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Supporting Information

Divergent CO_2 Activation by Tuning the Lewis Acid in Iron-Based Bimetallic Systems

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Supporting Information

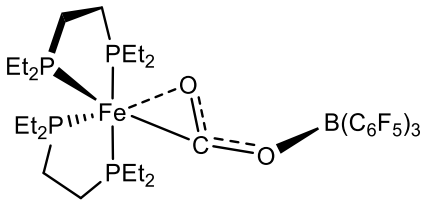
Table of Contents

1. General considerations

All preparations and manipulations were performed by using standard Schlenk and glovebox techniques, under an atmosphere of high purity nitrogen. All solvents were dried, stored over 4 Å molecular sieves, and degassed prior to use. Toluene (C_7H_8) and *n*-pentane (C_5H_{12}), THF and diethyl ether were distilled under nitrogen over sodium. Toluene-d_8, C_6D_6 and thf-d_8 were dried over sodium and distilled under argon. [AuCl(THT)] (THT = tetrahydrothiophene),[1] the phosphine ligand $PMe_2Ar^{Xyl_2}$,[2] $[Fe(N_2)(depe)_2]$,[3] $[Fe(CO_2)(depe)_2]$,[4] $Al(C_6F_5)_3$[5] and $[(PMe_2Ar^{Xyl2})Au]NTf_2$[6] were prepared as described previously. $B(C_6F_5)_3$ was purchased from TCI Chemicals and sublimated twice. All other reagents were used as received from commercial suppliers. Solution NMR spectra were recorded with Bruker AMX-300, DRX-400, and DRX-500 spectrometers. Spectra were referenced to external $SiMe_4$ (d: 0 ppm) by using the residual proton solvent peaks as internal standards (^{1}H NMR experiments), or the characteristic resonances of the solvent nuclei (^{13}C NMR experiments), while ^{31}P was referenced to H_3PO_4. ^{19}F is referenced to fluorotrichloromethane, and ^{11}B is referenced to $BF_3{\cdot}OEt_2$. The following abbreviations and their combinations are used: br, broad; s, singlet; d, doublet; t, triplet; m, multiplet. The ^{1}H and ^{13}C resonance signals were attributed by means of 2D HSQC and HMBC experiments. Infrared spectra were recorded with a Bruker Vector 22 spectrometer and preparation was made in Nujol or using a solid-state sample. For elemental analyses a LECO TruSpec CHN elementary analyzer was utilized.

2. Synthesis and characterization of new compounds

[(depe)$_2$Fe(μ-CO$_2$)B(C$_6$F$_5$)$_3$]



Compound 2. A solution of B(C$_6$F$_5$)$_3$ (20 mg, 0.039 mmol) in THF (5 mL) was added to a solution of [Fe(CO$_2$)(depe)$_2$] (20 mg, 0.039 mmol) in THF (5 mL) and stirred at room temperature under N_2 atmosphere for 5 minutes. The solution turns from red to deep pink. The solvent was removed under vacuum obtaining a pink powder (33 mg, 82%). Crystals suitable for X-ray diffraction studies were obtained from a concentrated solution of compound **2** in diethyl ether at -30 ºC.

Anal. Calcd. for $C_{39}H_{48}BF_{15}FeO_2P_4$: C, 45.73; H, 4.72; **Found:** C, 45.65; H, 4.99.

^{1}H NMR (400 MHz, C$_6$D$_6$, 25 ºC) δ, ppm: 1.56-0.60 (br m, depe).

^{13}C{^{1}H} NMR (126 MHz, thf-d_8, 25 ºC) δ, ppm: 214.8 (CO$_2$), 150.0 (d, $^1J_{CF}$ = 240 Hz, *o*-C$_6$F$_5$), 140.7 (d, $^1J_{CF}$ = 240 Hz, *p*-C$_6$F$_5$), 138.3 (d, $^1J_{CF}$ = 240 Hz, *m*-C$_6$F$_5$), 122.6 (br, *ipso*-C$_6$F$_5$), 26.5, 21.8, 20.1, 19.5, 15.1, 9.9, 8.9, 8.2, 7.5, 5.5 (depe).

^{11}B{^{1}H} NMR (128 MHz, C$_6$D$_6$, 25 ºC) δ, ppm: -1.6

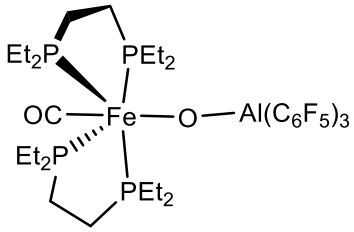
^{31}P{^{1}H} NMR (160 MHz, C$_6$D$_6$, 25 ºC) δ, ppm: 85.1, 80.4, 70.4 (relative intensities 1:1:2)

^{31}P{^{1}H} NMR (160 MHz, thf-d_8, -20 ºC) δ, ppm: 85.8, 80.7, 71.0, 70.1 (relative intensities 1:1:1:1)

^{19}F{^{1}H} NMR (377 MHz, C$_6$D$_6$, 25 ºC) δ, ppm: -130.6, -160.9, -166.3

IR cm^{-1} (Nujol): 1641, 1251 ν(CO$_2$)

[(depe)$_2$(CO)Fe(μ-O)Al(C$_6$F$_5$)$_3$]



Compound 3. A solution of Al(C$_6$F$_5$)$_3$ (30 mg, 0.039 mmol) in toluene (3 mL) was added to a solution of [Fe(CO$_2$)(depe)$_2$] (30 mg, 0.039 mmol) in toluene (3 mL) and stirred at room temperature under N_2 atmosphere for 5 minutes. The solution, which colour changes from red to orange, was introduced in the glovebox freezer (-30 ºC) obtaining yellow crystals after two days (16.2 mg, 27%).

Anal. Calcd. for $C_{39}H_{48}AlF_{15}FeO_2P_4$: C, 45.02; H, 4.65; **Found:** C, 45.23; H, 4.42.

^{1}H NMR (400 MHz, C_6D_6, 25 ºC) δ, ppm: 2.44 (br, 2H, -C*H*$_2$), 2.09 (br, 2H, -C*H*$_2$), 1.38 (br, 12H, -C*H*$_2$), 1.09 (br, 8H, -C*H*$_2$), 0.79 (br s, 12H -C*H*$_3$), 0.71 (br s, 12H, -C*H*$_3$).

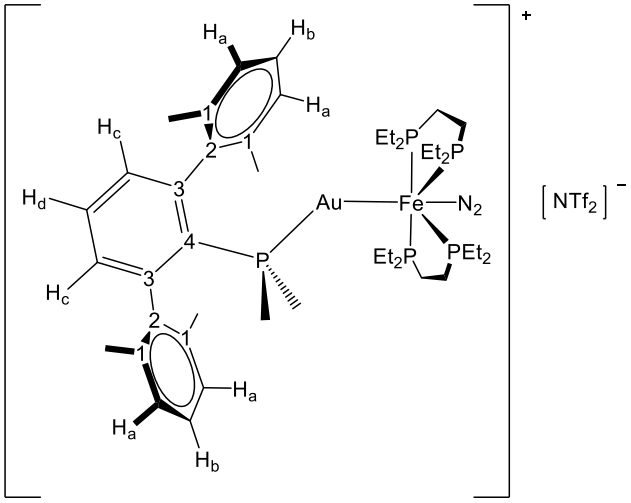
^{13}C{^{1}H} NMR (126 MHz, C_6D_6, 25 ºC) δ, ppm: 213.6 (*C*O), 150.7 (d, $^1J_{CF}$ = 240 Hz, *o*-C$_6$F$_5$), 140.9 (d, $^1J_{CF}$ = 240 Hz, *p*-C$_6$F$_5$), 138.1 (d, $^1J_{CF}$ = 240 Hz, *m*-C$_6$F$_5$), 22.5, 20.1, 16.1 (-*C*H$_2$), 9.2, 8.0 (-*C*H$_3$).

^{31}P{^{1}H} NMR (160 MHz, C_6D_6, 25 ºC) δ, ppm: 67.9

^{19}F{^{1}H} NMR (377 MHz, C_6D_6, 25 ºC) δ, ppm: -121.3, -156.0, -163.3

IR cm^{-1} (solid): 1914 ν(C≡O)

[(N$_2$)(depe)$_2$Fe-Au(PMe$_2$Ar^{Xyl2})]NTf$_2$



Compound 6. [Fe(depe)$_2$(N$_2$)] (50 mg, 0.100 mmol) and [(PMe$_2$Ar^{Xyl})Au(NTf$_2$)] (71 mg, 0.100 mmol) were placed in an ampoule inside the glovebox. Both solids were cooled down to -20 °C with an acetone/N$_2$ bath and toluene (8 mL) was added under N$_2$ pressure. A yellow solution was formed after stirring 5 minutes at low temperature. The solvent was removed under vacuum and the green residue was washed with 5 mL of pentane at low temperature. The residue was then dissolved in 2 mL of diethyl ether and 10 mL of pentane were added. The mixture was stirred for 30 min at -20 °C and then all the solvent was removed under vacuum to afford a green solid which was isolated in a 30 % yield (40 mg). Single crystals suitable for X-ray diffraction studies were obtained by dissolving compound **6** in toluene and resting 48h at -30ºC.

Anal. Calcd. for C$_{46}$H$_{75}$AuF$_6$FeN$_3$O$_4$P$_5$S$_2$**:** C, 41.86; H, 5.73; N, 3.18; S, 4.86; **Found:** C, 41.68; H, 6.08; N, 2.95; S, 4.72.

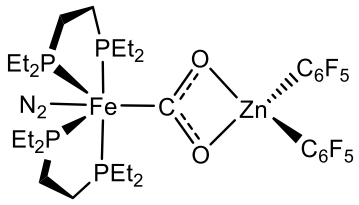
^{1}H NMR (400 MHz, C$_6$D$_6$, 25 ºC) δ, ppm: 7.03 (br, 6H, H$_a$, H$_b$), 6.76 (br, 1H, H$_d$), 6.62 (br, 2H, H$_c$), 2.12-0.73 (m, 66H, depe, Me^{Xyl}, PMe$_2$).

^{31}P{^{1}H} NMR (160 MHz, C$_6$D$_6$, 25 ºC) δ, ppm: 72.4 (m, $^3J_{PP}$ = 42 Hz, P^{depe}), 31.0 (q, $^3J_{PP}$ = 42 Hz, P^{Xyl}).

A clean **^{13}C{^{1}H} NMR** spectrum could not be obtained due to the quick decomposition of compound **6** in solution, forming free terphenyl phosphine among other undetermined by-products, even at low temperatures.

IR cm^{-1} (Nujol): 2057 ν(N≡N)

[(N_2)(depe)$_2$Fe(μ-CO_2)Zn(C_6F_5)$_2$]



Compound 7. A solution of $Zn(C_6F_5)_2$ (16 mg, 0.039 mmol) in toluene (5 mL) was added to a solution of [$Fe(CO_2)$(depe)$_2$] (20 mg, 0.039 mmol) in toluene (5 mL) and stirred at -20 ºC under N_2 atmosphere for 5 minutes. The solution colour changes from red to pink. Crystals suitable for X-ray diffraction studies were obtained from a concentrated solution of compound **7** in toluene at -30 ºC (12.8 mg, 35%).

Anal. Calcd. for $C_{33}H_{48}F_{10}FeN_2O_2P_4Zn$: C, 42.17; H, 5.15; N, 2.98; **Found:** C, 42.30; H, 5.31; N, 2.79.

^{1}H NMR (400 MHz, thf-d_8, -20 ºC) δ, ppm: 2.39-0.62 (m, depe).

^{31}P{^{1}H} NMR (160 MHz, thf-d_8, 25 ºC) δ, ppm: 77.8

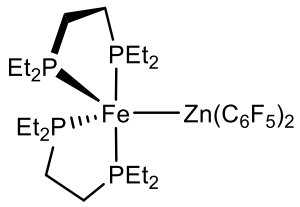
^{31}P{^{1}H} NMR (160 MHz, thf-d_8, -20 ºC) δ, ppm: 89.1, 80.9, 74.7, 67.9

^{19}F{^{1}H} NMR (377 MHz, thf-d_8, -20 ºC) δ, ppm: -116.2, -162.0, -165.0

A clean **^{13}C{^{1}H} NMR** spectrum could not be obtained due to the quick decomposition of compound **7** in solution even at low temperatures.

IR cm^{-1} (solid): 2105 ν(N≡N), 1633 ν(CO_2).

[(depe)$_2$Fe–Zn(C$_6$F$_5$)$_2$]



Compound 8. A solution of Zn(C$_6$F$_5$)$_2$ (16 mg, 0.039 mmol) in THF (5 mL) was added to a solution of [Fe(N$_2$)(depe)$_2$] (20 mg, 0.039 mmol) in toluene (5 mL) and stirred at room temperature under N$_2$ atmosphere for 5 minutes until the solution turns green. Crystals suitable for X-ray diffraction studies were obtained from a diethyl ether solution at -30 ºC (9.5 mg, 28 %).

Anal. Calcd. for C$_{32}$H$_{48}$F$_{10}$FeP$_4$Zn: C, 44.29; H, 5.58; **Found:** C, 44.45; H, 5.79

^{1}H NMR (400 MHz, C$_6$D$_6$, 25 ºC) δ, ppm: 1.97-0.84 (m, depe).

^{13}C{^{1}H} NMR (126 MHz, C$_6$D$_6$, 25 ºC) δ, ppm: 149.8 (d, $^1J_{CF}$ = 240 Hz, *p*-*C*$_6$F$_5$), 138.1 (d, $^1J_{CF}$ = 240 Hz, *o*-*C*$_6$F$_5$), 36.0, 34.6, 29.1, 28.5, 27.1, 25.6, 22.7, 14.3, 10.0, 9.3 (depe).

^{31}P{^{1}H} NMR (160 MHz, C$_6$D$_6$, 25 ºC) δ, ppm: 84.6 [Fe(N$_2$)(depe)$_2$]; 81.2, 78.7 (Compound **8**).

^{19}F{^{1}H} NMR (377 MHz, C$_6$D$_6$, 25 ºC) δ, ppm: -116.3, -159.4, -162.5 [Fe(N$_2$)(depe)$_2$]; -123.1, 156.2, -160.4 (Compound **8**).

3. General procedure for the hydrogenation of compounds 2 and 3

In a representative example, compound **2** (10 mg, 0.010 mmol) was placed in a J. Young NMR tube and dissolved in toluene-d_8 (0.6 mL). The solution was frozen and the inert gas was removed under high vacuum. Then, the atmosphere was replaced by 1 bar of H_2 and the resulting mixture was kept under H_2 atmosphere for 24 hours. The conversion of compound **2** into **4** was determined by $^{31}P\{^1H\}$ NMR spectroscopy by means of the disappearance of **2** and using triphenylphosphine oxide as internal standard. Besides, formation of compound **4** was also verified by infrared spectroscopy after solvent evaporation under vacuum inside the glovebox, giving rise to a yellow oil which was employed to record the corresponding infrared spectrum.

4. Spectroscopic data of compounds

Figure S1. $^{31}P\{^{1}H\}$ NMR (160 MHz, C_6D_6, 25 ºC) for compound **2**

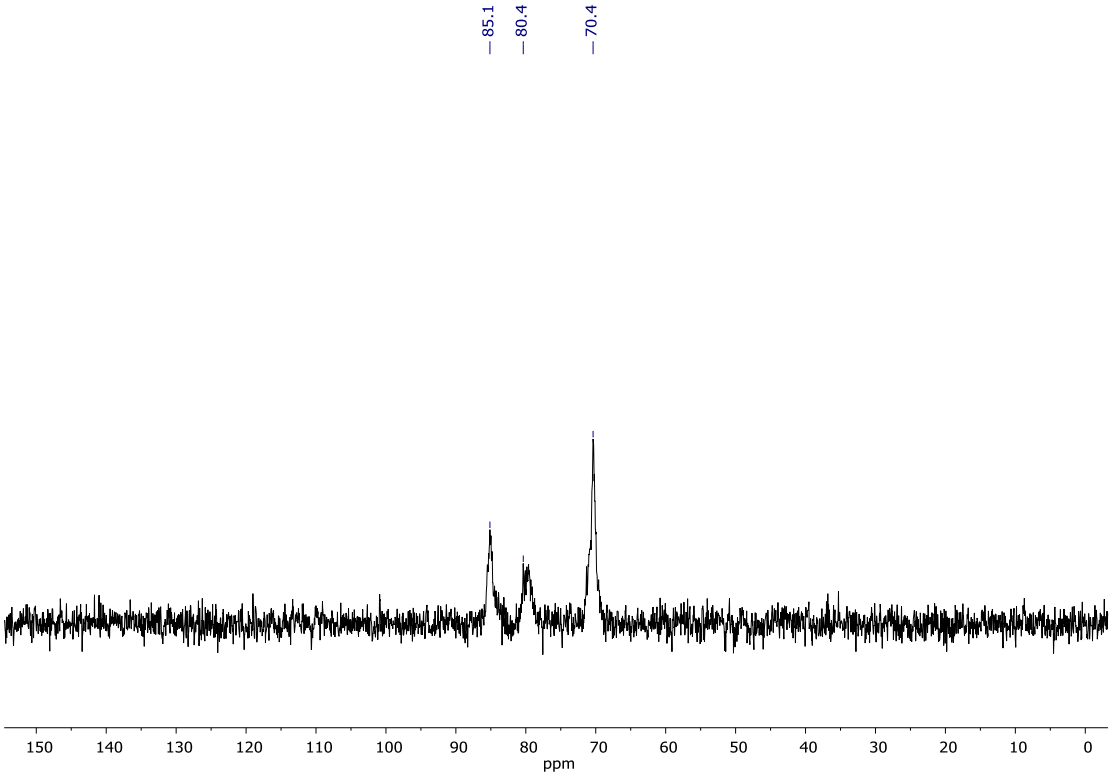


Figure S2. $^{31}P\{^{1}H\}$ NMR (160 MHz, thf-d_8, -30 ºC) for compound **2**

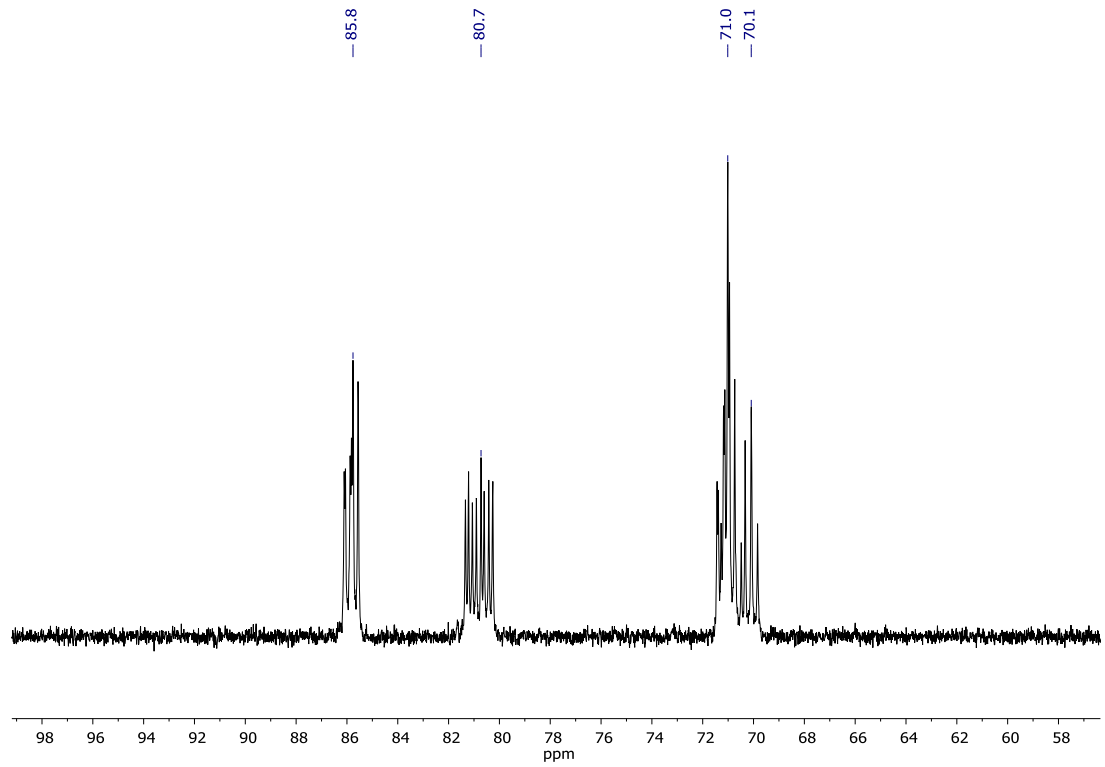


Figure S3. $^{11}B\{^{1}H\}$ NMR (128 MHz, C_6D_6, 25 ºC) for compound **2**

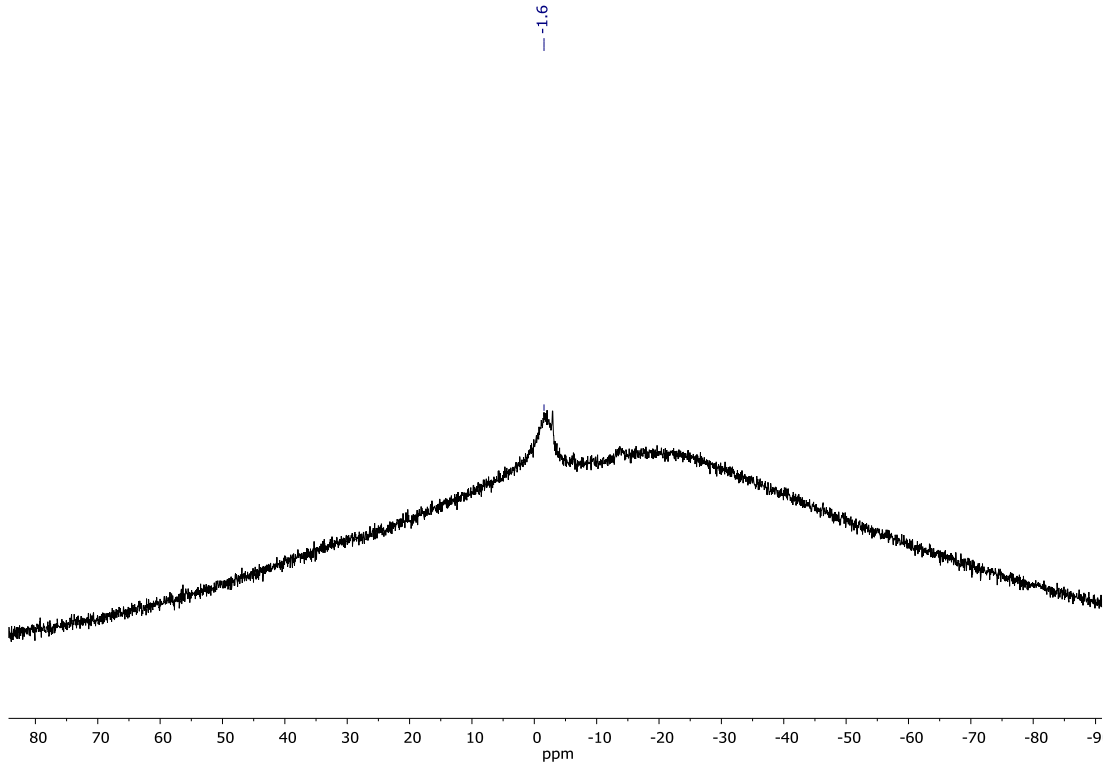


Figure S4. ^{1}H NMR (400 MHz, C_6D_6, 25 ºC) for compound **2**

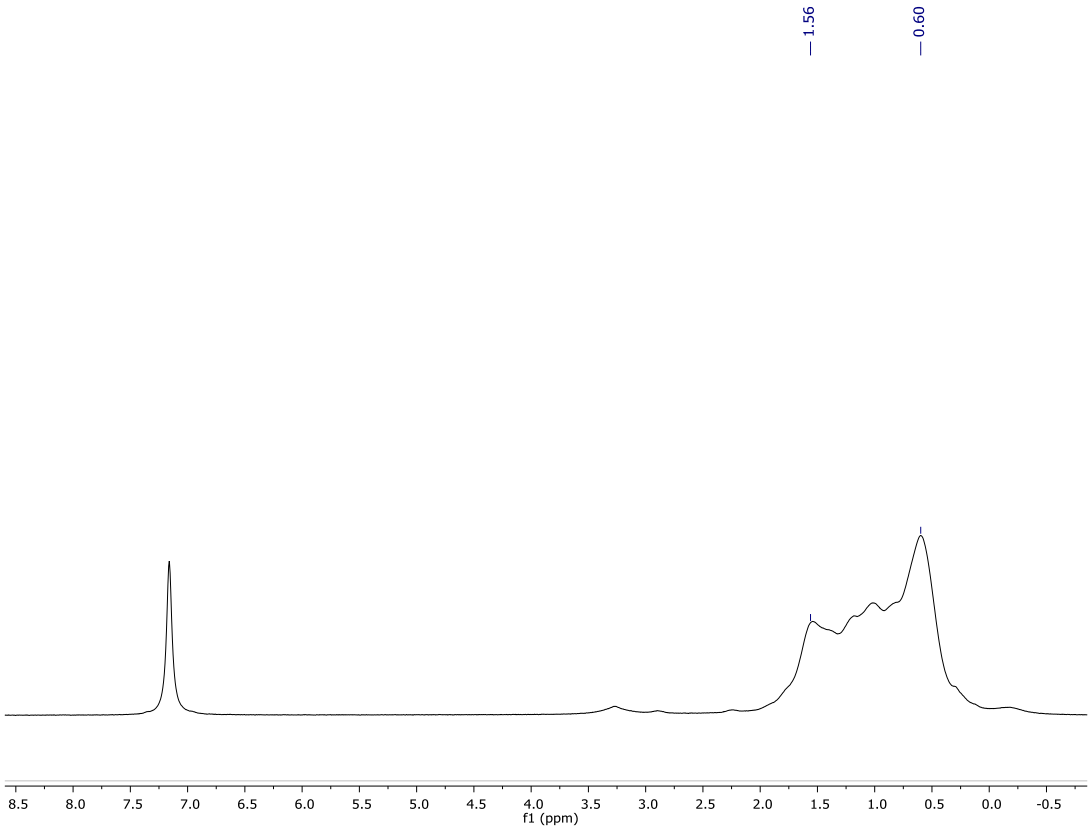


Figure S5. $^{19}F\{^{1}H\}$ NMR (377 MHz, C_6D_6, 25 ºC) for compound **2**

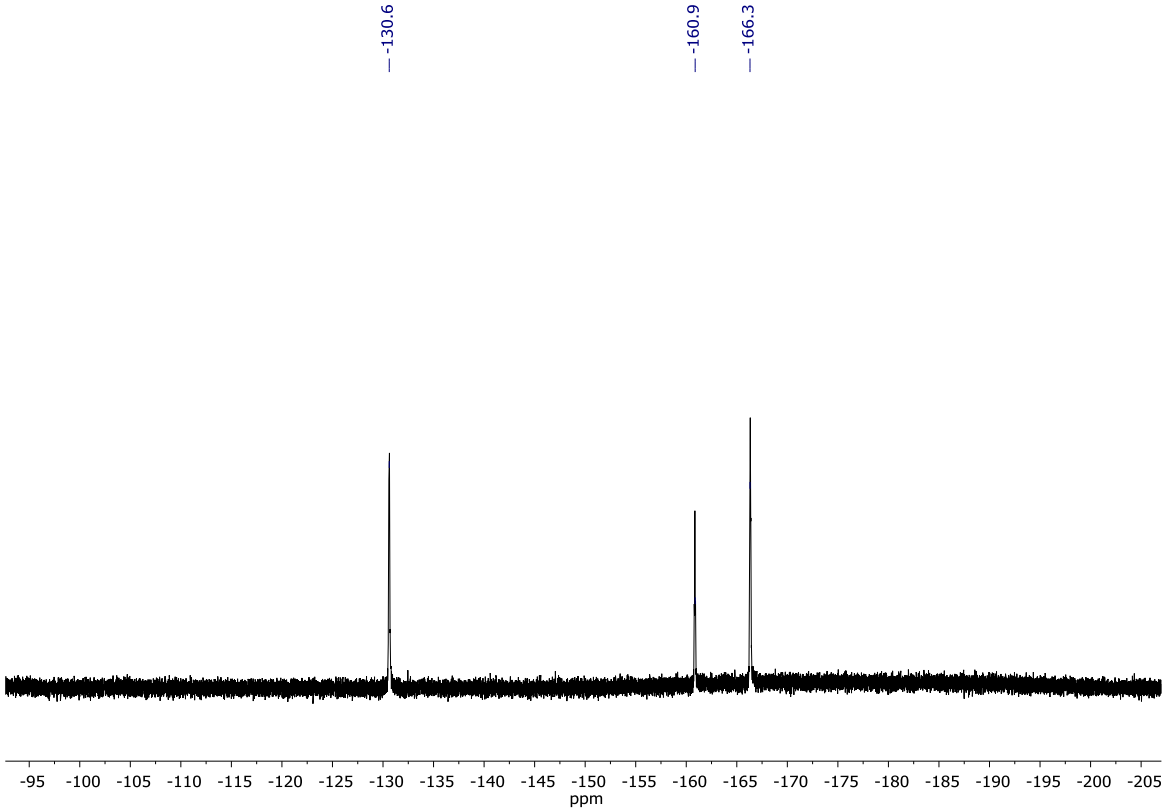


Figure S6. $^{13}C\{^{1}H\}$ NMR (126 MHz, thf-d_8, 25 ºC) for compound **2**

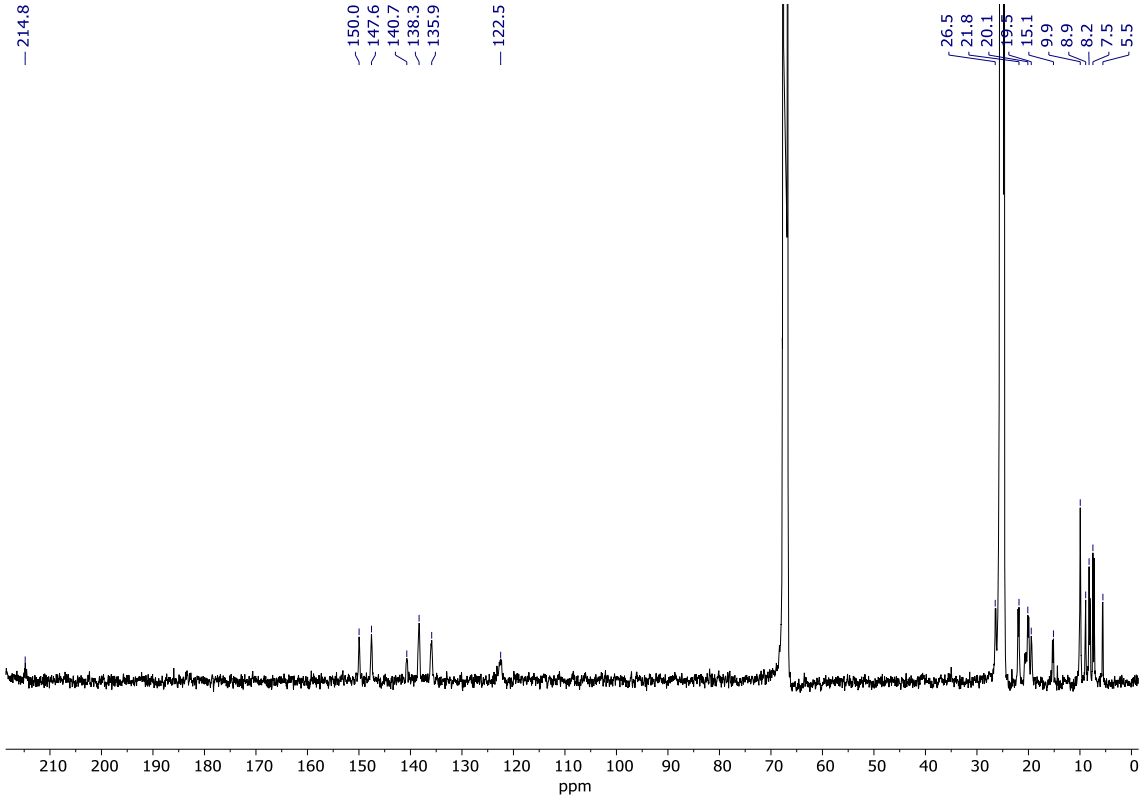


Figure S7. IR spectrum (Nujol) for compound **2**

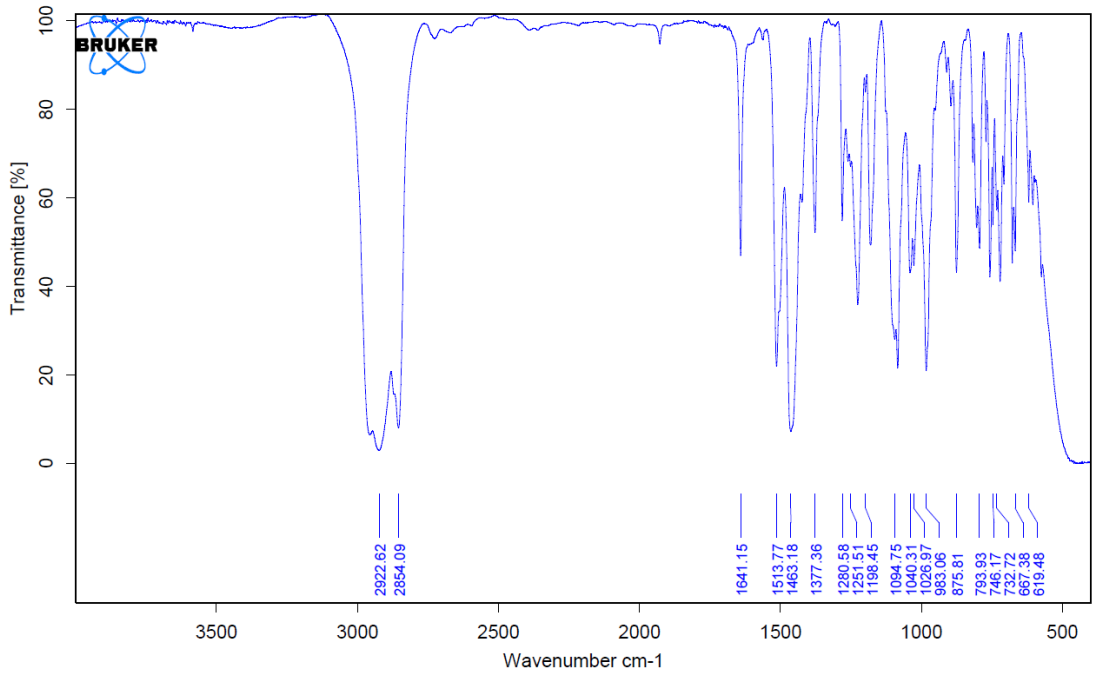


Figure S8. $^{31}P\{^{1}H\}$ NMR (160 MHz, C_6D_6, 25 ºC) for compound **3**

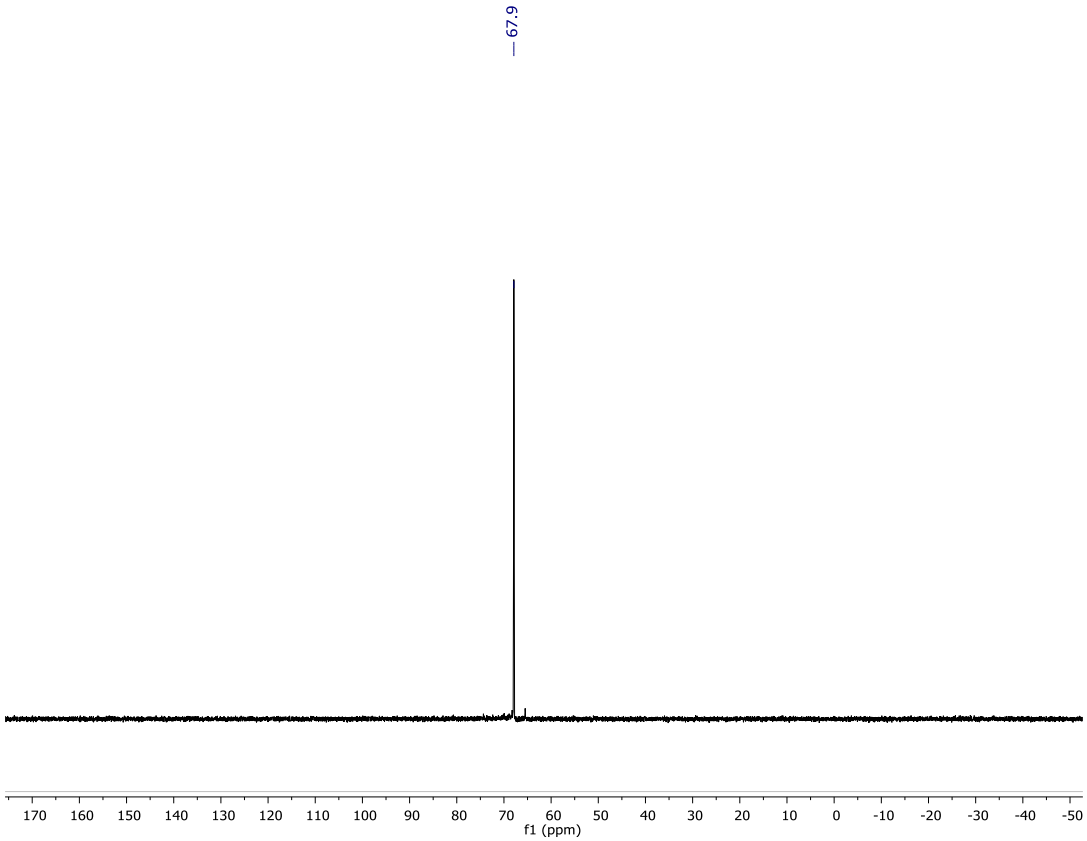


Figure S9. ^{1}H NMR (400 MHz, C_6D_6, 25 ºC) for compound **3**

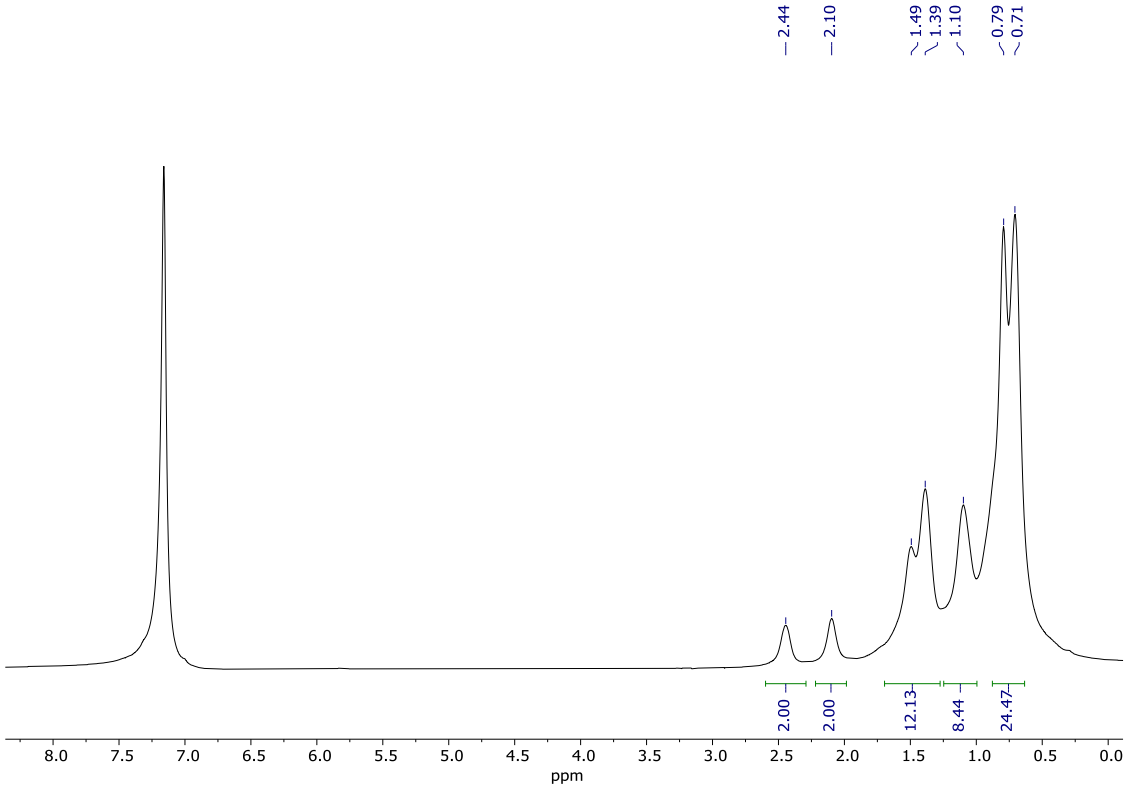


Figure S10. ^{19}F{^{1}H} NMR (377 MHz, C_6D_6, 25 ºC) for compound **3**

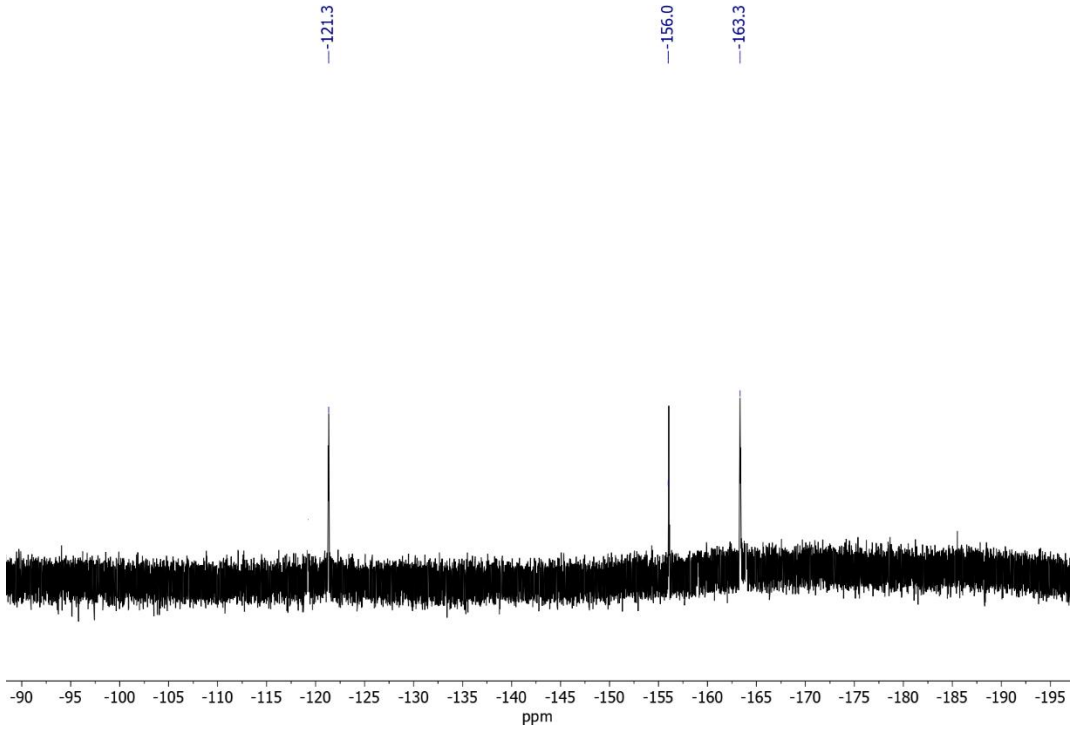


Figure S11. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6, 25 ºC) for compound **3**

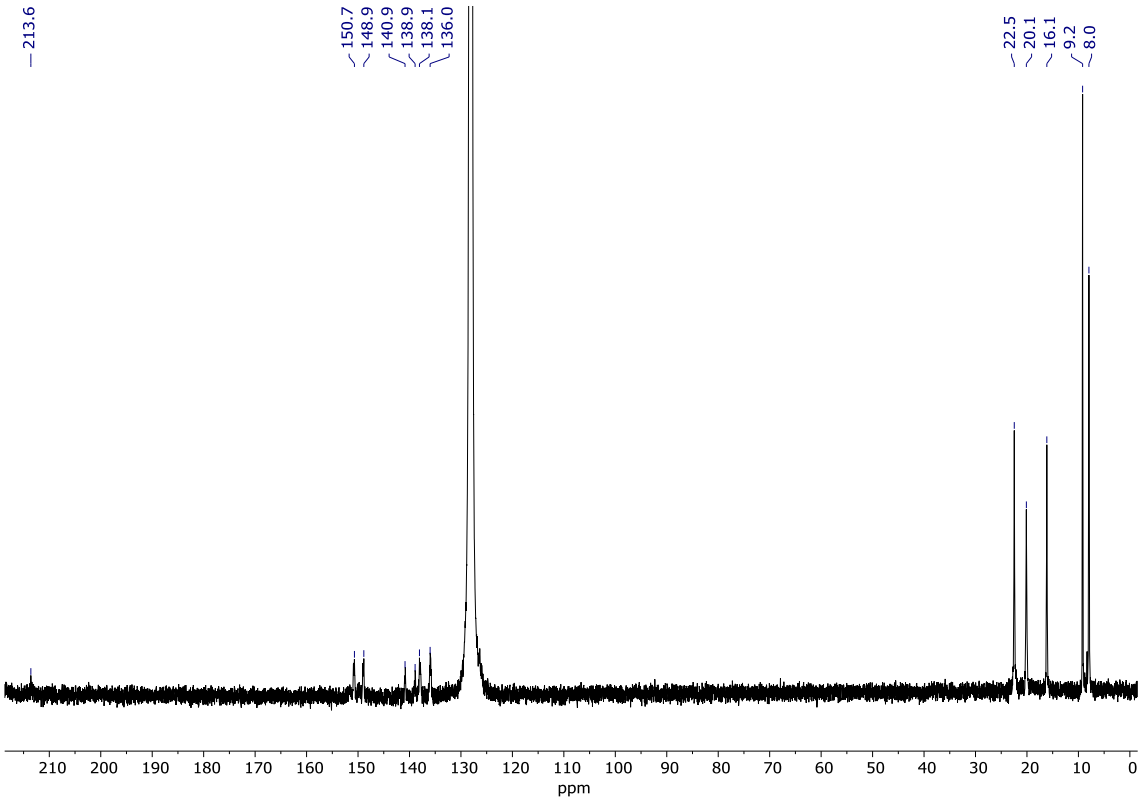


Figure S12. IR spectrum (solid) for compound **3**

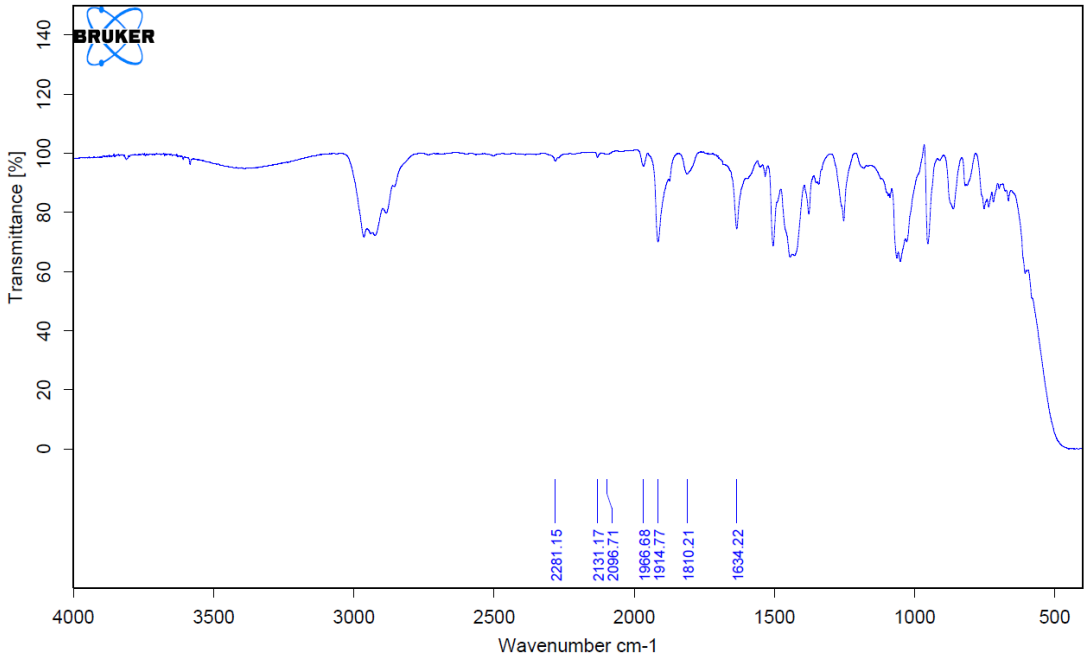


Figure S13. $^{31}P\{^{1}H\}$ NMR (160 MHz, tol-d_8, -80 ºC) for the reaction of compound **1** with $AlEt_3$.

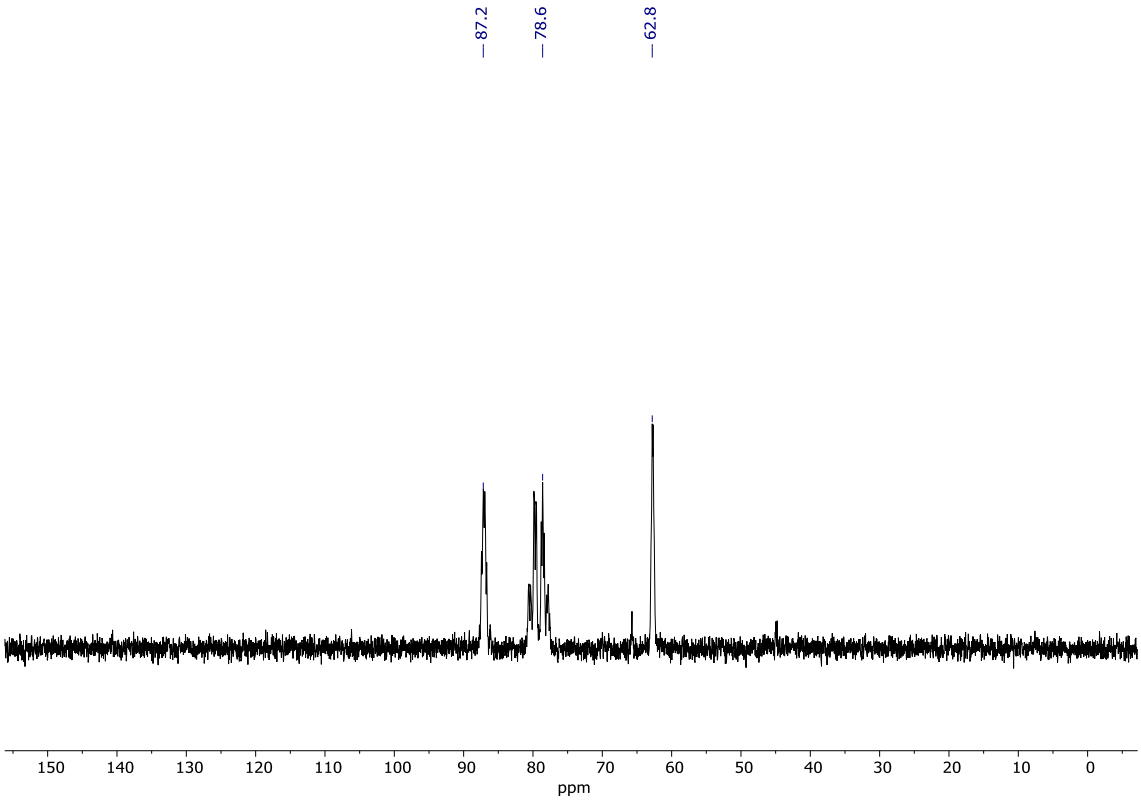


Figure S14. $^{31}P\{^{1}H\}$ NMR (160 MHz, tol-d_8, -20 ºC) for the reaction of complex **2** with H_2 (1 bar H_2, 25 ºC, 24 h).

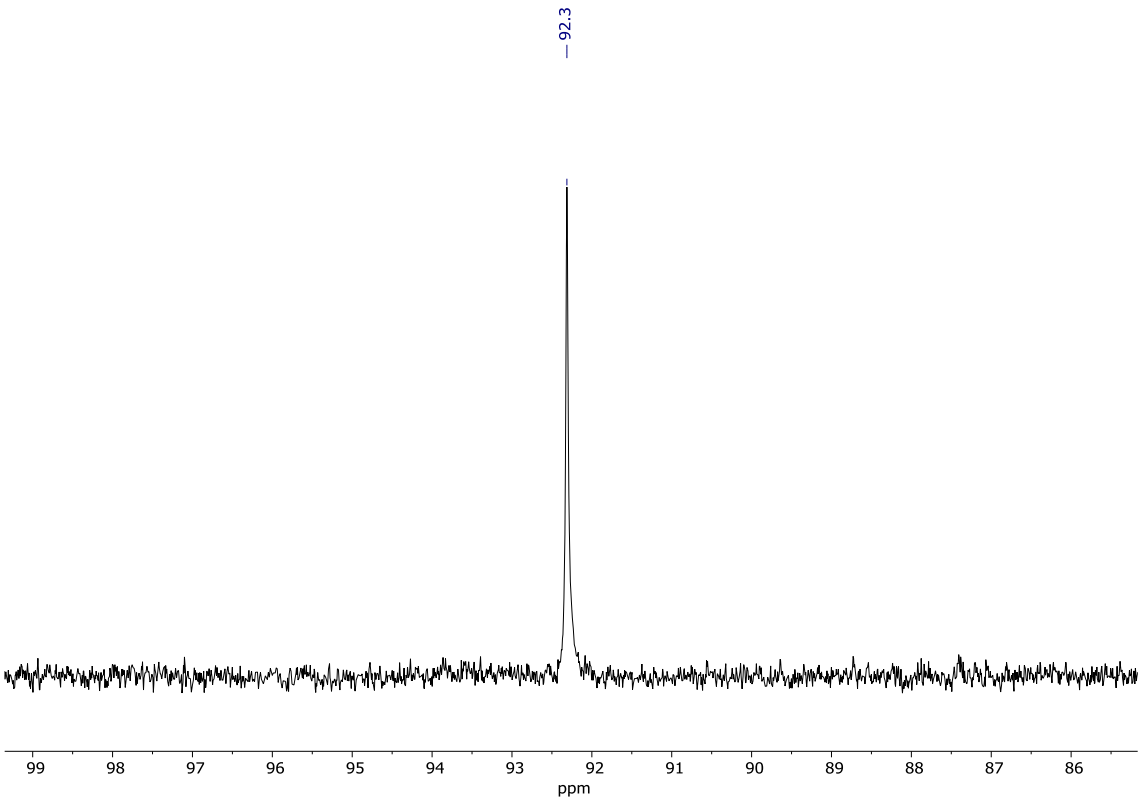


Figure S15. $^{11}B\{^{1}H\}$ NMR (128 MHz, tol-d_8, -20 ºC) for the reaction of complex **2** with H_2 (1 bar H_2, 25 ºC, 24 h).

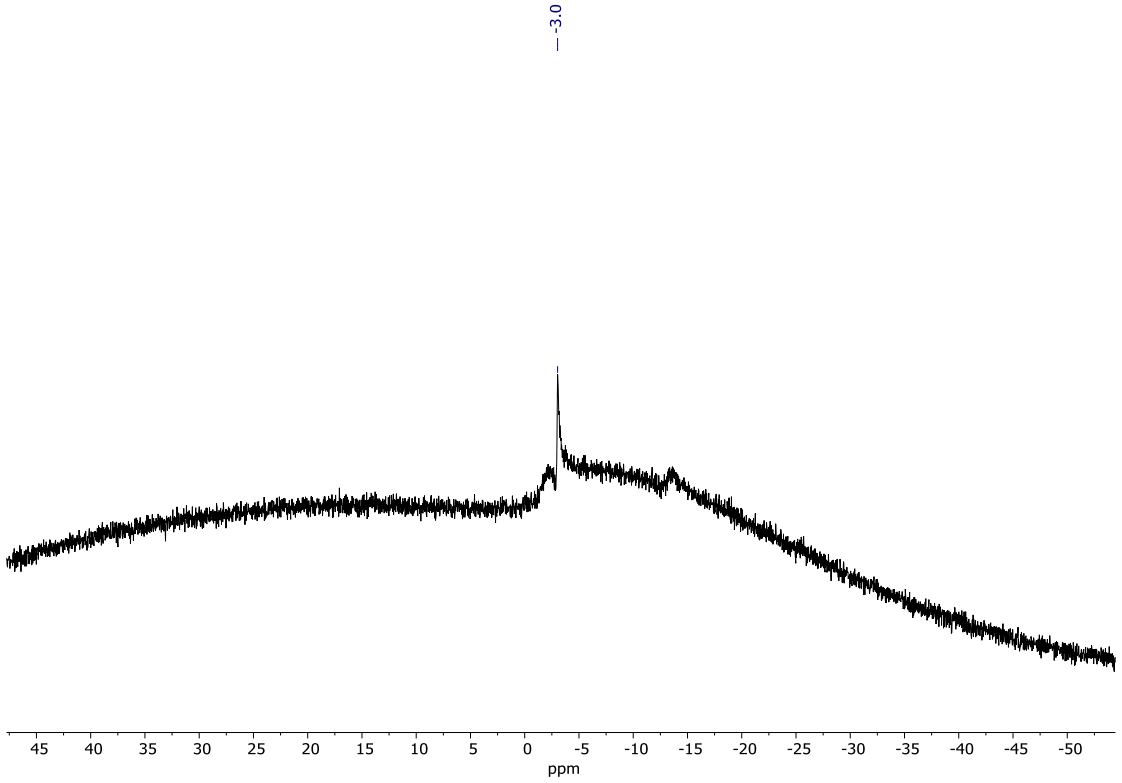


Figure S16. ^{1}H NMR (400 MHz, tol-d_8, -20 ºC) for the reaction of complex **2** with H_2 (1 bar H_2, 25 ºC, 24 h).

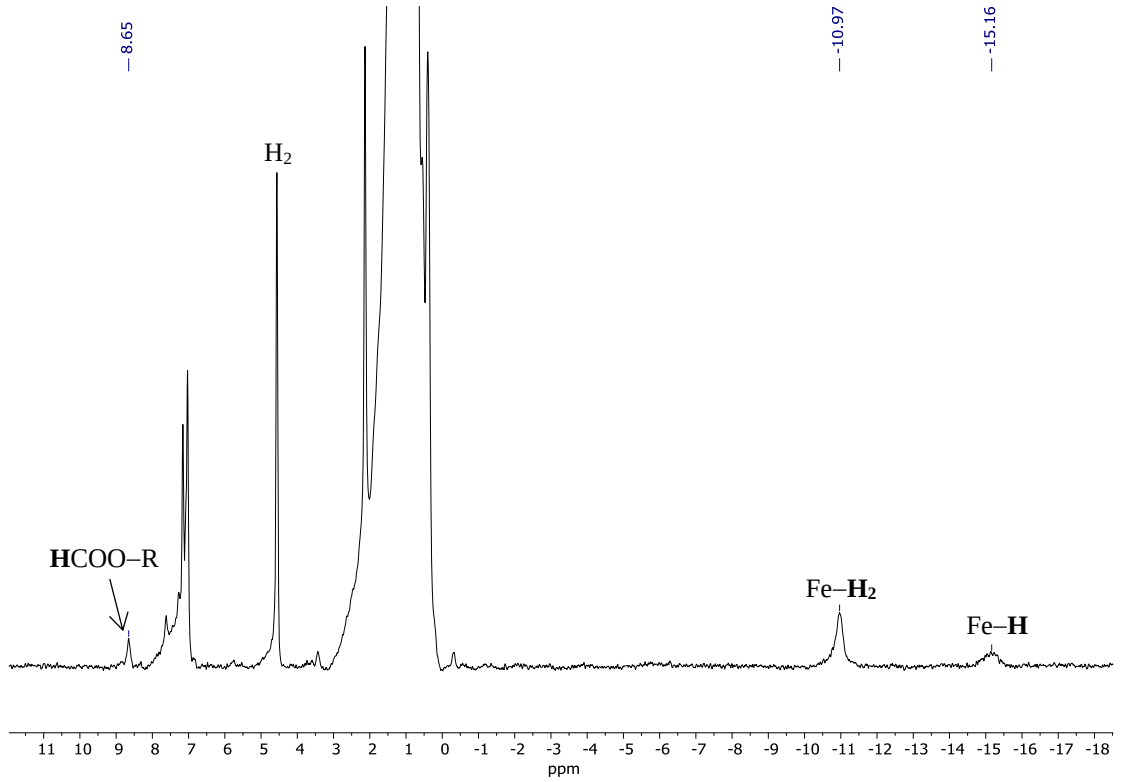


Figure S17. IR spectrum (neat) for the reaction of complex **2** with H_2

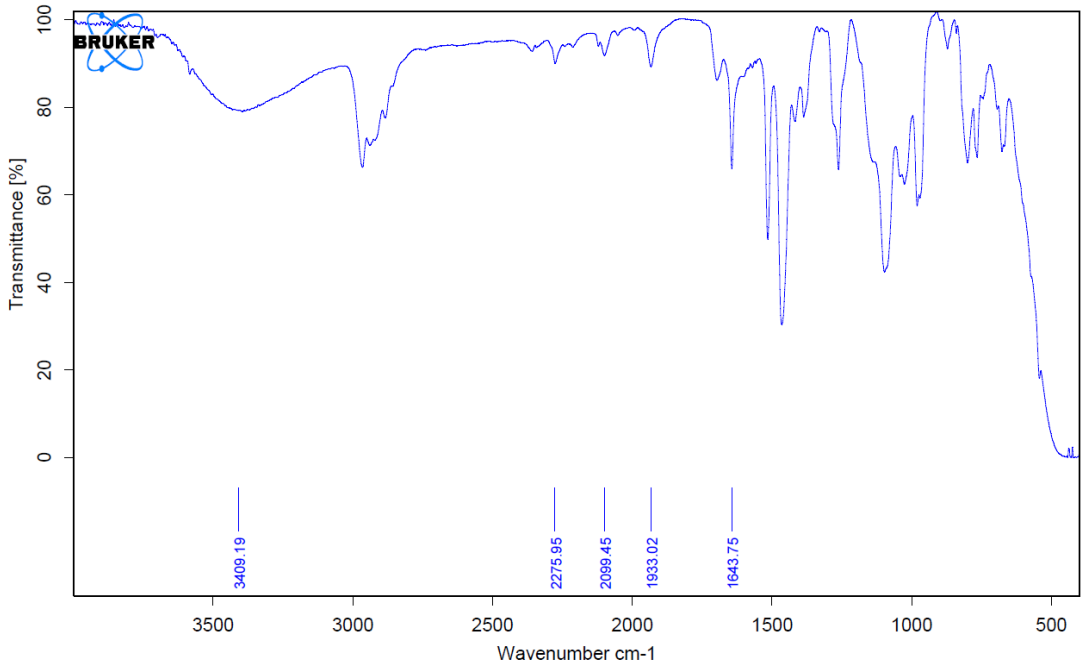


Figure S18. $^{31}P\{^{1}H\}$ NMR (160 MHz, tol-d_8, -20 ºC) for the reaction of complex **3** with H_2 (1 bar H_2, 25 ºC, 24 h).

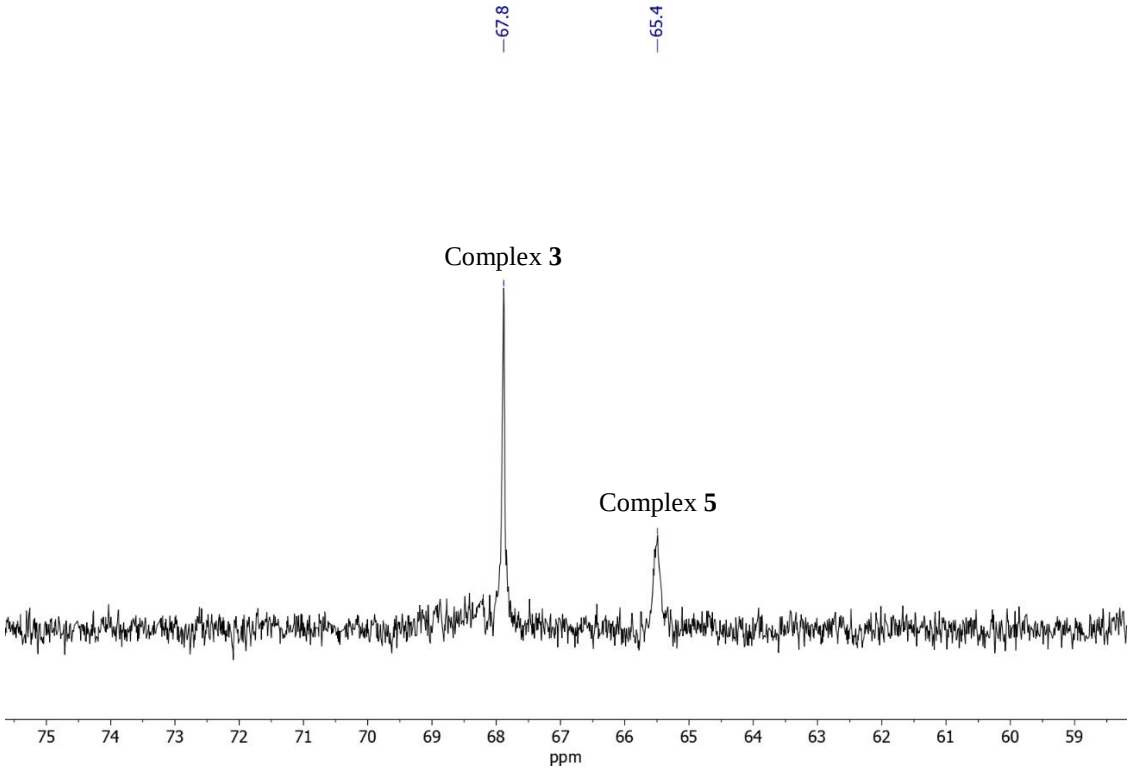


Figure S19. ^{1}H NMR (400 MHz, tol-d_8, -20 ºC) for the reaction of complex **3** with H_2 (1 bar H_2, 25 ºC, 24 h).

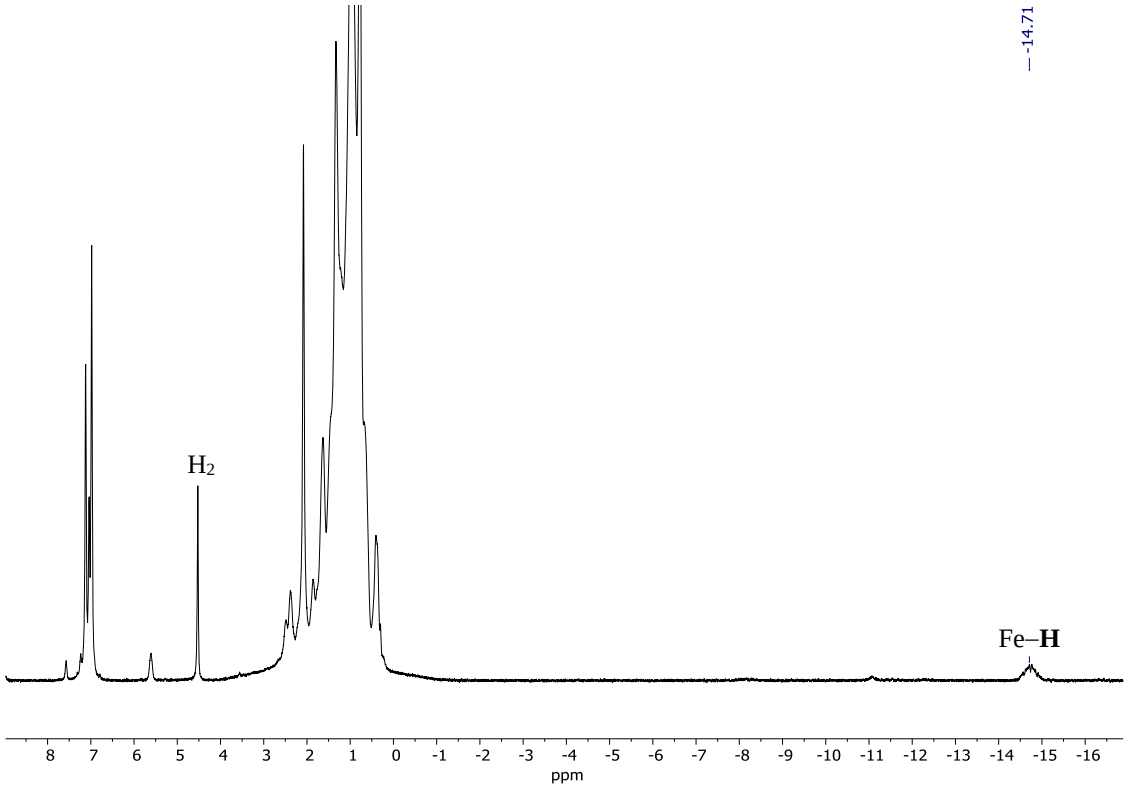


Figure S20. IR spectrum (neat) for the reaction of complex **3** with H_2

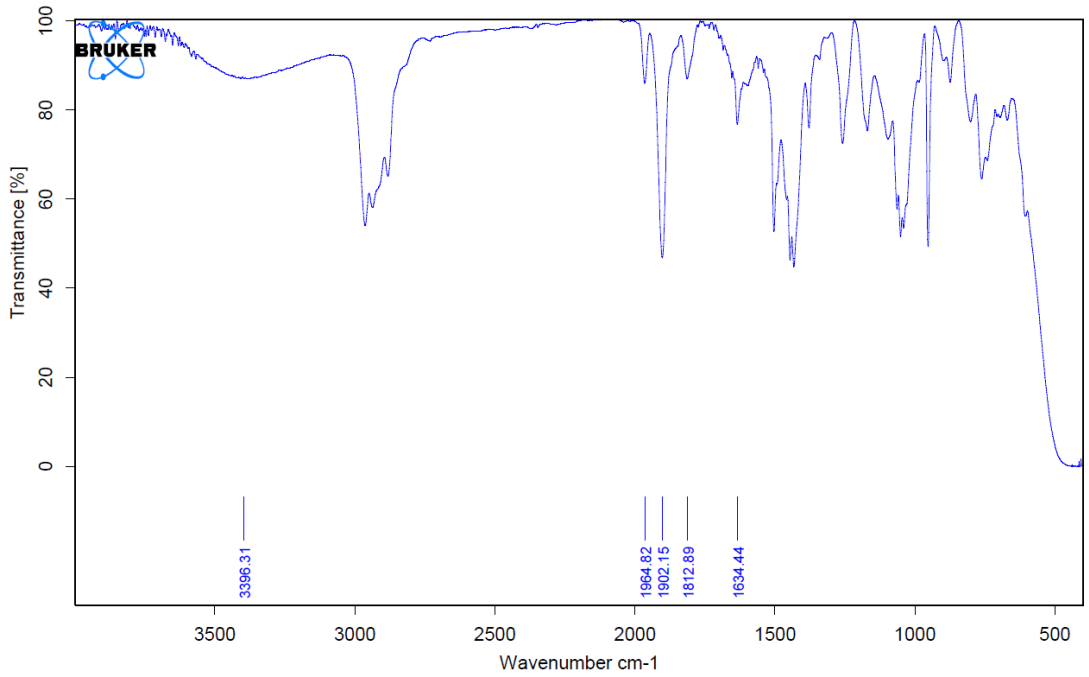


Figure S21. $^{31}P\{^{1}H\}$ NMR (160 MHz, CD_2Cl_2, -20 ºC) for: a) compound **3**, b) reaction of compound **3** with H_2 in CD_2Cl_2 (1 bar H_2, 25 ºC, 24 h).

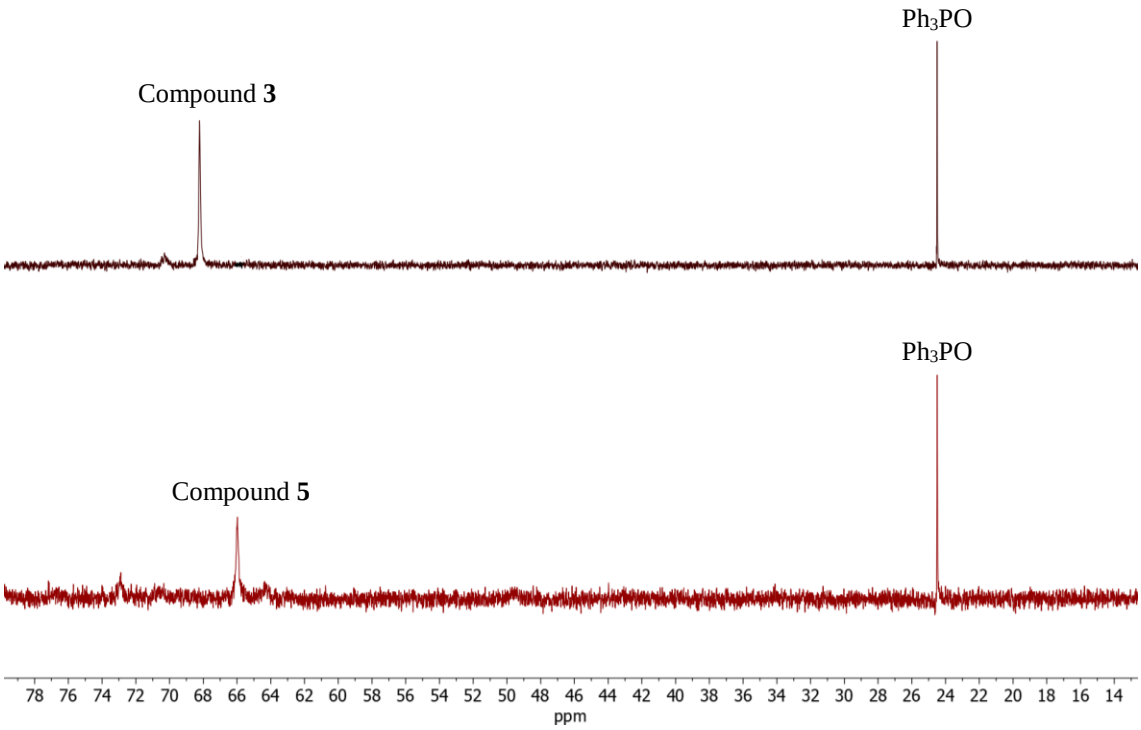


Figure S22. $^{31}P\{^{1}H\}$ NMR (160 MHz, C_6D_6, 25 ºC) for compound **6**

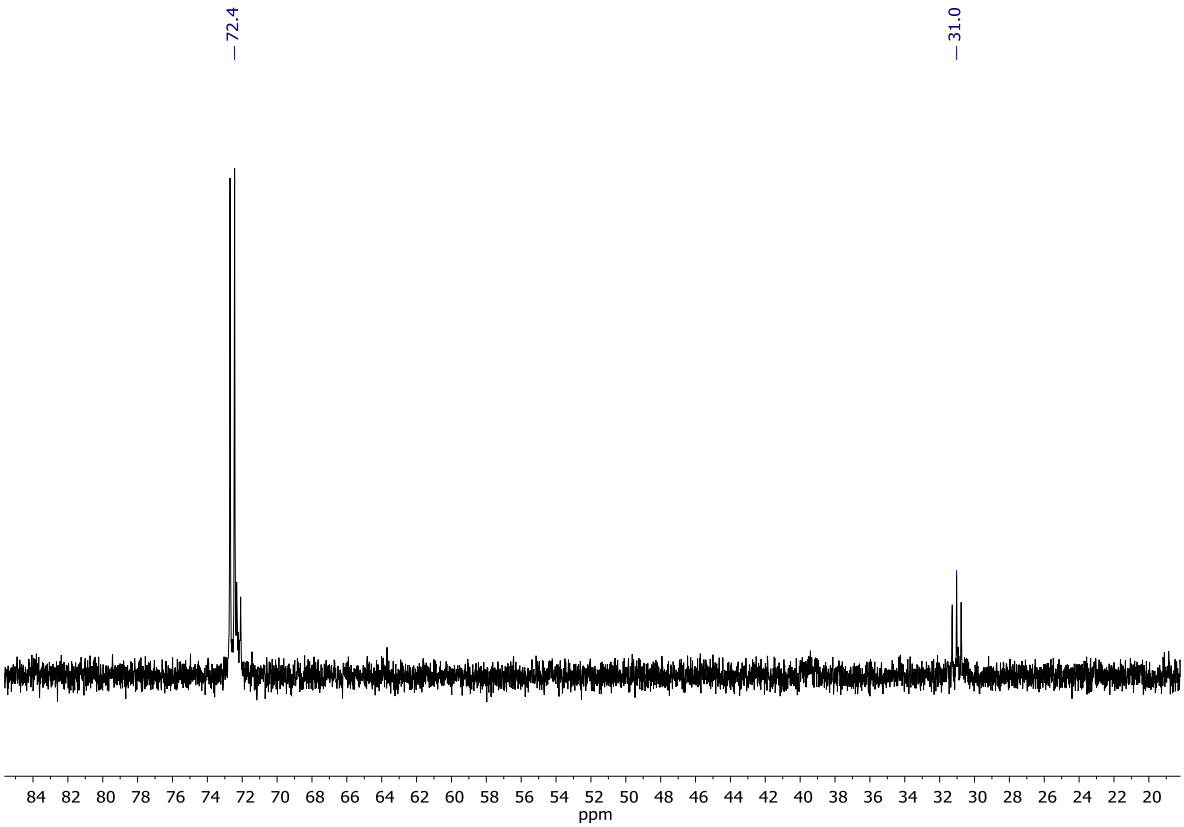


Figure S23. ^{1}H NMR (400 MHz, C_6D_6, 25 ºC) for compound **6**

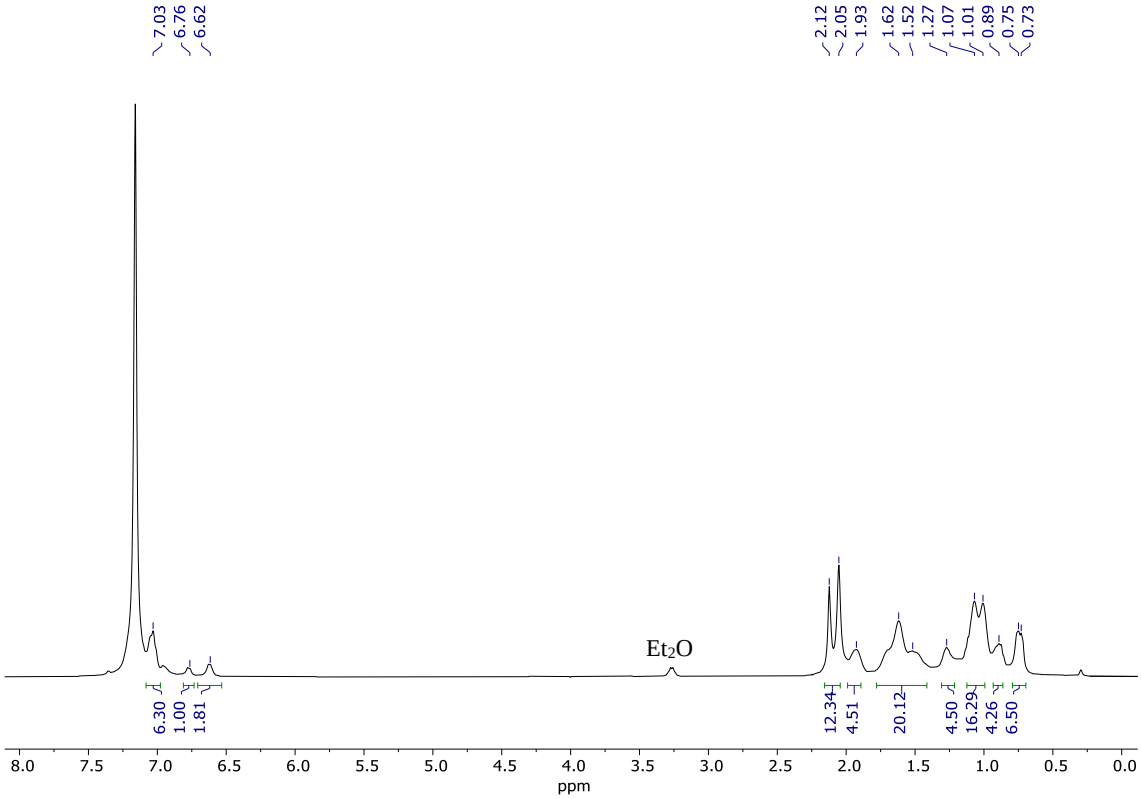


Figure S24. IR spectrum (Nujol) for compound **6**

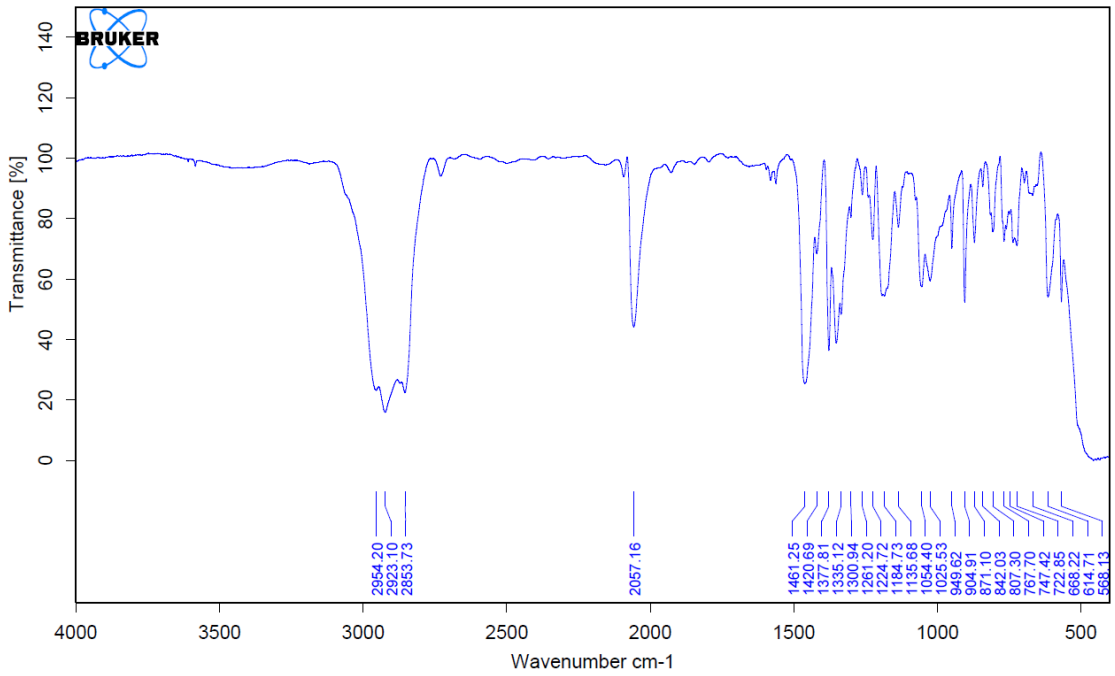


Figure S25. $^{31}P\{^{1}H\}$ NMR (160 MHz, thf-d_8, -20 ºC) for compound **7**

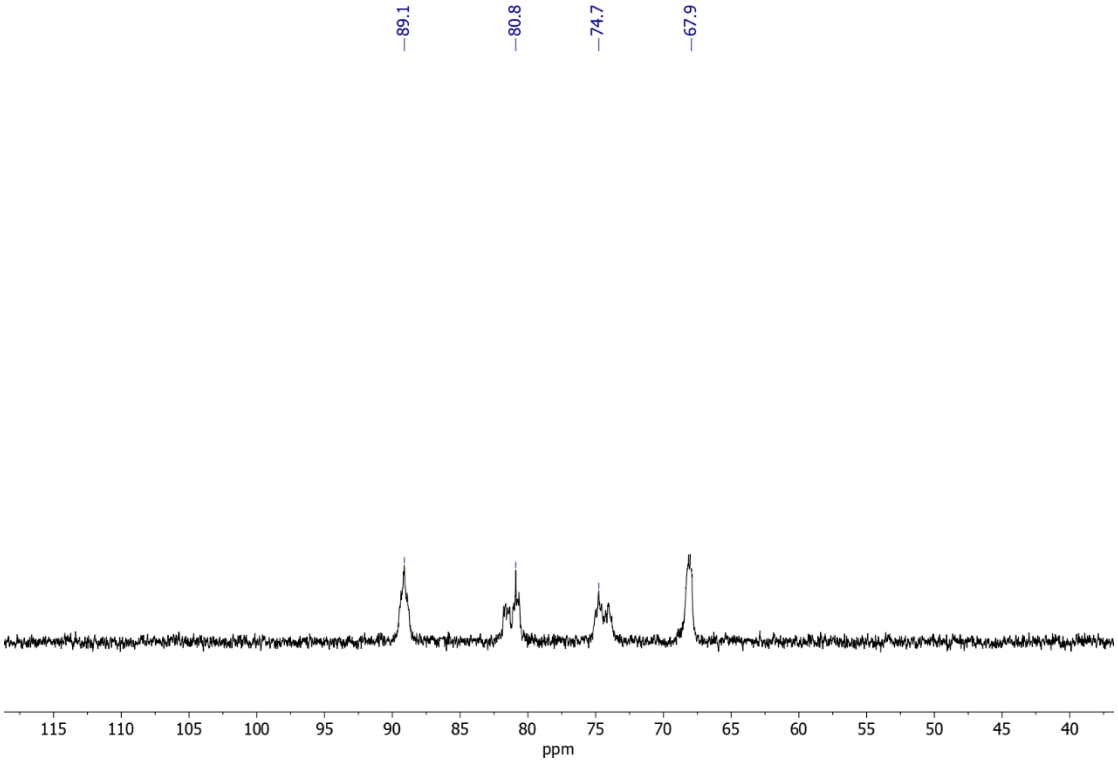


Figure S26. $^{31}P\{^{1}H\}$ NMR (160 MHz, thf-d_8, 25 ºC) for compound **7**

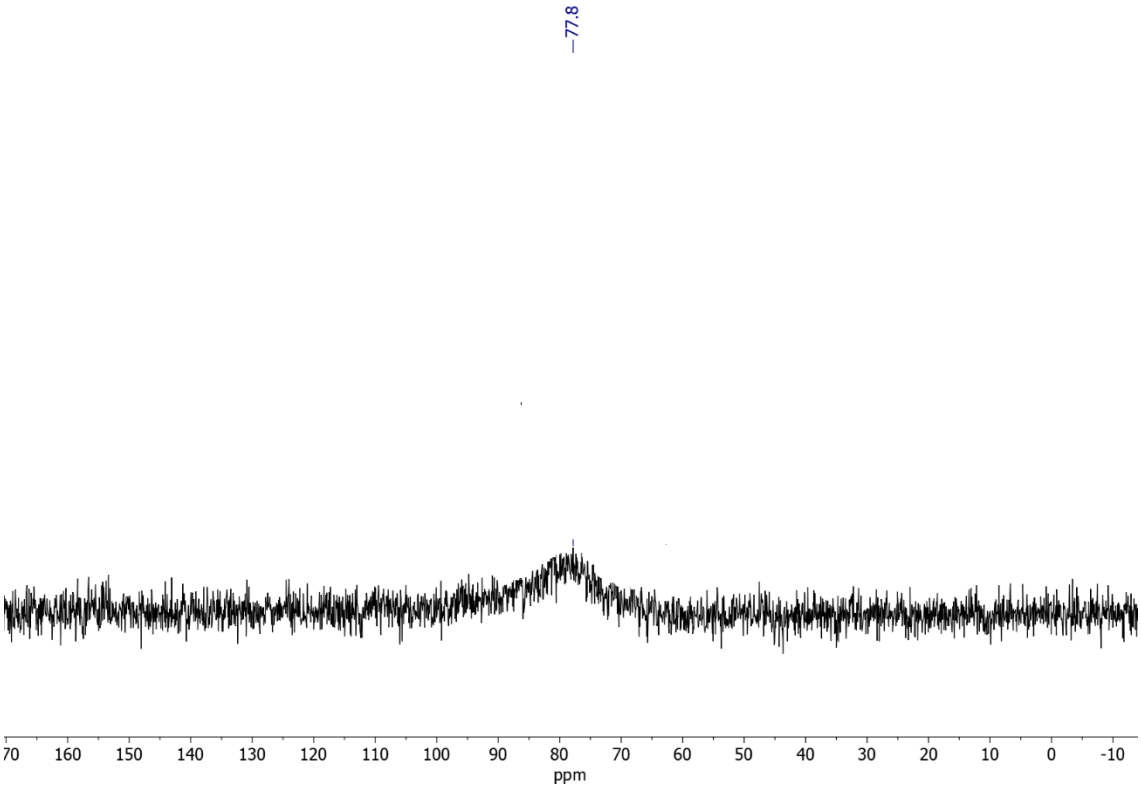


Figure S27. ^{1}H NMR (400 MHz, thf-d_8, -20 ºC) for compound **7**

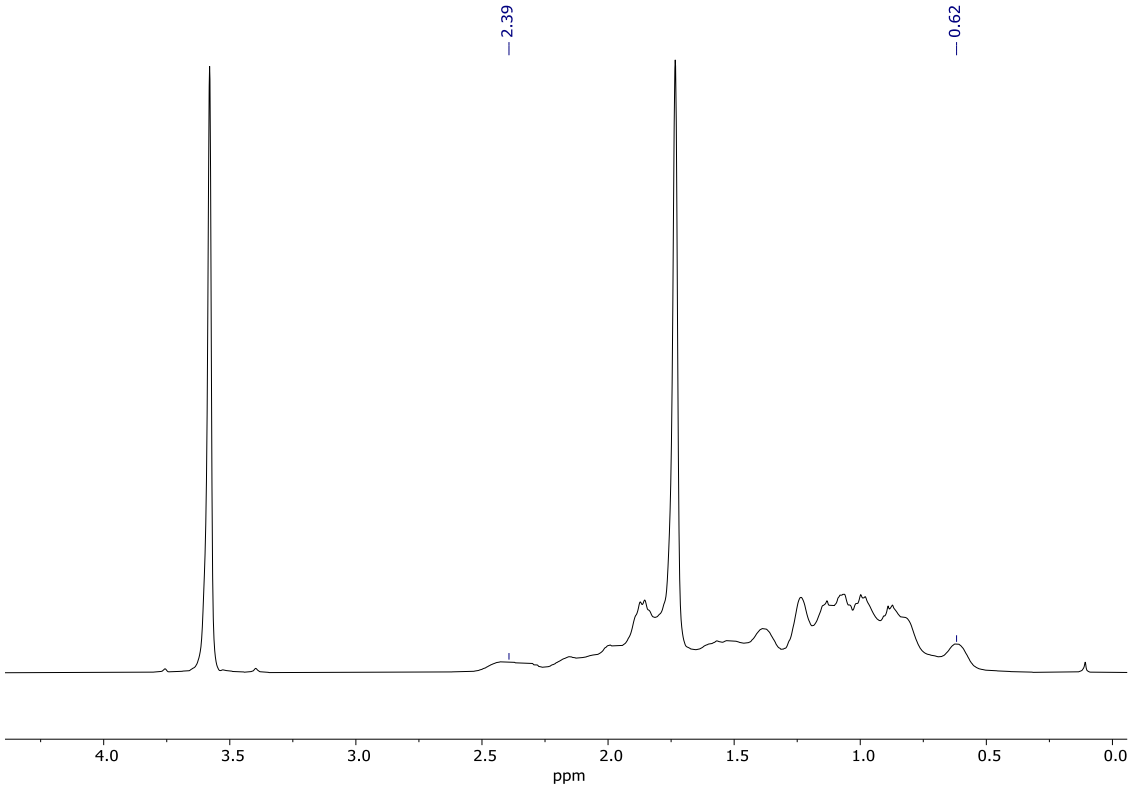


Figure S28. ^{19}F{^{1}H} NMR (377 MHz, thf-d_8, -20 ºC) for compound **7**

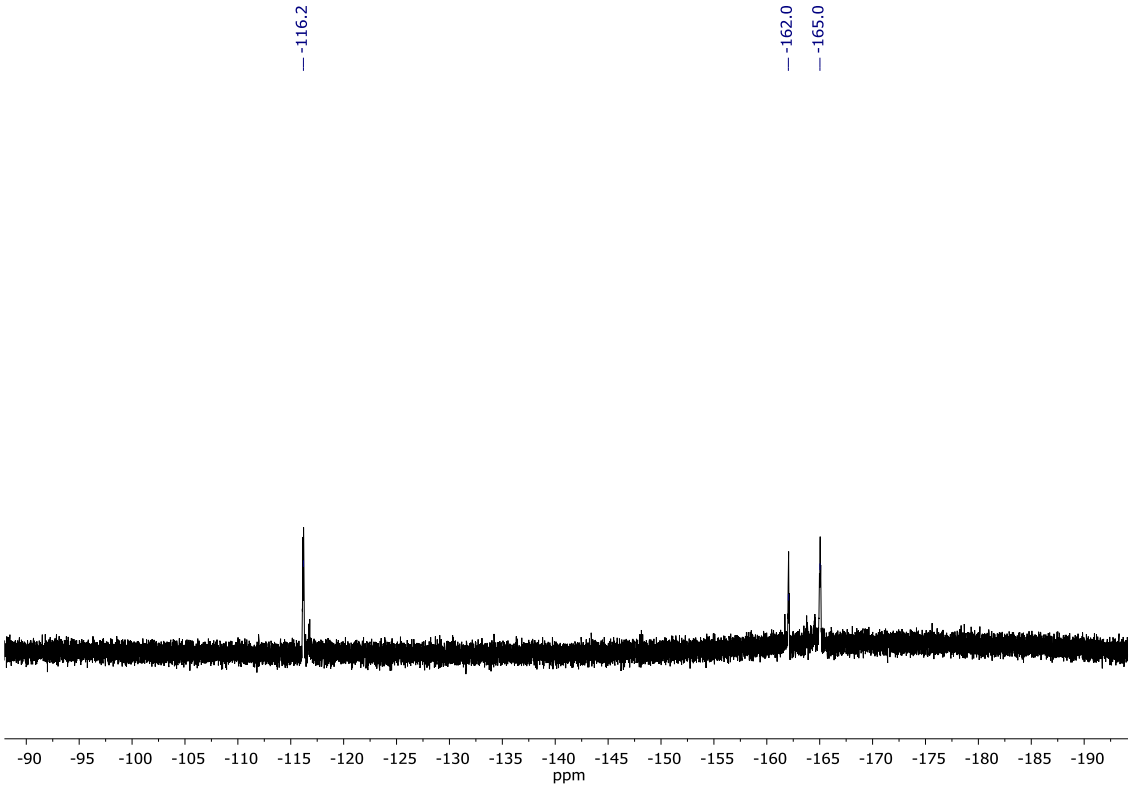


Figure S29. IR spectrum (solid) for compound **7**

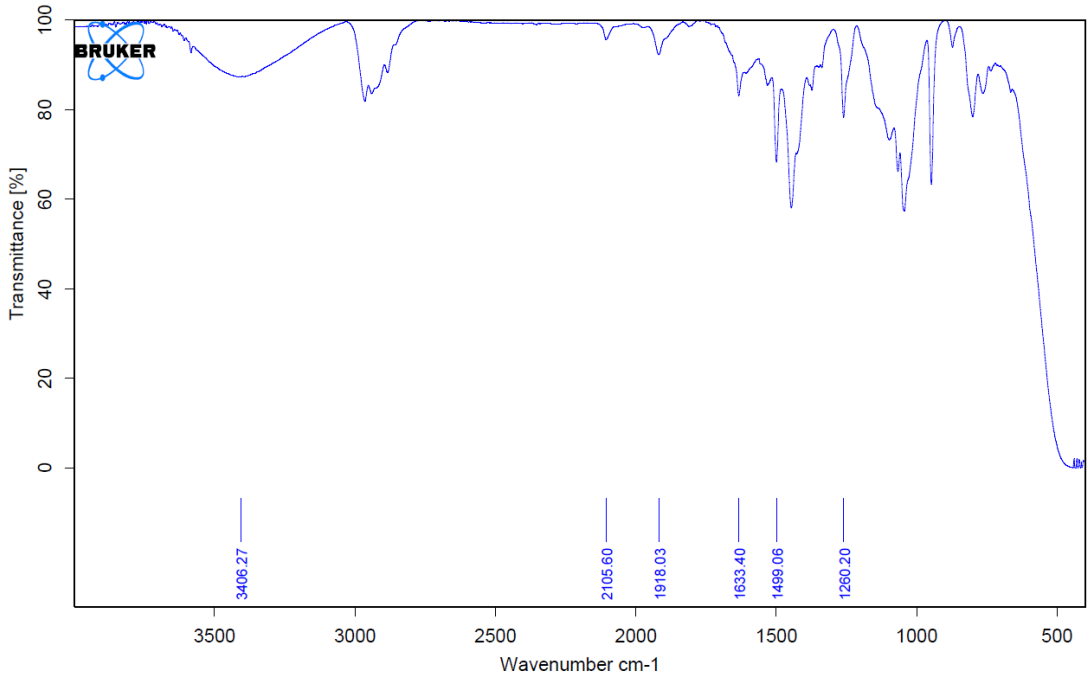


Figure S30. $^{31}P\{^{1}H\}$ NMR (160 MHz, C_6D_6, 25 ºC) for the mixture of $[Fe(N_2)(depe)_2]$ (●) and compound **8** (●).

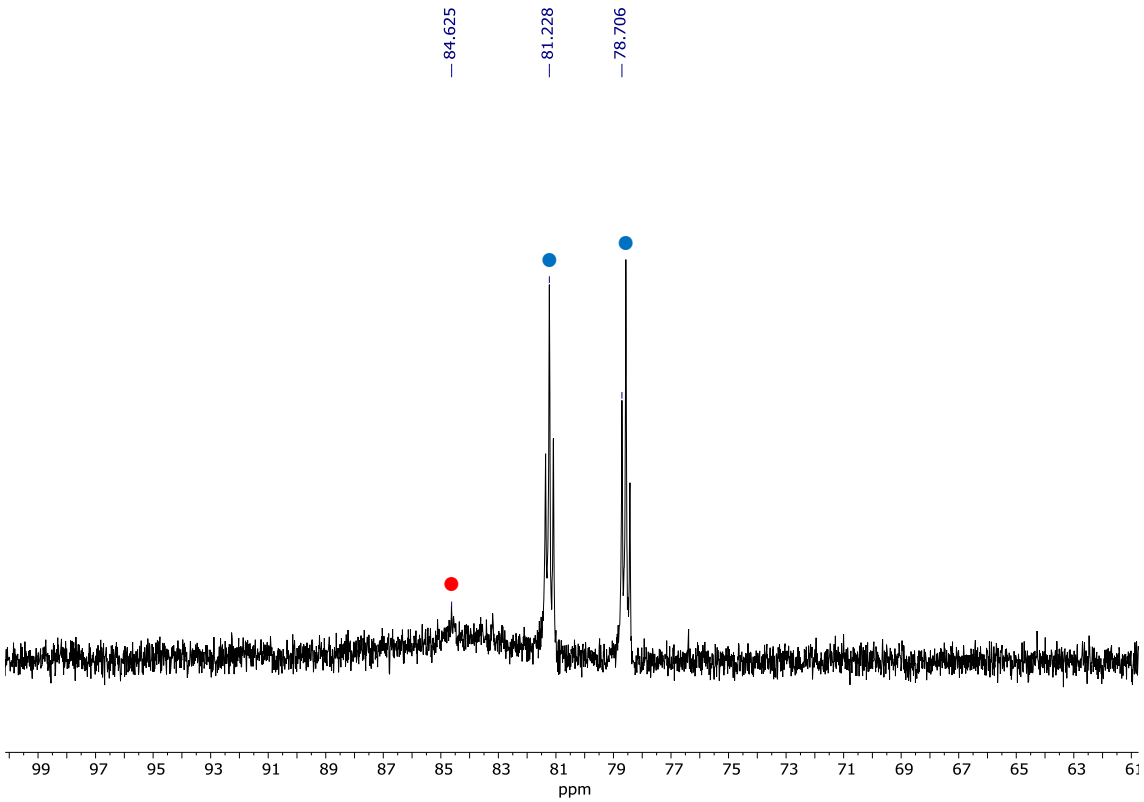


Figure S31. ^{1}H NMR (400 MHz, C_6D_6, 25 ºC) for the mixture of $[Fe(N_2)(depe)_2]$ and compound **8**.

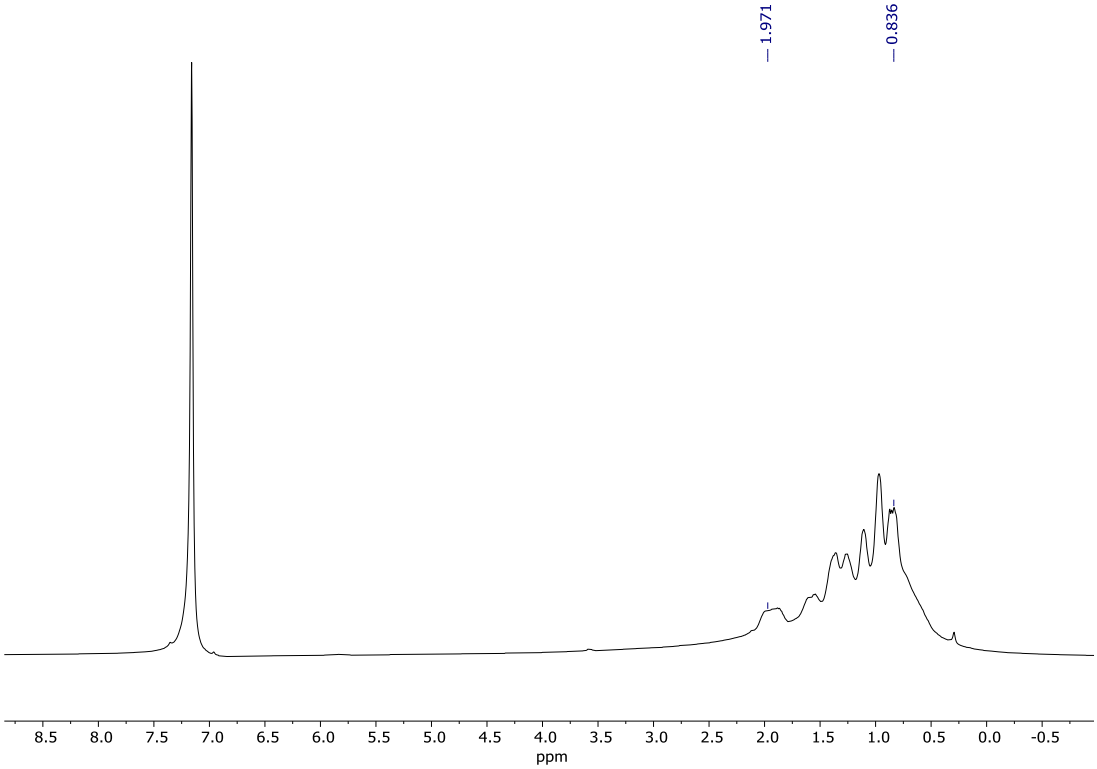


Figure S32. $^{19}F\{^{1}H\}$ NMR (377 MHz, C_6D_6, 25 ºC) for the mixture of $[Fe(N_2)(depe)_2]$ (●) and compound **8** (●).

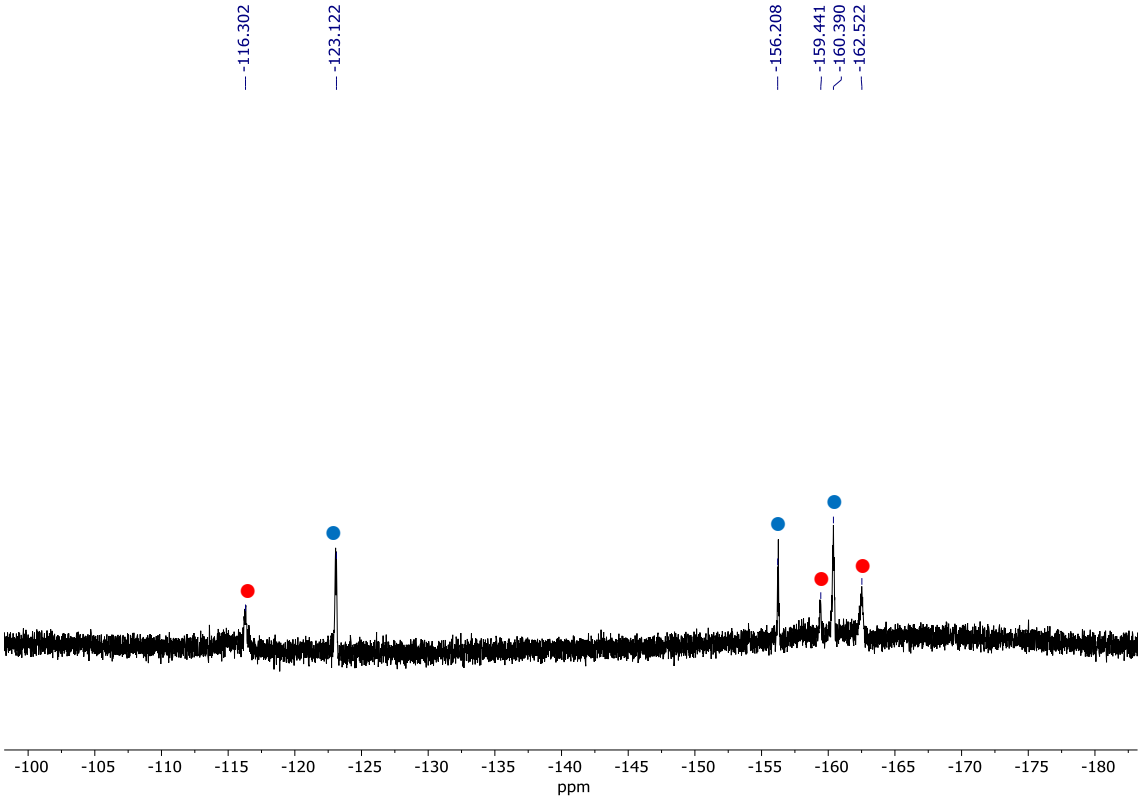
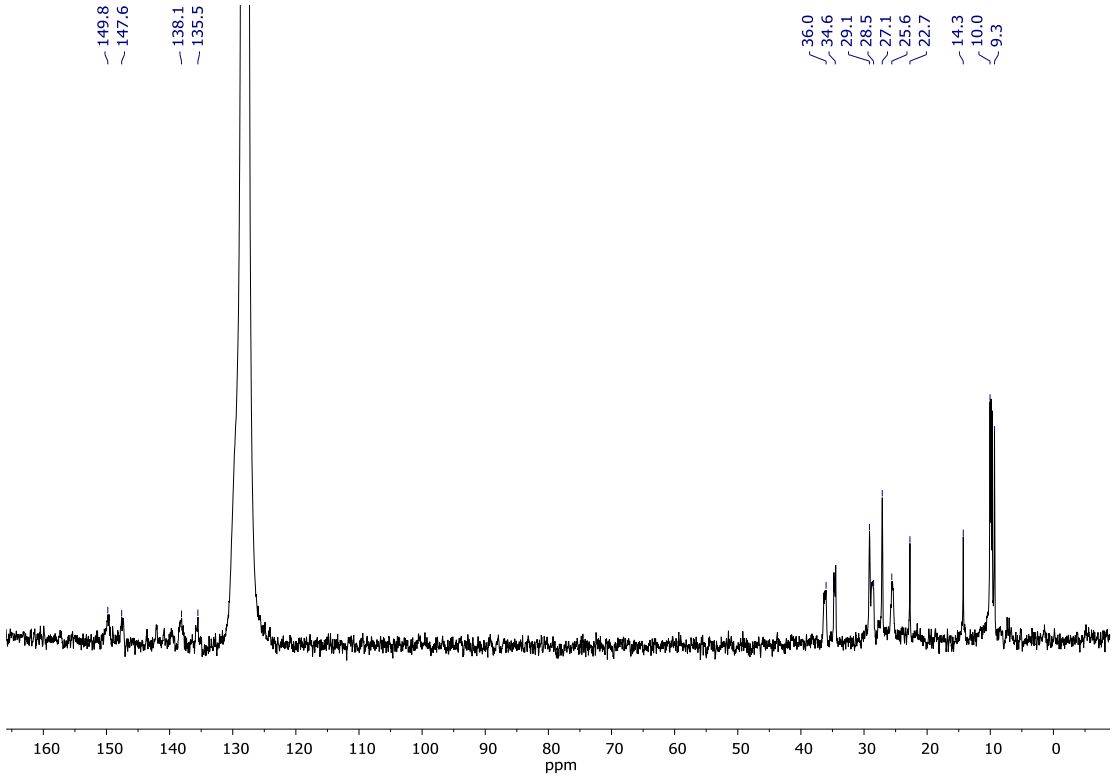


Figure S33. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6, 25 ºC) for the mixture of $[Fe(N_2)(depe)_2]$ and compound **8**.



5. Variable temperature experiments

Figure S34. Variable temperature $^{31}P\{^{1}H\}$ NMR spectra for the equilibrium process between [Fe(N_2)(depe)$_2$] (●) and compound **8** (●) in thf-d_8.

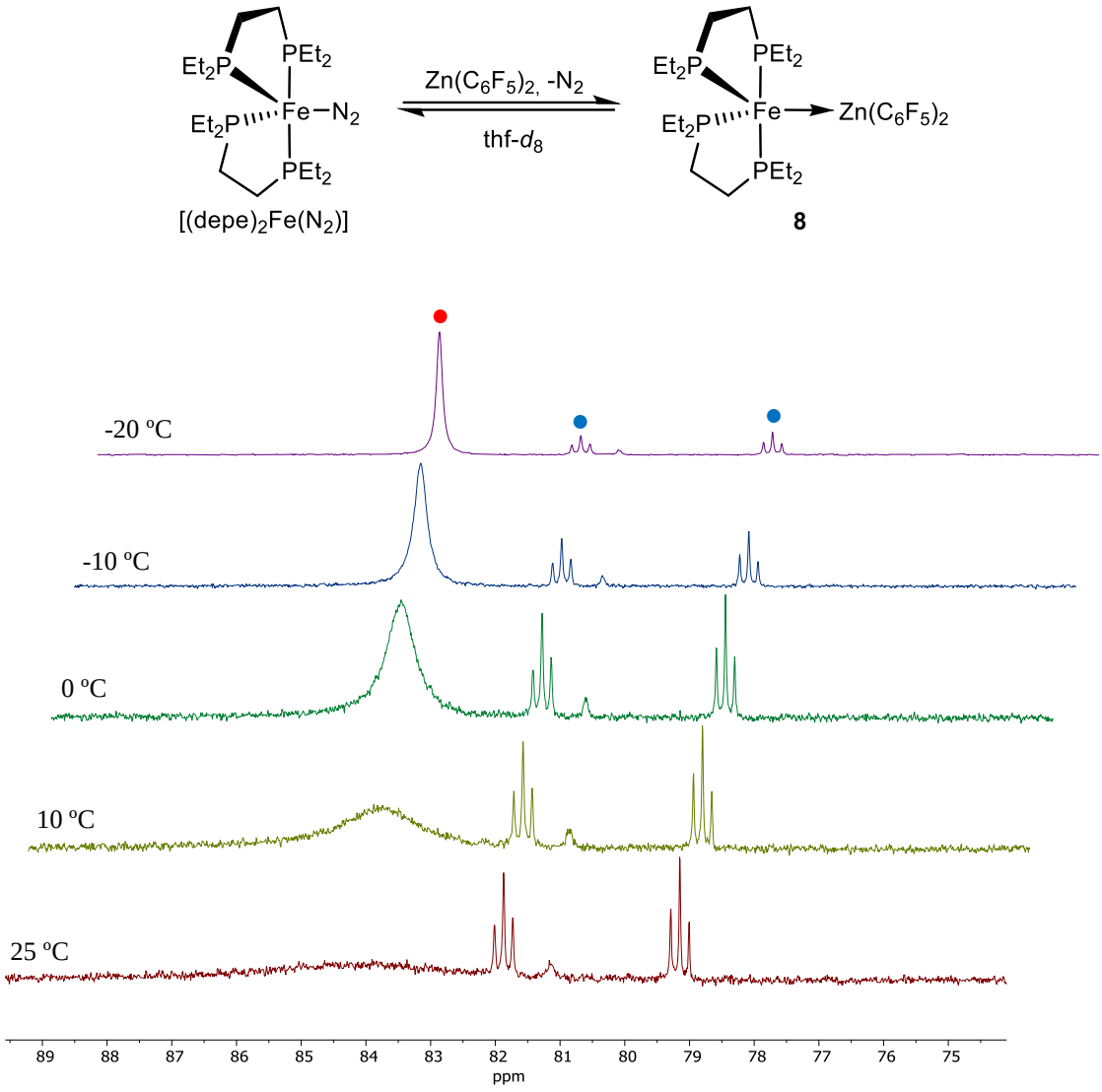
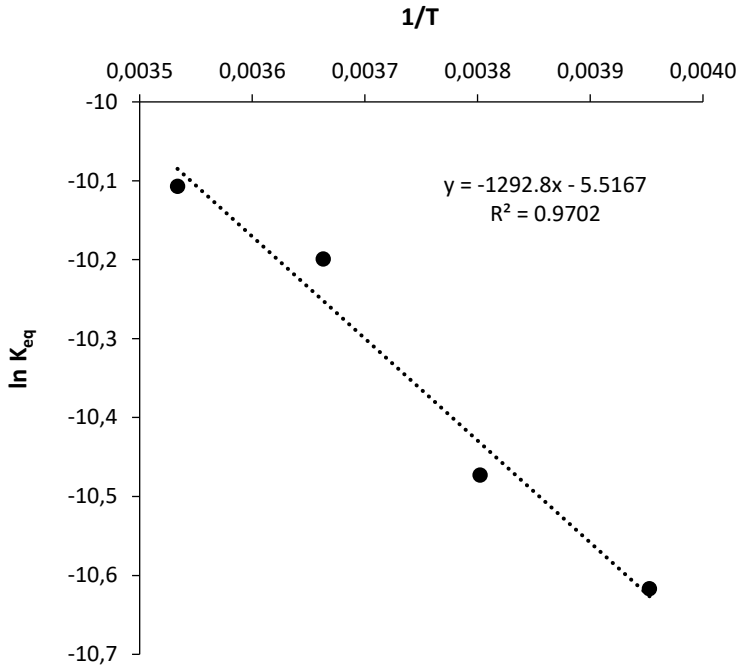


Figure S35. Van't Hoff plot for the equilibrium process over the temperature range -20 ºC to 25 ºC.



ΔH^0 = **2.6** kcal·mol^{-1}; ΔS^0 = **-11.0** cal·mol^{-1}·K^{-1}

6. Crystal structure determinations

Single crystals of suitable size, coated with dry perfluoropolyether or FOMBLIN oil were mounted on a glass fiber and fixed in a cold nitrogen stream [T = 193 K] to the goniometer head. Data collection was performed on a Bruker D8 Quest APEX-III CCD area detector PhotonIII using monochromatic radiation λ (Mo Kα1) = 0.71073 Å by a IμS 3.0 microfocus X-ray source. Data collections were processed with APEX-W2D-NT (Bruker, 2004), cell refinement and data reduction with SAINT-Plus (Bruker, 2004) and the absorption was corrected by multiscan method applied by SADABS.[7] The space-group assignment was based upon systematic absences, E statistics, and successful refinement of the structure. The structure was solved by direct methods and expanded through successive difference Fourier maps, F^2 (SHELXTL).[8] In the last cycles of refinement, ordered non-hydrogen atoms were refined anisotropically. Hydrogen atoms connected to carbon atoms were included in idealized positions and a riding model was used for their refinement.

	2	**3**	**6**
Formula	$C_{39}H_{48}BF_{15}FeO_2P_4$	$C_{54}H_{63}AlF_{15}FeO_2P_4$	$C_{138}H_{117}Au_3F_{18}Fe_3N_9O_{12}P_{15}S_6$
fw	1024.31	1235.75	3911.24
Crystal size, mm	0.1x0.1x0.1	0.08x0.04x0.03	0.08x0.01x0.01
Crystal system	monoclinic	triclinic	orthorhombic
Space group	C 1 c 1	P -1	P n m a
a, Å	14.7572(5)	11.580(2)	19.1095(5)
b, Å	14.9776(5)	12.520(2)	62.9956(16)
c, Å	20.2694(7)	21.393(4)	13.9182(4)
α, deg	90	73.425(4)	90
β, deg	102.6370(10)	86.006(5)	90
γ, deg	90	73.472(4)	90
V, Å^3	4371.6(3)	2849.6(9)	16754.9(8)
T, K	193.0	193.0	193.0
Z	4	2	4
ρcalc, g·cm^{-3}	1.556	1.440	1.551
μ, mm^{-1} (Mo1Kα)	0.590	0.481	3.163
F (000)	2096	1.440	7848
Absoption correction	multi-scan 0.6956-0.7456	multi-scan 0.6352-0.7453	multi-scan 0.6371-0.7454
θ range, deg	2.059-27.898	1.987-25.790	1.839-26.376
No. of rflns measd	10319	10897	17297
Rint	0.0489	0.2019	0.0759
No. of rlfns unique	10319	10897	17297
No. of params/restraints	567/2	702/8	981/148
R1 (I > 2σ(I))	0.0326	0.1065	0.0746
R1 (all data)	0.0428	0.1675	0.1040
wR2 (I > 2σ(I))	0.0675	0.2779	0.1742
wR2 (all data)	0.0727	0.3129	0.1901
Diff. Fourier peaks min/max, eÅ^{-3}	-0.267/0.287	-0.717/1.125	-2.896/1.735
CCDC number	2172177	2172178	2172179

	8	**7**
Formula	$C_{32}H_{48}F_{10}FeP_4Zn$	$C_{33}H_{48}F_{10}Fe\ N_2O_2P_4Zn$, C_6H_6
fw	867.80	1017.94
Crystal size, mm	0.1x0.1x0.1	0.1x0.1x0.1
Crystal system	monoclinic	monoclinic
Space group	C 1 2/c 1	P 1 21 1
a, Å	17.5085(16)	13.453(3)
b, Å	11.3314(16)	10.7351(19)
c, Å	20.086(3)	17.039(3)
α, deg	90	90
β, deg	111.281(6)	110.225(7)
γ, deg	90	90
V, $Å^3$	3713.2(8)	2309.1(8)
T, K	193.0	193.0
Z	4	2
ρcalc, $g \cdot cm^{-3}$	1.552	1.464
μ, mm^{-1} (Mo1Kα)	1.282	1.047
F (000)	1784	1048
Absoption correction	multi-scan 0.6694-0.7454	multi-scan 0.5387-0.7455
θ range, deg	2.176-25.350	2.285-25.654
No. of rflns measd	3417	8426
Rint	0.1746	0.1381
No. of rlfns unique	3417	8426
No. of params/restraints	222/0	541/1
R1 (I > 2σ(I))	0.0418	0.0916
R1 (all data)	0.0812	0.1754
wR2 (I > 2σ(I))	0.0829	0.1753
wR2 (all data)	0.1044	0.2193
Diff. Fourier peaks min/max, $eÅ^{-3}$	-0.489/0.810	-0.868/1.660
CCDC number	2172176	2172175

Figure S36. ORTEP structure of complex **8**. Hydrogen atoms have been excluded for clarity. Thermal ellipsoids are set at 50% probability. Selected bond distances (Å) and angles (º): Zn1–Fe1, 2.5607(12); Fe1–P1, 2.2426(11); Fe1–P2, 2.2426(12); Fe1–Zn1–C1, 129.88(12); C1–Zn1–C1, 100.2(2); P1–Fe1–Zn1, 89.87(4); P2–Fe1–Zn1, 125.79(3).

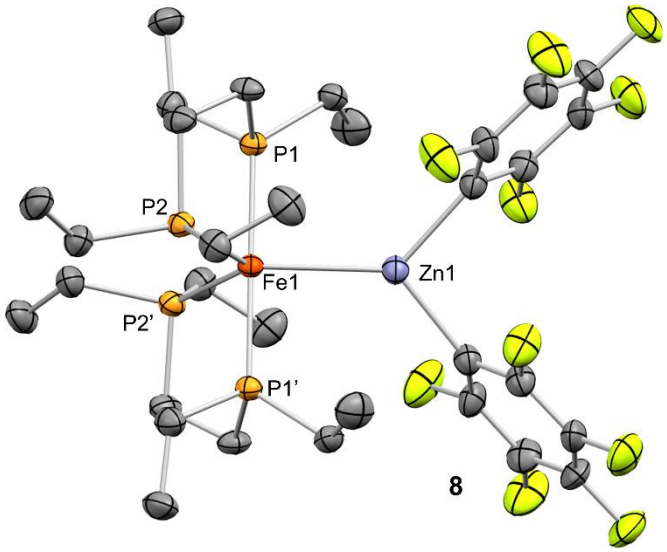


Figure S37. ORTEP structure of complex **2**. Hydrogen atoms have been excluded for clarity. Thermal ellipsoids are set at 50% probability. Selected bond distances (Å) and angles (º): Fe1–O2, 2.121(2); Fe1–C21, 1.861(3); C21–O2, 1.249(4); C21–O1, 1.305(4); O1–B1, 1.531(4); C21–Fe1–O2, 35.81(11); C21–O1–B1, 126.8(3); C21–O2–Fe1, 60.64(17).

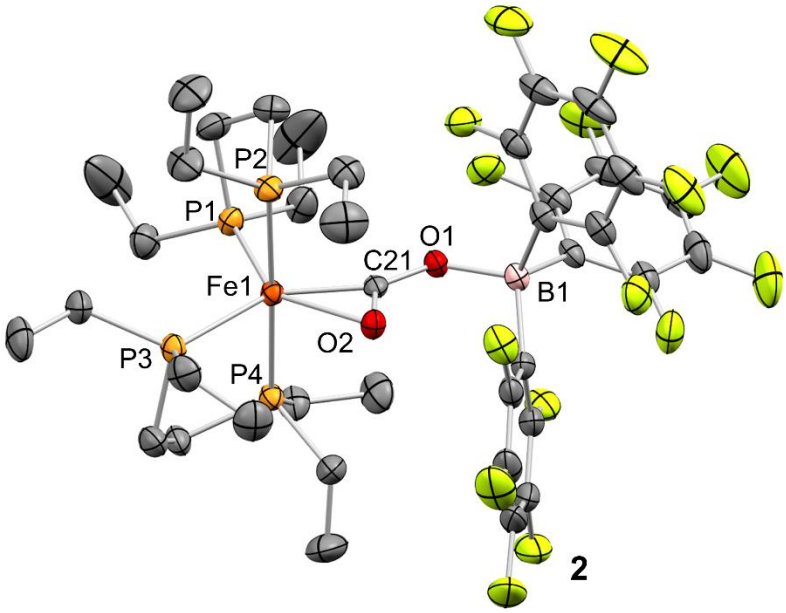


Figure S38. ORTEP structure of complex **3**. Hydrogen atoms have been excluded for clarity. Thermal ellipsoids are set at 50% probability. Selected bond distances (Å) and angles (º): Fe1–O1, 2.007(6); Fe1–C21, 1.724(10); C21–O2, 1.164(11); Al1–O1, 1.685(6); O2–C21–Fe1, 176.5(11); C21–Fe1–O1, 176.9(4); Fe1–O1–Al1, 171.9(4).

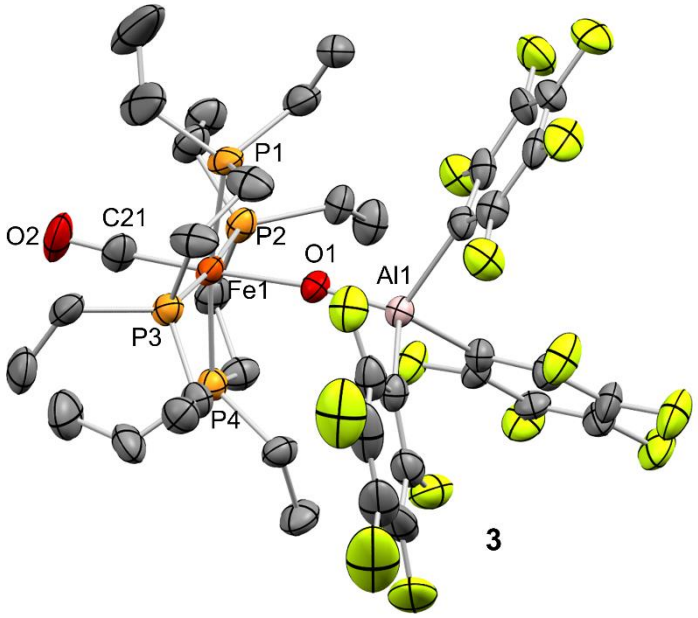


Figure S39. ORTEP structure of complex **6**. Hydrogen atoms have been excluded for clarity. Thermal ellipsoids are set at 50% probability. Selected bond distances (Å) and angles (º): N1–N2, 1.121(13); N1–Fe1, 1.827(10); Fe1–Au1, 2.5299(14); N2–N1–Fe1, 176.7(11); N1–Fe1–Au1, 178.0(4); Fe1–Au1–P1, 165.24(7).

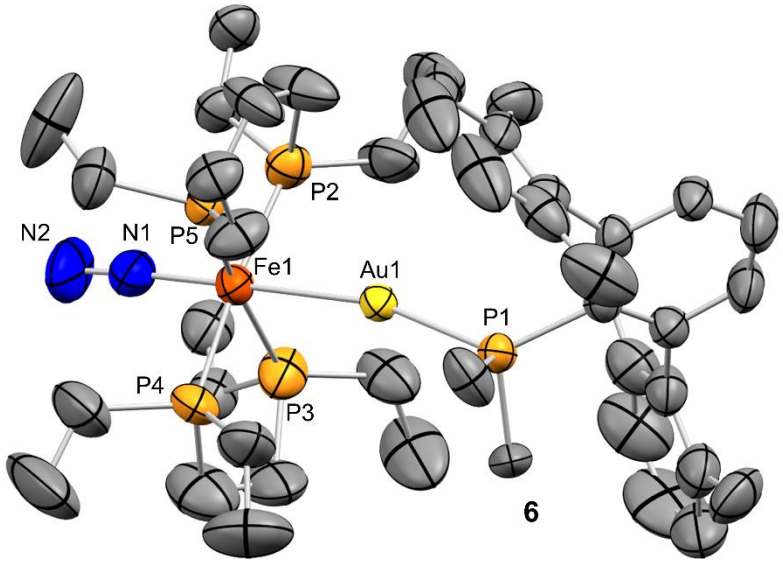
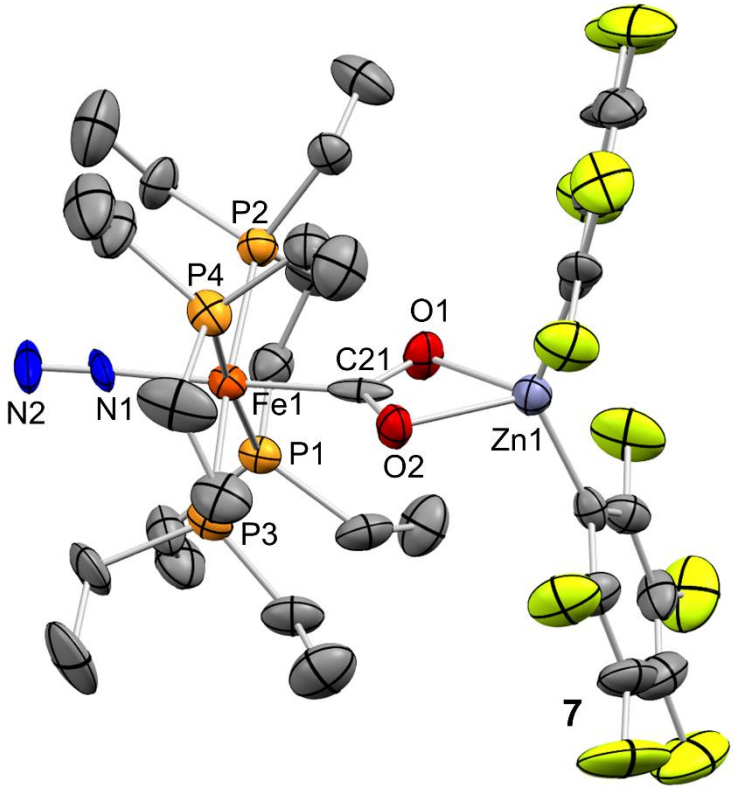


Figure S40. ORTEP structure of complex **7**. Hydrogen atoms have been excluded for clarity. Thermal ellipsoids are set at 50% probability. Selected bond distances (Å) and angles (º): N2–N1, 1.066(16); N1–Fe1, 1.862(14); Fe1–C21, 1.93(2); C21–O1, 1.27(2); C21–O2, 1.31(2); O1–Zn1, 2.106(10); O2–Zn1, 2.072(10); N2–N1–Fe1, 175.7(19); N1–Fe1–C21, 177.0(8); Fe1–C21–O1, 124.5(14); Fe1–C21–O2, 121.7(13); C21–O1–Zn1, 91.8(11); C21–O2–Zn1, 92.1(10); O1–Zn1–O2, 62.2(5).



7. Computational details

Geometry optimizations of the complexes were performed using the Gaussian09[9] suite of programs at the BP86[10]/def2-SVP[11] level of theory using the D3 dispersion correction suggested by Grimme et al.[12] Reactants and adducts were characterized by frequency calculations, and have positive definite Hessian matrices. Transition states (TS's) show only one negative eigenvalue in their diagonalized force constant matrices, and their associated eigenvectors were confirmed to correspond to the motion along the reaction coordinate under consideration using the Intrinsic Reaction Coordinate (IRC) method.[13] Energy refinements were carried out through single-point calculations at the same DFT level using the much larger triple-ζ basis-set def2-TZVPP[3] and including solvent effects (solvent = toluene) with the Polarization Continuum Model (PCM) method.[14] This level is denoted PCM(toluene)-BP86–D3/def2-TZVPP//BP86–D3/def2-SVP.
The interaction between the selected fragments in complexes $Fe(depe)_2(N_2)$ and **6+** has been investigated with the Energy Decomposition Analysis (EDA)[15] in combination with Natural Orbitals for Chemical Valence (NOCV)[16] method. Within this approach, the interaction energy can be decomposed into the following physically meaningful terms:

$$\Delta E_{int} = \Delta E_{elstat} + \Delta E_{Pauli} + \Delta E_{orb} + \Delta E_{disp}$$

The term ΔE_{elstat} corresponds to the classical electrostatic interaction between the unperturbed charge distributions of the deformed reactants and is usually attractive. The Pauli repulsion ΔE_{Pauli} comprises the destabilizing interactions between occupied orbitals and is responsible for any steric repulsion. The orbital interaction ΔE_{orb} accounts for charge transfer (interaction between occupied orbitals on one moiety with unoccupied orbitals on the other, including HOMO–LUMO interactions) and polarization (empty-occupied orbital mixing on one fragment due to the presence of another fragment). Finally, the ΔE_{disp} term takes into account the interactions which are due to dispersion forces.

The EDA-NOCV calculations were carried out using the BP86-D3/def2-TZVPP optimized geometries with the program package ADF 2020[17] using the same functional (BP86-D3) in conjunction with a triple-ζ-quality basis set using uncontracted Slater-type orbitals (STOs) augmented by two sets of polarization function with a frozen-core approximation for the core electrons.[18] An auxiliary set of s, p, d, f, and g STOs were used to fit the molecular densities and to represent the Coulomb and exchange potentials accurately in each SCF cycle.[19] Scalar relativistic effects were incorporated by applying the zeroth-order regular approximation (ZORA).[20] This level of theory is denoted ZORA-BP86-D3/TZ2P//BP86-D3/def2-SVP.

Table S1. EDA-NOCV results (in kcal/mol, ZORA-BP86-D3/TZ2P//BP86-D3/def2-SVP level) for complexes $Fe(depe)_2$-(N_2) and **6+**.

	$Fe(depe)_2$-(N_2)	$[(N_2)$-$Fe(depe)_2(Au)]^+$	$[(N_2)Fe(depe)_2$-$(Au)]^+$
	Fe-N_2 bond		(N_2)Fe-(Au+) bond
DE_{int}	-56.5	-40.9	-120.4
DE_{Pauli}	154.9	140.7	191.3
DE_{elstat}	-92.1	-83.1	-175.0
DE_{orb}	-109.6	-92.1	-100.0
$DE_{orb}(r_1)$	-42.8	-28.2	-68.4
$DE_{orb}(r_2)$	-27.2	-27.2	
$DE_{orb}(r_3)$	-26.9	-25.9	
DE_{disp}	-9.6	-6.4	-36.7
r(Fe···L) / Å[a]	1.766 (1.749)[a]	1.785 (1.834)	2.580 (2.530)
r (N-N) / Å[a]	1.154 (1.139)	1.143 (1.113)	

[a] Values within parenthesis refer to experimental values.

As stated in the main text, we performed additional calculations using $[Fe]^{2+}$ and $[Au]^{(-1)}$ as fragments, which is consistent with the relative electronegativies of iron and gold. The computed NBO-charges are not conclusive in that regard: q(Au) = -0.07 and q(Fe) = +0.27. Therefore, we computed the alternative EDA using the aforesaid fragmentation. Table S2 contains the corresponding EDA values:

Table S2. EDA-NOCV results (in kcal/mol, ZORA-BP86-D3/TZ2P//BP86-D3/def2-SVP level) for complex **6+**.

	$[(N_2)Fe(depe)_2$-$(Au)]^+$	
	$[Fe]^{(q=0)}$ and $[Au]^{(q=+1)}$	$[Fe]^{(q=+2)}$ and $[Au]^{(q=-1)}$
DE_{int}	-120.4	-267.5
DE_{Pauli}	191.3	212.7
DE_{elstat}	-175.0	-271.6
DE_{orb}	-100.0	-171.8
DE_{disp}	-36.7	-36.7

From the data in the above table, it can be concluded that the $[Fe]^{(q=0)}/Au^{(q=+1)}$ fragmentation better describes the bonding in $\mathbf{6}^+$ rather than the $[Fe]^{(q=+2)}/[Au]^{(q=-1)}$. This is based on the magnitude of the DE_{orb} term, which is lower in the former fragmentation scheme. According to the literature, the calculation that gives the smallest orbital term DE_{orb} and thus, the smallest change in the electronic structure of the fragments by the bond formation, indicates the more useful description of the bond.[21]

Cartesian coordinates (in Å) and total energies (in a. u., non corrected zero-point vibrational energy included) of all species discussed in the text (PCM(toluene)-BP86-D3/def2-TZVPP//BP86/def2-SVP level).

1: E= -3609.8000928

Fe	-0.033835000	-0.094335000	-0.358509000
P	-0.299042000	1.711525000	0.799487000
P	2.074835000	0.572011000	-0.649869000
P	0.366566000	-1.717855000	1.100565000
P	-2.141366000	-0.721236000	-0.201423000
O	-0.670724000	1.435908000	-2.872037000
O	-0.030720000	-0.731102000	-2.351613000
C	-1.128963000	3.111647000	-0.148377000
H	-1.000095000	2.819304000	-1.213352000
H	-2.215723000	3.015488000	0.062854000
C	-0.659355000	4.556292000	0.067837000
H	-0.751856000	4.901342000	1.117483000
H	-1.259162000	5.248322000	-0.561423000
H	0.399966000	4.692417000	-0.234431000
C	-1.170002000	1.737339000	2.464799000
H	-2.138816000	1.214713000	2.313252000
H	-0.565841000	1.063943000	3.109409000
C	-1.402655000	3.085597000	3.156184000
H	-1.868456000	2.941290000	4.154636000
H	-2.083225000	3.734889000	2.568668000
H	-0.456018000	3.643391000	3.312547000
C	2.262240000	2.315996000	0.019468000
H	3.324855000	2.570306000	0.216678000
H	1.905384000	2.985997000	-0.792901000
C	2.709367000	0.777844000	-2.395087000
H	1.911301000	1.340441000	-2.924092000
H	3.602363000	1.439627000	-2.346940000
C	3.017831000	-0.535360000	-3.124043000
H	3.803386000	-1.129886000	-2.610454000
H	3.380936000	-0.331589000	-4.153366000
H	2.099421000	-1.150151000	-3.200381000

C	3.508015000	-0.330784000	0.161594000
H	3.253310000	-0.397911000	1.240757000
H	3.443303000	-1.368241000	-0.228221000
C	4.923761000	0.223928000	-0.033161000
H	5.666796000	-0.394940000	0.513689000
H	5.024353000	1.262559000	0.345319000
H	5.222429000	0.227730000	-1.101291000
C	-1.229838000	-2.634116000	1.559138000
H	-1.322444000	-3.491882000	0.858349000
H	-1.163061000	-3.060031000	2.583180000
C	-2.416408000	-1.682310000	1.388361000
H	-2.454035000	-0.935856000	2.210616000
H	-3.395033000	-2.208370000	1.379781000
C	-2.600249000	-1.958523000	-1.522167000
H	-2.470739000	-1.415670000	-2.480604000
H	-1.770940000	-2.696156000	-1.515544000
C	-3.971188000	-2.632136000	-1.423374000
H	-4.085118000	-3.222165000	-0.489425000
H	-4.122819000	-3.333792000	-2.271113000
H	-4.802625000	-1.897337000	-1.457649000
C	-3.604015000	0.440901000	-0.204501000
H	-4.503503000	-0.119451000	0.134633000
H	-3.396480000	1.197043000	0.582739000
C	-3.839725000	1.113922000	-1.563992000
H	-4.588980000	1.928599000	-1.478178000
H	-4.225358000	0.387994000	-2.309612000
H	-2.903267000	1.538197000	-1.979514000
C	1.428318000	-3.180484000	0.586749000
H	2.486569000	-2.889654000	0.755655000
H	1.227572000	-4.043939000	1.258254000
C	1.190300000	-3.529121000	-0.886437000
H	0.164373000	-3.923027000	-1.048031000
H	1.901597000	-4.302365000	-1.244878000
H	1.279967000	-2.623669000	-1.520659000
C	1.029349000	-1.320900000	2.817390000
H	1.798409000	-0.534273000	2.665578000

H	0.179848000	-0.808532000	3.318620000
C	1.568832000	-2.462745000	3.684801000
H	1.845913000	-2.098813000	4.697343000
H	2.474743000	-2.923825000	3.240769000
H	0.818886000	-3.270505000	3.820729000
C	-0.361629000	0.496551000	-2.133766000
C	1.371317000	2.446386000	1.256264000
H	1.287959000	3.492628000	1.616148000
H	1.764501000	1.833838000	2.097344000

$B(C_6F_5)_3$: E= -2209.252418

F	-3.582717000	3.181884000	-1.428942000
F	-2.209201000	-1.280915000	1.435591000
F	-4.769978000	-0.421059000	1.433252000
F	-5.470277000	1.806536000	0.001791000
F	-1.012554000	2.349910000	-1.432401000
F	-0.002343000	2.559084000	1.430229000
F	2.028067000	4.341345000	1.427206000
F	4.306794000	3.825503000	-0.001967000
F	2.536708000	-0.302269000	-1.434101000
F	4.547639000	1.501588000	-1.431197000
F	1.165395000	-5.638519000	-0.000718000
F	-0.956693000	-4.685892000	-1.446846000
F	-1.518123000	-2.042425000	-1.448649000
F	2.735735000	-3.923007000	1.445989000
F	2.202222000	-1.274042000	1.449881000
B	-0.000473000	0.001757000	0.000000000
C	-1.492174000	0.495178000	0.001175000
C	-1.901925000	1.647236000	-0.709954000
C	-3.231431000	2.097854000	-0.729787000
C	-4.204581000	1.389466000	0.001837000
C	-3.843173000	0.241520000	0.733694000
C	-2.506378000	-0.187220000	0.712929000
C	1.174016000	1.045237000	-0.001230000
C	1.093268000	2.265868000	0.708914000
C	2.135529000	3.206244000	0.729111000
C	3.310119000	2.940908000	-0.001673000

C	3.433794000	1.743030000	-0.732335000
C	2.376115000	0.819969000	-0.711960000
C	0.317019000	-1.537131000	0.000534000
C	1.408736000	-2.076680000	0.719698000
C	1.704454000	-3.448997000	0.739444000
C	0.895421000	-4.333464000	-0.000330000
C	-0.198113000	-3.842015000	-0.739835000
C	-0.471313000	-2.465055000	-0.718908000

Al(C_6F_5)$_3$: E= -2426.8700527

Al	-0.016909000	-0.001747000	0.002006000
F	2.778577000	-0.691119000	1.259143000
F	4.182930000	-3.030815000	1.289087000
F	-0.739543000	-2.843435000	-1.128398000
F	0.661549000	-5.185557000	-1.069978000
F	3.118799000	-5.271106000	0.132233000
F	3.068856000	5.296701000	-0.130513000
F	0.625866000	5.181518000	1.097924000
F	-0.753040000	2.825722000	1.157789000
F	4.140820000	3.073133000	-1.312153000
F	2.757995000	0.719956000	-1.280259000
F	-4.783205000	0.566407000	-2.312504000
F	-4.790531000	-0.599085000	2.300593000
F	-2.038293000	-0.586769000	2.302334000
F	-6.143273000	-0.019831000	-0.008939000
F	-2.030600000	0.568218000	-2.301543000
C	0.975496000	-1.689235000	0.059738000
C	2.241425000	-1.778275000	0.666448000
C	2.982891000	-2.971213000	0.701985000
C	2.434055000	-4.126805000	0.109003000
C	1.167223000	-4.082536000	-0.507468000
C	0.464605000	-2.864752000	-0.518781000
C	0.959718000	1.694899000	-0.055491000
C	2.217882000	1.799058000	-0.675479000
C	2.947948000	2.998948000	-0.712216000
C	2.394974000	4.145957000	-0.106495000

C	1.135440000	4.086436000	0.523510000
C	0.444258000	2.862123000	0.535326000
C	-1.977143000	-0.009048000	0.000473000
C	-2.703067000	0.283254000	-1.159820000
C	-4.107938000	0.286881000	-1.192165000
C	-4.808213000	-0.016424000	-0.005980000
C	-4.111648000	-0.316109000	1.183303000
C	-2.706627000	-0.305281000	1.157538000

2-Al: E= -6036.7691607

Fe	2.318912000	-0.281921000	0.381120000
P	2.359104000	-0.142882000	2.547397000
P	2.512625000	1.950478000	0.357276000
P	4.380376000	-0.748281000	-0.352990000
P	2.013253000	-2.485930000	0.291857000
O	-0.647705000	0.031271000	0.548971000
F	-4.389701000	-1.586215000	4.385363000
F	-5.228722000	-0.138367000	-0.835006000
F	-7.327700000	-1.017208000	0.682658000
F	-6.906510000	-1.741695000	3.297979000
F	-2.310297000	-0.716425000	2.889919000
F	-3.005307000	-2.784346000	-0.838698000
F	-2.072432000	-4.500968000	-2.713819000
F	-0.534306000	-3.575542000	-4.784116000
F	-0.902572000	0.837307000	-3.139757000
F	0.047517000	-0.896624000	-4.982143000
F	-1.513713000	6.323165000	-1.131869000
F	-0.856103000	5.133424000	1.257975000
F	-1.425942000	2.515398000	1.671027000
F	-2.703323000	4.859310000	-3.120525000
F	-3.229874000	2.214767000	-2.735809000
O	0.860834000	-0.051933000	-1.181532000
C	0.733672000	-0.578459000	3.379195000
H	-0.001151000	-0.595617000	2.555691000
H	0.838733000	-1.624781000	3.738102000
C	0.197526000	0.325884000	4.494440000

H	0.880338000	0.408006000	5.365099000
H	-0.770211000	-0.079071000	4.855023000
H	-0.012380000	1.347707000	4.117546000
C	3.615891000	-1.074115000	3.572407000
H	3.513210000	-2.140009000	3.271203000
H	4.607377000	-0.744096000	3.195889000
C	3.532834000	-0.928048000	5.097121000
H	4.345850000	-1.499329000	5.593119000
H	2.571175000	-1.310797000	5.495401000
H	3.630787000	0.130543000	5.415016000
C	1.996134000	2.555950000	2.045858000
H	2.252217000	3.625866000	2.193113000
H	0.888989000	2.473500000	2.082284000
C	1.397504000	2.892685000	-0.794122000
H	0.381404000	2.489220000	-0.622959000
H	1.380749000	3.944469000	-0.434827000
C	1.741393000	2.797832000	-2.284604000
H	2.803283000	3.044964000	-2.498076000
H	1.111591000	3.504424000	-2.863271000
H	1.528484000	1.781679000	-2.666424000
C	4.158735000	2.821641000	0.139770000
H	4.794277000	2.459499000	0.976252000
H	4.619008000	2.414570000	-0.784221000
C	4.137958000	4.354658000	0.095431000
H	5.171613000	4.757892000	0.052638000
H	3.651217000	4.794193000	0.990662000
H	3.599366000	4.732814000	-0.796807000
C	4.607626000	-2.610481000	-0.603930000
H	4.346346000	-2.832600000	-1.660361000
H	5.671858000	-2.896370000	-0.467198000
C	3.666884000	-3.361872000	0.340853000
H	4.027513000	-3.316506000	1.391583000
H	3.561566000	-4.435743000	0.076407000
C	1.312109000	-2.945417000	-1.369713000
H	0.312200000	-2.469083000	-1.384064000
H	1.893086000	-2.361577000	-2.110769000

C	1.229803000	-4.428186000	-1.735599000
H	2.229565000	-4.908472000	-1.784872000
H	0.756169000	-4.546272000	-2.731667000
H	0.609734000	-5.002452000	-1.017030000
C	0.979752000	-3.502415000	1.461596000
H	1.238444000	-4.569085000	1.280955000
H	1.336463000	-3.265130000	2.486273000
C	-0.533184000	-3.276244000	1.334462000
H	-1.078929000	-3.881217000	2.087150000
H	-0.918953000	-3.570149000	0.338231000
H	-0.812545000	-2.218213000	1.494904000
C	4.836745000	-0.116955000	-2.055125000
H	5.069351000	0.962705000	-1.938839000
H	5.774715000	-0.609990000	-2.389607000
C	3.697468000	-0.311285000	-3.063127000
H	3.565000000	-1.379870000	-3.333966000
H	3.896338000	0.238868000	-4.005341000
H	2.737421000	0.045888000	-2.640728000
C	5.896259000	-0.355333000	0.684718000
H	5.713294000	0.635377000	1.149253000
H	5.844499000	-1.091181000	1.516719000
C	7.268987000	-0.395886000	0.003821000
H	8.081188000	-0.244902000	0.745930000
H	7.371490000	0.398906000	-0.762953000
H	7.459179000	-1.369098000	-0.496158000
C	0.531164000	-0.061308000	0.044021000
Al	-2.289750000	0.259847000	-0.298524000
C	-3.693881000	-0.396070000	0.961386000
C	-3.531712000	-0.775023000	2.297828000
C	-4.590580000	-1.231263000	3.104495000
C	-5.881408000	-1.312176000	2.549539000
C	-6.095504000	-0.940549000	1.207932000
C	-4.996819000	-0.491898000	0.454655000
C	-2.032360000	-0.887741000	-1.928474000
C	-2.309518000	-2.261427000	-1.881169000
C	-1.841851000	-3.181462000	-2.837156000

C	-1.046931000	-2.708064000	-3.895224000
C	-0.748034000	-1.337220000	-3.993084000
C	-1.256460000	-0.461868000	-3.017610000
C	-2.317929000	2.252065000	-0.534991000
C	-2.653513000	2.903863000	-1.729767000
C	-2.391695000	4.268889000	-1.956583000
C	-1.792212000	5.027284000	-0.932294000
C	-1.474399000	4.421619000	0.296814000
C	-1.772194000	3.060403000	0.471338000
C	2.666732000	1.638030000	3.073291000
H	2.309886000	1.827715000	4.105277000
H	3.769737000	1.785190000	3.080503000

2-B: E= -5819.114568

Fe	2.268390000	-0.043942000	0.325638000
P	2.457146000	0.827414000	2.302813000
P	2.341709000	2.061777000	-0.449957000
P	4.286129000	-0.658288000	-0.430165000
P	2.124994000	-2.157004000	1.015533000
O	-0.729329000	-0.006867000	0.558868000
F	-4.170229000	0.009720000	4.470291000
F	-4.802356000	-0.591135000	-0.925069000
F	-6.953881000	-0.775500000	0.692353000
F	-6.668564000	-0.473601000	3.416174000
F	-2.034178000	0.187520000	2.899824000
F	-2.766052000	-2.837291000	0.469478000
F	-2.080450000	-5.020388000	-0.902303000
F	-0.800418000	-4.809353000	-3.323133000
F	-0.991589000	-0.113151000	-3.057894000
F	-0.272784000	-2.313033000	-4.367701000
F	-2.520807000	5.364094000	-2.424467000
F	-1.432163000	4.922445000	0.074500000
F	-1.374875000	2.457618000	1.108675000
F	-3.513974000	3.245297000	-3.862342000
F	-3.410959000	0.752806000	-2.874649000
O	0.785442000	-0.413692000	-1.132127000

C	0.921351000	0.622909000	3.361591000
H	0.149391000	0.270818000	2.656765000
H	1.129917000	-0.220279000	4.054754000
C	0.370032000	1.830791000	4.125736000
H	1.082356000	2.245507000	4.868504000
H	-0.551299000	1.529049000	4.665152000
H	0.072873000	2.643145000	3.432328000
C	3.836448000	0.350777000	3.473590000
H	3.774734000	-0.756179000	3.565660000
H	4.780414000	0.559226000	2.925542000
C	3.847678000	1.012047000	4.857765000
H	4.722157000	0.670736000	5.451314000
H	2.937762000	0.763570000	5.441476000
H	3.908822000	2.117603000	4.786001000
C	1.889066000	3.188693000	0.965926000
H	2.093848000	4.253116000	0.726698000
H	0.795538000	3.084767000	1.120052000
C	1.159559000	2.513210000	-1.809422000
H	0.168501000	2.133995000	-1.494476000
H	1.087055000	3.622068000	-1.828335000
C	1.514073000	1.934334000	-3.183413000
H	2.536435000	2.212198000	-3.517446000
H	0.801569000	2.306681000	-3.947560000
H	1.431340000	0.831976000	-3.171596000
C	3.940033000	2.860130000	-1.023833000
H	4.608749000	2.836484000	-0.137008000
H	4.399700000	2.172724000	-1.762796000
C	3.849603000	4.280710000	-1.594343000
H	4.863536000	4.681136000	-1.805259000
H	3.359632000	4.984960000	-0.890519000
H	3.280162000	4.309259000	-2.545175000
C	4.642969000	-2.474965000	-0.041066000
H	4.327004000	-3.074411000	-0.920312000
H	5.733789000	-2.638321000	0.084922000
C	3.839934000	-2.883345000	1.195111000
H	4.276290000	-2.448177000	2.120468000

H	3.793708000	-3.984547000	1.334627000
C	1.334060000	-3.195274000	-0.310259000
H	0.309248000	-2.784691000	-0.394959000
H	1.817830000	-2.895661000	-1.260740000
C	1.306835000	-4.714768000	-0.137286000
H	2.324858000	-5.158231000	-0.130454000
H	0.745175000	-5.175972000	-0.976148000
H	0.794335000	-5.021356000	0.797496000
C	1.283002000	-2.763894000	2.562435000
H	1.624751000	-3.810890000	2.719873000
H	1.700976000	-2.172424000	3.404856000
C	-0.248882000	-2.685191000	2.535720000
H	-0.669292000	-3.052602000	3.494479000
H	-0.687280000	-3.304235000	1.728445000
H	-0.614048000	-1.652739000	2.385552000
C	4.505038000	-0.645513000	-2.292019000
H	4.545323000	0.422210000	-2.595974000
H	5.491937000	-1.087174000	-2.549030000
C	3.366725000	-1.361284000	-3.032271000
H	3.414892000	-2.461704000	-2.892323000
H	3.426522000	-1.173987000	-4.123783000
H	2.375202000	-1.020675000	-2.675306000
C	5.862914000	0.131270000	0.217661000
H	5.664782000	1.216727000	0.320695000
H	5.938924000	-0.260940000	1.255515000
C	7.164405000	-0.107416000	-0.556522000
H	8.032007000	0.312663000	-0.005199000
H	7.142245000	0.377652000	-1.553761000
H	7.368430000	-1.187628000	-0.714164000
C	0.451333000	-0.088105000	0.046117000
B	-2.090812000	-0.044055000	-0.214551000
C	-3.303016000	-0.199576000	0.886490000
C	-3.215526000	-0.048298000	2.279529000
C	-4.325411000	-0.139084000	3.142987000
C	-5.600500000	-0.384417000	2.610295000
C	-5.742846000	-0.537465000	1.219631000

C	-4.604867000	-0.435154000	0.401869000
C	-1.964247000	-1.334516000	-1.229933000
C	-2.219745000	-2.635721000	-0.753091000
C	-1.871031000	-3.808840000	-1.448017000
C	-1.211553000	-3.703533000	-2.681694000
C	-0.945614000	-2.429916000	-3.210007000
C	-1.335879000	-1.286885000	-2.490914000
C	-2.287512000	1.451271000	-0.876699000
C	-2.887480000	1.732990000	-2.119066000
C	-2.964280000	3.033439000	-2.656938000
C	-2.468173000	4.123127000	-1.919975000
C	-1.921849000	3.896636000	-0.646222000
C	-1.881098000	2.585320000	-0.145083000
C	2.676546000	2.693771000	2.183589000
H	2.367072000	3.199442000	3.119746000
H	3.766392000	2.879840000	2.058806000

TS1: E= -6036.7412422 (i = -272 cm-1)

Fe	2.475743000	-0.067811000	0.114810000
P	2.990845000	1.648362000	1.303684000
P	2.258627000	1.334346000	-1.647364000
P	4.496049000	-0.745080000	-0.236216000
P	2.370015000	-1.603147000	1.719135000
O	-0.256275000	-0.105586000	0.115646000
F	-2.768603000	1.549599000	4.901140000
F	-4.318942000	-2.161718000	1.164298000
F	-5.347169000	-2.259835000	3.673700000
F	-4.591945000	-0.407864000	5.547026000
F	-1.721469000	1.647277000	2.392057000
F	-1.729968000	-3.100949000	0.492557000
F	-1.598152000	-5.306023000	-1.097707000
F	-2.069217000	-5.076841000	-3.796974000
F	-2.810891000	-0.428248000	-3.310372000
F	-2.671161000	-2.631404000	-4.890036000
F	-4.004776000	5.332218000	-2.375609000
F	-1.549094000	5.186403000	-1.125619000

F	-0.686205000	2.843621000	-0.111054000
F	-5.563590000	3.086852000	-2.602511000
F	-4.692362000	0.714999000	-1.581761000
O	0.589795000	-1.739878000	-1.224554000
C	1.346922000	2.072621000	2.088520000
H	0.590127000	1.604635000	1.426634000
H	1.319720000	1.489985000	3.031431000
C	0.980894000	3.540257000	2.343349000
H	1.686728000	4.055038000	3.025726000
H	-0.027632000	3.570580000	2.803410000
H	0.915755000	4.122860000	1.403532000
C	4.215141000	1.737391000	2.710771000
H	3.833831000	1.007728000	3.457646000
H	5.163101000	1.305379000	2.327553000
C	4.468408000	3.101455000	3.366212000
H	5.214117000	3.007057000	4.183379000
H	3.545121000	3.524626000	3.808637000
H	4.866374000	3.840706000	2.641431000
C	2.420324000	3.085703000	-0.976148000
H	2.732205000	3.778307000	-1.784494000
H	1.393674000	3.379306000	-0.677575000
C	0.674344000	1.446057000	-2.623736000
H	-0.118062000	1.409833000	-1.856528000
H	0.625886000	2.458728000	-3.080683000
C	0.454110000	0.342009000	-3.667212000
H	1.150191000	0.426196000	-4.527740000
H	-0.581166000	0.401571000	-4.059038000
H	0.565258000	-0.663193000	-3.215551000
C	3.529353000	1.293348000	-3.024702000
H	4.528290000	1.318401000	-2.542205000
H	3.422659000	0.285800000	-3.478261000
C	3.426879000	2.379573000	-4.102418000
H	4.224159000	2.242990000	-4.863062000
H	3.548373000	3.399848000	-3.683593000
H	2.455433000	2.349097000	-4.635055000
C	5.011083000	-2.055204000	1.033626000

H	4.872396000	-3.042670000	0.543873000
H	6.092469000	-1.957129000	1.265993000
C	4.125135000	-1.955803000	2.275993000
H	4.422363000	-1.098406000	2.914783000
H	4.173080000	-2.868991000	2.905164000
C	1.712144000	-3.264939000	1.194936000
H	0.638654000	-3.097839000	0.968053000
H	2.165453000	-3.454418000	0.200966000
C	1.905557000	-4.442410000	2.153095000
H	2.976588000	-4.668623000	2.341365000
H	1.447540000	-5.358055000	1.724475000
H	1.418287000	-4.267307000	3.135004000
C	1.520724000	-1.317488000	3.351072000
H	1.800011000	-2.164343000	4.015754000
H	1.990341000	-0.411104000	3.790674000
C	0.003619000	-1.155782000	3.240662000
H	-0.450859000	-0.973034000	4.235977000
H	-0.484681000	-2.051593000	2.807097000
H	-0.252524000	-0.306428000	2.584360000
C	4.723460000	-1.714003000	-1.824647000
H	4.834133000	-0.973751000	-2.640745000
H	5.704724000	-2.229276000	-1.734712000
C	3.599707000	-2.707840000	-2.130167000
H	3.596609000	-3.547585000	-1.403303000
H	3.737505000	-3.153990000	-3.136538000
H	2.594140000	-2.239309000	-2.080624000
C	5.988229000	0.395328000	-0.273619000
H	5.657538000	1.297859000	-0.829696000
H	6.119947000	0.722612000	0.778772000
C	7.306736000	-0.146766000	-0.838581000
H	8.123375000	0.593539000	-0.704298000
H	7.233899000	-0.363840000	-1.923275000
H	7.623114000	-1.081190000	-0.329128000
C	0.739960000	-0.792263000	-0.445888000
Al	-2.087304000	-0.136561000	-0.124890000
C	-2.958100000	-0.266916000	1.684106000

C	-2.631343000	0.668375000	2.671964000
C	-3.145872000	0.646802000	3.977820000
C	-4.074419000	-0.357326000	4.311181000
C	-4.455247000	-1.310797000	3.348047000
C	-3.898905000	-1.238300000	2.055191000
C	-2.368199000	-1.700214000	-1.332533000
C	-2.049557000	-2.965872000	-0.828308000
C	-1.941317000	-4.115445000	-1.621484000
C	-2.167362000	-3.996536000	-3.006718000
C	-2.482033000	-2.743498000	-3.563588000
C	-2.575181000	-1.626284000	-2.712605000
C	-2.632050000	1.663001000	-0.858435000
C	-3.883250000	1.793669000	-1.478857000
C	-4.364289000	3.006415000	-2.006662000
C	-3.569767000	4.163463000	-1.884703000
C	-2.317560000	4.087358000	-1.247739000
C	-1.901145000	2.847444000	-0.736824000
C	3.375640000	3.129097000	0.223835000
H	3.273813000	4.073761000	0.797189000
H	4.437658000	3.043637000	-0.092614000

TS1-B: E= -5819.0823944 (i = -228 cm-1)

Fe	-2.328990000	-0.028563000	0.212009000
P	-3.028425000	-2.043246000	0.533401000
P	-2.222184000	-0.534007000	-1.997081000
P	-4.270725000	0.940795000	0.192325000
P	-2.180079000	0.692058000	2.317712000
O	0.453414000	0.044699000	0.235069000
F	2.865626000	-3.209144000	3.517271000
F	4.385529000	1.560095000	1.300614000
F	5.679188000	0.627064000	3.436551000
F	4.957967000	-1.760824000	4.592037000
F	1.588664000	-2.323796000	1.340992000
F	1.858256000	2.475406000	1.708672000
F	1.847137000	5.081522000	1.025969000
F	2.085757000	5.822711000	-1.616913000

F	2.394298000	1.291658000	-2.894730000
F	2.351964000	3.879323000	-3.554805000
F	3.928499000	-3.863978000	-3.840862000
F	1.351722000	-4.057357000	-2.834001000
F	0.425371000	-2.237576000	-1.142582000
F	5.515642000	-1.749440000	-3.081073000
F	4.573585000	0.114377000	-1.362384000
O	-0.480150000	2.016864000	-0.466563000
C	-1.430115000	-2.781063000	1.162997000
H	-0.643513000	-2.044847000	0.893391000
H	-1.508475000	-2.745041000	2.269488000
C	-1.002989000	-4.176466000	0.689965000
H	-1.744512000	-4.963776000	0.931507000
H	-0.045993000	-4.436384000	1.186887000
H	-0.805246000	-4.199770000	-0.398748000
C	-4.343122000	-2.721026000	1.673854000
H	-4.261289000	-2.121525000	2.606296000
H	-5.314069000	-2.440475000	1.213853000
C	-4.307001000	-4.222527000	1.988848000
H	-5.165654000	-4.505325000	2.633530000
H	-3.381692000	-4.506947000	2.529128000
H	-4.365707000	-4.840272000	1.069145000
C	-2.394104000	-2.401884000	-2.147166000
H	-2.711456000	-2.673806000	-3.174113000
H	-1.382234000	-2.821551000	-2.000151000
C	-0.727757000	-0.109926000	-3.033209000
H	0.147207000	-0.267487000	-2.378130000
H	-0.647472000	-0.856279000	-3.853364000
C	-0.707984000	1.328772000	-3.568826000
H	-1.477100000	1.511526000	-4.347639000
H	0.283587000	1.542283000	-4.014079000
H	-0.848048000	2.053227000	-2.742741000
C	-3.602879000	0.048018000	-3.127787000
H	-4.558197000	-0.151592000	-2.601719000
H	-3.490308000	1.150352000	-3.167329000
C	-3.641061000	-0.531110000	-4.546948000

H	-4.441773000	-0.040662000	-5.139581000
H	-3.855191000	-1.619452000	-4.551501000
H	-2.687086000	-0.374521000	-5.089861000
C	-4.708074000	1.664269000	1.884547000
H	-4.423884000	2.737650000	1.863228000
H	-5.806991000	1.618886000	2.037789000
C	-3.919031000	0.929291000	2.963059000
H	-4.328217000	-0.088106000	3.139874000
H	-3.917535000	1.463254000	3.935979000
C	-1.398203000	2.368727000	2.520618000
H	-0.331733000	2.224913000	2.251329000
H	-1.802723000	2.981845000	1.689610000
C	-1.540094000	3.064930000	3.876530000
H	-2.597541000	3.285702000	4.135393000
H	-0.996935000	4.032760000	3.863580000
H	-1.108171000	2.462360000	4.702988000
C	-1.431271000	-0.299987000	3.702112000
H	-1.714480000	0.199566000	4.654556000
H	-1.958832000	-1.278437000	3.694173000
C	0.080640000	-0.478596000	3.571001000
H	0.474419000	-1.181368000	4.333553000
H	0.623954000	0.481425000	3.678851000
H	0.331794000	-0.877631000	2.574150000
C	-4.463253000	2.478288000	-0.859531000
H	-4.582901000	2.145730000	-1.908365000
H	-5.433346000	2.932054000	-0.560842000
C	-3.317058000	3.485729000	-0.732110000
H	-3.294190000	3.951239000	0.276111000
H	-3.444831000	4.310333000	-1.463215000
H	-2.326723000	3.010469000	-0.890384000
C	-5.848057000	-0.017898000	-0.184719000
H	-5.591400000	-0.758693000	-0.970553000
H	-6.027344000	-0.607402000	0.739234000
C	-7.105099000	0.771343000	-0.569301000
H	-7.978778000	0.091758000	-0.657698000
H	-6.987461000	1.286902000	-1.543753000

H	-7.363251000	1.539663000	0.189606000
C	-0.575386000	0.856966000	-0.057585000
B	1.974027000	0.200932000	-0.080910000
C	2.832638000	-0.275697000	1.256564000
C	2.565385000	-1.524369000	1.846634000
C	3.230059000	-2.033160000	2.973469000
C	4.294155000	-1.299401000	3.522078000
C	4.649418000	-0.073556000	2.935573000
C	3.936099000	0.399888000	1.815106000
C	2.216239000	1.752902000	-0.541563000
C	2.072123000	2.784883000	0.401380000
C	2.027674000	4.145086000	0.076967000
C	2.133671000	4.525792000	-1.273460000
C	2.280089000	3.534824000	-2.256057000
C	2.323512000	2.182354000	-1.871237000
C	2.435991000	-0.924454000	-1.203736000
C	3.746837000	-0.889521000	-1.719739000
C	4.263633000	-1.847867000	-2.608254000
C	3.456921000	-2.935849000	-2.995485000
C	2.153569000	-3.030035000	-2.485636000
C	1.693215000	-2.043591000	-1.596226000
C	-3.371370000	-2.925717000	-1.086860000
H	-3.294277000	-4.026159000	-0.962373000
H	-4.426371000	-2.695479000	-1.356181000

INT1: E= -6036.7603105

Fe	2.150015000	0.046478000	-0.157078000
P	3.251331000	-1.476648000	1.097854000
P	2.129886000	1.290162000	1.737816000
P	3.530955000	1.273403000	-1.266539000
P	2.016883000	-1.278948000	-2.015682000
O	-0.207519000	0.153080000	-0.213167000
F	-1.733014000	-5.126355000	-1.199924000
F	-4.300390000	-0.404232000	-2.308319000
F	-4.850337000	-2.619939000	-3.778322000
F	-3.575411000	-4.984248000	-3.233992000

F	-1.150183000	-2.899657000	0.258214000
F	-2.160340000	1.206116000	-2.830768000
F	-2.548504000	3.737998000	-3.752425000
F	-3.104278000	5.765105000	-1.988949000
F	-2.934567000	2.722522000	1.626289000
F	-3.280374000	5.243933000	0.705696000
F	-2.947274000	-1.069037000	6.074044000
F	-0.490351000	-1.627835000	4.936794000
F	-0.102667000	-1.208055000	2.302035000
F	-4.974249000	-0.057097000	4.528887000
F	-4.568242000	0.389498000	1.867496000
O	0.362359000	1.965757000	-1.520092000
C	2.171801000	-2.984377000	1.435921000
H	1.170720000	-2.701448000	1.058526000
H	2.548711000	-3.778900000	0.757604000
C	2.053433000	-3.507542000	2.871035000
H	3.034478000	-3.776396000	3.313428000
H	1.422181000	-4.420929000	2.884725000
H	1.555769000	-2.771097000	3.532468000
C	4.905525000	-2.222557000	0.637605000
H	4.810018000	-2.568422000	-0.414232000
H	5.606776000	-1.361629000	0.605869000
C	5.449795000	-3.340711000	1.535016000
H	6.438325000	-3.692772000	1.171256000
H	4.774502000	-4.220615000	1.553269000
H	5.586107000	-3.000052000	2.582125000
C	2.497201000	0.163432000	3.193988000
H	2.731509000	0.761296000	4.098234000
H	1.567445000	-0.399374000	3.403589000
C	0.545522000	2.110891000	2.273660000
H	-0.244779000	1.357607000	2.090930000
H	0.604047000	2.247239000	3.375551000
C	0.200782000	3.426969000	1.564419000
H	0.963708000	4.213870000	1.741458000
H	-0.768270000	3.810002000	1.941139000
H	0.090380000	3.282780000	0.471297000

C	3.394927000	2.649690000	1.997464000
H	4.369632000	2.242860000	1.652550000
H	3.121317000	3.441204000	1.273973000
C	3.510487000	3.244300000	3.405503000
H	4.216129000	4.101518000	3.404958000
H	3.890820000	2.510530000	4.145239000
H	2.535202000	3.622723000	3.775303000
C	3.418734000	0.821532000	-3.083044000
H	2.471857000	1.278288000	-3.439195000
H	4.249731000	1.262963000	-3.669779000
C	3.347373000	-0.698663000	-3.191169000
H	4.296737000	-1.181006000	-2.869064000
H	3.135961000	-1.047696000	-4.223647000
C	0.439256000	-1.088689000	-2.996302000
H	-0.353242000	-1.505049000	-2.341300000
H	0.227521000	-0.001448000	-3.035161000
C	0.387888000	-1.705105000	-4.396823000
H	1.117842000	-1.236010000	-5.089300000
H	-0.619687000	-1.548515000	-4.835213000
H	0.578164000	-2.797947000	-4.394853000
C	2.306774000	-3.130950000	-2.097255000
H	2.665464000	-3.341441000	-3.128879000
H	3.166277000	-3.344975000	-1.428091000
C	1.109464000	-4.025067000	-1.762024000
H	1.406926000	-5.093818000	-1.765865000
H	0.293682000	-3.914010000	-2.503346000
H	0.674702000	-3.804260000	-0.771470000
C	3.265526000	3.134545000	-1.289071000
H	2.260261000	3.271483000	-0.845040000
H	4.014046000	3.565570000	-0.592758000
C	3.320086000	3.848042000	-2.644769000
H	4.278841000	3.688423000	-3.179042000
H	3.200180000	4.942082000	-2.497781000
H	2.492097000	3.518063000	-3.302216000
C	5.365724000	1.088930000	-0.934434000
H	5.483019000	1.203944000	0.165469000

H	5.579426000	0.019393000	-1.145560000
C	6.334767000	2.005763000	-1.690118000
H	7.386621000	1.778365000	-1.416043000
H	6.158511000	3.076084000	-1.457826000
H	6.249610000	1.883547000	-2.789697000
C	0.662825000	1.004008000	-0.817528000
Al	-2.025243000	0.047366000	0.034171000
C	-2.660713000	-1.550276000	-1.005216000
C	-2.070287000	-2.792181000	-0.743180000
C	-2.348386000	-3.960344000	-1.471334000
C	-3.289890000	-3.890055000	-2.515317000
C	-3.937379000	-2.671630000	-2.796490000
C	-3.622624000	-1.534575000	-2.025537000
C	-2.618170000	1.848290000	-0.578867000
C	-2.501965000	2.169051000	-1.938687000
C	-2.676655000	3.467090000	-2.442796000
C	-2.951435000	4.511071000	-1.538352000
C	-3.059156000	4.240350000	-0.162181000
C	-2.889695000	2.916773000	0.281092000
C	-2.309785000	-0.347554000	1.986902000
C	-3.543255000	-0.095913000	2.602744000
C	-3.783037000	-0.320806000	3.971785000
C	-2.745823000	-0.846985000	4.768424000
C	-1.498461000	-1.135737000	4.185627000
C	-1.328767000	-0.899069000	2.812987000
C	3.632936000	-0.780847000	2.800657000
H	3.789072000	-1.582043000	3.550697000
H	4.594428000	-0.229423000	2.703067000

INT1-B: E= -5819.1016235

Fe	2.062091000	0.003853000	-0.170607000
P	3.198804000	-1.733093000	0.745852000
P	2.181154000	0.892326000	1.907416000
P	3.405753000	1.440217000	-1.073541000
P	1.910214000	-0.954437000	-2.237080000

O	-0.305179000	0.141098000	-0.208486000
F	-1.961261000	-4.430490000	-2.041261000
F	-4.446708000	0.429032000	-1.584416000
F	-5.482353000	-1.444804000	-3.182849000
F	-4.268197000	-3.895262000	-3.449068000
F	-0.895112000	-2.550133000	-0.425808000
F	-2.138072000	1.574438000	-2.466897000
F	-2.697560000	4.189504000	-2.791629000
F	-3.106376000	5.800588000	-0.600598000
F	-2.440982000	2.124769000	2.276253000
F	-2.948266000	4.720832000	1.933023000
F	-3.101249000	-2.380244000	5.197734000
F	-0.524435000	-2.539939000	4.196364000
F	0.085981000	-1.450211000	1.855792000
F	-5.025041000	-1.033272000	3.763256000
F	-4.400950000	0.123293000	1.399473000
O	0.321105000	2.172613000	-1.126048000
C	2.162606000	-3.306312000	0.793525000
H	1.163428000	-2.982318000	0.451189000
H	2.571869000	-3.964248000	-0.001853000
C	2.034772000	-4.065191000	2.117075000
H	3.014450000	-4.397628000	2.518574000
H	1.412908000	-4.973194000	1.969721000
H	1.523619000	-3.451780000	2.885441000
C	4.852174000	-2.326744000	0.104725000
H	4.726659000	-2.465363000	-0.991223000
H	5.530002000	-1.454822000	0.221171000
C	5.451039000	-3.578365000	0.757882000
H	6.437767000	-3.824322000	0.311730000
H	4.799102000	-4.466061000	0.624290000
H	5.605829000	-3.437534000	1.847537000
C	2.533649000	-0.480040000	3.143318000
H	2.839441000	-0.047286000	4.117767000
H	1.594180000	-1.037831000	3.312789000
C	0.683188000	1.740881000	2.613184000
H	-0.182450000	1.111866000	2.327396000

H	0.760726000	1.693356000	3.721303000
C	0.465142000	3.180361000	2.127601000
H	1.319255000	3.846539000	2.371219000
H	-0.438479000	3.605113000	2.607933000
H	0.296193000	3.210911000	1.033295000
C	3.576575000	2.060943000	2.368456000
H	4.510945000	1.529377000	2.088202000
H	3.503104000	2.928640000	1.688099000
C	3.642338000	2.545734000	3.822170000
H	4.495123000	3.244449000	3.954110000
H	3.789371000	1.715596000	4.542702000
H	2.723207000	3.090210000	4.119822000
C	3.284398000	1.307702000	-2.938219000
H	2.332218000	1.798745000	-3.224846000
H	4.109512000	1.854394000	-3.438335000
C	3.244085000	-0.175802000	-3.288949000
H	4.199800000	-0.684588000	-3.034319000
H	3.049391000	-0.359286000	-4.366261000
C	0.347147000	-0.551824000	-3.171845000
H	-0.463599000	-1.042051000	-2.597979000
H	0.167359000	0.531905000	-3.020709000
C	0.283249000	-0.921680000	-4.656871000
H	1.029891000	-0.366256000	-5.262222000
H	-0.717327000	-0.663166000	-5.061738000
H	0.440654000	-2.004950000	-4.838423000
C	2.202306000	-2.752027000	-2.694113000
H	2.529592000	-2.729815000	-3.756909000
H	3.088599000	-3.083325000	-2.112320000
C	1.038905000	-3.733121000	-2.531532000
H	1.347808000	-4.749720000	-2.852437000
H	0.166542000	-3.448735000	-3.151522000
H	0.677469000	-3.802325000	-1.492106000
C	3.118038000	3.275143000	-0.752822000
H	2.255679000	3.309646000	-0.061902000
H	4.008826000	3.650137000	-0.205653000
C	2.812595000	4.162330000	-1.963839000

H	3.618554000	4.145027000	-2.725698000
H	2.688338000	5.215503000	-1.634855000
H	1.859503000	3.849264000	-2.432762000
C	5.255549000	1.241417000	-0.830031000
H	5.414100000	1.206826000	0.268319000
H	5.483920000	0.219471000	-1.201700000
C	6.179828000	2.275561000	-1.484902000
H	7.243810000	2.044834000	-1.266232000
H	5.984628000	3.303494000	-1.115842000
H	6.069545000	2.291690000	-2.588941000
C	0.579274000	1.081170000	-0.624054000
B	-1.833446000	0.142207000	0.051166000
C	-2.554312000	-0.925505000	-0.991519000
C	-2.010446000	-2.215393000	-1.126375000
C	-2.548389000	-3.221902000	-1.944465000
C	-3.728909000	-2.956335000	-2.659161000
C	-4.342122000	-1.699627000	-2.523561000
C	-3.762372000	-0.724378000	-1.686086000
C	-2.329961000	1.693833000	-0.088059000
C	-2.391795000	2.302432000	-1.356018000
C	-2.666688000	3.661606000	-1.556330000
C	-2.864335000	4.491337000	-0.437446000
C	-2.801577000	3.936031000	0.849251000
C	-2.537345000	2.561388000	0.993405000
C	-2.119185000	-0.543546000	1.527033000
C	-3.420126000	-0.517424000	2.066852000
C	-3.772347000	-1.112435000	3.290508000
C	-2.792791000	-1.807715000	4.025876000
C	-1.490035000	-1.887619000	3.512077000
C	-1.196679000	-1.283840000	2.276481000
C	3.617490000	-1.383414000	2.548077000
H	3.747386000	-2.317412000	3.130260000
H	4.603730000	-0.867770000	2.538300000

TS2: E= -6036.7445342 (i = -162 cm-1)

Fe	-2.273377000	-0.030567000	0.253906000

P	-2.600212000	-1.871751000	1.587599000
P	-2.296841000	-1.546445000	-1.457440000
P	-4.246297000	0.823372000	-0.059671000
P	-2.090689000	1.419845000	1.989663000
O	0.081830000	0.033827000	0.257967000
F	3.480639000	-1.673474000	4.624507000
F	4.304802000	2.100157000	0.727414000
F	5.806952000	2.140223000	2.975617000
F	5.417307000	0.260431000	4.934952000
F	1.978095000	-1.731987000	2.367938000
F	1.795358000	3.180355000	0.707142000
F	1.355939000	5.443383000	-0.715471000
F	1.229855000	5.343976000	-3.462804000
F	1.928759000	0.666030000	-3.355588000
F	1.528033000	2.943206000	-4.767793000
F	3.863413000	-4.831195000	-3.291062000
F	1.677600000	-5.064487000	-1.619528000
F	0.827069000	-2.927533000	-0.205162000
F	5.148495000	-2.420654000	-3.538741000
F	4.277597000	-0.259053000	-2.134210000
O	-0.995929000	1.928124000	-1.528201000
C	-0.932222000	-2.308884000	2.278853000
H	-0.238325000	-1.765152000	1.601360000
H	-0.866448000	-1.787348000	3.255298000
C	-0.526296000	-3.778853000	2.417211000
H	-1.200567000	-4.362416000	3.076269000
H	0.495348000	-3.818360000	2.846437000
H	-0.470464000	-4.287459000	1.434950000
C	-3.805231000	-1.961056000	3.008104000
H	-3.673609000	-1.018421000	3.581418000
H	-4.814945000	-1.897549000	2.548375000
C	-3.702054000	-3.174758000	3.940381000
H	-4.492594000	-3.137428000	4.719022000
H	-2.724012000	-3.204505000	4.461583000
H	-3.821804000	-4.131396000	3.391691000
C	-2.235981000	-3.277504000	-0.750281000

H	-2.566126000	-4.014280000	-1.510392000
H	-1.165194000	-3.475076000	-0.548348000
C	-0.826461000	-1.473288000	-2.586861000
H	-0.019397000	-1.137740000	-1.905144000
H	-0.574004000	-2.507273000	-2.904944000
C	-0.961636000	-0.525304000	-3.784321000
H	-1.659703000	-0.911638000	-4.555414000
H	0.029695000	-0.380805000	-4.255124000
H	-1.305820000	0.481398000	-3.475777000
C	-3.746237000	-1.625594000	-2.637229000
H	-4.673610000	-1.606142000	-2.027407000
H	-3.714725000	-0.662923000	-3.187496000
C	-3.765395000	-2.805941000	-3.617225000
H	-4.566082000	-2.668611000	-4.373742000
H	-3.963162000	-3.769624000	-3.105209000
H	-2.806307000	-2.907797000	-4.164791000
C	-4.553993000	2.248459000	1.138770000
H	-4.142413000	3.163717000	0.665384000
H	-5.642854000	2.415105000	1.274405000
C	-3.817112000	1.964490000	2.451053000
H	-4.292624000	1.131540000	3.012837000
H	-3.791975000	2.849005000	3.122010000
C	-1.227878000	2.988998000	1.515305000
H	-0.239332000	2.639764000	1.158399000
H	-1.747770000	3.362353000	0.608893000
C	-1.078376000	4.091539000	2.564844000
H	-2.055464000	4.486681000	2.915452000
H	-0.511216000	4.936519000	2.122830000
H	-0.508204000	3.750647000	3.452727000
C	-1.311611000	0.985371000	3.616990000
H	-1.579607000	1.792827000	4.333840000
H	-1.816814000	0.065755000	3.980989000
C	0.203790000	0.785684000	3.504175000
H	0.621014000	0.336542000	4.428258000
H	0.735218000	1.740459000	3.319859000
H	0.437650000	0.126988000	2.649353000

C	-4.582548000	1.597811000	-1.735749000
H	-3.575466000	1.797932000	-2.156807000
H	-5.028655000	0.795422000	-2.357726000
C	-5.446677000	2.865401000	-1.795162000
H	-6.439656000	2.729152000	-1.323228000
H	-5.617871000	3.155214000	-2.852893000
H	-4.953078000	3.726740000	-1.302494000
C	-5.732477000	-0.266102000	0.281591000
H	-5.485944000	-1.257419000	-0.154343000
H	-5.708803000	-0.411082000	1.383049000
C	-7.114774000	0.207885000	-0.179325000
H	-7.895032000	-0.526371000	0.111668000
H	-7.165692000	0.322462000	-1.281358000
H	-7.395389000	1.180533000	0.275175000
C	-1.348728000	1.098179000	-0.773752000
Al	1.802070000	0.155319000	-0.152129000
C	3.022243000	0.223423000	1.477874000
C	2.906030000	-0.737469000	2.487777000
C	3.669873000	-0.745736000	3.666202000
C	4.659461000	0.241348000	3.827377000
C	4.849159000	1.209491000	2.824171000
C	4.041324000	1.168363000	1.669788000
C	1.940657000	1.833592000	-1.267288000
C	1.785252000	3.081018000	-0.656684000
C	1.542350000	4.272764000	-1.357061000
C	1.464904000	4.222902000	-2.761328000
C	1.625721000	2.993815000	-3.426422000
C	1.856117000	1.836283000	-2.662122000
C	2.484720000	-1.484885000	-1.151066000
C	3.603000000	-1.422576000	-1.994236000
C	4.080626000	-2.524044000	-2.730346000
C	3.427928000	-3.765795000	-2.601069000
C	2.316124000	-3.883203000	-1.747440000
C	1.901512000	-2.746870000	-1.034466000
C	-3.068409000	-3.343162000	0.532203000
H	-2.906205000	-4.291719000	1.084681000

H	-4.157054000	-3.262720000	0.317812000

TS2-B: E= -5819.0765391 (i = -96 cm-1)

Fe	2.053572000	-0.115779000	-0.135345000
P	2.582238000	-2.147343000	0.805040000
P	2.221888000	0.664464000	1.997140000
P	3.974970000	0.674098000	-0.862058000
P	1.806924000	-1.085154000	-2.221616000
O	-0.289457000	-0.225819000	-0.357435000
F	-3.086987000	-4.289564000	-1.664410000
F	-3.984965000	1.097468000	-2.015443000
F	-5.295766000	-0.559893000	-3.631699000
F	-4.883550000	-3.276797000	-3.509883000
F	-1.794312000	-2.656409000	-0.004887000
F	-1.502535000	1.682099000	-2.594974000
F	-1.605502000	4.314969000	-3.021183000
F	-1.914099000	6.063547000	-0.911873000
F	-2.127748000	2.449282000	2.098189000
F	-2.151314000	5.058175000	1.649633000
F	-4.005443000	-1.517091000	5.101110000
F	-1.325281000	-2.028306000	4.555695000
F	-0.245075000	-1.192506000	2.267995000
F	-5.509021000	-0.126960000	3.265712000
F	-4.396086000	0.732491000	0.954007000
O	0.973331000	2.414020000	-1.098123000
C	1.084141000	-3.245031000	0.811215000
H	0.272000000	-2.547645000	0.528132000
H	1.221344000	-3.937753000	-0.044190000
C	0.732985000	-4.022342000	2.082749000
H	1.525581000	-4.737485000	2.386125000
H	-0.195077000	-4.603789000	1.903289000
H	0.518054000	-3.344981000	2.931412000
C	3.960026000	-3.248153000	0.176470000
H	3.869793000	-3.283391000	-0.929574000
H	4.903254000	-2.703759000	0.388161000
C	4.017055000	-4.667229000	0.757048000

H	4.878402000	-5.226097000	0.334715000
H	3.100988000	-5.245933000	0.522018000
H	4.136173000	-4.659792000	1.859995000
C	2.373390000	-0.750039000	3.225063000
H	2.881346000	-0.388466000	4.141116000
H	1.348597000	-1.042746000	3.513447000
C	0.798291000	1.680892000	2.617253000
H	-0.094136000	1.229465000	2.145842000
H	0.705665000	1.510080000	3.711359000
C	0.866694000	3.177202000	2.287140000
H	1.706940000	3.695025000	2.793624000
H	-0.071493000	3.665840000	2.614424000
H	0.951983000	3.351007000	1.196519000
C	3.700341000	1.711036000	2.484402000
H	4.607269000	1.186971000	2.115377000
H	3.609724000	2.639616000	1.888476000
C	3.847268000	2.058181000	3.972331000
H	4.668465000	2.791318000	4.115616000
H	4.093160000	1.171324000	4.591232000
H	2.924347000	2.510687000	4.388666000
C	4.038645000	0.460227000	-2.722849000
H	3.409336000	1.266932000	-3.153511000
H	5.070335000	0.609264000	-3.102911000
C	3.458071000	-0.903963000	-3.084286000
H	4.109471000	-1.731910000	-2.728655000
H	3.338877000	-1.030664000	-4.180946000
C	0.612641000	-0.181050000	-3.301957000
H	-0.346626000	-0.291381000	-2.754874000
H	0.853642000	0.895286000	-3.198821000
C	0.520531000	-0.581759000	-4.775776000
H	1.476267000	-0.432812000	-5.322716000
H	-0.243319000	0.048017000	-5.277007000
H	0.211603000	-1.637560000	-4.916443000
C	1.451232000	-2.874341000	-2.636663000
H	1.822782000	-2.989048000	-3.679159000
H	2.119013000	-3.502147000	-2.010407000

C	-0.001884000	-3.341513000	-2.536297000
H	-0.096216000	-4.383389000	-2.905264000
H	-0.685483000	-2.713026000	-3.139790000
H	-0.374980000	-3.316026000	-1.500487000
C	4.303132000	2.515789000	-0.655330000
H	3.331358000	2.954818000	-0.354854000
H	4.979756000	2.613067000	0.216732000
C	4.874065000	3.285444000	-1.854116000
H	5.833424000	2.864403000	-2.216292000
H	5.062822000	4.340194000	-1.564321000
H	4.166440000	3.307581000	-2.706191000
C	5.585588000	-0.122166000	-0.335015000
H	5.512567000	-0.260062000	0.765634000
H	5.539622000	-1.142474000	-0.768986000
C	6.898621000	0.569801000	-0.718122000
H	7.768039000	-0.028579000	-0.373837000
H	6.989207000	1.575070000	-0.258705000
H	6.999124000	0.690562000	-1.816404000
C	1.259227000	1.350060000	-0.692071000
B	-1.640745000	0.238698000	-0.015422000
C	-2.671927000	-0.663609000	-1.023410000
C	-2.590557000	-2.063975000	-0.937768000
C	-3.288081000	-2.959769000	-1.764071000
C	-4.199695000	-2.450150000	-2.702248000
C	-4.391844000	-1.060437000	-2.771165000
C	-3.656774000	-0.207151000	-1.921745000
C	-1.838876000	1.886384000	-0.232752000
C	-1.719117000	2.464371000	-1.509215000
C	-1.756028000	3.841710000	-1.770180000
C	-1.905967000	4.737572000	-0.698351000
C	-2.038880000	4.221383000	0.598058000
C	-2.012505000	2.827310000	0.794831000
C	-2.262521000	-0.191166000	1.486968000
C	-3.612656000	0.042177000	1.811489000
C	-4.215891000	-0.386065000	3.006983000
C	-3.451206000	-1.100652000	3.951073000

C	-2.100423000	-1.356400000	3.672633000
C	-1.564029000	-0.905577000	2.455507000
C	3.125438000	-1.915113000	2.582985000
H	3.001400000	-2.855937000	3.158139000
H	4.216755000	-1.705410000	2.530437000

INT2: E= -6036.752685

Fe	-2.114614000	0.230605000	0.237059000
P	-2.306346000	-1.379230000	2.267248000
P	-2.205016000	-1.732363000	-0.912114000
P	-4.223388000	0.881328000	0.080786000
P	-1.751635000	2.043852000	1.533199000
O	0.060078000	-0.334499000	0.522249000
F	4.342526000	-0.825387000	4.615569000
F	4.545479000	1.077316000	-0.518992000
F	6.730874000	1.259136000	1.063496000
F	6.654900000	0.307936000	3.640569000
F	2.158317000	-1.009725000	3.056283000
F	2.539310000	2.989266000	0.522772000
F	2.303911000	5.268070000	-0.908049000
F	1.302072000	5.199221000	-3.466841000
F	0.678166000	0.529424000	-3.123168000
F	0.494093000	2.808764000	-4.559908000
F	2.160996000	-5.360645000	-3.333266000
F	1.375449000	-5.325689000	-0.692629000
F	1.442338000	-3.002802000	0.707085000
F	2.989489000	-3.048054000	-4.552416000
F	3.033596000	-0.713900000	-3.168143000
O	-1.733421000	1.790326000	-2.169644000
C	-0.645526000	-1.560520000	3.039006000
H	-0.009811000	-1.157342000	2.206924000
H	-0.596189000	-0.827365000	3.870307000
C	-0.168459000	-2.948736000	3.478457000
H	-0.822433000	-3.438261000	4.229603000
H	0.842142000	-2.841588000	3.920001000
H	-0.051330000	-3.630939000	2.613265000

C	-3.542323000	-1.253167000	3.660280000
H	-3.543034000	-0.186128000	3.978319000
H	-4.541050000	-1.441440000	3.215071000
C	-3.309787000	-2.174875000	4.864887000
H	-4.114834000	-2.039874000	5.617723000
H	-2.344534000	-1.960362000	5.365244000
H	-3.305976000	-3.243890000	4.568843000
C	-1.756373000	-3.122428000	0.230670000
H	-1.848191000	-4.095359000	-0.294516000
H	-0.685226000	-2.966324000	0.466773000
C	-1.038423000	-1.922666000	-2.332071000
H	-0.129587000	-1.395114000	-1.986897000
H	-0.765927000	-2.997234000	-2.410220000
C	-1.519850000	-1.359305000	-3.672277000
H	-2.378620000	-1.924557000	-4.091312000
H	-0.692482000	-1.409572000	-4.408090000
H	-1.801208000	-0.291234000	-3.591475000
C	-3.846316000	-2.293006000	-1.614810000
H	-4.614470000	-2.128754000	-0.828754000
H	-4.077231000	-1.569967000	-2.423723000
C	-3.905683000	-3.732095000	-2.142628000
H	-4.873782000	-3.922917000	-2.651358000
H	-3.812100000	-4.476740000	-1.326032000
H	-3.099741000	-3.937314000	-2.877012000
C	-4.325750000	2.647071000	0.715715000
H	-3.959504000	3.300071000	-0.104580000
H	-5.377885000	2.934846000	0.917307000
C	-3.422123000	2.781885000	1.946885000
H	-3.826775000	2.206954000	2.808884000
H	-3.314054000	3.837460000	2.274520000
C	-0.861856000	3.388222000	0.625447000
H	0.051468000	2.876406000	0.266044000
H	-1.450694000	3.589418000	-0.293536000
C	-0.517591000	4.684465000	1.361933000
H	-1.420099000	5.258381000	1.660727000
H	0.092794000	5.330645000	0.697669000

H	0.090119000	4.500922000	2.270342000
C	-0.907187000	1.985416000	3.181044000
H	-1.135149000	2.947857000	3.691437000
H	-1.419633000	1.190124000	3.763963000
C	0.598092000	1.722326000	3.078081000
H	1.045416000	1.574264000	4.081400000
H	1.135101000	2.552744000	2.579586000
H	0.776583000	0.816257000	2.473584000
C	-4.990952000	0.959250000	-1.631445000
H	-4.148018000	0.878655000	-2.346589000
H	-5.578786000	0.023531000	-1.736315000
C	-5.852000000	2.183206000	-1.973284000
H	-6.689719000	2.329324000	-1.262796000
H	-6.290450000	2.065070000	-2.986075000
H	-5.252063000	3.114853000	-1.987690000
C	-5.528997000	0.023628000	1.103131000
H	-5.368181000	-1.064161000	0.941472000
H	-5.230729000	0.221702000	2.152726000
C	-6.995713000	0.405702000	0.874694000
H	-7.652896000	-0.152996000	1.573436000
H	-7.334266000	0.168362000	-0.154287000
H	-7.176811000	1.486318000	1.049823000
C	-1.821459000	1.134076000	-1.199057000
Al	1.673918000	-0.060525000	-0.132277000
C	3.228156000	0.061660000	1.198428000
C	3.260616000	-0.423621000	2.509570000
C	4.382390000	-0.349816000	3.355790000
C	5.565150000	0.226107000	2.861056000
C	5.598744000	0.715083000	1.542250000
C	4.440157000	0.611403000	0.750519000
C	1.687841000	1.635090000	-1.263274000
C	2.089050000	2.879447000	-0.759256000
C	1.972790000	4.087189000	-1.469125000
C	1.440577000	4.059669000	-2.770893000
C	1.034396000	2.834776000	-3.329781000
C	1.164632000	1.666762000	-2.558872000

C	2.152271000	-1.740912000	-1.198629000
C	2.596563000	-1.818519000	-2.524673000
C	2.589350000	-3.015782000	-3.269228000
C	2.171051000	-4.207010000	-2.646160000
C	1.773234000	-4.186939000	-1.295668000
C	1.814153000	-2.963263000	-0.608956000
C	-2.618296000	-3.045586000	1.496081000
H	-2.366087000	-3.853130000	2.214016000
H	-3.703453000	-3.132392000	1.266440000

INT2-B: E= -5819.0822867

Fe	-1.859882000	0.059199000	0.193951000
P	-2.167168000	-1.570058000	1.927625000
P	-1.897979000	-1.799350000	-1.149627000
P	-4.059209000	0.566763000	-0.086941000
P	-1.801688000	1.770671000	1.687648000
O	0.186193000	-0.157283000	0.595502000
F	4.229458000	-0.947064000	4.285969000
F	4.150297000	1.024173000	-0.798358000
F	6.445223000	0.957830000	0.533723000
F	6.557335000	-0.039855000	3.104408000
F	1.939738000	-0.876059000	3.015556000
F	2.298548000	2.808835000	1.063708000
F	2.133695000	5.166274000	-0.159646000
F	1.228989000	5.349976000	-2.758367000
F	0.515116000	0.695457000	-2.842532000
F	0.428836000	3.055886000	-4.069153000
F	2.867368000	-4.707864000	-3.199484000
F	1.879351000	-4.858131000	-0.616575000
F	1.479430000	-2.637752000	0.800533000
F	3.407288000	-2.241193000	-4.287014000
F	2.944424000	-0.009464000	-2.925732000
O	-1.818395000	1.974561000	-1.980236000
C	-0.594344000	-1.762068000	2.849206000
H	0.096694000	-1.282270000	2.114718000
H	-0.639968000	-1.069420000	3.713370000
C	-0.105468000	-3.148413000	3.274392000

H	-0.781352000	-3.668892000	3.984192000
H	0.881142000	-3.026336000	3.764934000
H	0.067450000	-3.810440000	2.403417000
C	-3.519785000	-1.525735000	3.218301000
H	-3.612454000	-0.468625000	3.549505000
H	-4.466475000	-1.771734000	2.698092000
C	-3.328102000	-2.450655000	4.426895000
H	-4.191546000	-2.363819000	5.119687000
H	-2.413875000	-2.198352000	5.000173000
H	-3.252413000	-3.514648000	4.122840000
C	-1.481863000	-3.271768000	-0.098593000
H	-1.566212000	-4.209694000	-0.683948000
H	-0.426391000	-3.160394000	0.209179000
C	-0.804582000	-1.931016000	-2.631008000
H	0.151994000	-1.485785000	-2.306118000
H	-0.613042000	-3.009401000	-2.818180000
C	-1.330941000	-1.220276000	-3.883107000
H	-2.209271000	-1.732338000	-4.328786000
H	-0.534484000	-1.189368000	-4.653595000
H	-1.599997000	-0.166182000	-3.670627000
C	-3.552794000	-2.336474000	-1.855038000
H	-4.313889000	-2.193972000	-1.061212000
H	-3.792607000	-1.600006000	-2.645707000
C	-3.625057000	-3.758486000	-2.425258000
H	-4.598194000	-3.921463000	-2.934151000
H	-3.536465000	-4.532006000	-1.635519000
H	-2.827350000	-3.947376000	-3.172780000
C	-4.316850000	2.256529000	0.683819000
H	-3.892951000	3.009873000	-0.011954000
H	-5.397867000	2.479496000	0.791129000
C	-3.568371000	2.282195000	2.016013000
H	-3.995897000	1.550742000	2.736043000
H	-3.605346000	3.279326000	2.502304000
C	-1.012625000	3.320034000	1.051710000
H	0.056344000	3.048703000	1.014542000
H	-1.316254000	3.446962000	-0.005959000

C	-1.207167000	4.612659000	1.848772000
H	-2.253958000	4.981259000	1.817430000
H	-0.562698000	5.406353000	1.417145000
H	-0.914770000	4.501325000	2.913335000
C	-1.108918000	1.656349000	3.405628000
H	-1.575659000	2.478370000	3.992464000
H	-1.491238000	0.710936000	3.840943000
C	0.421182000	1.713830000	3.438761000
H	0.810037000	1.382838000	4.422279000
H	0.798285000	2.737160000	3.247228000
H	0.837827000	1.051386000	2.660312000
C	-4.671058000	0.767186000	-1.861130000
H	-3.801450000	0.569859000	-2.515969000
H	-5.388500000	-0.060035000	-2.035116000
C	-5.300703000	2.112514000	-2.239645000
H	-6.168966000	2.372595000	-1.600991000
H	-5.658702000	2.076789000	-3.289688000
H	-4.560623000	2.934789000	-2.177104000
C	-5.484254000	-0.356917000	0.717172000
H	-5.309254000	-1.441880000	0.554813000
H	-5.356271000	-0.182999000	1.804088000
C	-6.905443000	0.031379000	0.289443000
H	-7.652505000	-0.534444000	0.884359000
H	-7.100507000	-0.191408000	-0.778736000
H	-7.109105000	1.110163000	0.449375000
C	-1.705556000	1.174522000	-1.126167000
B	1.477239000	0.112002000	-0.036925000
C	2.856042000	0.115727000	1.010052000
C	2.997467000	-0.396484000	2.310448000
C	4.207082000	-0.449948000	3.033595000
C	5.391161000	0.004376000	2.440489000
C	5.326475000	0.514805000	1.133757000
C	4.091141000	0.541315000	0.464411000
C	1.475165000	1.583248000	-0.838845000
C	1.870301000	2.787845000	-0.228790000
C	1.801107000	4.051561000	-0.840243000

C	1.324722000	4.153172000	-2.157277000
C	0.925117000	2.983748000	-2.822253000
C	1.005891000	1.754440000	-2.147962000
C	2.011233000	-1.175478000	-1.027365000
C	2.613953000	-1.158627000	-2.303337000
C	2.887007000	-2.324841000	-3.050068000
C	2.624502000	-3.589104000	-2.497859000
C	2.118747000	-3.660921000	-1.189518000
C	1.883830000	-2.468180000	-0.488572000
C	-2.406382000	-3.237392000	1.121230000
H	-2.173667000	-4.043775000	1.846061000
H	-3.475605000	-3.346992000	0.835663000

3: E= -6036.7855219

Fe	-2.401917000	-0.288491000	0.046861000
P	-2.503519000	-2.023249000	1.504649000
P	-2.319845000	1.035326000	1.892305000
P	-2.479258000	1.406759000	-1.474750000
P	-2.030057000	-1.591942000	-1.740046000
Al	1.291033000	0.012119000	-0.074804000
O	-0.414563000	-0.341009000	-0.022377000
F	3.543308000	0.159356000	-2.565608000
F	4.827083000	-1.810725000	-3.868096000
F	1.576324000	-3.075183000	0.349193000
F	2.846025000	-5.041037000	-0.988419000
F	4.503325000	-4.427259000	-3.103198000
F	1.428335000	5.843498000	-2.321218000
F	1.858993000	5.402297000	0.359367000
F	1.940245000	2.901717000	1.331804000
F	1.145429000	3.705184000	-4.029348000
F	1.243034000	1.198557000	-3.093743000
F	2.051029000	-0.257536000	5.371010000
F	5.792763000	0.912462000	2.659538000
F	4.253734000	0.671650000	0.438494000
F	4.710190000	0.464850000	5.143602000
F	0.543536000	-0.568816000	3.169947000

O	-5.282115000	-0.531366000	-0.104903000
C	-3.200715000	-1.333087000	3.094065000
H	-4.278886000	-1.150282000	2.894143000
H	-3.129877000	-2.073851000	3.916460000
C	-2.462038000	-0.034876000	3.428325000
H	-1.430487000	-0.253720000	3.758478000
H	-2.954743000	0.534970000	4.243286000
C	-3.648512000	2.312432000	2.192650000
H	-3.276223000	2.974293000	3.005284000
H	-3.689437000	2.933917000	1.274740000
C	-5.038900000	1.768303000	2.542183000
H	-5.426725000	1.073433000	1.771846000
H	-5.767830000	2.599316000	2.639715000
H	-5.034042000	1.224131000	3.509309000
C	-0.772164000	2.014210000	2.125534000
H	0.011743000	1.374594000	1.681660000
H	-0.861854000	2.889845000	1.452682000
C	-0.396888000	2.447775000	3.544461000
H	-1.188883000	3.048586000	4.040101000
H	0.519203000	3.069791000	3.493735000
H	-0.163770000	1.577564000	4.188470000
C	-0.919794000	-2.870054000	1.948062000
H	-0.838116000	-3.737420000	1.261373000
H	-0.152695000	-2.145849000	1.614359000
C	-0.697775000	-3.300380000	3.401715000
H	-0.680450000	-2.436009000	4.093149000
H	0.295450000	-3.788194000	3.485656000
H	-1.458451000	-4.022597000	3.761759000
C	-3.706589000	-3.379543000	1.084461000
H	-4.672391000	-2.871610000	0.877337000
H	-3.364845000	-3.794996000	0.112609000
C	-3.877413000	-4.503581000	2.113995000
H	-2.933550000	-5.064234000	2.270662000
H	-4.640436000	-5.232150000	1.768264000
H	-4.212557000	-4.119330000	3.099327000
C	-1.722305000	3.073321000	-1.143607000

H	-2.229402000	3.461148000	-0.234310000
H	-0.675505000	2.866809000	-0.850691000
C	-1.799732000	4.100080000	-2.279765000
H	-1.327523000	3.729654000	-3.211641000
H	-1.248825000	5.020715000	-1.997065000
H	-2.843077000	4.394151000	-2.516718000
C	-1.740484000	0.822349000	-3.108159000
H	-2.565943000	0.830029000	-3.850336000
H	-0.983818000	1.550798000	-3.457292000
C	-1.122873000	-0.572841000	-2.987707000
H	-0.090668000	-0.510635000	-2.598935000
H	-1.086933000	-1.093234000	-3.966627000
C	-3.576711000	-2.151801000	-2.621266000
H	-4.206449000	-2.633567000	-1.843344000
H	-4.113711000	-1.213017000	-2.879555000
C	-3.427549000	-3.057488000	-3.848170000
H	-2.996940000	-4.043019000	-3.578159000
H	-2.773827000	-2.605948000	-4.623163000
H	-4.415459000	-3.247154000	-4.318108000
C	-0.984133000	-3.107063000	-1.534762000
H	-0.327541000	-2.837969000	-0.688691000
H	-1.660735000	-3.920618000	-1.193781000
C	-0.126440000	-3.562594000	-2.725403000
H	-0.722647000	-3.822919000	-3.621988000
H	0.456362000	-4.459472000	-2.430040000
H	0.611079000	-2.786021000	-3.008422000
C	-4.185984000	1.884152000	-2.085986000
H	-4.031631000	2.443169000	-3.034113000
H	-4.686634000	0.931368000	-2.360081000
C	-5.068567000	2.690064000	-1.130145000
H	-5.299846000	2.124488000	-0.208145000
H	-6.037079000	2.932719000	-1.614616000
H	-4.598106000	3.653133000	-0.841710000
C	2.393284000	-1.366780000	-1.116559000
C	3.287683000	-1.104900000	-2.167710000
C	3.996398000	-2.111242000	-2.855787000

C	3.847621000	-3.451899000	-2.456895000
C	3.011164000	-3.759491000	-1.370599000
C	2.342302000	-2.708685000	-0.722741000
C	1.594697000	1.903811000	-0.827695000
C	1.437089000	2.196980000	-2.187891000
C	1.398837000	3.495605000	-2.722163000
C	1.530684000	4.590105000	-1.851659000
C	1.733571000	4.359953000	-0.479909000
C	1.765640000	3.032015000	-0.010349000
C	2.328768000	0.033335000	1.695393000
C	1.849964000	-0.198470000	2.982146000
C	2.603695000	-0.054238000	4.158458000
C	3.953258000	0.322324000	4.045614000
C	4.504188000	0.550347000	2.769419000
C	3.681568000	0.402875000	1.637380000
C	-4.110752000	-0.398878000	-0.016739000

3-B: E= -2209.252418

Fe	-2.170309000	-0.107118000	-0.176166000
P	-2.531407000	-2.297627000	0.435112000
P	-2.308264000	0.358738000	2.047997000
P	-2.135548000	2.040910000	-0.934725000
P	-1.793374000	-0.647526000	-2.337418000
B	1.301222000	0.079499000	0.023952000
O	-0.090407000	-0.185631000	-0.251108000
F	3.804994000	1.240352000	-1.670914000
F	5.074473000	-0.027779000	-3.606884000
F	1.400197000	-2.769784000	-0.666266000
F	2.675120000	-4.016199000	-2.627307000
F	4.561337000	-2.678480000	-4.148555000
F	1.944491000	5.982355000	0.405717000
F	2.127664000	4.434370000	2.682430000
F	1.998641000	1.802483000	2.557648000
F	1.670842000	4.735687000	-2.043781000
F	1.514450000	2.107250000	-2.214104000
F	1.094241000	-2.817982000	4.270745000

F	5.321785000	-1.029805000	2.973126000
F	4.147687000	0.230162000	0.907631000
F	3.833264000	-2.575301000	4.697372000
F	-0.049447000	-1.632947000	2.203579000
O	-5.029141000	-0.049259000	-0.570441000
C	-3.374379000	-2.225969000	2.107224000
H	-4.417574000	-1.918705000	1.875855000
H	-3.420121000	-3.230504000	2.573987000
C	-2.698472000	-1.203102000	3.023048000
H	-1.749427000	-1.598604000	3.424028000
H	-3.338542000	-0.943874000	3.891523000
C	-3.635157000	1.509984000	2.690157000
H	-3.320537000	1.783755000	3.721679000
H	-3.556174000	2.435405000	2.085332000
C	-5.076996000	0.988726000	2.697655000
H	-5.424137000	0.680334000	1.692763000
H	-5.769118000	1.775838000	3.062363000
H	-5.195879000	0.116129000	3.372529000
C	-0.794094000	1.105103000	2.788178000
H	0.012478000	0.762700000	2.120997000
H	-0.887110000	2.198335000	2.621536000
C	-0.484715000	0.791610000	4.253381000
H	-1.316960000	1.058803000	4.939057000
H	0.412884000	1.363836000	4.561749000
H	-0.250140000	-0.282077000	4.395768000
C	-1.164171000	-3.552446000	0.527756000
H	-1.241373000	-4.145565000	-0.408003000
H	-0.248119000	-2.949771000	0.443110000
C	-1.106826000	-4.459385000	1.761757000
H	-0.918355000	-3.874577000	2.683234000
H	-0.258778000	-5.167982000	1.656521000
H	-2.027482000	-5.062280000	1.903096000
C	-3.818226000	-3.193389000	-0.582347000
H	-4.695301000	-2.519305000	-0.664820000
H	-3.388041000	-3.269436000	-1.603712000
C	-4.240583000	-4.580918000	-0.081875000

H	-3.385499000	-5.285999000	-0.040678000
H	-4.998157000	-5.021613000	-0.763295000
H	-4.694399000	-4.538446000	0.929489000
C	-1.406110000	3.403163000	0.090740000
H	-2.031401000	3.430751000	1.008337000
H	-0.415757000	3.035346000	0.411368000
C	-1.331162000	4.792897000	-0.550431000
H	-0.766119000	4.784737000	-1.503466000
H	-0.792757000	5.490986000	0.123165000
H	-2.334900000	5.222727000	-0.747207000
C	-1.344387000	2.081188000	-2.646985000
H	-2.142488000	2.408065000	-3.345612000
H	-0.551903000	2.852572000	-2.678544000
C	-0.788096000	0.714306000	-3.057628000
H	0.211467000	0.550276000	-2.619641000
H	-0.715371000	0.616170000	-4.159988000
C	-3.332851000	-0.703983000	-3.393810000
H	-4.035787000	-1.399470000	-2.888603000
H	-3.794740000	0.300607000	-3.280849000
C	-3.176666000	-1.065070000	-4.875524000
H	-2.822314000	-2.107309000	-5.010414000
H	-2.460391000	-0.396052000	-5.396154000
H	-4.150592000	-0.979288000	-5.401789000
C	-0.872025000	-2.204716000	-2.727274000
H	-0.282557000	-2.394176000	-1.814289000
H	-1.633267000	-3.011372000	-2.806761000
C	0.052229000	-2.190364000	-3.954299000
H	-0.490999000	-2.025931000	-4.905800000
H	0.584552000	-3.161124000	-4.022906000
H	0.831985000	-1.409703000	-3.859297000
C	-3.789768000	2.800539000	-1.406034000
H	-3.541297000	3.669164000	-2.053458000
H	-4.292411000	2.058411000	-2.061278000
C	-4.732134000	3.234395000	-0.282696000
H	-5.054762000	2.378062000	0.337481000
H	-5.649850000	3.689371000	-0.710002000

H	-4.270909000	3.996104000	0.379325000
C	2.333032000	-0.615284000	-1.179426000
C	3.383804000	-0.019458000	-1.912992000
C	4.117897000	-0.678107000	-2.921418000
C	3.880295000	-2.035825000	-3.187102000
C	2.926525000	-2.708315000	-2.410873000
C	2.228123000	-1.994971000	-1.422652000
C	1.658245000	1.751711000	0.161449000
C	1.646033000	2.605281000	-0.957272000
C	1.768673000	4.002545000	-0.914930000
C	1.908743000	4.642250000	0.325221000
C	1.978735000	3.850383000	1.480142000
C	1.874687000	2.448079000	1.368363000
C	1.986862000	-0.666243000	1.396560000
C	1.301127000	-1.464939000	2.309237000
C	1.871478000	-2.106762000	3.421313000
C	3.248223000	-1.975058000	3.649191000
C	4.003558000	-1.183471000	2.762281000
C	3.363298000	-0.554264000	1.680288000
C	-3.863421000	-0.069367000	-0.375579000

(N_2)Fe(depe)$_2$: E= -3530.7042883

Fe	0.013702000	-0.146650000	-0.280674000
P	-0.464802000	1.913007000	0.303353000
P	2.092786000	0.572327000	-0.481882000
P	0.480297000	-1.711458000	1.167738000
P	-2.058299000	-0.908674000	-0.178676000
C	1.086414000	2.998926000	0.378757000
C	2.121643000	2.446897000	-0.597074000
C	-1.067749000	-2.653239000	1.718806000
C	-2.083672000	-2.629402000	0.580834000
C	-1.326006000	2.483958000	1.889697000
C	-1.198687000	3.958607000	2.296329000
C	-1.520640000	2.875441000	-0.931582000
C	-0.915191000	2.921634000	-2.337774000
C	3.015754000	0.139301000	-2.047278000

C	3.359256000	-1.346555000	-2.179251000
C	3.407485000	0.262360000	0.828402000
C	4.823828000	0.792620000	0.576314000
C	1.565056000	-3.144505000	0.594228000
C	1.001413000	-3.851679000	-0.642240000
C	1.262428000	-1.457712000	2.870156000
C	0.813731000	-0.152982000	3.526496000
C	-2.950841000	-1.253595000	-1.784313000
C	-3.328283000	-0.000195000	-2.579365000
C	-3.399197000	-0.058023000	0.826961000
C	-4.813011000	-0.650418000	0.812377000
N	0.025984000	-0.541995000	-2.002011000
N	0.036197000	-0.806926000	-3.125086000
H	1.468208000	2.940825000	1.422371000
H	0.836593000	4.062913000	0.180124000
H	1.850570000	2.683350000	-1.646441000
H	3.141877000	2.849017000	-0.420406000
H	-1.465018000	-2.116871000	2.608528000
H	-0.803038000	-3.683039000	2.043877000
H	-1.785566000	-3.318806000	-0.235640000
H	-3.107527000	-2.915599000	0.902621000
H	-0.946311000	1.820901000	2.692578000
H	-2.395286000	2.221559000	1.761292000
H	-1.826497000	4.176533000	3.187127000
H	-0.156645000	4.232810000	2.559325000
H	-1.529384000	4.646161000	1.489597000
H	-1.732935000	3.899525000	-0.552115000
H	-2.489892000	2.332119000	-0.954163000
H	-1.654470000	3.268829000	-3.089920000
H	-0.049695000	3.615843000	-2.384920000
H	-0.557431000	1.915907000	-2.641746000
H	3.924271000	0.777352000	-2.106537000
H	2.345844000	0.451910000	-2.875151000
H	3.862814000	-1.554786000	-3.146417000
H	4.039975000	-1.690698000	-1.371160000
H	2.441084000	-1.964101000	-2.140102000

H	3.436176000	-0.836749000	0.974496000
H	2.985336000	0.681056000	1.766677000
H	5.476491000	0.598608000	1.454052000
H	5.298896000	0.304068000	-0.299178000
H	4.838064000	1.887715000	0.395872000
H	1.729403000	-3.854571000	1.435949000
H	2.550542000	-2.690058000	0.355942000
H	1.758599000	-4.504996000	-1.124087000
H	0.131716000	-4.491658000	-0.384033000
H	0.658481000	-3.105496000	-1.390082000
H	2.364439000	-1.472111000	2.742234000
H	1.010436000	-2.340974000	3.498053000
H	1.330989000	0.029643000	4.492289000
H	1.012182000	0.700386000	2.843782000
H	-0.279769000	-0.151900000	3.724263000
H	-3.844028000	-1.875723000	-1.557958000
H	-2.256294000	-1.886796000	-2.374932000
H	-3.842723000	-0.271039000	-3.525219000
H	-4.013441000	0.662966000	-2.008979000
H	-2.427672000	0.586133000	-2.846912000
H	-3.425705000	0.993371000	0.472665000
H	-2.987441000	-0.020641000	1.858650000
H	-5.479997000	-0.089514000	1.501269000
H	-5.270518000	-0.602747000	-0.197277000
H	-4.829350000	-1.711927000	1.136073000

6+: E= -4939.1997082

Au	-0.105281000	0.034911000	-0.136894000
Fe	2.448825000	-0.274272000	0.051961000
P	-2.312603000	0.184339000	-0.983538000
P	2.038686000	0.027906000	2.235167000
P	2.546211000	1.987458000	-0.056812000
P	1.980594000	-2.493515000	0.062773000
P	2.644214000	-0.501015000	-2.182356000
C	-3.859357000	0.519438000	-0.007834000
N	4.189410000	-0.614421000	0.257701000

C	-4.794686000	-0.502017000	0.340659000
C	-5.309292000	2.166075000	1.094234000
C	-3.046852000	2.930158000	0.457710000
C	-4.564336000	-1.966214000	0.125437000
C	-4.091573000	1.851314000	0.455500000
C	-2.103849000	2.918244000	1.526983000
C	-5.989766000	-0.148187000	1.006131000
N	5.286787000	-0.896768000	0.408439000
C	-6.270644000	1.179373000	1.350323000
C	1.453137000	1.782030000	2.497253000
C	2.305885000	2.720079000	1.656463000
C	-5.309692000	-2.666360000	-0.862277000
C	-3.085396000	4.010980000	-0.461852000
C	-5.082729000	-4.046766000	-1.032437000
C	-1.169255000	5.016773000	0.681343000
C	-1.174294000	3.973190000	1.620820000
C	3.188497000	-2.266865000	-2.437725000
C	2.213608000	-3.164977000	-1.680443000
C	-2.117218000	5.033345000	-0.350712000
C	-4.162807000	-4.730870000	-0.222702000
C	-3.457081000	-4.036662000	0.771591000
C	-3.637679000	-2.650873000	0.958484000
H	-0.465242000	3.991891000	2.463215000
H	-0.437351000	5.834505000	0.770023000
H	-2.132528000	5.867829000	-1.070573000
H	-5.641317000	-4.592524000	-1.809757000
H	-4.006066000	-5.812556000	-0.357956000
H	-2.763642000	-4.578705000	1.434456000
C	-2.580911000	-1.336670000	-2.007862000
H	-2.495388000	-2.258225000	-1.405389000
H	-3.560658000	-1.319950000	-2.522236000
H	-1.772792000	-1.329237000	-2.767123000
C	-2.285838000	1.442107000	-2.341726000
H	-3.275339000	1.535203000	-2.830185000
H	-1.957065000	2.421997000	-1.954331000
H	-1.539874000	1.088852000	-3.081003000

H	-5.472667000	3.203939000	1.424943000
H	-7.214384000	1.437169000	1.855316000
H	-6.697253000	-0.950753000	1.267905000
C	-4.161151000	4.111324000	-1.521066000
H	-4.923006000	4.865312000	-1.226966000
H	-3.743032000	4.438511000	-2.495276000
H	-4.694949000	3.153519000	-1.669795000
C	-2.140483000	1.823020000	2.568851000
H	-1.483342000	2.056052000	3.428794000
H	-3.168774000	1.662002000	2.952248000
H	-1.811028000	0.853346000	2.138758000
C	-2.838284000	-1.917156000	2.010552000
H	-2.008621000	-1.340013000	1.541954000
H	-3.454696000	-1.184024000	2.568063000
H	-2.381718000	-2.619674000	2.735657000
C	-6.307125000	-1.939259000	-1.736500000
H	-7.225706000	-1.675921000	-1.170241000
H	-5.899766000	-0.978420000	-2.116186000
H	-6.615020000	-2.557137000	-2.602782000
H	1.210627000	-3.147360000	-2.160748000
H	2.542478000	-4.222625000	-1.659332000
H	3.249902000	-2.513882000	-3.517668000
H	4.215218000	-2.339314000	-2.020833000
H	3.313695000	2.847318000	2.105064000
H	1.856936000	3.731184000	1.560943000
H	1.451901000	2.046190000	3.575404000
H	0.404713000	1.785724000	2.141634000
C	3.185726000	-3.511959000	1.105146000
H	2.594051000	-4.283646000	1.640507000
H	3.562727000	-2.811780000	1.877357000
C	0.321546000	-3.255251000	0.477102000
H	0.058286000	-2.930843000	1.502764000
H	-0.398642000	-2.730503000	-0.187547000
C	3.986248000	0.428771000	-3.101976000
H	4.468170000	-0.285021000	-3.803775000
H	4.748493000	0.665934000	-2.330299000

C	1.163974000	-0.377330000	-3.320770000
H	0.341600000	-0.862517000	-2.755176000
H	0.898569000	0.701183000	-3.347298000
C	3.585327000	-0.056720000	3.285465000
H	4.366416000	0.478087000	2.706004000
H	3.903006000	-1.122439000	3.271646000
C	0.775235000	-0.883084000	3.279355000
H	0.480715000	-0.178192000	4.086287000
H	-0.116633000	-0.995093000	2.626859000
C	4.113468000	2.903093000	-0.535019000
H	4.210319000	2.871273000	-1.637382000
H	3.915225000	3.966048000	-0.278444000
C	1.236790000	2.900646000	-1.049447000
H	0.318807000	2.803888000	-0.429109000
H	1.044802000	2.278103000	-1.947465000
C	0.209060000	-4.776120000	0.325952000
H	0.895397000	-5.324283000	1.003716000
H	-0.821816000	-5.104023000	0.567164000
H	0.417107000	-5.112105000	-0.710072000
C	1.190561000	-2.225001000	3.890288000
H	0.344661000	-2.662168000	4.460336000
H	1.487451000	-2.968649000	3.127092000
H	2.040062000	-2.120401000	4.594833000
C	4.370754000	-4.173748000	0.390069000
H	5.020363000	-4.681568000	1.132680000
H	4.046435000	-4.944667000	-0.337838000
H	5.004184000	-3.436381000	-0.140757000
C	3.502113000	0.481421000	4.718585000
H	2.698763000	-0.003280000	5.310728000
H	4.457463000	0.305058000	5.255279000
H	3.317568000	1.575223000	4.737415000
C	5.408448000	2.431225000	0.133873000
H	5.300111000	2.312220000	1.232525000
H	5.758796000	1.461731000	-0.265236000
H	6.216433000	3.172930000	-0.032832000
C	1.483929000	4.365181000	-1.419904000

H	1.706096000	4.988618000	-0.529160000
H	2.320845000	4.489038000	-2.137123000
H	0.572297000	4.791534000	-1.886996000
C	1.296569000	-0.967356000	-4.729548000
H	2.175438000	-0.571300000	-5.278338000
H	1.390260000	-2.072213000	-4.703619000
H	0.396938000	-0.731532000	-5.335613000
C	3.548218000	1.689478000	-3.860229000
H	4.434031000	2.242409000	-4.234916000
H	2.918583000	1.446892000	-4.739155000
H	2.967408000	2.389114000	-3.227732000

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