

## Supporting Information

# Unprecedented 1,3-migration of aryl ligand in metallacyclic aryl $\alpha$ -naphthyl $\text{Pt}^{\text{IV}}$ difluorides to produce $\beta$ -arylnaphthyl $\text{Pt}^{\text{II}}$ complexes

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## General procedures:

All operations with air- and moisture- sensitive compounds were performed in a nitrogen-filled Innovative Technology glove box. All solvents were degassed and stored under high-purity nitrogen over activated 4Å molecular sieves. All deuterated solvents were stored under high-purity nitrogen on 3Å molecular sieves. Commercially available reagents (Aldrich and Strem) were used as received. The NMR spectra were recorded on Bruker AC 200MHz and Bruker AMX 400MHz spectrometers.  $^1\text{H}$  and  $^{13}\text{C}$  NMR signals are reported in ppm downfield from TMS.  $^1\text{H}$  signals are referenced to the residual proton of a deuterated solvent 7.26 ppm for  $\text{CDCl}_3$ , 1.94 ppm for  $\text{CD}_3\text{CN}$ .  $^{13}\text{C}$  NMR signals are referenced to the solvent signal:  $\text{CDCl}_3$  at 77.36 ppm,  $\text{CD}_3\text{CN}$  at 1.32 ppm.  $^{31}\text{P}$  chemical shifts are reported in ppm downfield from  $\text{H}_3\text{PO}_3$  and referenced to an external 85% phosphoric acid sample.  $^{19}\text{F}$  chemical shifts are reported in ppm downfield from  $\text{CClF}_3$ . All measurements were performed at 22 °C in  $\text{CDCl}_3$  unless stated otherwise. Elemental analysis was performed in the laboratory for microanalysis at the Hebrew University of Jerusalem. Mass Spectra were recorded on a VG-Autospec M-250 instrument.

**Computational details.** Theoretical calculations in this work have been performed using density functional theory (DFT) method,<sup>1</sup> specifically functional PBE,<sup>2</sup> and LACVP relativistic basis set with two polarization functions implemented in the Jaguar program<sup>3</sup> package. Full geometry optimization has been performed without constraints on symmetry. For all species under investigation frequency analysis has been carried out. All energy minima have been checked for the absence of imaginary frequencies. All transition states possessed just one imaginary frequency. Using the method of Intrinsic Reaction Coordinate, reactants, products and the corresponding transition states were proven to be connected by a single minimal energy reaction path.

The solvation of all complexes in Scheme 6 in MeCN solvent was modeled using a Poisson-Boltzmann continuum solvation model (PBF).<sup>3</sup> For MeCN and pyridine experimentally determined solvation Gibbs energies in MeCN solvent were used instead of calculated values, -1.3 kcal/mol for MeCN (determined as  $RT\ln(P_{298}, \text{ mm Hg}/760, \text{ mm Hg})$  where  $P_{298} = 90 \text{ mm Hg}^4$ ) and -1.7 kcal/mol for pyridine.<sup>5</sup>

## Synthesis of 1.<sup>6</sup>

In a Shlenck flask, 200 mg (1.1 mmol) of chloro-di-tert-butylphosphine, 2.2 mg (0.022 mmol, 2 mol%) of copper(I) chloride and 1.4 ml of tetrahydrofuran were placed. A solution of 2-methyl-1-naphthylmagnesium

bromide, 0.25M in tetrahydrofuran, 6.6 ml (1.5 equiv.) was added at room temperature and the mixture was stirred for 20 min. The resulting yellow mixture was heated at 80°C for 6 h. The formation of the product and the disappearance of the chloro-di-tert-butylphosphine were monitored by the  $^{31}\text{P}$  NMR spectroscopy. After the completion, 6 ml of toluene and 6 ml of saturated ammonium chloride aqueous solution were added to the reaction mixture under  $\text{N}_2$  atmosphere. The organic layer was separated, washed again with aq.  $\text{NH}_4\text{Cl}$  and dried over anhydrous  $\text{MgSO}_4$ . The solvent was evaporated to give a yellow oily material in a 80% yield.

$^1\text{H}$  NMR: 8.35 (1H, d,  $J_{\text{HH}}= 8.45$  Hz, Ar), 7.79 (1H, br-d,  $J_{\text{HH}}= 8.17$  Hz, Ar), 7.74 (1H, d,  $J_{\text{HH}}= 8.35$  Hz, Ar), 7.47 (1H, br-t,  $J_{\text{HH}}= 7.60$  Hz, Ar), 7.40 (1H, m, Ar), 7.38 (1H, m, Ar), 2.44 (3H, d,  $J_{\text{PH}}= 2.50$  Hz, Me-Ar), 1.32 (18H, d,  $J_{\text{PH}}= 12.73$  Hz,  $^t\text{Bu}$ );  $^{13}\text{C}\{^1\text{H}\}$  147.65 (d,  $J_{\text{PC}}= 37.61$  Hz, Ar), 136.34 (m, Ar), 131.47 (s, Ar), 130.08 (d,  $J_{\text{PC}}= 7.32$  Hz, Ar), 129.90 (s, Ar), 129.71 (s, Ar), 129.21 (d,  $J_{\text{PC}}= 13.16$  Hz, Ar), 128.61 (s, Ar), 124.63 (s, Ar), 124.45 (s, Ar), 34.00 (d,  $J_{\text{PC}}= 29.52$  Hz,  $^t\text{Bu}$ ), 32.16 (d,  $J_{\text{PC}}= 16.86$  Hz,  $^t\text{Bu}$ ), 26.70 (s, Me-Ar);  $^{31}\text{P}\{^1\text{H}\}$  22.5 (s); HRMS ASAP: found for  $\text{C}_{19}\text{H}_{27}\text{P} [\text{M}+\text{H}]^+$  (calc.) 287.1927 (287.1929).

## Synthesis of complex 2

A solution of 343 mg (0.92 mmol) of  $\text{CODPtCl}_2$  in 10 ml of toluene was heated with 1.2 equiv. (1.1 mmol) of **1** in the presence of 1.5 equiv. (0.2 ml) of  $\text{Et}_3\text{N}$  at 100°C for 8 h. The  $^{31}\text{P}$  NMR spectrum of the reaction mixture indicated the disappearance of the free ligand and formation of a new complex. The solution was concentrated by evaporation and pentane was added to precipitate the product. The resulting solid was dissolved in 1 ml of dichloromethane and 2 equiv. of pyridine was added followed by precipitation with 5 ml of pentane. Complex 2 was obtained as an off-white solid in 55% yield.

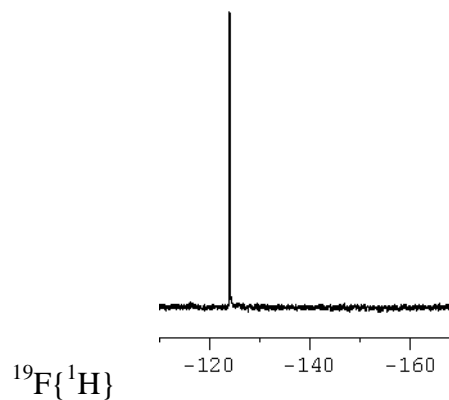
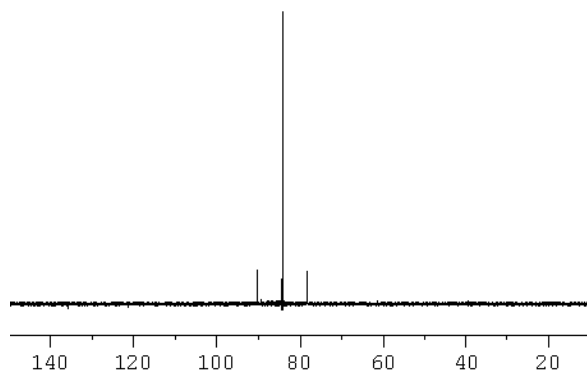
$^1\text{H}$  NMR: 8.94 (2H, m, Py), 7.84 (1H, m, Py), 7.68 (1H, br-d,  $J_{\text{HH}}= 8.20$  Hz, Ar), 7.44 (2H, m, Py), 7.44 (1H, m, Ar), 7.25 (1H, br-d,  $J_{\text{HH}}= 7.92$  Hz, Ar), 6.89 (1H, t,  $J_{\text{HH}}= 7.54$  Hz, Ar), 6.44 (1H, d,  $J_{\text{HH}}= 7.44$  Hz, ,  $J_{\text{PH}}= 57.60$  Hz, Ar), 2.78 (3H, s, Me-Ar), 1.63 (18H, d,  $J_{\text{PH}}= 14.97$  Hz,  $^t\text{Bu}$ );  $^{13}\text{C}\{^1\text{H}\}$  152.22 (d,  $J_{\text{PC}}= 26.60$  Hz, Ar), 151.63 (s, Py), 138.70 (s, Ar), 137.94 (s, Py), 137.41 (m, Ar), 132.76 (s, Ar), 132.34 (s, Ar), 132.06 (d,  $J_{\text{PC}}= 13.18$  Hz, Ar), 131.30 (m, Ar), 130.14 (d,  $J_{\text{PC}}= 8.82$  Hz, Ar), 125.80 (s, Py), 125.70 (s, Ar), 122.77 (s, Ar), 38.43 (d,  $J_{\text{PC}}= 23.00$  Hz,  $^t\text{Bu}$ ), 31.88 (m,  $J_{\text{PC}}= 4.52$  Hz,  $^t\text{Bu}$ ), 27.35 (br-s, Me-Ar);  $^{31}\text{P}\{^1\text{H}\}$  84.2 (s,  $J_{\text{PtP}}= 4183$  Hz); HRMS APPI: found for  $\text{C}_{24}\text{H}_{31}\text{ClNPPt} [\text{M}-\text{Cl}]^+$  (calc.) 558.1819 (558.1821).

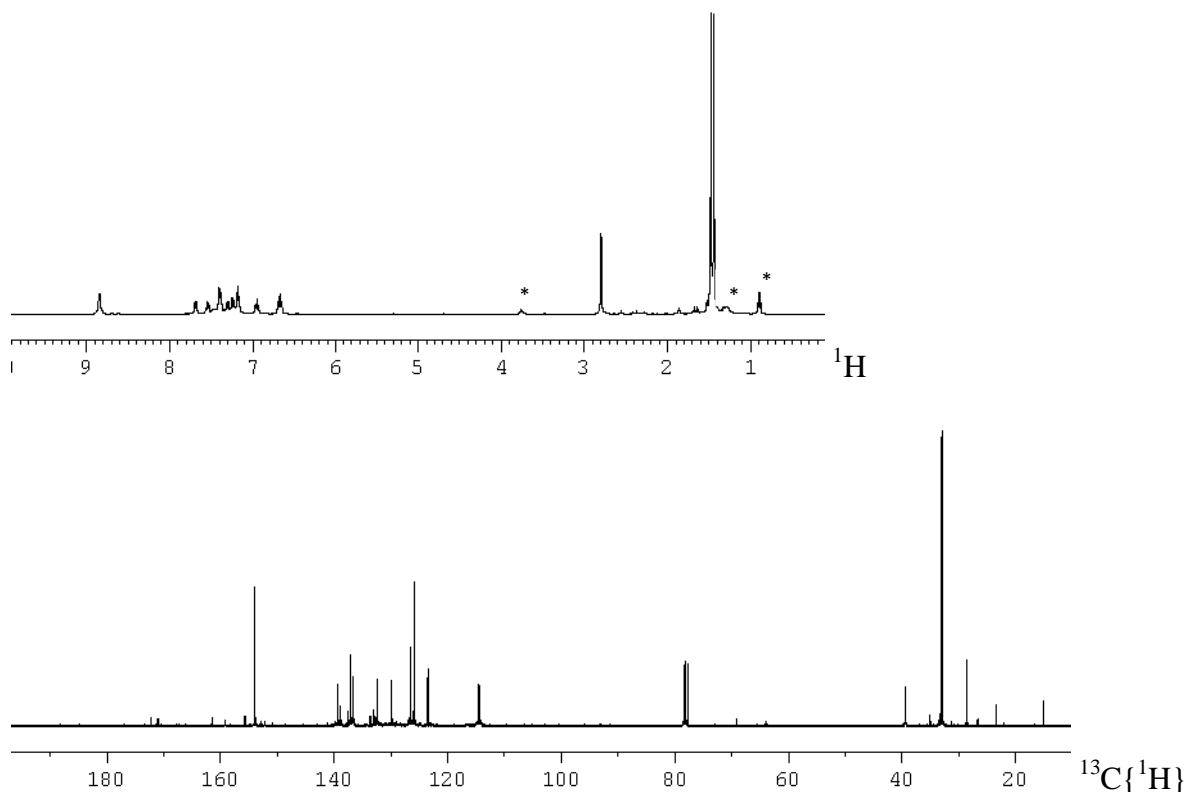
## General synthetic procedure for complexes 3

A solution of **2** (100 mg, 0.17 mmol) in 5 ml of tetrahydrofuran was treated with 3 equiv. (0.51 mmol) of an arylmagnesium halide (Grignard reagents) in the presence of 3 equiv. (0.04 ml) of pyridine at  $-30^{\circ}\text{C}$ , followed by stirring at room temperature for 5 min – 5 h. The  $^{31}\text{P}$  NMR spectrum indicated the disappearance of the starting material and formation of a new complex with a splitting of about 2000 Hz. The reaction was quenched with 5 ml of saturated  $\text{NH}_4\text{Cl}$  and 5 ml of toluene was added. The organic layer was separated, washed with aqueous  $\text{NH}_4\text{Cl}$  and dried over anhydrous  $\text{MgSO}_4$ . The solution was filtered through celite and concentrated in vacuum. The addition of pentane resulted in the precipitation of the desired **3**.

**3a**: After stirring for 3 h at room temperature with 4-fluorophenyl magnesium bromide (0.51 ml, 1M in THF) the complex was isolated as an off-white solid in 60% yield.

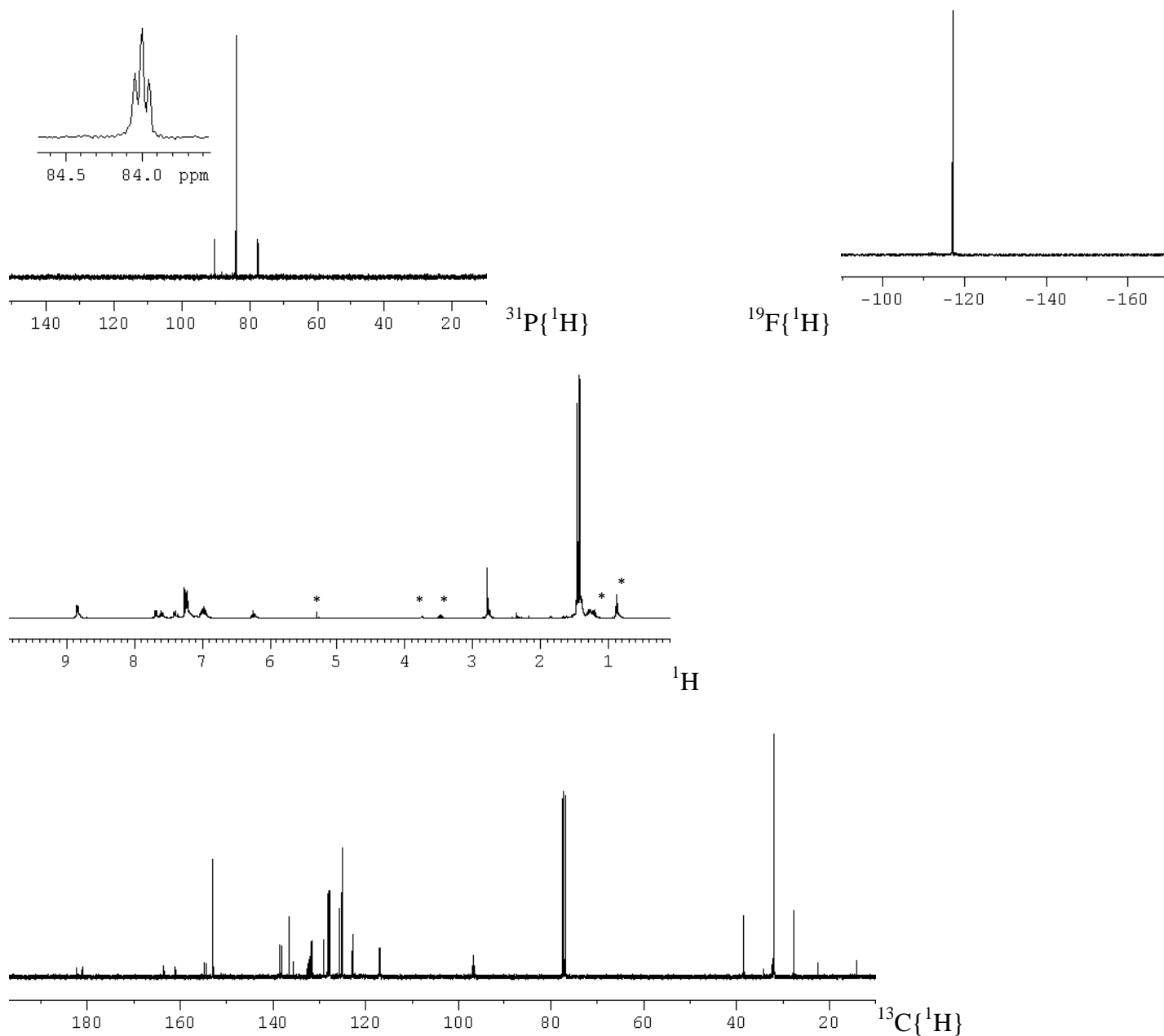
$^1\text{H}$  NMR 8.85 (2H, m, Py), 7.69 (1H, m, Ar), 7.55 (1H, m, Py), 7.40 (1H, m, Ar), 7.40 (2H, m, Py), 7.30 (1H, d,  $J_{\text{HH}} = 7.04$  Hz, Ar), 7.24 (1H, dd,  $J_{\text{HH}} = 8.00$  Hz,  $J_{\text{HH}} = 2.30$  Hz, Ar), 7.18 (2H, m, 4- $\text{FC}_6\text{H}_4$ ), 6.95 (1H, m, Ar), 6.68 (2H, m, 4- $\text{FC}_6\text{H}_4$ ), 2.80 (3H, br-s, Me-Ar), 1.46 (18H, d,  $J_{\text{PH}} = 13.68$  Hz,  $^t\text{Bu}$ );  $^{13}\text{C}\{^1\text{H}\}$  171.90 (dd,  $J_{\text{PC}} = 116.36$  Hz,  $J_{\text{FC}} = 4.00$  Hz, 4- $\text{FC}_6\text{H}_4$ ), 160.32 (dd,  $J_{\text{FC}} = 237.80$  Hz,  $J_{\text{PC}} = 1.48$  Hz, 4- $\text{FC}_6\text{H}_4$ ), 155.40 (d,  $J_{\text{PC}} = 35.21$  Hz, Ar), 153.09 (s, Py), 138.57 (d,  $J_{\text{PC}} = 3.09$  Hz,  $J_{\text{PtC}} = 72.96$  Hz, Ar), 136.80 (d,  $J_{\text{PC}} = 2.02$  Hz, Ar), 136.32 (s, Py), 135.76 (dd,  $J = 4.83$  Hz,  $J = 1.44$  Hz,  $J_{\text{PtC}} = 32.28$  Hz, 4- $\text{FC}_6\text{H}_4$ ), 132.87 (s, Ar), 132.67 (s, Ar), 132.19 (d,  $J_{\text{PC}} = 13.73$  Hz, Ar), 131.60 (d,  $J_{\text{PC}} = 2.42$  Hz, Ar), 129.00 (d,  $J_{\text{PC}} = 7.09$  Hz, Ar), 125.62 (s, Ar), 125.10 (s,  $J_{\text{PtC}} = 20.64$  Hz, Py), 122.64 (s, Ar), 113.63 (dd,  $J = 17.21$  Hz,  $J = 7.31$  Hz,  $J_{\text{PtC}} = 74.51$  Hz, 4- $\text{FC}_6\text{H}_4$ ), 38.51 (d,  $J_{\text{PC}} = 12.80$  Hz,  $^t\text{Bu}$ ), 32.04 (d,  $J_{\text{PC}} = 6.50$  Hz,  $^t\text{Bu}$ ), 27.71 (d,  $J_{\text{PC}} = 1.27$  Hz, Me-Ar);  $^{31}\text{P}\{^1\text{H}\}$  84.3 (s,  $J_{\text{PtP}} = 1961$  Hz);  $^{19}\text{F}$  NMR  $-124.0$  (1F, m, 4- $\text{FC}_6\text{H}_4$ ). APPI- MS: found for  $\text{C}_{30}\text{H}_{35}\text{FNPPtO}$   $[\text{M}+\text{O}]^+$  (calc.) 670.2 (670.2).





**3b:** After stirring for 45 min at room temperature with 3,5-difluorophenylmagnesium bromide (1.02 ml, 0.5M in ether) the complex was isolated as a yellow solid in 71% yield.

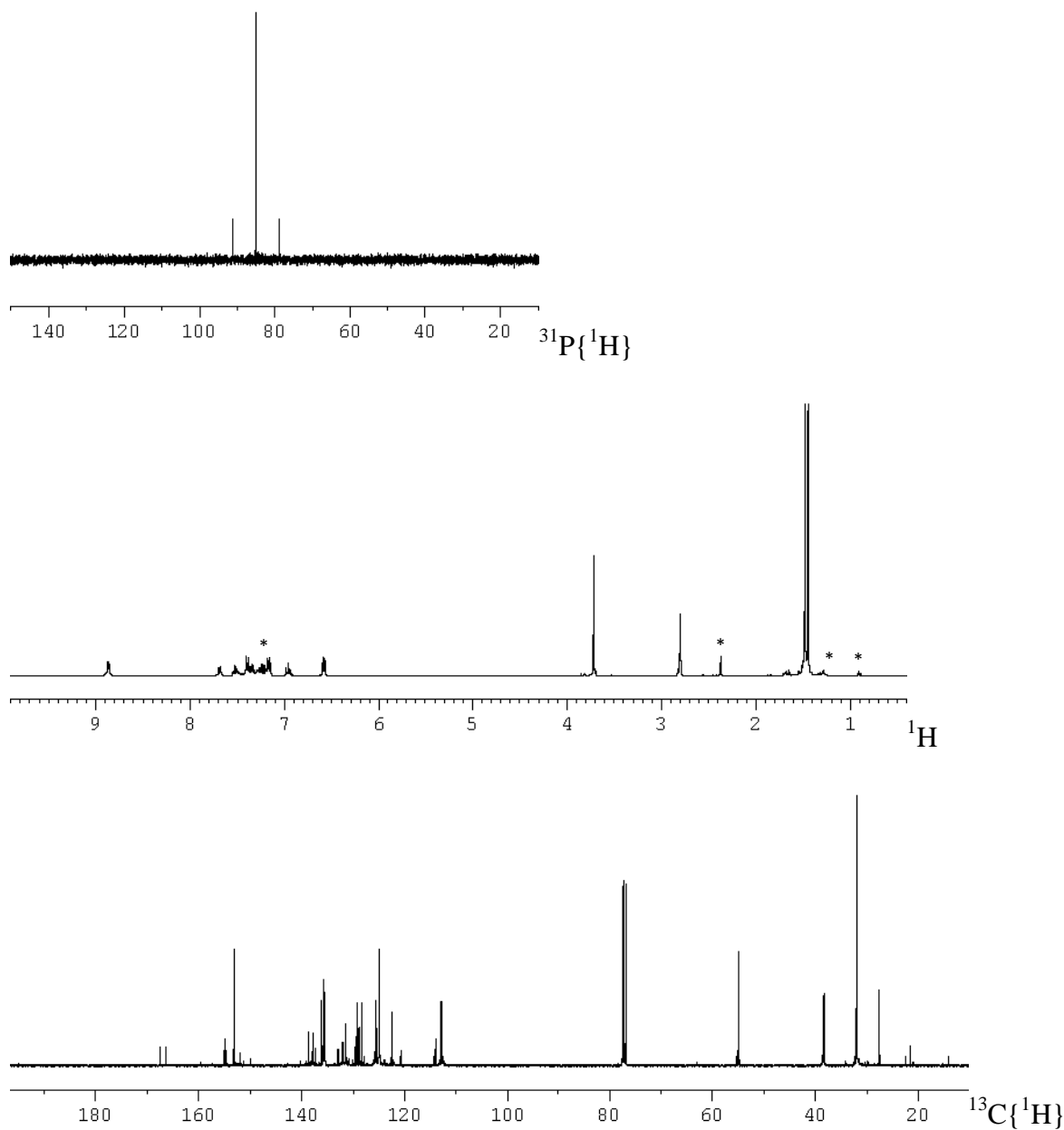
$^1\text{H}$  NMR 8.79 (2H, m, Py), 7.67 (1H, d,  $J_{\text{HH}}= 8.05$  Hz, Ar), 7.50 (1H, m, Py), 7.40 (1H, m, Ar), 7.27 (1H, d,  $J_{\text{HH}}= 7.36$  Hz, Ar), 7.21 (1H, dd,  $J_{\text{HH}}= 8.18$  Hz,  $J_{\text{HH}}= 2.48$  Hz, Ar), 7.13 (2H, m, Py), 7.03 (2H, m, 3,5- $\text{F}_2\text{C}_6\text{H}_3$ ), 6.96 (1H, t,  $J_{\text{HH}}= 7.58$  Hz, Ar), 6.25 (1H, tt,  $J_{\text{FH}}= 9.74$  Hz,  $J_{\text{HH}}= 2.15$  Hz, 3,5- $\text{F}_2\text{C}_6\text{H}_3$ ), 2.76 (3H, m, Me-Ar), 1.42 (18H, d,  $J_{\text{PH}}= 13.78$  Hz  $^t\text{Bu}$ );  $^{13}\text{C}\{^1\text{H}\}$  181.63 (dt,  $J_{\text{PC}}= 116.30$  Hz,  $J_{\text{FC}}= 2.16$  Hz, 3,5- $\text{F}_2\text{C}_6\text{H}_4$ ), 162.22 (dm,  $J_{\text{FC}}= 249.90$  Hz, 3,5- $\text{F}_2\text{C}_6\text{H}_4$ ), 154.62 (d,  $J_{\text{PC}}= 34.64$  Hz, Ar), 152.94 (s, Py), 138.55 (d,  $J_{\text{PC}}= 2.72$  Hz,  $J_{\text{PC}}= 74.52$  Hz, Ar), 136.53 (s, Py), 135.71 (d,  $J_{\text{PC}}= 2.28$  Hz, Ar), 132.63 (s, Ar), 132.28 (s, Ar), 132.19 (d,  $J_{\text{PC}}= 13.72$  Hz, Ar), 131.70 (d,  $J_{\text{PC}}= 2.25$  Hz, Ar), 129.07 (d,  $J_{\text{PC}}= 7.17$  Hz, Ar), 125.69 (s, Ar), 125.17 (s,  $J_{\text{PC}}= 20.88$  Hz, Py), 122.87 (s, Ar), 117.05 (dd,  $J= 13.91$  Hz,  $J= 2.69$  Hz, 3,5- $\text{F}_2\text{C}_6\text{H}_3$ ), 96.58 (t,  $J_{\text{FC}}= 25.49$  Hz, 3,5- $\text{F}_2\text{C}_6\text{H}_3$ ), 38.50 (d,  $J_{\text{PC}}= 13.50$  Hz,  $^t\text{Bu}$ ), 31.97 (d,  $J_{\text{PC}}= 6.28$  Hz,  $^t\text{Bu}$ ), 27.63 (d,  $J_{\text{PC}}= 1.44$  Hz, Me-Ar);  $^{31}\text{P}\{^1\text{H}\}$  84.0 (t,  $J_{\text{FP}}= 15$  Hz,  $J_{\text{PP}}= 2059$  Hz);  $^{19}\text{F}$  NMR  $-115.7$  (2F, m, 3,5- $\text{F}_2\text{C}_6\text{H}_3$ ).



**3c:** After stirring for 5 min at room temperature with 4-methoxyphenylmagnesium bromide (1.02 ml, 0.5M in THF) the complex was isolated as an off-white solid in a 50% yield.

$^1\text{H}$  NMR 8.87 (2H, m, Py), 7.69 (1H, d,  $J_{\text{HH}} = 8.15$  Hz, Ar), 7.53 (1H, m, Py), 7.40 (2H, d,  $J_{\text{HH}} = 7.43$  Hz, 4-OMeC<sub>6</sub>H<sub>4</sub>), 7.35 (2H, m, Py), 7.26 (1H, m, Ar), 7.23 (1H, m, Ar), 7.16 (1H, m, Ar), 6.97 (1H, t,  $J_{\text{HH}} = 7.43$  Hz, Ar), 6.59 (2H, d,  $J_{\text{HH}} = 7.35$  Hz, 4-OMeC<sub>6</sub>H<sub>4</sub>), 3.72 (3H, s, 4-OMeC<sub>6</sub>H<sub>4</sub>), 2.80 (3H, br-s, Me-Ar), 1.47 (18H, d,  $J_{\text{PH}} = 13.39$  Hz, <sup>t</sup>Bu);  $^{13}\text{C}\{^1\text{H}\}$  166.93 (d,  $J_{\text{PC}} = 115.62$  Hz, 4-OMeC<sub>6</sub>H<sub>4</sub>), 154.89 (d,  $J_{\text{PC}} = 36.00$  Hz, Ar), 154.36 (m, 4-OMeC<sub>6</sub>H<sub>4</sub>), 153.21 (s, Py), 138.71 (d,  $J_{\text{PC}} = 3.08$  Hz,  $J_{\text{PC}} = 76.55$  Hz, Ar), 137.29 (s, Ar), 136.14 (s, Py), 135.64 (m,  $J_{\text{PC}} = 31.39$  Hz, 4-OMeC<sub>6</sub>H<sub>4</sub>), 133.12 (s, Ar), 132.80 (s, Ar), 132.11 (d,  $J_{\text{PC}} = 13.71$  Hz, Ar), 131.50

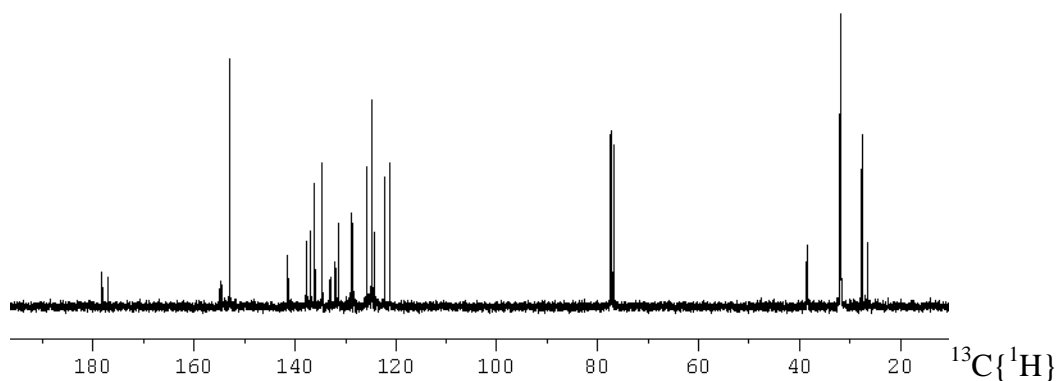
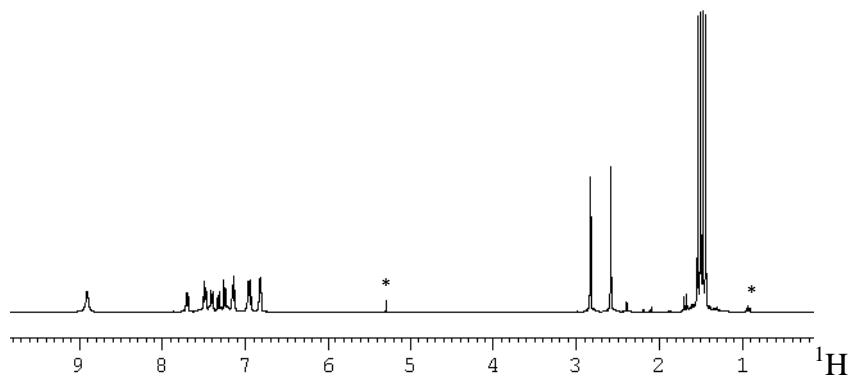
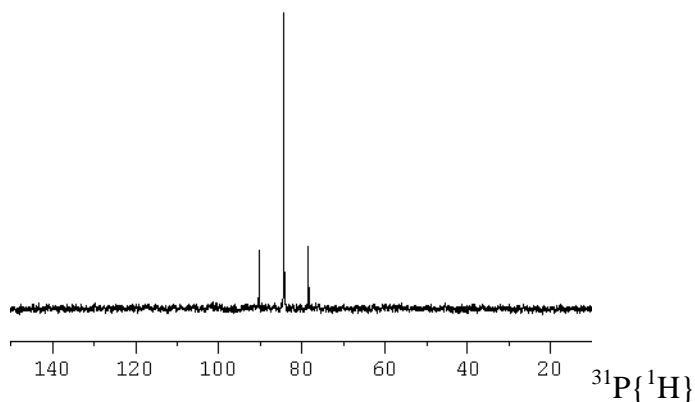
(m, Ar), 128.85 (d,  $J_{PC}= 6.95$  Hz, Ar), 125.43 (s, Ar), 124.94 (s,  $J_{PC}= 22.27$  Hz, Py), 122.43 (s, Ar), 112.90 (d,  $J_{PC}= 6.95$  Hz,  $J_{PC}= 70.92$  Hz, 4-OMeC<sub>6</sub>H<sub>4</sub>), 54.89 (s, 4-OMeC<sub>6</sub>H<sub>4</sub>), 38.44 (d,  $J_{PC}= 12.22$  Hz, <sup>t</sup>Bu), 32.00 (s,  $J_{PC}= 6.54$  Hz, <sup>t</sup>Bu), 27.68 (m, Me-Ar); <sup>31</sup>P{<sup>1</sup>H} 85.1 (s,  $J_{PtP}= 1919$  Hz).



**3d:** After stirring for 5 h at room temperature with *o*-tolylmagnesium chloride (0.51 ml, 1M in THF), the complex was isolated as an off-white solid in a 58% yield.

<sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$  8.91 (2H, m, Py), 7.70 (1H, br-d,  $J_{HH}= 7.48$  Hz, Ar), 7.49 (2H, m, Ar), 7.40 (1H, m, Py), 7.32 (1H, d,  $J_{HH}= 8.05$  Hz, Ar), 7.25 (1H, dd,  $J_{HH}= 7.94$  Hz,  $J_{HH}= 2.33$  Hz, Me-C<sub>6</sub>H<sub>4</sub>), 7.14 (2H, m, Py), 6.95 (1H, m, Me-C<sub>6</sub>H<sub>4</sub>), 6.95 (1H, m, Ar), 6.82 (2H, m, Me-C<sub>6</sub>H<sub>4</sub>), 2.83 (3H, s, Me-C<sub>6</sub>H<sub>4</sub>), 2.58 (3H, br-s, Me-Ar),

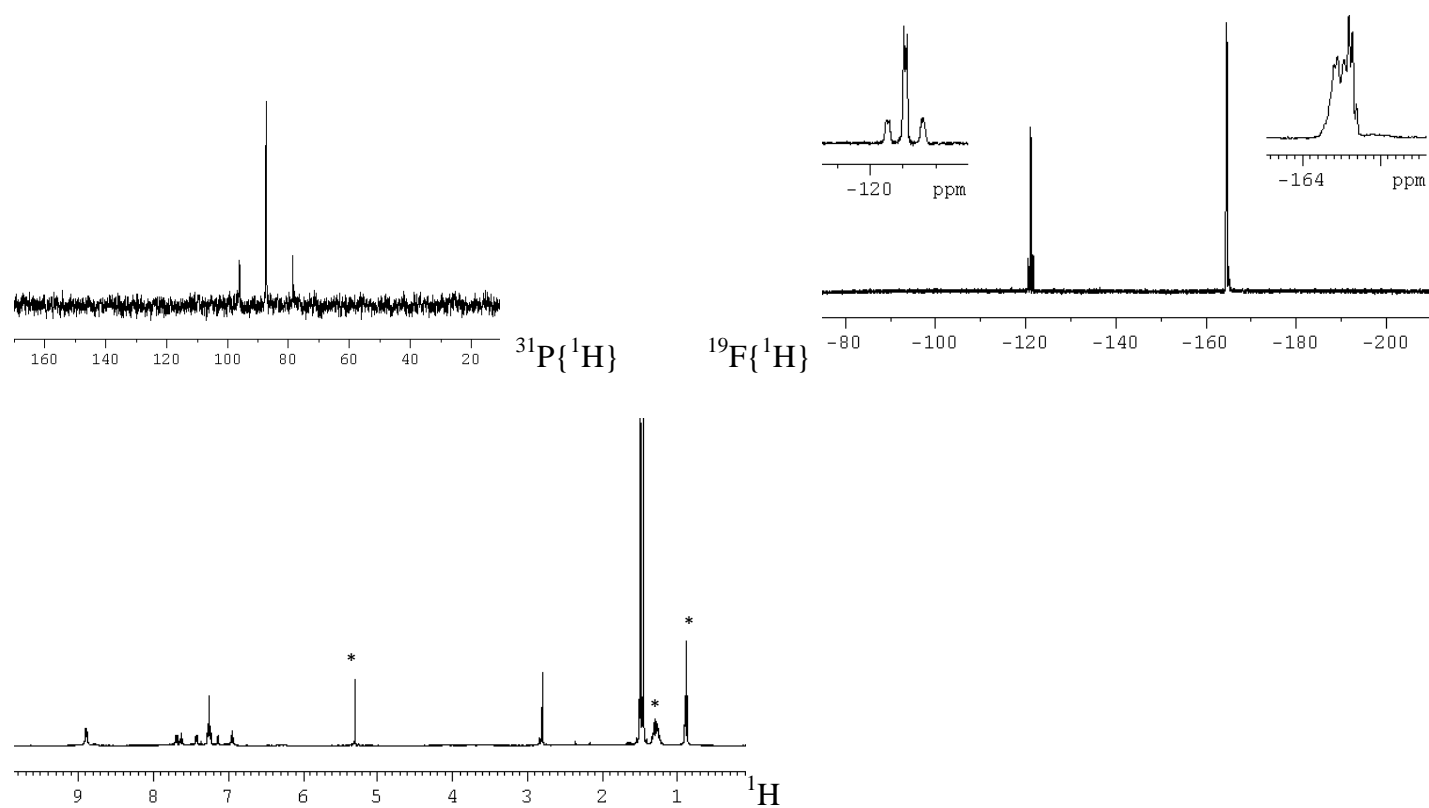
1.52 (9H, d,  $J_{\text{PH}} = 13.48$  Hz,  $^1\text{Bu}$ ), 1.46 (9H, d,  $J_{\text{PH}} = 13.58$  Hz,  $^1\text{Bu}$ );  $^{13}\text{C}\{^1\text{H}\}$  177.63 (d,  $J_{\text{PC}} = 112.66$  Hz, Me- $\text{C}_6\text{H}_4$ ), 154.68 (d,  $J_{\text{PC}} = 35.30$  Hz, Ar), 152.95 (s, Py), 141.44 (s, Me- $\text{C}_6\text{H}_4$ ), 137.83 (s, Ar), 137.07 (d,  $J_{\text{PC}} = 3.42$  Hz,  $J_{\text{PC}} = 76.68$  Hz, Ar), 136.15 (s, Py), 135.91 (m, Ar), 134.73 (s, Me- $\text{C}_6\text{H}_4$ ), 133.24 (s, Ar), 132.91 (s, Ar), 132.10 (d,  $J_{\text{PC}} = 13.81$  Hz, Ar), 131.48 (s, Ar), 128.75 (m, Ar), 125.82 (s, Ar), 124.84 (s, Py), 124.30 (d,  $J_{\text{PC}} = 6.55$  Hz, Me- $\text{C}_6\text{H}_4$ ), 122.35 (s, Ar), 121.42 (s, Me- $\text{C}_6\text{H}_4$ ), 38.62 (d,  $J_{\text{PC}} = 12.80$  Hz,  $^1\text{Bu}$ ), 38.45 (d,  $J_{\text{PC}} = 12.01$  Hz,  $^1\text{Bu}$ ), 32.02 (d,  $J_{\text{PC}} = 5.95$  Hz,  $^1\text{Bu}$ ), 31.89 (d,  $J_{\text{PC}} = 6.04$  Hz,  $^1\text{Bu}$ ), 27.73 (s, Me-Ar), 26.63 (m,  $J_{\text{PC}} = 74.17$  Hz, Me- $\text{C}_6\text{H}_4$ );  $^{31}\text{P}\{^1\text{H}\}$  84.8 (s,  $J_{\text{PP}} = 1923$  Hz); Elemental Analysis: Found: C, 57.07; H, 5.63; Calc. for  $\text{C}_{31}\text{H}_{38}\text{NPt}$ : C, 57.22; H, 5.89.

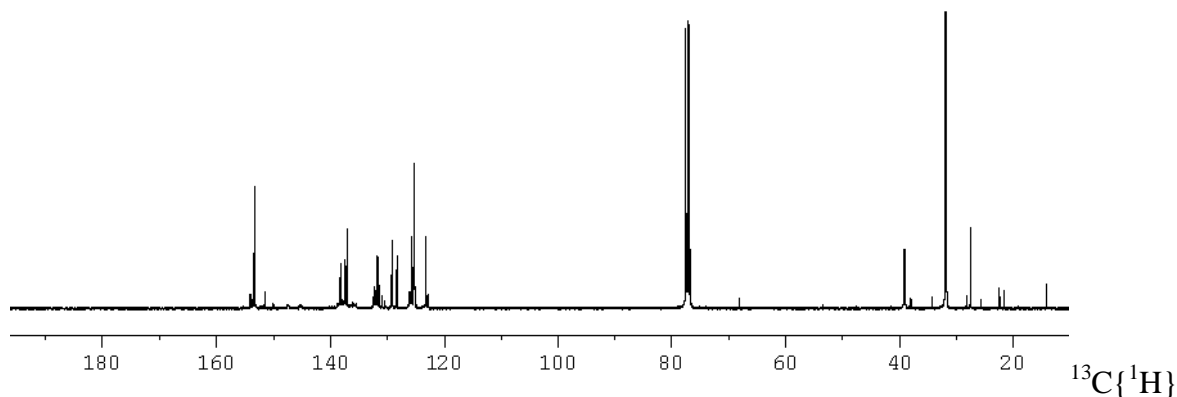




**3e:** After stirring for 5 h at room temperature with pentafluorophenylmagnesium bromide (1.02 ml, 0.5 M in ether), the complex was isolated as an off-white solid in a 40% yield.

$^1\text{H}$  NMR 8.90 (2H, m, Py), 7.70 (1H, br-d,  $J_{\text{HH}}=8.22$  Hz, Ar), 7.62 (1H, m, Py), 7.42 (2H, m, Ar), 7.26 (2H, m, Py), 7.14 (1H, m, Ar), 6.95 (1H, m, Ar), 2.80 (3H, br-s, Me-Ar), 1.48 (18H, d,  $J_{\text{PH}}=14.14$  Hz,  $^t\text{Bu}$ );  $^{13}\text{C}\{^1\text{H}\}$  154.03 (d,  $J_{\text{PC}}=33.10$  Hz, Ar), 153.38 (s, Py), 146.36 (dm,  $J_{\text{FC}}=220.05$  Hz,  $\text{C}_6\text{F}_5$ ), 138.29 (m, Ar), 138.04 (m,  $\text{C}_6\text{F}_5$ ), 137.22 (m, Ar), 137.07 (s, Py), 136.07 (m,  $\text{C}_6\text{F}_5$ ), 132.45 (s, Ar), 132.32 (d,  $J_{\text{PC}}=14.08$  Hz, Ar), 132.09 (s, Ar), 131.78 (m, Ar), 129.24 (m, Ar), 125.86 (s, Ar), 125.30 (s,  $J_{\text{PC}}=20.88$  Hz, Py), 123.30 (s, Ar), 39.13 (d,  $J_{\text{PC}}=17.18$  Hz,  $^t\text{Bu}$ ), 31.92 (d,  $J_{\text{PC}}=5.86$  Hz,  $^t\text{Bu}$ ), 27.56 (br-s, Me-Ar);  $^{31}\text{P}\{^1\text{H}\}$  85.9 (m,  $J_{\text{PP}}=2825$  Hz);  $^{19}\text{F}$  NMR  $-119.9$  (2F, m,  $J_{\text{PF}}=406$  Hz,  $\text{C}_6\text{F}_5$ ),  $-163.4$  (3F, m,  $\text{C}_6\text{F}_5$ ).

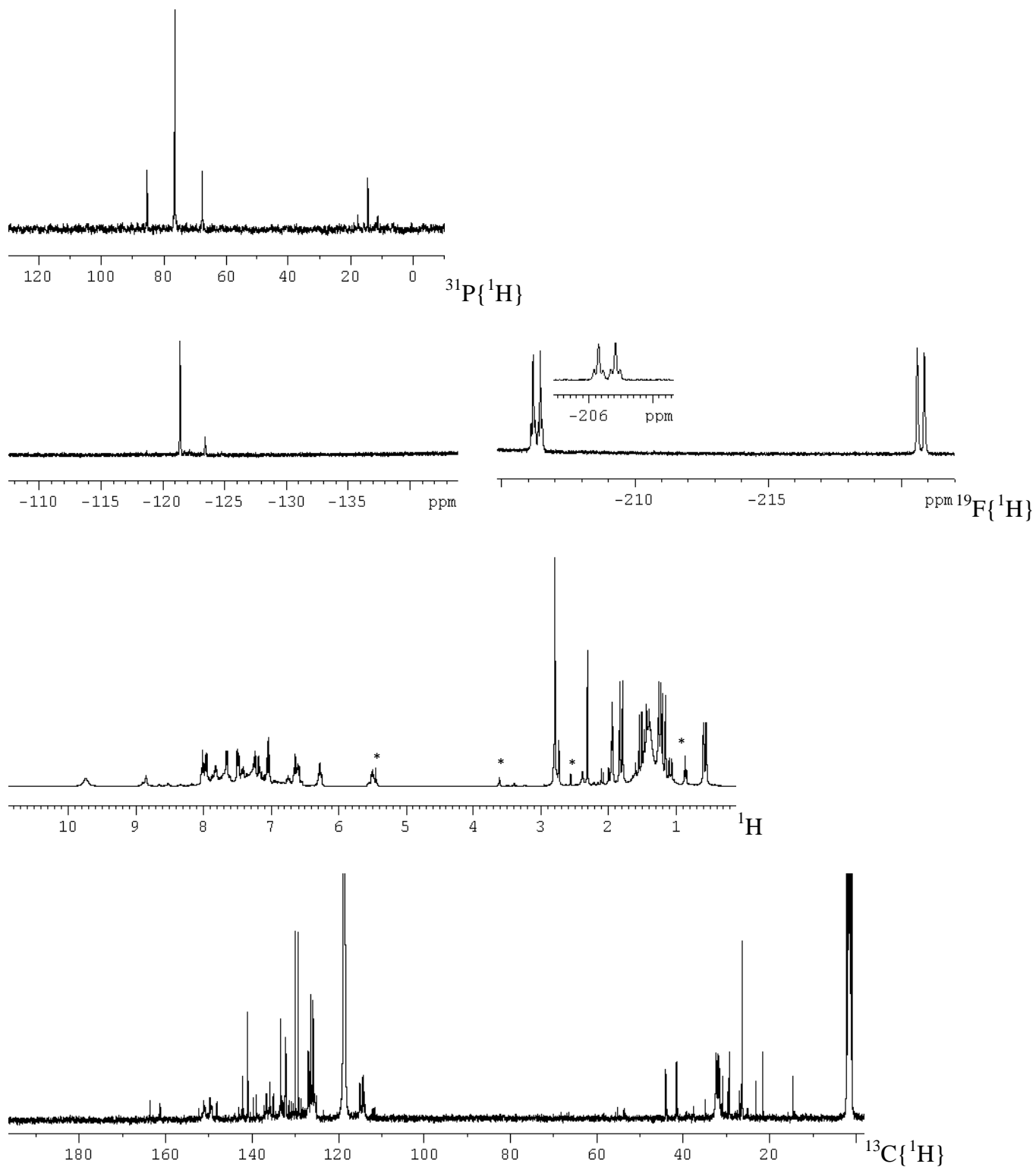




### Reactions with XeF<sub>2</sub>

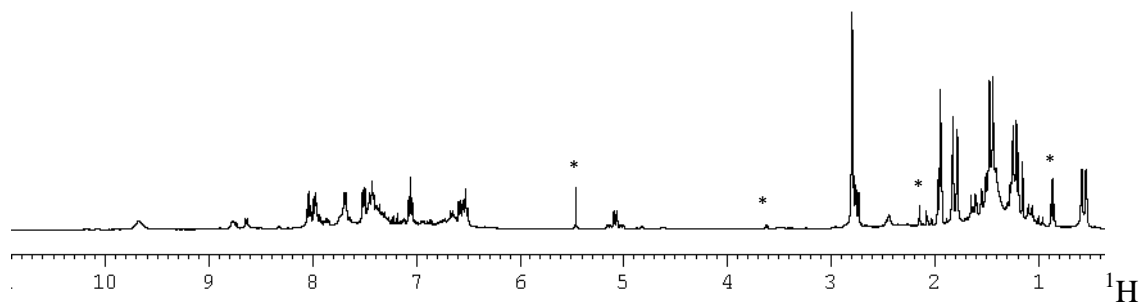
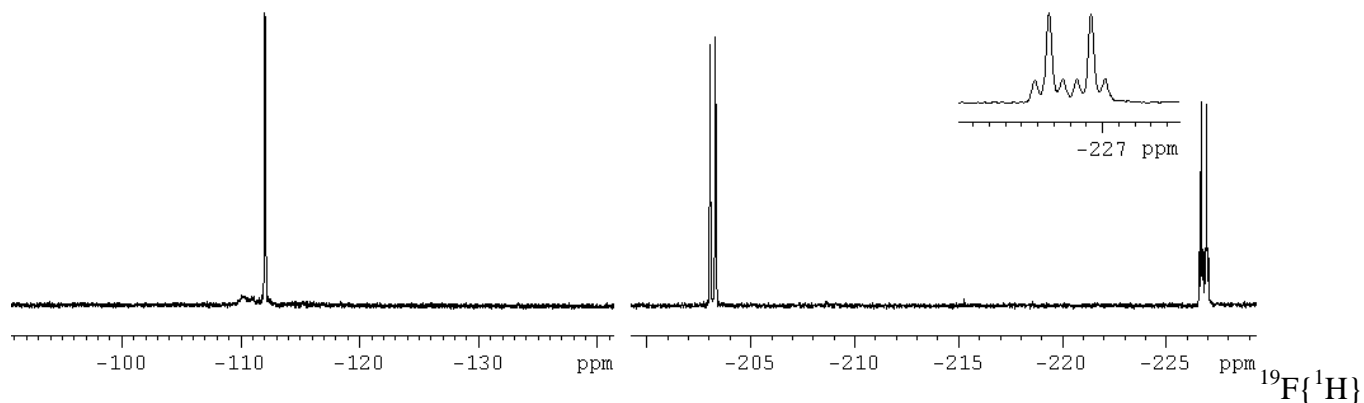
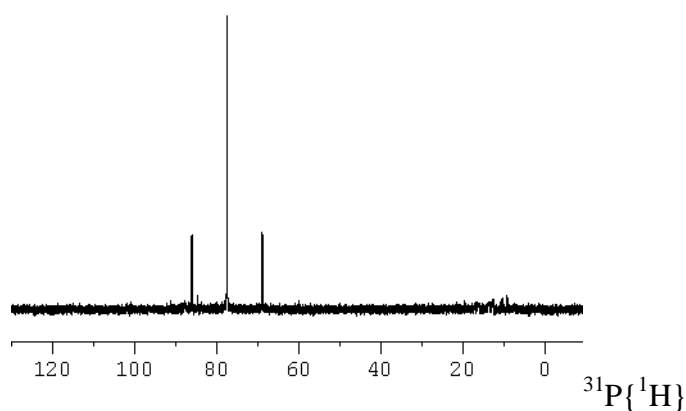
In a glove box, a cold (-30°C) freshly prepared solution of XeF<sub>2</sub> (1eq) in CD<sub>3</sub>CN or CH<sub>2</sub>Cl<sub>2</sub> was quickly added to a solution of **3** (10mg, 1eq) in a plastic vial at -30°C. The reaction mixture was left at this temperature for 10 min and then slowly warmed to room temperature. The <sup>31</sup>P{<sup>1</sup>H} and <sup>19</sup>F{<sup>1</sup>H}NMR analysis (in a PTFE liner) showed the formation of the corresponding complexes **4a-d**.

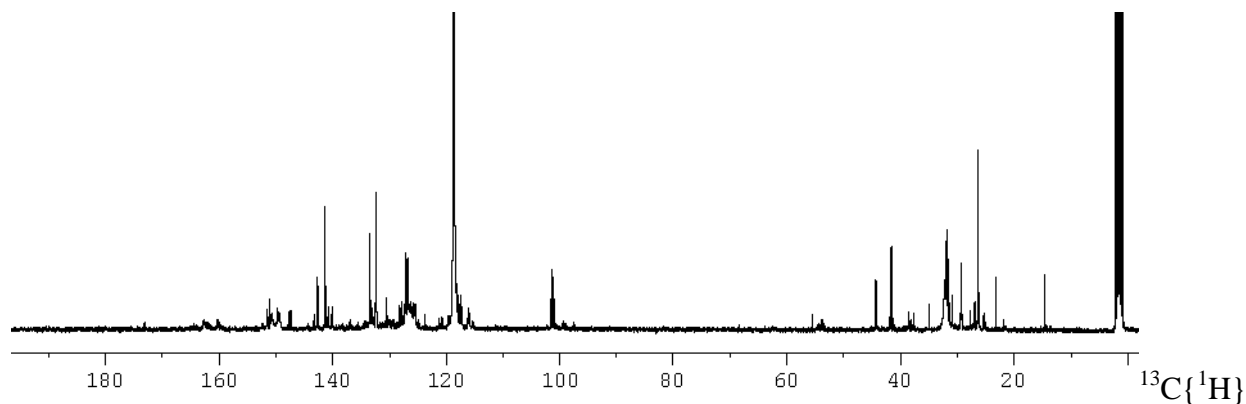
**4a** (263K): <sup>1</sup>H NMR (CD<sub>3</sub>CN) δ 9.74 (1H, m, Py), 8.01 (1H, m, Py), 7.96 (1H, dm, J<sub>HH</sub>= 8.23 Hz, Ar), 7.66 (2H, m, Ar), 7.66 (1H, m, Py), 7.49 (1H, m, Ar), 7.42 (1H, m, Py), 7.04 (1H, m, Py), 6.75 (1H, m, Ar), 6.64 (1H, m, 4-FC<sub>6</sub>H<sub>4</sub>), 6.60 (1H, m, 4-FC<sub>6</sub>H<sub>4</sub>), 6.28 (1H, m, 4-FC<sub>6</sub>H<sub>4</sub>), 5.50 (1H, m, 4-FC<sub>6</sub>H<sub>4</sub>), 2.79 (3H, br-s, Me-Ar), 1.81 (3H, d, J<sub>PH</sub>= 16.43 Hz, <sup>t</sup>Bu), 1.53 (3H, d, J<sub>PH</sub>= 15.73 Hz, <sup>t</sup>Bu), 1.46 (3H, m, <sup>t</sup>Bu), 1.24 (3H, d, J<sub>PH</sub>= 13.68 Hz, <sup>t</sup>Bu), 1.18 (3H, d, J<sub>PH</sub>= 15.04 Hz, <sup>t</sup>Bu), 0.58 (3H, dm, J<sub>PH</sub>= 15.73 Hz, <sup>t</sup>Bu); <sup>13</sup>C{<sup>1</sup>H} 178.17 (d, J<sub>PC</sub>= 137.56 Hz, 4-FC<sub>6</sub>H<sub>4</sub>), 162.18 (d, J<sub>FC</sub>= 240.50 Hz, 4-FC<sub>6</sub>H<sub>4</sub>), 152.03 (m, Ar), 150.97 (m, Ar), 150.03 (m, Ar), 149.54 (dm, J<sub>PC</sub>= 9.57 Hz, Ar), 147.89 (dm, J<sub>FC</sub>= 20.66 Hz, Ar), 142.01 (d, J<sub>PC</sub>= 2.19 Hz, J<sub>PC</sub>= 36.34 Hz, Ar), 140.75 (m, Ar), 136.41 (dm, J= 17.63 Hz, 4-FC<sub>6</sub>H<sub>4</sub>), 135.24 (dm, J= 85.09 Hz, 4-FC<sub>6</sub>H<sub>4</sub>), 133.13 (m, Ar), 132.06 (m, Ar), 131.97 (s, Ar), 131.88 (s, Ar), 126.71 (d, J<sub>PC</sub>= 3.46 Hz, Ar), 126.26 (m, Ar), 125.63 (s, Ar), 114.72 (dm, J<sub>FC</sub>= 20.77 Hz, 4-FC<sub>6</sub>H<sub>4</sub>), 114.05 (dm, J<sub>FC</sub>= 19.60 Hz, 4-FC<sub>6</sub>H<sub>4</sub>), 43.71 (dm, J<sub>PC</sub>= 22.16 Hz, <sup>t</sup>Bu), 41.22 (m, <sup>t</sup>Bu), 32.09 (m, <sup>t</sup>Bu), 31.66 (m, <sup>t</sup>Bu), 31.45 (m, <sup>t</sup>Bu), 31.38 (m, <sup>t</sup>Bu), 30.64 (m, <sup>t</sup>Bu), 29.12 (m, J<sub>PC</sub>= 23.57 Hz, <sup>t</sup>Bu), 26.12 (m, Me-Ar); <sup>31</sup>P{<sup>1</sup>H} 76.5 (s, J<sub>PP</sub>= 2855 Hz); <sup>19</sup>F NMR -121.4 (1F, m, 4-FC<sub>6</sub>H<sub>4</sub>), -206.3 (1F, dm, J<sub>FF</sub>= 100 Hz), -220.7 (1F, d, J<sub>FF</sub>= 100 Hz)



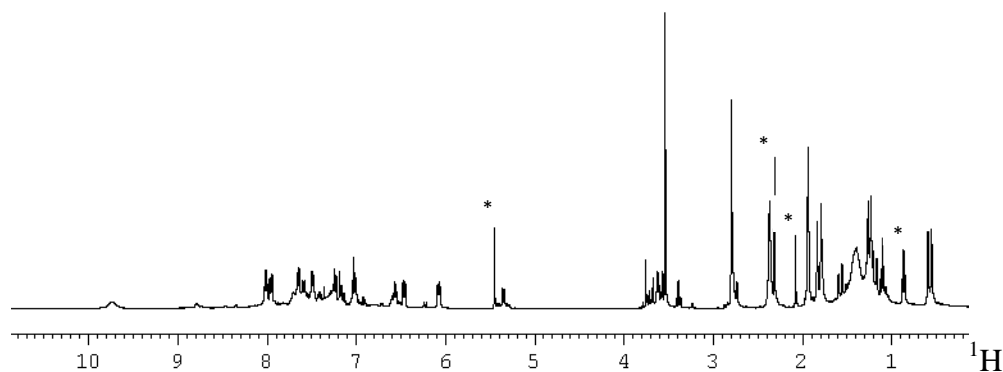
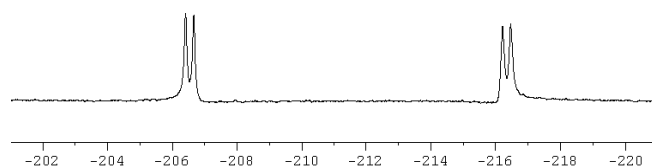
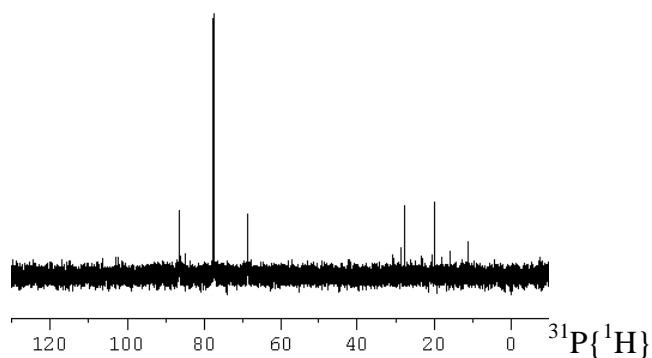
**4b** (263K):  $^1\text{H}$  NMR ( $\text{CD}_3\text{CN}$ )  $\delta$  9.68 (1H, m, Py), 8.04 (1H, m, Py), 7.99 (1H, dm,  $J_{\text{HH}} = 8.38$  Hz, Ar), 7.69 (2H, m, Ar), 7.69 (1H, m, Py), 7.52 (1H, m, Ar), 7.43 (1H, m, Py), 7.07 (1H, m, Py), 6.67 (1H, m, Ar), 6.59 (1H, m, 3,5- $\text{FC}_6\text{H}_4$ ), 6.54 (1H, m, 3,5- $\text{FC}_6\text{H}_4$ ), 5.08 (1H, m, 3,5- $\text{FC}_6\text{H}_4$ ), 2.80 (3H, m, Me-Ar), 1.81 (3H, d,  $J_{\text{PH}} =$

16.94 Hz, <sup>t</sup>Bu), 1.45 (6H, m, <sup>t</sup>Bu), 1.23 (3H, m, <sup>t</sup>Bu), 1.18 (3H, d, J<sub>PH</sub>= 16.20 Hz, <sup>t</sup>Bu), 0.57 (3H, dm, J<sub>PH</sub>= 16.11 Hz, <sup>t</sup>Bu); <sup>13</sup>C{<sup>1</sup>H} 180.41 (d, J<sub>PC</sub>= 116.34 Hz, 3,5-F<sub>2</sub>C<sub>6</sub>H<sub>4</sub>), 161.10 (dm, J<sub>FC</sub>= 243.94 Hz, 3,5-F<sub>2</sub>C<sub>6</sub>H<sub>4</sub>), 151.24 (m, Ar), 150.86 (dm, J<sub>FC</sub>= 4.70 Hz, Ar), 149.97 (m, Ar), 149.51 (dm, J<sub>PC</sub>= 10.24 Hz, Ar), 147.26 (dm, J<sub>FC</sub>= 19.90 Hz, Ar), 143.06 (m, Ar), 142.42 (d, J<sub>PC</sub>= 2.25 Hz, J<sub>FC</sub>= 35.33 Hz, Ar), 141.10 (m, Ar), 133.25 (m, Ar), 132.24 (m, Ar), 132.14 (m, Ar), 126.86 (d, J<sub>PC</sub>= 3.11 Hz, Ar), 126.53 (m, Ar), 125.97 (s, Ar), 117.30 (m, 3,5-F<sub>2</sub>C<sub>6</sub>H<sub>3</sub>), 115.84 (m, 3,5-F<sub>2</sub>C<sub>6</sub>H<sub>3</sub>), 101.12 (t, J<sub>FC</sub>= 25.24 Hz, 3,5-F<sub>2</sub>C<sub>6</sub>H<sub>3</sub>), 44.00 (dm, J<sub>PC</sub>= 21.75 Hz, <sup>t</sup>Bu), 41.39 (m, <sup>t</sup>Bu), 31.98 (m, <sup>t</sup>Bu), 31.63 (m, <sup>t</sup>Bu), 31.56 (m, <sup>t</sup>Bu), 31.34 (m, <sup>t</sup>Bu), 30.58 (m, <sup>t</sup>Bu), 29.07 (m, J<sub>PC</sub>= 22.23 Hz, <sup>t</sup>Bu), 26.12 (m, Me-Ar); <sup>31</sup>P{<sup>1</sup>H} 77.6 (s, J<sub>PP</sub>= 2771 Hz); <sup>19</sup>F NMR -112.0 (2F, m, 3,5-F<sub>2</sub>C<sub>6</sub>H<sub>3</sub>), -203.2 (1F, d, J<sub>FF</sub>= 98 Hz), -226.8 (1F, dm, J<sub>FF</sub>= 98 Hz)

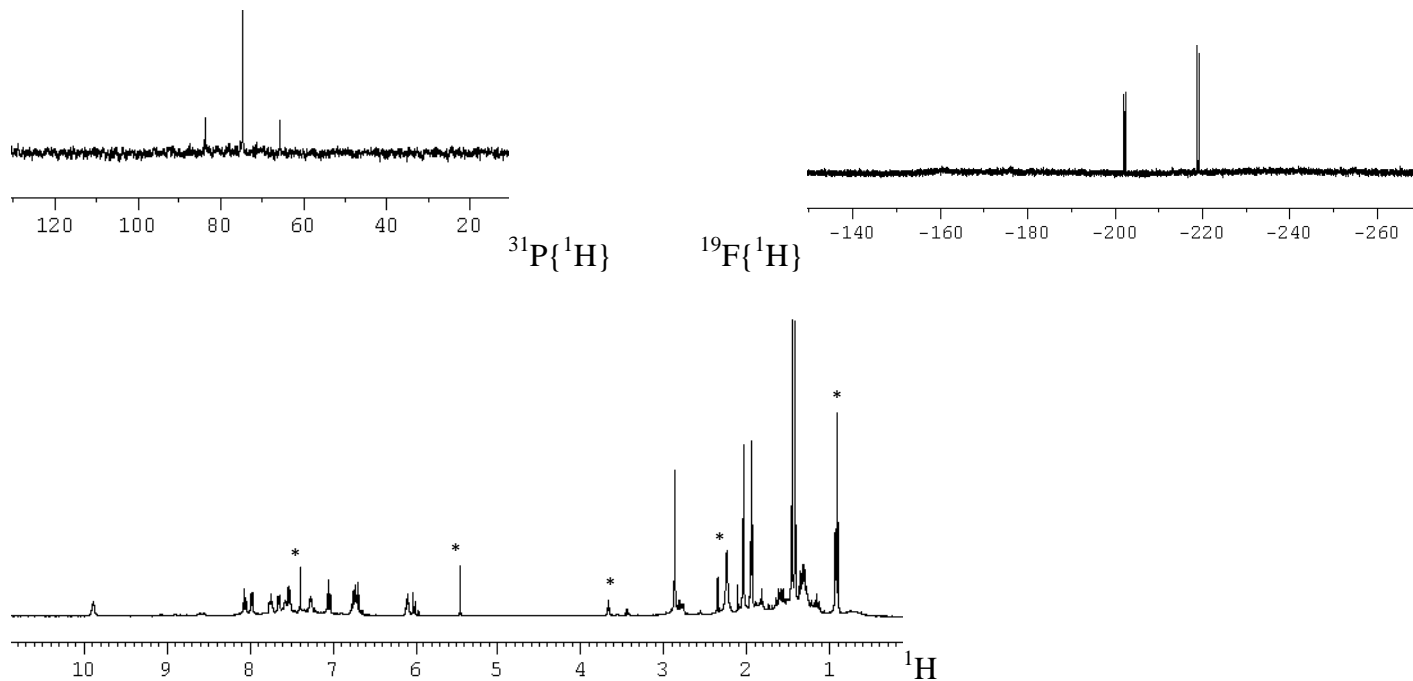




**4c** (263K):  $^1\text{H}$  NMR ( $\text{CD}_3\text{CN}$ )  $\delta$  8.01 (1H, m, Py), 7.96 (1H, dd,  $J_{\text{HH}} = 8.36$  Hz,  $J_{\text{HH}} = 2.05$  Hz, Ar), 7.66 (2H, m, Ar), 7.60 (1H, m, Py), 7.49 (1H, m, Ar), 7.42 (1H, m, Py), 7.25 (1H, m, Ar), 7.03 (2H, m, Py), 6.56 (1H, m, Ar), 6.47 (1H, dd,  $J_{\text{HH}} = 8.90$  Hz,  $J_{\text{HH}} = 2.98$  Hz, Ar), 6.08 (1H, m, dd,  $J_{\text{HH}} = 8.86$  Hz,  $J_{\text{HH}} = 3.11$  Hz, Ar), 5.35 (1H, d, dd,  $J_{\text{HH}} = 8.69$  Hz,  $J_{\text{PH}} = 42.53$  Hz, Ar), 3.54 (3H, s, OMe), 2.79 (3H, br-s, Me-Ar), 1.81 (3H, d,  $J_{\text{PH}} = 16.87$  Hz,  $^t\text{Bu}$ ), 1.57 (3H, d,  $J_{\text{PH}} = 16.87$  Hz,  $^t\text{Bu}$ ), 1.41 (3H, m,  $^t\text{Bu}$ ), 1.25 (3H, d,  $J_{\text{PH}} = 12.50$  Hz,  $^t\text{Bu}$ ), 1.19 (3H, d,  $J_{\text{PH}} = 15.62$  Hz,  $^t\text{Bu}$ ), 0.57 (3H, br-d,  $J_{\text{PH}} = 16.24$  Hz,  $^t\text{Bu}$ );  $^{31}\text{P}\{^1\text{H}\}$  77.6 (s,  $J_{\text{PH}} = 2771$  Hz);  $^{19}\text{F}$  NMR -206.5 (1F, d,  $J_{\text{FF}} = 98$  Hz), -216.5 (1F, d,  $J_{\text{FF}} = 98$  Hz);



**4d:**  $^1\text{H}$  NMR ( $\text{CD}_3\text{CN}$ )  $\delta$  9.89 (1H, m, Py), 8.07 (1H, m, Py), 7.98 (1H, dd,  $J_{\text{HH}}=8.30$  Hz,  $J_{\text{HH}}=2.46$  Hz, Ar), 7.75 (1H, m, Ar), 7.65 (1H, dm,  $J_{\text{HH}}=8.61$  Hz, Ar), 7.57 (1H, m, Py), 7.53 (1H, dd,  $J_{\text{HH}}=8.30$  Hz,  $J_{\text{HH}}=3.36$  Hz, Ar), 7.27 (2H, m, Py), 7.05 (1H, t,  $J_{\text{HH}}=7.69$  Hz, Ar), 6.63 (2H, m, Ar), 6.10 (1H, m, Ar), 6.02 (1H, m, Ar), 2.87 (3H, m, Me-Ar), 2.04 (3H, m, Me-Ar), 1.60 (3H, m,  $^t\text{Bu}$ ), 1.44 (9H,  $J_{\text{PH}}=15.26$  Hz,  $^t\text{Bu}$ ), 1.33 (6H, m,  $^t\text{Bu}$ );  $^{31}\text{P}\{^1\text{H}\}$  74.6 (s,  $J_{\text{PtP}}=2922.5$  Hz);  $^{19}\text{F}$  NMR  $-202.3$  (1F, d,  $J_{\text{FF}}=131$  Hz),  $-219.1$  (1F, d,  $J_{\text{FF}}=131$  Hz);

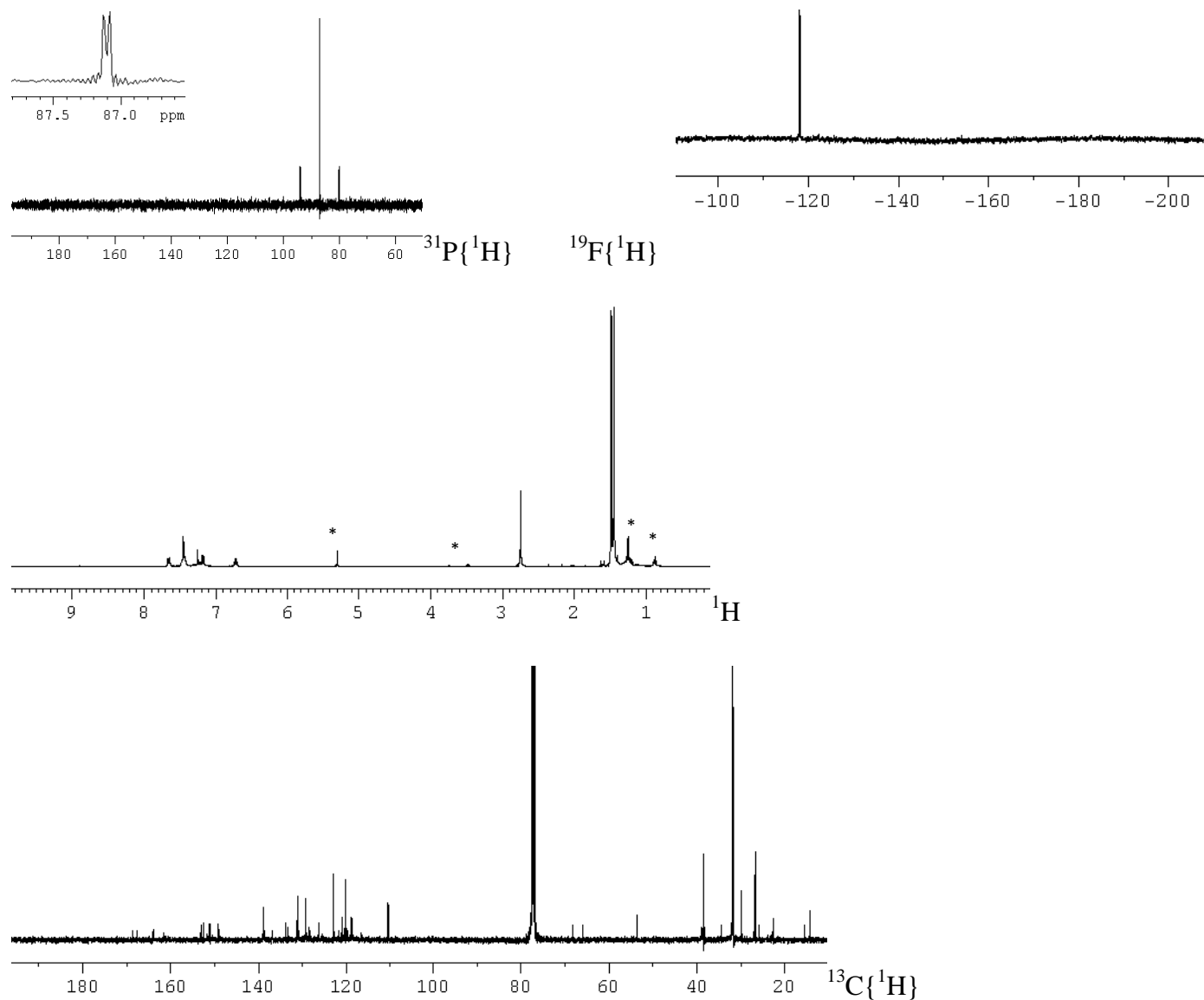


#### Preparation of complexes **5a-d**.

Solutions of complexes **4a-d** were left at room temperature (**4c,d**) or heated at  $60^\circ\text{C}$  (**4a,b**) in a Schlenk flask for 16 h. The formation of the doubly cyclometallated complexes **5** was confirmed by the  $^{31}\text{P}\{^1\text{H}\}$  NMR spectroscopy. The formation of complexes **6** accompanied the conversion of **4** to **5**.

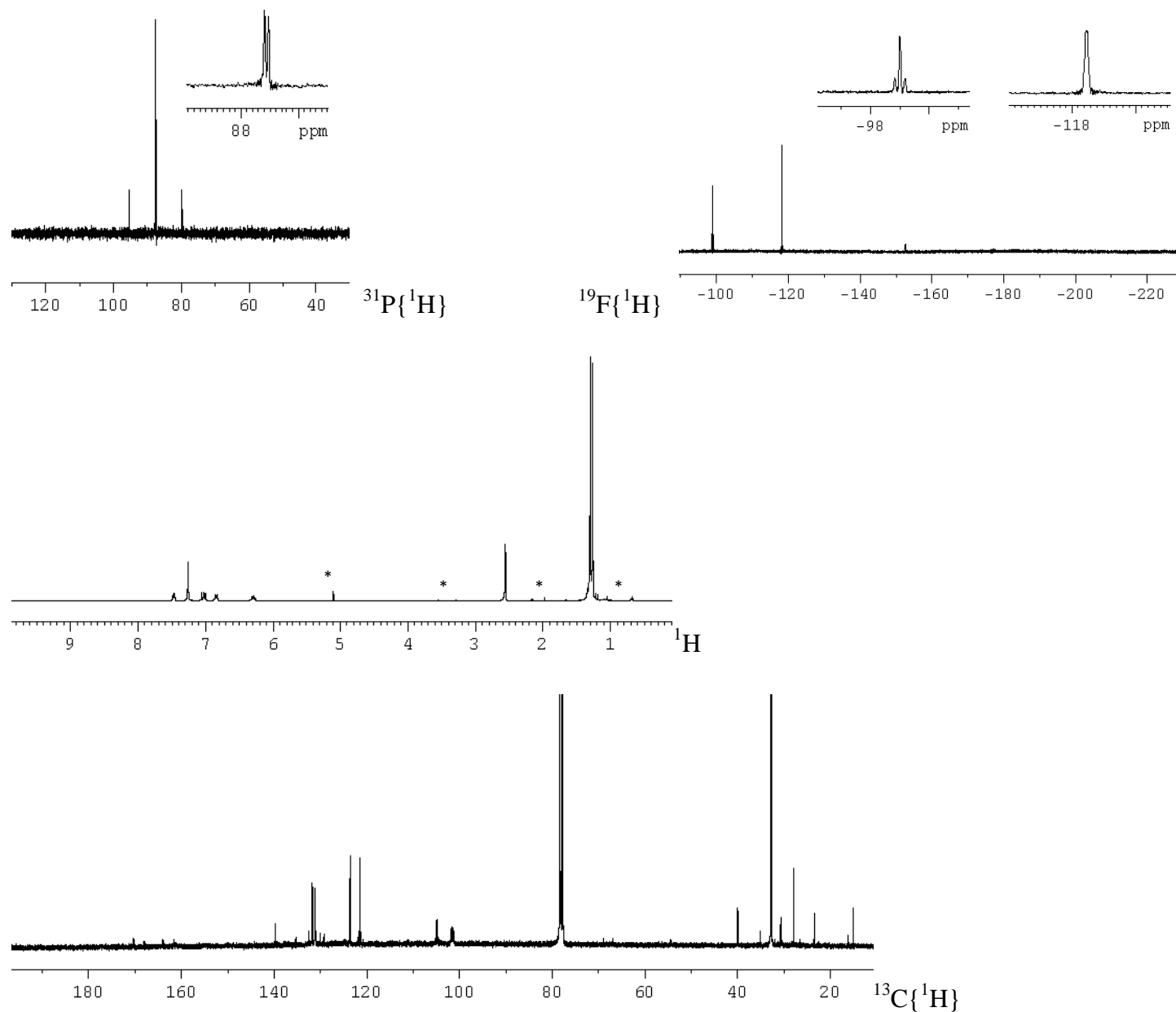
**5a:**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  7.66 (1H, dd,  $J_{\text{HH}}=8.35$  Hz,  $J_{\text{HH}}=2.25$  Hz, Ar), 7.45 (3H, m, Ar), 7.24 (1H, m, Ar), 7.18 (1H, dd,  $J_{\text{HH}}=8.37$  Hz,  $J_{\text{HH}}=2.41$  Hz, Ar), 6.73 (1H, m, Ar), 2.75 (3H, m, Me-Ar), 1.47 (18H, d,  $J_{\text{PH}}=14.26$  Hz,  $^t\text{Bu}$ );  $^{13}\text{C}\{^1\text{H}\}$  168.10 (d,  $J_{\text{PC}}=103.55$  Hz, Ar), 162.63 (dd,  $J_{\text{FC}}=247.70$  Hz,  $J_{\text{PC}}=10.06$  Hz, Ar), 152.47 (s, Ar), 151.22 (m, Ar), 151.07 (d,  $J_{\text{PC}}=22.49$  Hz, Ar), 149.10 (m, Ar), 138.83 (s,  $J_{\text{PC}}=30.61$  Hz, Ar), 133.58 (d,  $J_{\text{PC}}=34.44$  Hz, Ar), 131.30 (d,  $J_{\text{PC}}=13.39$  Hz, Ar), 130.98 (br-s, Ar), 129.26 (d,  $J_{\text{PC}}=7.84$  Hz, Ar), 123.02 (s, Ar), 120.97 (m, Ar), 120.15 (s,  $J_{\text{PC}}=64.53$  Hz, Ar), 118.77 (d,  $J=17.45$  Hz, Ar), 110.26 (d,  $J=21.45$  Hz, Ar), 38.42 (d,  $J_{\text{PC}}=12.45$  Hz,  $^t\text{Bu}$ ), 31.74 (d,  $J_{\text{PC}}=7.16$  Hz,  $^t\text{Bu}$ ), 26.67 (br-s, Me-Ar);  $^{31}\text{P}\{^1\text{H}\}$  87.1 (d,  $J_{\text{PF}}=7$  Hz,  $J_{\text{PtP}}=2232$  Hz);  $^{19}\text{F}$  NMR  $-118.1$  (1F, br-s, 4- $\text{FC}_6\text{H}_4$ ). HRMS ESI: found for  $\text{C}_{27}\text{H}_{31}\text{FNPPt}$  [ $\text{M-MeCN}$ ] $^+$

(calc.) 573.1618 (573.1618); Elemental Analysis: Found: C, 52.32; H, 5.38; Calc. for C<sub>27</sub>H<sub>28</sub>D<sub>3</sub>FNPPt: C, 52.51; H, 5.55.



**5b:** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.67 (1H, dd, J<sub>HH</sub>= 8.07 Hz, J<sub>HH</sub>= 2.07 Hz, Ar), 7.46 (2H, m, Ar), 7.22 (1H, dd, J<sub>HH</sub>= 8.30 Hz, J<sub>HH</sub>= 2.79 Hz, Ar), 7.05 (1H, m, Ar), 6.50 (1H, m, Ar), 2.76 (3H, m, Me-Ar), 1.48 (18H, d, J<sub>PH</sub>= 14.38 Hz, <sup>t</sup>Bu); <sup>13</sup>C{<sup>1</sup>H} 168.33 (dd, J<sub>FC</sub>= 234.56 Hz, J= 11.36 Hz, Ar), 161.89 (dd, J<sub>FC</sub>= 240.03 Hz, J= 13.73 Hz, Ar), 151.12 (m, Ar), 150.83 (m, Ar), 149.23 (m, Ar), 138.91 (s, J<sub>PC</sub>= 30.04 Hz, Ar), 134.52 (d, J<sub>PC</sub>= 34.44 Hz, Ar), 131.71 (d, J<sub>PC</sub>= 13.39 Hz, Ar), 130.89 (d, J<sub>PC</sub>= 2.03 Hz, Ar), 130.28 (d, J<sub>PC</sub>= 7.64 Hz, Ar), 129.19 (s, Ar), 128.38 (s, Ar), 122.78 (s, Ar), 120.63 (s, J<sub>PC</sub>= 57.90 Hz, Ar), 104.03 (m, Ar), 100.72 (ddd, J= 21.45 Hz, J=

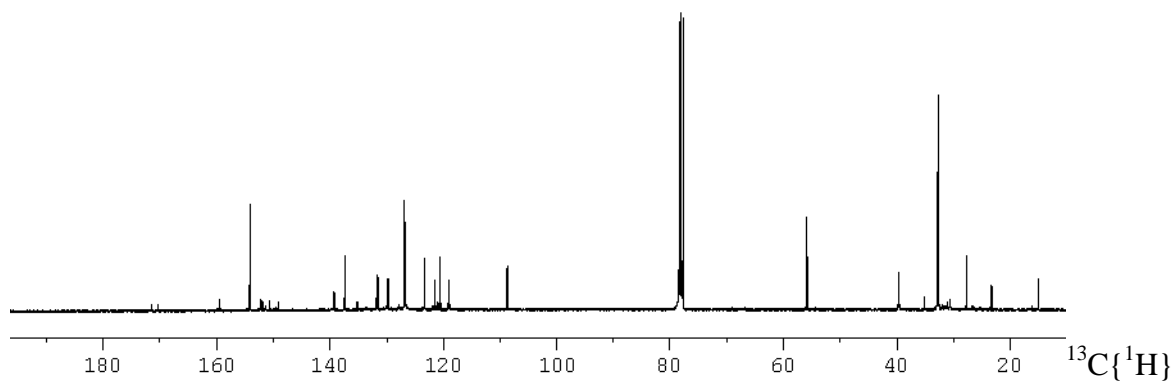
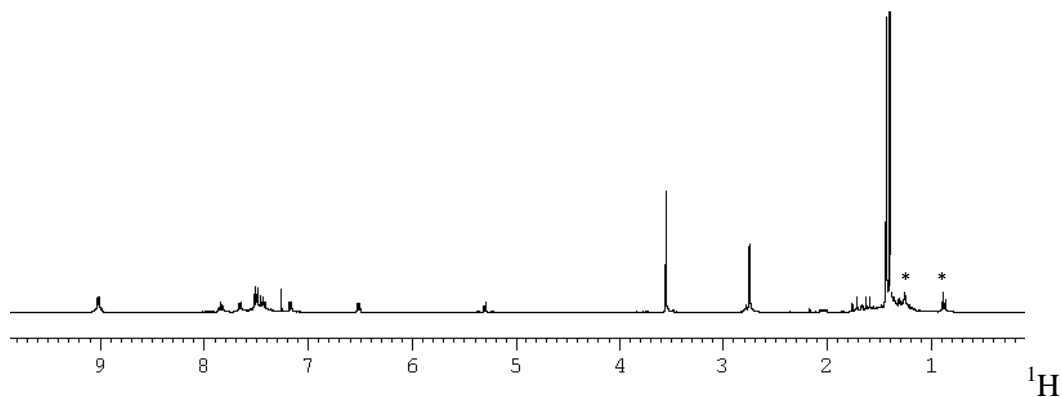
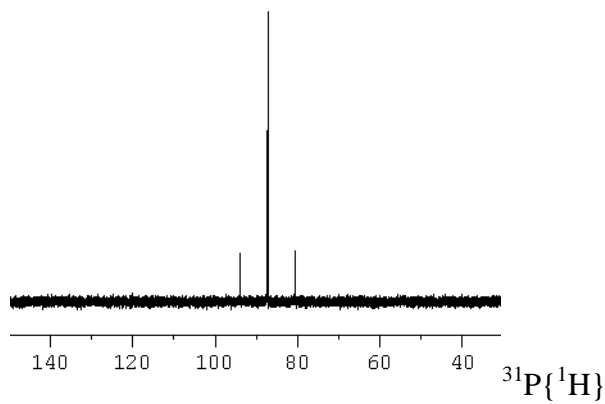
23.04 Hz,  $J = 4.59$  Hz, Ar), 39.12 (d,  $J_{PC} = 13.26$  Hz,  $^t$ Bu), 31.88 (m,  $J_{PC} = 6.39$  Hz,  $^t$ Bu), 27.07 (s, Me-Ar);  $^{31}\text{P}\{^1\text{H}\}$  87.6 (d,  $J_{PF} = 11$  Hz,  $J_{PiP} = 2499$  Hz);  $^{19}\text{F}$  NMR  $-99.0$  (1F, m,  $J_{PF} = 132$  Hz, 3,5- $\text{F}_2\text{C}_6\text{H}_3$ ),  $-118.2$  (1F, m, 3,5- $\text{F}_2\text{C}_6\text{H}_3$ ); HRMS APPI: found for  $\text{C}_{27}\text{H}_{30}\text{F}_2\text{NPt} [\text{M-MeCN}]^+$  (calc.) 591.1520 (591.1524).



**5c:**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  9.02 (2H, m, Py), 7.84 (1H, m, Py), 7.66 (1H, m, Ar), 7.51 (3H, m, Ar+ Py), 7.45 (1H, m, Ar), 7.42 (1H, m, Ar), 7.17 (1H, dd,  $J_{HH} = 8.33$  Hz,  $J_{HH} = 2.52$  Hz, Ar), 6.52 (1H, dd,  $J_{HH} = 8.18$  Hz,  $J_{HH} = 2.62$  Hz, Ar), 5.31 (1H, m,  $J_{PH} = 53.80$  Hz, Ar), 3.55 (3H, m, Ar-OMe), 2.75 (3H, m, Me-Ar), 1.42 (18H, d,  $J_{PH} = 14.28$  Hz  $^t$ Bu);  $^{13}\text{C}\{^1\text{H}\}$  170.03 (d,  $J_{FC} = 106.22$  Hz, Ar), 158.70 (d,  $J_{PC} = 8.90$  Hz,  $J_{PC} = 59.94$  Hz, Ar), 153.31 (m, Py), 151.31 (m, Ar), 151.14 (d,  $J_{PC} = 23.24$  Hz, Ar), 149.83 (m, Ar), 148.29 (m, Ar), 138.45 (m,  $J_{PC} = 27.45$

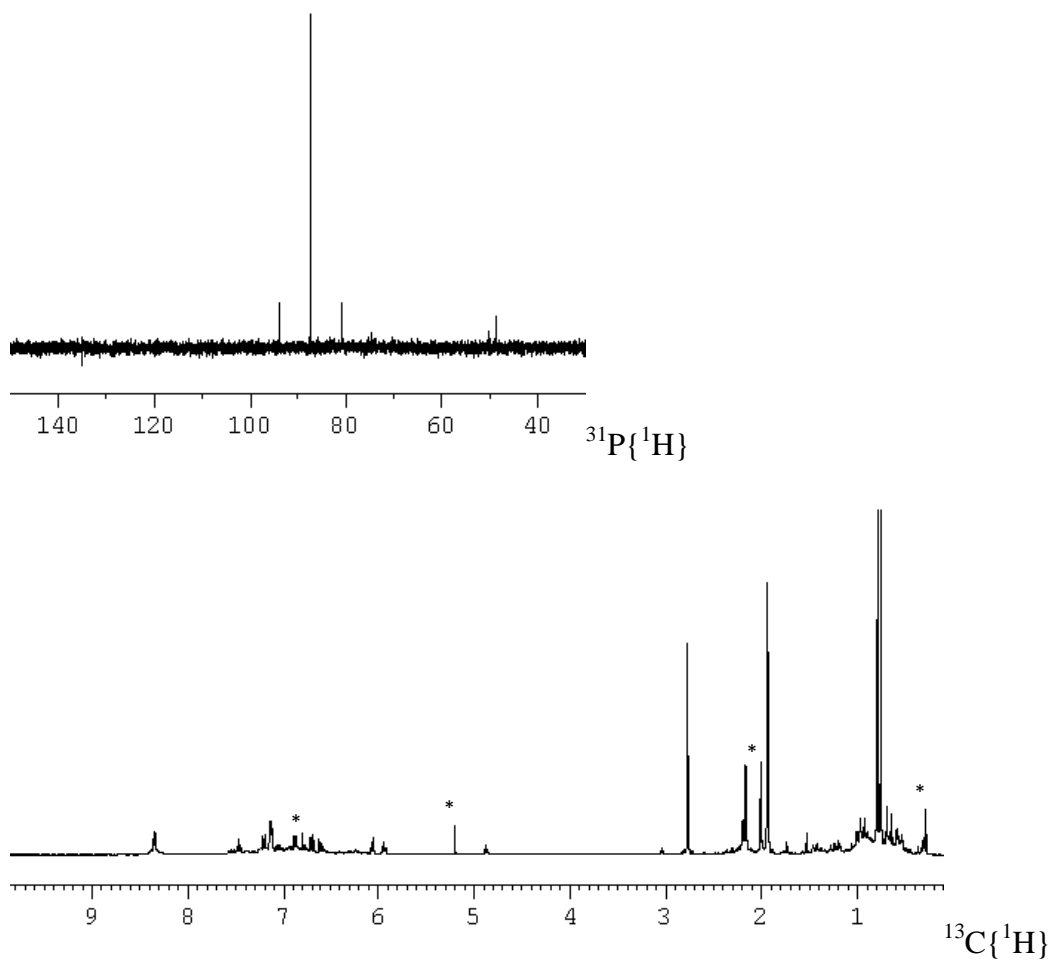


Hz, Ar), 136.62 (s, Py), 134.36 (d,  $J_{PC} = 32.53$  Hz, Ar), 131.00 (d,  $J_{PC} = 13.39$  Hz, Ar), 130.78 (d,  $J_{PC} = 2.03$  Hz, Ar), 129.00 (d,  $J_{PC} = 7.24$  Hz, Ar), 126.25 (s,  $J_{PtC} = 25.56$  Hz, Py), 122.57 (s, Ar), 120.77 (d,  $J_{PC} = 4.50$  Hz,  $J_{PtC} = 65.95$  Hz, Ar), 119.94 (s,  $J_{PtC} = 61.52$  Hz, Ar), 118.24 (m,  $J_{PtC} = 41.33$  Hz, Ar), 108.86 (s, Ar), 54.98 (s, Ar-OMe), 38.80 (d,  $J_{PC} = 11.65$  Hz,  $^t$ Bu), 31.80 (d,  $J_{PC} = 7.01$  Hz,  $^t$ Bu), 26.93 (m, Me-Ar);  $^{31}\text{P}\{^1\text{H}\}$  87.34 (s,  $J_{PtP} = 2167$  Hz); HRMS APPI: found for  $\text{C}_{28}\text{H}_{31}\text{D}_3\text{NOPt} [\text{M-CD}_3\text{CN}]^+$  (calc.) 585.1812 (585.1818).



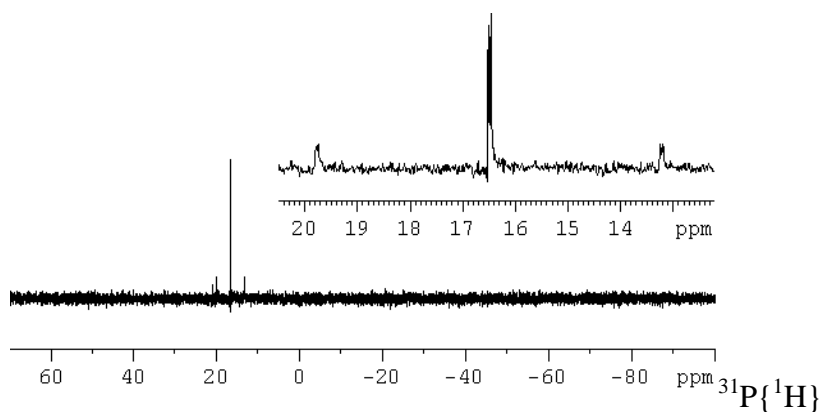
**5d:**  $^1\text{H}$  NMR ( $\text{CD}_3\text{CN}$ )  $\delta$  8.35 (2H, m, Py), 7.47 (1H, m, Py), 7.22 (1H, m, Ar), 7.14 (2H, m, Py), 6.88 (1H, br-d,  $J_{HH} = 8.65$  Hz, Ar), 6.71 (1H, m, Ar), 6.68 (1H, m, Ar), 6.61 (1H, m, Ar), 5.94 (1H, td,  $J_{HH} = 7.31$  Hz,  $J_{HH} =$

1.70 Hz, Ar), 4.87 (1H, t,  $J_{\text{HH}} = 6.70$  Hz,  $J_{\text{PtH}} = 47.36$  Hz, Ar), 2.77 (3H, s, Me-Ar), 2.01 (3H, s, Me-Ar), 0.78 (18H, d,  $J_{\text{PH}} = 14.03$  Hz  $^t\text{Bu}$ );  $^{31}\text{P}\{^1\text{H}\}$  87.26 (s,  $J_{\text{PtP}} = 2109.8$  Hz).



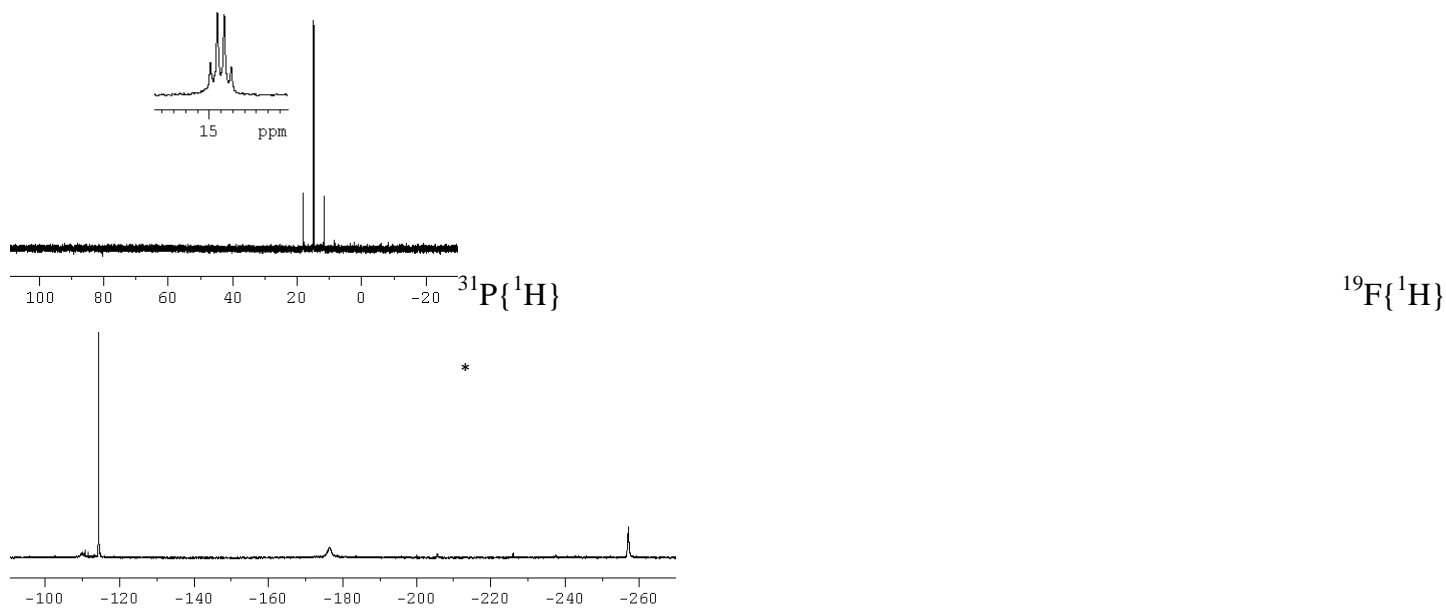
### Characterization of complexes 6

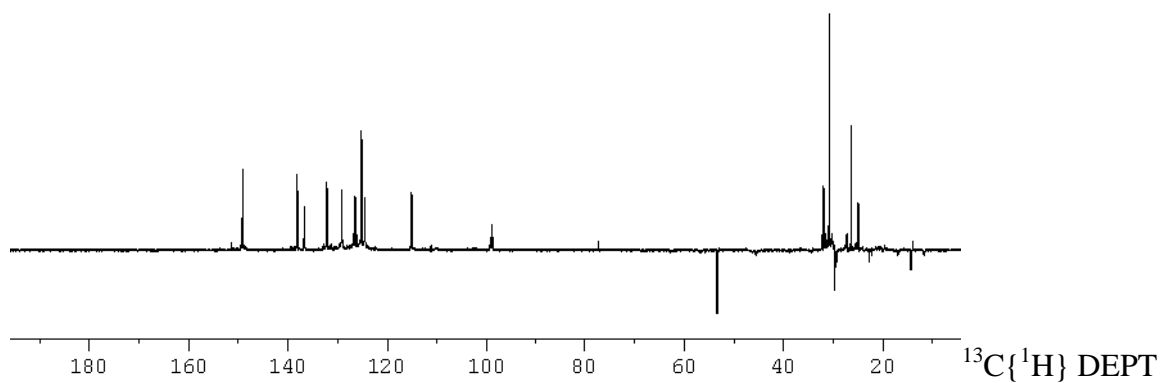
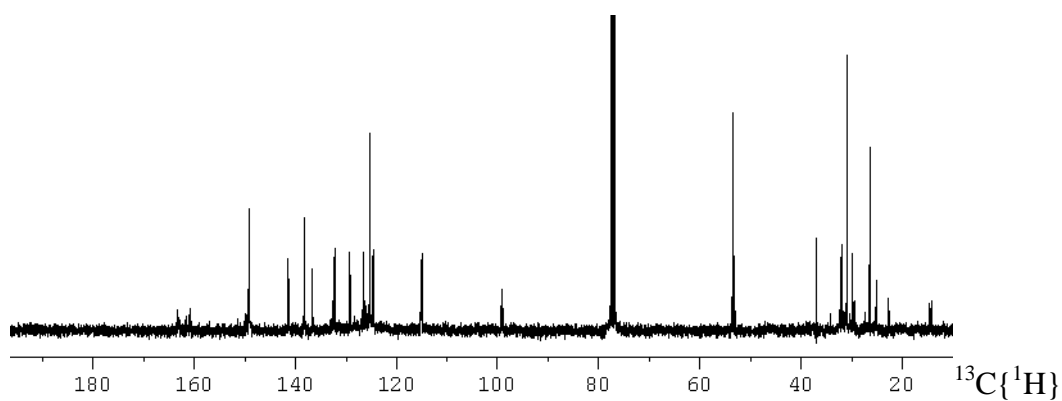
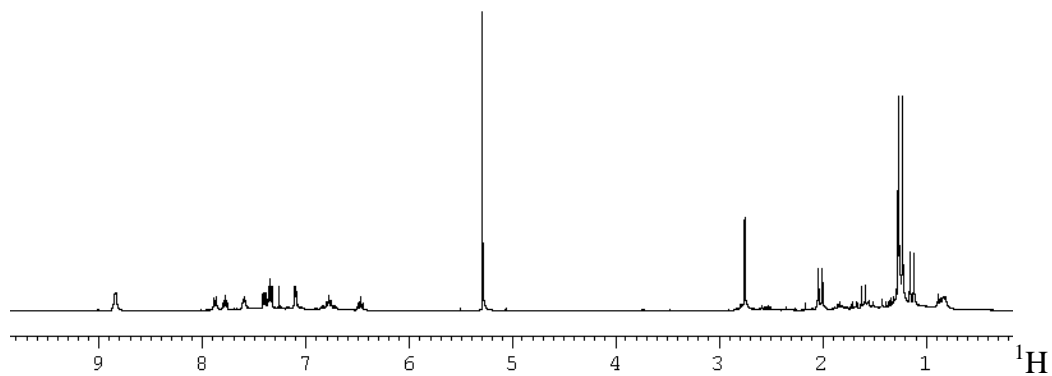
**6a:**  $^{31}\text{P}\{^1\text{H}\}$  16.5 (d,  $J_{\text{FP}} = 7$  Hz,  $J_{\text{PtP}} = 1061$  Hz);  $^{19}\text{F}$  NMR  $-122.6$  (1F, m, 4- $\text{FC}_6\text{H}_4$ ),  $-261.1$  (1F, m, Pt-F);



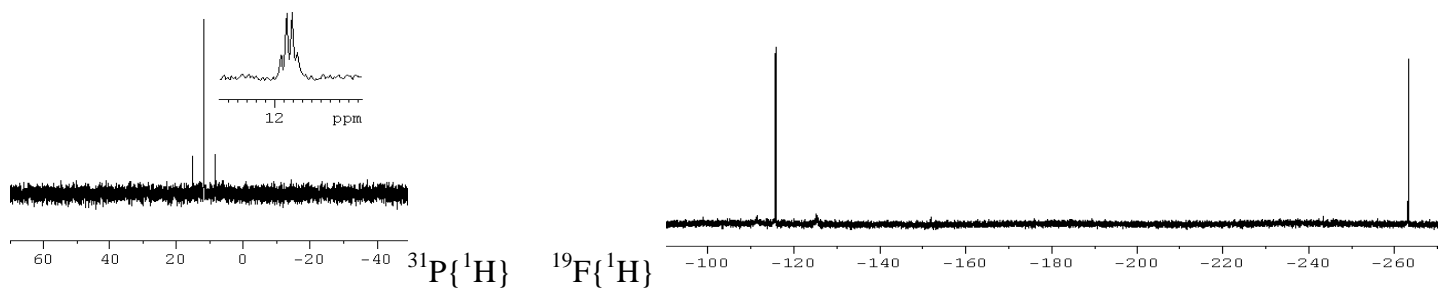


**6b:**  $^1\text{H}$  NMR  $\delta$  8.79 (2H, m, Py), 7.88 (1H, m, Ar), 7.80 (1H, m, Py), 7.60 (1H, m, Ar), 7.41 (1H, dd,  $J_{\text{HH}}=7.82$  Hz,  $J_{\text{HH}}=2.79$  Hz, Ar), 7.36 (2H, m, Py), 7.08 (2H, m, Ar), 6.77 (2H, m, 3,5- $\text{F}_2\text{C}_6\text{H}_3$ ), 6.49 (1H, tt,  $J_{\text{FH}}=9.19$  Hz,  $J_{\text{HH}}=2.07$  Hz, 3,5- $\text{F}_2\text{C}_6\text{H}_3$ ), 2.76 (3H, m, Me-Ar), 2.00 (3H, d,  $J_{\text{PH}}=15.60$  Hz,  $^t\text{Bu}$ ), 1.25 (9H, d,  $J_{\text{PH}}=15.60$  Hz,  $^t\text{Bu}$ ), 1.14 (3H, d,  $J_{\text{PH}}=15.60$  Hz,  $^t\text{Bu}$ ), 0.82 (2H, m,  $\text{CH}_2\text{-Pt}$ );  $^{13}\text{C}\{^1\text{H}\}$  162.14 (dm,  $J_{\text{FC}}=253.58$  Hz, 3,5- $\text{F}_2\text{C}_6\text{H}_4$ ), 161.74 (m, 3,5- $\text{F}_2\text{C}_6\text{H}_4$ ), 149.91 (d,  $J_{\text{PC}}=27.27$  Hz, Ar), 149.30 (m, Py), 141.48 (s,  $J_{\text{PC}}=18.32$  Hz, Ar), 138.37 (s, Ar), 136.78 (s, Py), 132.81 (d,  $J_{\text{PC}}=13.10$  Hz, Ar), 132.37 (m, Ar), 129.40 (d,  $J_{\text{PC}}=7.60$  Hz, Ar), 129.17 (s, Ar), 126.65 (m,  $J_{\text{PC}}=62.08$  Hz, Ar), 125.45 (m, Py), 124.78 (s, Ar), 115.23 (d,  $J_{\text{FC}}=18.02$  Hz, 3,5- $\text{F}_2\text{C}_6\text{H}_3$ ), 99.05 (t,  $J_{\text{FC}}=25.30$  Hz, 3,5- $\text{F}_2\text{C}_6\text{H}_3$ ), 37.00 (m,  $^t\text{Bu}$ ), 34.25 (m,  $^t\text{Bu}$ ), 32.09 (d,  $J_{\text{PC}}=4.20$  Hz,  $^t\text{Bu}$ ), 30.92 (d,  $J_{\text{PC}}=4.44$  Hz,  $^t\text{Bu}$ ), 26.51 (m, Me-Ar), 25.17 (d,  $J_{\text{PC}}=9.65$  Hz,  $^t\text{Bu}$ ), 14.33 (m,  $J_{\text{PC}}=521.47$  Hz,  $\text{CH}_2\text{-Pt}$ );  $^{31}\text{P}\{^1\text{H}\}$  14.9 (m,  $J_{\text{PtP}}=1051$  Hz);  $^{19}\text{F}$  NMR -114.3 (2F, m, 3,5- $\text{F}_2\text{C}_6\text{H}_3$ ), -176.3 (1F, br s, PtF-HF), -257.1 (1F, m, PtF-HF);



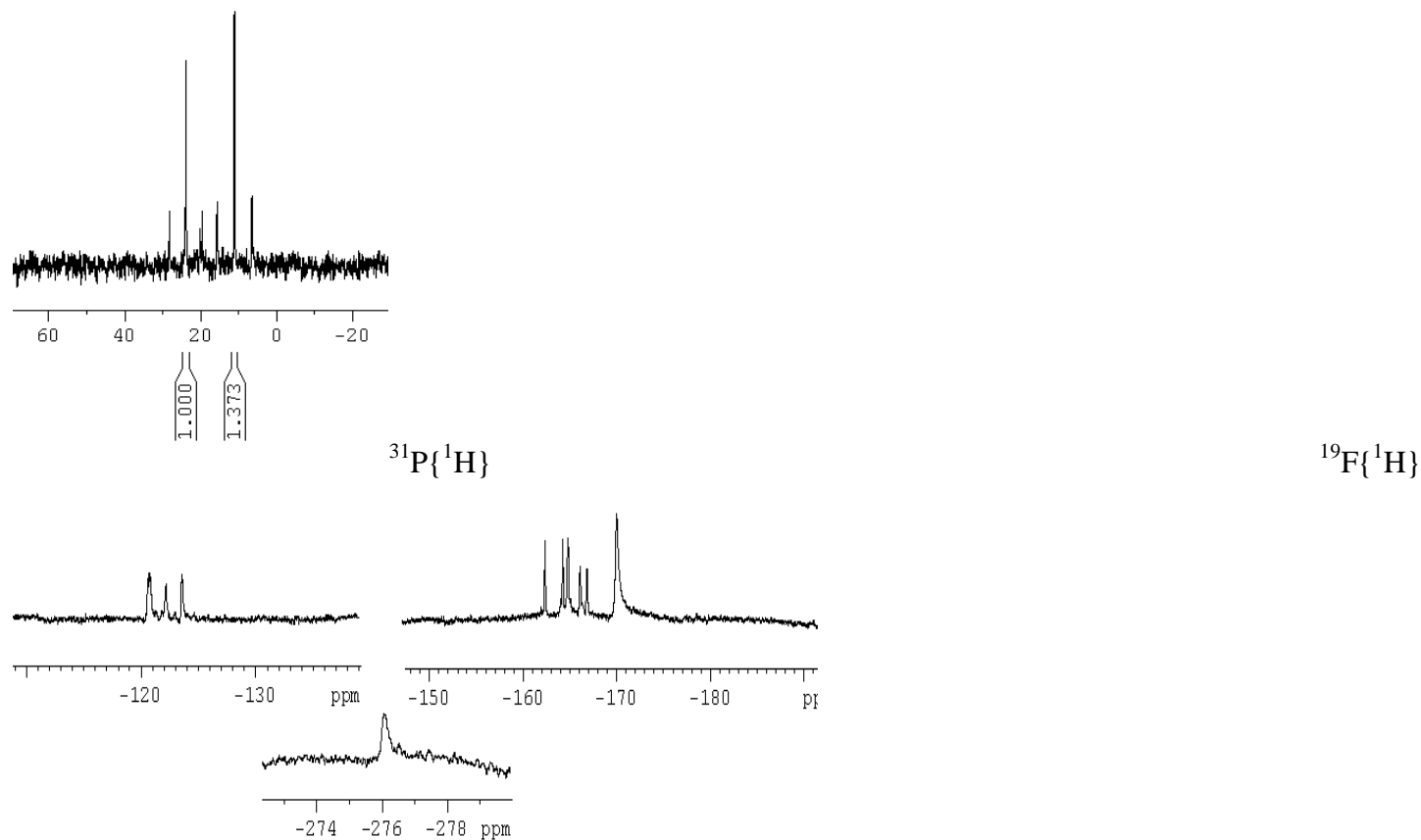


When 1 equiv. of  $(i\text{-Pr})_2\text{NEt}$  was added to a solution of **6b** in  $\text{CD}_3\text{CN}$ , complex **6b'** was formed as evident from the disappearance of the broad signal of  $\text{Pt-F}\cdots\text{HF}$  at  $-177$  ppm and X-ray analysis.

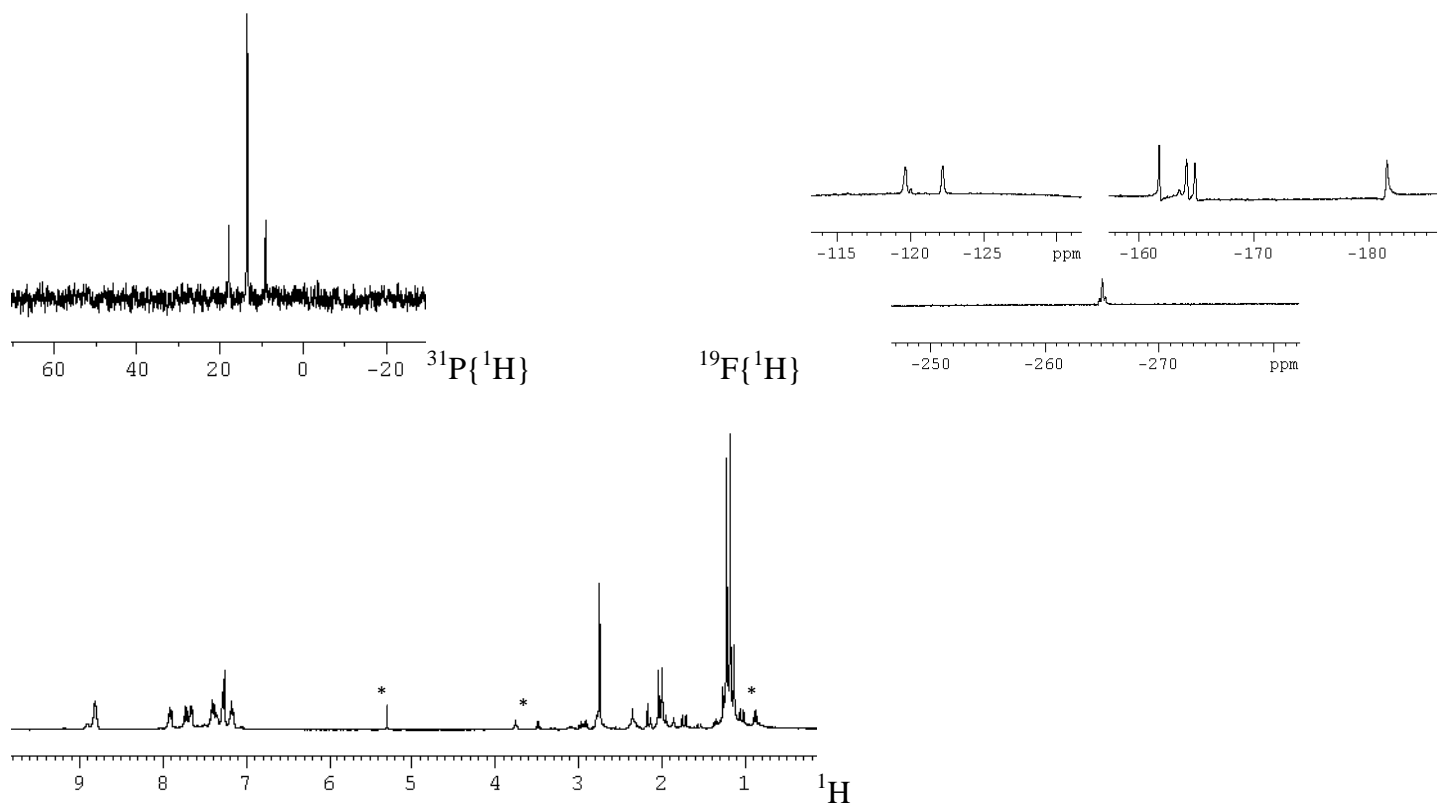


**6e:** This complex was obtained under a typical procedure for fluorination of **3** with XeF<sub>2</sub> and exists as a mixture of two compounds in acetonitrile while only one is observed in CH<sub>2</sub>Cl<sub>2</sub> or chloroform.

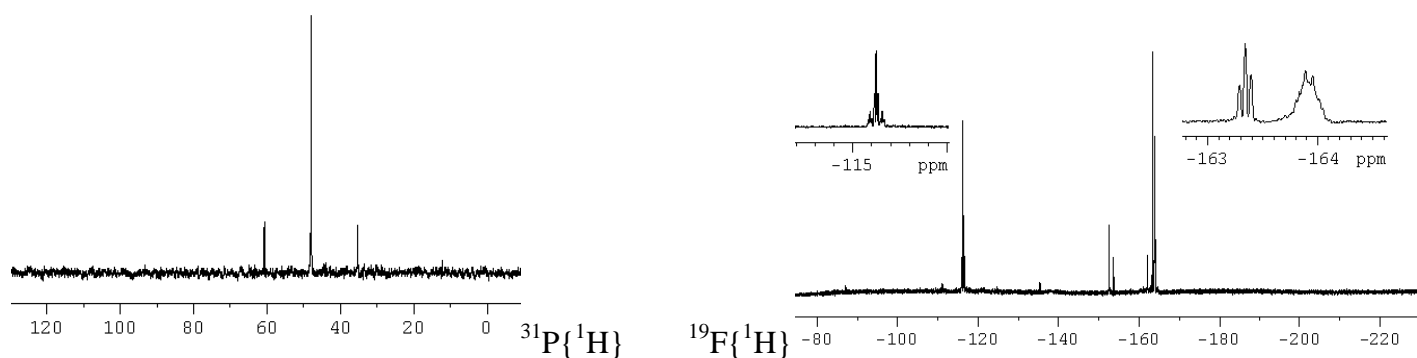
CD<sub>3</sub>CN: <sup>31</sup>P{<sup>1</sup>H} 21.7 (m, J<sub>PtP</sub>= 1379 Hz), 9.0 (m, J<sub>PtP</sub>= 1457 Hz); <sup>19</sup>F NMR -120.4 (2F, m, C<sub>6</sub>F<sub>5</sub>), -121.9 (1F, m, C<sub>6</sub>F<sub>5</sub>), -123.3 (1F, m, C<sub>6</sub>F<sub>5</sub>), -162.3 (1F, m, C<sub>6</sub>F<sub>5</sub>), -164.1 (1F, m, C<sub>6</sub>F<sub>5</sub>), -164.7 (2F, m, C<sub>6</sub>F<sub>5</sub>), -166.0 (1F, m, C<sub>6</sub>F<sub>5</sub>), -166.7 (1F, m, C<sub>6</sub>F<sub>5</sub>), -169.9 (1F, m, PtF-HF), -276.0 (1F, m, J<sub>PtF</sub>= 184 Hz, Pt-F);

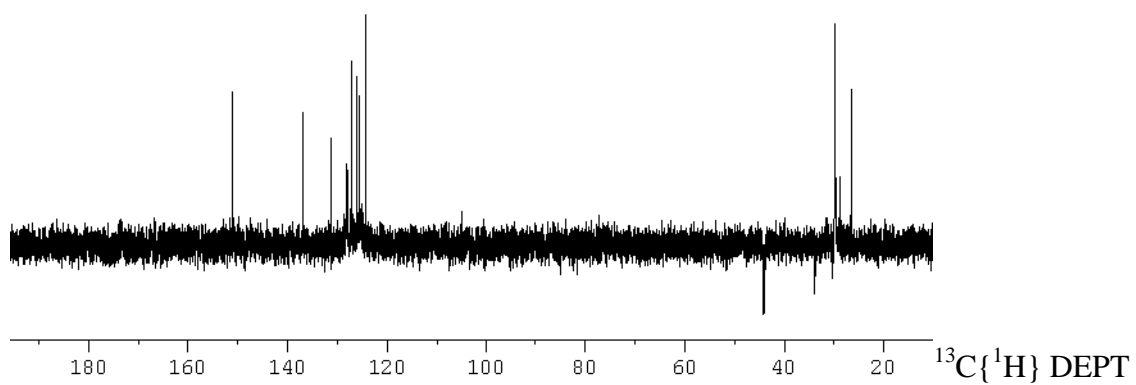
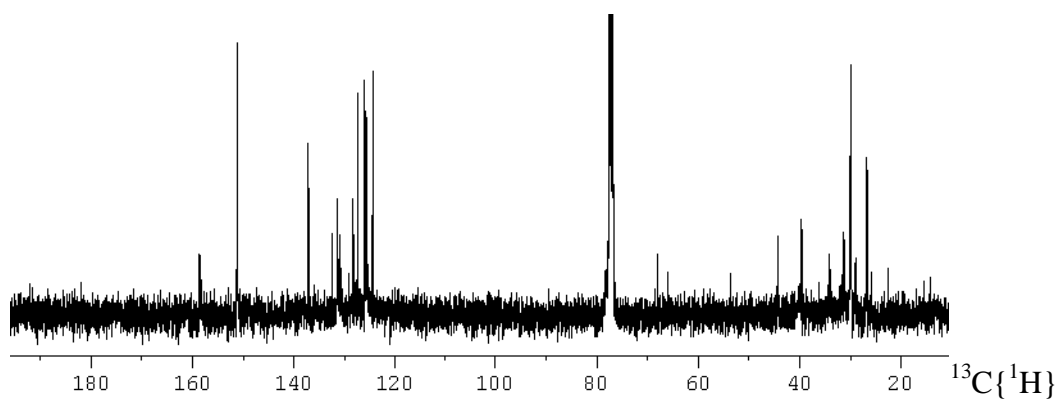
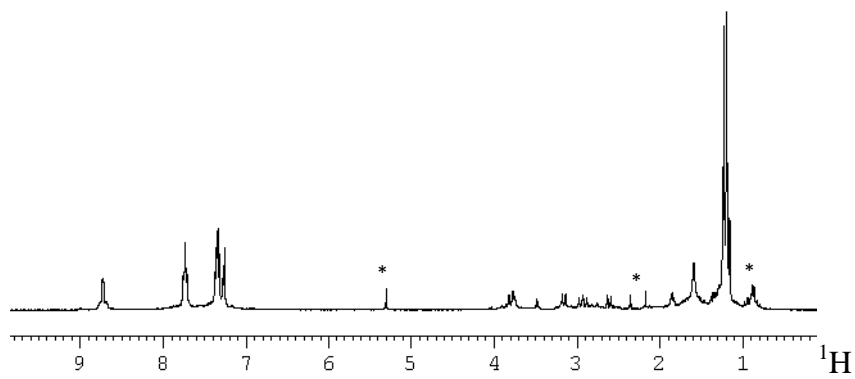


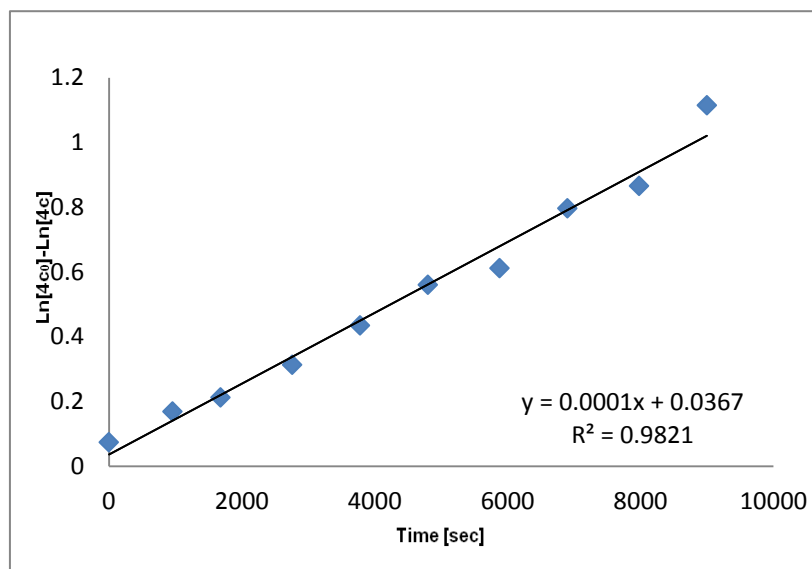
CDCl<sub>3</sub>: <sup>1</sup>H NMR δ 8.82 (2H, m, Py), 7.91 (1H, dm, J<sub>HH</sub>= 8.81 Hz, Ar), 7.73 (1H, m, Py), 7.66 (1H, m, Ar), 7.40 (1H, dd, J<sub>HH</sub>= 8.01 Hz, J<sub>HH</sub>= 2.80 Hz, Ar), 7.30 (2H, m, Py), 7.17 (2H, m, Ar), 2.75 (3H, m, Me-Ar), 2.02 (3H, d, J<sub>PH</sub>= 16.46 Hz, <sup>t</sup>Bu), 1.20 (9H, d, J<sub>PH</sub>= 16.15 Hz, <sup>t</sup>Bu), 1.16 (3H, m, <sup>t</sup>Bu), 1.04 (2H, m, CH<sub>2</sub>-Pt); <sup>31</sup>P{<sup>1</sup>H} 13.4 (m, J<sub>PtP</sub>= 1434 Hz); <sup>19</sup>F NMR -119.6 (1F, m, C<sub>6</sub>F<sub>5</sub>), -122.2 (1F, m, C<sub>6</sub>F<sub>5</sub>), -161.8 (1F, m, C<sub>6</sub>F<sub>5</sub>), -164.2 (1F, m, C<sub>6</sub>F<sub>5</sub>), -165.0 (1F, m, C<sub>6</sub>F<sub>5</sub>), -181.6 (1F, m, PtF-HF), -265.0 (1F, m, J<sub>PtF</sub>= 184 Hz, Pt-F);



**7:**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  8.73 (2H, m, Py), 7.74 (3H, Py+Ar), 7.35 (5H, m, Py+Ar), 3.78 (1H, m,  $-\text{CH}_2-$ ), 3.16 (1H, m,  $-\text{CH}_2-$ ), 2.93 (1H, m,  $-\text{CH}_2-$ ), 2.61 (1H, m,  $-\text{CH}_2-$ ), 1.22 (15H, m,  $^t\text{Bu}$ );  $^{13}\text{C}\{^1\text{H}\}$  158.38 (d,  $J_{\text{PC}}=20.17$  Hz, Ar), 151.10 (s, Py), 137.00 (s, Py), 132.44 (m, Ar), 131.30 (s, Ar), 130.89 (m, Ar), 129.08 (m, Ar), 128.13 (d,  $J_{\text{PC}}=15.30$  Hz, Ar), 127.27 (m, Ar), 126.07 (m, Ar), 125.60 (d,  $J_{\text{PC}}=2.79$  Hz, Ar), 124.31 (s, Py), 44.19 (m,  $-\text{CH}_2-$ ), 39.73 (m,  $^t\text{Bu}$ ), 33.92 (m,  $\text{CH}_2\text{-Pt}$ ), 31.35 (m,  $^t\text{Bu}$ ), 29.85 (m,  $^t\text{Bu}$ ), 26.60 (m,  $^t\text{Bu}$ );  $^{31}\text{P}\{^1\text{H}\}$  48.0 (s,  $J_{\text{PP}}=4144$  Hz); problem  $^{19}\text{F}$  NMR -116.2 (2F, m,  $J_{\text{PF}}=243$  Hz,  $\text{C}_6\text{F}_5$ ), -163.3 (1F, m,  $\text{C}_6\text{F}_5$ ), -163.9 (2F, m,  $\text{C}_6\text{F}_5$ );







**Figure S1.** First-order kinetics in the conversion of **4c** to **5c** followed by the  $^{31}\text{P}$  NMR spectroscopy in  $\text{CD}_3\text{CN}$  at 298 K.



**DFT-optimized geometries for MeCN, pyridine, py-HF, py-(HF)<sub>2</sub>, complexes 4b, 4c, 5b, 8-15, TS<sub>Pt-C8</sub>, TS<sub>σ-π</sub>, TS<sub>C8-C7</sub> (Ar = 3,5-difluorophenyl and Ar = 4-methoxyphenyl), TS<sub>CHF</sub> and TS<sub>CH-Pt</sub> for gas phase and MeCN solutions**

Drawings are given for all metal complexes with geometry optimized in MeCN solution.

Total solution phase Gibbs energy in MeCN (G<sub>tot</sub>) for 298K is given in Hartrees (1 Hartree = 627.51 kcal/mol).

Reaction Gibbs energies in kcal/mol were calculated as  $627.51 * [\Sigma(G_{tot})_{products} - \Sigma(G_{tot})_{reactants}]$

**MeCN, gas phase**

Total Gibbs free energy, G<sub>tot</sub> (H<sub>tot</sub> - T\*S): -132.563057 hartrees

C1	-0.0020533289	-0.1622928395	0.0000000000
N2	-0.0174520205	-1.3352946620	0.0000000000
C3	0.0169133719	1.2970889583	0.0000000000
H4	1.0544888475	1.6670986946	0.0000000000
H5	-0.4944701739	1.6870650366	0.8943243650
H6	-0.4944701739	1.6870650366	-0.8943243650

**MeCN, acetonitrile solution**

Total Gibbs free energy, G<sub>tot</sub> (H<sub>tot</sub> - T\*S): -132.575749 hartrees

The solvation energy: -7.9133 kcal/mol

C1	-0.0017362016	-0.1590720835	0.0000000000
N2	-0.0173501115	-1.3339031188	0.0000000000
C3	0.0170394715	1.2949070476	0.0000000000
H4	1.0595115977	1.6579469403	0.0000000000
H5	-0.4967337234	1.6776139855	0.8989389092
H6	-0.4967337234	1.6776139855	-0.8989389092

**Pyridine, gas phase**

Total Gibbs free energy, G<sub>tot</sub> (H<sub>tot</sub> - T\*S): -247.910559 hartrees

C1	-0.3439527491	1.0579033802	0.3774567028
C2	-1.3116173257	0.0454499612	0.3649277710
H3	-0.6059566806	2.0788555713	0.6725994617
C4	0.9665971142	0.7342308982	0.0043120277
C5	-0.9218155627	-1.2452254897	-0.0214617056
H6	-2.3488642932	0.2482803553	0.6478058414
H7	1.7579314295	1.4897412574	-0.0019294058
C8	1.2476139066	-0.5894368093	-0.3645924451
N9	0.3320998522	-1.5767209618	-0.3835828042
H10	-1.6570338769	-2.0600972382	-0.0415817569
H11	2.2650382191	-0.8743770347	-0.6623020925

### Pyridine, acetonitrile solution

Total Gibbs free energy, Gtot (Htot - T\*S): -247.919329 hartrees

The solvation energy: -5.5562 kcal/mol

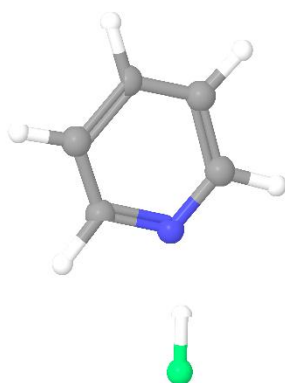
C1	-0.3457435132	1.0607581179	0.3715667745
C2	-1.3152834968	0.0468947626	0.3588991846
H3	-0.6076431645	2.0823682417	0.6675716909
C4	0.9669858765	0.7369457345	-0.0025053746
C5	-0.9282647677	-1.2451957325	-0.0270711965
H6	-2.3542893756	0.2475200413	0.6418587734
H7	1.7607137978	1.4918025987	-0.0096145004
C8	1.2511539210	-0.5863691062	-0.3717164259
N9	0.3314206414	-1.5780040439	-0.3904588061
H10	-1.6668430603	-2.0569278883	-0.0457164970
H11	2.2699884242	-0.8669786012	-0.6682394335

### Pyridine-HF, gas phase

Total Gibbs free energy, Gtot (Htot - T\*S): -348.251826 hartrees

C1	-0.3778691852	1.3627226528	0.4010723263
C2	-1.4374985220	0.4465980386	0.4300921754
H3	-0.5391822925	2.4083533342	0.6801962670
C4	0.8908012824	0.9163748774	0.0085384037
C5	-1.1850826325	-0.8816216425	0.0646763893
H6	-2.4436389265	0.7515027736	0.7299738861
H7	1.7456740436	1.5968230584	-0.0284400683
C8	1.0475585841	-0.4293684604	-0.3389572221
N9	0.0313789383	-1.3161381389	-0.3131629581
H10	-1.9850839190	-1.6302210647	0.0733800221
H11	2.0074069390	-0.8511035163	-0.6547947305
H12	0.8172167415	-2.7027048571	-0.8082831719
F13	1.5915604140	-3.2063848869	-1.0980019868

### Pyridine-HF, acetonitrile solution



Total Gibbs free energy, Gtot (Htot - T\*S): -348.266784 hartrees

C1	-0.3649159705	1.4090490546	0.4179763721
C2	-1.2961224156	0.3592392706	0.3901775417

H3	-0.6696922616	2.4166138932	0.7214385045
C4	0.9637464046	1.1469120960	0.0495827489
C5	-0.8599930384	-0.9110227990	-0.0045065376
H6	-2.3423971608	0.5177799619	0.6697928991
H7	1.7221469369	1.9361577074	0.0571103277
C8	1.3125025127	-0.1553911937	-0.3317742446
N9	0.4183248923	-1.1676553770	-0.3596187575
H10	-1.5467219419	-1.7647773740	-0.0442474053
H11	2.3387127093	-0.4043727090	-0.6270069388
H12	0.6193563627	-2.6582089366	-0.7450219911
F13	0.5849325005	-3.6315285993	-0.9573986226

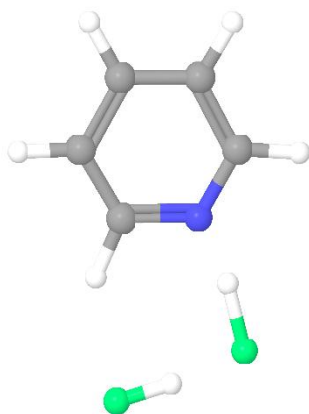
### Pyridine-(HF)<sub>2</sub>, gas phase

Total Gibbs free energy, Gtot (Htot - T\*S): -448.604169 hartrees

C1	-0.6078906333	1.3408526575	0.2628994939
C2	-1.2762377546	0.1281328050	0.0537400820
H3	-1.1684316330	2.2543877181	0.4829696531
C4	0.7916019179	1.3681612106	0.1866393200
C5	-0.5266674012	-1.0194408800	-0.2247032868
H6	-2.3660928136	0.0648084791	0.1047606926
H7	1.3515993539	2.2934383576	0.3436049938
C8	1.4687563037	0.1783981992	-0.0963455878
N9	0.8229325654	-0.9869564381	-0.2970086423
H10	-0.9730540284	-2.0083222623	-0.4001480210
H11	2.5608361076	0.1444601182	-0.1665617200
H12	1.4062302036	-2.2896652247	-0.5911404075
F13	1.6307564185	-3.2752347438	-0.7993214064
H14	0.2171654537	-3.8169702629	-0.8274677549
F15	-0.7446609656	-3.9607571682	-0.8012752274

### Pyridine-(HF)<sub>2</sub>, acetonitrile solution

Time: pyridine\_HF2\_in\_MCN



Total Gibbs free energy, Gtot (Htot - T\*S): -448.620652 hartrees

C1	-0.5949202932	1.3551747629	0.2697749578
C2	-1.2943888055	0.1557791436	0.0609080873
H3	-1.1373639895	2.2797836696	0.4952488273

C4	0.8075165953	1.3582372036	0.1869660850
C5	-0.5690239380	-1.0031081127	-0.2237524449
H6	-2.3864058159	0.1135374356	0.1179380630
H7	1.3843908051	2.2744310950	0.3445824324
C8	1.4701509772	0.1611361358	-0.1016810528
N9	0.7821503149	-0.9847965312	-0.3003305251
H10	-1.0254775088	-1.9847224010	-0.3970834099
H11	2.5610879697	0.0979654072	-0.1800161405
H12	1.3005778125	-2.0917406200	-0.5470694359
F13	1.5941981332	-3.2140163590	-0.7786762608
H14	0.3012781742	-3.7709531726	-0.8182658772
F15	-0.6568445603	-4.0595606882	-0.8208964392

#### 4b, gas phase

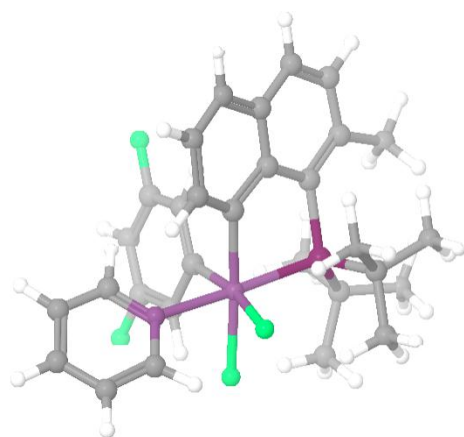
Total Gibbs free energy, Gtot (Htot - T\*S): -2075.756885 hartrees

Pt1	8.0454877703	9.2165679353	4.2555212392
P2	7.9591163806	8.2166426067	2.1363063340
F3	6.1374329408	8.8238280725	5.0243670179
F4	8.5613559611	7.4553583167	5.2505676791
C5	8.6017245732	6.3967590815	2.2240321940
C6	8.8206148889	5.7994655534	0.8183183561
H7	9.2024430481	4.7714147754	0.9522398517
H8	9.5896984303	6.3576057885	0.2606358730
H9	7.9096134514	5.7313442279	0.2089955804
C10	9.9685342064	6.3826309438	2.9439766112
H11	9.8682437539	6.7605811627	3.9717950309
H12	10.7343063648	6.9533437592	2.3961372771
H13	10.3036509088	5.3299032134	2.9845066047
C14	7.5933106686	5.5670763213	3.0439472907
H15	7.9905898172	4.5403782426	3.1417891332
H16	6.6066256845	5.4915259514	2.5606187719
H17	7.4917696967	5.9972829540	4.0530579699
C18	6.2022619835	8.3403690304	1.3219251378
C19	5.1418886803	8.0108626342	2.4024555824
H20	4.1648799917	8.3608671098	2.0219126013
H21	5.3402052878	8.4756635064	3.3832710714
H22	5.0571134303	6.9244735072	2.5637319759
C23	5.9446193132	7.3773364868	0.1429245238
H24	5.9788915862	6.3234962789	0.4574444856
H25	6.6107657686	7.5149151859	-0.7174629365
H26	4.9142910399	7.5702115472	-0.2063049526
C27	6.0072011888	9.8022312402	0.8617178573
H28	6.8133271717	10.1699576213	0.2088415061
H29	5.9314209282	10.4849683722	1.7179749078
H30	5.0593009923	9.8593342145	0.2976610949
N31	8.2031630597	10.0672917949	6.2417595685
C32	7.8176673999	9.2334528838	7.2322163554
H33	7.6107891017	8.2106383687	6.9066878531
C34	7.7350872309	9.6796344858	8.5535914021
H35	7.4192835995	8.9831301818	9.3343689555
C36	8.0537159248	11.0104462026	8.8482485221
H37	7.9890192501	11.3838094475	9.8749332533
C38	8.4563593831	11.8589107457	7.8084128488
H39	8.7142198175	12.9049464084	7.9919901815
C40	8.5156627249	11.3518458698	6.5084444513
H41	8.8062673908	11.9636492667	5.6501837652
C42	7.3886789138	11.0704575444	3.6231062273
C43	6.1090085573	11.4449637757	4.0883082117
H44	5.5173184468	10.7290667329	4.6660440304
C45	5.6197968415	12.7187614994	3.7903598330
C46	6.3385078390	13.6593254178	3.0453064472
H47	5.9372795919	14.6493102440	2.8240836884

C48	7.6026987591	13.2600052179	2.6089918627
C49	8.1440325817	11.9972803328	2.8785550514
H50	9.1385338856	11.7724976711	2.4938817296
F51	4.3885825602	13.0691960300	4.2405352909
F52	8.3429873760	14.1398891136	1.8870086941
C53	9.9429066598	9.6235314865	3.6727451910
C54	10.9233817859	9.9629500393	4.5995157788
H55	10.6987391031	9.9206781449	5.6681567604
C56	12.2183772942	10.3764789816	4.1921307729
H57	12.9580564658	10.6441796119	4.9539222344
C58	12.5351055161	10.4666234003	2.8496485663
H59	13.5169946057	10.8222429651	2.5211865292
C60	11.5796654474	10.0830918214	1.8667757088
C61	11.8646039598	10.1599785401	0.4786790898
H62	12.8374682285	10.5467403336	0.1568490576
C63	10.9301054919	9.7562569784	-0.4524291772
H64	11.1622412567	9.8361146952	-1.5195854790
C65	9.6682935196	9.1987875974	-0.0847281723
C66	9.3501133303	9.1190560082	1.2832113783
C67	10.2791126533	9.6083596340	2.2745453939
C68	8.7924972721	8.7407240771	-1.2296573968
H69	8.5911670335	7.6586509455	-1.1933111553
H70	9.2893294276	8.9451042520	-2.1903813793
H71	7.8213873683	9.2594218908	-1.2484045262

#### 4b, acetonitrile solution

Totals: 2075.781772 hartrees



Total Gibbs free energy, Gtot (Htot - T\*S): -2075.781772 hartrees

Pt1	8.0350016631	9.1880121935	4.2809769573
P2	7.9526824158	8.2171605155	2.1219640327
F3	6.1041465663	8.7714548632	5.0673628510
F4	8.5547796001	7.4138866736	5.2983785765
C5	8.5975152549	6.3930672389	2.1704905771
C6	8.8390658265	5.8282319842	0.7542179513
H7	9.2286772012	4.8002797526	0.8722378250
H8	9.6091908991	6.4044407032	0.2166576502
H9	7.9359483241	5.7650245154	0.1329400006
C10	9.9518820989	6.3687218959	2.9119565428

H11	9.8293768669	6.7275666436	3.9442436540
H12	10.7199498930	6.9612394446	2.3911188811
H13	10.2953664451	5.3179036506	2.9324287371
C14	7.5852948751	5.5355214437	2.9569311120
H15	7.9892017131	4.5089792241	3.0338151631
H16	6.6043384847	5.4639487330	2.4612646799
H17	7.4682436701	5.9405268893	3.9748296167
C18	6.1975159854	8.3534439959	1.2934283837
C19	5.1338342509	8.0143829590	2.3677096103
H20	4.1557728497	8.3570892876	1.9822342606
H21	5.3270093740	8.4816714383	3.3475242044
H22	5.0583351639	6.9261514884	2.5243378610
C23	5.9502179906	7.3985535245	0.1039410410
H24	5.9861751642	6.3402245806	0.4043550658
H25	6.6205613298	7.5508465059	-0.7510219711
H26	4.9212261556	7.5938332645	-0.2503864331
C27	5.9981741062	9.8165315808	0.8372348294
H28	6.8025299590	10.1851774403	0.1832759211
H29	5.9186068105	10.4984008529	1.6935814981
H30	5.0506818478	9.8692411150	0.2708994652
N31	8.2196720928	10.0942678712	6.2606034434
C32	7.8493376233	9.3106687686	7.2987794020
H33	7.6154196652	8.2773691839	7.0328807011
C34	7.8104895954	9.8056026301	8.6061201511
H35	7.5059393727	9.1429413021	9.4227370081
C36	8.1630637682	11.1425377664	8.8421534694
H37	8.1358521615	11.5559066687	9.8565420342
C38	8.5554315667	11.9411598683	7.7573852150
H39	8.8450191470	12.9883191247	7.8920513431
C40	8.5690732814	11.3826812954	6.4759142085
H41	8.8613786008	11.9610727368	5.5952991767
C42	7.3731873189	11.0300806422	3.6268849378
C43	6.0881632966	11.4031255528	4.0780698836
H44	5.5001609214	10.6943307534	4.6674247892
C45	5.5847363838	12.6632386376	3.7464354845
C46	6.2885598016	13.5992572553	2.9812682370
H47	5.8739806048	14.5799515837	2.7318021370
C48	7.5599883931	13.1998029599	2.5643677745
C49	8.1182551160	11.9515803178	2.8650698194
H50	9.1165694374	11.7312977684	2.4871622085
F51	4.3416192362	13.0031222171	4.1852443439
F52	8.2965067576	14.0708179890	1.8222298944
C53	9.9382389630	9.5986475936	3.7001860535
C54	10.9185555370	9.9172865113	4.6367504641
H55	10.6908010570	9.8707369594	5.7049797171
C56	12.2226329752	10.3259164931	4.2423102768
H57	12.9611942171	10.5765818526	5.0128792571
C58	12.5416515148	10.4367548605	2.8998178634
H59	13.5273836437	10.7918306861	2.5766895598
C60	11.5820797272	10.0783046395	1.9077078476

C61	11.8746032263	10.1849199485	0.5203099036
H62	12.8522937478	10.5728257470	0.2090145271
C63	10.9390928320	9.8076158152	-0.4226994296
H64	11.1763053188	9.9101698327	-1.4881798418
C65	9.6711479046	9.2461954679	-0.0721722092
C66	9.3482115709	9.1375236402	1.2946359774
C67	10.2760108650	9.6022082612	2.3011984111
C68	8.8062849870	8.8170942549	-1.2389301218
H69	8.5866965447	7.7378316338	-1.2236464727
H70	9.3252153597	9.0258367791	-2.1879045244
H71	7.8439158301	9.3527747268	-1.2733077293



#### 4c, gas phase

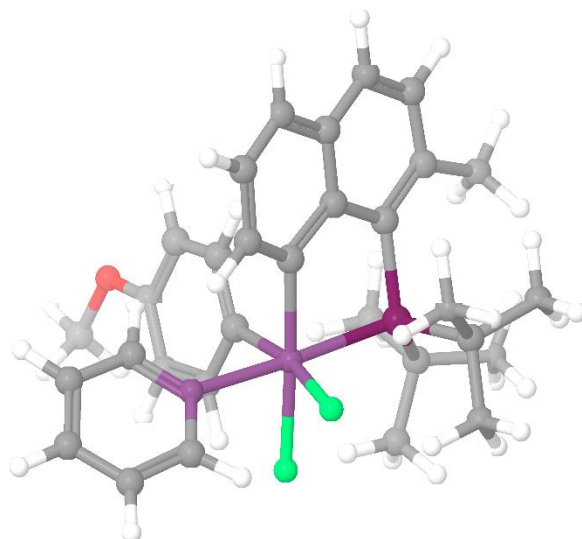
Total Gibbs free energy, Gtot (Htot - T\*S): -1991.807605 hartrees

Pt1	-0.1383296831	-0.1021379548	1.3976141363
P2	-0.2915956453	-1.0355184472	-0.7429037621
F3	-2.0361357771	-0.4979035722	2.1906148530
F4	0.3717323612	-1.8969379814	2.3577912798
C5	0.2826331504	-2.8789071637	-0.7066660334
C6	0.4496673030	-3.4674752122	-2.1228425045
H7	0.7913043514	-4.5119273771	-2.0077000675
H8	1.2311362599	-2.9352251628	-2.6885384194
H9	-0.4741390512	-3.4912322066	-2.7159632035
C10	1.6631560776	-2.9553675549	-0.0166090941
H11	1.5974922447	-2.5932901278	1.0201769294
H12	2.4374155021	-2.4026100680	-0.5711930333
H13	1.9608116395	-4.0200562603	-0.0013259690
C14	-0.7390337048	-3.6794675713	0.1261102719
H15	-0.3869823052	-4.7250943236	0.1925044544
H16	-1.7419958133	-3.6993681674	-0.3288411263
H17	-0.7911682121	-3.2654741409	1.1460164863
C18	-2.0495041740	-0.8224551291	-1.5374628598
C19	-3.1130215483	-1.1229724868	-0.4513148734
H20	-4.0744487508	-0.7096210375	-0.8073800471
H21	-2.8765866009	-0.7021858418	0.5408423986
H22	-3.2545426014	-2.2078567027	-0.3201269252
C23	-2.3610308166	-1.7556284483	-2.7273363747
H24	-2.3670140688	-2.8148223549	-2.4292714761
H25	-1.6997745735	-1.6321026646	-3.5935901257
H26	-3.3863553684	-1.5146456226	-3.0614904572
C27	-2.1832666700	0.6529882964	-1.9774360006
H28	-1.3701328138	0.9891794186	-2.6386067484
H29	-2.2116862375	1.3295574593	-1.1136538711
H30	-3.1354202990	0.7599625835	-2.5273779698
N31	0.0720008924	0.7088680979	3.3925723181
C32	-0.2976762715	-0.1357669442	4.3795743369
H33	-0.5227485186	-1.1511637001	4.0419343290
C34	-0.3411520487	0.2915586222	5.7092219945
H35	-0.6457073635	-0.4123937681	6.4878479523
C36	0.0029474656	1.6136437317	6.0153150978
H37	-0.0290464609	1.9718471924	7.0490195180
C38	0.3894541017	2.4728533612	4.9781718986
H39	0.6672804674	3.5122522321	5.1706036894
C40	0.4070537280	1.9854161385	3.6694005008
H41	0.6782265135	2.6065146533	2.8115603454
C42	-0.7829730419	1.7795304995	0.8220219578
C43	-2.0473231145	2.1659928123	1.3095957045
H44	-2.6248426783	1.4298733698	1.8778102326
C45	-2.5685900817	3.4486761790	1.0707422361
C46	-1.8190731244	4.3847415468	0.3358489001
O47	-2.2261803607	5.6632425955	0.0383185207

C48	-0.5485448127	4.0172187809	-0.1438805617
C49	-0.0395013366	2.7341567729	0.0956444984
H50	0.9490286200	2.4905844382	-0.2997846856
H51	-3.5570339070	3.7001779361	1.4649779362
H52	0.0293324542	4.7536884841	-0.7109119295
C53	1.7532908240	0.2864836514	0.7925775009
C54	2.7561277085	0.5852862217	1.7102470807
H55	2.5454763509	0.5304335047	2.7810901779
C56	4.0568714004	0.9689009500	1.2926945309
H57	4.8136397218	1.2030962853	2.0489104348
C58	4.3599411653	1.0688569180	-0.0522959263
H59	5.3485868832	1.3977623289	-0.3886876371
C60	3.3811662089	0.7269748397	-1.0275822095
C61	3.6542641410	0.8099718984	-2.4175048096
H62	4.6364403967	1.1674928597	-2.7453562494
C63	2.6983723029	0.4444237848	-3.3424646632
H64	2.9231328066	0.5257182659	-4.4111210387
C65	1.4236989138	-0.0769796094	-2.9669519155
C66	1.1171496991	-0.1631756938	-1.5967829243
C67	2.0715097151	0.2855615243	-0.6103470275
C68	0.5247111270	-0.4942159937	-4.1102298534
H69	0.2676737074	-1.5639674349	-4.0704860136
H70	1.0314371691	-0.3190938050	-5.0718237291
H71	-0.4188124275	0.0737217514	-4.1317048892
C72	-3.5131347401	6.0568450187	0.5004743328
H73	-3.6535811184	7.0928670237	0.1594064957
H74	-4.3153250670	5.4227731823	0.0766080925
H75	-3.5831962478	6.0256460980	1.6048130659

#### 4c, acetonitrile solution

Titled: rpl0\_Pf2\_06HOMe\_pfc\_MeCN



Total Gibbs free energy, Gtot (Htot - T\*S): -1991.836051 hartrees

Pt1	-0.1522772157	-0.1234628855	1.4148551663
P2	-0.3012623667	-1.0273355747	-0.7650673628
F3	-2.0699443695	-0.5533509492	2.2292147247

F4	0.3619169198	-1.9351199141	2.4024215767
C5	0.2632115971	-2.8781721611	-0.7686489999
C6	0.4507052645	-3.4351948431	-2.1958958290
H7	0.7903719411	-4.4828978474	-2.0982293136
H8	1.2396036359	-2.8913251562	-2.7399130985
H9	-0.4647334216	-3.4451360705	-2.8022004538
C10	1.6296394291	-2.9739212878	-0.0553438441
H11	1.5410039756	-2.6317883657	0.9866787580
H12	2.4115449325	-2.4030473754	-0.5800864549
H13	1.9295338977	-4.0383717241	-0.0629103062
C14	-0.7707974647	-3.6993011920	0.0283569411
H15	-0.4208735904	-4.7474772307	0.0718857623
H16	-1.7678808402	-3.7068026069	-0.4399272382
H17	-0.8370050514	-3.3108405564	1.0574400543
C18	-2.0525193231	-0.7888951585	-1.5779553519
C19	-3.1256019362	-1.0894792107	-0.5010807562
H20	-4.0820266085	-0.6660083386	-0.8596525757
H21	-2.8889369006	-0.6773079475	0.4938653192
H22	-3.2745386063	-2.1754592588	-0.3835209744
C23	-2.3579180544	-1.7105731494	-2.7800797967
H24	-2.3713940968	-2.7745045505	-2.4980649730
H25	-1.6891079844	-1.5761632420	-3.6393350060
H26	-3.3791026139	-1.4586184967	-3.1210636077
C27	-2.1740504909	0.6887988392	-2.0148076058
H28	-1.3565360373	1.0151348816	-2.6753133875
H29	-2.2004817429	1.3653628343	-1.1511089864
H30	-3.1230356260	0.8013783255	-2.5699854086
N31	0.0947854643	0.7524400389	3.3994126017
C32	-0.2514414303	-0.0407850068	4.4380066348
H33	-0.5071282452	-1.0668432827	4.1630951409
C34	-0.2382473775	0.4356132284	5.7529621980
H35	-0.5255990836	-0.2336065284	6.5704194442
C36	0.1449394175	1.7630024147	5.9949335111
H37	0.1609580834	2.1614190592	7.0155117141
C38	0.5119369365	2.5718067855	4.9085533727
H39	0.8248514763	3.6114670183	5.0491444758
C40	0.4702585021	2.0336808195	3.6190262343
H41	0.7358114687	2.6185369190	2.7344678541
C42	-0.8080262293	1.7501210648	0.8239870866
C43	-2.0754465809	2.1313026156	1.3086939693
H44	-2.6446877394	1.3966274316	1.8861595643
C45	-2.6156792049	3.4045374290	1.0564277306
C46	-1.8792042555	4.3401480819	0.3055952709
O47	-2.3061039103	5.6103277776	-0.0072073341
C48	-0.6039250486	3.9799543213	-0.1730981104
C49	-0.0780041534	2.7046452332	0.0831907838
H50	0.9122004477	2.4675578674	-0.3122918302
H51	-3.6064992454	3.6494963442	1.4515415542
H52	-0.0307015256	4.7128296718	-0.7531864874
C53	1.7453302054	0.2627011043	0.8125483577

C54	2.7469408184	0.5324324782	1.7424931300
H55	2.5306363591	0.4744858382	2.8123364953
C56	4.0600464116	0.8992092564	1.3410092339
H57	4.8149212901	1.1097551931	2.1081478677
C58	4.3726111299	1.0143725291	-0.0019757318
H59	5.3694734185	1.3317860652	-0.3289665113
C60	3.3919447370	0.7044773775	-0.9886939137
C61	3.6818346299	0.8079636497	-2.3762839691
H62	4.6736657518	1.1556928876	-2.6903300150
C63	2.7272762800	0.4731806607	-3.3158354232
H64	2.9633855034	0.5700306607	-4.3821916269
C65	1.4399583389	-0.0395321853	-2.9608511474
C66	1.1203954323	-0.1469000333	-1.5923215425
C67	2.0713858502	0.2752321599	-0.5893170556
C68	0.5534803059	-0.4215131732	-4.1279236808
H69	0.2562281412	-1.4811161191	-4.1024714291
H70	1.0917146231	-0.2612981731	-5.0755584492
H71	-0.3675078158	0.1825149813	-4.1750493527
C72	-3.6027908062	6.0043450020	0.4658991676
H73	-3.7528485443	7.0351396312	0.1115818024
H74	-4.3998926767	5.3573721861	0.0552025209
H75	-3.6559821703	5.9859988200	1.5702267525

## 5b, gas phase

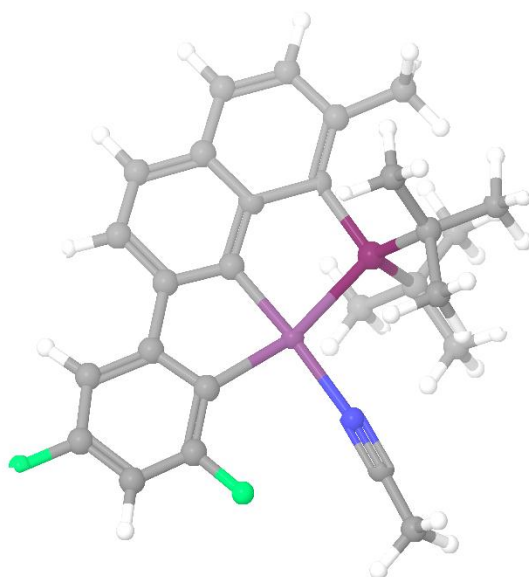
Total Gibbs free energy, Gtot (Htot - T\*S): -1759.759898 hartrees

Pt1	0.3219128838	1.7190485523	2.6368652457
P2	-0.9410316860	2.3254215406	4.5542990134
C3	-0.9610133278	4.2377220892	4.8701409820
C4	-2.1547347488	4.8204578710	5.6504574931
H5	-2.2076258829	4.4770600909	6.6926825650
H6	-3.1193117931	4.6067944981	5.1625418575
H7	-2.0464411741	5.9204137545	5.6826419975
C8	0.3656350717	4.5674941240	5.5865124188
H9	0.4888754336	5.6649943420	5.6288147801
H10	1.2290918622	4.1506278124	5.0409271063
H11	0.3960866610	4.1802977555	6.6161870462
C12	-0.9338079955	4.9099061164	3.4785764799
H13	-0.8749407565	6.0058253707	3.6129142127
H14	-1.8397998426	4.6902443547	2.8909148058
H15	-0.0609105606	4.5805115505	2.8934011885
C16	-2.6868774345	1.5193146531	4.4726963630
C17	-3.5305989428	1.5414381699	5.7588208083
H18	-3.7664933018	2.5601052190	6.1047401516
H19	-3.0404653909	0.9902714893	6.5754738767
H20	-4.4926782238	1.0354346724	5.5555313793
C21	-2.4148595434	0.0441466392	4.0954525806
H22	-3.3806258595	-0.4780263365	3.9652547486
H23	-1.8478869044	-0.4782476276	4.8835175138
H24	-1.8377720934	-0.0336643121	3.1585632322
C25	-3.4660285704	2.1966626669	3.3276337196
H26	-2.8956305523	2.1740129242	2.3864983315
H27	-3.7247003180	3.2441494429	3.5559497890
H28	-4.4138271322	1.6515266071	3.1660933732
C29	1.3828154540	0.6794583090	3.9621206559
C30	2.4547343326	-0.0861321350	3.4633945873
C31	3.2397207013	-0.8842172484	4.3394731989
H32	4.0664936780	-1.4820456085	3.9419140574
C33	2.9713423368	-0.9111685423	5.6963889254
H34	3.5783422762	-1.5197712464	6.3752872954
C35	1.9077591262	-0.1381344073	6.2397052631
C36	1.6311629302	-0.1202652285	7.6311519304
H37	2.2438642610	-0.7316437951	8.3028501559
C38	0.6159399156	0.6669152174	8.1345264474
H39	0.4265550475	0.6857450773	9.2138751899
C40	-0.2089272751	1.4764815971	7.2962491028
C41	0.0075729295	1.4569741487	5.9089366637
C42	1.0884424180	0.6672915607	5.3620569243
C43	-1.2142008905	2.3345828024	8.0292476715
H44	-0.7059547281	3.1714137698	8.5436644452
H45	-1.7287753537	1.7514045975	8.8123430831
H46	-1.9798732908	2.7600744768	7.3751805893
C47	2.6633510952	0.0291835540	2.0117074058

C48	3.6937787879	-0.6361465920	1.3217327670
H49	4.4049538894	-1.2940643132	1.8268160615
C50	3.8111377822	-0.4414637749	-0.0544739344
C51	2.9406498153	0.3911430756	-0.7546667660
H52	3.0443656660	0.5439236454	-1.8306905578
C53	1.9265611465	1.0328881538	-0.0251599073
C54	1.7311425556	0.8925926743	1.3509823228
F55	4.8025508862	-1.0760079926	-0.7332153895
F56	1.1127037091	1.8452587579	-0.7731135423
N57	-0.7501676351	2.6764001437	1.1060314026
C58	-1.2495944717	3.1029111126	0.1365117710
C59	-1.7771920601	3.5810773880	-1.1299978181
H60	-1.7951100303	4.6826070315	-1.1555693889
H61	-2.8001316485	3.2057479020	-1.2947908821
H62	-1.1264874474	3.2149973024	-1.9417996849

### 5b, acetonitrile solution

Title: nprth\_7\_CSHF92\_P1\_NCM6\_MeCN



Total Gibbs free energy, Gtot (Htot - T\*S): -1759.780807 hartrees

Pt1	0.3511995849	1.7214251235	2.6288884399
P2	-0.9427837425	2.3338350880	4.5445377775
C3	-1.0187196850	4.2479480949	4.8539952549
C4	-2.2426835853	4.8026649330	5.6102584047
H5	-2.3046507881	4.4744250173	6.6571191751
H6	-3.1920432775	4.5549838305	5.1090429377
H7	-2.1639749893	5.9057959858	5.6267859278
C8	0.2863435378	4.6253664062	5.5871364717
H9	0.3777278847	5.7262551751	5.6192869339
H10	1.1704245813	4.2294598404	5.0584536467
H11	0.3132749259	4.2519171560	6.6218483189
C12	-0.9972134741	4.9087681787	3.4570435270
H13	-0.9552511895	6.0065416098	3.5789176295
H14	-1.8963772488	4.6684190221	2.8679387593

H15	-0.1194669568	4.5840546422	2.8771512523
C16	-2.6671149308	1.4825861389	4.4567530709
C17	-3.5099447167	1.4959073700	5.7449305157
H18	-3.7681491109	2.5114513059	6.0835587736
H19	-3.0090301527	0.9599994584	6.5660542394
H20	-4.4600771624	0.9674173456	5.5407839909
C21	-2.3647517352	0.0113552052	4.0894351915
H22	-3.3195919893	-0.5284134261	3.9530538693
H23	-1.7948477705	-0.4981968095	4.8840680369
H24	-1.7809518209	-0.0548557637	3.1555013067
C25	-3.4589663305	2.1366354867	3.3051344126
H26	-2.8820660668	2.1341682002	2.3671419346
H27	-3.7578196951	3.1739294265	3.5306579838
H28	-4.3855418899	1.5577362827	3.1373526800
C29	1.3887421319	0.6715520441	3.9659129878
C30	2.4448394345	-0.1277048973	3.4765809677
C31	3.2193680004	-0.9321611616	4.3600493463
H32	4.0333243659	-1.5542203877	3.9697281895
C33	2.9572371669	-0.9300521928	5.7199766728
H34	3.5560654683	-1.5390499948	6.4072745498
C35	1.9081112922	-0.1267845432	6.2542393709
C36	1.6433204435	-0.0870328501	7.6508720075
H37	2.2565846916	-0.6935465891	8.3291521823
C38	0.6342651498	0.7149425849	8.1457540089
H39	0.4478311722	0.7500650733	9.2264230473
C40	-0.1958997171	1.5140565708	7.2974873246
C41	0.0196504448	1.4822313807	5.9087032501
C42	1.0956095704	0.6791378633	5.3696686937
C43	-1.2129513057	2.3625488585	8.0255334644
H44	-0.7112734906	3.1850390891	8.5699932088
H45	-1.7454486132	1.7635153618	8.7851004434
H46	-1.9631354923	2.8035580646	7.3638940436
C47	2.6575411325	-0.0349120660	2.0219203199
C48	3.6636248616	-0.7458696370	1.3363714144
H49	4.3496623832	-1.4295111870	1.8461687599
C50	3.7854926464	-0.5648445584	-0.0426470319
C51	2.9509080727	0.2941260560	-0.7564959339
H52	3.0614990240	0.4336917582	-1.8360076030
C53	1.9608815309	0.9780696029	-0.0281424441
C54	1.7555094037	0.8569013255	1.3510757090
F55	4.7547602481	-1.2455848101	-0.7156663661
F56	1.1741327797	1.8139567995	-0.7738163042
N57	-0.7249570625	2.7270251341	1.0784675442
C58	-1.2451641171	3.2112928385	0.1469605617
C59	-1.8531822793	3.8038539097	-1.0325789201
H60	-1.7077381613	4.8984412007	-1.0256984076
H61	-2.9340020897	3.5810814783	-1.0590054983
H62	-1.3814441291	3.3889618206	-1.9411903601

## 8, gas phase

Total Gibbs free energy, Gtot (Htot - T\*S): -1827.823794 hartrees

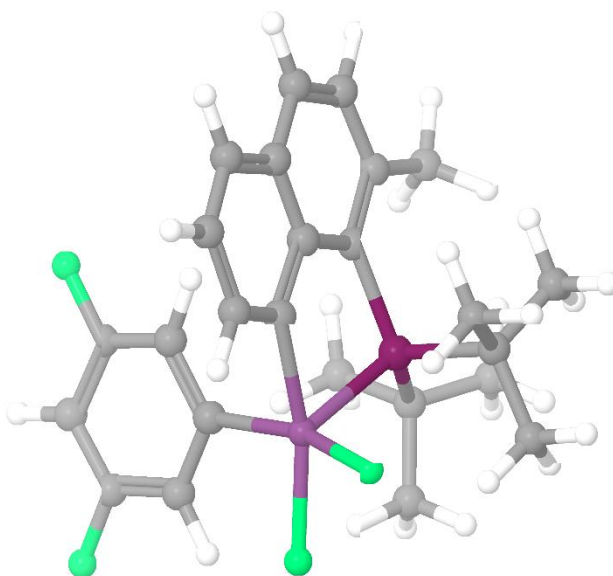
Pt1	7.9702495933	9.1471781748	4.1634972855
P2	7.9883568413	8.2178730776	2.0904172711
F3	6.2401948122	8.9527109267	5.2009624912
F4	8.5491071806	7.5148259758	5.2567333878
C5	8.6275350950	6.4018684336	2.2387649506
C6	8.8581565815	5.8095429093	0.8296788911
H7	9.2462495538	4.7851761288	0.9693523879
H8	9.6266052302	6.3725940126	0.2765196596
H9	7.9509923419	5.7321881597	0.2156617022
C10	9.9847079581	6.4020634928	2.9745769583
H11	9.8640693748	6.7919100725	3.9973627594
H12	10.7584542294	6.9657136754	2.4313919761
H13	10.3180048604	5.3500905353	3.0327102983
C14	7.6193224032	5.5708720003	3.0553869842
H15	8.0254690879	4.5485694917	3.1565883663
H16	6.6347237293	5.4834961260	2.5703323910
H17	7.5139604323	5.9994853165	4.0654145565
C18	6.2079901168	8.3507463020	1.3525069453
C19	5.1792770830	8.0462304254	2.4707095641
H20	4.1849800013	8.3264604962	2.0794222633
H21	5.3566317603	8.5927019702	3.4109945119
H22	5.1466047947	6.9735743316	2.7149910139
C23	5.9498951751	7.3530348894	0.2006458407
H24	5.9951961841	6.3067703150	0.5373440346
H25	6.6172521085	7.4826129209	-0.6617028867
H26	4.9191652326	7.5311539269	-0.1531492164
C27	6.0005400110	9.7961131707	0.8537434387
H28	6.7780860209	10.1328111670	0.1513687255
H29	5.9664677572	10.5087412094	1.6880671494
H30	5.0295909766	9.8368707351	0.3298800759
C42	7.3506948292	11.0357488590	3.5974282829
C43	6.1494540481	11.4855257089	4.1893707602
H44	5.5698328685	10.8131154335	4.8257508294
C45	5.7250262226	12.7981641805	3.9680419280
C46	6.4258488558	13.7028647139	3.1659672767
H47	6.0750353117	14.7229753948	3.0041263360
C48	7.6068667356	13.2277173406	2.5919546639
C49	8.0800301389	11.9265378269	2.7817808215
H50	9.0106410733	11.6492475517	2.2879116823
F51	4.5731986995	13.2161768650	4.5472487105
F52	8.3253355862	14.0689054659	1.8056845495
C53	9.8713257548	9.5703658336	3.6262897172
C54	10.7774848903	9.9355709645	4.6116415143
H55	10.4907024581	9.8830112075	5.6669529161
C56	12.0714302536	10.4056542892	4.2593031656
H57	12.7620326615	10.7091082271	5.0524762552
C58	12.4556263680	10.4979952470	2.9318234243



H59	13.4429397767	10.8839699408	2.6594914071
C60	11.5665818486	10.0899660352	1.8977236557
C61	11.8874304337	10.1723665905	0.5164902396
H62	12.8614765863	10.5747952647	0.2184881039
C63	10.9808310404	9.7634554567	-0.4445775323
H64	11.2448278000	9.8509036532	-1.5036836355
C65	9.7072728251	9.2039029367	-0.1212835014
C66	9.3671136082	9.1130869580	1.2378978920
C67	10.2674365323	9.5884329680	2.2519556697
C68	8.8444928922	8.7536876259	-1.2780989690
H69	8.6415032132	7.6708598883	-1.2499477092
H70	9.3485582778	8.9638071769	-2.2334881087
H71	7.8732297610	9.2730040116	-1.3011043151

## 8, acetonitrile solution

Title: rpt0\_Pf2\_OHf\_a\_MeCN



Total Gibbs free energy, Gtot (Htot - T\*S): -1827.851932 hartrees

Pt1	7.9898519763	9.1370483250	4.1808069757
P2	7.9823388094	8.2158323496	2.0655583735
F3	6.2860494975	8.9635994742	5.3297262961
F4	8.5914349703	7.5260777711	5.3378610164
C5	8.6139763702	6.3938387832	2.2153188383
C6	8.8492513482	5.8050087656	0.8031354352
H7	9.2238281864	4.7752416695	0.9480116938
H8	9.6305331510	6.3569536587	0.2564055349
H9	7.9463790834	5.7366499604	0.1817727836
C10	9.9669062550	6.3830365404	2.9585789800
H11	9.8496178193	6.7660650064	3.9834510093
H12	10.7442247944	6.9501774970	2.4237749908
H13	10.2959732456	5.3290298196	3.0076252437
C14	7.5957030266	5.5599868160	3.0173058102
H15	7.9971017855	4.5342093635	3.1080392981
H16	6.6125029966	5.4829658476	2.5272244068

H17	7.4844615822	5.9744271842	4.0322002775
C18	6.1981760181	8.3661088919	1.3300049450
C19	5.1742904344	8.0853678570	2.4596816523
H20	4.1791213694	8.3645406803	2.0681493014
H21	5.3584188653	8.6543361781	3.3841118346
H22	5.1368180051	7.0167137359	2.7236097017
C23	5.9270141264	7.3553785887	0.1901363318
H24	5.9607792866	6.3104095798	0.5336995082
H25	6.5903668832	7.4727145471	-0.6776332846
H26	4.8964658371	7.5454768414	-0.1612335386
C27	6.0024419320	9.8056100557	0.8075228154
H28	6.7690710754	10.1172965871	0.0820199705
H29	5.9867188656	10.5367256345	1.6259670470
H30	5.0236472559	9.8445858880	0.2969086994
C42	7.3545521458	11.0111460905	3.5969974855
C43	6.1417741792	11.4562018141	4.1708032238
H44	5.5568662280	10.7856621066	4.8044843258
C45	5.7023469792	12.7608531933	3.9271792742
C46	6.3971440406	13.6724207473	3.1271622830
H47	6.0328946082	14.6876667028	2.9470949018
C48	7.5918267477	13.2007254016	2.5769013752
C49	8.0812786506	11.9075601205	2.7845715810
H50	9.0182553759	11.6362939669	2.2995353741
F51	4.5328266159	13.1637405336	4.4902820642
F52	8.3144554405	14.0423466578	1.7921037092
C53	9.8815867342	9.5664137597	3.6125879521
C54	10.7834605384	9.9485968952	4.5970935214
H55	10.4974808524	9.9106959852	5.6544843865
C56	12.0754245423	10.4302914078	4.2423882843
H57	12.7630608525	10.7474493092	5.0351371497
C58	12.4549108570	10.5151520819	2.9112836163
H59	13.4403282028	10.9060970717	2.6328532763
C60	11.5640836792	10.0951609233	1.8800013450
C61	11.8848235060	10.1808564122	0.4964681408
H62	12.8592725992	10.5865532176	0.1967298315
C63	10.9771247225	9.7699371811	-0.4645295985
H64	11.2428436337	9.8570617801	-1.5248623764
C65	9.7006288162	9.2090464235	-0.1425064098
C66	9.3637341882	9.1132700798	1.2205582294
C67	10.2677843615	9.5836785133	2.2352938130
C68	8.8437535397	8.7646872343	-1.3073273042
H69	8.5993007768	7.6909469600	-1.2643232126
H70	9.3767572568	8.9360755720	-2.2555678182
H71	7.8937589964	9.3215967384	-1.3654842747

## 9, gas phase

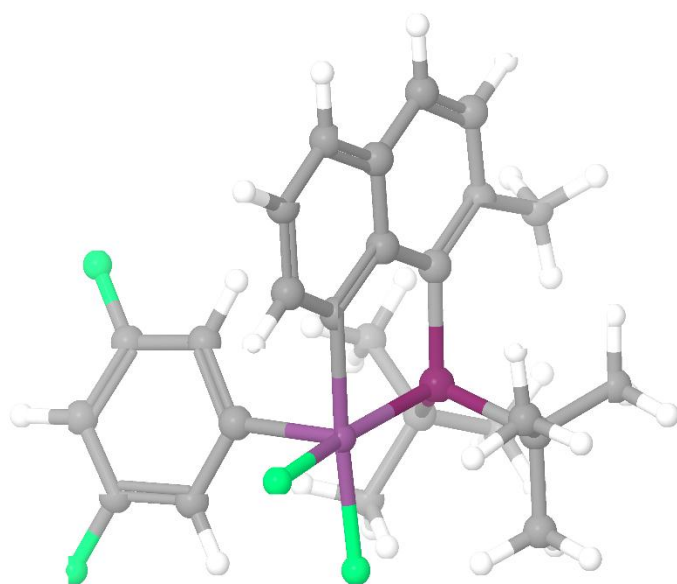
Total Gibbs free energy, Gtot (Htot - T\*S): -1827.833866 hartrees

Pt1	8.2790136371	9.0836984783	4.0860203668
P2	8.0303022825	8.2831663197	1.9340511360
F3	8.7843518970	9.4919259641	5.9826011785
F4	6.6347179269	8.0620104047	4.8453992601
C5	8.4028215254	6.4199708280	2.2404250407
C6	8.7873174454	5.6546681117	0.9637678861
H7	9.0394193951	4.6160376868	1.2444815771
H8	9.6716995307	6.0906287059	0.4724593406
H9	7.9618272909	5.6030801705	0.2374555831
C10	9.6115780103	6.4155770029	3.2092404070
H11	9.3536924216	6.8321093329	4.2051294350
H12	10.4802503326	6.9674858913	2.8170479883
H13	9.9173554651	5.3692051778	3.3902503901
C14	7.2034759819	5.7607751137	2.9539549413
H15	7.5190996067	4.7612499513	3.3037375649
H16	6.3445378355	5.6113884023	2.2818117515
H17	6.8774791216	6.3579931318	3.8248852565
C18	6.3426741238	8.6155774030	1.0640444422
C19	5.2912479733	8.7950643356	2.1926472233
H20	4.2863894070	8.6196721592	1.7706746636
H21	5.3210739452	9.8217797511	2.5840076341
H22	5.4460454638	8.1374390788	3.0630383060
C23	5.8652574799	7.4844141730	0.1280649662
H24	5.6841522229	6.5419723053	0.6644475829
H25	6.5397683544	7.2844188735	-0.7168607457
H26	4.9002270953	7.8012036291	-0.3059118499
C27	6.4632165076	9.9327338436	0.2696474956
H28	7.1391678545	9.8520271668	-0.5947409985
H29	6.8070245355	10.7622274689	0.9070958042
H30	5.4596986219	10.1987387663	-0.1077224467
C42	7.3288745887	10.8512290466	3.9536118336
C43	6.2478812555	10.9620409257	4.8398487945
H44	5.9376765964	10.1192378909	5.4593217770
C45	5.5567126220	12.1786939331	4.8592083687
C46	5.8944758778	13.2643908735	4.0452181768
H47	5.3369830336	14.2011219355	4.0812325177
C48	6.9831343308	13.0923504970	3.1892060446
C49	7.7249246711	11.9047524226	3.1203347941
H50	8.5799712573	11.8439342011	2.4478017109
F51	4.5033385270	12.3074674951	5.6963773132
F52	7.3469065818	14.1198701051	2.3861226254
C53	10.0007842673	9.8789644240	3.4136651667
C54	10.8430968877	10.5487735747	4.2937173951
H55	10.5364264750	10.6183045938	5.3419260315
C56	12.0580736012	11.1181120281	3.8399167588
H57	12.7037546315	11.6434204459	4.5512578420
C58	12.4210547903	11.0230614788	2.5066918072

H59	13.3514130178	11.4720107248	2.1441399369
C60	11.5882755642	10.3377276344	1.5784923588
C61	11.9347602469	10.2184447263	0.2055499612
H62	12.8665376014	10.6740144133	-0.1467296967
C63	11.1163556478	9.5353789497	-0.6698009999
H64	11.4009226466	9.4473578854	-1.7239730935
C65	9.8987574926	8.9190286804	-0.2520585021
C66	9.5141995802	9.0296676668	1.0927933559
C67	10.3522932584	9.7452297366	2.0294005457
C68	9.1276861879	8.1976235738	-1.3310115655
H69	8.3153422493	7.5794529585	-0.9360745985
H70	9.7981693904	7.5374608256	-1.9071878389
H71	8.6920549525	8.9126011241	-2.0520989688

## 9, acetonitrile solution

Title: nqth\_Pf2\_O5H4F\_b\_MeCN



Total Gibbs free energy, Gtot (Htot - T\*S): -1827.860665 hartrees

Pt1	8.2592339309	9.0705232924	4.0925912093
P2	8.0116201640	8.2833922886	1.9182597926
F3	8.7749568115	9.4542320288	6.0361851819
F4	6.6185908558	8.0496146397	4.9220355284
C5	8.4068200386	6.4262547397	2.2390083369
C6	8.8126433063	5.6667221677	0.9643591775
H7	9.0748166944	4.6320577209	1.2532552745
H8	9.6978133522	6.1108605558	0.4811934222
H9	7.9938120462	5.6036152722	0.2309318356
C10	9.6048687783	6.4377564890	3.2228850227
H11	9.3361399372	6.8627188582	4.2165191119
H12	10.4772906107	6.9869157638	2.8344921526
H13	9.9111116389	5.3942186901	3.4243925369
C14	7.2053941055	5.7513541101	2.9347044789
H15	7.5298656532	4.7533174835	3.2814846298

H16	6.3556338198	5.5981829772	2.2518043001
H17	6.8679466226	6.3386902353	3.8063111984
C18	6.3171340276	8.6122101259	1.0487421271
C19	5.2652540249	8.7977512363	2.1727126197
H20	4.2601345764	8.6845607916	1.7296816881
H21	5.3351634849	9.8051809105	2.6066295645
H22	5.3775108269	8.0883228556	3.0069217309
C23	5.8441779361	7.4672961696	0.1241136525
H24	5.6403627165	6.5357994627	0.6724425444
H25	6.5287123635	7.2437793226	-0.7067562099
H26	4.8903773587	7.7914962242	-0.3308369334
C27	6.4333277685	9.9229126921	0.2411450444
H28	7.1021490366	9.8325284928	-0.6277409491
H29	6.7802874087	10.7605273786	0.8667003643
H30	5.4264737246	10.1824559471	-0.1339515560
C42	7.3225417400	10.8474968315	3.9593416757
C43	6.2373192406	10.9853072915	4.8407598947
H44	5.8980656302	10.1539637895	5.4609206809
C45	5.5687122652	12.2159856674	4.8520254863
C46	5.9221997907	13.2964710442	4.0376219596
H47	5.3804185095	14.2460271816	4.0688506434
C48	7.0081955689	13.0942806486	3.1835462177
C49	7.7301518689	11.8938374523	3.1193111817
H50	8.5781320082	11.8156682160	2.4395345508
F51	4.5144059839	12.3612997829	5.6905405292
F52	7.3951187828	14.1103629201	2.3745400293
C53	9.9832280243	9.8702297761	3.4098019122
C54	10.8285813541	10.5371873899	4.2911620048
H55	10.5339415632	10.6063184461	5.3428498612
C56	12.0442834754	11.1132979971	3.8397197500
H57	12.6912468294	11.6345173619	4.5549898857
C58	12.4034254397	11.0275018133	2.5033007317
H59	13.3342866267	11.4788091489	2.1398475746
C60	11.5655359772	10.3472749007	1.5729233949
C61	11.9121641642	10.2389352302	0.1963105668
H62	12.8453584040	10.6960099032	-0.1552987010
C63	11.0903397876	9.5616314936	-0.6820463019
H64	11.3739917990	9.4787604374	-1.7383126934
C65	9.8702427540	8.9414898731	-0.2671433914
C66	9.4888699506	9.0442414066	1.0818227628
C67	10.3297075717	9.7501396466	2.0223510263
C68	9.1076550479	8.2237975399	-1.3545706143
H69	8.2852533051	7.6092753950	-0.9744634858
H70	9.7852820519	7.5605551665	-1.9202679598
H71	8.6905153529	8.9441881230	-2.0826471989

## 10, gas phase

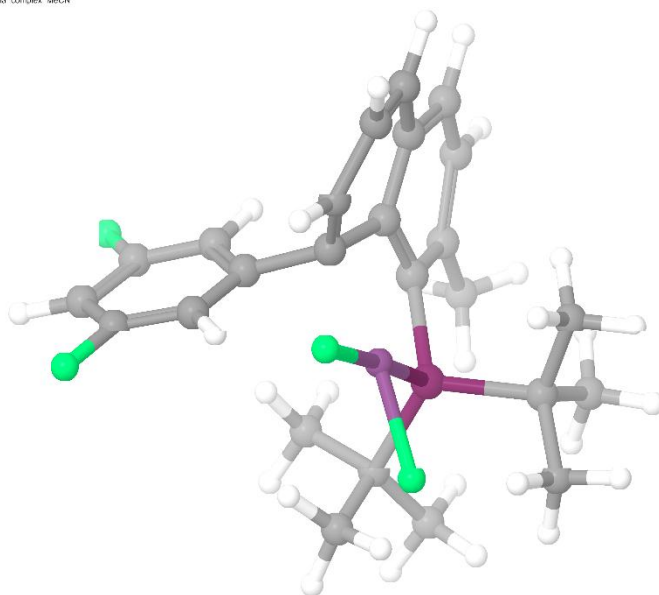
Total Gibbs free energy, Gtot (Htot - T\*S): -1827.811182 hartrees

Pt1	0.1756009483	-0.7895306430	1.8882434429
P2	0.2134616470	-0.5925698111	-0.3854851395
F3	0.4779625236	-0.9559169359	3.8957900117
F4	0.5005179232	-2.7467508770	1.8134577746
C5	1.9036235171	-1.3099050018	-0.9966348043
C6	2.2325239781	-0.9484556146	-2.4569385171
H7	3.2147391365	-1.3906945348	-2.7031618734
H8	2.3188704949	0.1394127482	-2.6038235926
H9	1.5061562650	-1.3520804378	-3.1774798991
C10	2.9894226976	-0.6928214437	-0.0853414053
H11	2.8312596746	-0.9530058923	0.9730507837
H12	3.0349877389	0.4046582208	-0.1688380701
H13	3.9686830403	-1.0967804838	-0.3984757449
C14	1.9162170401	-2.8410785545	-0.7974806449
H15	2.9436222675	-3.2017655503	-0.9850058969
H16	1.2550414532	-3.3676868931	-1.5031744874
H17	1.6219689208	-3.1055589023	0.2302085727
C18	-1.3175743526	-1.4078464005	-1.2455291684
C19	-1.7683395987	-2.5179056553	-0.2618508195
H20	-2.5506540977	-3.1259365485	-0.7500508946
H21	-2.1908128855	-2.0762395681	0.6544953680
H22	-0.9471520755	-3.1748482183	0.0619263639
C23	-1.0498432452	-2.0466916081	-2.6234782748
H24	-0.2862508142	-2.8361669961	-2.5854090587
H25	-0.7639336523	-1.3228397941	-3.4021545180
H26	-1.9899128384	-2.5179302683	-2.9615086428
C27	-2.4575263838	-0.3792120148	-1.3754142004
H28	-2.2182301344	0.4480113493	-2.0616539778
H29	-2.7386057864	0.0436530110	-0.4002087565
H30	-3.3459899103	-0.8985954435	-1.7776510248
C31	-1.0789428642	1.0241231401	2.2857008595
C32	-1.5469982512	0.8302333463	3.6184372415
H33	-0.9115617803	0.3091988562	4.3401762193
C34	-2.8469025273	1.1898173605	3.9514659341
C35	-3.7524247358	1.7580168087	3.0456448007
H36	-4.7656467073	2.0361563432	3.3370660662
C37	-3.2730519928	1.9433176048	1.7487045150
C38	-1.9815955971	1.6026021456	1.3512975809
H39	-1.6754823676	1.8617966584	0.3394288670
F40	-3.2716158394	0.9692912276	5.2166664218
F41	-4.0957556485	2.4949292275	0.8220895486
C42	0.5463912231	1.2779575190	1.9453503975
C43	1.2877226201	1.7502624405	3.0614841344
H44	1.1680747754	1.2060664754	4.0021666390
C45	2.0862742450	2.8989402189	2.9778918444
H46	2.6188481022	3.2489032888	3.8672368304
C47	2.1466557985	3.6253111269	1.7921886636

H48	2.6876788251	4.5758435122	1.7424247392
C49	1.5337509735	3.1256640196	0.6079941391
C50	1.6294031301	3.8204450562	-0.6295042637
H51	2.1417070019	4.7881485642	-0.6538327851
C52	1.0872748170	3.2849742222	-1.7799128334
H53	1.1392252590	3.8444328053	-2.7199894374
C54	0.5200430254	1.9770412438	-1.8032167883
C55	0.4391770959	1.2503251852	-0.5996284156
C56	0.8345838636	1.8718639465	0.6373570094
C57	0.0283738647	1.4853152943	-3.1426130197
H58	-0.1455577804	0.4044210970	-3.1633886269
H59	0.7445328576	1.7301237838	-3.9444963259
H60	-0.9237744954	1.9831403375	-3.4026398906

## 10, acetonitrile solution

TiSe: opt63 8 CBHF2 PF2 c c sigma complex MeCN



Total Gibbs free energy, Gtot (Htot - T\*S): -1827.846614 hartrees

Pt1	0.5307518907	-0.7986810439	1.9228925472
P2	0.2742309904	-0.6285541036	-0.3442991333
F3	0.5953455007	-0.9533234183	3.9971161138
F4	0.6733319340	-2.8418763086	1.9592317670
C5	1.8971089341	-1.2783917622	-1.1642333054
C6	2.0438283593	-1.0435122100	-2.6791870539
H7	2.9991031299	-1.5016040314	-2.9970058132
H8	2.1020441555	0.0267328633	-2.9294877073
H9	1.2454644247	-1.5101611530	-3.2748958936
C10	3.0441538090	-0.5346514654	-0.4420817840
H11	2.9821114109	-0.6775769946	0.6497859946
H12	3.0314337325	0.5479675719	-0.6484695885
H13	4.0080214066	-0.9367802607	-0.8022521491
C14	1.9856064865	-2.7890816998	-0.8419957926
H15	3.0167793221	-3.1275242754	-1.0521862240
H16	1.3109610788	-3.3872175724	-1.4759563700

H17	1.7450335336	-2.9974673876	0.2146984339
C18	-1.3481097346	-1.4650139693	-0.9844775040
C19	-1.7469295797	-2.5115195309	0.0824916058
H20	-2.6015126216	-3.0998791762	-0.2976359274
H21	-2.0529495778	-2.0083674520	1.0151541273
H22	-0.9227188588	-3.1905662411	0.3483686681
C23	-1.2232543932	-2.1557025873	-2.3573103016
H24	-0.4943509619	-2.9802269989	-2.3564858627
H25	-0.9685130637	-1.4615567817	-3.1741213329
H26	-2.2089174072	-2.5910146333	-2.6047882721
C27	-2.4466932493	-0.3850890689	-1.0548339332
H28	-2.2609389480	0.3589100493	-1.8456893857
H29	-2.5603685748	0.1470191023	-0.0978608377
H30	-3.4082943029	-0.8810907189	-1.2820780557
C31	-1.3951162447	1.4137003845	2.1846576845
C32	-1.9874524752	0.7182074821	3.2616762068
H33	-1.3865857621	0.0332149119	3.8719524649
C34	-3.3432589856	0.9145996167	3.5255019277
C35	-4.1633023949	1.7643537275	2.7720884096
H36	-5.2249944361	1.8972011505	2.9997072194
C37	-3.5395050016	2.4382946968	1.7208030668
C38	-2.1831609660	2.2885259926	1.4086789618
H39	-1.7645170078	2.8701555685	0.5848746466
F40	-3.9048137759	0.2391388045	4.5595847351
F41	-4.2804432262	3.2869865983	0.9651047061
C42	0.1100368228	1.2927493771	1.9264441789
C43	0.9316540233	1.6461420578	3.0711204581
H44	0.6695421182	1.2010440732	4.0379282603
C45	1.9488598651	2.6159027609	3.0024242377
H46	2.5457766894	2.8456320288	3.8911564731
C47	2.0637231800	3.3989006709	1.8534610250
H48	2.7192783029	4.2793232326	1.8521633074
C49	1.3943100206	3.0411585224	0.6415453214
C50	1.5956212989	3.7414280732	-0.5830523044
H51	2.1986356616	4.6575951991	-0.5871686707
C52	1.0408810033	3.2502543063	-1.7552975282
H53	1.1464629176	3.8158934303	-2.6886942105
C54	0.4261476313	1.9621456051	-1.8096904665
C55	0.3005718857	1.2209852728	-0.6097018176
C56	0.6015517681	1.8527171412	0.6285574443
C57	-0.0806976004	1.5014222739	-3.1539966312
H58	-0.3050928929	0.4283599296	-3.1880863967
H59	0.6333919793	1.7375842243	-3.9610455642
H60	-1.0161468402	2.0443416490	-3.3906386733



## 11, gas phase

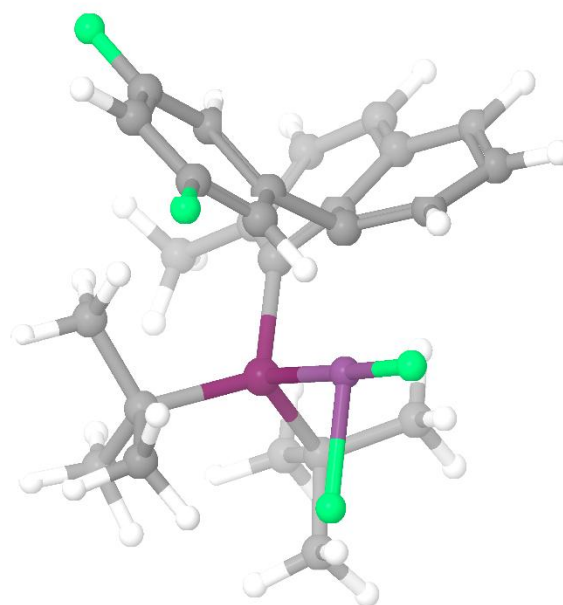
Total Gibbs free energy, Gtot (Htot - T\*S): -1827.816800 hartrees

Pt1	8.1931178502	8.8264038704	4.3122434147
P2	8.0181452106	8.2060202560	2.0837136895
F3	8.0361478055	9.4586744941	6.2392176671
F4	6.8965065695	7.4022496837	4.8229814008
C5	8.7695089279	6.4358477723	1.9232835165
C6	9.0035450399	5.9220158495	0.4922653528
H7	9.3969734540	4.8916492773	0.5633474265
H8	9.7563476179	6.5192905577	-0.0437642972
H9	8.0836793775	5.8757005108	-0.1087773545
C10	10.1334536755	6.5043811868	2.6482935996
H11	10.0172233677	6.8191391931	3.6982347919
H12	10.8339372599	7.1965252599	2.1529465545
H13	10.5850086337	5.4961304709	2.6326774041
C14	7.8345224324	5.4762010989	2.6944995885
H15	8.3691286240	4.5206798048	2.8433256294
H16	6.9163790926	5.2498824637	2.1287691156
H17	7.5456528350	5.8864646096	3.6766145154
C18	6.2278298270	8.4082593034	1.3914341260
C19	5.2473858081	8.3524688755	2.5833176282
H20	4.2154057114	8.3672896189	2.1898124501
H21	5.3815878901	9.2270763120	3.2396796142
H22	5.3889651451	7.4663876424	3.2174592944
C23	5.8328687803	7.3433531203	0.3512383494
H24	5.8271444755	6.3256792742	0.7686019132
H25	6.4739908034	7.3518226894	-0.5446138945
H26	4.8055216362	7.5636637514	0.0100279579
C27	6.1483751040	9.8077735245	0.7478404878
H28	6.7787486323	9.8987286967	-0.1512819988
H29	6.4385867922	10.6019873646	1.4529031855
H30	5.1020011381	9.9938173847	0.4456058319
C42	8.2137598204	11.6508845777	3.3507733067
C43	7.3327024636	11.9351285810	4.4178487384
H44	7.3026696025	11.2884972265	5.3046262134
C45	6.4973299719	13.0458701540	4.3136662882
C46	6.4852064473	13.8916811068	3.1978118441
H47	5.8176459674	14.7526774957	3.1410847299
C48	7.3708523080	13.5822031727	2.1656710258
C49	8.2345866214	12.4840499043	2.2146017383
H50	8.9169314207	12.3022543764	1.3820032457
F51	5.6484092236	13.3207031831	5.3290254324
F52	7.3993306256	14.3808711058	1.0721934414
C53	9.1923990453	10.5100307975	3.4669110896
C54	9.9615185696	10.3588328816	4.6674875162
H55	9.5216882183	10.6790541908	5.6185831727
C56	11.3867734363	10.1546726957	4.6195554666
H57	11.9345849569	10.0788186655	5.5628762768
C58	12.0532061570	10.2504566429	3.4217232232

H59	13.1480080083	10.2737792328	3.3884349966
C60	11.3252347966	10.1763579168	2.1749227350
C61	11.9436735474	9.9836063846	0.9148861073
H62	13.0299179103	10.0904892961	0.8254835218
C63	11.1780795125	9.6185803161	-0.1894348104
H64	11.6526545108	9.5298161705	-1.1725195668
C65	9.8231240907	9.2182989727	-0.0535978677
C66	9.2258862318	9.3351548602	1.2242306365
C67	9.9129760388	10.0407838273	2.2450073200
C68	9.0912292441	8.7369722441	-1.2832260422
H69	8.2289125261	8.1019328985	-1.0430799895
H70	9.7538257181	8.1788394459	-1.9641892876
H71	8.7061130243	9.6072651599	-1.8465389812

## 11, acetonitrile solution

Title: nphh\_8\_C6H12F2\_Pf2\_u\_pi\_complex\_MeCN



Total Gibbs free energy, Gtot (Htot - T\*S): -1827.846906 hartrees

Pt1	8.1423003660	8.7800470381	4.2835049774
P2	8.0026171471	8.2042248701	2.0729229669
F3	8.1496605320	9.4099507065	6.2650500352
F4	6.8308529776	7.3537342972	4.9408433380
C5	8.7095168976	6.4149867969	1.8965578802
C6	8.9344821155	5.9007873114	0.4625521594
H7	9.3085580688	4.8624834630	0.5352149661
H8	9.7023246649	6.4817544459	-0.0707703263
H9	8.0168129550	5.8740135212	-0.1434564427
C10	10.0741732652	6.4387014992	2.6226525832
H11	9.9654255379	6.7973351852	3.6599439786
H12	10.8040976756	7.0851515769	2.1092076510
H13	10.4834135719	5.4126832927	2.6384322460
C14	7.7414343497	5.4781647949	2.6569183434
H15	8.2486813702	4.5082449112	2.8111947580
H16	6.8236242692	5.2773310917	2.0804867863

H17	7.4525633416	5.8953045311	3.6368906761
C18	6.2358708720	8.4517627944	1.3277341982
C19	5.2515229352	8.4111945291	2.5196905152
H20	4.2180318254	8.4265566831	2.1289795205
H21	5.3968352930	9.2937353359	3.1645395580
H22	5.3886262973	7.5267184433	3.1599408001
C23	5.8213313189	7.3939145432	0.2851890908
H24	5.7839407180	6.3755924681	0.7010584303
H25	6.4658271177	7.3855019994	-0.6084057427
H26	4.8014418860	7.6440287123	-0.0604310185
C27	6.1813488119	9.8524306520	0.6836166855
H28	6.8066591652	9.9281050051	-0.2201414216
H29	6.4907855543	10.6415610007	1.3864100916
H30	5.1369224317	10.0568902839	0.3843315403
C42	8.2730011939	11.5866995979	3.4090098929
C43	7.3791740658	11.8959114979	4.4575857770
H44	7.3571301315	11.2786275479	5.3632768694
C45	6.5259696628	12.9895381275	4.3124232311
C46	6.5040915831	13.8066875362	3.1758864938
H47	5.8187988628	14.6544835019	3.0854765018
C48	7.4115747736	13.4779211316	2.1681383440
C49	8.2963842424	12.3972489859	2.2562595544
H50	8.9893564276	12.2133288497	1.4322591921
F51	5.6622871512	13.2744112124	5.3193330298
F52	7.4452974159	14.2459073621	1.0504395567
C53	9.2790526011	10.4441095039	3.5705613299
C54	10.1436648395	10.5886648487	4.7262734183
H55	9.6747079015	10.8519786695	5.6805680216
C56	11.5470439516	10.5282646662	4.6355626333
H57	12.1573305569	10.6364756921	5.5379710553
C58	12.1457208633	10.5121796345	3.3764814142
H59	13.2304583570	10.6500465446	3.2810875899
C60	11.3832410411	10.2508537792	2.1955774109
C61	11.9855208500	10.0936819698	0.9142424836
H62	13.0592335673	10.2832131716	0.7955263707
C63	11.2122425796	9.6894581320	-0.1635380165
H64	11.6607144040	9.6233023053	-1.1620367787
C65	9.8651606770	9.2478169530	0.0026655286
C66	9.2897954663	9.3093366005	1.2946840498
C67	9.9835038664	9.9965953880	2.3298160075
C68	9.1361309362	8.7811648050	-1.2331547625
H69	8.2420098630	8.1858011282	-1.0106667408
H70	9.7933857552	8.1942085934	-1.8965325947
H71	8.8081164976	9.6661149336	-1.8124633942

## 12, gas phase

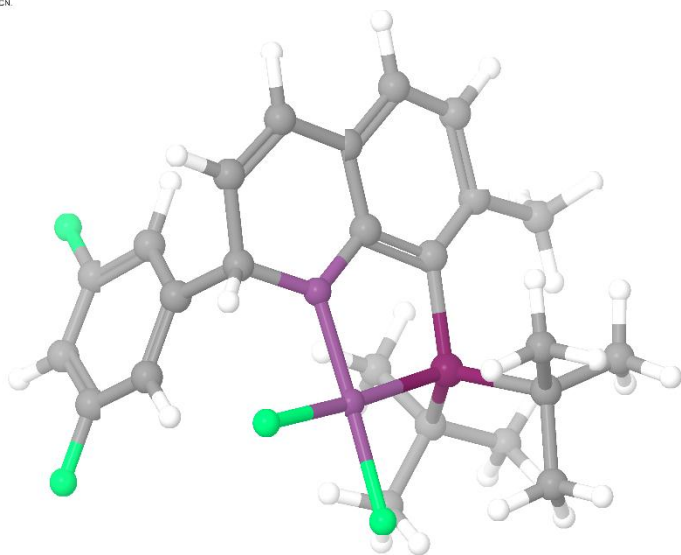
Total Gibbs free energy, Gtot (Htot - T\*S): -1827.839494 hartrees

Pt1	1.8373932546	0.5607515022	-1.1764819704
P2	-0.0781902882	-0.6001252693	-0.8577365368
F3	3.4570028665	1.7315291588	-1.5962440478
F4	2.9642819531	-1.0351148400	-1.6765136254
C5	-0.5065551442	-1.4985824668	-2.4983337131
C6	-1.9105345025	-2.1219340865	-2.5820247283
H7	-1.9950722505	-2.6347712023	-3.5571248871
H8	-2.7058937991	-1.3616389601	-2.5454225579
H9	-2.0965792570	-2.8768066000	-1.8030697535
C10	-0.3814832676	-0.4183852764	-3.5984152141
H11	0.6334723115	0.0084854081	-3.6354717094
H12	-1.0985993319	0.4069647478	-3.4523787792
H13	-0.5983003918	-0.8881969381	-4.5744700278
C14	0.5800445085	-2.5761841548	-2.7153625742
H15	0.4988854239	-2.9447214257	-3.7538987163
H16	0.4390873388	-3.4438872774	-2.0498596462
H17	1.5942477978	-2.1672011652	-2.5552807773
C18	0.0160653240	-1.7154042090	0.7053204051
C19	1.5113356672	-2.0870970156	0.8649382772
H20	1.6039689727	-2.8453750775	1.6629420212
H21	2.1023318394	-1.2033230216	1.1530493875
H22	1.9685592959	-2.4719185196	-0.0589387579
C23	-0.8227580324	-3.0058974529	0.6534523836
H24	-0.5153669507	-3.6714965228	-0.1674044751
H25	-1.9052558890	-2.8235007148	0.5713956197
H26	-0.6635693388	-3.5572428109	1.5974358241
C27	-0.4102471081	-0.8484068194	1.9079833474
H28	-1.4885329262	-0.6234491706	1.9080129827
H29	0.1437614116	0.1048385565	1.9373642089
H30	-0.1779549634	-1.3968533004	2.8380407554
C31	2.1185705420	3.4518659412	0.8631836433
C32	3.3926601345	2.8962019964	1.0722582951
H33	3.9228082183	2.4276221790	0.2341479897
C34	3.9196584229	2.9220984156	2.3649838307
C35	3.2366737139	3.4703109788	3.4559264389
H36	3.6737625887	3.4823980784	4.4556853795
C37	1.9701076961	4.0004763265	3.2054378563
C38	1.3918107867	4.0028061537	1.9336568569
H39	0.4018579757	4.4417083167	1.7931839385
F40	5.1461158512	2.3951085442	2.5829816493
F41	1.2748469489	4.5389017341	4.2371741028
C42	0.8153595246	2.1104971432	-0.7747920325
C43	1.5098380307	3.4332132111	-0.5683861551
H44	2.3927602959	3.3956547189	-1.2461950633
C45	0.6601638565	4.6438769645	-0.7905358117
H46	1.1704307943	5.6118955009	-0.8386039832
C47	-0.6909226471	4.5664375798	-0.8486395195

H48	-1.3041542677	5.4648176583	-0.9759307917
C49	-1.3783915384	3.2910899022	-0.7072053817
C50	-2.7813180920	3.2135504324	-0.5926350873
H51	-3.3759497136	4.1329338558	-0.6110076327
C52	-3.4037145258	1.9819707644	-0.4247833081
H53	-4.4910739119	1.9454780500	-0.2919633901
C54	-2.6888213855	0.7552032105	-0.4167912747
C55	-1.2967700109	0.8030735269	-0.6142125830
C56	-0.6355271156	2.0715562853	-0.6998670955
C57	-3.4908278884	-0.4931871974	-0.1356231631
H58	-2.9021281279	-1.4104253948	-0.2384829880
H59	-4.3606766700	-0.5711977220	-0.8099094383
H60	-3.8882180474	-0.4622308175	0.8947311744

## 12, acetonitrile solution

Title: nphb\_h\_h7\_C0H9F2\_Pf2\_MeCN



Total Gibbs free energy, Gtot (Htot - T\*S): -1827.870346 hartrees

Pt1	1.8426041901	0.6081069728	-1.2313171594
P2	-0.0771464532	-0.5679180993	-0.8504098539
F3	3.4928132737	1.7854869471	-1.6967094883
F4	3.0475684453	-0.9487389389	-1.7927586592
C5	-0.5047003381	-1.5386566793	-2.4531801622
C6	-1.8953842601	-2.1984082620	-2.4990049972
H7	-1.9674470297	-2.7523062912	-3.4533723278
H8	-2.7081628604	-1.4562127498	-2.4937052619
H9	-2.0616514356	-2.9245952545	-1.6888334080
C10	-0.4186997617	-0.5007974323	-3.5958777891
H11	0.5781013290	-0.0325827270	-3.6389815738
H12	-1.1705793667	0.2984746941	-3.4852275596
H13	-0.6093519548	-1.0162909873	-4.5543408459
C14	0.6005028039	-2.6041731825	-2.6387569772
H15	0.5059536539	-3.0224702872	-3.6576578988
H16	0.4900354621	-3.4418784114	-1.9301544342
H17	1.6082335778	-2.1685108644	-2.5215914283

C18	0.0518990642	-1.6264542000	0.7558365057
C19	1.5484850286	-1.9904514558	0.9078464497
H20	1.6596646676	-2.6696075760	1.7721508139
H21	2.1510869848	-1.0860047188	1.0919261818
H22	1.9650891036	-2.4823941218	0.0158369997
C23	-0.7847207472	-2.9217660301	0.7640669100
H24	-0.4879807372	-3.6208127944	-0.0332373922
H25	-1.8691913564	-2.7457823686	0.6937739900
H26	-0.6060357052	-3.4325412252	1.7281269916
C27	-0.3615244651	-0.7196209683	1.9344497682
H28	-1.4415096539	-0.5017540294	1.9392003551
H29	0.1864548958	0.2380884340	1.9266406861
H30	-0.1155192939	-1.2382752969	2.8788202532
C31	2.0853843476	3.4045567590	0.9028545298
C32	3.3565205710	2.8328104100	1.0932456873
H33	3.8989729520	2.4225234405	0.2337525815
C34	3.8687168472	2.7684612125	2.3909392817
C35	3.1795900061	3.2424575467	3.5122060956
H36	3.6048864171	3.1845019880	4.5184403917
C37	1.9177773815	3.7938081411	3.2757361673
C38	1.3506376899	3.8862947850	2.0011293826
H39	0.3633321154	4.3400901910	1.8829471312
F40	5.0952587718	2.2189193900	2.5796062213
F41	1.2111384156	4.2663993459	4.3336324456
C42	0.8005461081	2.1438576008	-0.7862481186
C43	1.4931980126	3.4651859599	-0.5354070568
H44	2.3765377867	3.4856669968	-1.2076534639
C45	0.6446541038	4.6875833817	-0.7090411499
H46	1.1601979104	5.6551481911	-0.7179939812
C47	-0.7063776629	4.6093980813	-0.7803816001
H48	-1.3223212841	5.5108715321	-0.8784714903
C49	-1.3887278553	3.3272873617	-0.6813086043
C50	-2.7941532022	3.2472383405	-0.5742506516
H51	-3.3928280390	4.1659397417	-0.5797868463
C52	-3.4133873260	2.0105191283	-0.4239347493
H53	-4.5027272825	1.9705513366	-0.2950013469
C54	-2.6963988775	0.7792857062	-0.4211791662
C55	-1.3047883822	0.8313668463	-0.6260120880
C56	-0.6437848048	2.1041885387	-0.7013965491
C57	-3.5082578870	-0.4620523050	-0.1389224008
H58	-2.9221657321	-1.3852787485	-0.1955848022
H59	-4.3550972986	-0.5504016887	-0.8422799670
H60	-3.9434769777	-0.3981567099	0.8754840183

### 13, gas phase

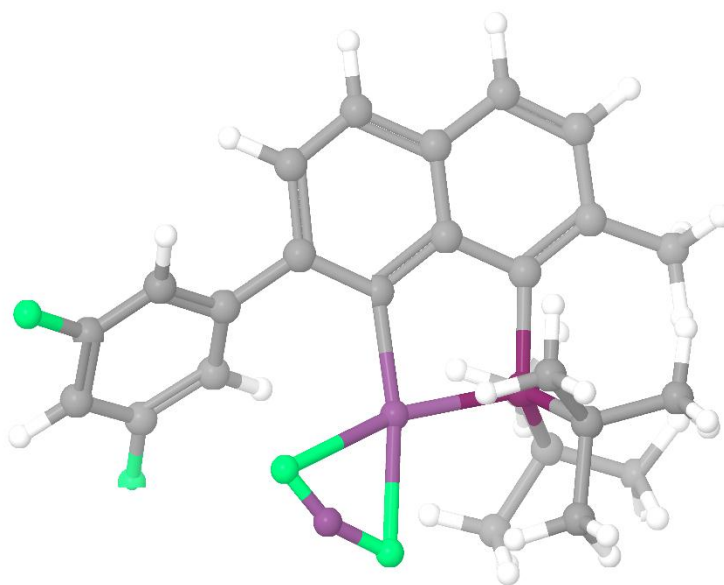
Total Gibbs free energy, Gtot (Htot - T\*S): -1827.891255 hartrees

Pt1	1.4712264069	-0.1463177329	-0.4685376678
P2	-0.4857748351	-1.1435178871	-0.1432198910
F3	3.5249929724	0.3295980263	-1.2727644167
F4	2.8667030678	-1.7941630771	-0.9003024193
C5	-0.8472061175	-2.1140155419	-1.7617907743
C6	-2.2613162666	-2.7170315882	-1.8522861867
H7	-2.3383813260	-3.2558575189	-2.8138486011
H8	-3.0400928957	-1.9395782189	-1.8519838736
H9	-2.4776625761	-3.4449236219	-1.0555734812
C10	-0.6865297336	-1.0846793134	-2.9047188023
H11	0.3344693589	-0.6710806565	-2.9345159365
H12	-1.3927390894	-0.2443126142	-2.8033607587
H13	-0.8914875885	-1.5911341091	-3.8649721227
C14	0.2159768734	-3.2224450299	-1.9157905009
H15	0.1058525043	-3.6700233349	-2.9199173672
H16	0.0813882309	-4.0344843226	-1.1821715741
H17	1.2424066106	-2.8320754123	-1.8223019184
C18	-0.4220135155	-2.2204875574	1.4517962430
C19	1.0420620946	-2.6920172769	1.6188225196
H20	1.1024933278	-3.3294844096	2.5195720368
H21	1.7237970020	-1.8368115393	1.7486347291
H22	1.4084589837	-3.2728416267	0.7593110988
C23	-1.3370324215	-3.4604328333	1.4606151651
H24	-1.0920456892	-4.1682805510	0.6536903908
H25	-2.4079955824	-3.2168415697	1.4040882725
H26	-1.1812740645	-3.9924641613	2.4163420868
C27	-0.7793006142	-1.2804838621	2.6214688039
H28	-1.8352716553	-0.9685957559	2.6037345458
H29	-0.1531129109	-0.3726731748	2.6136386611
H30	-0.5939159391	-1.8108464957	3.5723006852
C31	2.5884044012	2.9204847417	-0.0074415444
C32	3.3143147661	3.8226403131	-0.8117042285
H33	2.8282666376	4.3898211250	-1.6087157221
C34	4.6887803532	3.9569550094	-0.6116351736
C35	5.3843796882	3.2378622281	0.3639502745
H36	6.4603956246	3.3548133639	0.5006284313
C37	4.6376961533	2.3570232993	1.1489928108
C38	3.2609165364	2.1928712850	0.9959229474
H39	2.7196329084	1.5025733352	1.6474569569
F40	5.3818392352	4.8185968785	-1.3936986117
F41	5.2778441903	1.6428546975	2.1050183239
C42	0.4606169059	1.5399186210	-0.2157163850
C43	1.1146144406	2.7869592299	-0.1606255779
C44	0.3504670889	3.9922253704	-0.1980008301
H45	0.8922722023	4.9435963623	-0.1803929892
C46	-1.0299500159	3.9824938996	-0.2046974698
H47	-1.5990387826	4.9174744025	-0.2155826796

C48	-1.7256488906	2.7462213207	-0.1281547196
C49	-3.1397638258	2.6826688289	-0.0046069479
H50	-3.7133519389	3.6159042130	-0.0136750241
C51	-3.7797706979	1.4718071775	0.1638054053
H52	-4.8670564567	1.4436278180	0.2958878907
C53	-3.0670201815	0.2361901116	0.1934679295
C54	-1.6798822491	0.2647839323	-0.0041711856
C55	-0.9790963614	1.5157803764	-0.1374138910
C56	-3.8890595457	-0.9910980452	0.5094307438
H57	-3.3365298759	-1.9277377719	0.3858079902
H58	-4.7859524865	-1.0436701696	-0.1315692936
H59	-4.2497361187	-0.9484631154	1.5534344970
H60	3.4673216972	-0.7634225931	-1.2022218021

### 13, acetonitrile solution

Title: n0th\_7\_C0H3F2\_Pf\_a\_McCN



Total Gibbs free energy, Gtot (Htot - T\*S): -1827.908637 hartrees

Pt1	1.4671391425	-0.1398737163	-0.4856237072
P2	-0.4963423083	-1.1516365262	-0.1289179175
F3	3.5320689304	0.3497793771	-1.3817572308
F4	2.9171446186	-1.7767690908	-0.9360817519
C5	-0.8550524092	-2.1428842300	-1.7402982655
C6	-2.2650940399	-2.7591167268	-1.8245898308
H7	-2.3275905857	-3.3117401419	-2.7803330388
H8	-3.0511345940	-1.9888586642	-1.8428878524
H9	-2.4792305617	-3.4780027656	-1.0189879901
C10	-0.7009179473	-1.1282304834	-2.8965123560
H11	0.3130242154	-0.6954218360	-2.9101189954
H12	-1.4258117541	-0.3013773673	-2.8183336766
H13	-0.8793903683	-1.6509966849	-3.8533944850
C14	0.2141508790	-3.2486078661	-1.8814124481
H15	0.1043277887	-3.7061692046	-2.8814671540



H16	0.0856474494	-4.0540240958	-1.1394542693
H17	1.2376840725	-2.8497718547	-1.7961737922
C18	-0.4173777105	-2.2127612076	1.4800223594
C19	1.0448313788	-2.6938741264	1.6330592122
H20	1.1180290622	-3.2947309171	2.5575238162
H21	1.7364102974	-1.8395459036	1.7116065980
H22	1.3771720027	-3.3207871226	0.7918713465
C23	-1.3401550388	-3.4486425691	1.5054723622
H24	-1.1092358671	-4.1641474174	0.7005852214
H25	-2.4112759656	-3.2014585012	1.4645888458
H26	-1.1696697102	-3.9729507096	2.4637643450
C27	-0.7565092848	-1.2639221207	2.6486722252
H28	-1.8106931144	-0.9448334895	2.6370363624
H29	-0.1207178985	-0.3617833691	2.6400703968
H30	-0.5709953314	-1.7977211063	3.5981766738
C31	2.5996099716	2.9199264419	0.0111144365
C32	3.3264313345	3.8563538416	-0.7566918012
H33	2.8421815748	4.4584414364	-1.5314527869
C34	4.6988366177	3.9946052833	-0.5373180768
C35	5.4017521170	3.2500223589	0.4153413162
H36	6.4767110179	3.3790686084	0.5701951983
C37	4.6518152317	2.3355044183	1.1589690295
C38	3.2770331023	2.1624568509	0.9916105860
H39	2.7392166685	1.4486658797	1.6219061653
F40	5.3884958208	4.8951047714	-1.2833160160
F41	5.2903135737	1.5910113874	2.0982181086
C42	0.4610666148	1.5447835968	-0.2098168874
C43	1.1229146458	2.7900644406	-0.1438460043
C44	0.3611197104	4.0008844017	-0.1623818156
H45	0.9017364917	4.9541815630	-0.1330363457
C46	-1.0210754617	3.9932860211	-0.1656499266
H47	-1.5877657836	4.9312915258	-0.1647190045
C48	-1.7215954560	2.7558474906	-0.1029009600
C49	-3.1392065484	2.6975333151	0.0178364639
H50	-3.7120063690	3.6329898614	0.0146854363
C51	-3.7808596730	1.4845655107	0.1750046468
H52	-4.8700168558	1.4564437234	0.3027545158
C53	-3.0704427931	0.2439227219	0.1995920237
C54	-1.6818461353	0.2700878706	0.0026759128
C55	-0.9797372278	1.5221120390	-0.1248553540
C56	-3.9004336890	-0.9809920269	0.5020930227
H57	-3.3457751273	-1.9197556114	0.4034475751
H58	-4.7790397839	-1.0359413844	-0.1647847227
H59	-4.2905501035	-0.9255877971	1.5355400980
H60	3.4689449453	-0.7446537715	-1.2723963641

## 14, gas phase

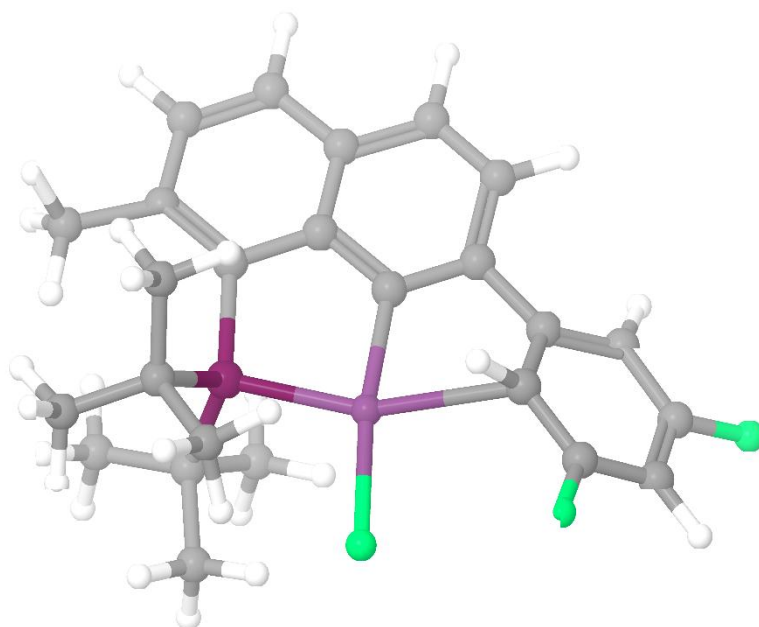
Total Gibbs free energy, Gtot (Htot - T\*S): -1727.534057 hartrees

Pt1	1.4546989970	0.2175686769	0.2347590622
P2	-0.4778979630	-0.9014443552	0.1585449125
F3	2.7834099792	-1.3192041729	-0.0054220557
C4	-0.5624223183	-1.7760799432	-1.5440753414
C5	-1.9091609839	-2.4446602501	-1.8741266101
H6	-1.8195064239	-2.9227698335	-2.8663436370
H7	-2.7287872919	-1.7120507260	-1.9369429255
H8	-2.1868594224	-3.2335813842	-1.1590071460
C9	-0.2948506033	-0.6643433789	-2.5844613725
H10	0.6944477379	-0.2039177784	-2.4298800399
H11	-1.0563449842	0.1323031491	-2.5453833844
H12	-0.3211414061	-1.1147917892	-3.5931570745
C13	0.5908401748	-2.8040155182	-1.5875590239
H14	0.7153094888	-3.1417714752	-2.6324868745
H15	0.3685179877	-3.6981872305	-0.9820409330
H16	1.5453245812	-2.3700355191	-1.2328670456
C17	-0.5924998017	-2.0747988367	1.6867597236
C18	0.8616899834	-2.4142480966	2.1006376071
H19	0.8350994963	-3.2343845685	2.8408080950
H20	1.3403576195	-1.5390545201	2.5677459972
H21	1.5119832147	-2.6963887855	1.2587063941
C22	-1.3617798707	-3.3886334506	1.4464961882
H23	-0.8850519518	-4.0188381631	0.6804714609
H24	-2.4168641925	-3.2380511457	1.1720583168
H25	-1.3567201985	-3.9634924871	2.3900529388
C26	-1.2534096224	-1.2730682394	2.8266462639
H27	-2.3236767125	-1.0839804044	2.6518254836
H28	-0.7516350201	-0.3030179001	2.9782429603
H29	-1.1571355835	-1.8516004509	3.7627141260
C30	2.4086540763	3.0486215541	0.0446743705
C31	3.1127974779	3.9160092782	-0.8079652961
H32	2.6091402011	4.7279487196	-1.3371240123
C33	4.4688726514	3.6768334724	-1.0498174182
C34	5.1772566690	2.6038566001	-0.4932260879
H35	6.2337951133	2.4438274988	-0.7120096791
C36	4.4736078033	1.7704625559	0.3743682486
C37	3.1099392527	1.9634114589	0.6660594349
H38	2.7057607002	1.4891679257	1.5813549525
F39	5.1302535221	4.5077733298	-1.8825558213
F40	5.1295708276	0.7706252935	0.9844324750
C41	0.3253665650	1.8290180410	0.2739675385
C42	0.9436615005	3.0934461980	0.1944936676
C43	0.1668405876	4.2855606464	0.1450680868
H44	0.6707475102	5.2572172126	0.0936573502
C45	-1.2159315747	4.2230991584	0.1854899879
H46	-1.8163919412	5.1383407356	0.1755788268
C47	-1.8838328682	2.9619497925	0.2359284098

C48	-3.2995674069	2.8392859810	0.2643767802
H49	-3.9146819418	3.7458626262	0.2563130633
C50	-3.8972166034	1.5933005627	0.3039693390
H51	-4.9902367262	1.5189682331	0.3343705468
C52	-3.1456991732	0.3785589078	0.3001765611
C53	-1.7484934849	0.4665500816	0.2527924857
C54	-1.1064937034	1.7538539081	0.2556553929
C55	-3.9429419838	-0.9018095923	0.3838374386
H56	-3.3208673868	-1.7998827913	0.3025333749
H57	-4.7043936177	-0.9485674347	-0.4141094884
H58	-4.4880351258	-0.9547203845	1.3436078039

#### 14, acetonitrile solution

Title: mpth\_7\_08H9F2\_PIF\_MoCN



Total Gibbs free energy, Gtot (Htot - T\*S): -1727.553372 hartrees

Pt1	1.4586886235	0.2023023709	0.2192556697
P2	-0.4956070235	-0.9149447546	0.1570794009
F3	2.8587033236	-1.3127266281	-0.0520993254
C4	-0.5945899859	-1.7830996806	-1.5496980598
C5	-1.9393031566	-2.4636826310	-1.8678783559
H6	-1.8517772584	-2.9329973217	-2.8653184026
H7	-2.7652804507	-1.7371280913	-1.9201276327
H8	-2.2035686551	-3.2591853917	-1.1546724150
C9	-0.3530683518	-0.6637453830	-2.5878250915
H10	0.6194979056	-0.1726192630	-2.4189243213
H11	-1.1395806822	0.1083016719	-2.5538658012
H12	-0.3572143604	-1.1115575551	-3.5976924984
C13	0.5658701840	-2.8027246673	-1.6112741988
H14	0.6803769995	-3.1342282711	-2.6597767914
H15	0.3580220555	-3.7007712732	-1.0056275771
H16	1.5197157767	-2.3615653542	-1.2664238398
C17	-0.6070603545	-2.0852753810	1.6905799689
C18	0.8460856797	-2.4370330538	2.0916827302

H19	0.8164195150	-3.2095957242	2.8813625198
H20	1.3594961421	-1.5462577881	2.4884077064
H21	1.4561219035	-2.8013089211	1.2516887357
C22	-1.3875977794	-3.3946961560	1.4573469354
H23	-0.9227936211	-4.0284430439	0.6860557581
H24	-2.4444216886	-3.2375284991	1.1937301072
H25	-1.3753601203	-3.9686021847	2.4021963351
C26	-1.2499352690	-1.2749000794	2.8355850289
H27	-2.3175508950	-1.0696483096	2.6625269131
H28	-0.7328543534	-0.3123500914	2.9891096587
H29	-1.1624380473	-1.8568341488	3.7709979173
C30	2.4087066091	3.0459896453	0.0302890545
C31	3.1142489897	3.9253732389	-0.8119042271
H32	2.6119555003	4.7346517750	-1.3505070207
C33	4.4816612236	3.7118383366	-1.0166570390
C34	5.2040632523	2.6551336102	-0.4425377716
H35	6.2732697193	2.5216476520	-0.6313075507
C36	4.4902123111	1.8119402274	0.4066680666
C37	3.1165212422	1.9757966408	0.6702584323
H38	2.7085194639	1.5040405787	1.5848015792
F39	5.1466257202	4.5587534307	-1.8319258819
F40	5.1496838084	0.8186656621	1.0360415571
C41	0.3196531751	1.8129832477	0.2556258472
C42	0.9404739739	3.0772124931	0.1673096620
C43	0.1649544967	4.2725469930	0.1107420666
H44	0.6710776337	5.2441870000	0.0518487749
C45	-1.2187872911	4.2142079478	0.1540253440
H46	-1.8175073643	5.1321077616	0.1375962652
C47	-1.8890895447	2.9532543554	0.2172768715
C48	-3.3077506715	2.8391508913	0.2527746664
H49	-3.9199411133	3.7494520078	0.2395988093
C50	-3.9092426600	1.5942866812	0.3058792428
H51	-5.0036723516	1.5235992760	0.3410248772
C52	-3.1615441638	0.3739863466	0.3083205049
C53	-1.7621105072	0.4571590636	0.2537505040
C54	-1.1141863390	1.7415996969	0.2435883463
C55	-3.9705998200	-0.8981812655	0.4003114493
H56	-3.3607237393	-1.8052023456	0.3237589494
H57	-4.7331951422	-0.9373123842	-0.3978970232
H58	-4.5170301270	-0.9357299437	1.3610131809

## 15, gas phase

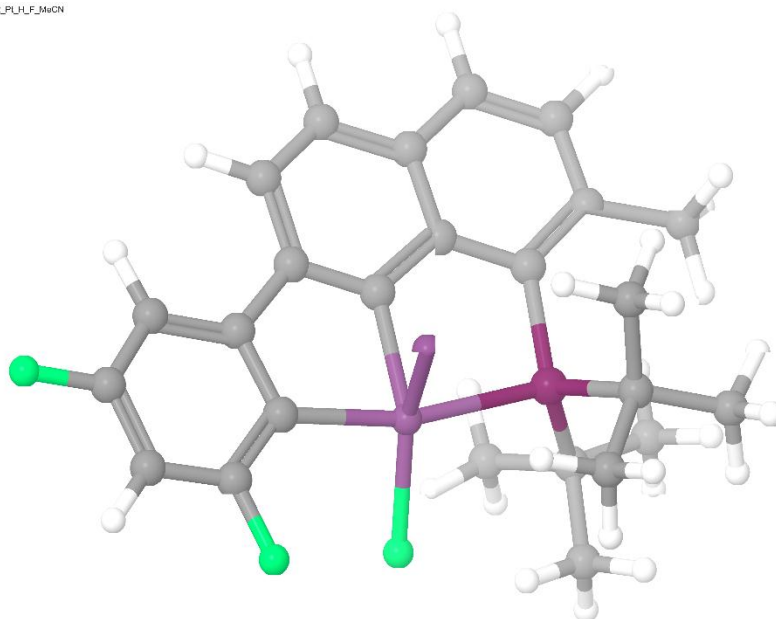
Total Gibbs free energy, Gtot (Htot - T\*S): -1727.512258 hartrees

Pt1	1.5803834345	0.0887643930	-0.0719700199
P2	-0.4905050716	-1.1484989944	-0.0565178023
F3	2.6274761638	-1.2208065424	1.0483352885
C4	-0.6778165385	-2.1699632141	-1.6798023369
C5	-1.6071654251	-3.3976926414	-1.6248692592
H6	-1.5516302086	-3.9192012914	-2.5977065050
H7	-2.6627365061	-3.1354153012	-1.4640344081
H8	-1.3029013078	-4.1205540856	-0.8523888332
C9	-1.1640830717	-1.1922692680	-2.7702442086
H10	-0.5227579646	-0.2971821747	-2.8361007860
H11	-2.1981370864	-0.8545765656	-2.5988631438
H12	-1.1280012440	-1.7013417244	-3.7499732772
C13	0.7476720552	-2.6544577801	-2.0400271435
H14	0.7080471523	-3.2055863360	-2.9970735819
H15	1.1685513636	-3.3279305866	-1.2778085412
H16	1.4462002619	-1.8102143595	-2.1608180911
C17	-0.6352610145	-2.1627198721	1.5602404691
C18	0.4126117288	-3.2942094013	1.4725985834
H19	0.4564912188	-3.8041858358	2.4521982937
H20	1.4097323829	-2.8725572919	1.2592037712
H21	0.1518731108	-4.0575414249	0.7214800906
C22	-2.0268159239	-2.7259518565	1.8893282561
H23	-2.4020136570	-3.4231154481	1.1235881109
H24	-2.7690065293	-1.9268842926	2.0416417168
H25	-1.9543404391	-3.2913291837	2.8363423397
C26	-0.2049724783	-1.1826605282	2.6782767933
H27	-0.8269486858	-0.2721709002	2.7005021428
H28	0.8535316253	-0.9019269304	2.5604717345
H29	-0.3184487206	-1.6911357000	3.6528488220
C30	2.5377637167	2.8471970568	0.0780607079
C31	3.4023581061	3.9567504674	0.1465077209
H32	3.0382495794	4.9800546874	0.2647701235
C33	4.7770245617	3.7300570201	0.0541702307
C34	5.3196671007	2.4525079894	-0.1089635329
H35	6.3982506615	2.3041182098	-0.1898473114
C36	4.4292346365	1.3707640510	-0.1702420013
C37	3.0486809730	1.5264468690	-0.0642376848
F38	5.6216991978	4.7894054529	0.1155560719
F39	4.9552288404	0.1368112756	-0.3531313353
C40	0.3996120152	1.6949036207	0.0381957960
C41	1.0684833176	2.9222747953	0.1532208161
C42	0.2929567110	4.0979183313	0.3543370177
H43	0.7927935165	5.0646159569	0.4684555119
C44	-1.0880041406	4.0262279874	0.4020248342
H45	-1.6838771812	4.9343802118	0.5382511398
C46	-1.7702902515	2.7823034961	0.2720719808
C47	-3.1863277616	2.6906215154	0.2906951260

H48	-3.7755657118	3.6047203355	0.4226930180
C49	-3.8138042503	1.4714910954	0.1327852906
H50	-4.9082078372	1.4215162275	0.1286235774
C51	-3.0875320847	0.2519578099	-0.0230945206
C52	-1.6846691755	0.2870702688	-0.0072630548
C53	-1.0133512252	1.5650287501	0.1004962526
C54	-3.9278026027	-0.9826561566	-0.2447341196
H55	-3.3541966426	-1.9114569048	-0.1735468947
H56	-4.3986592135	-0.9496831145	-1.2444416947
H57	-4.7499108561	-1.0371132600	0.4891696789
H58	1.2346390004	0.6343722089	-1.4837264220

## 15, acetonitrile solution

Title: nphh\_7\_C8H2F2\_PLH\_F\_MeCN



Total Gibbs free energy, Gtot (Htot - T\*S): -1727.531243 hartrees

Pt1	1.5788966129	0.0833484192	-0.0258107707
P2	-0.5012603960	-1.1561446770	-0.0485018502
F3	2.6465111400	-1.1893611184	1.1668843858
C4	-0.6530094232	-2.1453980538	-1.6995956722
C5	-1.5917301895	-3.3689583698	-1.6823931713
H6	-1.5136845550	-3.8715629104	-2.6640918292
H7	-2.6501669019	-3.1045325520	-1.5415417258
H8	-1.3069225128	-4.1084610086	-0.9173776195
C9	-1.1121688135	-1.1463291568	-2.7839366283
H10	-0.4597143351	-0.2569676786	-2.8380323716
H11	-2.1460751397	-0.8019794435	-2.6225186504
H12	-1.0682142134	-1.6489987342	-3.7671626776
C13	0.7759562964	-2.6349695275	-2.0400595324
H14	0.7556123263	-3.1448837183	-3.0202073195
H15	1.1625583805	-3.3493733248	-1.2968413679
H16	1.4871332752	-1.7939740807	-2.1053005489
C17	-0.6610853742	-2.2047688223	1.5491294423
C18	0.3951012208	-3.3289115329	1.4506605515

H19	0.4301514455	-3.8558560841	2.4220637459
H20	1.3918987170	-2.8996990850	1.2553065287
H21	0.1475634468	-4.0802419696	0.6833016899
C22	-2.0511317656	-2.7912837937	1.8481676706
H23	-2.4149370214	-3.4656829532	1.0568906716
H24	-2.8021682007	-2.0056102931	2.0258368857
H25	-1.9738759599	-3.3877094455	2.7762758870
C26	-0.2551122558	-1.2477977189	2.6954439208
H27	-0.8921818506	-0.3481349221	2.7340361148
H28	0.7991709087	-0.9463550850	2.5885160494
H29	-0.3665841190	-1.7821521942	3.6569136925
C30	2.5400804922	2.8538247619	0.0315746344
C31	3.4024787100	3.9692360735	0.0364350159
H32	3.0374252584	4.9986872641	0.1107847093
C33	4.7771285094	3.7380563097	-0.0689229460
C34	5.3303481648	2.4586115136	-0.1809632865
H35	6.4106852185	2.3106281199	-0.2742309954
C36	4.4353455894	1.3777453669	-0.1768770694
C37	3.0548996039	1.5270990171	-0.0609655390
F38	5.6189565383	4.8055513786	-0.0717587940
F39	4.9660087202	0.1298657526	-0.3092510884
C40	0.3990328088	1.6964732486	0.0371733823
C41	1.0688720618	2.9277103888	0.1170324259
C42	0.2960195083	4.1115442817	0.2962411736
H43	0.7951678427	5.0827484361	0.3862676245
C44	-1.0862618958	4.0387467374	0.3562770813
H45	-1.6821101855	4.9503526904	0.4791424701
C46	-1.7697928862	2.7904209553	0.2533761263
C47	-3.1897313478	2.7044621443	0.2804787784
H48	-3.7777114819	3.6221605470	0.4055258465
C49	-3.8179645358	1.4826643673	0.1342014244
H50	-4.9137587203	1.4329183481	0.1331452675
C51	-3.0933379054	0.2575511069	-0.0188950314
C52	-1.6891785619	0.2890925588	0.0015251358
C53	-1.0153522104	1.5672160085	0.0996060211
C54	-3.9387457832	-0.9727532828	-0.2432004360
H55	-3.3641238519	-1.9038758709	-0.2162354649
H56	-4.4403760145	-0.9107223831	-1.2272821394
H57	-4.7383234172	-1.0443150567	0.5149820615
H58	1.2413959038	0.5668405175	-1.4593602196

### TS<sub>Pt-C8</sub>, gas phase

Total Gibbs free energy, G<sub>tot</sub> (H<sub>tot</sub> - T\*S): -1827.809325 hartrees

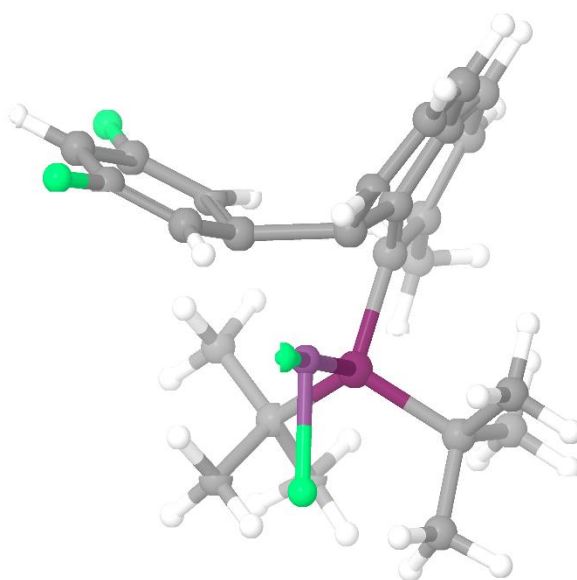
Pt1	0.3571679267	-0.5964633776	1.9318272841
P2	0.2608364263	-0.5970728906	-0.3508417162
F3	0.7766893356	-0.5514423516	3.9243384917
F4	0.9211243115	-2.4990282171	1.9937627397
C5	1.9961212327	-1.1573308646	-1.0004064074
C6	2.2040414059	-0.8849758357	-2.5018198571
H7	3.2202187936	-1.2253691868	-2.7709509591
H8	2.1465226557	0.1888809957	-2.7383531651
H9	1.4985758711	-1.4327294676	-3.1436897027
C10	3.0394931156	-0.3370728796	-0.2073178216
H11	2.9704394158	-0.5249094201	0.8756839530
H12	2.9406448409	0.7467309375	-0.3774767720
H13	4.0449396440	-0.6426105158	-0.5477465711
C14	2.2107806086	-2.6526761480	-0.6816742348
H15	3.2651778416	-2.9006304207	-0.8998253641
H16	1.5880098084	-3.3147026084	-1.3032031672
H17	2.0024384330	-2.8614984018	0.3792153409
C18	-1.1943616791	-1.6675906059	-1.0507723575
C19	-1.4488882385	-2.7363394257	0.0428039461
H20	-2.1692009742	-3.4766193164	-0.3486243196
H21	-1.8798015532	-2.2738689985	0.9448006482
H22	-0.5351265011	-3.2560736342	0.3677477051
C23	-0.9128224521	-2.3845063295	-2.3872021012
H24	-0.0509786936	-3.0641542970	-2.3329030471
H25	-0.7639140908	-1.7003462989	-3.2367856352
H26	-1.7982372686	-2.9989256033	-2.6291508463
C27	-2.4645443469	-0.8072067160	-1.1958145926
H28	-2.3677943525	-0.0158745856	-1.9553462846
H29	-2.7561198694	-0.3450940710	-0.2418696914
H30	-3.2931266363	-1.4680475546	-1.5083490548
C31	-1.1043088374	1.0391700390	2.2612888564
C32	-1.4790612593	0.9241132045	3.6308402026
H33	-0.7532116432	0.5451676821	4.3557398280
C34	-2.7914737728	1.1808536363	4.0087661355
C35	-3.7969594535	1.5662325934	3.1124293611
H36	-4.8182117159	1.7655396098	3.4383421844
C37	-3.4060355576	1.6774509106	1.7779989616
C38	-2.1071961006	1.4330068434	1.3350339671
H39	-1.8823279740	1.6259974922	0.2877344065
F40	-3.1254999923	1.0378766134	5.3118736981
F41	-4.3284897648	2.0528027630	0.8570193821
C42	0.4869096950	1.4876024501	1.7978734960
C43	1.1904678844	2.1532672659	2.8329129972
H44	1.1912148189	1.6787023072	3.8179252008
C45	1.8076906549	3.3941107784	2.6164096227
H46	2.3173669052	3.8918831685	3.4468210841
C47	1.7194762410	4.0146643893	1.3743695011



H48	2.1188063528	5.0223891312	1.2202820977
C49	1.1348532813	3.3353824805	0.2679813065
C50	1.0770794636	3.9265081089	-1.0247331069
H51	1.4499868769	4.9476200298	-1.1569859048
C52	0.5582084980	3.2250096665	-2.0937693105
H53	0.4893083543	3.7023154707	-3.0772305397
C54	0.1664889961	1.8588084670	-1.9797781107
C55	0.2440761426	1.2340274984	-0.7212980513
C56	0.6183385329	2.0047781746	0.4365711654
C57	-0.3232950283	1.1964153658	-3.2443842767
H58	-0.3638902923	0.1048886223	-3.1668917050
H59	0.3188806322	1.4528321843	-4.1033502674
H60	-1.3405442755	1.5530765132	-3.4894367219

### TS<sub>Pt-C8</sub>, acetonitrile solution

Title: nphh\_u\_06H3F2\_Pf2\_pLd\_C8\_ar\_migration\_c\_c\_sigma\_TS\_MeCN



Total Gibbs free energy, G<sub>tot</sub> (H<sub>tot</sub> - T\*S): -1827.836675 hartrees

Pt1	0.3651718158	-0.6057515706	1.9281263101
P2	0.2634005173	-0.5904599028	-0.3739287007
F3	0.8015753425	-0.6276877471	3.9587763400
F4	0.8683106117	-2.5492375865	2.0298561612
C5	2.0035856507	-1.1643603018	-1.0044559035
C6	2.2180108119	-0.9083977451	-2.5091240474
H7	3.2398701351	-1.2467174174	-2.7617271741
H8	2.1587152496	0.1623470223	-2.7595770697
H9	1.5220069960	-1.4684239390	-3.1508051834
C10	3.0456390830	-0.3345716982	-0.2193617366
H11	2.9519972738	-0.4856074568	0.8684053330
H12	2.9608719048	0.7444206160	-0.4236530537
H13	4.0533282434	-0.6619459694	-0.5328120209
C14	2.2111540420	-2.6584011558	-0.6724369460
H15	3.2690615072	-2.9072227308	-0.8732748273
H16	1.5965322339	-3.3232329364	-1.2993051962

H17	1.9884966924	-2.8646425535	0.3855105655
C18	-1.1983255435	-1.6638261235	-1.0770178915
C19	-1.4686809997	-2.7292489303	0.0138595474
H20	-2.2160854327	-3.4450066530	-0.3721032984
H21	-1.8735679163	-2.2549407120	0.9222431105
H22	-0.5658905671	-3.2812155792	0.3140888036
C23	-0.9009742953	-2.3857623596	-2.4096026252
H24	-0.0419593467	-3.0691984956	-2.3465221088
H25	-0.7470019853	-1.7053632903	-3.2615870091
H26	-1.7877242965	-2.9995166389	-2.6523084656
C27	-2.4685054648	-0.8052435869	-1.2421828704
H28	-2.3586197068	-0.0056997756	-1.9908184302
H29	-2.7905505005	-0.3599445613	-0.2899367206
H30	-3.2828965661	-1.4692043040	-1.5850778708
C31	-1.1024417794	0.9943519849	2.2743643774
C32	-1.4636857071	0.9308837275	3.6497206243
H33	-0.7402945596	0.5802046664	4.3891939050
C34	-2.7658093963	1.2384351359	4.0309652352
C35	-3.7745159718	1.6252240534	3.1390611516
H36	-4.7881260040	1.8667016420	3.4699673951
C37	-3.3891980826	1.6816850338	1.7989046829
C38	-2.1017826136	1.3864850525	1.3485243784
H39	-1.8845754642	1.5347461825	0.2922214115
F40	-3.0822300431	1.1481952877	5.3479769163
F41	-4.3098557755	2.0532547008	0.8727550141
C42	0.5324012317	1.4710263991	1.7834468266
C43	1.1980584355	2.1570469104	2.8286161039
H44	1.1990700791	1.7015001835	3.8232467746
C45	1.7776889659	3.4210064808	2.6228550344
H46	2.2610507207	3.9352780264	3.4607650977
C47	1.6800508836	4.0397259393	1.3789620068
H48	2.0524981034	5.0603758545	1.2301738877
C49	1.1135648400	3.3500582965	0.2676639800
C50	1.0364789677	3.9556322137	-1.0205762242
H51	1.3877272293	4.9875928675	-1.1443612682
C52	0.5255434100	3.2529708957	-2.0947389361
H53	0.4438405158	3.7367063630	-3.0756170175
C54	0.1551211788	1.8762577037	-1.9888452272
C55	0.2499135030	1.2418927338	-0.7329757683
C56	0.6306300008	2.0042235620	0.4281815934
C57	-0.3221067956	1.2194329437	-3.2611337766
H58	-0.3509529286	0.1261067873	-3.1984720509
H59	0.3222967857	1.4954706529	-4.1133790323
H60	-1.3414802972	1.5716523158	-3.5087257463

**TS<sub>σ-π</sub>, gas phase**

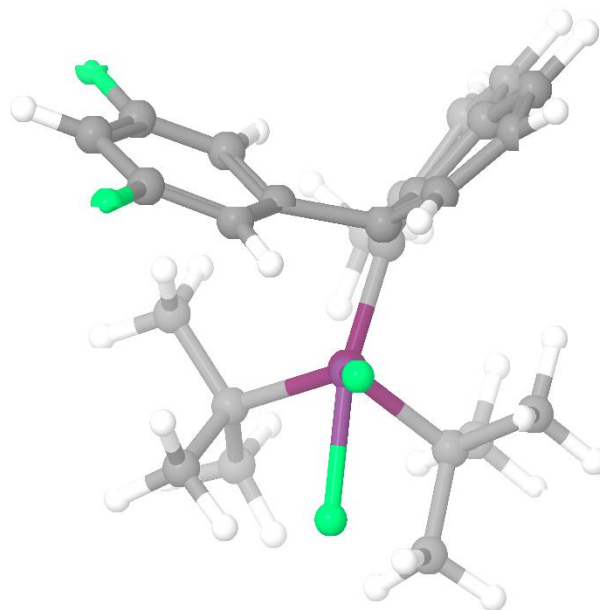
Total Gibbs free energy, Gtot (Htot - T\*S): -1827.808221 hartrees

Pt1	0.3348348806	-0.8097850313	1.8935817423
P2	0.2367982172	-0.6242952100	-0.3545561080
F3	0.5064629201	-0.8929575470	3.9239895201
F4	0.6022338869	-2.8049724077	1.8533429802
C5	1.8922733576	-1.3123231209	-1.0789806661
C6	2.1439360107	-1.0034190627	-2.5647127018
H7	3.1031233135	-1.4709328940	-2.8526137618
H8	2.2419549316	0.0770911646	-2.7518371116
H9	1.3710145934	-1.4153907420	-3.2302132186
C10	3.0183019712	-0.6596681283	-0.2440787674
H11	2.9065846788	-0.8820882495	0.8295803706
H12	3.0511780725	0.4350763374	-0.3690287829
H13	3.9855323903	-1.0688746625	-0.5874545146
C14	1.9150925406	-2.8366327050	-0.8277480203
H15	2.9376794069	-3.2036770322	-1.0300791330
H16	1.2361333186	-3.3823635994	-1.5021511160
H17	1.6438119905	-3.0721221538	0.2159429419
C18	-1.3476688456	-1.4235657250	-1.1132999865
C19	-1.7762528759	-2.5056527724	-0.0896297325
H20	-2.5849838620	-3.1144786345	-0.5322116924
H21	-2.1555917982	-2.0359212213	0.8320884699
H22	-0.9494129664	-3.1616721434	0.2237088751
C23	-1.1716417294	-2.0815889551	-2.4956027837
H24	-0.4373467873	-2.9000654919	-2.4849680393
H25	-0.8915278127	-1.3735246427	-3.2914869056
H26	-2.1433895639	-2.5176049798	-2.7890007714
C27	-2.4505469750	-0.3501525216	-1.1896767438
H28	-2.2453268070	0.4225079836	-1.9477238763
H29	-2.6011378849	0.1473550566	-0.2194043751
H30	-3.4009846580	-0.8429929885	-1.4640768527
C31	-1.1869539451	1.2975405527	2.2379818887
C32	-1.7233932562	0.7643641357	3.4373318973
H33	-1.0928883544	0.1528944663	4.0961961533
C34	-3.0762514330	0.9470888308	3.7137796198
C35	-3.9511761033	1.6467102559	2.8735452590
H36	-5.0054713461	1.7790704913	3.1189272241
C37	-3.3907317505	2.1700518807	1.7087767652
C38	-2.0438250393	2.0167587302	1.3716640759
H39	-1.6793893075	2.4979808863	0.4641144853
F40	-3.5798435497	0.4128134375	4.8492731079
F41	-4.1802998179	2.8813916247	0.8676028249
C42	0.3445180042	1.3339658590	1.9461855845
C43	1.1370405410	1.7475425094	3.0706126051
H44	0.9312411553	1.2480369462	4.0225827351
C45	2.0905136475	2.7664996912	2.9716718228
H46	2.6720237095	3.0557099056	3.8515861277
C47	2.2066902579	3.4855326882	1.7818505731

H48	2.8422451721	4.3766954251	1.7332430441
C49	1.5486969777	3.0562843830	0.5922887600
C50	1.7320573457	3.7211901359	-0.6515091815
H51	2.3315047390	4.6368801621	-0.6846431313
C52	1.1631040234	3.2071589448	-1.8007505879
H53	1.2673044456	3.7458216792	-2.7486127172
C54	0.5180760242	1.9362842137	-1.8129917735
C55	0.3864285647	1.2263217998	-0.6012627711
C56	0.7506408500	1.8682889017	0.6265105614
C57	-0.0099990350	1.4573725603	-3.1421525304
H58	-0.2211871433	0.3827601136	-3.1551197789
H59	0.6915306110	1.6827037868	-3.9617860286
H60	-0.9539748096	1.9839368892	-3.3742732726

### TS<sub>σ-π</sub>, acetonitrile solution

Title: nphh\_8\_C043FZ\_Pf2\_c\_c\_egme\_complex



Total Gibbs free energy, Gtot (Htot - T\*S): -1827.839456 hartrees

Pt1	0.3547510884	-0.7924296249	1.9099744899
P2	0.2787573229	-0.5770884761	-0.3572435456
F3	0.6083545918	-0.9497372852	3.9703316878
F4	0.5620906984	-2.8196748899	1.9222694979
C5	1.9404783836	-1.2881089131	-1.0507678605
C6	2.2067607066	-0.9965354342	-2.5394892242
H7	3.1764353036	-1.4586499105	-2.8029319345
H8	2.2988449723	0.0820457801	-2.7411268756
H9	1.4489041366	-1.4259837114	-3.2113566979
C10	3.0632951062	-0.6287196913	-0.2173244606
H11	2.9196772116	-0.8071614427	0.8612361381
H12	3.1194222136	0.4597254970	-0.3806059710
H13	4.0295363440	-1.0675266984	-0.5251429306
C14	1.9514936018	-2.8112352827	-0.7873199447
H15	2.9758498711	-3.1837154664	-0.9719685120
H16	1.2795790603	-3.3595216859	-1.4672365945

H17	1.6636563617	-3.0412878582	0.2520817254
C18	-1.3038453255	-1.3645924457	-1.1568305928
C19	-1.7794592506	-2.4255138160	-0.1340246439
H20	-2.6134692882	-2.9988316228	-0.5771512052
H21	-2.1376197758	-1.9336858107	0.7853511441
H22	-0.9815004221	-3.1201534910	0.1700647498
C23	-1.0925424164	-2.0477805925	-2.5240277023
H24	-0.3689121440	-2.8752634601	-2.4826422321
H25	-0.7877885759	-1.3551526340	-3.3244244933
H26	-2.0631799226	-2.4785858717	-2.8315517366
C27	-2.3998761499	-0.2889878767	-1.2914158174
H28	-2.1601375276	0.4766626481	-2.0452460182
H29	-2.6011815753	0.2122334088	-0.3329824360
H30	-3.3338581172	-0.7873612253	-1.6101080027
C31	-1.0941051018	1.2614523964	2.2835620815
C32	-1.5965896482	0.8258611543	3.5397989026
H33	-0.9464054129	0.2865228042	4.2368899029
C34	-2.9482216412	0.9948883643	3.8308518700
C35	-3.8692323767	1.5946226536	2.9621731849
H36	-4.9242966136	1.7176875569	3.2208575239
C37	-3.3405818721	2.0273511625	1.7461234269
C38	-1.9968665993	1.8863293734	1.3904273412
H39	-1.6695344080	2.3082828180	0.4407794473
F40	-3.4048317829	0.5418061665	5.0265381405
F41	-4.1666227269	2.6355776614	0.8570840531
C42	0.4480365769	1.3387656499	1.9739463131
C43	1.2119016583	1.8111371133	3.1049808373
H44	1.0336670938	1.3272028560	4.0705243959
C45	2.0896647507	2.8934245837	3.0128042600
H46	2.6355259300	3.2329407629	3.8994109593
C47	2.1780303476	3.6085999022	1.8132532690
H48	2.7592850072	4.5380280278	1.7658384633
C49	1.5527132521	3.1359350611	0.6239206467
C50	1.7086216165	3.8217231380	-0.6156702918
H51	2.2653270572	4.7664132150	-0.6379577108
C52	1.1672575082	3.2919483257	-1.7718335774
H53	1.2536535835	3.8397722751	-2.7176568808
C54	0.5648931720	1.9974619039	-1.7918955513
C55	0.4537666786	1.2735157185	-0.5805322943
C56	0.8151602772	1.9056048658	0.6521558190
C57	0.0686930386	1.5166288030	-3.1329677110
H58	-0.1207167251	0.4378958980	-3.1657639979
H59	0.7836435490	1.7668865551	-3.9350870693
H60	-0.8782274405	2.0333907838	-3.3817688873

**TS<sub>C8-c7</sub> (Ar = 3,5-difluorophenyl), gas phase**

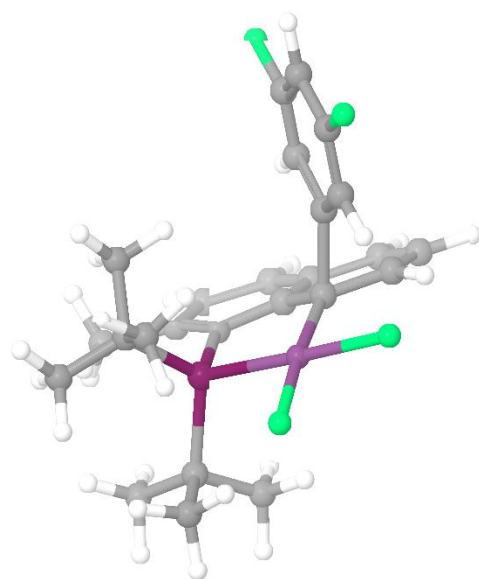
Total Gibbs free energy, G<sub>tot</sub> (H<sub>tot</sub> - T\*S): -1827.795683 hartrees

Pt1	7.9264768571	8.7178641207	4.1633781746
P2	7.9434586586	8.0126886549	2.0466453476
F3	8.0486268742	9.4690320190	6.0774584191
F4	6.6961363393	7.2491352544	4.8411309835
C5	8.6151228456	6.2103181629	1.9905422845
C6	8.9442255118	5.6438581443	0.5987119513
H7	9.2842566869	4.6000548624	0.7270282550
H8	9.7642052050	6.1923600549	0.1090823809
H9	8.0744680444	5.6187465436	-0.0753449150
C10	9.9137750469	6.2345014369	2.8305234688
H11	9.7207842232	6.5844623414	3.8574078793
H12	10.6859016733	6.8826866336	2.3826131965
H13	10.3192540292	5.2074820794	2.8768226544
C14	7.5702613161	5.3241946405	2.7054771530
H15	8.0321631758	4.3416789227	2.9130190680
H16	6.6852758943	5.1403170522	2.0739733072
H17	7.2381446506	5.7806050865	3.6570280126
C18	6.2366364048	8.2807696328	1.1963336502
C19	5.1967376229	8.2295795519	2.3456862462
H20	4.1826874706	8.1889562984	1.9086167764
H21	5.2744856854	9.1317629319	2.9731356582
H22	5.3416188260	7.3806945786	3.0323906115
C23	5.8427928555	7.2505901838	0.1213902406
H24	5.7812941788	6.2294000419	0.5268182455
H25	6.5143149421	7.2393890947	-0.7511553945
H26	4.8380750301	7.5130615613	-0.2559712182
C27	6.2429241215	9.7026520185	0.5982285714
H28	6.8914413927	9.7903696324	-0.2881792271
H29	6.5677516536	10.4512415538	1.3404176858
H30	5.2142924208	9.9634406128	0.2908531328
C42	8.4844301720	11.6037413816	3.6846945515
C43	7.5307713305	11.8498607270	4.6981584924
H44	7.4207761135	11.1208417493	5.5190268069
C45	6.7569970574	13.0031461304	4.6064420766
C46	6.8823523989	13.9300952954	3.5643001573
H47	6.2549027276	14.8211748236	3.5111052064
C48	7.8508097122	13.6574324157	2.5955431124
C49	8.6740011073	12.5314628541	2.6374661775
H50	9.4112193768	12.3914278431	1.8474898836
F51	5.8381497655	13.2462184357	5.5652744891
F52	8.0037228609	14.5263839062	1.5696206879
C53	9.2644229032	10.0992059442	3.5948220654
C54	10.0459649341	10.8154958711	4.5858409600
H55	9.6494764645	10.7580836423	5.6065000835
C56	11.3187882379	11.3902313217	4.2953272968
H57	11.8656245672	11.9147349170	5.0838161868
C58	11.8455957427	11.2643676870	3.0305870568

H59	12.8210118259	11.7038480362	2.7918064694
C60	11.1608935969	10.5416005643	1.9880772486
C61	11.7168953694	10.4265846472	0.6902506840
H62	12.6781395183	10.9030741348	0.4702438309
C63	11.0279378664	9.7384004312	-0.2952253177
H64	11.4357771648	9.6928043783	-1.3109600315
C65	9.8073420446	9.0633060261	-0.0291098008
C66	9.2842354141	9.0883526976	1.2850194164
C67	9.9133095623	9.9064293090	2.2639950107
C68	9.1302771140	8.4129756850	-1.2102899915
H69	8.3118120313	7.7464417600	-0.9214233665
H70	9.8475772040	7.8355643328	-1.8169577756
H71	8.7103757307	9.1933907458	-1.8705721441

### TS<sub>C8-C7</sub> (Ar = 3,5-difluorophenyl), acetonitrile solution

TIN: P/F2\_rpf/h/ORH/F2\_C8\_Iu\_C7\_ury\_mrg/atom\_TS\_MvCN - TS G0603



Total Gibbs free energy, G<sub>tot</sub> (H<sub>tot</sub> - T\*S): -1827.831917 hartrees

Pt1	7.9474114989	8.7019700819	4.1888276845
P2	7.9503003643	8.0255996925	2.0395158643
F3	8.0443887983	9.4122290452	6.1546642051
F4	6.6789342525	7.2492762921	4.9460671730
C5	8.5987071287	6.2126864646	1.9633250794
C6	8.8901363485	5.6428485304	0.5628400333
H7	9.2252599627	4.5966948745	0.6898480327
H8	9.7055334640	6.1819106909	0.0564689173
H9	8.0077528745	5.6239659652	-0.0942602393
C10	9.9193719604	6.2237155578	2.7666427502
H11	9.7570423727	6.6104464345	3.7864485303
H12	10.6910339962	6.8450541475	2.2823960169
H13	10.3055706154	5.1905883485	2.8295160701
C14	7.5601795889	5.3342387633	2.6980284159
H15	8.0183659130	4.3480996259	2.8980582551
H16	6.6627872872	5.1576425468	2.0820607789

H17	7.2461462980	5.7912201688	3.6540592159
C18	6.2389076645	8.3129612837	1.1939566885
C19	5.2003163130	8.2827981873	2.3426684407
H20	4.1850176431	8.3086884152	1.9070399424
H21	5.3308080263	9.1612426200	2.9957205596
H22	5.2981817615	7.3974794743	2.9901840243
C23	5.8276535945	7.2781681303	0.1274068178
H24	5.7465997494	6.2602431528	0.5389975959
H25	6.4963081501	7.2492448918	-0.7468473473
H26	4.8267496008	7.5589552268	-0.2485005875
C27	6.2570897301	9.7293304656	0.5808175646
H28	6.9058272762	9.7988038592	-0.3066215380
H29	6.5886439986	10.4858351084	1.3122978714
H30	5.2299626896	9.9925590273	0.2684400070
C42	8.5088493144	11.6273433916	3.6764014260
C43	7.5097522966	11.8410596588	4.6550181465
H44	7.3972802426	11.1190654029	5.4765690075
C45	6.7004881451	12.9683648195	4.5388728021
C46	6.8268700023	13.9014077799	3.5035754061
H47	6.1703419552	14.7725893583	3.4279805886
C48	7.8424108143	13.6613530474	2.5709794125
C49	8.6993245466	12.5630993273	2.6364559341
H50	9.4739706495	12.4544614264	1.8756422550
F51	5.7414536620	13.1718645582	5.4722959398
F52	8.0037331317	14.5384092142	1.5535538963
C53	9.2724121247	10.0976049033	3.5972924413
C54	10.0368893210	10.8642451849	4.5711353314
H55	9.6683258374	10.8476726279	5.6025792370
C56	11.3087241298	11.4481253125	4.2731059616
H57	11.8386643733	12.0013434308	5.0549000530
C58	11.8484198486	11.2926858278	3.0164049919
H59	12.8255513326	11.7300893647	2.7756611309
C60	11.1646900376	10.5540237826	1.9829587615
C61	11.7163379043	10.4455706298	0.6806243841
H62	12.6742421351	10.9300620590	0.4567096702
C63	11.0239771121	9.7599724393	-0.3053910926
H64	11.4268003769	9.7214087943	-1.3249887544
C65	9.8040604306	9.0794541215	-0.0381016404
C66	9.2912588157	9.0945937380	1.2831186981
C67	9.9220542124	9.9074474793	2.2651725689
C68	9.1354901003	8.4336753010	-1.2272494169
H69	8.2865655334	7.7966623463	-0.9573800112
H70	9.8534981588	7.8276485838	-1.8072415590
H71	8.7642390374	9.2212788475	-1.9109246815



**TS<sub>C8-c7</sub> (Ar = 4-methoxyphenyl), gas phase**

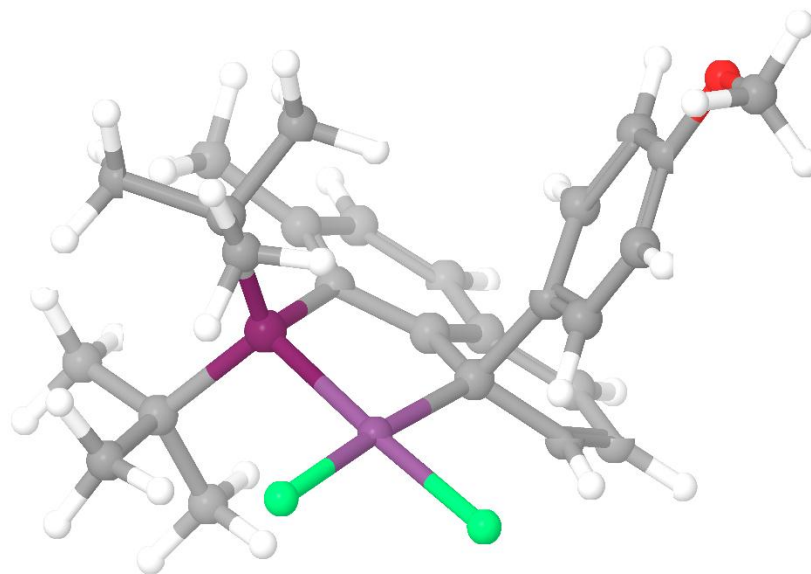
Total Gibbs free energy, G<sub>tot</sub> (H<sub>tot</sub> - T\*S): -1743.853758 hartrees

Pt1	-0.3250472185	-0.4036042256	2.1383071324
P2	-0.3841592146	-1.0864014014	0.0206005809
F3	-0.1624611963	0.3584381119	4.0416274544
F4	-1.5764368509	-1.8606049364	2.8379266270
C5	0.2297439475	-2.9090620164	-0.0763195706
C6	0.5060577712	-3.4738061210	-1.4800245305
H7	0.8134247883	-4.5298403503	-1.3690938580
H8	1.3323907777	-2.9489234484	-1.9847408735
H9	-0.3796979209	-3.4630039030	-2.1333486472
C10	1.5487401993	-2.9322169346	0.7308078470
H11	1.3911025265	-2.5819318410	1.7637381144
H12	2.3293546466	-2.3047346826	0.2682012571
H13	1.9229939782	-3.9717987927	0.7611828565
C14	-0.8228657093	-3.7684512525	0.6597834799
H15	-0.3853316882	-4.7653531123	0.8516003779
H16	-1.7280641914	-3.9229943166	0.0493096580
H17	-1.1175235366	-3.3064394329	1.6218111618
C18	-2.1006187539	-0.7593296845	-0.7903804641
C19	-3.1110854239	-0.7675634367	0.3859458677
H20	-4.1378581133	-0.7781686143	-0.0229660107
H21	-2.9850469296	0.1366864695	1.0027292660
H22	-2.9731900759	-1.6149453051	1.0767314596
C23	-2.5578862153	-1.7783805084	-1.8505462981
H24	-2.6490314252	-2.7947694415	-1.4389343316
H25	-1.9055933356	-1.8198748722	-2.7370403875
H26	-3.5595451373	-1.4793590825	-2.2087909052
C27	-2.0601905894	0.6581130227	-1.3985911607
H28	-1.4320668452	0.7164285079	-2.3022596524
H29	-1.6903791903	1.4010520068	-0.6721519520
H30	-3.0865295136	0.9527033977	-1.6835804411
C42	0.2255239909	2.4299034338	1.5249038640
C43	-0.6675106353	2.7653895223	2.5681842250
H44	-0.7728205434	2.0548366983	3.4027222378
C45	-1.3987432935	3.9540109789	2.5311888103
C46	-1.2387934845	4.8481855170	1.4533087458
O47	-1.9111208644	6.0266951670	1.3057171527
C48	-0.3211152280	4.5396087720	0.4287552806
C49	0.4206895640	3.3601984195	0.4763818223
H50	1.1182012241	3.1479557642	-0.3364626501
H51	-2.0918411000	4.1706583712	3.3472573892
H52	-0.2128133794	5.2384938154	-0.4055759231
C53	1.0113579459	1.0052390639	1.5248235854
C54	1.8886117749	1.5861100852	2.5326453511
H55	1.4648148323	1.5997402551	3.5442436057
C56	3.1921270215	2.0492752748	2.2454971405
H57	3.7971004865	2.5072496909	3.0331848416
C58	3.6845234177	1.9244609272	0.9584401823

H59	4.6835822038	2.3041679632	0.7127555011
C60	2.9377959222	1.2802136756	-0.0849103778
C61	3.4710615318	1.1409595283	-1.3917020137
H62	4.4627665492	1.5484600804	-1.6162834738
C63	2.7268178315	0.5118420739	-2.3747076914
H64	3.1177218920	0.4474467974	-3.3960135717
C65	1.4713062220	-0.0919149582	-2.0931178270
C66	0.9688138047	-0.0494271781	-0.7713897928
C67	1.6503561876	0.7323135198	0.2014139445
C68	0.7437878699	-0.6997034337	-3.2668976824
H69	-0.1091778093	-1.3175555200	-2.9688391175
H70	1.4192733377	-1.3163891998	-3.8831861747
H71	0.3629080839	0.1058181549	-3.9213173522
C72	-2.8604338136	6.3765892373	2.3137911597
H73	-3.2907902716	7.3373797938	1.9983141048
H74	-3.6649394567	5.6227753091	2.3934512622
H75	-2.3794017099	6.4979958661	3.3016342156

### TS<sub>C8-C7</sub> (Ar = 4-methoxyphenyl), acetonitrile solution

Title: Pff2\_nphn\_C8H4OMe\_migration\_TS\_MeCN



Total Gibbs free energy, G<sub>tot</sub> (H<sub>tot</sub> - T\*S): -1743.892514 hartrees

Pt1	-0.3035355130	-0.4300503019	2.1562919678
P2	-0.3731746098	-1.0799859354	0.0067463901
F3	-0.1528035920	0.2752477459	4.1183390800
F4	-1.5853724253	-1.8747485168	2.9590379680
C5	0.2061664086	-2.9148497862	-0.1033139241
C6	0.4342565460	-3.4981036814	-1.5099853824
H7	0.7255392166	-4.5585575774	-1.3907794959
H8	1.2587401310	-2.9968560108	-2.0400255823
H9	-0.4656701312	-3.4779916705	-2.1432387071
C10	1.5494168085	-2.9565539770	0.6612166443
H11	1.4323413630	-2.5503112810	1.6795538292

H12	2.3330200467	-2.3740443122	0.1485690334
H13	1.8921169762	-4.0051706694	0.7244635844
C14	-0.8444530969	-3.7538830995	0.6602017201
H15	-0.4221100918	-4.7596705773	0.8426433915
H16	-1.7662754797	-3.8898657477	0.0697771314
H17	-1.1123045481	-3.2880109548	1.6269067232
C18	-2.0883244963	-0.7242040400	-0.8074777337
C19	-3.1016227072	-0.7061361316	0.3632117286
H20	-4.1245699774	-0.6328863760	-0.0481633947
H21	-2.9129542002	0.1643270133	1.0128560255
H22	-3.0280510235	-1.5954612461	1.0088911756
C23	-2.5644465388	-1.7417664733	-1.8630442577
H24	-2.6798512050	-2.7553000772	-1.4485758658
H25	-1.9132599881	-1.7992320869	-2.7491796480
H26	-3.5595696572	-1.4197142367	-2.2216563966
C27	-2.0237680099	0.6875696013	-1.4278135820
H28	-1.3894857203	0.7252832347	-2.3276658437
H29	-1.6461764131	1.4326567249	-0.7076387706
H30	-3.0445984972	0.9924071693	-1.7233990064
C42	0.2362112773	2.4523690946	1.5087062007
C43	-0.6766861278	2.7721609902	2.5467198799
H44	-0.7815244452	2.0597641083	3.3763850453
C45	-1.4250937925	3.9500944047	2.5203165157
C46	-1.2660801431	4.8556149544	1.4483077050
O47	-1.9491870716	6.0230553087	1.3074047945
C48	-0.3371599342	4.5644759446	0.4205950241
C49	0.4178309459	3.3957998084	0.4625468860
H50	1.1198830219	3.2026260072	-0.3524361901
H51	-2.1265946236	4.1540700628	3.3339120788
H52	-0.2308214725	5.2687747744	-0.4121721220
C53	0.9896866366	1.0182399764	1.5098787872
C54	1.8514595721	1.6729086556	2.5009424369
H55	1.4635637557	1.7097221561	3.5243738278
C56	3.1465413193	2.1660392887	2.2024834766
H57	3.7293805781	2.6683637369	2.9814278554
C58	3.6602131896	1.9983787403	0.9289905307
H59	4.6606947341	2.3786821149	0.6836933958
C60	2.9279514402	1.3126569095	-0.1010616948
C61	3.4773733598	1.1562646357	-1.4009929560
H62	4.4659804027	1.5754493255	-1.6247304616
C63	2.7479209411	0.5025751114	-2.3816550140
H64	3.1475728666	0.4291418173	-3.4005736441
C65	1.4921101613	-0.1041869923	-2.1044353602
C66	0.9844926117	-0.0535699918	-0.7796919058
C67	1.6487786176	0.7433087596	0.1893005292
C68	0.7783789895	-0.7155963169	-3.2850766511
H69	-0.0925681988	-1.3173694703	-3.0049912370
H70	1.4604267129	-1.3466710509	-3.8810604531
H71	0.4299042887	0.0916476341	-3.9571296045
C72	-2.8973576144	6.3857251470	2.3314203109

H73	-3.3172046135	7.3514664488	2.0153678911
H74	-3.7057687017	5.6375069812	2.4090670149
H75	-2.4009663612	6.5005477675	3.3110477795

### TS<sub>CHF</sub>, gas phase

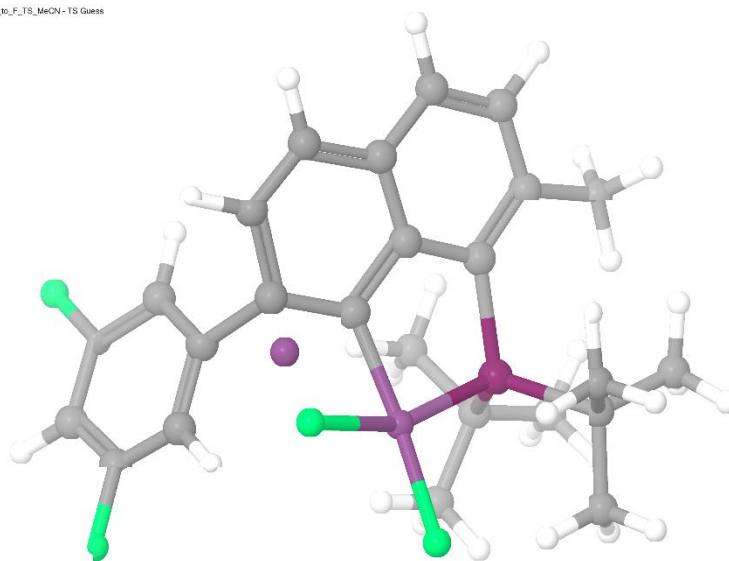
Total Gibbs free energy, G<sub>tot</sub> (H<sub>tot</sub> - T\*S): -1827.834699 hartrees

Pt1	1.7367543420	0.5857221749	-0.9368471399
P2	-0.1399553633	-0.5991307583	-0.6851869401
F3	3.0949736876	2.2190111965	-1.5144934587
F4	2.9813945568	-0.8163116499	-1.6901600754
C5	-0.4386449284	-1.5448455802	-2.3254373086
C6	-1.8196950553	-2.2082359841	-2.4722187309
H7	-1.8254440405	-2.7577005766	-3.4306456142
H8	-2.6331434361	-1.4685999727	-2.5175578907
H9	-2.0396917907	-2.9393952129	-1.6796576837
C10	-0.2818979295	-0.4895192227	-3.4450596325
H11	0.7243618487	-0.0420870125	-3.4438050936
H12	-1.0241069465	0.3212618785	-3.3550370748
H13	-0.4401541859	-0.9895459648	-4.4173154980
C14	0.6853400927	-2.5965586186	-2.4497687033
H15	0.6466749631	-3.0209388480	-3.4692408694
H16	0.5488764797	-3.4333407258	-1.7445423751
H17	1.6801653243	-2.1385866916	-2.2922745011
C18	-0.0850473260	-1.6827506221	0.8988033896
C19	1.3956790208	-2.0941118200	1.0830484176
H20	1.4683520014	-2.7710688402	1.9534156274
H21	2.0278274370	-1.2115971390	1.2697022386
H22	1.8133785649	-2.6076310722	0.2037995830
C23	-0.9632322688	-2.9473745126	0.8651951083
H24	-0.6703129230	-3.6396531397	0.0609823648
H25	-2.0376284549	-2.7277967920	0.7690076281
H26	-0.8312052860	-3.4841056755	1.8217216512
C27	-0.5037957460	-0.7726478750	2.0713819633
H28	-1.5719898517	-0.5050158121	2.0331449236
H29	0.0867281788	0.1585565031	2.0925708198
H30	-0.3192520374	-1.3079766837	3.0195097925
C31	2.2665210324	3.3834739491	1.1666726567
C32	3.6064414035	2.9549602277	1.1782451564
H33	4.0772071602	2.5738417280	0.2706007953
C34	4.3262316332	3.0274760830	2.3731808735
C35	3.7828092669	3.5146569172	3.5646073805
H36	4.3692573405	3.5648650228	4.4832636865
C37	2.4518897792	3.9331925961	3.5193246670
C38	1.6852708589	3.8786464273	2.3537458399
H39	0.6450504974	4.2110953349	2.3785121617
F40	5.6153188219	2.6168782872	2.3803102951
F41	1.8808046278	4.4063451232	4.6535991093
C42	0.6835520805	2.0886572547	-0.3845042432
C43	1.3691101995	3.3490202173	-0.0778390942

C44	0.5693570469	4.5684077929	-0.2421500937
H45	1.0758160130	5.5273352939	-0.0849255128
C46	-0.7721264965	4.5399224216	-0.5163848365
H47	-1.3401665926	5.4684682985	-0.6340809887
C48	-1.4846388906	3.2872657038	-0.5614255491
C49	-2.8972667356	3.2003454069	-0.6156989381
H50	-3.4934377334	4.1168880558	-0.6708141500
C51	-3.5219875725	1.9644865556	-0.5415954374
H52	-4.6169575534	1.9190381751	-0.5228899069
C53	-2.8055573787	0.7335097662	-0.4707518884
C54	-1.4045411880	0.7863914101	-0.5351568583
C55	-0.7488223461	2.0633650447	-0.5230229191
C56	-3.6296194420	-0.5136138806	-0.2554018554
H57	-3.0314150878	-1.4307121655	-0.2738565600
H58	-4.4240087766	-0.6108668787	-1.0152543150
H59	-4.1337714588	-0.4625675455	0.7263829710
H60	2.2905064963	3.0654364999	-0.9916842857

### TS<sub>CHF</sub>, acetonitrile solution

file: nptc1\_7\_OHQP2\_Pf2\_H1transfer\_to\_P\_TS\_MeCN - TS Gauss



Total Gibbs free energy, G<sub>tot</sub> (H<sub>tot</sub> - T\*S): -1827.859203 hartrees

Pt1	1.7059690263	0.6564843421	-1.0104223421
P2	-0.1500783912	-0.5834672134	-0.6986334306
F3	2.9730473210	2.4353217287	-1.6035655763
F4	3.0511268395	-0.5676087814	-1.9644358370
C5	-0.3893044438	-1.6493802118	-2.2772514364
C6	-1.7288809385	-2.3994442830	-2.3998221943
H7	-1.6663838313	-3.0299077040	-3.3056804231
H8	-2.5773400232	-1.7142353439	-2.5422704963
H9	-1.9410847818	-3.0694345427	-1.5531788322
C10	-0.2735407628	-0.6708724389	-3.4676831603
H11	0.7085145467	-0.1727046137	-3.4856736738
H12	-1.0599852124	0.1019085175	-3.4434315764
H13	-0.3928087723	-1.2469572530	-4.4030325146

C14	0.7867108503	-2.6519528188	-2.3195628565
H15	0.7622736093	-3.1569991293	-3.3027555303
H16	0.6942133793	-3.4361721253	-1.5494703173
H17	1.7581743258	-2.1365121851	-2.2169032962
C18	-0.0824114653	-1.5590136442	0.9599023869
C19	1.3878295522	-1.9839356997	1.1732333733
H20	1.4610981193	-2.5198243219	2.1366051549
H21	2.0489741843	-1.1025181348	1.2075601453
H22	1.7543869135	-2.6566423099	0.3821550409
C23	-0.9832485353	-2.8087790095	1.0106445737
H24	-0.7018016978	-3.5617372942	0.2577100458
H25	-2.0539878572	-2.5773171904	0.9016054695
H26	-0.8549794829	-3.2763163299	2.0037890468
C27	-0.4843845181	-0.5726874836	2.0763430964
H28	-1.5457780192	-0.2834216639	2.0170786016
H29	0.1283885608	0.3441080855	2.0532261142
H30	-0.3176539084	-1.0644214772	3.0512263716
C31	2.2629714212	3.2972896084	1.2536217521
C32	3.6031917045	2.8726626505	1.1602982739
H33	4.0243813910	2.5647927747	0.2014744474
C34	4.3944425310	2.8656744733	2.3124998195
C35	3.9311939783	3.2729105663	3.5671010120
H36	4.5741027643	3.2659553823	4.4518799401
C37	2.5988405682	3.6925410736	3.6224989241
C38	1.7578605038	3.7133548156	2.5058080875
H39	0.7220643119	4.0449382130	2.6202756203
F40	5.6841034433	2.4549993737	2.2066538508
F41	2.0980409842	4.0948666647	4.8185359963
C42	0.6283789500	2.0960673986	-0.3227474573
C43	1.2995936217	3.3403378174	0.0629732207
C44	0.4889496004	4.5619056059	0.0024596303
H45	0.9889738094	5.5097342914	0.2357780277
C46	-0.8503294855	4.5417476463	-0.2907829685
H47	-1.4279427650	5.4718691061	-0.3432216295
C48	-1.5462561692	3.2885479310	-0.4482160351
C49	-2.9584421546	3.1967864477	-0.5513951549
H50	-3.5633908149	4.1112605910	-0.5618427693
C51	-3.5709343755	1.9523852492	-0.5836802759
H52	-4.6668174149	1.8964751495	-0.6043514088
C53	-2.8445811182	0.7196618343	-0.5649190057
C54	-1.4417477556	0.7862423868	-0.5900892225
C55	-0.7984668609	2.0683959396	-0.4837186607
C56	-3.6799439416	-0.5332755771	-0.4560576037
H57	-3.0831423435	-1.4477030256	-0.3731942529
H58	-4.3562630942	-0.6410544571	-1.3232337988
H59	-4.3230946197	-0.4689004112	0.4403895686
H60	2.1736580377	3.1583662821	-0.9346507226

### TS<sub>CH-Pt</sub>, gas phase

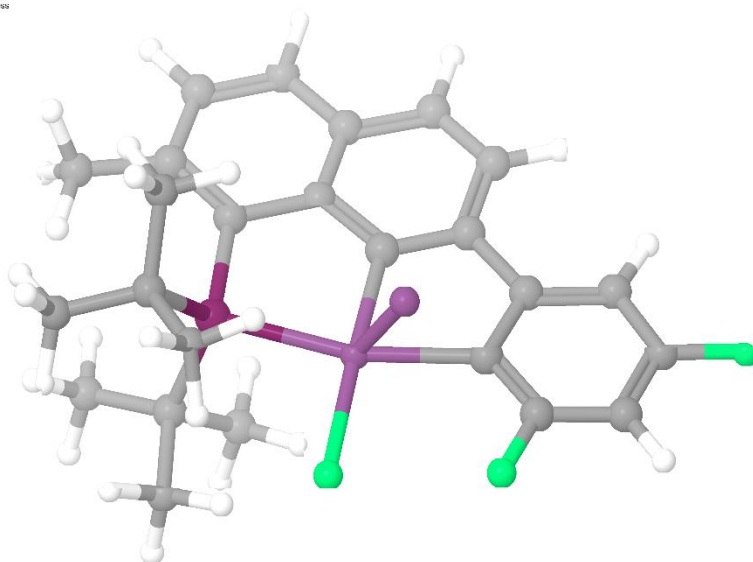
Total Gibbs free energy, G<sub>tot</sub> (H<sub>tot</sub> - T\*S): -1727.505864 hartrees

Pt1	1.5490591304	0.2744005193	0.0862408394
P2	-0.4817582613	-0.9578991473	0.1808761811
F3	2.7236039249	-1.3702501004	-0.2871979418
C4	-0.6659115804	-1.8865026310	-1.4850895330
C5	-2.0445656121	-2.5053189761	-1.7673084842
H6	-2.0069505653	-3.0040708670	-2.7530078447
H7	-2.8378435588	-1.7430015532	-1.8144535255
H8	-2.3268093691	-3.2704401980	-1.0276365278
C9	-0.3744594591	-0.8068739070	-2.5542866571
H10	0.6444987042	-0.3924053372	-2.4511801792
H11	-1.0918918127	0.0290863531	-2.5124651041
H12	-0.4437988774	-1.2690160947	-3.5554702176
C13	0.4446541180	-2.9589603008	-1.5411681019
H14	0.5039528795	-3.3463364336	-2.5746021439
H15	0.2248630767	-3.8174872641	-0.8858736219
H16	1.4276722838	-2.5380827168	-1.2581579869
C17	-0.5392683941	-2.0711784433	1.7511348939
C18	0.9373698877	-2.4000914470	2.0878083346
H19	0.9610667111	-3.1852723211	2.8647369329
H20	1.4501129963	-1.5092172895	2.4842142419
H21	1.5281976788	-2.7272287819	1.2185353865
C22	-1.3261550099	-3.3881942748	1.6077404509
H23	-0.9019820185	-4.0479256600	0.8358060794
H24	-2.3951194659	-3.2398645419	1.3920150583
H25	-1.2663694667	-3.9309940563	2.5684317199
C26	-1.1309345514	-1.2218610567	2.8943328095
H27	-2.2065927610	-1.0267643818	2.7652842401
H28	-0.6148603620	-0.2518055037	2.9873124479
H29	-0.9943720189	-1.7668949518	3.8454268370
C30	2.4305913753	3.0761843289	-0.1192125353
C31	3.2601487314	4.1924925214	-0.3234293980
H32	2.8617115815	5.2009141345	-0.4577382468
C33	4.6448925872	3.9984129275	-0.3568215707
C34	5.2393300732	2.7453065760	-0.1904960737
H35	6.3242609247	2.6247920798	-0.2069430642
C36	4.3914595662	1.6461680001	0.0093247895
C37	2.9999874349	1.7739892090	0.0165797052
H38	2.1189767736	0.9592124508	1.3727001539
F39	5.4470078065	5.0723068929	-0.5466010735
F40	4.9629497698	0.4414858066	0.1973891295
C41	0.3406299227	1.8603816443	0.0793821173
C42	0.9564258493	3.1160087684	-0.0555097398
C43	0.1544078499	4.2877909565	-0.1370398754
H44	0.6271480299	5.2685943792	-0.2499173913
C45	-1.2259520014	4.1972471325	-0.0705994476
H46	-1.8434997810	5.0997153241	-0.1200410953
C47	-1.8738290419	2.9350542204	0.0663593116

C48	-3.2861065261	2.8096994582	0.1548205942
H49	-3.9046401679	3.7128548020	0.1098808694
C50	-3.8738432345	1.5686274777	0.3045571394
H51	-4.9639920762	1.4914632255	0.3850619339
C52	-3.1119717991	0.3615213749	0.3561135377
C53	-1.7169478453	0.4407205687	0.2461597363
C54	-1.0789800350	1.7325594749	0.1295132957
C55	-3.8988732051	-0.9108351234	0.5634391646
H56	-3.2784291240	-1.8113881286	0.5022832519
H57	-4.7037440604	-1.0054556864	-0.1860597149
H58	-4.3892734851	-0.9039638403	1.5537308845

### TS<sub>CH-Pt</sub>, acetonitrile solution

Title: nphh\_7\_084F2\_H\_PIF\_OA\_TS\_MuCN - TS Guess



Total Gibbs free energy, G<sub>tot</sub> (H<sub>tot</sub> - T\*S): -1727.526026 hartrees

Pt1	1.5544667779	0.2661696652	0.0823796195
P2	-0.4920674924	-0.9669257290	0.1774284194
F3	2.7968949545	-1.3658454012	-0.3030476785
C4	-0.6736640264	-1.8970012285	-1.4891039367
C5	-2.0489300453	-2.5250403146	-1.7723375673
H6	-2.0013809956	-3.0259248298	-2.7571968762
H7	-2.8457869468	-1.7667500680	-1.8279939216
H8	-2.3304358978	-3.2889257899	-1.0307069883
C9	-0.3861140716	-0.8195614192	-2.5620475308
H10	0.6226542547	-0.3813822980	-2.4440341182
H11	-1.1216631590	0.0015357205	-2.5378315194
H12	-0.4302163505	-1.2889959213	-3.5616563990
C13	0.4403941371	-2.9673418225	-1.5367373883
H14	0.5001597396	-3.3605732036	-2.5684121995
H15	0.2227614522	-3.8212920825	-0.8740370865
H16	1.4215801171	-2.5411870767	-1.2578745623
C17	-0.5514964760	-2.0668182903	1.7617933429
C18	0.9212132788	-2.4068047278	2.0988920471



H19	0.9380104071	-3.1385236818	2.9269015638
H20	1.4612447032	-1.5022449601	2.4227832386
H21	1.4792876565	-2.8180297295	1.2441905364
C22	-1.3518833494	-3.3780723521	1.6332308446
H23	-0.9369661803	-4.0522777559	0.8677449597
H24	-2.4201727458	-3.2216198744	1.4199729643
H25	-1.2930318117	-3.9083805758	2.6016174215
C26	-1.1289714314	-1.1989702190	2.8994677908
H27	-2.2024876153	-0.9927276991	2.7700956969
H28	-0.5995748843	-0.2345779265	2.9837387647
H29	-0.9989518419	-1.7381508462	3.8552313319
C30	2.4281839338	3.0766243464	-0.1001410186
C31	3.2475891533	4.2023758967	-0.3062798160
H32	2.8400657348	5.2098212579	-0.4347334900
C33	4.6342562172	4.0188991042	-0.3501302786
C34	5.2470080604	2.7722519340	-0.1947020452
H35	6.3353519399	2.6622902410	-0.2191347063
C36	4.4032256615	1.6695046387	0.0048767226
C37	3.0094248361	1.7765178767	0.0256802455
H38	2.1749150492	0.9255440294	1.3644451022
F39	5.4246493507	5.1037123510	-0.5426692934
F40	4.9912412073	0.4624569776	0.1804110456
C41	0.3396743097	1.8506104049	0.0963980137
C42	0.9539772991	3.1098192546	-0.0291352563
C43	0.1549233065	4.2869598616	-0.1001107461
H44	0.6286825685	5.2699542981	-0.2036895802
C45	-1.2263381364	4.1972333686	-0.0354784400
H46	-1.8434750593	5.1018584331	-0.0779715696
C47	-1.8743093598	2.9321433382	0.0892221593
C48	-3.2902237672	2.8138457361	0.1723962309
H49	-3.9055870817	3.7213944391	0.1328317784
C50	-3.8815452456	1.5721917473	0.3102089700
H51	-4.9733093948	1.4967598441	0.3874202668
C52	-3.1222794796	0.3596128704	0.3539816967
C53	-1.7247104460	0.4351953518	0.2464997198
C54	-1.0822180545	1.7260487727	0.1432220841
C55	-3.9208318569	-0.9068891989	0.5508350692
H56	-3.3120289902	-1.8151108453	0.4849198988
H57	-4.7261040863	-0.9843896197	-0.2011270348
H58	-4.4140713571	-0.8980173307	1.5407438391

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