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DOI
10.1002/open.201700027

Publication date
2017

Document Version
Other version

Published in
ChemistryOPEN

ChemistryOPEN

Supporting Information

Metalate-Mediated Functionalization of P_4 by Trapping Anionic $[Cp^*Fe(CO)_2(\eta^1\text{-}P_4)]^-$ with Lewis Acids

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Supporting Information

1. Experimental Details

All manipulations regarding the preparation of air-sensitive compounds were carried out under an atmosphere of dry nitrogen, using standard Schlenk and drybox techniques. Solvents were purified, dried and degassed according to standard procedures.

^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were recorded on a Bruker Avance 400 and internally referenced to the residual solvent resonances (THF-d_8: ^{1}H δ 3.58, 1.72 ppm, $^{13}C\{^{1}H\}$ δ 67.2, 25.3 ppm). $^{31}P\{^{1}H\}$, ^{31}P, $^{11}B\{^{1}H\}$, ^{11}B and ^{7}Li NMR spectra were recorded on a Bruker Avance 400 and externally referenced (85% H_3PO_4, $BF_3{\cdot}OEt_2$ and LiCl, respectively). ^{19}F NMR spectra were recorded on a Bruker Avance 250 and externally referenced ($CFCl_3$). Chemical shifts are reported in ppm. Melting points were measured on samples in sealed capillaries and are uncorrected. ESI Mass spectra were recorded on a Bruker Daltonics micrOTOF spectrometer in negative (capillary potential of 4500 V) ion mode and the IR spectra were recorded on a Shimadzu FTIR-8400S spectrophotometer.

White phosphorus was sublimed prior to use (40 ^{o}C, 1 x 10^{-3} mbar) and triphenylborane (BPh_3) and $[Me_3NH][BPh_4]$ were prepared according to previously published procedures.[S1] $[Cp^*Fe(CO)_2]_2$ and $B(C_6F_5)_3$ were purchased from commercial resources and used without further purification.

Preparation of Li[Cp*Fe(CO)$_2$]

Freshly cut lithium (0.084 g, 12.1 mmol, 10.0 equiv.) was added to a solution of $[Cp^*Fe(CO)_2]_2$ (0.600 g, 1.21 mmol, 1.0 equiv.) in THF (10 mL) which was heated to 70 ^{o}C in a closed vessel and subsequently stirred for 40 h. The resulting dark brown mixture was cooled to room temperature and separated from the excess lithium by filtration through a cannula. The solvent was removed *in vacuo* and the resulting sticky red residue was further dried at 80 ^{o}C for 1 h to give a brown solid. Washing with *n*-pentane (3 x 10 mL) afforded **Li[Cp*Fe(CO)$_2$]** as a fine dark orange powder in 68% yield (0.420 g, 1.65 mmol).

^{1}H NMR (400.1 MHz, THF-d_8, 293 K): δ 1.85 (s, 15H; $(C_5(CH_3)_5)$.

^{7}Li (155.5 MHz, THF-d_8, 293 K): δ –0.8 (s).

$^{13}C\{^{1}H\}$ NMR (100.6 MHz, THF-d_8, 293 K): δ 88.5 (s; $C_5(CH_3)_5$), 12.5 (s; $C_5(CH_3)_5$), not observed (*C*O).

Preparation of [Li(Tol)][Cp*Fe(CO)$_2$(η^1-P$_4$·B(C$_6$F$_5$)$_3$)] (1a)

A cool solution of P_4 (0.054 g, 0.433 mmol, 1.1 equiv.) in toluene (10 mL, 0 ^{o}C) was added to a cooled (0 ^{o}C) mixture of $Li[Cp^*Fe(CO)_2]$ (0.100 g, 0.394 mmol, 1.0 equiv.) and $B(C_6F_5)_3$ (0.222 g, 0.433 mmol, 1.1 equiv.). The resulting brown suspension was warmed to room temperature and stirred for 1 h. The mixture was concentrated to about 3 mL and *n*-pentane (20 mL) was added after which the brown precipitate was collected by filtration through a cannula. Washing with toluene (3 x 5 mL) and subsequent drying *in vacuo* afforded **[Li(Tol)][Cp*Fe(CO)$_2$(η^1-P$_4$·B(C$_6$F$_5$)$_3$)]** as a dark yellow powder in 55% yield (0.213 g, 0.217 mmol). X-ray suitable crystals were obtained after slow (1 minute) addition of 12-crown-4 to a saturated solution of **[Li(Tol)][Cp*Fe(CO)$_2$(η^1-P$_4$·B(C$_6$F$_5$)$_3$)]** in Et_2O at room temperature.

Mp. (nitrogen, sealed capillary): 118 °C (decomposition).

^{1}H NMR (400.1 MHz, THF-d_8, 297 K): δ 1.74 (s, 15H; $C_5(CH_3)_5$).

^{7}Li (155.5 MHz, THF-d_8, 297 K): δ –2.4 (s).

^{11}B NMR (128.4 MHz, THF-d_8, 297 K): δ –15.6 (br. d, $^{1}J_{B,P}$ = 25.7 Hz).

^{13}C{^{1}H} NMR (100.6 MHz, THF-d_8, 297 K): δ 216.5 (s; *C*O), 148.5 (dm, $^{1}J_{C,F}$ = 239.4 Hz; *o*-B(C_6F_5)$_3$), 138.3 (dm, $^{1}J_{C,F}$ = 256.5 Hz; *p*-B(C_6F_5)$_3$), 137.1 (dm, $^{1}J_{C,F}$ = 253.5 Hz; *m*-B(C_6F_5)$_3$), 95.9 (s; $C_5(CH_3)_5$), 9.3 (d, $^{3}J_{C,P}$ = 7.0 Hz; $C_5(CH_3)_5$), not observed (*ipso*-B(C_6F_5)$_3$).

^{19}F NMR (235.4 MHz, THF-d_8, 292 K): δ –128.7 (br. d, $^{3}J_{F,F}$ = 56.5 Hz, 6F; *o*-B(C_6F_5)$_3$), –167.8 (br. t, $^{3}J_{F,F}$ = 21.2 Hz, 3F; *p*-B(C_6F_5)$_3$), –170.2 (br. t, $^{3}J_{F,F}$ = 18.8 Hz, 6F; *m*-B(C_6F_5)$_3$).

^{31}P{^{1}H} NMR (162.0 MHz, THF-d_8, 297 K): δ –65.0 (m, 1P; *P*-Fe), –107.1 (m, 1P; *P*-B(C_6F_5)$_3$), –340.7 (ddm, $^{1}J_{P,P}$ = –175.5 Hz, $^{1}J_{P,P}$ = –175.5 Hz; *P*-bridgehead).

HR-MS (ESI): 882.9270 [M]$^-$. Calcd.: for $C_{30}H_{15}BF_{15}FeO_2P_4$ 882.9231; 854.9318 [M – CO]$^-$. Calcd.: for $C_{29}H_{15}BF_{15}FeOP_4$ 854.9282.

IR (cm^{-1}): 2982 (w), 2914 (w), 2033 (w), 1996 (s), 1956 (s), 1747 (w), 1641 (m), 1512 (s), 1456 (s), 1381 (m), 1279 (m), 1153 (w), 1084 (s), 1030 (w), 964 (s), 816 (w), 785 (m), 771 (m), 761 (m), 677 (m), 621 (m), 582 (s), 569 (s), 501 (m).

Preparation of [Li(THF)$_x$][Cp*Fe(CO)$_2$(η^1-P$_4$·BPh$_3$)] (1b)

A solution of Li[Cp*Fe(CO)$_2$] (0.150 g, 0.590 mmol, 1.0 equiv.) in THF (5 mL) was added to a cooled solution of P_4 (0.081 g, 0.650 mmol, 1.1 equiv.) and BPh_3 (0.157 g, 0.650 mmol, 1.1 equiv.) in THF (10 mL, 0 °C). The resulting dark red brown solution was stirred at 0 °C for 15 min. and then allowed to warm to room temperature. The reaction solution was concentrated *in vacuo* to approximately one fifth of the initial volume after which *n*-pentane (30 mL) was added rapidly. The resulting sticky red precipitate was collected by filtration and washed with *n*-pentane (2 x 10 mL). Drying under reduced pressure at 60 °C afforded **[Li(THF)$_x$][Cp*Fe(CO)$_2$(η^1-P$_4$·BPh$_3$)]** as a brown powder in 86% yield (0.387 g, 0.506 mmol; for x = 2).

Mp. (nitrogen, sealed capillary): 64 °C (decomposition).

^{1}H NMR (400.1 MHz, THF-d_8, 297 K): δ 7.27 (d, $^{3}J_{H,H}$ = 7.2 Hz, 6H; *o*-B(C_6H_5)$_3$), 6.88 (t, $^{3}J_{H,H}$ = 7.2 Hz, 6H; *m*-B(C_6H_5)$_3$), 6.74 (t, $^{3}J_{H,H}$ = 7.2 Hz, 3H; *p*-B(C_6H_5)$_3$), 1.73 (s, 15H; $C_5(CH_3)_5$).

^{7}Li (155.5 MHz, THF-d_8, 297 K): δ –0.5 (s).

^{11}B NMR (128.4 MHz, THF-d_8, 297 K): δ –4.3 (br. s).

^{13}C{^{1}H} NMR (100.6 MHz, THF-d_8, 297 K): δ 217.2 (s; *C*O), 159.4 (s; *ipso*-B(C_6H_5)$_3$), 136.3 (s; *o*-B(C_6H_5)$_3$), 125.9 (s; *m*-B(C_6H_5)$_3$), 122.6 (s; *p*-B(C_6H_5)$_3$), 95.6 (s; $C_5(CH_3)_5$), 9.6 (d, $^{3}J_{C,P}$ = 5.0 Hz; $C_5(CH_3)_5$).

^{31}P{^{1}H} NMR (162.0 MHz, THF-d_8, 297 K): δ –46.6 (dt, $^{2}J_{P,P}$ = 186.0 Hz, $^{1}J_{P,P}$ = –177.9 Hz, 1P; *P*-B(C_6H_5)$_3$), –84.3 (dt, $^{2}J_{P,P}$ = 186.0 Hz, $^{1}J_{P,P}$ = –186.7 Hz, 1P; *P*-Fe), –337.0 (dd, $^{1}J_{P,P}$ = –177.9 Hz, $^{1}J_{P,P}$ = –186.7 Hz, 2P; *P*-bridgehead).

Despite numerous attempts, we were unable to obtain satisfactory analytical data for **1b** using IR spectroscopy and HR-MS spectrometry.

*Comment on the stability of **1b**:*

The product is stable in THF but slowly decomposes in Et_2O, benzene and toluene, as well as after the addition of 12-crown-4 or Ph_4PBr (to affect either encapsulation or exchange of the Li^+ cation) to a THF solution of **1b**. In addition, similar to white phosphorus, **1b** starts smoking immediately upon contact with air and may also ignite spontaneously.

Protonation experiments

Protonation of $[Li(THF)_x][Cp^*Fe(CO)_2(\eta^1\text{-}P_4{\cdot}BPh_3)]$ (1b) using $[Me_3NH][BPh_4]$:

$[Li(THF)_x][Cp^*Fe(CO)_2(\eta^1\text{-}P_4{\cdot}BPh_3)]$ (0.020 g, 0.026 mmol, 1.0 equiv.; for x = 2) and $[Me_3NH][BPh_4]$ (0.010 g, 0.026 mmol, 1.0 equiv.) were loaded in an NMR tube and THF-d_8 (0.6 mL) was added to give a dark red suspension which was directly analyzed using $^{31}P\{^1H\}$ (Figure S1), ^{31}P (Figure S2), $^{11}B\{^1H\}$, ^1H and $1H\{^{31}P\}$ NMR spectroscopy.

The $^{31}P\{^1H\}$ NMR spectrum revealed full conversion of the starting material and the formation of two new bicyclic tetraphosphabutane species (Figure S1). The $^{31}P\{^1H\}$ resonances of the two products were simulated[S2] as AMX_2 spin systems (inset; inverted), consistent with those expected for the neutral *exo,endo* and *exo,exo* isomers of $Cp^*Fe(CO)_2(\eta^1\text{-}P_4H)$ (1:1.2 ratio respectively). The former was distinguished from the latter by the smaller $^2J_{P,P}$ coupling constant (27.6 Hz vs. 243.3 Hz). The ^{31}P NMR spectrum (Figure S2) showed additional splitting of most signals into doublets (*exo,endo*-$Cp^*Fe(CO)_2(\eta^1\text{-}P_4H)$: $^1J_{P,H}$ = 145.9 Hz, $^2J_{P,H}$ = not resolved, $^3J_{P,H}$ = not resolved; *exo,exo*-$Cp^*Fe(CO)_2(\eta^1\text{-}P_4H)$: $^1J_{P,H}$ = 109.3 Hz, $^2J_{P,H}$ = 8.7 Hz, $^3J_{P,H}$ = 85.0 Hz). The $^{11}B\{^1H\}$ NMR spectrum showed two signals at 27.3 ppm and –8.4 ppm, corresponding to $Me_3N{\cdot}BPh_3$ in equilibrium with its constituents (the signal is observed at 52.0 ppm in Tol-d_8[S1]) and $[Li][BPh_4]$ respectively,[S3] confirming both neutral P_4 derivatives to be devoid of Lewis acid.

The products decomposed within 24h, revealing only three singlet resonance signals at –55.8, –67.2 and –345.6 ppm in the $^{31}P\{^1H\}$ NMR spectrum, corresponding to unidentified products.

***Exo,endo*-$Cp^*Fe(CO)_2(\eta^1\text{-}P_4H)$:**

$^{31}P\{^1H\}$ NMR (162.0 MHz, THF-d_8, 297 K): AMX_2 spin system, δ_{P_A} 70.6, δ_{P_M} –41.8, δ_{P_X} –335.5 ppm, $^1J_{P_A,P_X}$ = –194.5, $^1J_{P_M,P_X}$ = –198.4, $^2J_{P_A,P_M}$ = 27.6 Hz.

^1H NMR (400.1 MHz, THF-d_8, 297 K): δ 1.81 (s, 15H; $C_5(CH_3)_5$), –1.14 (br. d, $^1J_{H,P}$ = 152.9 Hz; P*H*).

***Exo,exo*-$Cp^*Fe(CO)_2(\eta^1\text{-}P_4H)$:**

$^{31}P\{^1H\}$ NMR (162.0 MHz, THF-d_8, 297 K): AMX_2 spin system, δ_{P_A} –19.8, δ_{P_M} –226.7, δ_{P_X} –355.2 ppm, $^1J_{P_A,P_X}$ = –166.4, $^1J_{P_M,P_X}$ = –149.9, $^2J_{P_A,P_M}$ = 243.3 Hz.

^1H NMR (400.1 MHz, THF-d_8, 297 K): δ 1.80 (s, 15H; $C_5(CH_3)_5$), not observed (P*H*).

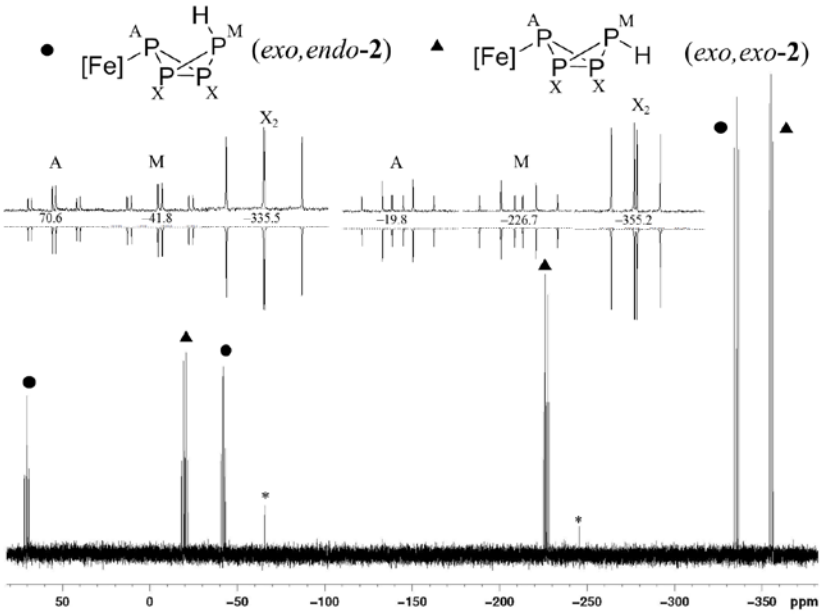

Figure S1. $^{31}P\{^{1}H\}$ NMR spectrum (162.0 MHz, THF-d_8, 297 K) recorded directly after mixing $[Li(THF)_x][Cp^*Fe(CO)_2(\eta^1\text{-}P_4{\cdot}BPh_3)]$ and $[Me_3NH][BPh_4]$: expansion (inset) shows the experimental (top) and simulated[S2] (inverted) spectrum. The resonance signals marked with an asterisk (*) correspond to unidentified side products. [Fe] = $Cp^*Fe(CO)_2$.

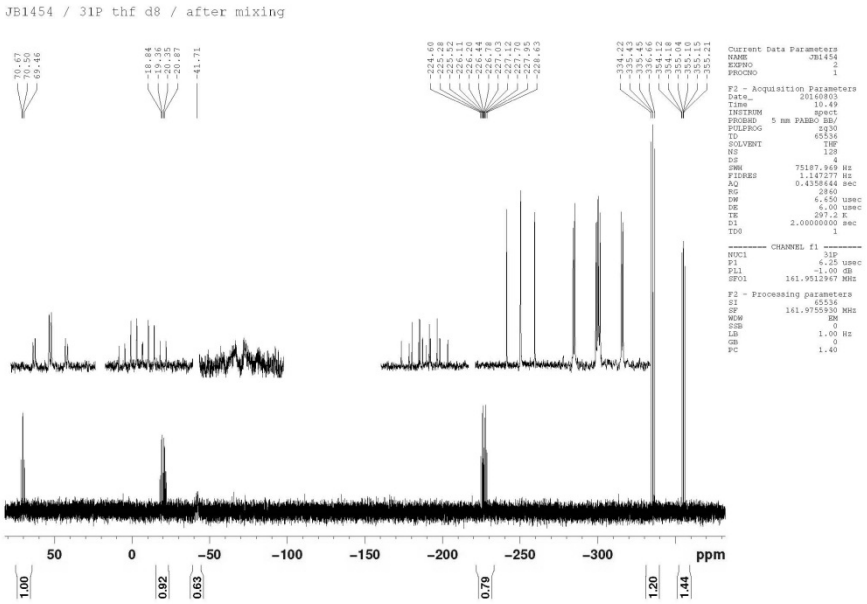

Figure S2. ^{31}P NMR spectrum (162.0 MHz, THF-d_8, 297 K) recorded directly after mixing $[Li(THF)_x][Cp^*Fe(CO)_2(\eta^1\text{-}P_4{\cdot}BPh_3)]$ and $[Me_3NH][BPh_4]$.

Protonation of [Li(Tol)][Cp*Fe(CO)$_2$(η^1-P$_4$·B(C$_6$F$_5$)$_3$)] (1a) using [Me$_3$NH][BPh$_4$]:

[Li(Tol)][Cp*Fe(CO)$_2$(η^1-P$_4$·B(C$_6$F$_5$)$_3$)] (0.010 g, 0.010 mmol, 1.0 equiv.) and [Me$_3$NH][BPh$_4$] (0.004 g, 0.010 mmol, 1.0 equiv.) were loaded in an NMR tube and THF-d_8 (0.6 mL) was added to give a dark brown solution which was directly analyzed using ^{31}P{^{1}H} and ^{11}B{^{1}H} NMR spectroscopy.

The ^{31}P{^{1}H} NMR spectrum revealed the *exo,endo*- and *exo,exo* isomers of Cp*Fe(CO)$_2$(η^1-P$_4$H) (see above) in a ca. 1:1.2 ratio respectively. The ^{11}B{^{1}H} NMR spectrum showed a singlet signal at –3.0 ppm, attributed to the amine-borane adduct Me$_3$N–B(C$_6$F$_5$)$_3$, and a large sharp one at –6.6 ppm corresponding to [Li][BPh$_4$].

Reaction of Li[Cp*Fe(CO)$_2$] with P$_4$

Li[Cp*Fe(CO)$_2$] (0.015 g, 0.059 mmol, 1 equiv.) and P$_4$ (0.007 g, 0.059 mmol, 1 equiv.) were loaded in an NMR tube and THF-d_8 (0.6 mL) was added to give a deep red mixture which was analyzed using ^{31}P{^{1}H} NMR spectroscopy (Figure S3). The obtained spectrum showed no bicyclic tetraphosphorus species but only several broad signals between 100 and –200 ppm indicative of a mixture of iron polyphosphides.

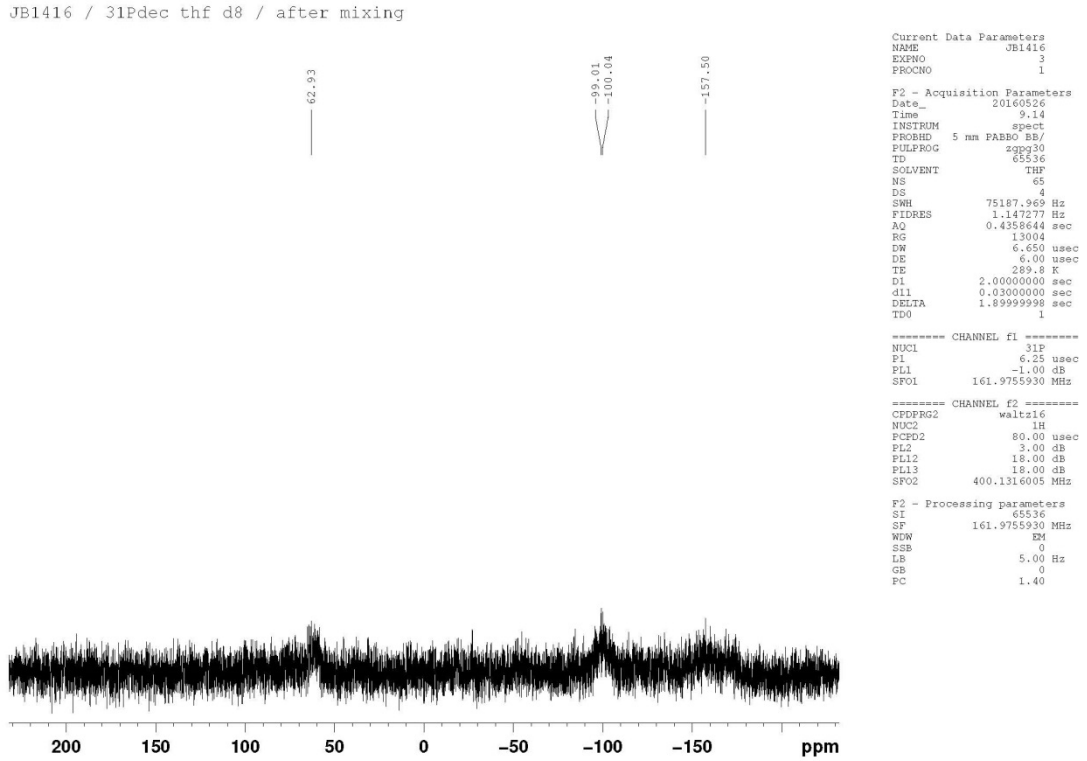

Figure S3. ^{31}P{^{1}H} NMR spectrum recorded directly after mixing of the reagents in THF-d_8 (LB = 5 Hz).

2. Computational Details

Density functional calculations were performed at the ωB97X-D[S4] level of theory using Gaussian09, revision D.01.[S5] Geometry optimizations were performed using the 6-31G(d) basis set[S6, S7] and uncorrected energies were obtained from single point calculations using the 6-311+G(2d,p) basis set.[S7, S8, S9] The nature of each stationary point was confirmed by frequency calculations. The ETS-NOCV[S10] analyses were performed at the ZORA-BP86-D3/TZ2P[S11] level of theory using ADF2014.[S12]

P_4

E: –1365.46676513 a.u.

Cartesian coordinates:

P	-0.449954000	-0.636325000	1.102058000
P	1.349861000	0.000022000	0.000000000
P	-0.449954000	-0.636325000	-1.102058000
P	-0.449954000	1.272629000	0.000000000

$B(C_6F_5)_3$

E: –2208.32982445 a.u.

Cartesian coordinates:

B	0.000065000	-0.000242000	0.003527000
C	0.136622000	1.560172000	0.002733000
C	-0.724753000	2.378935000	-0.732176000
C	1.127830000	2.219021000	0.734769000
C	-0.613010000	3.760853000	-0.753411000
C	1.258121000	3.599402000	0.752002000
C	0.383125000	4.372130000	-0.001859000
C	-1.419455000	-0.662317000	0.002948000
C	-1.699251000	-1.816058000	-0.734037000
C	-2.484542000	-0.135101000	0.737979000
C	-2.952235000	-2.409500000	-0.755833000
C	-3.745457000	-0.711792000	0.754688000
C	-3.978698000	-1.853864000	-0.001818000
C	1.283233000	-0.898442000	0.002518000
C	1.359010000	-2.084743000	0.736896000
C	2.422462000	-0.563007000	-0.733679000
C	2.489324000	-2.887740000	0.754301000
C	3.563216000	-1.350955000	-0.755028000

C	3.595345000	-2.517854000	-0.001261000
F	4.679732000	-3.277453000	-0.003069000
F	2.524184000	-3.999665000	1.481040000
F	0.327459000	-2.476757000	1.487918000
F	-0.750447000	-2.380395000	-1.484435000
F	2.436712000	0.541100000	-1.483718000
F	4.618456000	-1.002869000	-1.483777000
F	-1.689345000	1.839287000	-1.480641000
F	-2.307881000	0.953305000	1.490270000
F	-4.725948000	-0.185933000	1.481307000
F	-5.179089000	-2.412299000	-0.004601000
F	-3.178933000	-3.496737000	-1.485445000
F	1.984528000	1.521517000	1.484006000
F	2.205121000	4.185777000	1.476681000
F	0.498678000	5.691039000	-0.003904000
F	-1.443855000	4.500790000	-1.480081000

BPh_3

E: –719.761820912 a.u.

Cartesian coordinates:

B	-0.003002000	-0.001125000	0.000212000
C	0.973861000	-1.228024000	-0.000521000
C	0.641630000	-2.431150000	0.647674000
C	2.220134000	-1.168356000	-0.649162000
C	1.513219000	-3.514940000	0.660755000
H	-0.313990000	-2.512419000	1.159073000
C	3.085956000	-2.256317000	-0.663293000
H	2.509046000	-0.253674000	-1.160256000
C	2.735704000	-3.430440000	-0.001232000
H	1.238258000	-4.427761000	1.181572000
H	4.036995000	-2.187520000	-1.183622000
H	3.414877000	-4.278539000	-0.001228000
C	-1.554029000	-0.231377000	0.000640000
C	-2.427077000	0.663751000	0.644035000
C	-2.128823000	-1.341686000	-0.643146000
C	-3.802131000	0.456240000	0.656951000
H	-2.016453000	1.532709000	1.151720000

C	-3.504815000	-1.542398000	-0.657378000
H	-1.482931000	-2.053953000	-1.149941000
C	-4.343835000	-0.645461000	-0.000762000
H	-4.453004000	1.156127000	1.173115000
H	-3.923796000	-2.400642000	-1.174857000
H	-5.418590000	-0.804838000	-0.001462000
C	0.573906000	1.457314000	0.001191000
C	-0.096594000	2.510592000	-0.645689000
C	1.784396000	1.764279000	0.647952000
C	0.419829000	3.801772000	-0.659543000
H	-1.035112000	2.308927000	-1.155419000
C	2.294239000	3.057969000	0.661290000
H	2.329118000	0.973698000	1.157289000
C	1.614594000	4.078334000	0.000530000
H	-0.111027000	4.594533000	-1.178904000
H	3.224658000	3.270404000	1.180040000
H	2.015977000	5.087950000	0.000071000

Me_3N

E: –174.470260294 a.u.

Cartesian coordinates:

N	0.000000000	-0.000195000	-0.376536000
C	1.210678000	-0.665777000	0.061560000
H	1.231612000	-1.689502000	-0.326602000
H	2.085940000	-0.136712000	-0.329642000
H	1.303514000	-0.714704000	1.165071000
C	-1.182053000	-0.715210000	0.061572000
H	-1.271593000	-0.768978000	1.165095000
H	-2.078975000	-0.222217000	-0.328125000
H	-1.161653000	-1.738684000	-0.327292000
C	-0.028559000	1.381091000	0.061552000
H	-0.925806000	1.874157000	-0.327225000
H	-0.029536000	1.485739000	1.165098000
H	0.846103000	1.911644000	-0.328730000

$[Me_3NH]^+$

E: –174.848070054 a.u.

Cartesian coordinates:

N	0.000030000	-0.000025000	-0.339872000
C	-0.360474000	1.384687000	0.103123000
H	0.381302000	2.084741000	-0.282367000
H	-1.349244000	1.634217000	-0.282755000
H	-0.366496000	1.406511000	1.193829000
C	1.379502000	-0.380200000	0.103161000
H	1.401002000	-0.386467000	1.193866000
H	1.614917000	-1.372379000	-0.282877000
H	2.089948000	0.351682000	-0.282162000
C	-1.018976000	-1.004508000	0.103153000
H	-0.742193000	-1.985295000	-0.284575000
H	-1.033348000	-1.021937000	1.193853000
H	-1.996438000	-0.710827000	-0.280505000
H	0.000022000	0.000057000	-1.363829000

$Me_3N{\cdot}B(C_6F_5)_3$

E: –2382.82812511 a.u.

Cartesian coordinates:

B	-0.001676000	-0.001016000	0.606918000
N	-0.000273000	-0.001874000	2.418094000
C	-0.085545000	1.375818000	2.993657000
H	-0.862658000	1.940788000	2.488677000
H	-0.322452000	1.293336000	4.059020000
H	0.873487000	1.874975000	2.887806000
C	1.235141000	-0.617392000	2.993130000
H	1.282647000	-0.372445000	4.058862000
H	1.187594000	-1.697246000	2.885817000
H	2.113571000	-0.226570000	2.489728000
C	-1.150529000	-0.764387000	2.993551000
H	-0.961040000	-0.928788000	4.058924000
H	-2.062275000	-0.183637000	2.887808000
H	-1.251554000	-1.720321000	2.489604000
C	0.348317000	1.538012000	0.126197000
C	-0.418230000	2.293449000	-0.764212000
C	1.523046000	2.184113000	0.516254000
C	-0.087678000	3.584908000	-1.171732000

C	1.892818000	3.464624000	0.146279000
C	1.070852000	4.182805000	-0.710340000
C	-1.509076000	-0.466902000	0.125457000
C	-1.777594000	-1.506168000	-0.768362000
C	-2.657527000	0.224013000	0.517249000
C	-3.060459000	-1.867273000	-1.176731000
C	-3.950720000	-0.097270000	0.145677000
C	-4.159101000	-1.166422000	-0.713876000
C	1.155816000	-1.072500000	0.123521000
C	2.190583000	-0.783978000	-0.769104000
C	1.133857000	-2.412484000	0.515336000
C	3.147577000	-1.712148000	-1.175983000
C	2.061586000	-3.369720000	0.145814000
C	3.092262000	-3.013914000	-0.712461000
F	-0.882939000	4.241134000	-2.013492000
F	1.397671000	5.413198000	-1.086331000
F	3.029528000	3.999022000	0.589618000
F	2.411830000	1.544536000	1.306787000
F	-0.804505000	-2.230511000	-1.333328000
F	-3.229014000	-2.882480000	-2.020938000
F	-5.387178000	-1.500340000	-1.091197000
F	-4.983333000	0.616731000	0.590648000
F	-1.534925000	1.816537000	-1.326644000
F	-2.550561000	1.310876000	1.311961000
F	0.138307000	-2.865280000	1.307768000
F	2.329410000	0.420934000	-1.334609000
F	4.110814000	-1.348233000	-2.019331000
F	3.997871000	-3.908944000	-1.087960000
F	1.961534000	-4.621070000	0.591111000

$Me_3N{\cdot}BPh_3$

E: –894.251953079 a.u.

Cartesian coordinates:

B	-0.002113000	-0.005752000	0.169218000
N	-0.025077000	-0.060925000	2.025021000
C	1.293982000	-0.454030000	2.578752000
H	2.067093000	0.214471000	2.205173000

H	1.264216000	-0.394545000	3.673547000
H	1.535324000	-1.469955000	2.271444000
C	-1.019587000	-1.041738000	2.525542000
H	-0.944360000	-1.115025000	3.617301000
H	-2.023573000	-0.727156000	2.246370000
H	-0.826485000	-2.019118000	2.087503000
C	-0.377677000	1.256215000	2.608671000
H	-0.464539000	1.162837000	3.698005000
H	0.387259000	1.989938000	2.362015000
H	-1.329183000	1.594659000	2.202643000
C	1.102119000	-1.119767000	-0.281193000
C	2.227207000	-0.770182000	-1.042644000
C	0.982051000	-2.489575000	0.024714000
C	3.180423000	-1.704939000	-1.445032000
H	2.365253000	0.263340000	-1.342716000
C	1.927689000	-3.434086000	-0.360212000
H	0.108732000	-2.846795000	0.564641000
C	3.042333000	-3.042772000	-1.097161000
H	4.033509000	-1.381151000	-2.035598000
H	1.787306000	-4.478807000	-0.095099000
H	3.783946000	-3.774337000	-1.405288000
C	0.431312000	1.515161000	-0.235137000
C	-0.348428000	2.288807000	-1.107865000
C	1.632740000	2.113790000	0.190974000
C	0.016829000	3.577003000	-1.497945000
H	-1.266932000	1.873035000	-1.509050000
C	2.007195000	3.401252000	-0.177975000
H	2.323169000	1.551668000	0.814639000
C	1.191425000	4.147576000	-1.024121000
H	-0.623554000	4.134119000	-2.176717000
H	2.942241000	3.818192000	0.187186000
H	1.476495000	5.153522000	-1.319380000
C	-1.527015000	-0.370851000	-0.281999000
C	-1.826454000	-1.493466000	-1.067159000
C	-2.627109000	0.441836000	0.055163000
C	-3.128324000	-1.811364000	-1.453777000
H	-1.021330000	-2.138968000	-1.402533000

C	-3.932406000	0.135209000	-0.313448000
H	-2.462582000	1.369281000	0.598082000
C	-4.192470000	-1.006272000	-1.067565000
H	-3.306638000	-2.693996000	-2.062477000
H	-4.745350000	0.795481000	-0.022573000
H	-5.208927000	-1.252296000	-1.361853000

$[Cp^*Fe(CO)_2]^-$

E: –1880.53497021 a.u.

Cartesian coordinates:

Fe	-0.004244000	0.647735000	-0.024286000
C	0.929497000	-0.994399000	0.791799000
C	-0.441678000	-0.977962000	1.174555000
C	0.995541000	-1.038719000	-0.644378000
C	-1.221164000	-0.994022000	-0.029713000
C	-0.335016000	-1.052141000	-1.155239000
C	1.276230000	1.785380000	-0.050933000
O	2.225369000	2.482946000	-0.061715000
C	-1.226469000	1.849238000	-0.049847000
O	-2.116434000	2.620258000	-0.058788000
C	2.114431000	-1.031627000	1.710951000
H	2.462622000	-2.060688000	1.885658000
H	2.951704000	-0.460390000	1.296958000
H	1.875875000	-0.587359000	2.682707000
C	2.261422000	-1.122051000	-1.445910000
H	3.028533000	-0.450492000	-1.046437000
H	2.674241000	-2.141673000	-1.450535000
H	2.089462000	-0.825669000	-2.485605000
C	-0.743957000	-1.211390000	-2.589024000
H	0.006555000	-0.791553000	-3.266490000
H	-0.885860000	-2.269756000	-2.859149000
H	-1.684320000	-0.688625000	-2.790438000
C	-2.720156000	-1.025861000	-0.095853000
H	-3.086462000	-0.548424000	-1.010490000
H	-3.106285000	-2.055068000	-0.073678000
H	-3.164593000	-0.482285000	0.744263000
C	-0.980385000	-1.042532000	2.572322000

H	-1.925505000	-0.496945000	2.657166000
H	-1.162891000	-2.080341000	2.892738000
H	-0.284000000	-0.590954000	3.286408000

$[Cp^*Fe(CO)_2(\eta^1\text{-}P_4)]^-$

E: –3246.02661568 a.u.

Cartesian coordinates:

Fe	0.757985000	-0.208992000	-0.338182000
C	1.461714000	1.538758000	0.541824000
C	1.079869000	0.644944000	1.580221000
C	2.495170000	0.907375000	-0.235484000
C	1.813497000	-0.565723000	1.412825000
C	2.710333000	-0.389507000	0.302603000
C	0.102061000	0.581524000	-1.748990000
O	-0.171898000	1.179648000	-2.699581000
C	0.674931000	-1.808335000	-1.004277000
O	0.729409000	-2.885500000	-1.428167000
P	-1.461352000	-0.677955000	0.448538000
P	-3.037058000	-0.587199000	-1.123407000
P	-4.361199000	-0.325512000	0.624358000
P	-2.764150000	1.122325000	0.179851000
C	1.710034000	-1.762810000	2.309942000
H	2.243874000	-1.598374000	3.254724000
H	0.662192000	-1.979219000	2.542355000
H	2.131271000	-2.654754000	1.836751000
C	0.153029000	0.952309000	2.714901000
H	-0.458500000	0.086656000	2.985067000
H	0.734852000	1.254399000	3.595830000
H	-0.534395000	1.762837000	2.461714000
C	0.937740000	2.932113000	0.355390000
H	-0.136953000	2.976813000	0.555487000
H	1.445849000	3.635958000	1.026881000
H	1.086921000	3.278843000	-0.671188000
C	3.242193000	1.542846000	-1.370547000
H	2.583897000	2.167498000	-1.981629000
H	4.057854000	2.176845000	-0.999598000
H	3.677081000	0.788802000	-2.033106000

C	3.733399000	-1.382833000	-0.164292000
H	3.944661000	-1.265437000	-1.231220000
H	4.676159000	-1.258673000	0.383226000
H	3.390114000	-2.410458000	-0.015348000

$[Cp^*Fe(CO)_2(\eta^1\text{-}P_4{\cdot}B(C_6F_5)_3)]^-$ ($1a^-$)

E: –5454.45125054 a.u.

Cartesian coordinates:

Fe	-4.626487000	-0.331640000	-0.316234000
C	-5.246901000	1.638594000	-0.043994000
C	-4.920562000	1.460598000	-1.415388000
C	-6.304266000	0.716544000	0.283884000
C	-5.714252000	0.392450000	-1.929020000
C	-6.593886000	-0.043877000	-0.879935000
C	-3.975308000	-0.481985000	1.307998000
O	-3.676141000	-0.515620000	2.417799000
C	-4.689785000	-2.049499000	-0.631331000
O	-4.817760000	-3.169770000	-0.870961000
P	-2.503763000	-0.415034000	-1.304367000
P	-1.039698000	-1.335867000	0.095449000
P	0.410476000	-0.206099000	-1.149736000
P	-1.187877000	0.843081000	-0.022051000
C	2.491824000	1.535152000	0.205624000
C	3.095571000	2.049177000	1.352794000
C	2.261255000	2.491625000	-0.780321000
C	3.370061000	3.395784000	1.549374000
C	2.521142000	3.848617000	-0.631719000
C	3.077491000	4.309157000	0.549295000
C	1.972783000	-0.894078000	1.370337000
C	1.190740000	-0.379688000	2.410136000
C	2.466069000	-2.173022000	1.630721000
C	0.888754000	-1.059100000	3.580347000
C	2.184443000	-2.893349000	2.787951000
C	1.385604000	-2.338183000	3.771298000
C	3.301699000	-0.707774000	-1.047429000
C	4.562706000	-0.157273000	-1.271979000
C	3.059591000	-1.870092000	-1.784776000

C	5.484597000	-0.670918000	-2.180849000
C	3.946652000	-2.416796000	-2.699512000
C	5.174969000	-1.807097000	-2.905519000
B	2.168674000	-0.062824000	-0.031050000
C	-5.687944000	-0.091275000	-3.347620000
H	-6.234754000	0.595413000	-4.005300000
H	-4.659285000	-0.167963000	-3.713641000
H	-6.144340000	-1.080640000	-3.442652000
C	-3.981817000	2.304196000	-2.220447000
H	-3.380045000	1.703254000	-2.908543000
H	-4.559360000	3.025984000	-2.811013000
H	-3.290811000	2.859232000	-1.582163000
C	-4.663690000	2.674396000	0.870884000
H	-3.596437000	2.816084000	0.678948000
H	-5.169175000	3.638437000	0.737461000
H	-4.764833000	2.383586000	1.919954000
C	-7.019866000	0.643122000	1.600197000
H	-6.336944000	0.808281000	2.438184000
H	-7.806674000	1.405193000	1.653721000
H	-7.487340000	-0.334375000	1.747581000
C	-7.673295000	-1.076648000	-1.017782000
H	-7.875894000	-1.575474000	-0.066054000
H	-8.604023000	-0.610190000	-1.361606000
H	-7.399386000	-1.850501000	-1.739705000
F	1.919276000	-2.552327000	-1.609135000
F	3.639581000	-3.532066000	-3.371140000
F	6.047854000	-2.316569000	-3.780210000
F	6.673443000	-0.078410000	-2.348661000
F	4.991996000	0.923814000	-0.600603000
F	2.255594000	4.708028000	-1.623272000
F	3.338163000	5.609819000	0.717767000
F	1.771225000	2.128346000	-1.977597000
F	3.484041000	1.239203000	2.349649000
F	3.937683000	3.818015000	2.686137000
F	0.692066000	0.864343000	2.327990000
F	3.281931000	-2.805365000	0.771578000
F	2.694852000	-4.118746000	2.961879000

F	1.109979000	-3.016808000	4.889519000
F	0.132590000	-0.491301000	4.524842000

$[Cp^*Fe(CO)_2(\eta^1\text{-}P_4{\cdot}BPh_3)]^-$ ($1b^-$)

E: –3965.84436085 a.u.

Cartesian coordinates:

Fe	-3.507173000	-0.349890000	-0.046259000
C	-4.153258000	1.570768000	0.434120000
C	-3.864957000	1.533799000	-0.956488000
C	-5.184680000	0.601209000	0.700434000
C	-4.656623000	0.506010000	-1.550094000
C	-5.495141000	-0.049092000	-0.523577000
C	-2.779823000	-0.628541000	1.526213000
O	-2.435962000	-0.752456000	2.617117000
C	-3.543694000	-2.030296000	-0.512911000
O	-3.657305000	-3.127857000	-0.850412000
P	-1.421334000	-0.306142000	-1.125459000
P	0.133091000	-1.313248000	0.112477000
P	1.507590000	-0.047588000	-1.099766000
P	-0.049847000	0.852697000	0.199716000
C	3.883862000	1.528106000	-0.253976000
C	4.593539000	2.197558000	0.755468000
C	3.795915000	2.199091000	-1.486403000
C	5.161004000	3.456528000	0.561906000
H	4.707508000	1.716201000	1.723575000
C	4.352031000	3.457780000	-1.694142000
H	3.281835000	1.715645000	-2.315360000
C	5.038151000	4.099444000	-0.665501000
H	5.700978000	3.935648000	1.376585000
H	4.251245000	3.939414000	-2.664778000
H	5.475907000	5.083046000	-0.821376000
C	3.076283000	-0.390252000	1.510689000
C	2.467703000	0.500029000	2.414796000
C	3.446881000	-1.636574000	2.039740000
C	2.232412000	0.172661000	3.746382000
H	2.173267000	1.486440000	2.062431000
C	3.218911000	-1.978936000	3.371548000

H	3.929412000	-2.362835000	1.390801000
C	2.608153000	-1.075781000	4.235476000
H	1.750128000	0.893758000	4.402962000
H	3.522841000	-2.958659000	3.735520000
H	2.425705000	-1.339489000	5.274861000
C	4.249554000	-1.063507000	-0.843779000
C	5.600785000	-0.787706000	-1.106957000
C	3.792904000	-2.329082000	-1.250350000
C	6.442593000	-1.706713000	-1.729688000
H	6.006088000	0.178626000	-0.816594000
C	4.620732000	-3.257890000	-1.876469000
H	2.754909000	-2.600356000	-1.066685000
C	5.956066000	-2.950589000	-2.122215000
H	7.484191000	-1.448830000	-1.912046000
H	4.218448000	-4.223573000	-2.175969000
H	6.607702000	-3.669739000	-2.613753000
B	3.299817000	0.012332000	-0.052117000
C	-4.662014000	0.158181000	-3.008216000
H	-5.226380000	0.899644000	-3.587063000
H	-3.641442000	0.121353000	-3.402584000
H	-5.116681000	-0.821022000	-3.183747000
C	-2.961852000	2.470746000	-1.696045000
H	-2.418267000	1.963309000	-2.497884000
H	-3.558534000	3.277361000	-2.140222000
H	-2.218205000	2.919340000	-1.033464000
C	-3.557502000	2.524249000	1.427421000
H	-2.491879000	2.679471000	1.235725000
H	-4.062316000	3.496869000	1.382982000
H	-3.648413000	2.143240000	2.448325000
C	-5.852447000	0.385800000	2.026322000
H	-5.138288000	0.465047000	2.850905000
H	-6.638779000	1.132929000	2.190027000
H	-6.311267000	-0.604879000	2.087884000
C	-6.559289000	-1.086317000	-0.731326000
H	-6.751969000	-1.651688000	0.184630000
H	-7.498397000	-0.612288000	-1.040806000
H	-6.275499000	-1.805837000	-1.503986000

$Cp^*Fe(CO)_2(\eta^1\text{-}P_4H\cdot B(C_6F_5)_3)$ (1aH)

E: –5454.95142403 a.u.

Cartesian coordinates:

Fe	4.721769000	-0.478240000	-0.148341000
C	5.451362000	0.915235000	1.216661000
C	5.044062000	-0.243948000	1.931011000
C	6.478143000	0.520476000	0.285507000
C	5.758895000	-1.367601000	1.414572000
C	6.674038000	-0.880063000	0.420681000
C	4.171842000	0.766764000	-1.267081000
O	3.889465000	1.636288000	-1.960787000
C	4.778412000	-1.774548000	-1.339054000
O	4.889218000	-2.635139000	-2.090254000
P	2.590371000	-1.194798000	0.391546000
P	1.164285000	-0.599466000	-1.213917000
P	-0.322913000	-0.747843000	0.373370000
P	1.349328000	0.639930000	0.621410000
H	-0.011491000	-1.890924000	1.124162000
C	5.653569000	-2.771200000	1.930737000
H	6.226642000	-2.884715000	2.857809000
H	4.613555000	-3.037343000	2.142100000
H	6.036924000	-3.495645000	1.207606000
C	7.711445000	-1.692653000	-0.294804000
H	8.646105000	-1.683682000	0.276599000
H	7.403334000	-2.734064000	-0.415165000
H	7.922231000	-1.292403000	-1.289760000
C	7.271856000	1.445132000	-0.588195000
H	8.146167000	1.820093000	-0.044422000
H	7.628552000	0.940352000	-1.489645000
H	6.681695000	2.308925000	-0.905274000
C	4.989314000	2.318944000	1.472016000
H	5.607202000	2.787459000	2.246168000
H	5.055360000	2.935542000	0.571920000
H	3.949350000	2.345042000	1.808372000
C	4.109252000	-0.278308000	3.100471000
H	4.693647000	-0.229173000	4.026486000

H	3.416481000	0.566454000	3.097296000
H	3.518606000	-1.198150000	3.127453000
B	-2.204460000	-0.009165000	0.016404000
C	-2.977010000	0.190898000	1.438878000
C	-2.996617000	-0.828594000	2.386824000
C	-3.797293000	1.278082000	1.739181000
C	-3.718873000	-0.780651000	3.569978000
C	-4.540824000	1.367541000	2.910705000
C	-4.501612000	0.333666000	3.834335000
C	-1.768803000	1.342134000	-0.784220000
C	-1.724899000	1.430997000	-2.175554000
C	-1.322588000	2.483570000	-0.115463000
C	-1.308880000	2.569406000	-2.856770000
C	-0.896977000	3.637098000	-0.755336000
C	-0.895877000	3.682974000	-2.142305000
C	-3.068498000	-1.085745000	-0.847802000
C	-4.304729000	-0.674248000	-1.343941000
C	-2.761084000	-2.417607000	-1.084023000
C	-5.170411000	-1.507345000	-2.035328000
C	-3.596231000	-3.291390000	-1.771150000
C	-4.812366000	-2.832173000	-2.250925000
F	-2.278345000	-1.949427000	2.171772000
F	-1.596022000	-2.940275000	-0.649848000
F	-3.235638000	-4.558952000	-1.966374000
F	-5.627707000	-3.649749000	-2.909860000
F	-6.335920000	-1.052321000	-2.490560000
F	-4.697687000	0.593190000	-1.163354000
F	-2.057620000	0.385580000	-2.943145000
F	-1.292696000	2.590825000	-4.187939000
F	-0.486101000	4.775901000	-2.777066000
F	-0.474760000	4.687591000	-0.053750000
F	-1.243324000	2.489258000	1.224540000
F	-3.915600000	2.307632000	0.896679000
F	-5.297893000	2.437016000	3.147553000
F	-5.207467000	0.408026000	4.958286000
F	-3.674919000	-1.790437000	4.438366000

$Cp^*Fe(CO)_2(\eta^1\text{-}P_4H\cdot BPh_3)$ (1bH)

E: –3966.36401689 a.u.

Cartesian coordinates:

Fe	-3.546573000	-0.355544000	0.064339000
C	-4.260934000	1.592817000	0.208722000
C	-3.877970000	1.356363000	-1.139678000
C	-5.291425000	0.643919000	0.547392000
C	-4.604754000	0.227666000	-1.623204000
C	-5.505899000	-0.188534000	-0.583036000
C	-2.992824000	-0.396720000	1.734897000
O	-2.714693000	-0.357447000	2.848062000
C	-3.579667000	-2.099760000	-0.159883000
O	-3.677025000	-3.230049000	-0.339678000
P	-1.409319000	-0.395972000	-0.822050000
P	0.028949000	-1.251034000	0.649300000
P	1.537669000	-0.137524000	-0.484186000
P	-0.134392000	0.950038000	0.417315000
H	1.178507000	-0.297114000	-1.840852000
C	-4.523934000	-0.321260000	-3.015736000
H	-5.122456000	0.286821000	-3.703756000
H	-3.492044000	-0.327494000	-3.379271000
H	-4.896139000	-1.347899000	-3.066397000
C	-6.546022000	-1.262346000	-0.703831000
H	-7.485459000	-0.830256000	-1.065857000
H	-6.243408000	-2.041582000	-1.407631000
H	-6.743779000	-1.744409000	0.257032000
C	-6.064816000	0.615919000	1.831903000
H	-6.886679000	1.339701000	1.791930000
H	-6.495187000	-0.370898000	2.019945000
H	-5.437910000	0.871893000	2.690227000
C	-3.773181000	2.711857000	1.080008000
H	-4.334332000	3.630282000	0.873826000
H	-3.893460000	2.476884000	2.140669000
H	-2.712610000	2.917533000	0.910442000
C	-2.953511000	2.204395000	-1.957506000
H	-3.549300000	2.881657000	-2.580398000
H	-2.298182000	2.812929000	-1.330099000

H	-2.322790000	1.607437000	-2.622307000
B	3.588264000	0.025377000	-0.001485000
C	3.932060000	1.527389000	-0.498997000
C	3.680627000	1.941993000	-1.818721000
C	4.519334000	2.471587000	0.353383000
C	3.980310000	3.225909000	-2.261050000
H	3.257620000	1.232823000	-2.529733000
C	4.831816000	3.759057000	-0.079475000
H	4.740993000	2.194491000	1.380045000
C	4.557330000	4.144311000	-1.387302000
H	3.769904000	3.507938000	-3.289397000
H	5.289553000	4.463302000	0.610337000
H	4.795079000	5.149021000	-1.725999000
C	3.617507000	-0.221716000	1.595027000
C	4.369611000	-1.254262000	2.171046000
C	2.905759000	0.606657000	2.480004000
C	4.403630000	-1.458169000	3.549213000
H	4.947937000	-1.912475000	1.528899000
C	2.921571000	0.406550000	3.856095000
H	2.335999000	1.446044000	2.083382000
C	3.673044000	-0.633290000	4.397700000
H	5.002124000	-2.267272000	3.959594000
H	2.348834000	1.063273000	4.505308000
H	3.692202000	-0.794815000	5.472001000
C	4.187680000	-1.168770000	-0.918036000
C	5.206597000	-0.937941000	-1.852450000
C	3.738215000	-2.495042000	-0.792124000
C	5.744643000	-1.967322000	-2.622553000
H	5.593610000	0.069461000	-1.977576000
C	4.261126000	-3.529410000	-1.560708000
H	2.967441000	-2.729442000	-0.059076000
C	5.269432000	-3.267197000	-2.484965000
H	6.536199000	-1.749942000	-3.334890000
H	3.883385000	-4.540796000	-1.436004000
H	5.681946000	-4.070366000	-3.089341000

***exo,endo*-Cp*Fe(CO)$_2$(η^1-P$_4$H) (2)**

E: –3246.59390724 a.u.

Cartesian coordinates:

Fe	0.720031000	-0.215175000	-0.302417000
C	1.489620000	1.564047000	0.450699000
C	1.135817000	0.729418000	1.545974000
C	2.481046000	0.870761000	-0.331209000
C	1.843372000	-0.502961000	1.418932000
C	2.700960000	-0.396849000	0.270101000
C	0.099345000	0.535514000	-1.766168000
O	-0.219387000	1.093045000	-2.718679000
C	0.693370000	-1.857991000	-0.920804000
O	0.753884000	-2.942688000	-1.296910000
P	-1.391293000	-0.631857000	0.545292000
P	-2.927314000	-0.707236000	-1.064338000
P	-4.430188000	-0.219292000	0.493503000
P	-2.703498000	1.122616000	0.125968000
C	1.782018000	-1.640837000	2.393211000
H	2.394173000	-1.426690000	3.276901000
H	0.755484000	-1.818900000	2.727591000
H	2.148589000	-2.569745000	1.948569000
C	0.255299000	1.110250000	2.695588000
H	-0.314179000	0.257488000	3.074686000
H	0.877742000	1.492359000	3.513185000
H	-0.457245000	1.891287000	2.420092000
C	1.007103000	2.965596000	0.222545000
H	-0.039844000	3.080682000	0.516278000
H	1.605012000	3.675418000	0.805491000
H	1.081806000	3.249045000	-0.830465000
C	3.211786000	1.433806000	-1.513490000
H	2.573282000	2.092691000	-2.107940000
H	4.077976000	2.017468000	-1.181409000
H	3.573401000	0.643333000	-2.176174000
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H	3.880789000	-1.373616000	-1.248585000
H	4.666570000	-1.235587000	0.331500000
H	3.391981000	-2.433738000	0.072072000

H	-3.881576000	-0.980432000	1.566609000

***exo,exo*-Cp*Fe(CO)$_2$(η^1-P$_4$H) (2)**

E: –3246.59421743 a.u.

Cartesian coordinates:

Fe	0.716558000	-0.214097000	-0.302830000
C	1.471586000	1.560896000	0.475505000
C	1.131225000	0.705535000	1.559033000
C	2.465444000	0.889006000	-0.322030000
C	1.849898000	-0.517650000	1.409812000
C	2.700658000	-0.385453000	0.258721000
C	0.091193000	0.549942000	-1.757900000
O	-0.230685000	1.117113000	-2.703622000
C	0.702982000	-1.850875000	-0.942223000
O	0.771822000	-2.929655000	-1.332433000
P	-1.399009000	-0.649055000	0.536085000
P	-2.924003000	-0.676798000	-1.087328000
P	-4.302371000	-0.334371000	0.627820000
P	-2.693760000	1.121432000	0.128769000
C	1.803541000	-1.671218000	2.366280000
H	2.412436000	-1.462194000	3.253434000
H	0.779383000	-1.868104000	2.697209000
H	2.183049000	-2.588073000	1.907721000
C	0.248823000	1.057867000	2.716184000
H	-0.315807000	0.194621000	3.078403000
H	0.869485000	1.427494000	3.540872000
H	-0.468493000	1.839722000	2.456196000
C	0.973540000	2.960537000	0.271089000
H	-0.072157000	3.060295000	0.574705000
H	1.568543000	3.668077000	0.859754000
H	1.037080000	3.259921000	-0.778312000
C	3.185000000	1.478383000	-1.498355000
H	2.538841000	2.145396000	-2.075186000
H	4.050369000	2.060093000	-1.160829000
H	3.546032000	0.703068000	-2.179031000
C	3.717640000	-1.386877000	-0.201961000
H	3.882647000	-1.326295000	-1.280804000

H	4.675720000	-1.202253000	0.296665000
H	3.413844000	-2.411401000	0.027181000
H	-5.322608000	0.307825000	-0.141087000

$Cp^*Fe(CO)_2(\eta^1\text{-}P_4H)$ ($[TS_{inv}]^{\ddagger}$: trigonal**)**

E: –3246.50839098 a.u.

Cartesian coordinates:

Fe	0.694951000	-0.230922000	-0.278313000
C	1.478415000	1.586800000	0.364102000
C	1.147333000	0.810814000	1.508568000
C	2.452648000	0.853047000	-0.402005000
C	1.854937000	-0.426716000	1.431425000
C	2.686516000	-0.381365000	0.260140000
C	0.072679000	0.441059000	-1.781312000
O	-0.188004000	0.949759000	-2.779225000
C	0.659671000	-1.903985000	-0.804033000
O	0.715780000	-3.008511000	-1.119293000
P	-1.397608000	-0.640274000	0.660503000
P	-2.874951000	-0.794026000	-1.012027000
P	-4.332272000	-0.166071000	0.443054000
P	-2.648171000	1.132865000	0.102120000
C	1.817615000	-1.514016000	2.462667000
H	2.468732000	-1.266174000	3.308938000
H	0.803299000	-1.660701000	2.845514000
H	2.153414000	-2.469014000	2.049974000
C	0.292431000	1.251492000	2.656584000
H	-0.229001000	0.412583000	3.124341000
H	0.927430000	1.721540000	3.416745000
H	-0.459808000	1.981776000	2.349094000
C	1.000059000	2.976987000	0.068621000
H	0.009583000	3.155831000	0.494860000
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C	3.159647000	1.353972000	-1.625565000
H	2.516750000	2.001654000	-2.227301000
H	4.045999000	1.932762000	-1.341254000
H	3.487403000	0.530574000	-2.265611000

C	3.686360000	-1.422523000	-0.146507000
H	3.835244000	-1.438515000	-1.229323000
H	4.653742000	-1.215374000	0.324516000
H	3.375406000	-2.425432000	0.156928000
H	-5.552526000	-0.403808000	1.073213000

$Cp^*Fe(CO)_2(\eta^1\text{-}P_4H)$ ($[TS_{inv}]^{\ddagger}$: turnstile**)**

E: –3246.50104171 a.u.

Cartesian coordinates:

P	1.387388000	-0.642707000	0.660577000
P	2.703073000	1.092511000	0.088571000
P	4.392089000	-0.219058000	0.425856000
P	2.837565000	-0.800634000	-1.012967000
H	5.381065000	0.150642000	1.339549000
Fe	-0.707282000	-0.237685000	-0.279736000
C	-0.708997000	-1.918903000	-0.782367000
C	-0.080789000	0.407066000	-1.791254000
C	-1.886490000	-0.413226000	1.420047000
C	-1.139560000	0.798656000	1.517819000
C	-1.433621000	1.598486000	0.378922000
C	-2.428054000	0.907634000	-0.401110000
C	-2.707898000	-0.325938000	0.243007000
O	-0.791913000	-3.026132000	-1.081279000
O	0.198727000	0.900082000	-2.792140000
C	-1.897010000	-1.514958000	2.436575000
C	-0.282490000	1.200648000	2.678463000
C	-0.902731000	2.973544000	0.104259000
C	-3.109466000	1.449765000	-1.621579000
C	-3.741063000	-1.326003000	-0.182593000
H	-0.896417000	-1.685850000	2.844262000
H	-2.566024000	-1.266408000	3.268499000
H	-2.239247000	-2.457796000	2.001700000
H	0.500358000	1.903391000	2.383588000
H	-0.909374000	1.690903000	3.432559000
H	0.200987000	0.340859000	3.148917000
H	-1.559267000	3.732692000	0.544926000
H	0.098243000	3.104601000	0.523076000

H	-0.832295000	3.171138000	-0.968674000
H	-3.457556000	0.648487000	-2.278652000
H	-3.979522000	2.050436000	-1.332462000
H	-2.443046000	2.088596000	-2.206788000
H	-3.462416000	-2.345147000	0.097351000
H	-4.700200000	-1.098404000	0.295894000
H	-3.893166000	-1.312237000	-1.264947000

ETS-NOCV analyses: Table S1 summarizes the results obtained from the ETS-NOCV analyses of the Fe–P bonds in **1a**$^-$ and **1b**$^-$.

Table S1 ETS-NOCV results using ZORA-BP86-D3/TZ2P (kcal mol^{-1})

	1a$^-$ ([Cp*Fe(CO)$_2$(η^1-P$_4$·B(C$_6$F$_5$)$_3$)]$^-$)	**1b**$^-$ ([Cp*Fe(CO)$_2$(η^1-P$_4$·BPh$_3$)]$^-$)
ΔE_{total}	–223.2	–236.9
ΔE_{Pauli}	156.4	169.4
ΔE_{elstat}	–234.3	–254.0
ΔE_{orb}	–132.7	–140.0
σ	**–101.6**	**–107.0**
$\pi^{\parallel}$	**–5.9**	**–6.0**
$\pi^{\perp}$	**–4.7**	**–4.9**

3. X-ray Structure Determinations

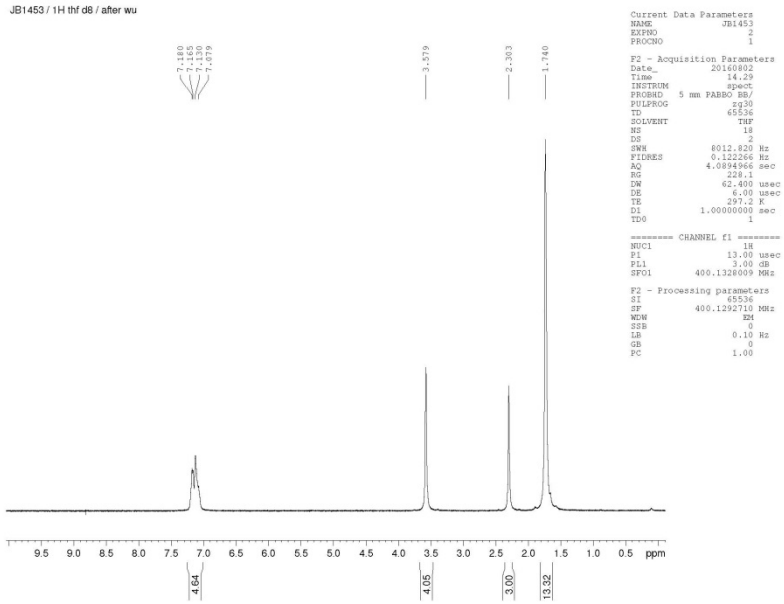
X-ray crystal structure determination of compound 1a

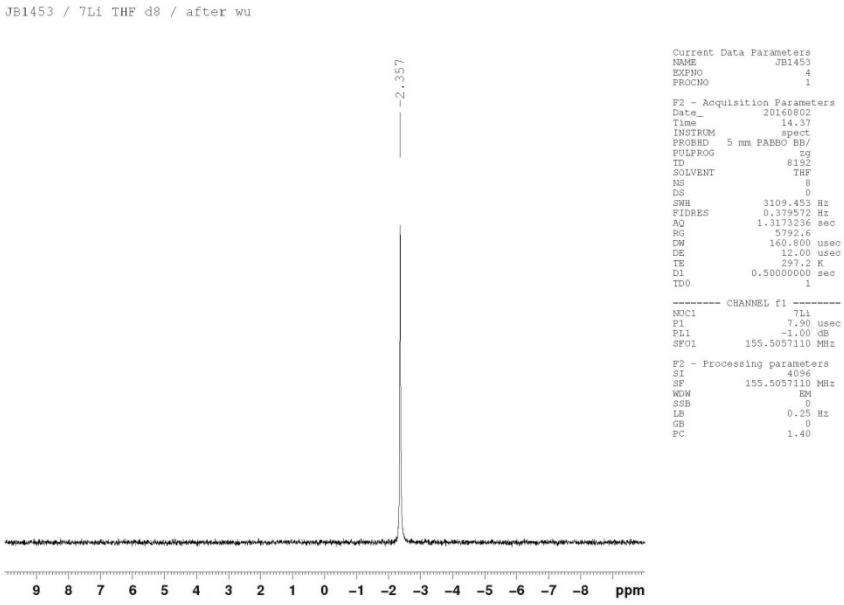
$[C_{16}H_{32}LiO_8][C_{30}H_{15}BF_{15}FeO_2P_4] \cdot 1.5(C_4H_{10}O)$, Fw = 1353.49, yellow plate, 0.34 × 0.12 × 0.04 mm^3, triclinic, $P\overline{1}$ (no. 2), a = 14.6890(10), b = 15.7521(11), c = 16.3286(11) Å, α = 62.487(2), β = 64.960(2), γ = 86.391(2) °, V = 2994.3(3) $Å^3$, Z = 2, D_x = 1.501 g/cm^3, μ = 0.46 mm^{-1}. 51426 Reflections were measured on a Bruker Kappa ApexII diffractometer with sealed tube and Triumph monochromator (λ = 0.71073 Å) at a temperature of 150(2) K up to a resolution of $(\sin\theta/\lambda)_{max}$ = 0.65 $Å^{-1}$. The Eval15 software[13] was used for the integration of the intensities. A model for large mosaicity was used for the prediction of the reflection profiles. Multiscan absorption correction and scaling was performed with SADABS[14] (correction range 0.61-0.75). 13736 Reflections were unique (R_{int} = 0.055), of which 8187 were observed [I>2σ(I)]. The structure was solved with Patterson superposition methods using SHELXT.[15] Least-squares refinement was performed with SHELXL-2014[16] against F^2 of all reflections. The coordinated crown ether and the co-crystallized diethyl ether molecules were refined with disorder models. Non-hydrogen atoms of the main molecules and the major disorder components were refined freely with anisotropic displacement parameters. The minor disorder component of a diethyl ether was refined with fixed isotropic displacement parameters. Hydrogen atoms were introduced in calculated positions and refined with a riding model. 1031 Parameters were refined with 696 restraints (distances, angles and displacement parameters of the disordered moieties). R1/wR2 [I > 2σ(I)]: 0.0626 / 0.1630. R1/wR2 [all refl.]: 0.1169 / 0.1901. S = 1.048. Residual electron density between -0.42 and 0.76 e/$Å^3$. Geometry calculations and checking for higher symmetry were performed with the PLATON program.[17]

CCDC 1509067 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

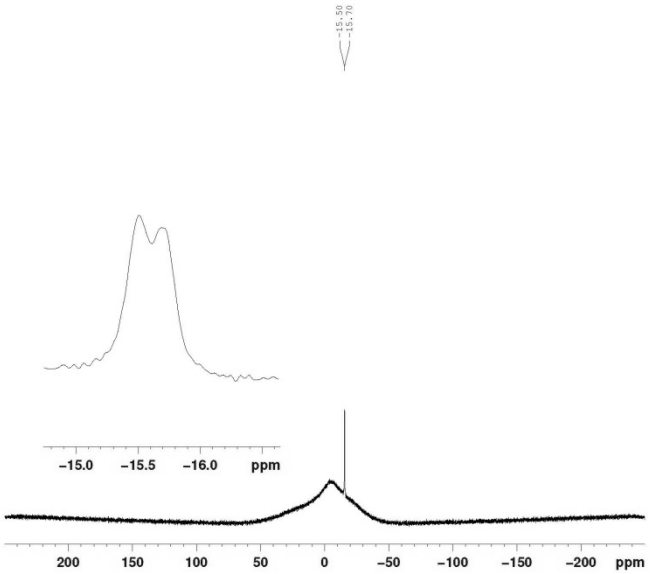
4. NMR Spectra

[Li(Tol)][Cp*Fe(CO)$_2$(η^1-P$_4$·B(C$_6$F$_5$)$_3$)] (1a)





JB1453 / 11Bdec thf d8 / after wu

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EXPNO                      3
PROCNO                     1

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PULPROG               zgpg
TD                   16384
SOLVENT                THF
NS                      32
DS                       0
SWH              64102.563 Hz
FIDRES            3.912510 Hz
AQ                0.1278452 sec
RG                     512
DW                  7.800 usec
DE                  6.00 usec
TE                  297.2 K
D1               3.00000000 sec
d11              0.03000000 sec
DELTA            2.90000010 sec
TD0                        1

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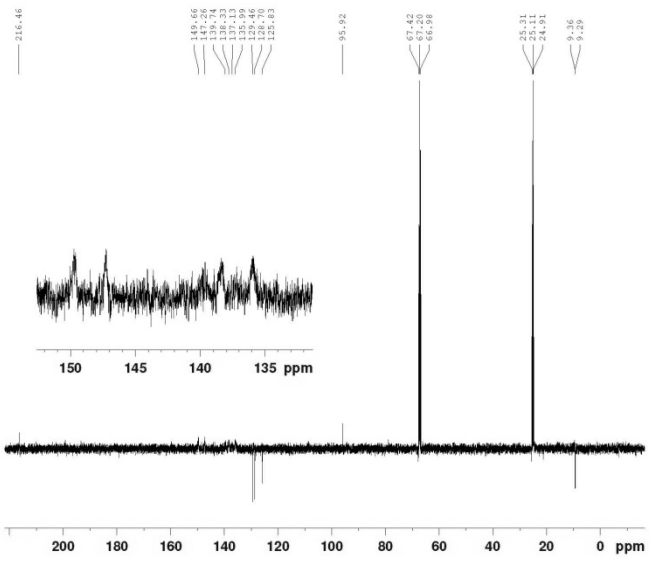
NUC1                     11B
P1                    8.90 usec
PL1                  -1.00 dB
SFO1          128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                80.00 usec
PL2                   3.00 dB
PL12                 18.00 dB
PL13                 18.00 dB
SFO2          400.1304001 MHz

F2 - Processing parameters
SI                       32768
SF            128.3776050 MHz
WDW                         EM
SSB                          0
LB                    1.00 Hz
GB                           0
PC                    4.00
```

JB1453 / 13C APT THF d8 / after wu



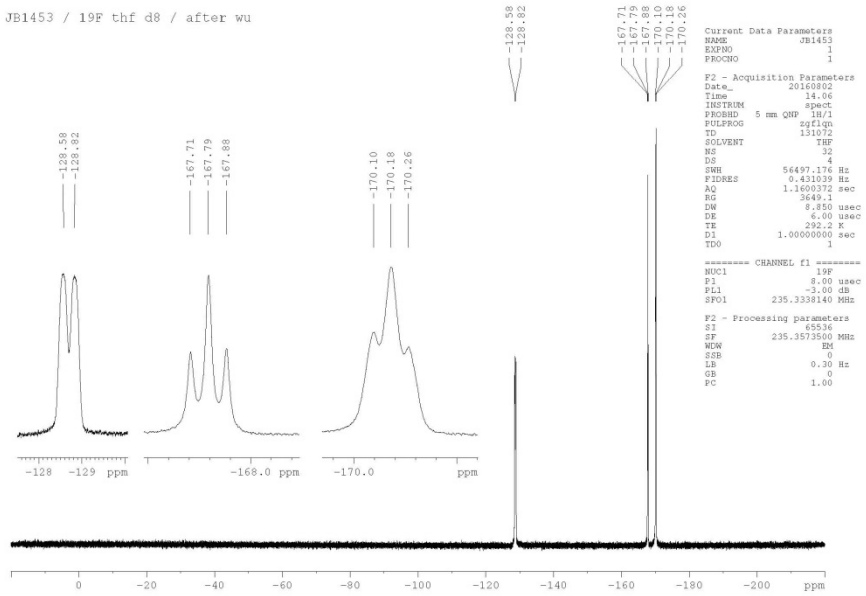

```
Current Data Parameters
NAME                  JB1453
EXPNO                      6
PROCNO                     1

F2 - Acquisition Parameters
Date_              20160803
Time                   6.33
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg6
TD                   65536
SOLVENT                THF
NS                   13312
DS                       2
SWH              23980.814 Hz
FIDRES            0.365918 Hz
AQ                1.36644756 sec
RG                     16384
DW                  20.850 usec
DE                   6.00 usec
TE                  297.2 K
CNST2           145.0000000
CNST11            1.0000000
D1                2.00000000 sec
d20               0.00689655 sec
DELTA             0.00001120 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                    8.80 usec
p2                   17.60 usec
PL1                  -1.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                80.00 usec
PL2                   3.00 dB
PL12                 18.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                        65536
SF            100.6125026 MHz
WDW                         EM
SSB                          0
LB                    1.00 Hz
GB                           0
PC                    1.40
```

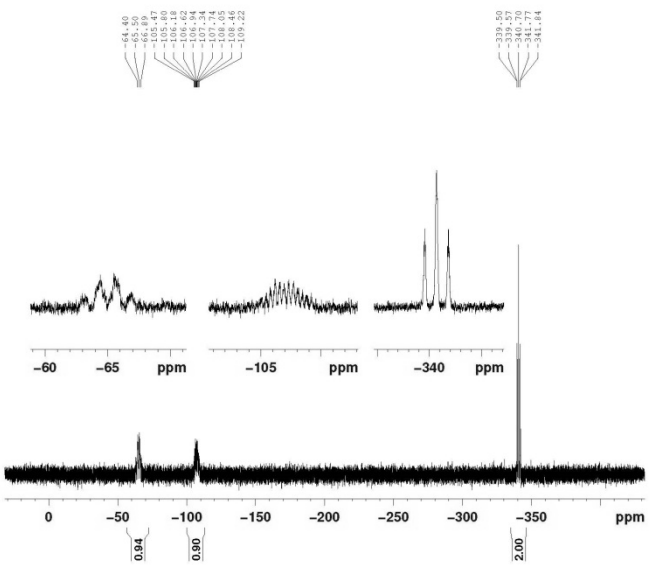



```
Current Data Parameters
NAME                  JB1453
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20160802
Time                  14.06
INSTRUM               spect
PROBHD   5 mm QNP  1H/1
PULPROG             zgflqn
TD                  131072
SOLVENT                THF
NS                      32
DS                       4
SWH               56497.176 Hz
FIDRES             0.431039 Hz
AQ                1.1600372 sec
RG                   3649.1
DW                    8.850 usec
DE                    6.00 usec
TE                  292.2 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     19F
P1                    8.00 usec
PL1                  -3.00 dB
SFO1           235.3338140 MHz

F2 - Processing parameters
SI                     65536
SF              235.3573500 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```




```
Current Data Parameters
NAME                  JB1453
EXPNO                      1
PROCNO                     1

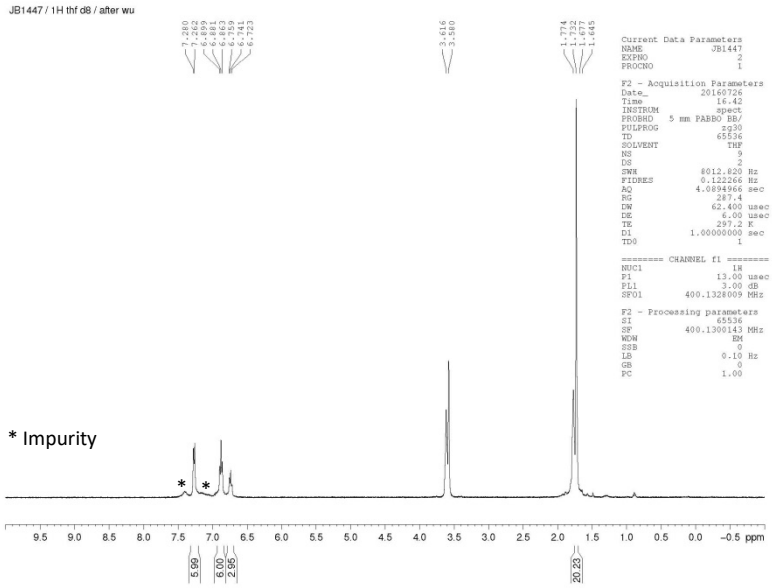
F2 - Acquisition Parameters
Date_              20160802
Time                  14.21
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                     65536
SOLVENT                THF
NS                     418
DS                       4
SWH               75187.969 Hz
FIDRES             1.147277 Hz
AQ                0.4358644 sec
RG                   14596.5
DW                    6.650 usec
DE                    6.00 usec
TE                  297.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1

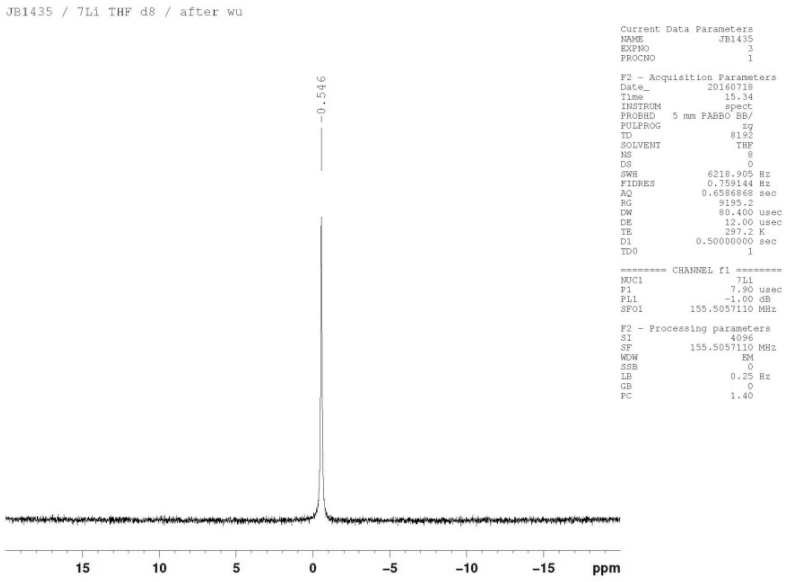
======== CHANNEL f1 ========
NUC1                    31P
P1                    6.25 usec
PL1                  -1.00 dB
SFO1           161.9431979 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   3.00 dB
PL12                 18.00 dB
PL13                 18.00 dB
SFO2           400.1316005 MHz

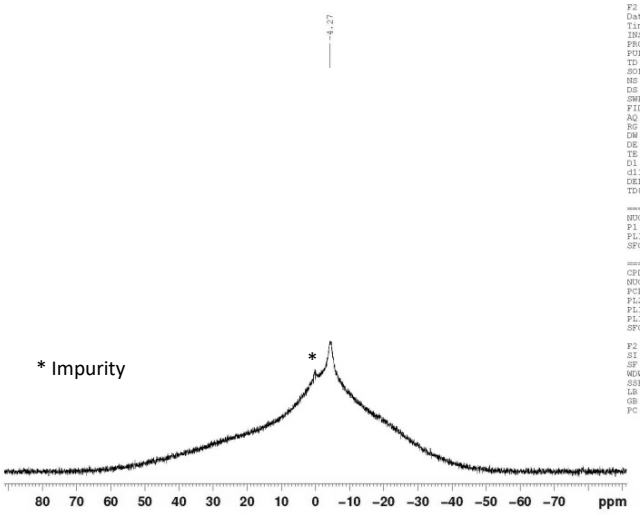
F2 - Processing parameters
SI                     65536
SF              161.9755930 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

$[Li(THF)_x][Cp^*Fe(CO)_2(\eta^1\text{-}P_4\cdot BPh_3)]$ (1b)





JB1435 / 11Bdec thf d8 / after wu



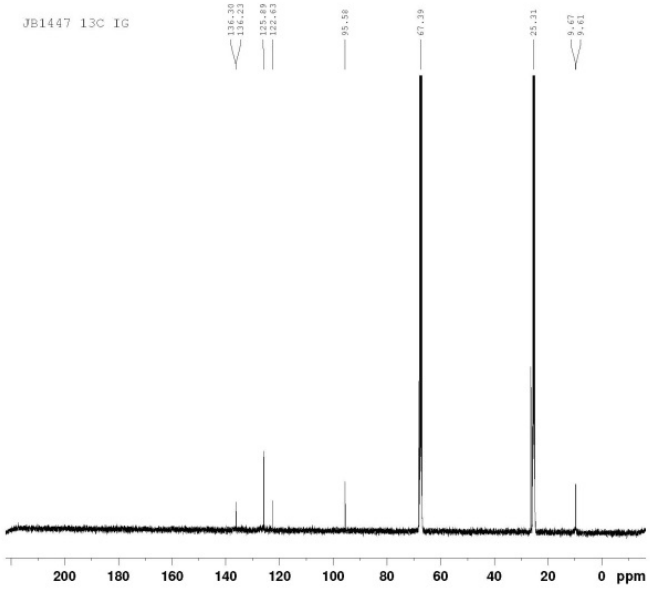

```
Current Data Parameters
NAME                  JB1435
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20160718
Time                   15.32
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg
TD                    16384
SOLVENT                 THF
NS                       32
DS                        0
SWH                75187.969 Hz
FIDRES              4.589109 Hz
AQ                  0.1090036 sec
RG                      574.7
DW                     6.650 usec
DE                     6.00 usec
TE                    297.2 K
D1                 3.00000000 sec
d11                0.03000000 sec
DELTA              2.90000010 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     11B
P1                      8.90 usec
PL1                    -1.00 dB
SFO1             128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                    3.00 dB
PL12                  18.00 dB
PL13                  18.00 dB
SFO2             400.1304001 MHz

F2 - Processing parameters
SI                       32768
SF               128.3776050 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        4.00
```



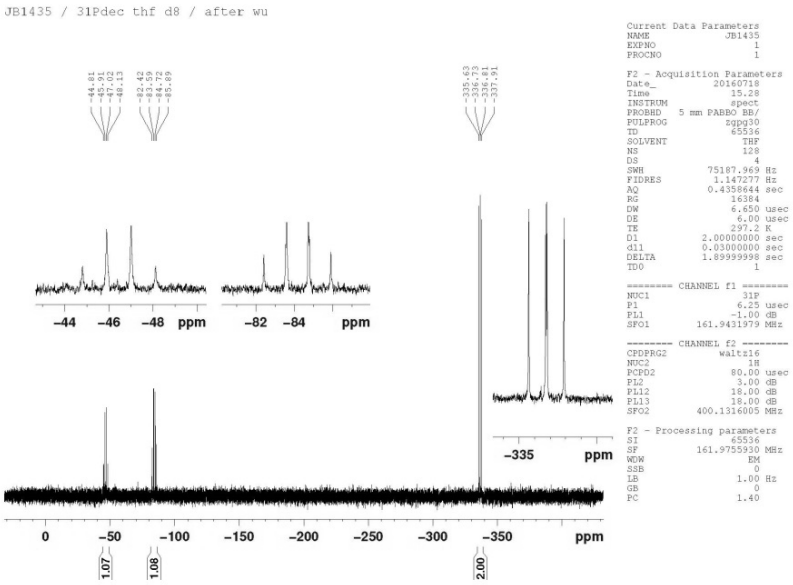

```
Current Data Parameters
NAME                  JB1447
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_               20160728
Time                    6.15
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgig30
TD                    65536
SOLVENT                 THF
NS                       12288
DS                        4
SWH                23980.814 Hz
FIDRES              0.365918 Hz
AQ                  1.3664756 sec
RG                      13004
DW                    20.850 usec
DE                     6.00 usec
TE                    297.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      8.80 usec
PL1                    -1.00 dB
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                    3.00 dB
PL12                  18.00 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF               100.6124838 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```




```
Current Data Parameters
NAME                  JB1435
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20160718
Time                  15.28
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT                THF
NS                     128
DS                       4
SWH               75187.969 Hz
FIDRES             1.147277 Hz
AQ                0.4358644 sec
RG                     16384
DW                  6.650 usec
DE                    6.00 usec
TE                   297.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                    31P
P1                    6.25 usec
PL1                  -1.00 dB
SFO1          161.9431979 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   3.00 dB
PL12                 18.00 dB
PL13                 18.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                     65536
SF            161.9755930 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

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