC$(CH_3)_3$), 139.3 ($C^3$), 138.3 ($C^{para}$Mes), 136.3 ($C^{ipso}$Mes), 135.7 ($C^5$), 134.8 ($C^{ortho}$Mes), 129.3 ($C^{meta}$Mes), 127.4 (br, $C^6$), 123.0 ($C^{imid}$), 111.4 ($C^4$), 53.4 (CN$C$$(CH_3)_3$), 29.7 (CNC$(CH_3)_3$), 21.3 ($Me^{para}$Mes), 18.1 ($Me^{ortho}$Mes), 2.2 ($SiMe_3$), $C^2$ was not detected; ESI-MS: m/z = 887.8 (calcd. = 887.4).

**2-Py**



**1** in $C_6D_6$ (5.9 mg, 0.006 mmol, 8 mol/L), Pyridine (0.5 mg, 0.006 mmol); $\delta_H$ ($C_6D_6$) 8.08 (dd, $J_{H-H}$ = 7.1 and 1.6 Hz, 1H, $H^3$), 7.83 (ddd, $J_{H-H}$ = 10.1, 6.8 and 1.5 Hz, 1H, $H^5$), 7.42 (t, $J_{H-H}$ = 7.6 Hz, 1H, $H^{para}$Py), 7.04 (d, $J_{H-H}$ = 10.3 Hz, 1H, $H^6$), 6.87 (t, $J_{H-H}$ = 7.1 Hz, 1H, $H^4$), 6.78 (d, $J_{H-H}$ = 5.4 Hz, 2H, $H^{ortho}$Py), 6.72 (s, 8H, $H^{meta}$Mes), 6.59 (dd, $J_{H-H}$ = 7.2 and 5.6 Hz, 2H, $H^{meta}$Py), 5.93 (s, 4H, $H^{imid}$), 2.32 (s, 12H, $Me^{para}$Mes), 1.52 (s, 24H, $Me^{ortho}$Mes), 0.86 (s, 9H, $SiMe_3$), -20.10 (s, $^1J_{Pt-H}$ = 1348 Hz, H-Pt); $\delta_B$ ($C_6D_6$) 37.5 (br); $\delta_C$ ($C_6D_6$) 173.3 (carbene), 150.3 ($C^{ortho}$Py), 139.4 ($C^3$), 139.0 ($C^{para}$Py), 138.8 ($C^{para}$Mes), 136.4 ($C^{ipso}$Mes), 136.0 ($C^5$), 135.3 ($C^{ortho}$Mes), 129.3 ($C^{meta}$Mes), 127.5 (br, $C^6$), 125.9 ($C^{meta}$Py), 122.0 ($C^{imid}$), 111.6 ($C^4$), 21.3 ($Me^{para}$Mes), 17.9 ($Me^{ortho}$Mes), 2.2 ($SiMe_3$), $C^2$ was not detected; HRMS : m/z (cation) = 883.3999 (calcd. = 883.4031), m/z (anion) = 183.0694 (calcd. = 183.0570).

**2-$PMe_3$**




**1** in $C_6D_6$ (5.9 mg, 0.006 mmol), $PMe_3$ (0.5 mg, 0.006 mmol); $\delta_H$ ($C_6D_6$) 7.95 (dd, $J_{H-H}$ = 7.1 and 1.5 Hz, 1H, $H^3$), 7.71 (ddd, $J_{H-H}$ = 10.4, 6.7 and 1.5 Hz, 1H, $H^5$), 6.90 (dd, $J_{H-H}$ = 10.2 and 1.1, Hz, 1H, $H^6$), 6.75 (td, $J_{H-H}$ = 6.7, 1.1 Hz, 1H, $H^4$), 6.64 (s, 8H, $H^{meta}$Mes), 6.06 (s, 4H, $H^{imid}$), 2.24 (s, 12H, $Me^{para}$Mes), 1.74 (s, 24H, $Me^{ortho}$Mes), 0.79 (s, 9H, $SiMe_3$), 0.55 (d, $J_{H-P}$ = 8.8 Hz, 9H, $PMe_3$), -5.61 (d, $J_{P-H}$ = 187.9 Hz, $^1J_{Pt-H}$ = 1060 Hz, H-Pt); $\delta_P$ ($C_6D_6$) -23.2 (s, $^1J_{P-Pt}$ = 1694 Hz, P-Pt); $\delta_B$ ($C_6D_6$) 39.7 (br); $\delta_C$ ($C_6D_6$) 139.4

($C_3$), 138.4 ($C^{para}$Mes), 136.3 ($C^{ipso}$Mes), 135.7 ($C^5$), 135.7 ($C^{ortho}$Mes), 129.7 ($C^{meta}$Mes), 127.2 (br, $C^6$), 123.5 ($C^{imid}$), 111.4 ($C^4$), 21.3 ($Me^{para}$Mes), 18.8 ($Me^{ortho}$Mes), 16.6 (br, $PMe_3$), 2.2 ($SiMe_3$), carbenic carbon and $C^2$ were not detected; ESI-MS: m/z = 880.1 (calcd. = 880.4).

**c. Synthesis of borabenzene adducts (4-L)**

**1-tertbutylisocyanide-2-(trimethylsilyl)borabenzene (4-BuNC)** 54µL (0.5 mmol) of (*tert*-butyl)isocyanide was added to a solution of 1-chloro-2,6-di(trimethylsilyl)-2,4-boracyclohexadiene and 1-chloro-2,2-di(trimethylsilyl)-3,5-boracyclohexadiene (120 mg, 0.47 mmol) in 3 mL of benzene. The reaction mixture was stirred for three hours to become a brown solution. The solvent was evaporated *in vacuo* and the residue washed two times with pentane to afford 18 mg (18%) of a light brown solid. $\delta_H$ ($C_6D_6$) 8.13 (d, $J_{H\text{-}H}$ = 7.3 Hz, 1H), 8.06-7.93 (ov. m, 2H), 7.46 (td, $J_{H\text{-}H}$ = 7.0 and 1.7 Hz, 1H), 0.68 (s, CNtBu), 0.48 (s, 9H); $\delta_B$ ($C_6D_6$) 14.6 (s); $\delta_C$ ($C_6D_6$) 138.7, 134.8, 122.9, 54.5, 28.6, 1.4, $C^{2/6}$ and *C*NC($CH_3$)$_3$ were not detected; no MS signal could be observed.

**1-trimethylphosphine-2-(trimethylsilyl)borabenzene (4-$PMe_3$)** 34µL (0.2 mmol) of trimethylphosphine was added to a solution of 1-chloro-2,6-di(trimethylsilyl)-2,4-boracyclohexadiene and 1-chloro-2,2-di(trimethylsilyl)-3,5-boracyclohexadiene (85 mg, 0.2 mmol) in 2 mL of pentane. The reaction mixture was stirred for eight hours during which the product precipitated as a pale solid. The solid was washed two times with pentane and dried *in vacuo* to afford 26 mg (35%) of a light brown solid. A significant portion of the 1-trimethylphosphine-borabenzene was observed as side-product, but no rational explication could be found to explain the loss of the other TMS group.[S2] $\delta_H$ ($C_6D_6$) 8.17 (t, $J_{H\text{-}H}$ = 6.6 Hz, 1H), 8.00 (br m, 1H), 7.40 (tdd, $J_{H\text{-}H}$ = 7.3, 2.3 and 1.1 Hz,

1H), 7.02 (td, $J_{H-H}$ = 9.9 and 1.1 Hz, 1H), 0.79 (d, $J_{H-P}$ = 11.0 Hz, 9H)  0.41 (s, 9H); $\delta_P$ ($C_6D_6$) -22.8 (br, P-B); $\delta_B$ ($C_6D_6$) 24.3 (d, $^1J_{P-B}$ = 80.7 Hz); $\delta_C$ ($C_6D_6$) 140.3 ($J_{C-P}$ = 19.2 Hz), 134.8 ($J_{C-P}$ = 18.1 Hz), 120.8, 12.3 ($J_{C-P}$ = 40.7 Hz), 2.9; HRMS: m/z = 224.1378 (calcd. = 224.1324).

**1-acetonitrile-2-(trimethylsilyl)borabenzene (4-MeCN)** could not be made using the same methodology and evidences point towards the instability of the species.

**d. Reactions with $AgBF_4$**

$(IMes)_2Pt(H)(Cl)$ (**3**) can be isolated form degraded samples of **1** and **2**. Old reaction mixtures were concentrated *in vacuo* and washed with successive portions of ethyl ether. The dried residue is pure **3**.

To a dilute solution of **3** in $C_6D_6$ were added an excess of L ligand and an excess of solid $AgBF_4$. A large amount of solid was present in the NMR tube which can be attributed to the limited solubility of $[(IMes)_2Pt(H)(L)]BF_4$ in $C_6D_6$. $^1$H NMR spectra were compared to spectra of corresponding 2-L to characterize the cation.

## 2. NMR Characterization

Fig. S1- $^{1}$H NMR spectrum of **2-MeCN** (400 MHz, $C_6D_6$)

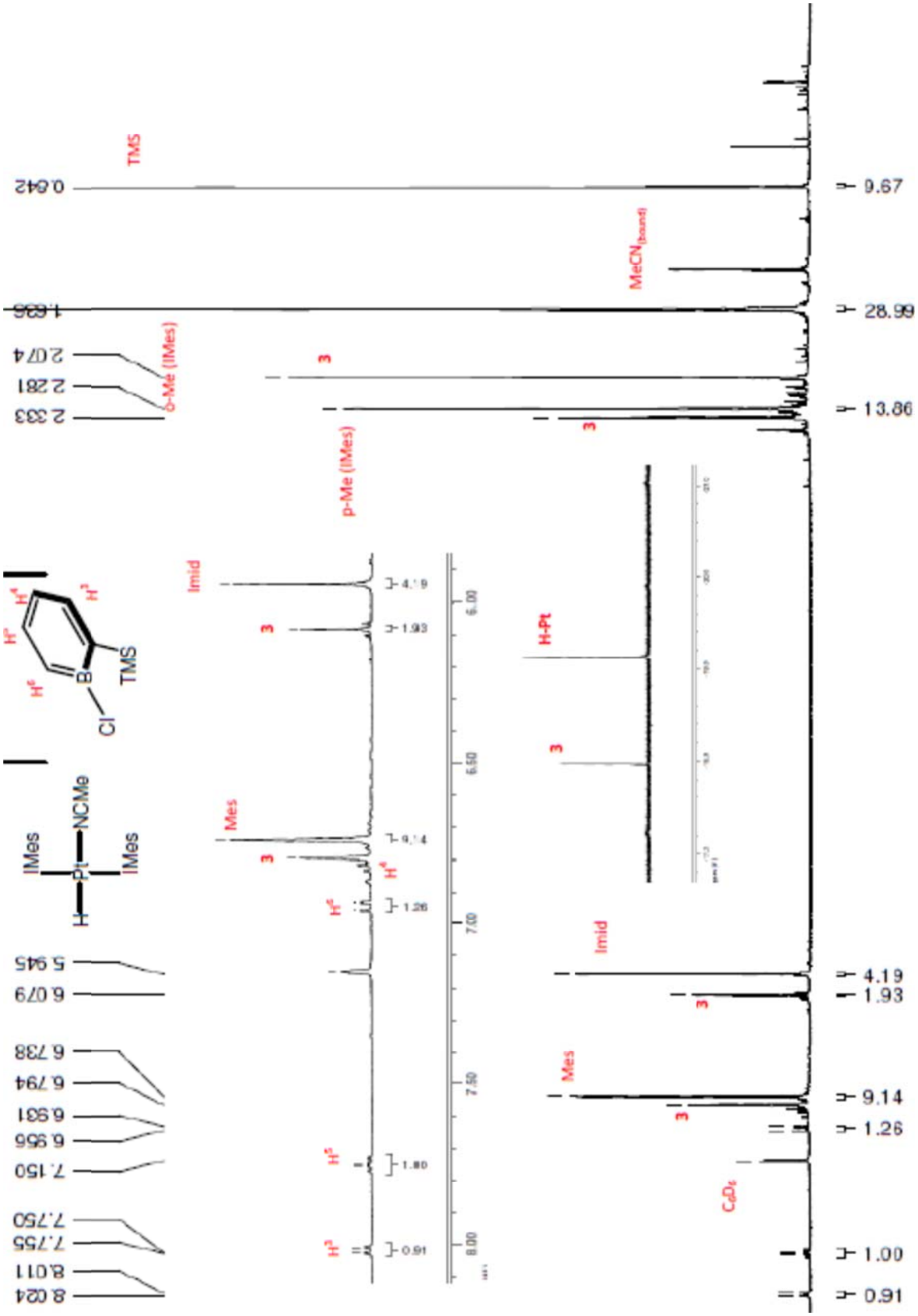


Fig. S2- $^{1}$H NMR spectrum of **2-BuNC** (400 MHz, $C_6D_6$)

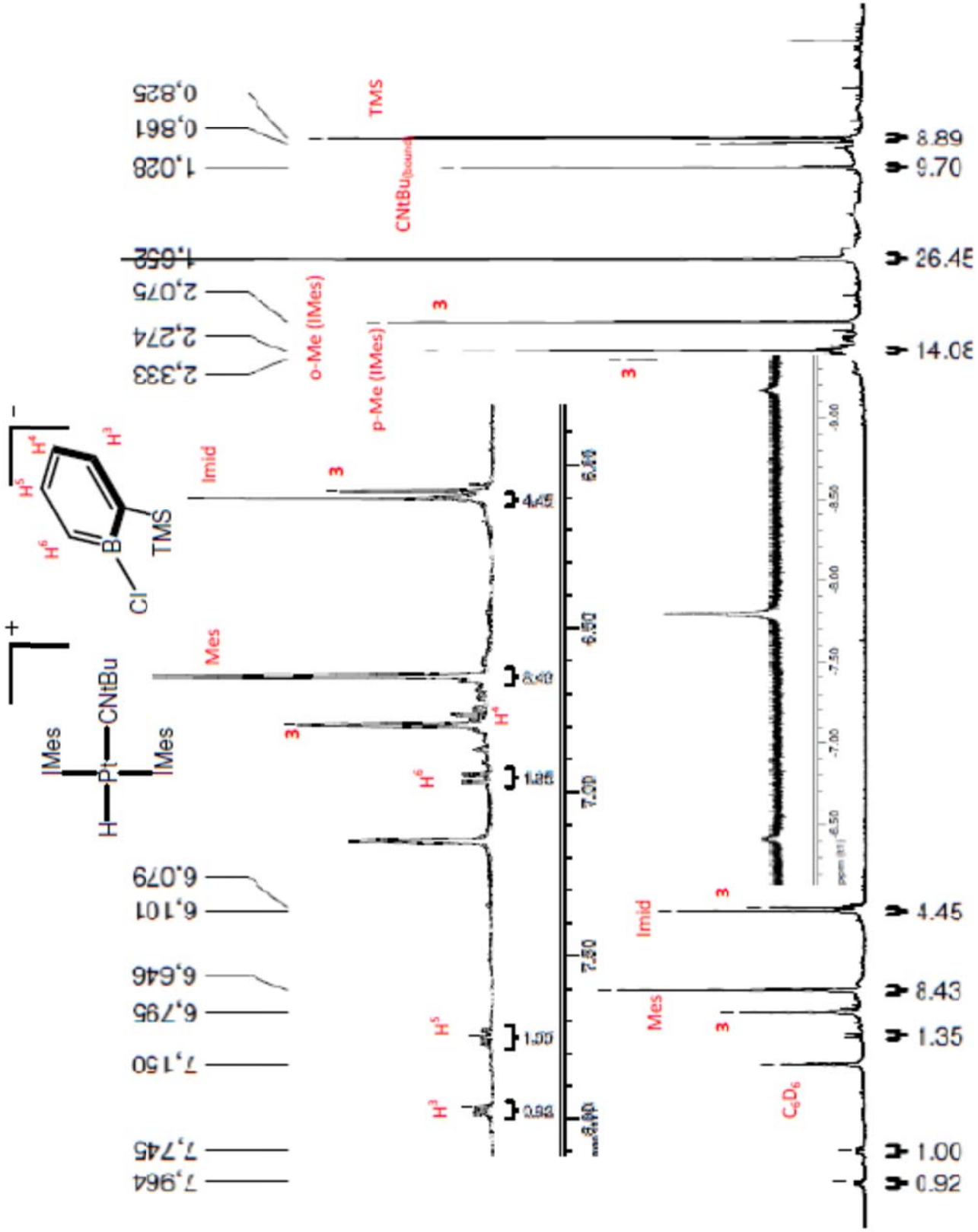


Fig. S3- $^{1}$H NMR spectrum of **2-Py** (400 MHz, $C_6D_6$)

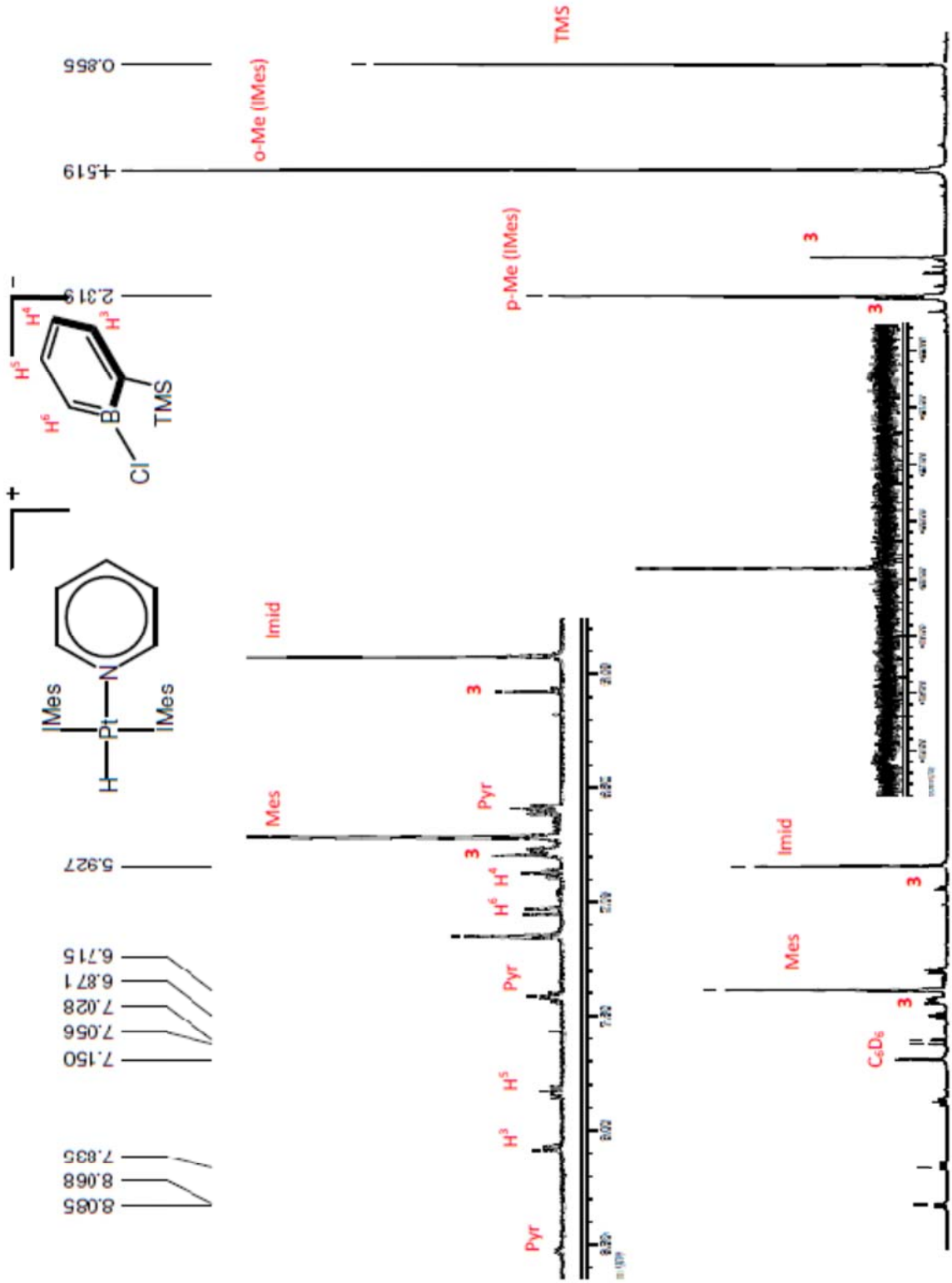


Fig. S4- $^{1}$H NMR spectrum of **2-PMe$_3$** (400 MHz, $C_6D_6$)

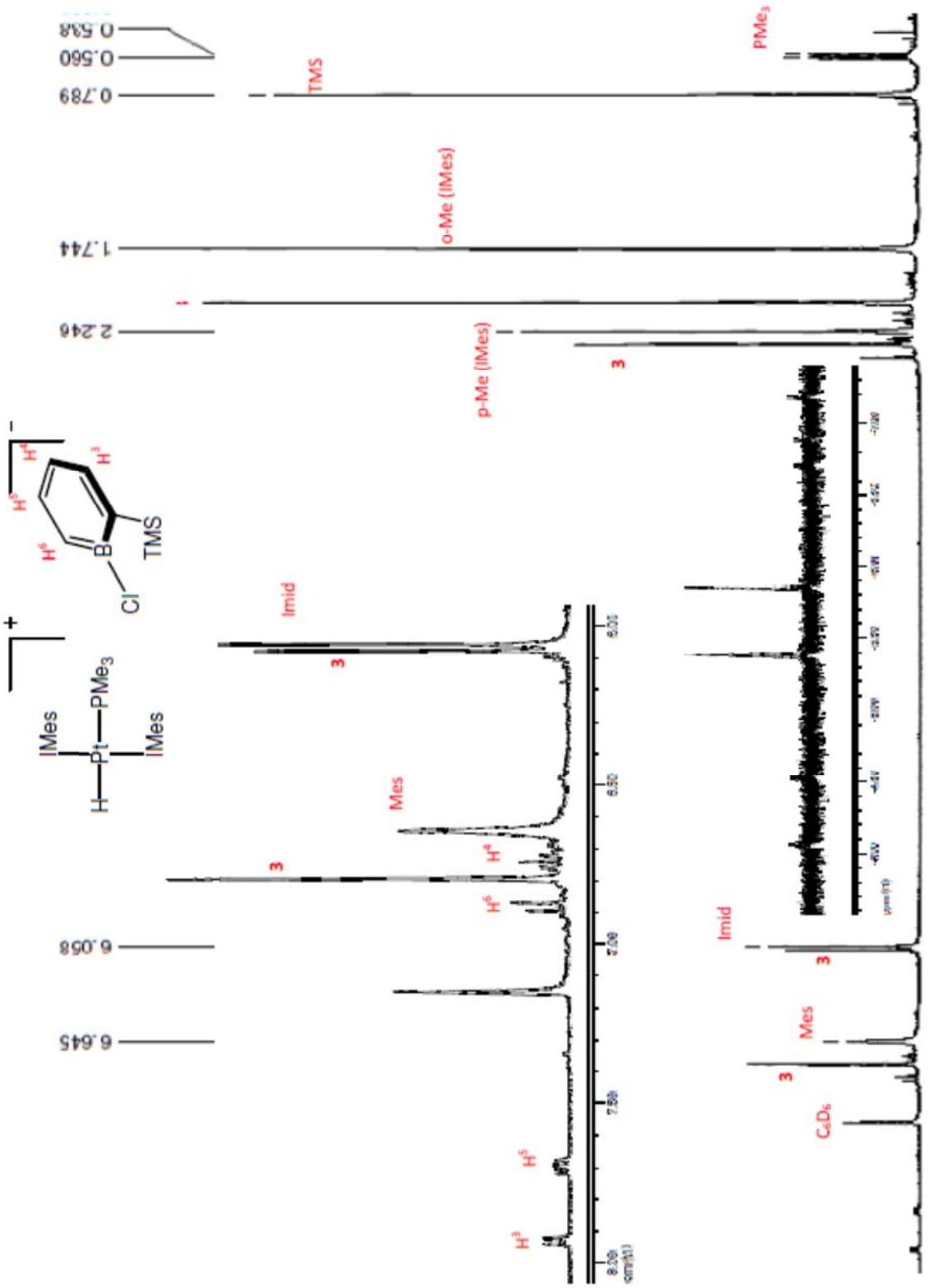


Fig. S5- $^{1}$H NMR spectrum of the hydride region for **2-MeCN** and the reaction of **3** with $AgBF_4$ and MeCN. (400 MHz, $C_6D_6$)

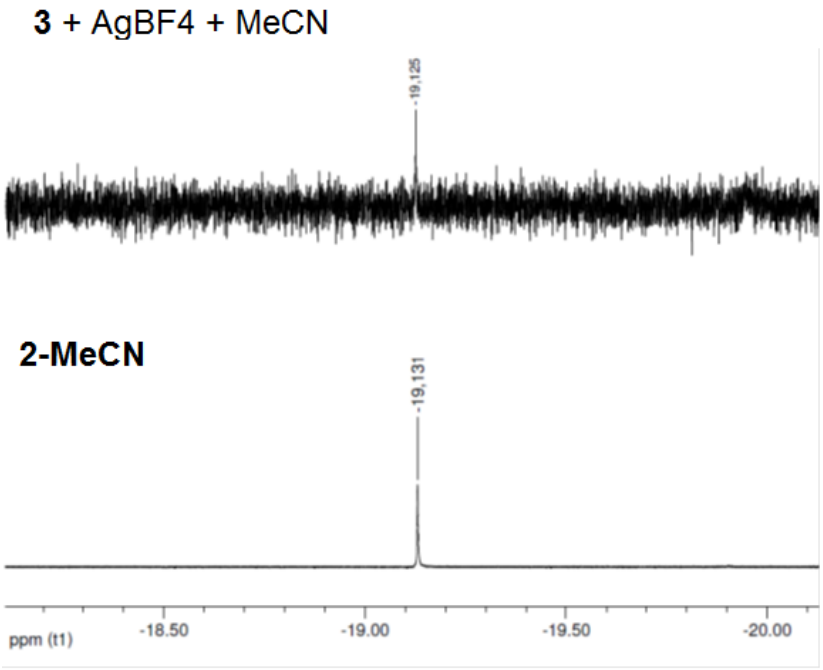



Fig. S6- $^{1}$H NMR spectrum of the hydride region for **2-BuNC** and the reaction of **3** with $AgBF_4$ and *t*BuNC. (400 MHz, $C_6D_6$)

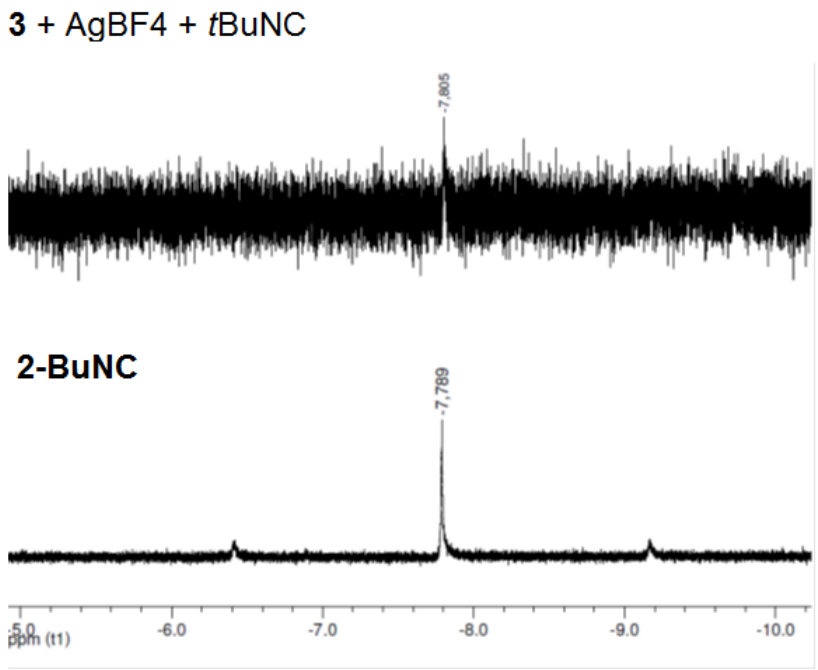


Fig. S7- $^{1}$H NMR spectrum of the hydride region for **2-Py** and the reaction of **3** with $AgBF_4$ and pyridine. (400 MHz, $C_6D_6$)

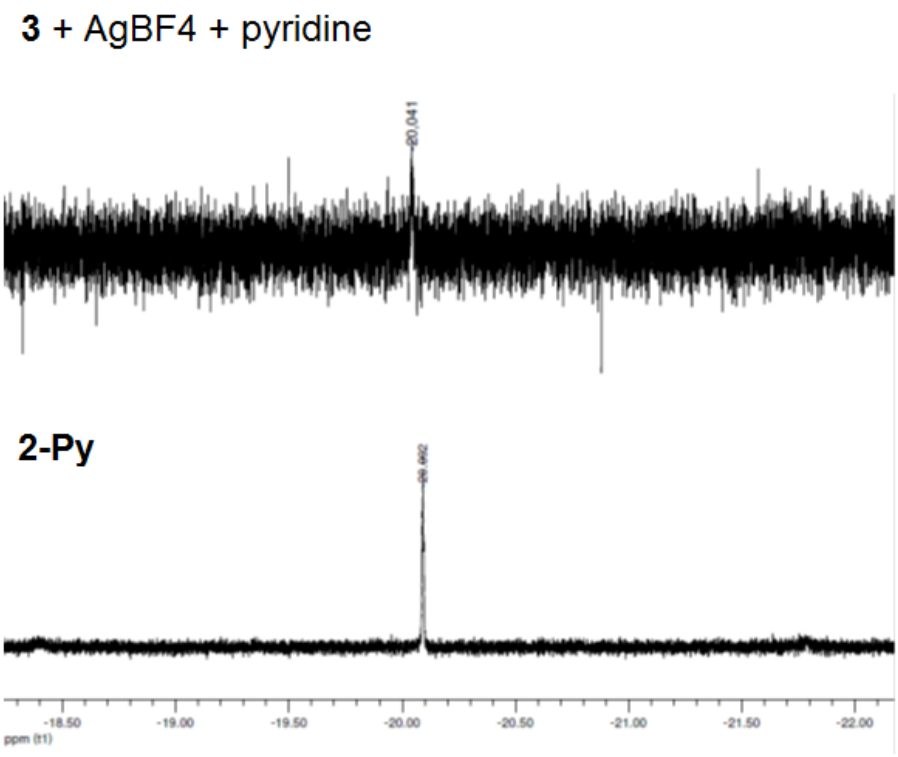
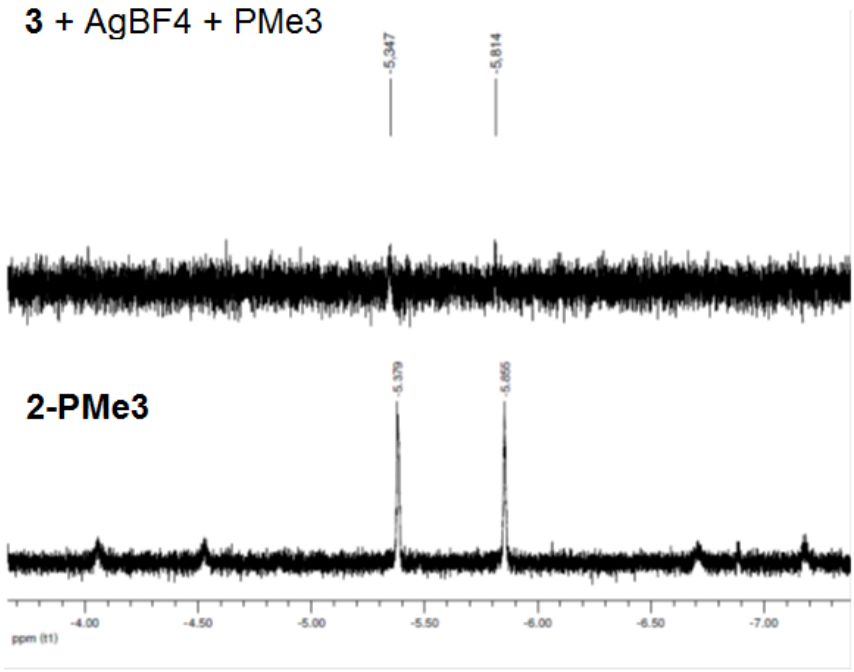



Fig. S8- $^{1}$H NMR spectrum of the hydride region for **2-PMe$_3$** and the reaction of **3** with $AgBF_4$ and $PMe_3$. (400 MHz, $C_6D_6$)



## 3. MS Characterization

Fig. S9 - Experimental ESI-MS spectrum for the cationic fragment of **2-CN*t*Bu**

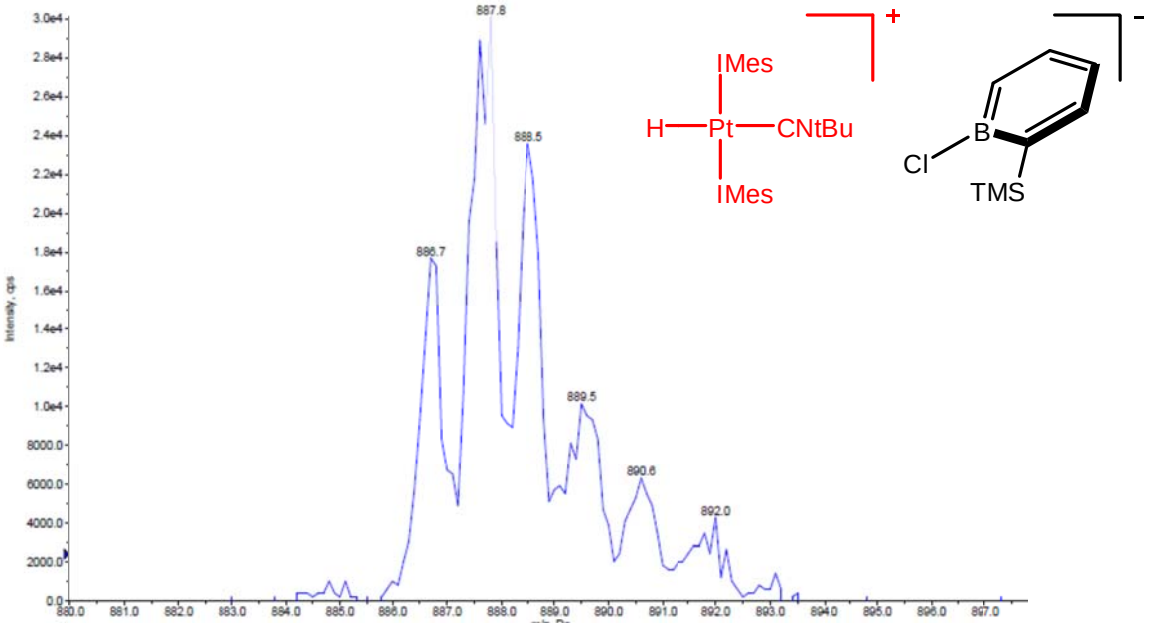



Fig. S10 - Simulated spectrum for the $C_{47}H_{58}N_5Pt_1$. [S3]

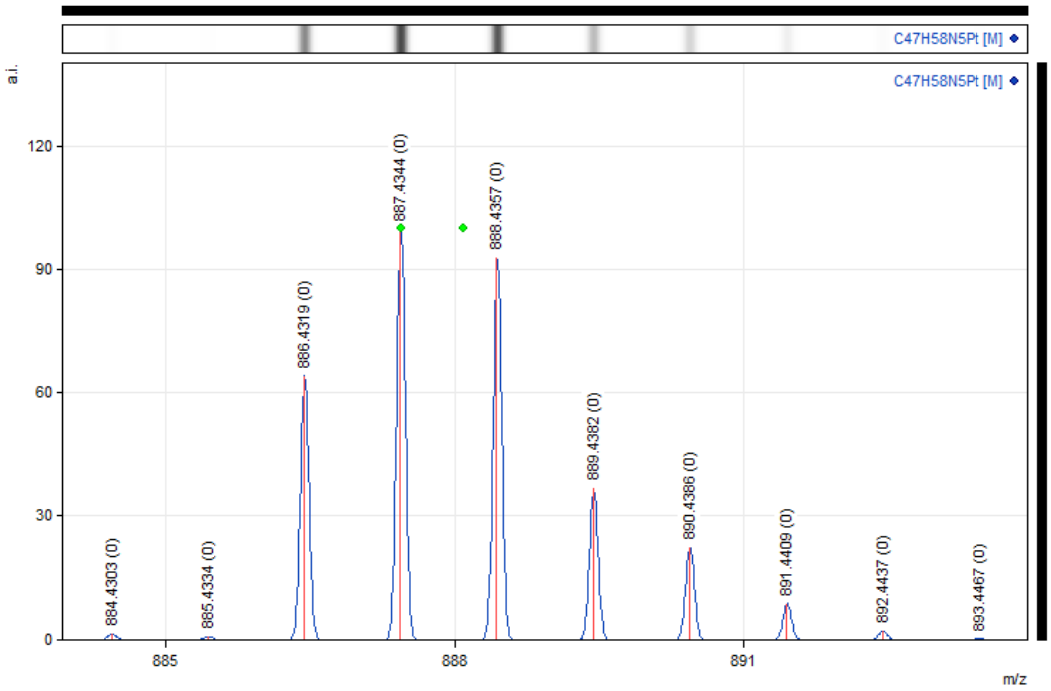


Fig. S11 - Experimental HRMS spectrum for the cationic fragment of **2-Py**

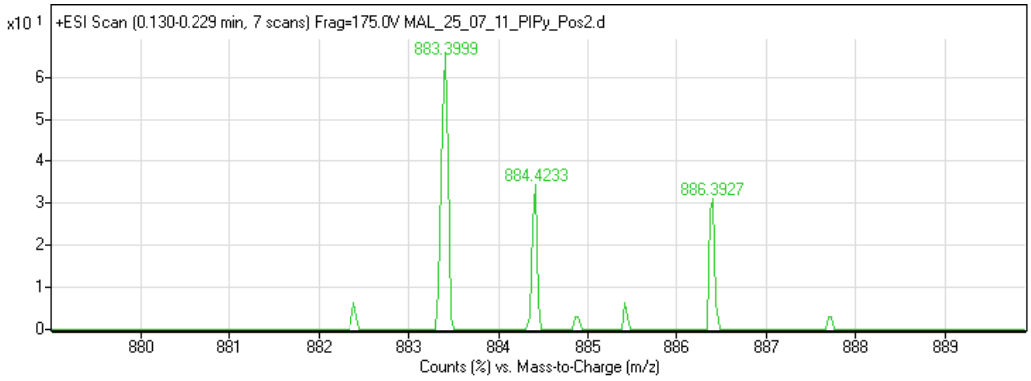



Fig. S12 - Simulated spectrum for the $C_{47}H_{54}N_5Pt_1$. [3S]

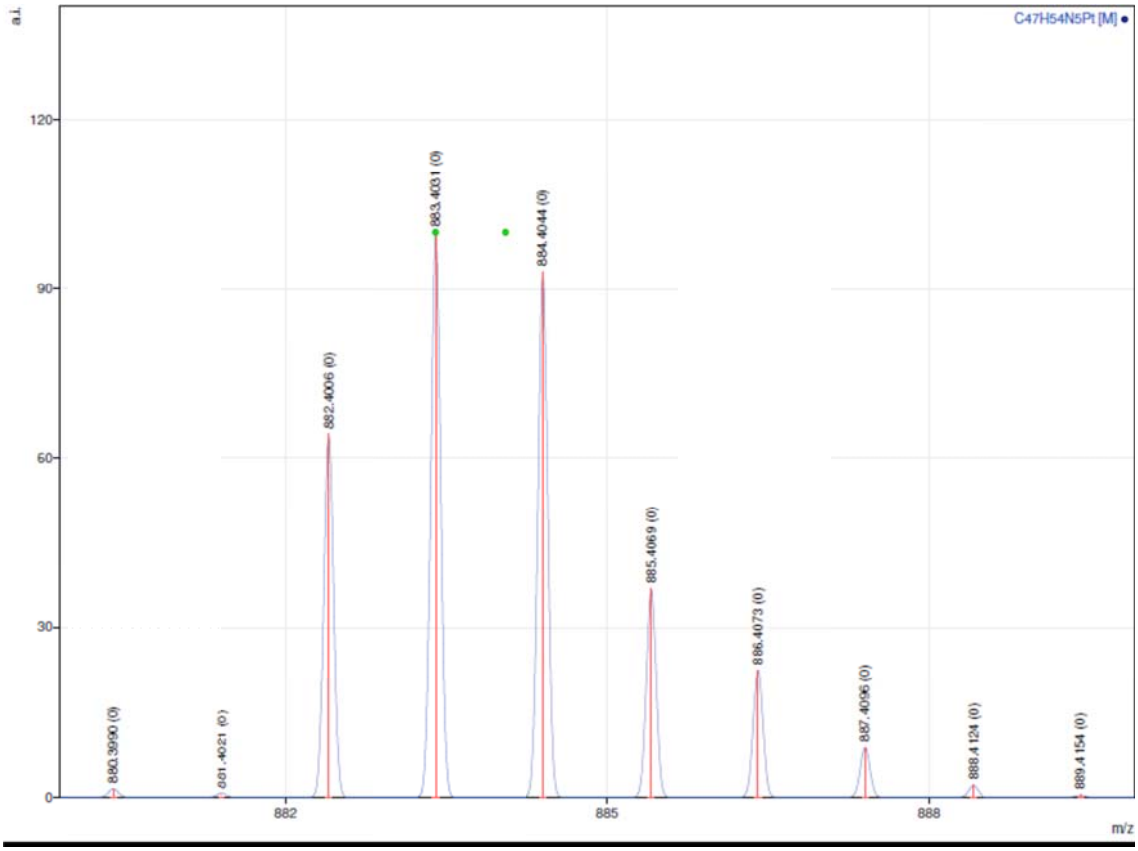


Fig. S13 - Experimental ESI-MS spectrum for the cationic fragment of **2-PMe$_3$**

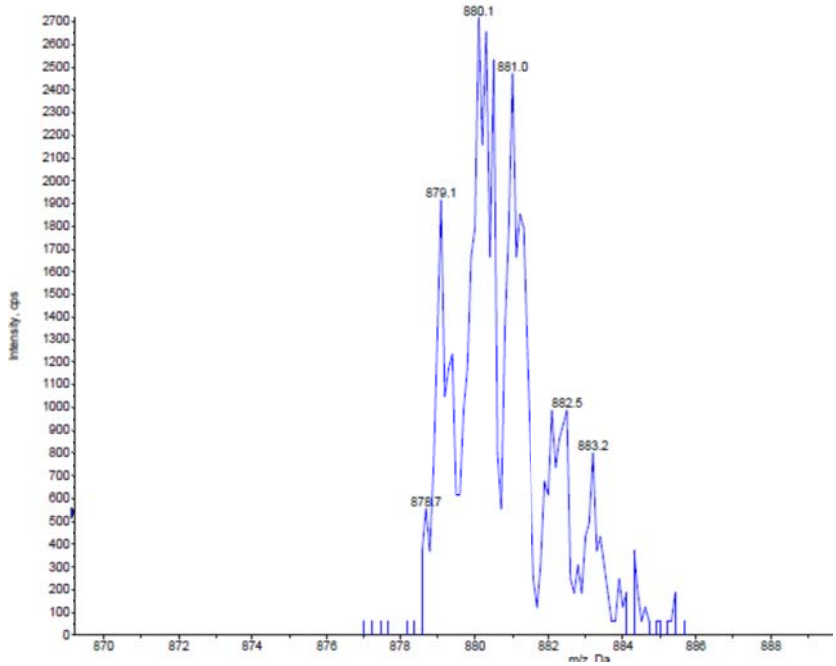



Fig. S14 - Simulated spectrum for the $C_{45}H_{58}N_4P_1Pt_1$. [3S]

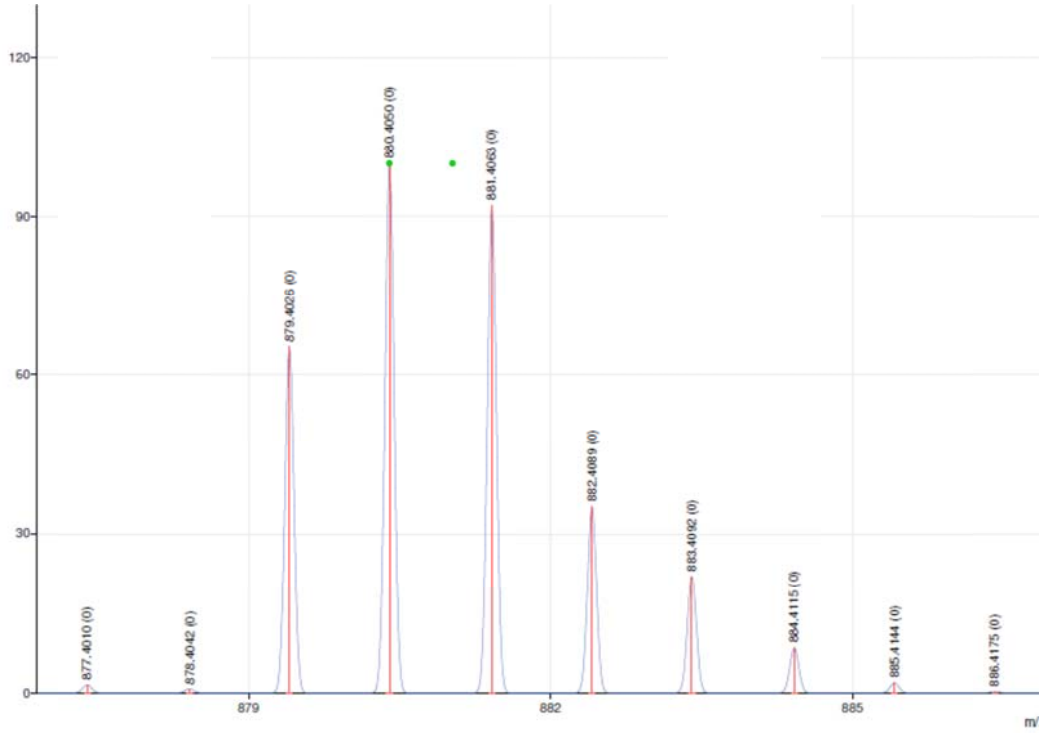


Fig. S15 - Experimental HRMS spectrum for the 1-Cl-2-TMS-boratabenzene fragment (taken from sample **2-Py**).

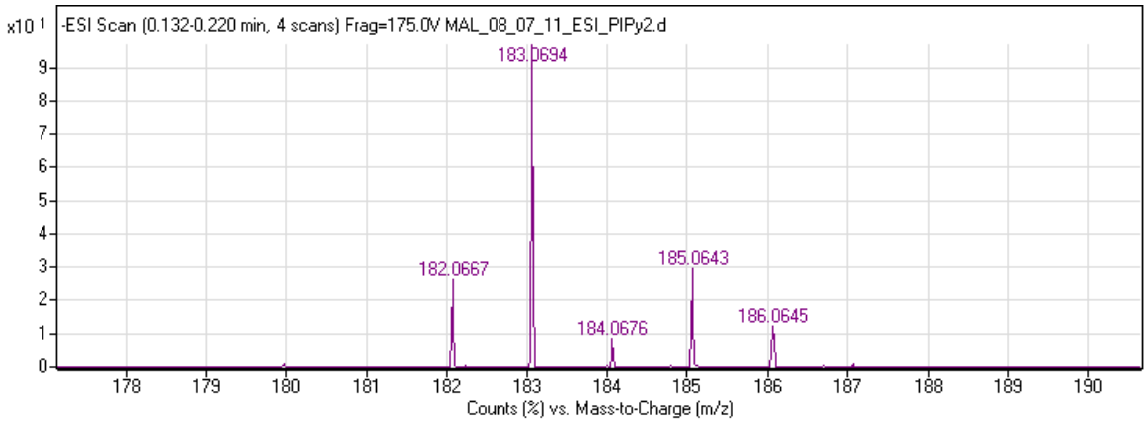
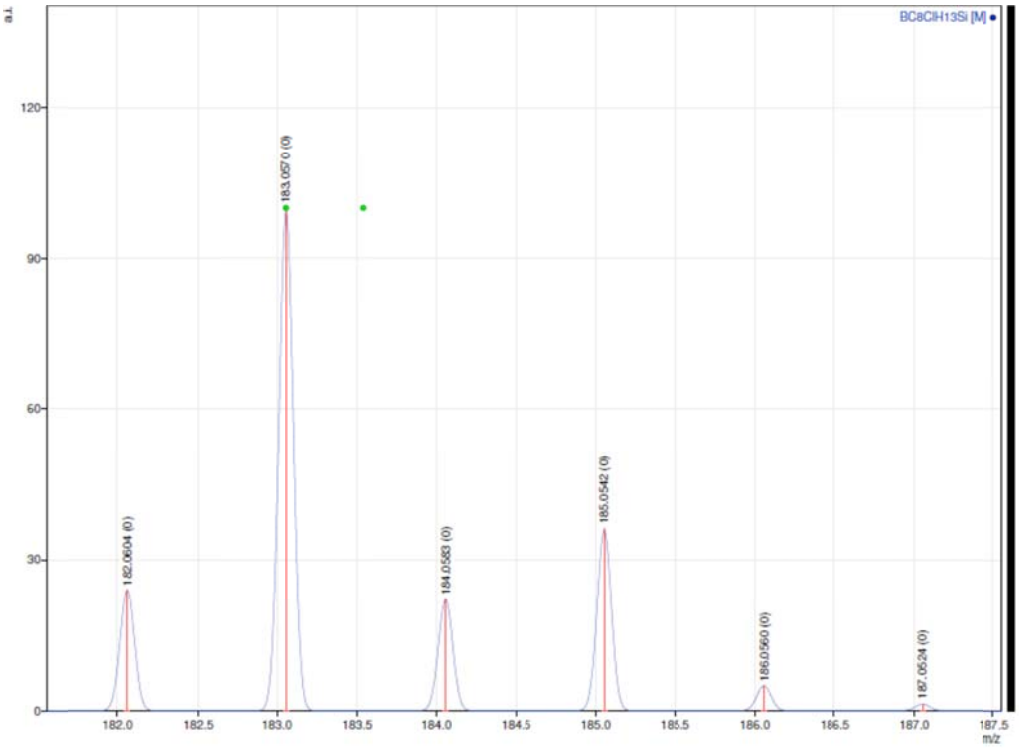



Fig. S16 - Simulated spectrum for the $C_8H_{13}B_1Cl_1Si_1$.[3S]



## 4. Variable Temperature NMR and WINDNMR simulations[S4]

Fig. S16 – $^{1}$H NMR of the aromatic region for the reaction between **1** and a subequivalent of pyridine at -30 °C and 20 °C in $C_6D_6$.

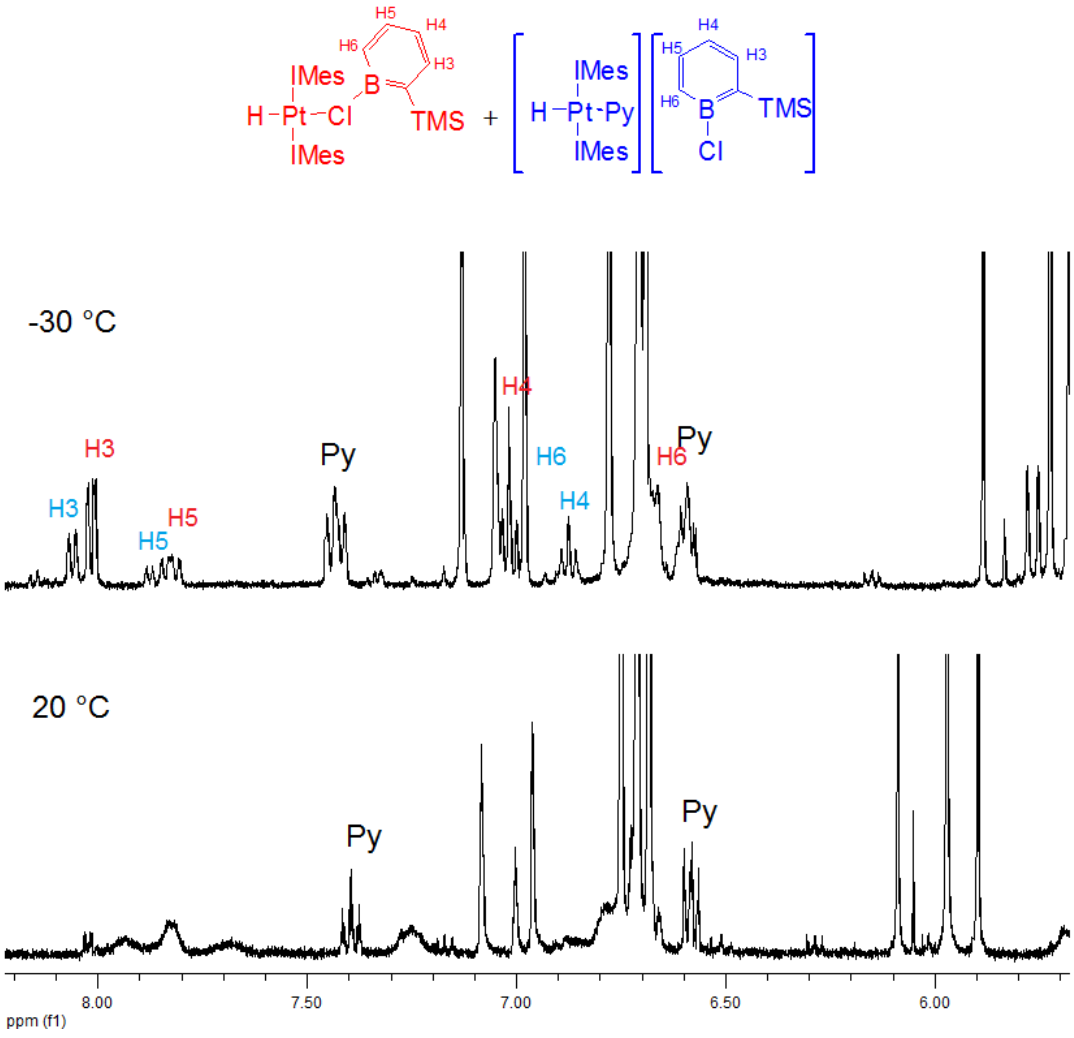
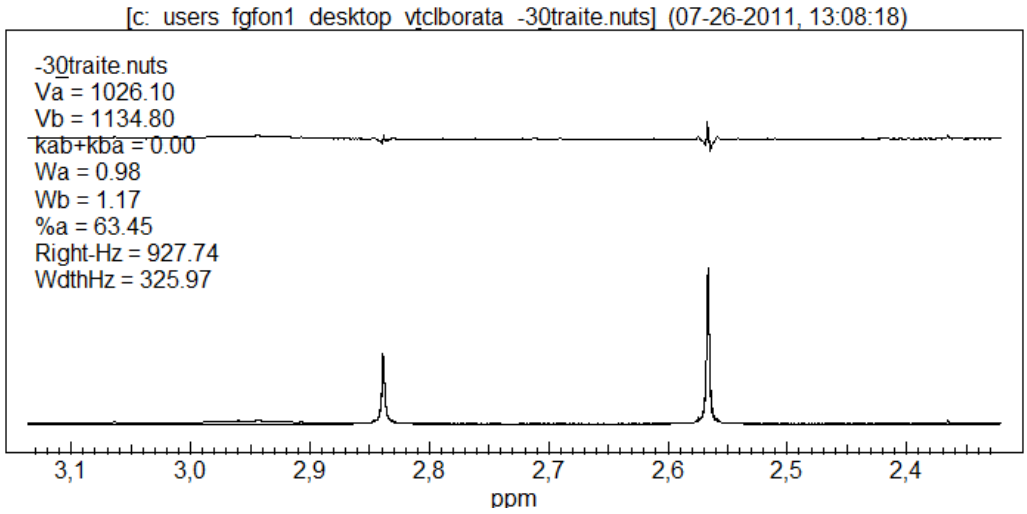
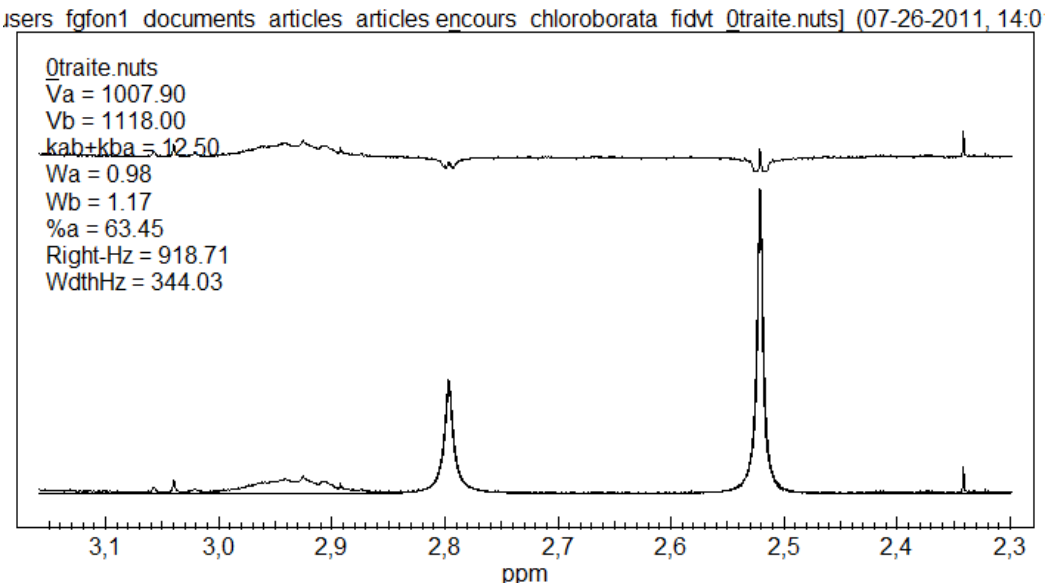


Fig. S17. Experimental and simulated (WINDNMR-pro) $^{1}$H NMR spectra (down) and difference spectra (up) of the $SiMe_3$ region for a 63.45 : 36.55 ratio of **1** to **2-Py** at various temperatures. The ppm scale is downfield by 2 ppm because of a glitch when importing the experimental data from MestRec. The Va and Vb values were not kept constant in order to account for the drifting of the chemical shift of **1** and **2-Py** with temperature, which can be seen by the IMes resonances on Fig S16. At low temperature, the difference spectra are not exactly flat because of the presence of $^{29}$Si satellites that could not be accounted for in the simulation.

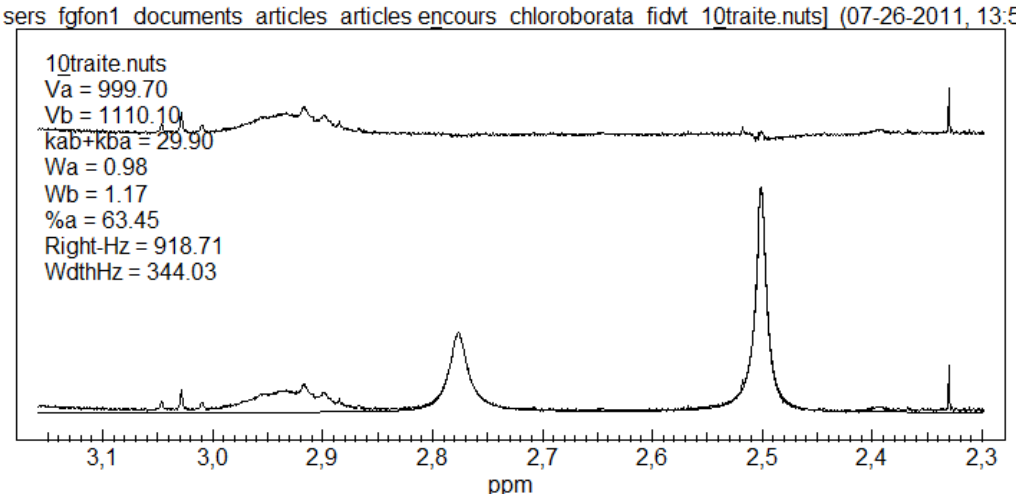
a) -30°C (k = 0, no exchange)



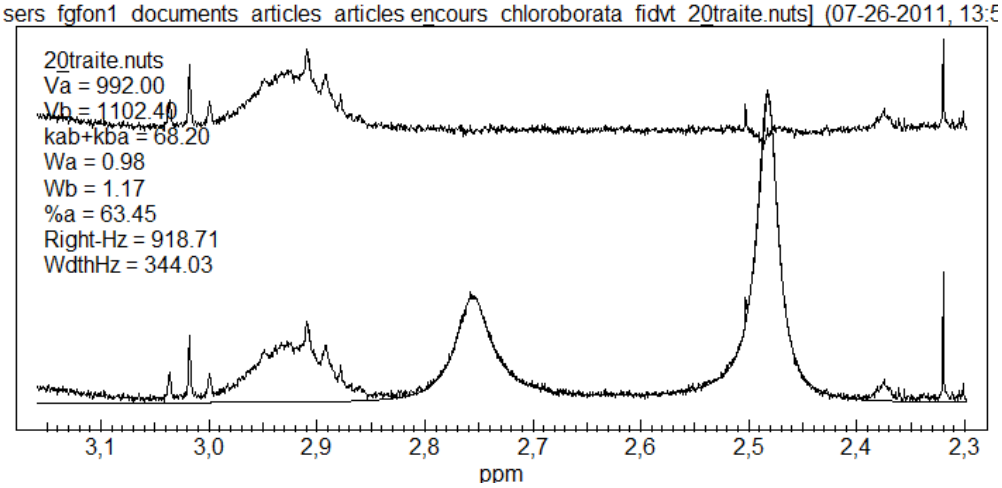

b) 0°C (k = 4.49 $sec^{-1}$)



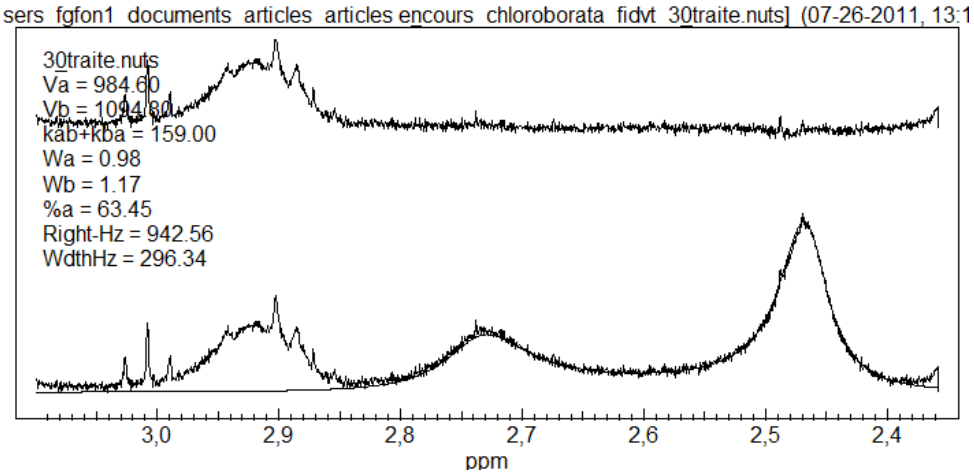
c) 10°C (k = 10.7 $sec^{-1}$)



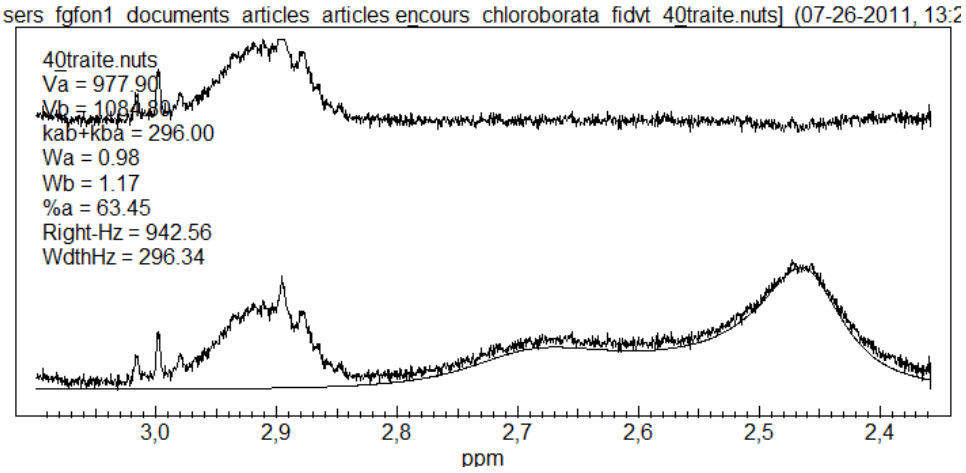

d) 20°C (k = 24.5 $sec^{-1}$)



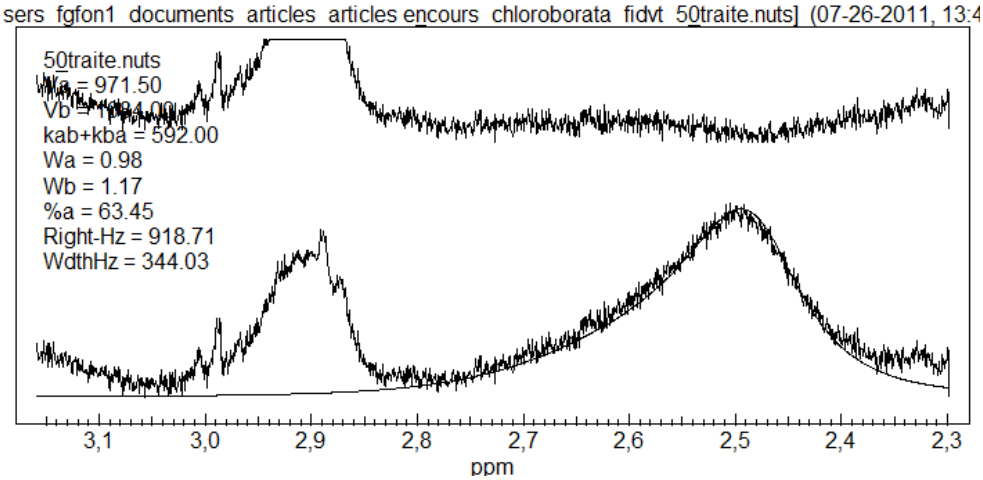

e) 30°C (k = 57.1 $sec^{-1}$)



f) 40°C (k = 106 $sec^{-1}$)




g) 50°C (k = 213 $sec^{-1}$)




h) 60°C (k = 382 $sec^{-1}$)

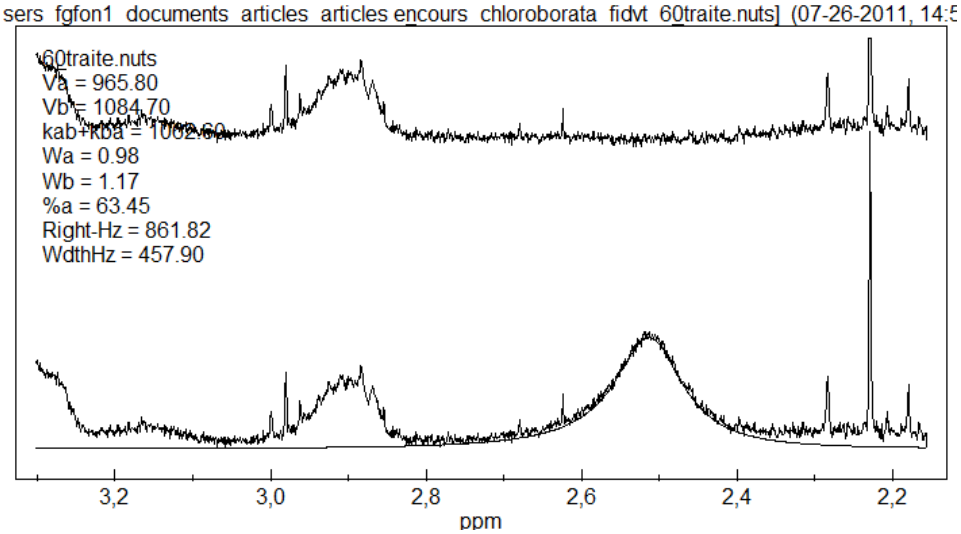


Fig. S18. Excel sheet with Eyring plot for the determination of the rate constant for the exchange of the 1-Cl-2-TMS-boratabenzene moiety in **1** and **2-L**. Model taken from an online workshop by William D. Jones.[S5]

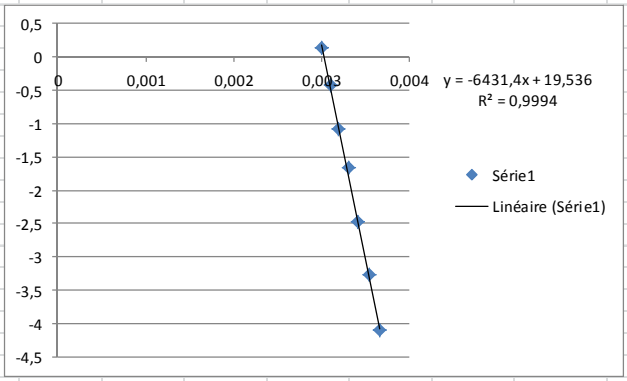
| | WINDNMR | | | | | | | | [A] | 0,0041 | M |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | ka+kb | ka | | | | | | | [B] | 0,0023 | M |
| | 6 | 2,15625 | | | | | | | | | |
| | 12,5 | 4,492188 | | | | | | | | | |
| | 29,9 | 10,74531 | | | | | | | | | |
| | 68,2 | 24,50938 | | | | | | | | | |
| | 159 | 57,14063 | | | | | | | | | |
| | 296 | 106,375 | | | | | | | | | |
| | 592 | 212,75 | | | | | | | | | |
| | 1085 | 389,9219 | | | | | | | | | |

Eyring Plot for the exchange between Cl-boratabenzene

| T(°C) | K | 1/T | ln(K/T) | calc | Statistiques: | | | |
|---|---|---|---|---|---|---|---|---|
| 59,07 | 381,6500 | 0,00301 | 0,138767 | 0,175545 | -6431,41 | 19,53561 | pente m | ordonnée b |
| 49,08 | 212,7500 | 0,003104 | -0,41509 | -0,42471 | 70,50906 | 0,234847 | std error m | std error b |
| 39,09 | 106,3750 | 0,003203 | -1,07674 | -1,06337 | 0,999399 | 0,041204 | r2 | std error y |
| 29,09 | 57,1406 | 0,003309 | -1,66564 | -1,74496 | 8319,996 | 5 | F | d.f. |
| 19,1 | 24,5094 | 0,003422 | -2,47849 | -2,47244 | 14,12528 | 0,008489 | reg sum sq | res sum sq |
| 9,11 | 10,7453 | 0,003543 | -3,26829 | -3,25143 | | | | |
| -0,89 | 4,4922 | 0,003673 | -4,10434 | -4,08845 | | | | |

95% confidence limits:

$\Delta H^0$ = 12,78 ± 0,34 kcal/mol
$\Delta S^0$ = -8,47 ± 1,14 e.u.

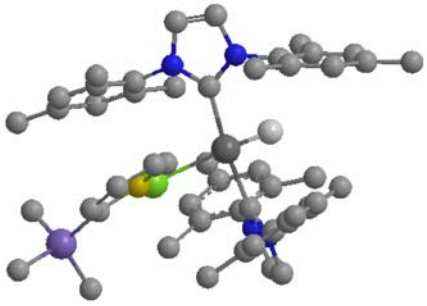


## 4. Computational details

Calculations were carried out using Gaussian 03 package at the DFT level by means of the hybrid density functional B3PW91.[S6] For the Cl, P and Si atoms,[S7] the Stuttgart-Dresden pseudopotentials were used in combination with their associated basis sets. For the N, B, C, and H atoms the all electron 6-311G(d,p)[8] basis sets were used. The nature of the optimized stationary point, minima, has been verified by means of analytical frequency calculation at 298.15 K and 1 atm. The geometry optimizations have been achieved without any geometrical constraints. The energy data presented correspond to the free enthalpy in gas phase of the computed compounds in which thermal, vibrational, translational and rotational contributions have been included.

**Cartesian coordinates of the optimized structures**

**Complex 1**



**120**

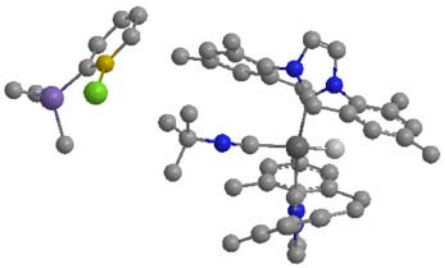
**E: -2324.294086 a.u.**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 0.262075 | 0.584633 | 0.517492 | N | -0.802630 | 1.760216 | 2.384116 |
| C | 0.204019 | 0.860529 | 1.890827 | C | -0.647361 | 3.094755 | 2.629653 |
| C | 1.036536 | 0.213771 | 2.817113 | N | -1.849218 | 3.476983 | 3.147062 |
| C | 1.964923 | -0.707530 | 2.329215 | C | -2.730444 | 2.408737 | 3.214922 |
| C | 2.069536 | -0.998906 | 0.966689 | C | -2.073848 | 1.328063 | 2.733997 |
| C | 1.207835 | -0.347759 | 0.082179 | Pt | 1.033364 | 4.199516 | 2.354537 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Cl | 0.155248 | 4.903607 | 0.050498 | C | 4.052200 | 2.568037 | 0.689275 |
| C | -2.202377 | 4.789789 | 3.621005 | C | 4.199726 | 3.501778 | 5.024200 |
| C | -2.990878 | 5.623307 | 2.815874 | C | 1.976693 | 5.816321 | 8.915345 |
| C | -3.353471 | 6.868921 | 3.335835 | C | 1.997614 | 8.016080 | 4.375134 |
| C | -2.968890 | 7.282628 | 4.609952 | H | 5.341883 | 6.728698 | 3.745588 |
| C | -2.211036 | 6.406348 | 5.391223 | H | 5.653281 | 6.248046 | 1.022302 |
| C | -1.818727 | 5.152653 | 4.922614 | H | 3.204201 | 6.195792 | -3.203415 |
| C | -3.443641 | 5.249670 | 1.432554 | H | 3.939154 | 2.154862 | -1.980515 |
| C | -3.356379 | 8.644655 | 5.121991 | H | 3.319930 | 3.872708 | 7.561618 |
| C | -1.021808 | 4.226081 | 5.798748 | H | 1.445150 | 7.687880 | 7.005676 |
| C | 0.929099 | 0.489642 | 4.291624 | H | 4.401307 | 2.766247 | 5.806977 |
| C | 3.093594 | -1.982832 | 0.465271 | H | 3.662701 | 3.002905 | 4.210535 |
| C | -0.661759 | 1.256067 | -0.459531 | H | 5.161833 | 3.832102 | 4.616791 |
| C | 2.817629 | 5.183558 | 2.300195 | H | 1.496183 | 7.703674 | 3.456099 |
| N | 3.462136 | 5.733594 | 3.379338 | H | 1.342753 | 8.715110 | 4.900020 |
| C | 4.697583 | 6.251468 | 3.024506 | H | 2.900620 | 8.562229 | 4.077580 |
| C | 4.847231 | 6.021449 | 1.701713 | H | 1.131454 | 6.482908 | 9.108153 |
| N | 3.699026 | 5.373954 | 1.272713 | H | 1.717995 | 4.821579 | 9.290828 |
| C | 3.028103 | 5.732836 | 4.749308 | H | 2.821845 | 6.178686 | 9.513423 |
| C | 3.408068 | 4.658330 | 5.569933 | H | 3.145725 | 2.392970 | 1.280602 |
| C | 3.037627 | 4.700929 | 6.914791 | H | 4.365526 | 1.615988 | 0.254311 |
| C | 2.328499 | 5.779534 | 7.451348 | H | 4.833553 | 2.899932 | 1.381930 |
| C | 1.989464 | 6.835791 | 6.604569 | H | 3.071425 | 7.941228 | -1.678586 |
| C | 2.334797 | 6.842011 | 5.249985 | H | 2.139794 | 7.456198 | -0.259441 |
| C | 3.582517 | 4.935479 | -0.093076 | H | 3.872706 | 7.772189 | -0.110511 |
| C | 3.370479 | 5.899398 | -1.092057 | H | 3.807445 | 2.639058 | -4.313157 |
| C | 3.374233 | 5.464353 | -2.417170 | H | 2.540572 | 3.835303 | -4.628943 |
| C | 3.567376 | 4.123068 | -2.759642 | H | 4.235869 | 4.284471 | -4.807626 |
| C | 3.774997 | 3.201615 | -1.733597 | H | -3.733851 | 2.527216 | 3.591523 |
| C | 3.798541 | 3.584101 | -0.389480 | H | -2.381780 | 0.302669 | 2.604250 |
| C | 3.106917 | 7.343241 | -0.764988 | H | -3.944050 | 7.535548 | 2.711745 |
| C | 3.539873 | 3.693576 | -4.202193 | H | -1.922663 | 6.701132 | 6.397950 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.614988 | -1.218905 | 3.036184 | C | -0.335279 | 7.590465 | 1.086706 |
| H | 1.263084 | -0.573752 | -0.980478 | C | -0.806551 | 8.899007 | 0.968307 |
| H | -2.914181 | 5.863345 | 0.693848 | C | -1.451185 | 9.346325 | -0.192097 |
| H | -3.254970 | 4.202929 | 1.190578 | C | -1.666464 | 8.491205 | -1.277836 |
| H | -4.515577 | 5.441688 | 1.316792 | C | -1.254771 | 7.139581 | -1.325396 |
| H | -1.433784 | 3.211189 | 5.797303 | H | 0.121056 | 7.276545 | 2.023921 |
| H | 0.015633 | 4.159156 | 5.454729 | H | -0.684599 | 9.602691 | 1.794827 |
| H | -1.012828 | 4.586745 | 6.830163 | H | -1.802271 | 10.374794 | -0.249922 |
| H | -3.152342 | 8.746141 | 6.191725 | H | -2.193241 | 8.917142 | -2.134225 |
| H | -2.798333 | 9.429490 | 4.598436 | Si | -1.689781 | 6.137263 | -2.850653 |
| H | -4.420512 | 8.845238 | 4.959472 | C | -2.658561 | 7.189058 | -4.110515 |
| H | 1.611741 | -0.150721 | 4.855790 | C | -0.149201 | 5.475886 | -3.754729 |
| H | 1.173314 | 1.533863 | 4.512790 | C | -2.788908 | 4.638934 | -2.424652 |
| H | -0.086038 | 0.311808 | 4.662970 | H | -2.909755 | 6.583687 | -4.988888 |
| H | -0.490972 | 2.336761 | -0.485553 | H | -3.595235 | 7.568222 | -3.688372 |
| H | -0.508634 | 0.863743 | -1.467668 | H | -2.074120 | 8.048343 | -4.456156 |
| H | -1.713322 | 1.103133 | -0.193846 | H | -3.004862 | 4.042350 | -3.318882 |
| H | 2.775785 | -2.449109 | -0.471689 | H | -2.299309 | 3.991697 | -1.690812 |
| H | 4.054069 | -1.488577 | 0.274613 | H | -3.742630 | 4.969793 | -1.999600 |
| H | 3.277520 | -2.776967 | 1.195088 | H | -0.434333 | 4.848776 | -4.607999 |
| H | 1.499999 | 3.681789 | 3.724572 | H | 0.457181 | 6.306954 | -4.130961 |
| B | -0.541034 | 6.696560 | -0.083621 | H | 0.473516 | 4.883887 | -3.077704 |

**Complex 2-CNtBu**



**135**

**E :-2574.9066588 a.u.**

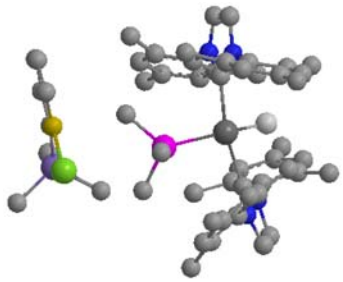
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 7.451171 | 7.491069 | 4.128576 | C | 5.955979 | 9.436912 | 4.220840 |
| C | 6.821523 | 8.587511 | 3.518837 | C | 5.730119 | 9.160855 | 5.572169 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 6.340751 | 8.085700 | 6.220929 | C | 4.953998 | 4.232929 | -2.921388 |
| C | 7.188904 | 7.258035 | 5.479507 | C | 4.080615 | 4.777022 | -1.977127 |
| N | 7.164906 | 8.907191 | 2.161200 | C | 1.755699 | 6.975244 | 2.731461 |
| C | 6.465231 | 8.586510 | 1.034932 | C | 2.380459 | 7.115068 | 3.977662 |
| N | 7.214718 | 9.102564 | 0.019631 | C | 1.882557 | 8.090996 | 4.844925 |
| C | 8.353429 | 9.725722 | 0.505980 | C | 0.794576 | 8.898727 | 4.508397 |
| C | 8.322041 | 9.607808 | 1.851862 | C | 0.178680 | 8.698243 | 3.269946 |
| C | 6.916850 | 9.072864 | -1.389162 | C | 0.635485 | 7.738137 | 2.365950 |
| C | 6.528305 | 10.268652 | -2.011749 | C | 5.395981 | 3.079660 | 1.201135 |
| C | 6.284615 | 10.240873 | -3.387986 | C | 6.850270 | 2.719119 | -3.617164 |
| C | 6.434660 | 9.070582 | -4.134598 | C | 3.008260 | 5.747041 | -2.389215 |
| C | 6.856243 | 7.909499 | -3.478998 | C | 3.528967 | 6.236491 | 4.386333 |
| C | 7.115255 | 7.884297 | -2.107561 | C | 0.298435 | 9.963588 | 5.449804 |
| C | 6.392761 | 11.563020 | -1.255010 | C | -0.076626 | 7.515542 | 1.059190 |
| C | 7.611020 | 6.630750 | -1.440883 | C | 4.078440 | 14.301316 | -3.279758 |
| C | 6.179164 | 9.078212 | -5.618416 | B | 2.727668 | 14.039251 | -3.877898 |
| Pt | 4.772385 | 7.443815 | 0.952012 | Cl | 1.200869 | 14.535373 | -2.889040 |
| C | 3.611364 | 8.880119 | 0.152452 | C | 5.197583 | 13.918983 | -4.018521 |
| N | 2.942020 | 9.709876 | -0.324149 | C | 5.085418 | 13.281011 | -5.266626 |
| C | 2.222043 | 10.777706 | -1.002652 | C | 3.830116 | 13.030320 | -5.834791 |
| C | 5.293684 | 10.608858 | 3.550999 | C | 2.605852 | 13.374209 | -5.225178 |
| C | 6.120125 | 7.840027 | 7.690338 | Si | 1.011018 | 13.091272 | -6.169985 |
| C | 8.381117 | 6.596816 | 3.355310 | C | 1.349015 | 12.258018 | -7.855845 |
| C | 3.315794 | 6.019874 | 1.022046 | C | -0.210045 | 11.947080 | -5.249690 |
| N | 3.293922 | 4.840137 | 0.339926 | C | 0.107037 | 14.727888 | -6.525495 |
| C | 2.206547 | 4.062695 | 0.711988 | H | 8.996947 | 9.955393 | 2.617671 |
| C | 1.529858 | 4.764054 | 1.648410 | H | 9.067371 | 10.191195 | -0.154254 |
| N | 2.213462 | 5.958642 | 1.824451 | H | 5.960198 | 11.156444 | -3.882526 |
| C | 4.243048 | 4.387155 | -0.640249 | H | 7.000457 | 6.995133 | -4.051003 |
| C | 5.239849 | 3.485753 | -0.239036 | H | 7.669150 | 6.412046 | 5.966611 |
| C | 6.088023 | 2.973564 | -1.223011 | H | 5.067268 | 9.815980 | 6.132985 |
| C | 5.956289 | 3.325981 | -2.568463 | H | 8.706242 | 5.752967 | 3.968684 |

| | | | |
|---|---|---|---|
| H | 7.889891 | 6.204828 | 2.458924 |
| H | 9.276660 | 7.133543 | 3.022819 |
| H | 4.754847 | 11.218518 | 4.279890 |
| H | 6.022545 | 11.250954 | 3.045466 |
| H | 4.578195 | 10.272878 | 2.793279 |
| H | 5.198428 | 8.310871 | 8.043280 |
| H | 6.064311 | 6.770438 | 7.914908 |
| H | 6.945136 | 8.252040 | 8.283974 |
| H | 6.842134 | 6.189926 | -0.797165 |
| H | 7.894010 | 5.886115 | -2.187975 |
| H | 8.485693 | 6.830363 | -0.811855 |
| H | 7.369710 | 12.038325 | -1.102223 |
| H | 5.777353 | 12.270806 | -1.817541 |
| H | 5.951364 | 11.415345 | -0.265078 |
| H | 5.701916 | 8.150161 | -5.948907 |
| H | 5.539625 | 9.917971 | -5.901792 |
| H | 7.118818 | 9.176012 | -6.175984 |
| H | 0.637177 | 4.533304 | 2.207458 |
| H | 2.023481 | 3.095798 | 0.270981 |
| H | -0.686571 | 9.299890 | 3.000411 |
| H | 2.356828 | 8.211756 | 5.816064 |
| H | 6.867905 | 2.274852 | -0.928103 |
| H | 4.839087 | 4.522735 | -3.963352 |
| H | -0.805775 | 8.307399 | 0.877000 |
| H | 0.621245 | 7.495199 | 0.217362 |
| H | -0.618279 | 6.562724 | 1.051873 |
| H | 3.313397 | 5.180390 | 4.191813 |
| H | 4.436692 | 6.492073 | 3.829671 |
| H | 3.740665 | 6.351611 | 5.451195 |
| H | 0.591155 | 9.754472 | 6.482487 |
| H | 0.710366 | 10.944238 | 5.182848 |
| H | -0.791522 | 10.052086 | 5.416569 |
| H | 6.271038 | 2.437809 | 1.328048 |
| H | 5.516152 | 3.957750 | 1.844060 |
| H | 4.522084 | 2.528429 | 1.566472 |
| H | 3.219538 | 6.748611 | -2.000803 |
| H | 2.945134 | 5.815476 | -3.477431 |
| H | 2.024920 | 5.449477 | -2.009923 |
| H | 7.817147 | 2.424579 | -3.199483 |
| H | 6.392671 | 1.819945 | -4.047448 |
| H | 7.032464 | 3.414812 | -4.441318 |
| H | 5.701792 | 6.305027 | 1.577739 |
| C | 2.595166 | 10.704384 | -2.485728 |
| C | 0.719274 | 10.554298 | -0.809184 |
| C | 2.644746 | 12.107992 | -0.371032 |
| H | 4.241582 | 14.811347 | -2.328865 |
| H | 6.202619 | 14.131124 | -3.642280 |
| H | 5.985855 | 13.025141 | -5.823949 |
| H | 3.826513 | 12.560381 | -6.821987 |
| H | 0.407092 | 12.099418 | -8.393486 |
| H | 1.993566 | 12.875545 | -8.490494 |
| H | 1.832424 | 11.281804 | -7.737416 |
| H | -0.839600 | 14.561234 | -7.053193 |
| H | -0.105409 | 15.252302 | -5.589253 |
| H | 0.732055 | 15.382187 | -7.142685 |
| H | -1.142153 | 11.832031 | -5.815696 |
| H | 0.220392 | 10.949703 | -5.104660 |
| H | -0.455569 | 12.362694 | -4.267814 |
| H | 2.128079 | 12.920756 | -0.889077 |
| H | 2.383664 | 12.132144 | 0.691987 |
| H | 3.717386 | 12.271965 | -0.482165 |
| H | 0.187117 | 11.364964 | -1.313390 |
| H | 0.400129 | 9.606047 | -1.250223 |
| H | 0.451900 | 10.566297 | 0.251473 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.117910 | 11.524844 | -3.026470 | H | 2.269254 | 9.752701 | -2.917124 |
| H | 3.671798 | 10.806619 | -2.626618 | | | | |

**Complex 2-$PMe_3$**



**133**

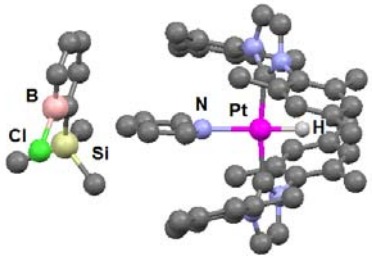
**E: -2450.5807641 a.u.**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 4.624000 | 4.089000 | -1.056000 | C | 2.132000 | 5.112000 | 4.309000 |
| C | 3.732000 | 5.164000 | -1.193000 | C | 2.672000 | 7.036000 | -2.534000 |
| C | 3.556000 | 5.826000 | -2.418000 | C | 5.892000 | 3.776000 | -4.645000 |
| C | 4.256000 | 5.344000 | -3.527000 | C | 4.926000 | 3.479000 | 0.287000 |
| C | 5.120000 | 4.250000 | -3.442000 | C | -1.170000 | 3.624000 | -1.548000 |
| C | 5.289000 | 3.637000 | -2.198000 | N | -1.251000 | 2.619000 | -2.483000 |
| N | 3.112000 | 5.702000 | -0.014000 | C | -2.489000 | 2.611000 | -3.113000 |
| C | 1.865000 | 5.435000 | 0.492000 | C | -3.212000 | 3.608000 | -2.564000 |
| N | 1.802000 | 6.219000 | 1.612000 | N | -2.400000 | 4.220000 | -1.622000 |
| C | 2.966000 | 6.950000 | 1.784000 | C | -0.250000 | 1.664000 | -2.871000 |
| C | 3.792000 | 6.625000 | 0.767000 | C | 0.884000 | 2.113000 | -3.573000 |
| Pt | 0.385000 | 4.325000 | -0.409000 | C | 1.815000 | 1.164000 | -3.992000 |
| P | 0.754000 | 2.274000 | 0.811000 | C | 1.637000 | -0.204000 | -3.765000 |
| C | 0.722000 | 6.349000 | 2.560000 | C | 0.473000 | -0.614000 | -3.118000 |
| C | -0.374000 | 7.159000 | 2.228000 | C | -0.493000 | 0.295000 | -2.670000 |
| C | -1.378000 | 7.312000 | 3.185000 | C | 1.071000 | 3.564000 | -3.910000 |
| C | -1.312000 | 6.696000 | 4.437000 | C | -1.751000 | -0.252000 | -2.042000 |
| C | -0.179000 | 5.942000 | 4.750000 | C | 2.674000 | -1.202000 | -4.207000 |
| C | 0.871000 | 5.789000 | 3.840000 | C | -2.893000 | 5.378000 | -0.921000 |
| C | -0.447000 | 7.894000 | 0.919000 | C | -3.408000 | 5.233000 | 0.373000 |
| C | -2.405000 | 6.871000 | 5.455000 | C | -4.044000 | 6.339000 | 0.944000 |

| | | | |
|---|---|---|---|
| C | -4.181000 | 7.550000 | 0.264000 |
| C | -3.631000 | 7.657000 | -1.017000 |
| C | -2.986000 | 6.584000 | -1.634000 |
| C | -3.278000 | 3.946000 | 1.134000 |
| C | -4.925000 | 8.705000 | 0.880000 |
| C | -2.406000 | 6.731000 | -3.015000 |
| H | 4.789000 | 6.953000 | 0.519000 |
| H | 3.087000 | 7.622000 | 2.618000 |
| H | -0.100000 | 5.467000 | 5.727000 |
| H | -2.232000 | 7.940000 | 2.943000 |
| H | 4.127000 | 5.848000 | -4.483000 |
| H | 5.975000 | 2.797000 | -2.105000 |
| H | 2.662000 | 7.411000 | -3.560000 |
| H | 1.645000 | 6.802000 | -2.236000 |
| H | 3.018000 | 7.845000 | -1.882000 |
| H | 5.376000 | 2.489000 | 0.174000 |
| H | 5.638000 | 4.099000 | 0.845000 |
| H | 4.034000 | 3.385000 | 0.908000 |
| H | 6.037000 | 2.692000 | -4.627000 |
| H | 5.385000 | 4.038000 | -5.578000 |
| H | 6.888000 | 4.235000 | -4.676000 |
| H | -0.627000 | 7.208000 | 0.085000 |
| H | -1.258000 | 8.625000 | 0.937000 |
| H | 0.487000 | 8.427000 | 0.706000 |
| H | 2.720000 | 5.805000 | 4.924000 |
| H | 1.883000 | 4.257000 | 4.944000 |
| H | 2.773000 | 4.781000 | 3.490000 |
| H | -3.338000 | 7.207000 | 4.993000 |
| H | -2.587000 | 5.932000 | 5.985000 |
| H | -2.121000 | 7.617000 | 6.208000 |
| H | -2.726000 | 1.897000 | -3.885000 |
| H | -4.222000 | 3.942000 | -2.742000 |
| H | 0.298000 | -1.676000 | -2.956000 |
| H | 2.695000 | 1.505000 | -4.532000 |
| H | -3.711000 | 8.598000 | -1.557000 |
| H | -4.452000 | 6.238000 | 1.947000 |
| H | -1.509000 | -1.028000 | -1.310000 |
| H | -2.349000 | 0.510000 | -1.543000 |
| H | -2.386000 | -0.718000 | -2.804000 |
| H | 0.182000 | 3.971000 | -4.405000 |
| H | 1.237000 | 4.157000 | -3.004000 |
| H | 1.927000 | 3.697000 | -4.573000 |
| H | 3.123000 | -0.914000 | -5.163000 |
| H | 3.486000 | -1.273000 | -3.475000 |
| H | 2.247000 | -2.202000 | -4.320000 |
| H | -2.454000 | 7.773000 | -3.342000 |
| H | -1.359000 | 6.412000 | -3.036000 |
| H | -2.942000 | 6.126000 | -3.755000 |
| H | -2.234000 | 3.781000 | 1.419000 |
| H | -3.873000 | 3.962000 | 2.049000 |
| H | -3.594000 | 3.085000 | 0.535000 |
| H | -4.470000 | 9.664000 | 0.613000 |
| H | -5.964000 | 8.731000 | 0.532000 |
| H | -4.950000 | 8.631000 | 1.971000 |
| H | 0.145000 | 5.657000 | -1.248000 |
| C | 1.950000 | 1.139000 | -0.041000 |
| C | 1.455000 | 2.349000 | 2.516000 |
| C | -0.716000 | 1.193000 | 1.114000 |
| H | 2.198000 | 0.300000 | 0.617000 |
| H | 1.513000 | 0.762000 | -0.965000 |
| H | 2.856000 | 1.693000 | -0.290000 |
| H | 1.544000 | 1.336000 | 2.918000 |
| H | 2.437000 | 2.824000 | 2.502000 |
| H | 0.786000 | 2.914000 | 3.167000 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -0.390000 | 0.175000 | 1.344000 | H | 1.209000 | 1.909000 | 5.880000 |
| H | -1.258000 | 1.571000 | 1.984000 | H | 1.784000 | 3.510000 | 7.651000 |
| H | -1.371000 | 1.184000 | 0.245000 | H | 0.067000 | 4.771000 | 8.870000 |
| Cl | -1.533000 | 1.056000 | 4.692000 | H | -2.298000 | 4.473000 | 8.437000 |
| B | -1.055000 | 2.272000 | 6.056000 | H | -5.984000 | 3.760000 | 7.791000 |
| C | 0.400000 | 2.460000 | 6.363000 | H | -4.641000 | 3.692000 | 8.940000 |
| C | 0.736000 | 3.359000 | 7.377000 | H | -4.700000 | 4.974000 | 7.723000 |
| C | -0.238000 | 4.083000 | 8.083000 | H | -5.557000 | 0.853000 | 6.953000 |
| C | -1.601000 | 3.900000 | 7.819000 | H | -3.957000 | 0.297000 | 6.410000 |
| C | -2.104000 | 3.022000 | 6.836000 | H | -4.211000 | 0.739000 | 8.105000 |
| Si | -3.956000 | 2.784000 | 6.685000 | H | -5.688000 | 3.052000 | 4.863000 |
| C | -4.904000 | 3.912000 | 7.900000 | H | -4.386000 | 4.247000 | 4.688000 |
| C | -4.605000 | 3.203000 | 4.937000 | H | -4.111000 | 2.562000 | 4.201000 |
| C | -4.476000 | 0.994000 | 7.074000 | | | | |

**Complex 2-Py**




**131**

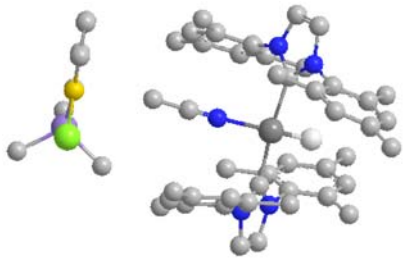
**E:-2572.5040936 a.u.**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 6.541686 | 10.464068 | -1.886135 | N | 7.438745 | 9.161666 | -0.021343 |
| C | 7.064090 | 9.253397 | -1.404632 | C | 6.641933 | 8.760129 | 1.014629 |
| C | 7.317791 | 8.164799 | -2.249801 | N | 7.454755 | 8.859567 | 2.106709 |
| C | 6.994713 | 8.299541 | -3.602994 | C | 8.718464 | 9.308314 | 1.758041 |
| C | 6.454902 | 9.478296 | -4.120036 | C | 8.711181 | 9.496538 | 0.418951 |
| C | 6.237334 | 10.547098 | -3.245660 | C | 7.094812 | 8.577432 | 3.471674 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 7.542443 | 7.383835 | 4.058328 | C | 1.816042 | 8.075609 | 4.235452 |
| C | 7.199109 | 7.142967 | 5.390838 | C | 3.070181 | 7.972139 | -2.499823 |
| C | 6.454064 | 8.062048 | 6.134869 | C | 3.813707 | 3.106522 | -3.606161 |
| C | 6.051297 | 9.249773 | 5.518257 | C | 1.815299 | 4.363357 | 0.845767 |
| C | 6.363012 | 9.536273 | 4.187412 | C | 8.095145 | 3.001674 | 5.846563 |
| C | 8.361758 | 6.373730 | 3.299884 | C | 7.604547 | 3.765256 | 6.919960 |
| C | 5.926892 | 10.830206 | 3.557165 | C | 6.269731 | 3.654917 | 7.330216 |
| C | 6.120099 | 7.778965 | 7.574614 | C | 5.323907 | 2.805719 | 6.718549 |
| Pt | 4.671132 | 8.252145 | 0.942367 | B | 5.853599 | 1.976295 | 5.574370 |
| N | 5.043314 | 6.210326 | 1.589270 | Cl | 4.745575 | 0.800894 | 4.614793 |
| C | 7.958480 | 6.903604 | -1.737723 | C | 7.285409 | 2.110482 | 5.144963 |
| C | 6.152206 | 9.613948 | -5.589075 | Si | 3.587663 | 2.714845 | 7.422000 |
| C | 6.334109 | 11.643381 | -0.976611 | C | 3.380393 | 3.924151 | 8.887630 |
| C | 2.657409 | 7.996022 | 0.807472 | C | 2.259035 | 3.200123 | 6.139526 |
| N | 1.690711 | 8.732541 | 1.432851 | C | 3.166618 | 0.976071 | 8.067934 |
| C | 0.419395 | 8.330946 | 1.051487 | H | 9.478048 | 9.832018 | -0.260970 |
| C | 0.580111 | 7.324741 | 0.163683 | H | 9.491805 | 9.449913 | 2.496038 |
| N | 1.946595 | 7.128031 | 0.026052 | H | 7.492053 | 6.197655 | 5.845477 |
| C | 1.892816 | 9.797829 | 2.376825 | H | 5.479861 | 9.980067 | 6.087336 |
| C | 1.939122 | 11.118404 | 1.905217 | H | 5.827966 | 11.477828 | -3.632860 |
| C | 2.063932 | 12.141198 | 2.846779 | H | 7.182190 | 7.460975 | -4.270237 |
| C | 2.125536 | 11.880362 | 4.218740 | H | 5.934695 | 12.495085 | -1.532562 |
| C | 2.062314 | 10.552290 | 4.644319 | H | 5.637410 | 11.399532 | -0.168275 |
| C | 1.936799 | 9.491411 | 3.743596 | H | 7.273202 | 11.957808 | -0.507809 |
| C | 2.474676 | 6.128812 | -0.861489 | H | 9.033416 | 7.044809 | -1.572649 |
| C | 2.996844 | 6.524587 | -2.101875 | H | 7.529249 | 6.586559 | -0.784307 |
| C | 3.446841 | 5.522725 | -2.965528 | H | 7.841671 | 6.089155 | -2.456812 |
| C | 3.366327 | 4.167288 | -2.635552 | H | 6.018786 | 8.637923 | -6.063794 |
| C | 2.828103 | 3.818533 | -1.394713 | H | 5.245459 | 10.202383 | -5.758923 |
| C | 2.374598 | 4.779334 | -0.487994 | H | 6.970745 | 10.122939 | -6.112360 |
| C | 1.842298 | 11.429654 | 0.436979 | H | 5.132976 | 10.660225 | 2.821941 |
| C | 2.217649 | 13.008024 | 5.212525 | H | 5.545235 | 11.516370 | 4.316550 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 6.754548 | 11.324581 | 3.036675 | H | 2.828630 | 13.831145 | 4.830143 |
| H | 9.410387 | 6.686875 | 3.223105 | H | 1.224197 | 13.417035 | 5.433443 |
| H | 8.339882 | 5.408430 | 3.810923 | H | 2.650148 | 12.674175 | 6.159708 |
| H | 7.991445 | 6.230340 | 2.280543 | H | 4.413727 | 9.718648 | 0.479942 |
| H | 5.246733 | 8.348107 | 7.906155 | H | 7.743237 | 1.529447 | 4.342397 |
| H | 5.922921 | 6.714393 | 7.727808 | H | 9.151742 | 3.105445 | 5.585456 |
| H | 6.957388 | 8.050514 | 8.229058 | H | 8.281944 | 4.415357 | 7.472688 |
| H | -0.135987 | 6.734469 | -0.385421 | H | 5.972838 | 4.254851 | 8.195307 |
| H | -0.467076 | 8.797663 | 1.450593 | H | 2.361679 | 3.862449 | 9.287556 |
| H | 2.764176 | 2.769298 | -1.115640 | H | 4.071526 | 3.692295 | 9.705084 |
| H | 3.856858 | 5.813912 | -3.930138 | H | 3.555825 | 4.962900 | 8.585872 |
| H | 2.105234 | 13.170620 | 2.496845 | H | 2.142843 | 0.928048 | 8.457503 |
| H | 2.101291 | 10.329999 | 5.708253 | H | 3.268079 | 0.239840 | 7.265359 |
| H | 1.999790 | 3.302807 | 1.028343 | H | 3.852361 | 0.691871 | 8.873249 |
| H | 2.270198 | 4.927652 | 1.664898 | H | 1.251401 | 3.123472 | 6.565254 |
| H | 0.733135 | 4.526081 | 0.903929 | H | 2.403645 | 4.232277 | 5.799464 |
| H | 2.110534 | 8.478002 | -2.347749 | H | 2.316246 | 2.542823 | 5.267081 |
| H | 3.816784 | 8.504143 | -1.899129 | C | 4.951998 | 5.866699 | 2.889235 |
| H | 3.344394 | 8.069152 | -3.552571 | C | 5.235403 | 4.588324 | 3.350427 |
| H | 4.598125 | 3.475764 | -4.273071 | C | 5.630448 | 3.616290 | 2.433463 |
| H | 4.195104 | 2.222651 | -3.086822 | C | 5.718843 | 3.966474 | 1.088346 |
| H | 2.978596 | 2.776940 | -4.236229 | C | 5.416138 | 5.267085 | 0.706205 |
| H | 1.911531 | 12.506501 | 0.265079 | H | 4.667327 | 6.662586 | 3.568101 |
| H | 2.643960 | 10.937449 | -0.123006 | H | 5.175692 | 4.344529 | 4.409042 |
| H | 0.893019 | 11.082559 | 0.013459 | H | 5.859747 | 2.615663 | 2.786412 |
| H | 2.485908 | 7.402380 | 3.695142 | H | 6.014904 | 3.243851 | 0.334782 |
| H | 2.052744 | 8.009999 | 5.299530 | H | 5.452294 | 5.576392 | -0.332997 |
| H | 0.798309 | 7.691740 | 4.097425 | | | | |

**Complex 2-MeCN**



**126**

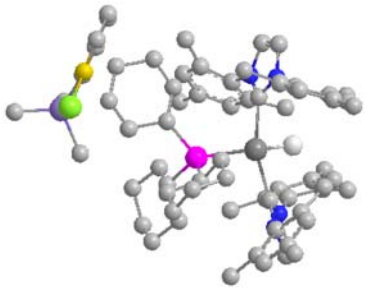
**E:-2457.0147322 a.u.**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 6.567000 | 10.565000 | -1.901000 | C | 7.099000 | 2.649000 | -3.394000 |
| C | 7.096000 | 9.356000 | -1.427000 | C | 1.524000 | 7.754000 | 1.808000 |
| C | 7.356000 | 8.269000 | -2.273000 | C | 1.884000 | 7.784000 | 3.162000 |
| C | 7.035000 | 8.411000 | -3.624000 | C | 1.367000 | 8.818000 | 3.947000 |
| C | 6.470000 | 9.584000 | -4.132000 | C | 0.513000 | 9.791000 | 3.424000 |
| C | 6.243000 | 10.649000 | -3.257000 | C | 0.171000 | 9.715000 | 2.071000 |
| N | 7.430000 | 9.238000 | -0.031000 | C | 0.661000 | 8.706000 | 1.239000 |
| C | 6.678000 | 8.612000 | 0.918000 | C | 2.789000 | 6.743000 | 3.761000 |
| N | 7.406000 | 8.744000 | 2.062000 | C | -0.019000 | 10.904000 | 4.288000 |
| C | 8.585000 | 9.440000 | 1.830000 | C | 0.266000 | 8.656000 | -0.213000 |
| C | 8.598000 | 9.748000 | 0.512000 | C | 7.034000 | 8.257000 | 3.361000 |
| Pt | 4.897000 | 7.658000 | 0.679000 | C | 6.282000 | 9.086000 | 4.204000 |
| C | 3.234000 | 6.509000 | 0.455000 | C | 5.980000 | 8.612000 | 5.483000 |
| N | 3.142000 | 5.345000 | -0.251000 | C | 6.409000 | 7.360000 | 5.928000 |
| C | 1.871000 | 4.799000 | -0.165000 | C | 7.158000 | 6.566000 | 5.054000 |
| C | 1.144000 | 5.631000 | 0.614000 | C | 7.489000 | 6.994000 | 3.767000 |
| N | 1.984000 | 6.670000 | 0.983000 | C | 5.806000 | 10.438000 | 3.750000 |
| C | 4.183000 | 4.721000 | -1.021000 | C | 6.106000 | 6.888000 | 7.325000 |
| C | 4.922000 | 3.685000 | -0.432000 | C | 8.302000 | 6.125000 | 2.848000 |
| C | 5.879000 | 3.040000 | -1.219000 | C | 7.957000 | 6.991000 | -1.755000 |
| C | 6.095000 | 3.393000 | -2.553000 | C | 6.136000 | 9.718000 | -5.593000 |
| C | 5.336000 | 4.431000 | -3.097000 | C | 6.371000 | 11.763000 | -1.011000 |
| C | 4.371000 | 5.114000 | -2.353000 | H | 9.288000 | 9.647000 | 2.621000 |
| C | 4.700000 | 3.282000 | 1.000000 | H | 9.320000 | 10.276000 | -0.091000 |
| C | 3.576000 | 6.236000 | -2.961000 | H | 5.783000 | 11.563000 | -3.632000 |

| | | | |
|---|---|---|---|
| H | 7.231000 | 7.579000 | -4.297000 |
| H | 7.501000 | 5.587000 | 5.383000 |
| H | 5.398000 | 9.244000 | 6.150000 |
| H | 8.585000 | 5.194000 | 3.344000 |
| H | 7.736000 | 5.877000 | 1.944000 |
| H | 9.221000 | 6.627000 | 2.524000 |
| H | 5.290000 | 10.960000 | 4.559000 |
| H | 6.638000 | 11.069000 | 3.417000 |
| H | 5.113000 | 10.344000 | 2.907000 |
| H | 5.224000 | 7.388000 | 7.735000 |
| H | 5.931000 | 5.809000 | 7.355000 |
| H | 6.945000 | 7.099000 | 8.000000 |
| H | 7.234000 | 6.436000 | -1.148000 |
| H | 8.266000 | 6.349000 | -2.583000 |
| H | 8.835000 | 7.181000 | -1.128000 |
| H | 7.311000 | 12.314000 | -0.881000 |
| H | 5.649000 | 12.453000 | -1.457000 |
| H | 6.024000 | 11.483000 | -0.013000 |
| H | 5.981000 | 8.743000 | -6.063000 |
| H | 5.234000 | 10.320000 | -5.732000 |
| H | 6.948000 | 10.219000 | -6.135000 |
| H | 0.117000 | 5.590000 | 0.942000 |
| H | 1.610000 | 3.884000 | -0.671000 |
| H | -0.500000 | 10.459000 | 1.645000 |
| H | 1.632000 | 8.853000 | 5.002000 |
| H | 6.464000 | 2.237000 | -0.777000 |
| H | 5.492000 | 4.719000 | -4.135000 |
| H | -0.104000 | 9.627000 | -0.552000 |
| H | 1.108000 | 8.380000 | -0.852000 |
| H | -0.529000 | 7.922000 | -0.389000 |
| H | 2.461000 | 5.730000 | 3.506000 |
| H | 3.814000 | 6.857000 | 3.390000 |
| H | 2.809000 | 6.831000 | 4.850000 |
| H | 0.107000 | 10.682000 | 5.351000 |
| H | 0.502000 | 11.846000 | 4.082000 |
| H | -1.083000 | 11.080000 | 4.100000 |
| H | 5.402000 | 2.499000 | 1.295000 |
| H | 4.834000 | 4.136000 | 1.673000 |
| H | 3.685000 | 2.901000 | 1.163000 |
| H | 3.854000 | 7.197000 | -2.515000 |
| H | 3.755000 | 6.301000 | -4.036000 |
| H | 2.500000 | 6.105000 | -2.806000 |
| H | 7.899000 | 2.222000 | -2.782000 |
| H | 6.621000 | 1.820000 | -3.932000 |
| H | 7.555000 | 3.301000 | -4.145000 |
| H | 5.663000 | 6.326000 | 0.920000 |
| N | 3.894000 | 9.468000 | 0.375000 |
| C | 3.383000 | 10.500000 | 0.257000 |
| C | 2.762000 | 11.794000 | 0.111000 |
| H | 2.935000 | 12.207000 | -0.899000 |
| H | 1.681000 | 11.708000 | 0.239000 |
| H | 3.168000 | 12.484000 | 0.856000 |
| C | 2.555000 | 13.820000 | -2.520000 |
| C | 3.731000 | 14.162000 | -3.194000 |
| C | 4.076000 | 13.580000 | -4.422000 |
| C | 3.233000 | 12.642000 | -5.035000 |
| C | 2.020000 | 12.188000 | -4.484000 |
| Si | 0.971000 | 10.979000 | -5.461000 |
| C | 0.770000 | 9.311000 | -4.553000 |
| B | 1.658000 | 12.796000 | -3.152000 |
| Cl | 0.095000 | 12.287000 | -2.227000 |
| C | -0.766000 | 11.666000 | -5.821000 |
| C | 1.771000 | 10.585000 | -7.150000 |
| H | 2.323000 | 14.358000 | -1.598000 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 4.397000 | 14.925000 | -2.782000 | H | -1.374000 | 10.943000 | -6.377000 |
| H | 4.985000 | 13.896000 | -4.932000 | H | -1.280000 | 11.911000 | -4.888000 |
| H | 3.549000 | 12.271000 | -6.014000 | H | -0.697000 | 12.582000 | -6.417000 |
| H | 1.130000 | 9.902000 | -7.720000 | H | 0.148000 | 8.615000 | -5.128000 |
| H | 1.906000 | 11.491000 | -7.751000 | H | 1.749000 | 8.845000 | -4.393000 |
| H | 2.750000 | 10.106000 | -7.042000 | H | 0.302000 | 9.468000 | -3.577000 |

**Complex 2-$PCy_3$**



**172**

**E:-3036.431158 a.u.**

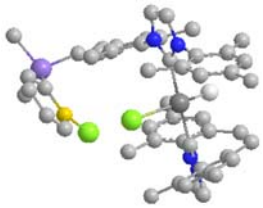
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 4.826479 | 4.065155 | -0.219219 | C | 0.163326 | 7.221340 | 5.266869 |
| C | 3.812015 | 4.957114 | -0.616690 | C | 0.467271 | 6.988244 | 3.920783 |
| C | 3.485516 | 5.132902 | -1.967518 | C | 4.196958 | 6.173731 | 4.245172 |
| C | 4.224547 | 4.427635 | -2.921866 | C | 0.778002 | 7.418339 | 7.709306 |
| C | 5.248781 | 3.548703 | -2.569498 | C | -0.664612 | 7.016579 | 2.924732 |
| C | 5.533812 | 3.385586 | -1.211849 | C | 2.352205 | 6.014450 | -2.396200 |
| N | 2.913531 | 5.435373 | 0.414287 | C | 6.032212 | 2.808926 | -3.620398 |
| C | 2.988884 | 6.510236 | 1.281233 | C | 5.130913 | 3.802432 | 1.229466 |
| N | 2.069819 | 6.169964 | 2.258963 | C | 6.194202 | 8.997719 | 0.757566 |
| C | 1.441135 | 4.962246 | 1.970718 | N | 7.104499 | 9.246914 | 1.757513 |
| C | 1.959305 | 4.512901 | 0.816836 | C | 8.322829 | 9.671917 | 1.247018 |
| Pt | 4.370193 | 8.053841 | 1.031926 | C | 8.194609 | 9.683264 | -0.095111 |
| P | 2.767007 | 10.041714 | 0.911728 | N | 6.903390 | 9.275411 | -0.387996 |
| C | 1.428705 | 9.911037 | -0.408105 | C | 6.985071 | 9.009118 | 3.171364 |
| C | 1.799080 | 6.692996 | 3.578724 | C | 6.618674 | 10.066966 | 4.019129 |
| C | 2.798559 | 6.606092 | 4.567908 | C | 6.617781 | 9.835206 | 5.395371 |
| C | 2.440002 | 6.857791 | 5.892258 | C | 7.008401 | 8.608804 | 5.940398 |
| C | 1.127865 | 7.156794 | 6.269575 | C | 7.418015 | 7.600973 | 5.067165 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 7.426533 | 7.778296 | 3.680307 | H | 8.148437 | 5.781877 | 3.342673 |
| C | 6.307858 | 11.432991 | 3.476414 | H | 7.235239 | 6.462151 | 1.979606 |
| C | 7.947133 | 6.694786 | 2.776794 | H | 8.880918 | 6.999716 | 2.290411 |
| C | 7.021962 | 8.402267 | 7.432129 | H | 5.986389 | 12.104608 | 4.275828 |
| C | 6.493882 | 9.150217 | -1.769281 | H | 7.189024 | 11.877665 | 3.000057 |
| C | 6.385912 | 7.860047 | -2.315657 | H | 5.522629 | 11.399591 | 2.719311 |
| C | 5.978724 | 7.744701 | -3.643519 | H | 6.047809 | 8.635047 | 7.875539 |
| C | 5.726358 | 8.865965 | -4.442259 | H | 7.273975 | 7.370867 | 7.692494 |
| C | 5.974619 | 10.127726 | -3.904182 | H | 7.757628 | 9.056064 | 7.914393 |
| C | 6.405051 | 10.292869 | -2.580718 | H | 6.201695 | 6.450281 | -0.681085 |
| C | 6.836390 | 6.652300 | -1.545696 | H | 6.827624 | 5.769405 | -2.185779 |
| C | 5.286363 | 8.720466 | -5.873691 | H | 7.860136 | 6.790194 | -1.176020 |
| C | 6.878378 | 11.659417 | -2.167405 | H | 7.870990 | 11.837078 | -2.600912 |
| C | 1.822856 | 10.144233 | 2.560268 | H | 6.227923 | 12.432393 | -2.587197 |
| C | 3.293876 | 11.883975 | 0.748337 | H | 6.961607 | 11.787218 | -1.088791 |
| Cl | 2.334887 | 13.487035 | -4.227705 | H | 4.536007 | 7.930451 | -5.983840 |
| B | 3.966103 | 13.316535 | -5.154293 | H | 4.869058 | 9.658170 | -6.248669 |
| C | 4.046422 | 12.650442 | -6.506437 | H | 6.134632 | 8.455100 | -6.516845 |
| Si | 2.591728 | 12.158767 | -7.579936 | H | 0.703188 | 4.540232 | 2.632615 |
| C | 1.491080 | 13.660858 | -7.980543 | H | 1.768769 | 3.617583 | 0.247074 |
| C | 5.205277 | 13.868504 | -4.514813 | H | -0.868363 | 7.443586 | 5.531651 |
| C | 6.417727 | 13.701456 | -5.186061 | H | 3.209358 | 6.781700 | 6.657192 |
| C | 6.499062 | 13.032826 | -6.416316 | H | 6.316719 | 2.692768 | -0.911050 |
| C | 5.346133 | 12.549700 | -7.047027 | H | 3.968660 | 4.555469 | -3.971107 |
| C | 3.177844 | 11.439037 | -9.250859 | H | -1.239262 | 7.942504 | 3.028427 |
| C | 1.460941 | 10.837081 | -6.794672 | H | -0.324606 | 6.944434 | 1.892579 |
| H | 9.151363 | 9.918638 | 1.891618 | H | -1.362169 | 6.190101 | 3.105078 |
| H | 8.889249 | 9.944999 | -0.876607 | H | 4.197089 | 5.201561 | 3.740451 |
| H | 5.857902 | 11.013953 | -4.526063 | H | 4.693526 | 6.883392 | 3.575354 |
| H | 5.888485 | 6.749060 | -4.073050 | H | 4.791564 | 6.085419 | 5.156344 |
| H | 7.757962 | 6.650219 | 5.472378 | H | 1.337065 | 6.760373 | 8.381571 |
| H | 6.328469 | 10.646922 | 6.059462 | H | 1.020508 | 8.450522 | 7.989613 |

| | | | |
|---|---|---|---|
| H | -0.288907 | 7.269702 | 7.896505 |
| H | 5.944456 | 3.079665 | 1.326822 |
| H | 5.425730 | 4.722260 | 1.743942 |
| H | 4.259723 | 3.400341 | 1.759445 |
| H | 2.595476 | 7.064715 | -2.221862 |
| H | 2.143906 | 5.892460 | -3.461366 |
| H | 1.434115 | 5.796917 | -1.841267 |
| H | 6.908346 | 3.388243 | -3.936574 |
| H | 6.396047 | 1.847546 | -3.246420 |
| H | 5.428241 | 2.621986 | -4.512805 |
| H | 5.330083 | 6.822172 | 1.168427 |
| H | 5.215005 | 14.428609 | -3.577686 |
| H | 7.341025 | 14.102249 | -4.758866 |
| H | 7.464301 | 12.918960 | -6.906812 |
| H | 5.485508 | 12.085462 | -8.026678 |
| H | 2.312530 | 11.171108 | -9.868230 |
| H | 3.775871 | 12.163507 | -9.813775 |
| H | 3.784554 | 10.535961 | -9.119974 |
| H | 0.634933 | 13.377280 | -8.604433 |
| H | 1.114918 | 14.108843 | -7.055705 |
| H | 2.066094 | 14.424954 | -8.514456 |
| H | 0.631385 | 10.581572 | -7.464870 |
| H | 2.016592 | 9.918115 | -6.576915 |
| H | 1.043517 | 11.217483 | -5.858267 |
| C | 0.668033 | 11.156024 | 2.609882 |
| C | -0.028755 | 11.159657 | 3.975645 |
| H | 1.057807 | 12.164755 | 2.431374 |
| H | -0.064700 | 10.956896 | 1.819904 |
| C | 0.965413 | 11.463815 | 5.095875 |
| H | -0.842762 | 11.894551 | 3.969981 |
| H | -0.490568 | 10.179175 | 4.158602 |
| C | 2.114872 | 10.456631 | 5.077938 |
| H | 1.359961 | 12.481393 | 4.961141 |
| H | 0.462326 | 11.452043 | 6.070462 |
| C | 2.808434 | 10.398087 | 3.713357 |
| H | 2.854626 | 10.702665 | 5.849979 |
| H | 1.724035 | 9.464168 | 5.322426 |
| H | 3.315580 | 11.358199 | 3.554684 |
| H | 3.588700 | 9.627967 | 3.714948 |
| H | 1.410552 | 9.137211 | 2.691990 |
| C | 2.277387 | 12.832704 | 0.079494 |
| H | 3.371475 | 12.186648 | 1.801704 |
| C | 2.704677 | 14.294257 | 0.269017 |
| H | 2.223654 | 12.628000 | -0.995978 |
| H | 1.268156 | 12.703554 | 0.478866 |
| C | 4.100548 | 14.545994 | -0.297096 |
| H | 1.973594 | 14.947761 | -0.220339 |
| H | 2.686234 | 14.543595 | 1.341166 |
| C | 5.113395 | 13.564260 | 0.291356 |
| H | 4.068778 | 14.427251 | -1.387239 |
| H | 4.412580 | 15.578733 | -0.100945 |
| C | 4.663199 | 12.108314 | 0.112216 |
| H | 6.095551 | 13.712304 | -0.171356 |
| H | 5.240750 | 13.768000 | 1.365859 |
| H | 4.603940 | 11.870576 | -0.954960 |
| H | 5.402310 | 11.427226 | 0.543550 |
| C | 0.470890 | 8.733872 | -0.219730 |
| H | 0.838590 | 10.828271 | -0.296243 |
| C | -0.654445 | 8.783727 | -1.262289 |
| H | 1.023043 | 7.789259 | -0.308459 |
| H | 0.037284 | 8.756990 | 0.785036 |
| C | -0.108042 | 8.824230 | -2.690838 |
| H | -1.326041 | 7.925703 | -1.129719 |
| H | -1.261110 | 9.682670 | -1.081983 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 0.912242 | 9.948695 | -2.875689 | H | 1.352567 | 9.909095 | -3.876013 |
| H | 0.361292 | 7.859927 | -2.924690 | H | 0.403995 | 10.919982 | -2.812946 |
| H | -0.931258 | 8.944397 | -3.404869 | H | 2.655428 | 9.023246 | -1.950315 |
| C | 2.025837 | 9.912709 | -1.822255 | H | 2.687391 | 10.770014 | -1.977913 |

**Complex 2-Cl**



**121**

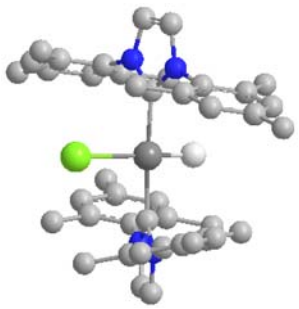
**E: -2339.455327 a.u.**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 5.993187 | 10.736310 | -1.400530 | Pt | 4.270669 | 8.313219 | 1.336713 |
| C | 6.692801 | 9.696844 | -0.771515 | C | 2.490610 | 7.390147 | 1.095791 |
| C | 7.296671 | 8.658839 | -1.495898 | N | 1.474140 | 7.312375 | 2.002738 |
| C | 7.180636 | 8.688217 | -2.887872 | C | 0.403890 | 6.585564 | 1.505444 |
| C | 6.495867 | 9.706318 | -3.554215 | C | 0.742092 | 6.198708 | 0.255355 |
| C | 5.903540 | 10.716396 | -2.793857 | N | 2.017797 | 6.693013 | 0.016757 |
| N | 6.876580 | 9.755417 | 0.650396 | C | 1.427693 | 7.905120 | 3.313791 |
| C | 6.012795 | 9.299478 | 1.607504 | C | 0.773394 | 9.136480 | 3.459880 |
| N | 6.617809 | 9.642802 | 2.781607 | C | 0.615301 | 9.639921 | 4.751134 |
| C | 7.825311 | 10.285951 | 2.558730 | C | 1.087842 | 8.954044 | 5.874224 |
| C | 7.991019 | 10.358546 | 1.218620 | C | 1.749086 | 7.738409 | 5.682325 |
| C | 6.101656 | 9.453455 | 4.113226 | C | 1.928876 | 7.188998 | 4.409335 |
| C | 6.533976 | 8.351109 | 4.867155 | C | 2.682359 | 6.467921 | -1.235434 |
| C | 6.082538 | 8.248228 | 6.183762 | C | 2.710954 | 7.498553 | -2.184772 |
| C | 5.244254 | 9.208239 | 6.760693 | C | 3.277403 | 7.224144 | -3.431641 |
| C | 4.851703 | 10.294359 | 5.975419 | C | 3.795588 | 5.967282 | -3.745375 |
| C | 5.265054 | 10.440571 | 4.650024 | C | 3.738918 | 4.965583 | -2.774640 |
| C | 7.451104 | 7.311649 | 4.284402 | C | 3.189126 | 5.187904 | -1.510696 |
| C | 4.822827 | 11.623794 | 3.832582 | C | 0.259188 | 9.894288 | 2.265331 |
| C | 4.787539 | 9.062681 | 8.184072 | C | 0.901061 | 9.517346 | 7.257673 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 2.627637 | 5.869790 | 4.230845 | H | 5.561661 | 10.299640 | -5.411776 |
| C | 2.151679 | 8.858821 | -1.876355 | H | 7.322404 | 10.205027 | -5.487684 |
| C | 4.421822 | 5.699418 | -5.089114 | H | 4.212935 | 11.300321 | 2.982256 |
| C | 3.169492 | 4.094166 | -0.480221 | H | 4.226811 | 12.309128 | 4.440989 |
| C | 8.027863 | 7.545610 | -0.801841 | H | 5.675093 | 12.183379 | 3.428963 |
| C | 6.428933 | 9.733162 | -5.059254 | H | 8.394454 | 7.750603 | 3.937031 |
| C | 5.352874 | 11.836004 | -0.600105 | H | 7.689264 | 6.552931 | 5.034118 |
| Cl | 5.444950 | 6.133397 | 1.426412 | H | 6.984481 | 6.815919 | 3.425288 |
| C | 5.394091 | 5.539385 | 9.371258 | H | 4.124572 | 8.198321 | 8.310302 |
| C | 5.118855 | 6.221094 | 10.562330 | H | 5.631774 | 8.885734 | 8.857004 |
| C | 3.826186 | 6.618443 | 10.962164 | H | 4.256382 | 9.955107 | 8.527150 |
| B | 2.716242 | 6.256160 | 10.006266 | H | 0.207796 | 5.627102 | -0.486686 |
| Cl | 0.923558 | 6.709215 | 10.360590 | H | -0.483574 | 6.414302 | 2.093617 |
| C | 4.361580 | 5.190292 | 8.486109 | H | 4.138227 | 3.978763 | -3.000930 |
| C | 3.028686 | 5.515752 | 8.739452 | H | 3.307402 | 8.016819 | -4.176115 |
| Si | 3.607133 | 7.480894 | 12.605773 | H | 0.100543 | 10.590321 | 4.882971 |
| C | 5.286512 | 7.726918 | 13.491727 | H | 2.125773 | 7.195632 | 6.547016 |
| C | 2.835679 | 9.218799 | 12.440244 | H | 3.595669 | 3.174245 | -0.889423 |
| C | 2.509231 | 6.483423 | 13.805667 | H | 3.764863 | 4.397656 | 0.388821 |
| H | 8.781758 | 10.774814 | 0.614907 | H | 2.155899 | 3.871867 | -0.129812 |
| H | 8.440935 | 10.626596 | 3.376005 | H | 1.116030 | 8.798647 | -1.523321 |
| H | 6.384971 | 7.391868 | 6.782363 | H | 2.737172 | 9.335756 | -1.082216 |
| H | 4.203628 | 11.054657 | 6.406376 | H | 2.175514 | 9.497600 | -2.763229 |
| H | 5.361944 | 11.516436 | -3.295061 | H | 4.072167 | 6.410644 | -5.843694 |
| H | 7.641683 | 7.888355 | -3.463972 | H | 5.514370 | 5.784125 | -5.037585 |
| H | 4.884728 | 12.573801 | -1.257327 | H | 4.193664 | 4.689143 | -5.444379 |
| H | 4.587485 | 11.426393 | 0.067845 | H | -0.201460 | 10.836054 | 2.575999 |
| H | 6.083807 | 12.355334 | 0.029558 | H | 1.074870 | 10.122769 | 1.570292 |
| H | 8.472479 | 6.863170 | -1.531253 | H | -0.490050 | 9.322633 | 1.704890 |
| H | 8.829256 | 7.926577 | -0.159016 | H | 3.517436 | 5.974970 | 3.600320 |
| H | 7.342848 | 6.975749 | -0.160766 | H | 2.935497 | 5.469338 | 5.198971 |
| H | 6.365387 | 8.723041 | -5.474999 | H | 1.975730 | 5.132099 | 3.747446 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -0.032558 | 10.084719 | 7.333555 | H | 5.782148 | 6.769881 | 13.688448 |
| H | 0.890920 | 8.730527 | 8.016572 | H | 5.971090 | 8.340787 | 12.895903 |
| H | 1.719921 | 10.200964 | 7.512153 | H | 2.373556 | 7.006554 | 14.760396 |
| H | 3.524278 | 9.684028 | 1.291731 | H | 1.525503 | 6.313316 | 13.358089 |
| H | 2.275675 | 5.187577 | 8.020454 | H | 2.958743 | 5.505668 | 14.011463 |
| H | 4.628498 | 4.637674 | 7.581085 | H | 2.696606 | 9.690057 | 13.421202 |
| H | 6.420642 | 5.255789 | 9.141780 | H | 3.478472 | 9.870066 | 11.837614 |
| H | 5.974145 | 6.444302 | 11.206386 | H | 1.862730 | 9.152610 | 11.944827 |
| H | 5.138367 | 8.230636 | 14.454445 | | | | |

**Complex 3-Cl**



**97**

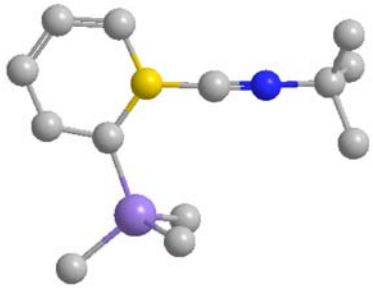
**E: -1982.960561 a.u.**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -0.524605 | 0.756065 | -0.043048 | C | -2.456564 | 4.746686 | 3.496006 |
| C | -0.230449 | 0.931565 | 1.315800 | C | -3.493010 | 5.396342 | 2.811594 |
| C | 0.795843 | 0.220275 | 1.956357 | C | -3.938817 | 6.621313 | 3.311757 |
| C | 1.538704 | -0.677566 | 1.187205 | C | -3.385442 | 7.192127 | 4.460093 |
| C | 1.284826 | -0.877318 | -0.171201 | C | -2.346675 | 6.516038 | 5.103474 |
| C | 0.250593 | -0.153216 | -0.765997 | C | -1.863501 | 5.288323 | 4.645201 |
| N | -1.081428 | 1.778762 | 2.106148 | C | -4.099921 | 4.800475 | 1.571193 |
| C | -1.039239 | 3.141205 | 2.200539 | C | -3.921226 | 8.487113 | 5.012367 |
| N | -2.058728 | 3.438047 | 3.058922 | C | -0.746942 | 4.577970 | 5.356783 |
| C | -2.714131 | 2.292582 | 3.487886 | C | 1.104289 | 0.421403 | 3.413045 |
| C | -2.100587 | 1.249344 | 2.885882 | C | 2.119258 | -1.839802 | -0.974987 |
| Pt | 0.202039 | 4.452536 | 1.294935 | C | -1.639508 | 1.514965 | -0.706748 |
| Cl | 2.051612 | 3.874188 | 2.832345 | C | 1.348407 | 5.803175 | 0.323740 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | 1.939085 | 5.657361 | -0.898583 | H | -0.458732 | 5.121472 | 6.260226 |
| C | 2.637630 | 6.798220 | -1.267211 | H | -1.038978 | 3.563378 | 5.650381 |
| C | 2.482991 | 7.686884 | -0.260485 | H | -3.132737 | 9.075998 | 5.490134 |
| N | 1.697497 | 7.068863 | 0.703005 | H | -4.376728 | 9.100017 | 4.228892 |
| C | 1.898221 | 4.491090 | -1.734993 | H | -4.692450 | 8.302536 | 5.770570 |
| C | 2.903846 | 3.523474 | -1.593662 | H | -1.410605 | 2.585860 | -0.729015 |
| C | 2.896708 | 2.449437 | -2.485823 | H | -1.784299 | 1.169884 | -1.733510 |
| C | 1.935942 | 2.327408 | -3.492418 | H | -2.586454 | 1.394755 | -0.168779 |
| C | 0.948706 | 3.309858 | -3.591265 | H | 1.896735 | -0.259127 | 3.735176 |
| C | 0.911049 | 4.405190 | -2.725592 | H | 1.438865 | 1.451633 | 3.583061 |
| C | 3.946882 | 3.634644 | -0.517681 | H | 0.228933 | 0.245989 | 4.047869 |
| C | -0.160390 | 5.453331 | -2.850253 | H | 1.586010 | -2.187357 | -1.864838 |
| C | 1.985992 | 1.182185 | -4.469602 | H | 3.049689 | -1.366713 | -1.312185 |
| C | 1.340406 | 7.745494 | 1.919918 | H | 2.400367 | -2.717315 | -0.384292 |
| C | 2.298108 | 7.842494 | 2.941579 | H | 2.848721 | 8.693283 | -0.132500 |
| C | 1.967741 | 8.595276 | 4.069697 | H | 3.172386 | 6.860360 | -2.201652 |
| C | 0.736382 | 9.242269 | 4.194863 | H | 2.699790 | 8.679536 | 4.870295 |
| C | -0.183587 | 9.123966 | 3.152164 | H | -1.144497 | 9.627782 | 3.226695 |
| C | 0.095472 | 8.383121 | 2.001372 | H | 0.188544 | 3.229081 | -4.365738 |
| C | 3.629675 | 7.153425 | 2.840407 | H | 3.669266 | 1.689469 | -2.390719 |
| C | 0.409387 | 10.035264 | 5.433043 | H | 3.485414 | 6.068199 | 2.782068 |
| C | -0.910334 | 8.280523 | 0.889161 | H | 4.187061 | 7.465213 | 1.950102 |
| H | -3.543078 | 2.335730 | 4.176334 | H | 4.243620 | 7.374763 | 3.717270 |
| H | -2.285432 | 0.187864 | 2.931234 | H | -0.475141 | 8.559835 | -0.076758 |
| H | 2.337173 | -1.237909 | 1.669304 | H | -1.272537 | 7.250844 | 0.798237 |
| H | 0.031117 | -0.301824 | -1.820827 | H | -1.765678 | 8.933511 | 1.079510 |
| H | -4.743722 | 7.137023 | 2.791836 | H | -0.405092 | 10.742909 | 5.252745 |
| H | -1.897930 | 6.950324 | 5.994109 | H | 0.099164 | 9.375978 | 6.252960 |
| H | -4.889448 | 5.445437 | 1.177029 | H | 1.276960 | 10.601192 | 5.787215 |
| H | -3.338304 | 4.670399 | 0.794706 | H | -0.834792 | 5.221510 | -3.678544 |
| H | -4.534806 | 3.813404 | 1.763607 | H | -0.749184 | 5.513279 | -1.928395 |
| H | 0.135649 | 4.484539 | 4.712306 | H | 0.262693 | 6.448472 | -3.027328 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 3.489180 | 3.606629 | 0.478492 | H | 1.008547 | 1.000729 | -4.926071 |
| H | 4.664859 | 2.813691 | -0.590137 | H | 2.692550 | 1.388580 | -5.283180 |
| H | 4.501954 | 4.576693 | -0.591917 | H | -0.965512 | 4.820714 | 0.325322 |
| H | 2.312479 | 0.256795 | -3.985671 | | | | |

**4-CNtBu**

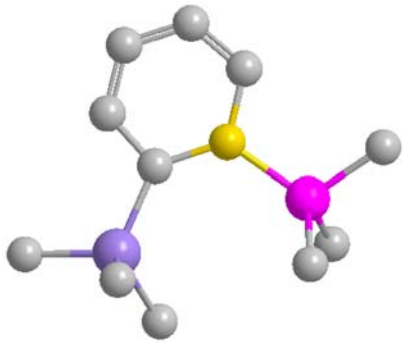


**38**

**E: -591.956657 a.u.**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -1.440025 | 0.243921 | 4.745198 | H | -2.246845 | 2.579929 | 2.596363 |
| Si | -1.868390 | 0.121087 | 2.898303 | H | -3.128877 | 1.676662 | 1.362556 |
| C | -2.849125 | 1.682542 | 2.421304 | H | -2.355133 | 0.330891 | 5.341163 |
| C | -2.998810 | -1.392761 | 2.661976 | H | -0.900912 | -0.643453 | 5.092669 |
| C | -0.317311 | -0.034619 | 1.842242 | H | -0.819587 | 1.120421 | 4.958648 |
| B | -0.279579 | -0.143419 | 0.332665 | N | -2.459616 | -0.131215 | -1.253980 |
| C | -1.535096 | -0.130120 | -0.536616 | C | -3.573591 | -0.053488 | -2.159937 |
| C | 0.940642 | -0.056361 | 2.462829 | C | -4.822773 | -0.545517 | -1.416251 |
| C | 2.147682 | -0.168618 | 1.759624 | C | -3.734145 | 1.410561 | -2.595668 |
| C | 2.192096 | -0.269606 | 0.364675 | C | -3.261388 | -0.954080 | -3.363344 |
| C | 1.028146 | -0.263232 | -0.399907 | H | -4.095739 | -0.915840 | -4.069393 |
| H | 1.129729 | -0.344617 | -1.481971 | H | -2.356442 | -0.618326 | -3.876760 |
| H | 1.012312 | 0.016702 | 3.549013 | H | -3.119677 | -1.990962 | -3.047404 |
| H | 3.080465 | -0.177212 | 2.320094 | H | -5.686223 | -0.488599 | -2.085015 |
| H | 3.167151 | -0.354142 | -0.115846 | H | -4.701188 | -1.582745 | -1.093095 |
| H | -3.915499 | -1.298717 | 3.254987 | H | -5.023055 | 0.072913 | -0.537390 |
| H | -3.288053 | -1.522171 | 1.613890 | H | -4.576009 | 1.493190 | -3.289176 |
| H | -2.484375 | -2.306704 | 2.976297 | H | -3.929617 | 2.053986 | -1.733722 |
| H | -3.768315 | 1.770760 | 3.011384 | H | -2.832066 | 1.767595 | -3.099706 |

**4-PMe$_3$**

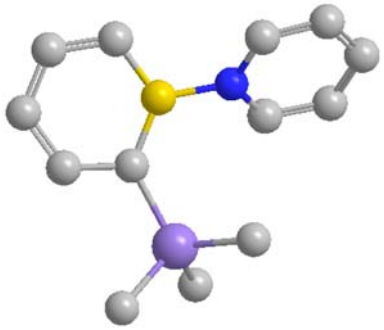


**36**

**E: -467.633663 a.u.**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -1.312515 | 0.209540 | 4.888458 | H | -3.924889 | 1.074868 | 3.440576 |
| Si | -1.780251 | -0.161456 | 3.081580 | H | -2.748598 | 2.111750 | 2.623776 |
| C | -3.155916 | 1.095575 | 2.660037 | H | -3.663368 | 0.900114 | 1.710430 |
| C | -2.540660 | -1.909680 | 3.072090 | H | -2.215036 | 0.199764 | 5.509840 |
| C | -0.276927 | -0.044226 | 1.949091 | H | -0.623833 | -0.535011 | 5.300000 |
| B | -0.160444 | 0.018526 | 0.442555 | H | -0.845369 | 1.194259 | 4.991651 |
| P | -1.628915 | 0.152027 | -0.835771 | C | -1.052875 | -0.184894 | -2.555918 |
| C | 0.965599 | -0.072946 | 2.615839 | C | -3.061007 | -1.002227 | -0.656688 |
| C | 2.209401 | -0.047137 | 1.975192 | C | -2.399043 | 1.827881 | -0.976387 |
| C | 2.315150 | 0.006157 | 0.585066 | H | -1.894988 | -0.131754 | -3.250429 |
| C | 1.179524 | 0.039040 | -0.226515 | H | -0.301363 | 0.553844 | -2.840003 |
| H | 1.355076 | 0.075878 | -1.301761 | H | -0.601300 | -1.178070 | -2.596409 |
| H | 0.990113 | -0.116321 | 3.705379 | H | -3.169703 | 1.841729 | -1.752237 |
| H | 3.112740 | -0.071082 | 2.581161 | H | -2.834824 | 2.109807 | -0.016713 |
| H | 3.310542 | 0.019757 | 0.139264 | H | -1.611938 | 2.543796 | -1.224425 |
| H | -3.424461 | -1.960439 | 3.718231 | H | -3.777650 | -0.847521 | -1.467777 |
| H | -2.834070 | -2.240284 | 2.071329 | H | -2.686536 | -2.027992 | -0.688002 |
| H | -1.807765 | -2.631282 | 3.448330 | H | -3.555896 | -0.840275 | 0.301515 |

**4-Py**

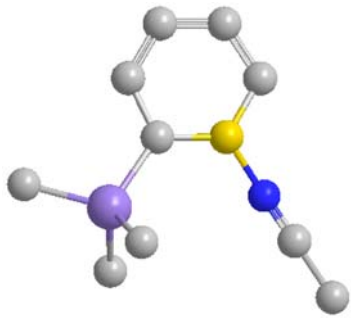


**34**

**E: -589.558907 a.u.**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -1.293755 | -0.614254 | 4.632520 | H | -2.439682 | -2.357756 | 2.105836 |
| Si | -1.869695 | -0.054587 | 2.907714 | H | -3.664232 | 1.323482 | 3.990529 |
| C | -2.928150 | 1.510056 | 3.200064 | H | -2.296182 | 2.344138 | 3.522732 |
| C | -3.009279 | -1.433613 | 2.249190 | H | -3.483501 | 1.838306 | 2.314880 |
| C | -0.383774 | 0.234069 | 1.778496 | H | -2.161879 | -0.881780 | 5.245292 |
| B | -0.268358 | 0.148243 | 0.277754 | H | -0.640898 | -1.490602 | 4.571021 |
| N | -1.504124 | 0.006032 | -0.641399 | H | -0.749143 | 0.173867 | 5.162488 |
| C | 0.855388 | 0.405589 | 2.431464 | C | -1.488709 | -0.883320 | -1.661660 |
| C | 2.086434 | 0.503208 | 1.774822 | C | -2.550246 | -1.006286 | -2.540543 |
| C | 2.186290 | 0.406302 | 0.382015 | C | -3.680353 | -0.208174 | -2.364528 |
| C | 1.058520 | 0.214539 | -0.411574 | C | -3.693035 | 0.702864 | -1.309619 |
| H | 1.200295 | 0.190387 | -1.494204 | C | -2.590504 | 0.793317 | -0.477190 |
| H | 0.888249 | 0.450533 | 3.521015 | H | -0.593240 | -1.489476 | -1.727633 |
| H | 2.988192 | 0.645229 | 2.366495 | H | -2.491166 | -1.733094 | -3.343356 |
| H | 3.173751 | 0.492326 | -0.073051 | H | -4.529618 | -0.293011 | -3.034953 |
| H | -3.806845 | -1.640910 | 2.971548 | H | -4.542210 | 1.354552 | -1.135334 |
| H | -3.487041 | -1.184810 | 1.296776 | H | -2.523951 | 1.506059 | 0.335235 |

**4-MeCN**

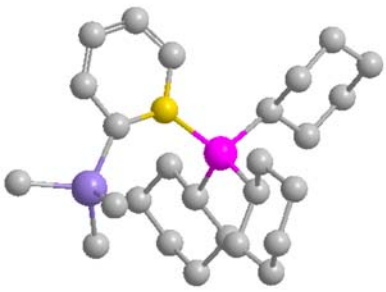


**29**

**E: -474.055910 a.u.**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -1.475959 | 0.000595 | 4.731483 | H | -3.835480 | -1.538220 | 3.063643 |
| Si | -1.849691 | -0.000137 | 2.869055 | H | -3.160664 | -1.612006 | 1.428881 |
| C | -2.901636 | 1.543019 | 2.489517 | H | -2.350294 | -2.453273 | 2.751206 |
| C | -2.901348 | -1.543774 | 2.490678 | H | -3.835811 | 1.537689 | 3.062415 |
| C | -0.264644 | -0.000351 | 1.856535 | H | -2.350773 | 2.452804 | 2.749451 |
| B | -0.164380 | -0.000873 | 0.353544 | H | -3.160881 | 1.610465 | 1.427653 |
| N | -1.390047 | -0.001325 | -0.488140 | H | -2.407977 | 0.000715 | 5.307271 |
| C | 0.977939 | -0.000002 | 2.513305 | H | -0.902836 | -0.884460 | 5.026376 |
| C | 2.208051 | -0.000117 | 1.844232 | H | -0.903012 | 0.885982 | 5.025720 |
| C | 2.294151 | -0.000601 | 0.446144 | C | -2.330635 | -0.001533 | -1.166400 |
| C | 1.154351 | -0.000995 | -0.353474 | C | -3.505966 | -0.002416 | -2.011246 |
| H | 1.283137 | -0.001364 | -1.435770 | H | -3.199768 | -0.000520 | -3.061470 |
| H | 1.013787 | 0.000383 | 3.603718 | H | -4.111915 | -0.894459 | -1.822124 |
| H | 3.124144 | 0.000181 | 2.431234 | H | -4.114845 | 0.887126 | -1.819800 |
| H | 3.285202 | -0.000663 | -0.008668 | | | | |

**4-$PCy_3$**



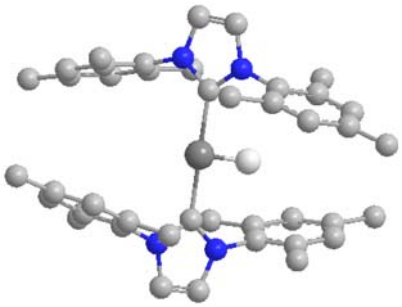
**75**

**E: -1053.522691 a.u.**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -0.983627 | 1.028759 | 4.986558 | H | -2.973396 | -0.540830 | -3.630031 |
| Si | -1.658555 | 0.223235 | 3.393670 | H | -2.496806 | 1.149294 | -3.509173 |
| C | -3.208611 | 1.273718 | 3.013058 | C | -0.746309 | -1.296118 | -5.243046 |
| C | -2.223793 | -1.522518 | 3.914100 | H | -2.129232 | 0.286270 | -5.792222 |
| C | -0.320278 | 0.169247 | 2.049909 | H | -0.639326 | 0.845885 | -5.045047 |
| B | -0.292135 | 0.040899 | 0.532476 | C | 0.202806 | -1.645993 | -4.097960 |
| P | -1.829942 | -0.050807 | -0.731281 | H | -1.521943 | -2.071601 | -5.321202 |
| C | 0.964215 | 0.243838 | 2.638481 | H | -0.212533 | -1.292085 | -6.200690 |
| C | 2.177152 | 0.220346 | 1.945305 | C | -0.518544 | -1.601535 | -2.747168 |
| C | 2.208209 | 0.133646 | 0.555962 | H | 0.637625 | -2.641277 | -4.247373 |
| C | 1.028633 | 0.046643 | -0.183588 | H | 1.043199 | -0.937687 | -4.085391 |
| H | 1.162823 | -0.002898 | -1.262481 | H | -1.311469 | -2.361603 | -2.757408 |
| H | 1.049943 | 0.335809 | 3.721113 | H | 0.173850 | -1.863146 | -1.941847 |
| H | 3.106653 | 0.285097 | 2.506948 | C | -4.113055 | 1.754508 | -1.398221 |
| H | 3.174930 | 0.138155 | 0.050539 | H | -3.034682 | 1.586076 | 0.443803 |
| H | -2.945223 | -1.470571 | 4.737492 | C | -4.788291 | 3.064145 | -0.969226 |
| H | -2.684414 | -2.087451 | 3.098922 | H | -3.923178 | 1.804453 | -2.474521 |
| H | -1.358186 | -2.097354 | 4.260255 | H | -4.796169 | 0.913841 | -1.248246 |
| H | -3.817860 | 1.332892 | 3.922518 | C | -3.868515 | 4.264260 | -1.204888 |
| H | -2.921990 | 2.296940 | 2.746810 | H | -5.729737 | 3.190533 | -1.517334 |
| H | -3.852744 | 0.879673 | 2.223741 | H | -5.051373 | 3.006597 | 0.096307 |
| H | -1.812127 | 1.179880 | 5.687958 | C | -2.520467 | 4.078801 | -0.505500 |
| H | -0.237175 | 0.410737 | 5.494818 | H | -3.703305 | 4.382324 | -2.285652 |
| H | -0.532097 | 2.005685 | 4.785733 | H | -4.350958 | 5.187165 | -0.861998 |
| C | -1.146231 | -0.218727 | -2.491776 | C | -1.849608 | 2.754963 | -0.891011 |
| C | -3.013950 | -1.516246 | -0.534466 | H | -1.849393 | 4.913449 | -0.740173 |
| C | -2.795574 | 1.568974 | -0.627141 | H | -2.669441 | 4.096964 | 0.582915 |
| C | -2.107968 | 0.137074 | -3.635331 | H | -1.582178 | 2.781864 | -1.957097 |
| H | -0.338699 | 0.525211 | -2.494062 | H | -0.916445 | 2.624019 | -0.332279 |
| C | -1.406347 | 0.059702 | -4.999304 | C | -4.209532 | -1.300266 | 0.406836 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -3.403459 | -1.688571 | -1.549217 | H | -4.098586 | -3.732462 | 1.842096 |
| C | -5.137629 | -2.521679 | 0.392676 | H | -5.065722 | -4.666466 | 0.708933 |
| H | -3.840268 | -1.145543 | 1.426249 | C | -2.245305 | -2.770011 | -0.073073 |
| H | -4.782588 | -0.407986 | 0.142581 | H | -2.585109 | -4.876353 | 0.271475 |
| C | -4.397944 | -3.800272 | 0.787250 | H | -3.457752 | -4.226285 | -1.109996 |
| H | -5.983608 | -2.345750 | 1.067722 | H | -1.858879 | -2.587854 | 0.937052 |
| H | -5.562458 | -2.639238 | -0.614826 | H | -1.368733 | -2.955882 | -0.696618 |
| C | -3.152472 | -4.005238 | -0.076685 | | | | |

**Complex $Imes_2PtH^+$**



**96**

**E: -1967.709321 a.u.**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 0.953946 | 0.301272 | 1.815844 | C | -3.462532 | 6.799715 | 2.385349 |
| C | 0.291338 | 0.918277 | 2.887020 | C | -3.741146 | 7.110211 | 1.050608 |
| C | 0.711166 | 0.769987 | 4.216635 | C | -3.485386 | 6.142257 | 0.075764 |
| C | 1.836577 | -0.022420 | 4.454953 | C | -2.973827 | 4.883301 | 0.398808 |
| C | 2.527516 | -0.658027 | 3.420300 | C | -2.678350 | 5.241031 | 4.210111 |
| C | 2.072955 | -0.479185 | 2.110236 | C | -4.338355 | 8.440919 | 0.680241 |
| N | -0.885541 | 1.700789 | 2.615819 | C | -2.722058 | 3.854395 | -0.670851 |
| C | -0.900110 | 3.017484 | 2.273526 | C | -0.014786 | 1.441593 | 5.350896 |
| N | -2.218601 | 3.314406 | 2.116013 | C | 3.710572 | -1.542277 | 3.709195 |
| C | -3.013484 | 2.205851 | 2.354788 | C | 0.485778 | 0.477527 | 0.397190 |
| C | -2.172728 | 1.189730 | 2.669585 | C | 2.177000 | 5.612512 | 1.829364 |
| Pt | 0.630957 | 4.318932 | 2.039855 | N | 2.553830 | 6.232117 | 0.677180 |
| C | -2.712771 | 4.615093 | 1.751356 | C | 3.652735 | 7.048877 | 0.884960 |
| C | -2.953464 | 5.556805 | 2.765148 | C | 3.972889 | 6.939000 | 2.197809 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | 3.063464 | 6.058498 | 2.760850 | H | 4.192890 | -1.273864 | 4.652836 |
| C | 1.910870 | 6.047811 | -0.596712 | H | 3.400617 | -2.591176 | 3.787338 |
| C | 2.303625 | 4.965497 | -1.400545 | H | -1.614564 | 5.036996 | 4.374239 |
| C | 1.691926 | 4.830949 | -2.647805 | H | -2.968518 | 6.076967 | 4.850327 |
| C | 0.730366 | 5.737955 | -3.103834 | H | -3.232202 | 4.356371 | 4.542389 |
| C | 0.371754 | 6.800399 | -2.270196 | H | -2.974084 | 4.252928 | -1.655652 |
| C | 0.948822 | 6.981058 | -1.010925 | H | -1.672253 | 3.543700 | -0.692224 |
| C | 3.345336 | 3.983425 | -0.939279 | H | -3.321358 | 2.951246 | -0.512996 |
| C | 0.550264 | 8.142147 | -0.139536 | H | -5.430083 | 8.415388 | 0.779202 |
| C | 0.127115 | 5.593348 | -4.475020 | H | -3.973200 | 9.240659 | 1.330743 |
| C | 3.084348 | 5.680956 | 4.149407 | H | -4.111971 | 8.710461 | -0.354829 |
| C | 2.283512 | 6.389771 | 5.056392 | H | 4.099034 | 7.621537 | 0.087166 |
| C | 2.351488 | 6.025097 | 6.402054 | H | 4.753256 | 7.401407 | 2.781515 |
| C | 3.189209 | 4.999503 | 6.850388 | H | -0.372019 | 7.517182 | -2.610270 |
| C | 3.969213 | 4.321530 | 5.910210 | H | 1.985206 | 4.000489 | -3.285888 |
| C | 3.938583 | 4.644266 | 4.551673 | H | 4.626946 | 3.521314 | 6.241463 |
| C | 1.376882 | 7.500537 | 4.601393 | H | 1.738810 | 6.564859 | 7.120625 |
| C | 3.274723 | 4.660396 | 8.314152 | H | 0.127682 | 7.805262 | 0.812990 |
| C | 4.792337 | 3.897806 | 3.562047 | H | 1.404908 | 8.784581 | 0.097734 |
| H | -2.365445 | 0.158860 | 2.921876 | H | -0.200078 | 8.758316 | -0.639082 |
| H | -4.088880 | 2.245269 | 2.280051 | H | 4.279307 | 4.484442 | -0.663171 |
| H | -3.697800 | 6.366916 | -0.966805 | H | 3.001212 | 3.431532 | -0.057644 |
| H | -3.658672 | 7.541124 | 3.156511 | H | 3.572188 | 3.261419 | -1.726808 |
| H | 2.176876 | -0.150163 | 5.479908 | H | 0.764328 | 6.068735 | -5.230203 |
| H | 2.598830 | -0.967337 | 1.292822 | H | 0.019530 | 4.542386 | -4.757838 |
| H | 0.465354 | 1.213600 | 6.304819 | H | -0.856510 | 6.066788 | -4.534775 |
| H | -0.024466 | 2.529984 | 5.228927 | H | 5.377263 | 3.124114 | 4.063910 |
| H | -1.058251 | 1.114761 | 5.416502 | H | 4.182070 | 3.413404 | 2.792229 |
| H | 0.573521 | 1.523327 | 0.081956 | H | 5.493359 | 4.562798 | 3.046063 |
| H | 1.080336 | -0.134030 | -0.285071 | H | 0.590643 | 7.119754 | 3.939943 |
| H | -0.564267 | 0.190176 | 0.276917 | H | 0.897744 | 7.983305 | 5.456010 |
| H | 4.458881 | -1.484471 | 2.913613 | H | 1.923847 | 8.269169 | 4.044900 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 2.311953 | 4.795299 | 8.815195 | H | 3.998190 | 5.309919 | 8.821197 |
| H | 3.599256 | 3.628022 | 8.469686 | H | 1.442663 | 3.513480 | 3.022344 |

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