Supporting Information

Electron-Rich, Diiron Bis(monothiolato) Carbonyls: C-S Bond Homolysis in a Mixed Valence Diiron Dithiolate

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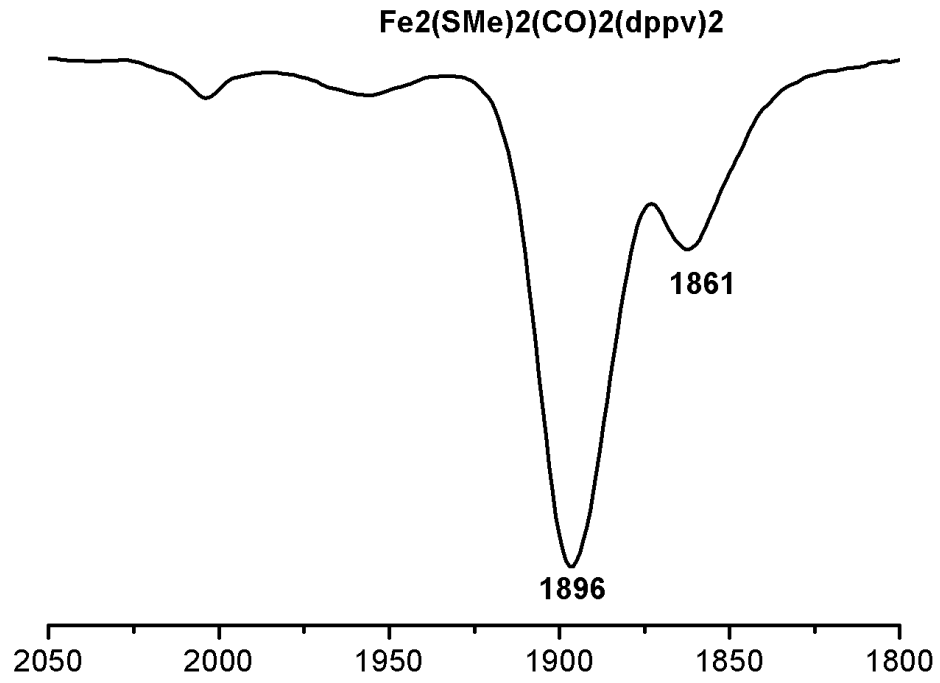


Figure S1. FT-IR spectrum of $Fe_2(SMe)_2(CO)_2(dppv)_2$ ([**1**]^0) in CH_2Cl_2 solution. *Assignments:* ν_{CO} = 1896, 1861.

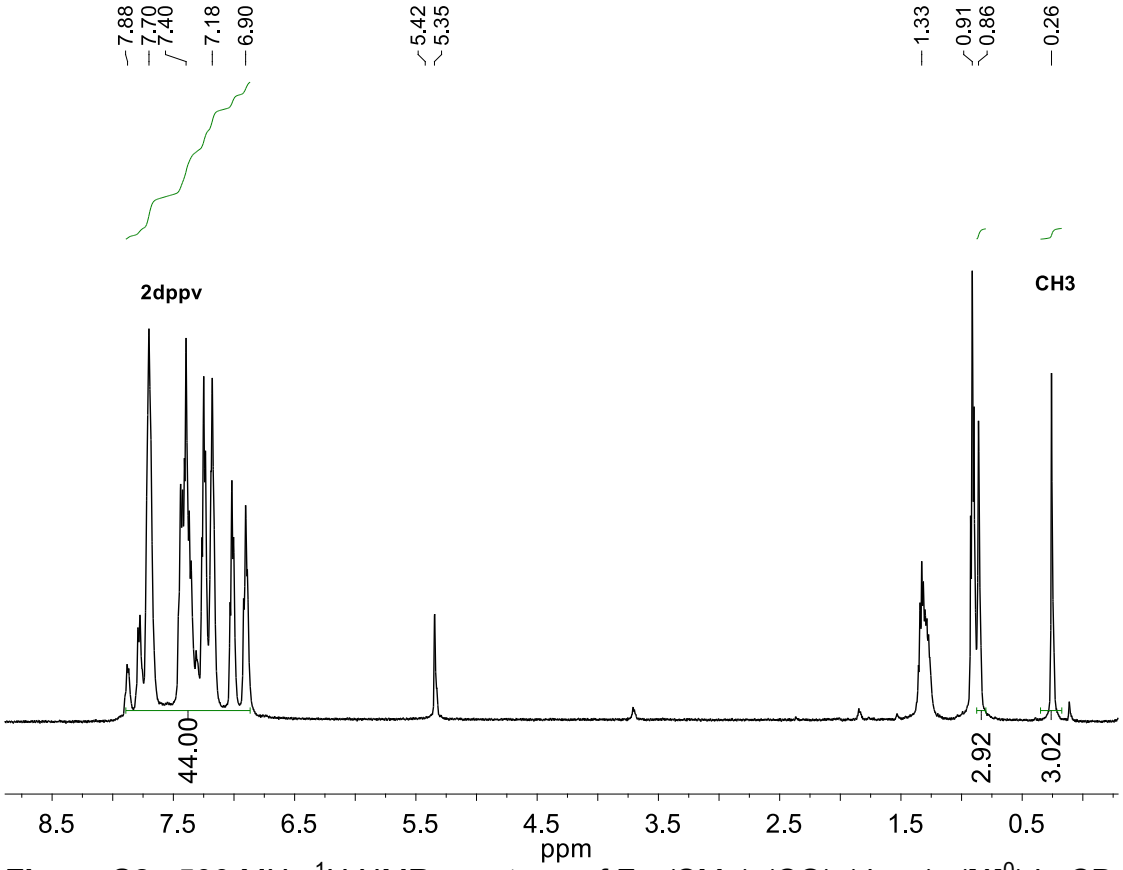


Figure S2. 500 MHz ^{1}H NMR spectrum of $Fe_2(SMe)_2(CO)_2(dppv)_2$ ([**1**]^{0}) in CD_2Cl_2 solution. *Assignments:* δ = 6.90-7.88, (m, 44H, 8C$_6$*H*$_5$, 2PC*H*=C*H*P); 0.26, 0.86 (s, 6H, 2C*H*$_3$).

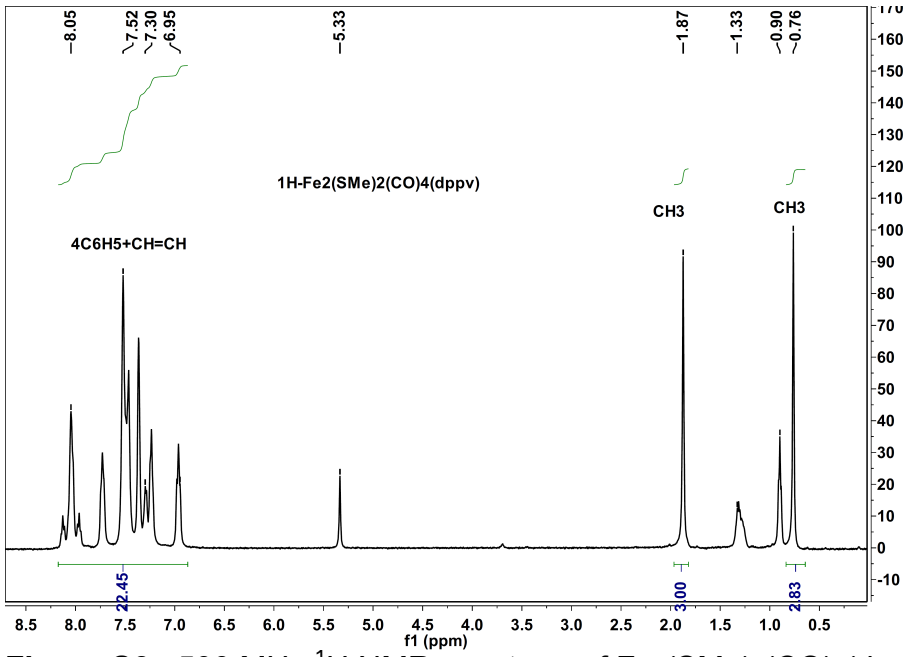


Figure S3. 500 MHz ^{1}H NMR spectrum of $Fe_2(SMe)_2(CO)_4(dppv)$ in CD_2Cl_2 solution.

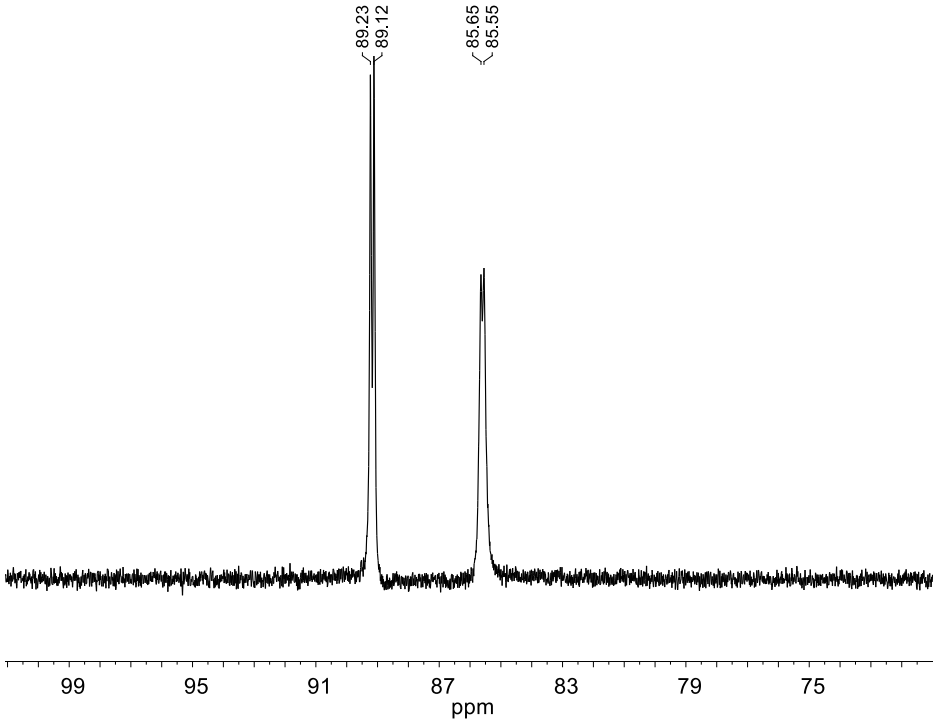


Figure S4. 202 MHz ^{31}P NMR spectrum of $Fe_2(SMe)_2(CO)_2(dppv)_2$ ([**1**]^0) in CD_2Cl_2 solution. *Assignments:* δ = 89.2 (d, $J_{p\text{-}p}$ = 20 Hz), 85.6 (d, $J_{p\text{-}p}$ = 20 Hz).

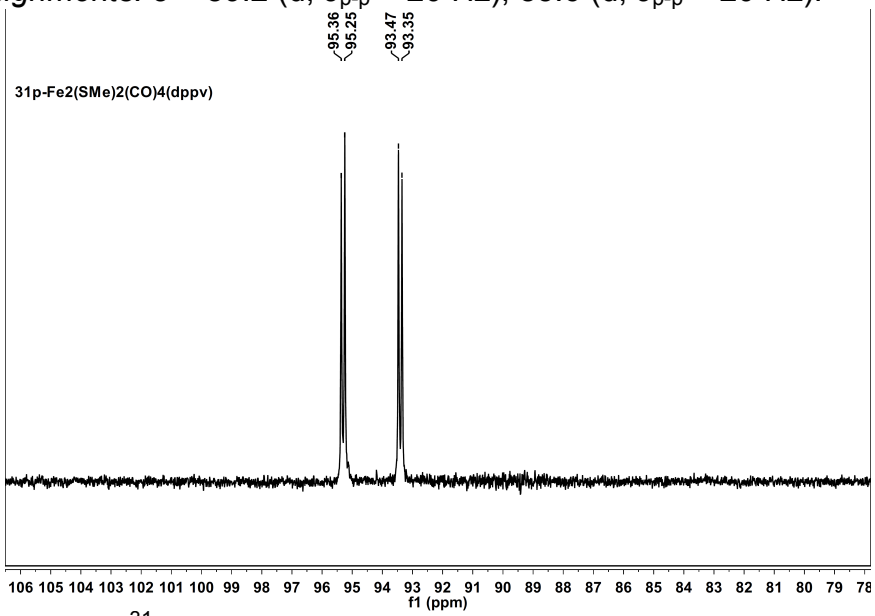


Figure S5. 202 MHz ^{31}P NMR spectrum of $Fe_2(SMe)_2(CO)_4(dppv)$ in CD_2Cl_2 solution.

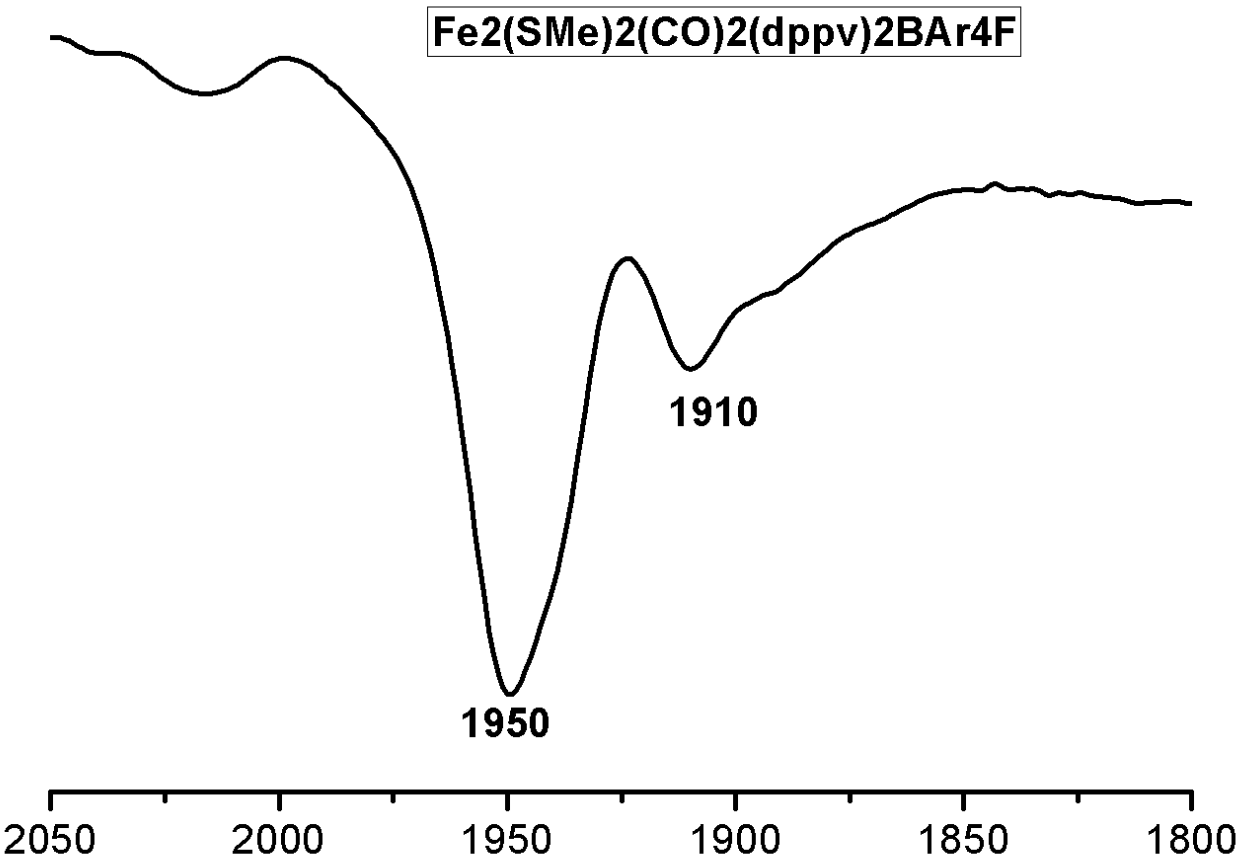


Figure S6. FT-IR spectrum of $[Fe_2(SMe)_2(CO)_2(dppv)_2]BAr^F{}_4$ ([**1**]$BAr^F{}_4$) generated *in situ* by combining **1** and $FcBAr^F{}_4$ in THF solution. *Assignments:* ν_{CO} = 1950, 1910 cm^{-1}.

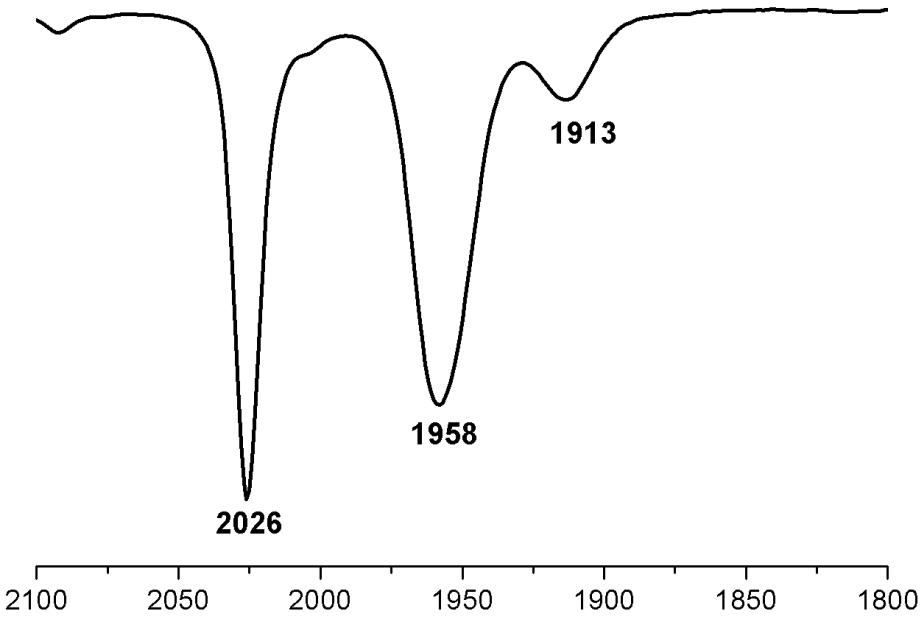


Figure S7. FT-IR spectrum of $Fe_2(SPh)_2(CO)_4$(dppv) in CH_2Cl_2 solution. *Assignments:* ν_{CO} = 2026, 1958, 1913 cm^{-1}.

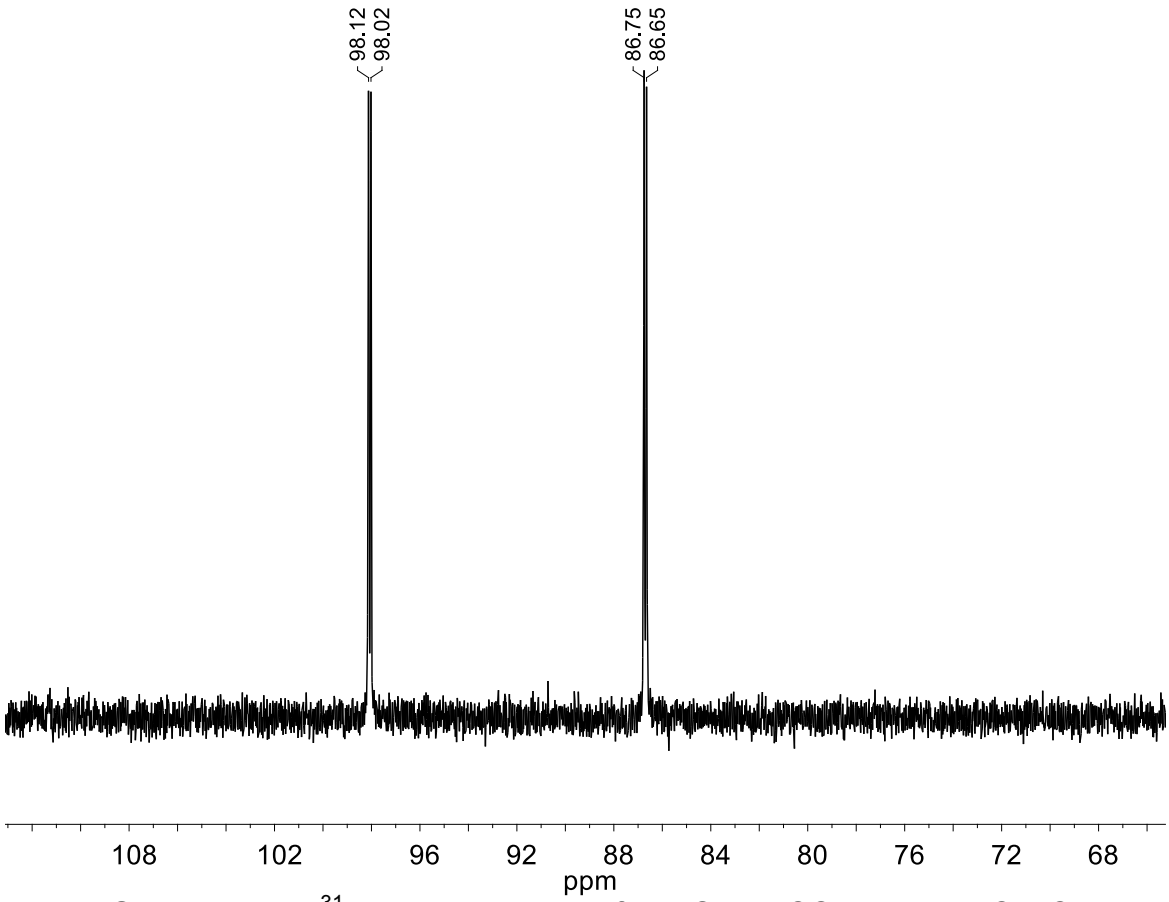


Figure S8. 202 MHz ^{31}P NMR spectrum of $Fe_2(SPh)_2(CO)_4$(dppv) in CD_2Cl_2 solution. *Assignments:* δ = 98.1 (d, $J_{p\text{-}p}$ = 20 Hz), 86.7 (d, $J_{p\text{-}p}$ = 20 Hz).

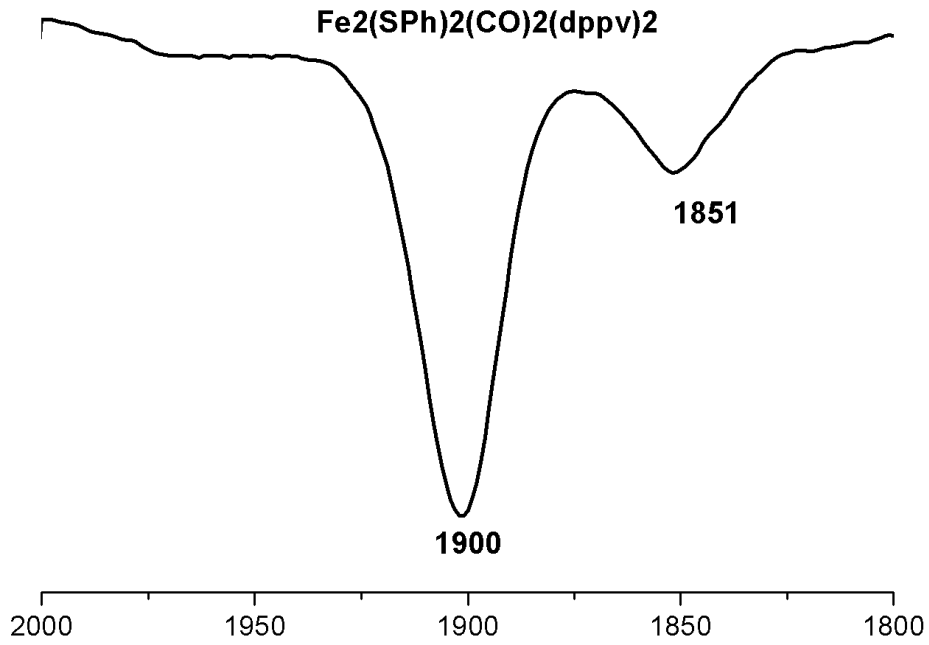


Figure S9. FT-IR spectrum of $Fe_2(SPh)_2(CO)_2(dppv)_2$ ([**2**]^0) in CH_2Cl_2 solution. *Assignments:* ν_{CO} = 1900, 1851 cm^{-1}.

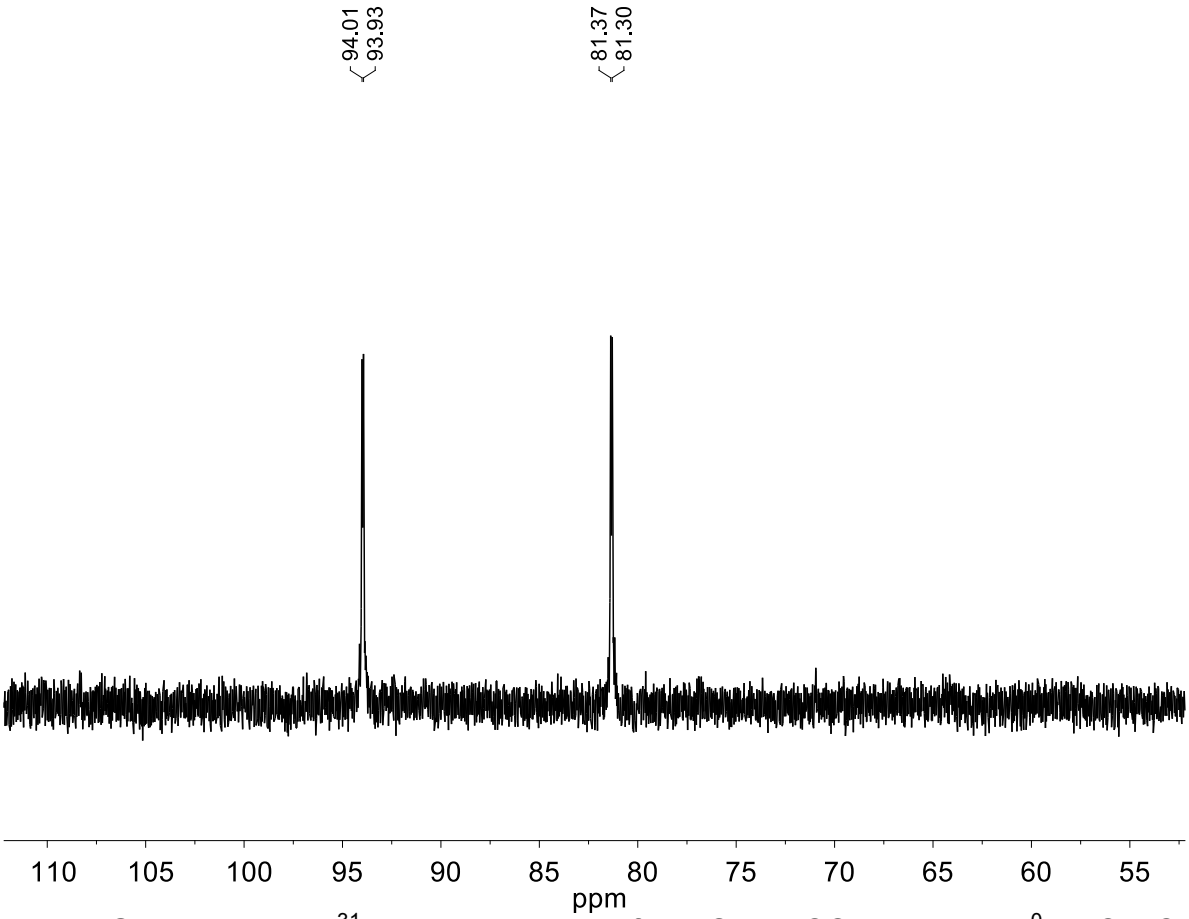


Figure S10. 202 MHz ^{31}P NMR spectrum of $Fe_2(SPh)_2(CO)_2(dppv)_2$ ([**2**]^0) in CD_2Cl_2 solution. *Assignments:* δ = 94.0 (d, $J_{p\text{-}p}$ = 20 Hz), 81.3 (d, $J_{p\text{-}p}$ = 20 Hz).

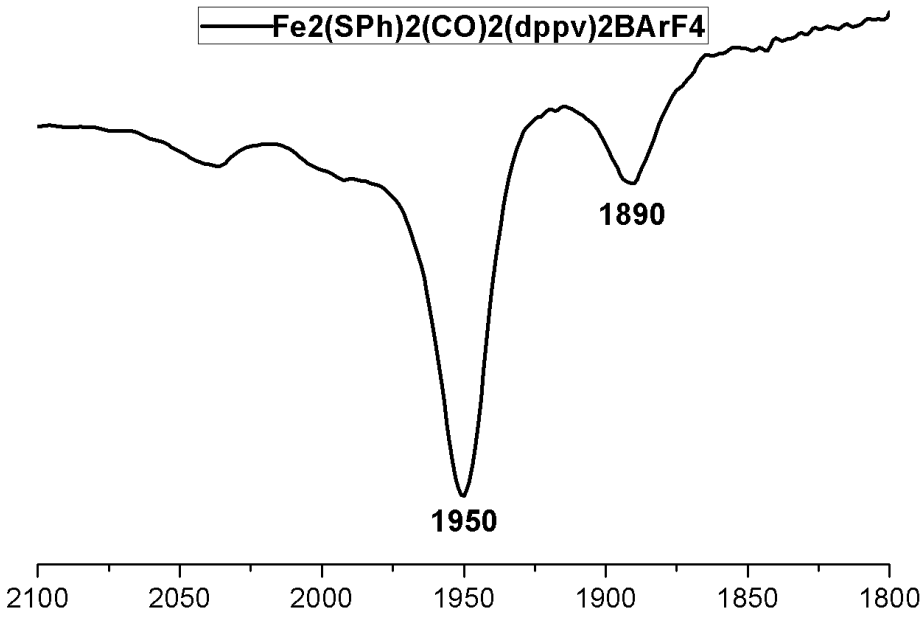


Figure S11. FT-IR spectrum of $[Fe_2(SPh)_2(CO)_2(dppv)_2]BAr^F_4$ ([**2**]BAr^F_4) generated in situ by combining **2** and $FcBAr^F_4$ in THF solution. *Assignments:* ν_{CO} = 1950, 1890 cm^{-1}.

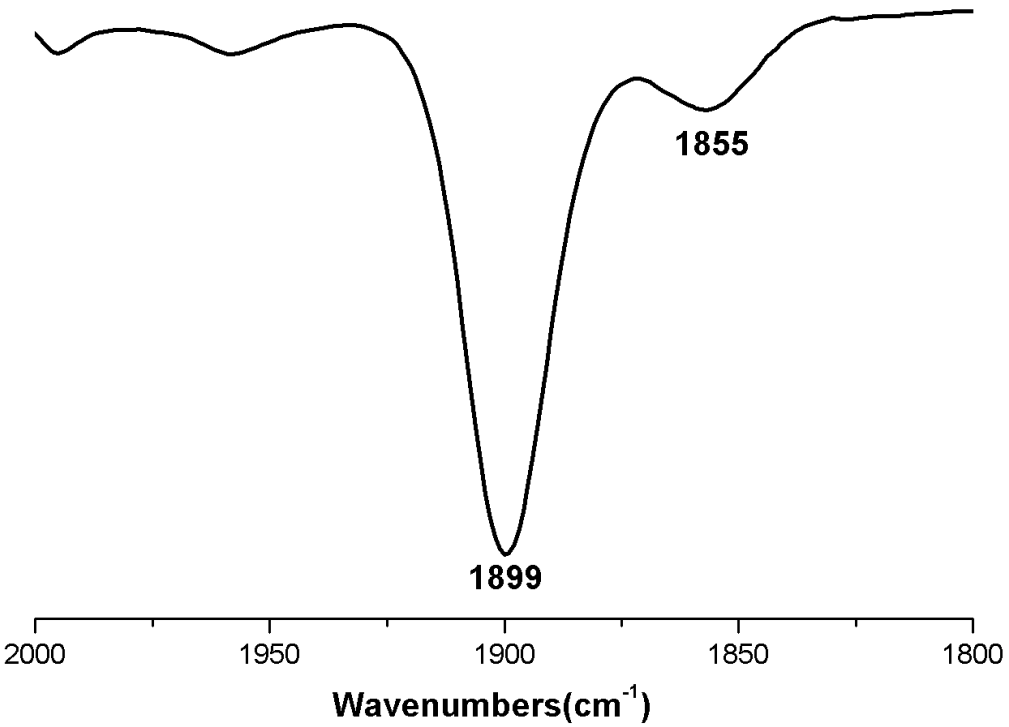


Figure S12. FT-IR spectrum of $Fe_2(SBn)_2(CO)_2(dppv)_2$ ([**3**]^0) in CH_2Cl_2 solution. *Assignments:* ν_{CO} = 1899, 1855 cm^{-1}.

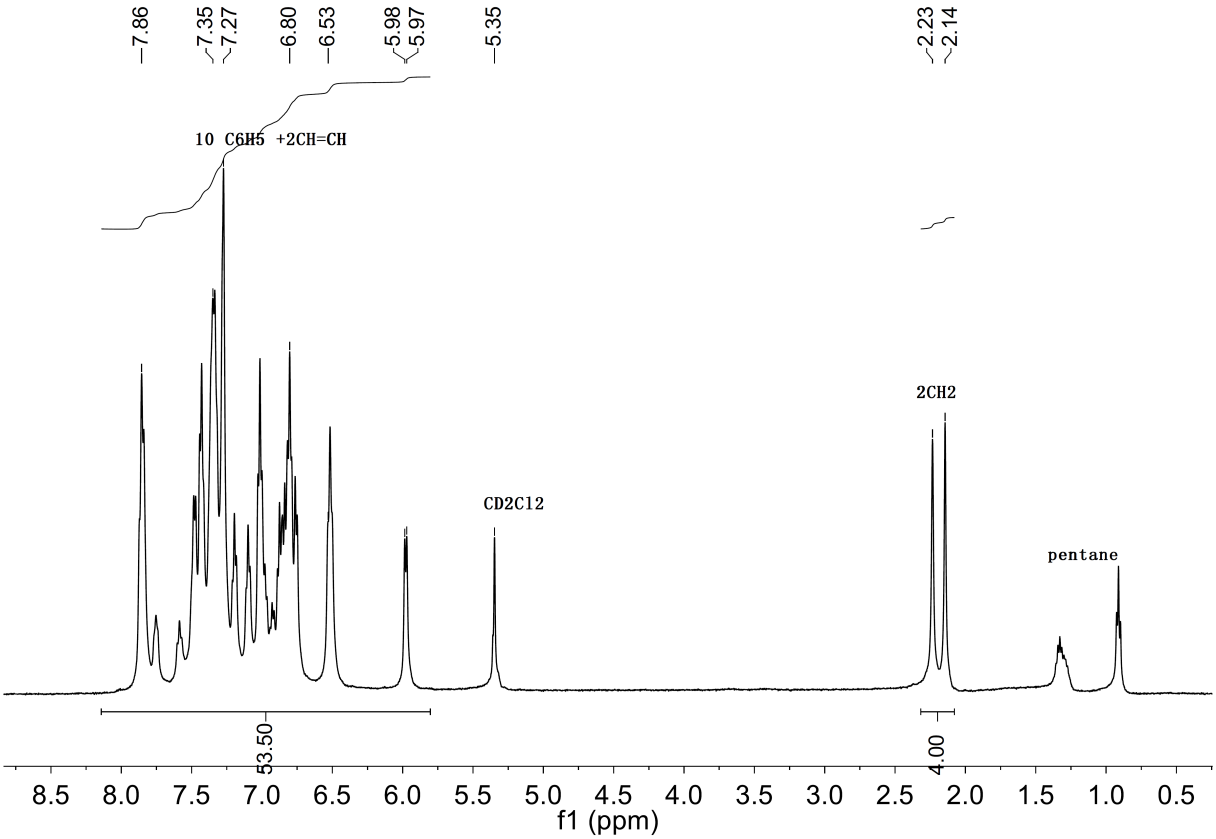


Figure S13. 500 MHz ^{1}H NMR spectrum of $Fe_2(SBn)_2(CO)_2(dppv)_2$ ([**3**]^0) in CD_2Cl_2 solution. *Assignments:* δ =5.97-7.86, (m, 54H, C_6H_5, 2C*H*=C*H*); 2.14, 2.23 (s, 4H, 2CH_2).

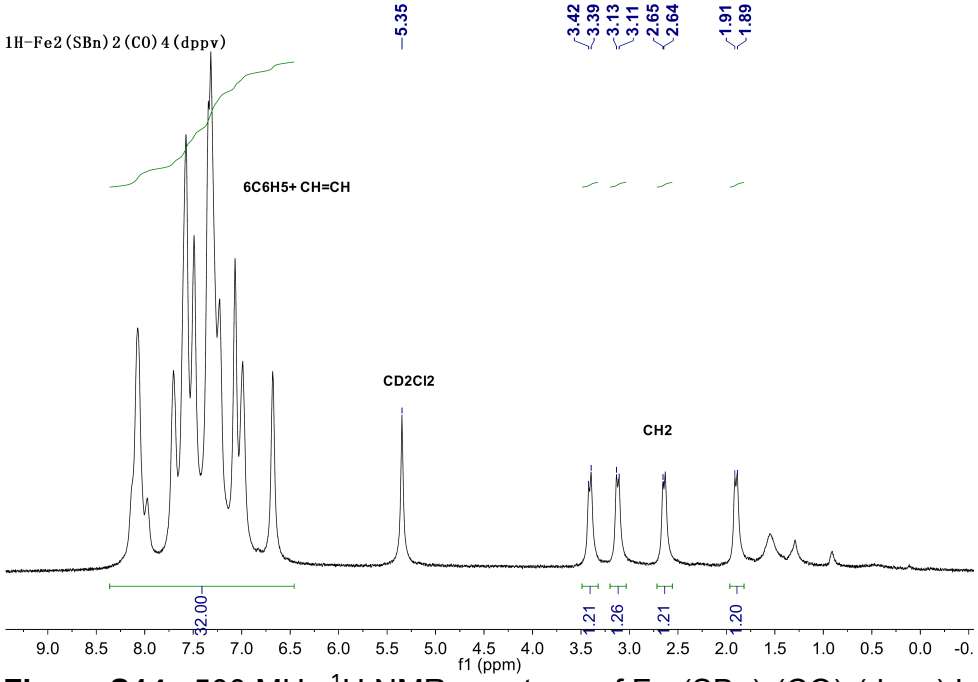


Figure S14. 500 MHz ^{1}H NMR spectrum of $Fe_2(SBn)_2(CO)_4(dppv)$ in CD_2Cl_2 solution. *Assignments:* signals in the range δ 3.4-1.8 SCH_2Ph (signals in the range δ 1.7 - 0.9 are from pentane).

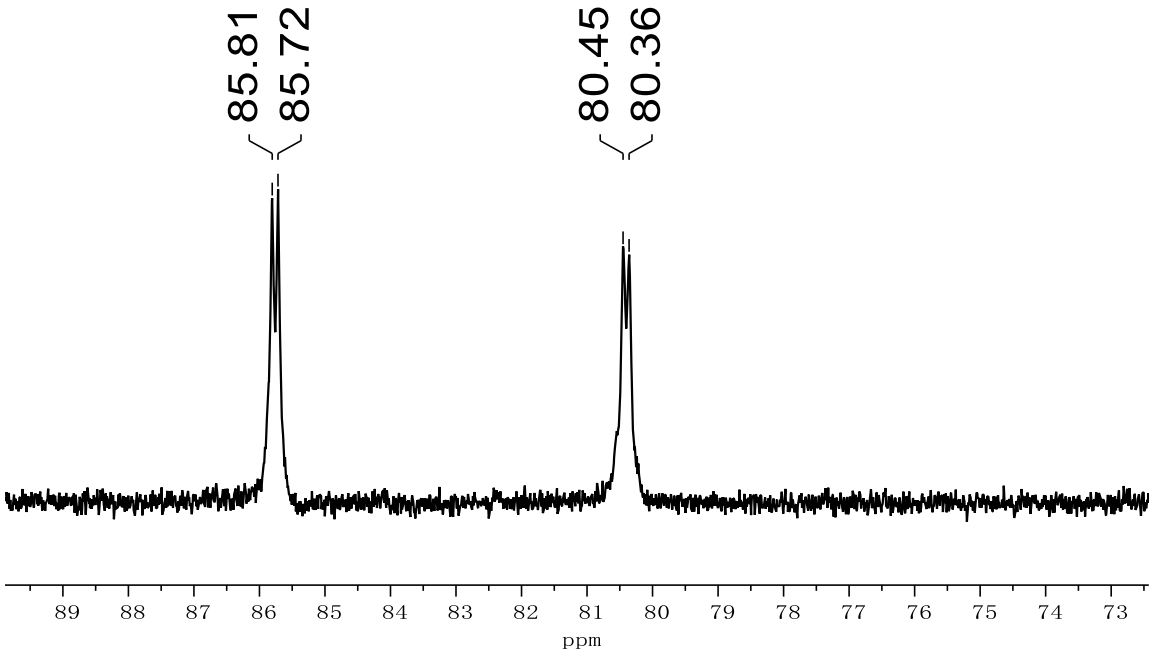


Figure S15. 202 MHz ^{31}P NMR spectrum of $Fe_2(SBn)_2(CO)_2(dppv)_2$ ([**3**]^0) in CD_2Cl_2 solution. *Assignments:* δ = 85.7 (d, $J_{p\text{-}p}$ = 20 Hz), 80.3 (d, $J_{p\text{-}p}$ = 20 Hz).

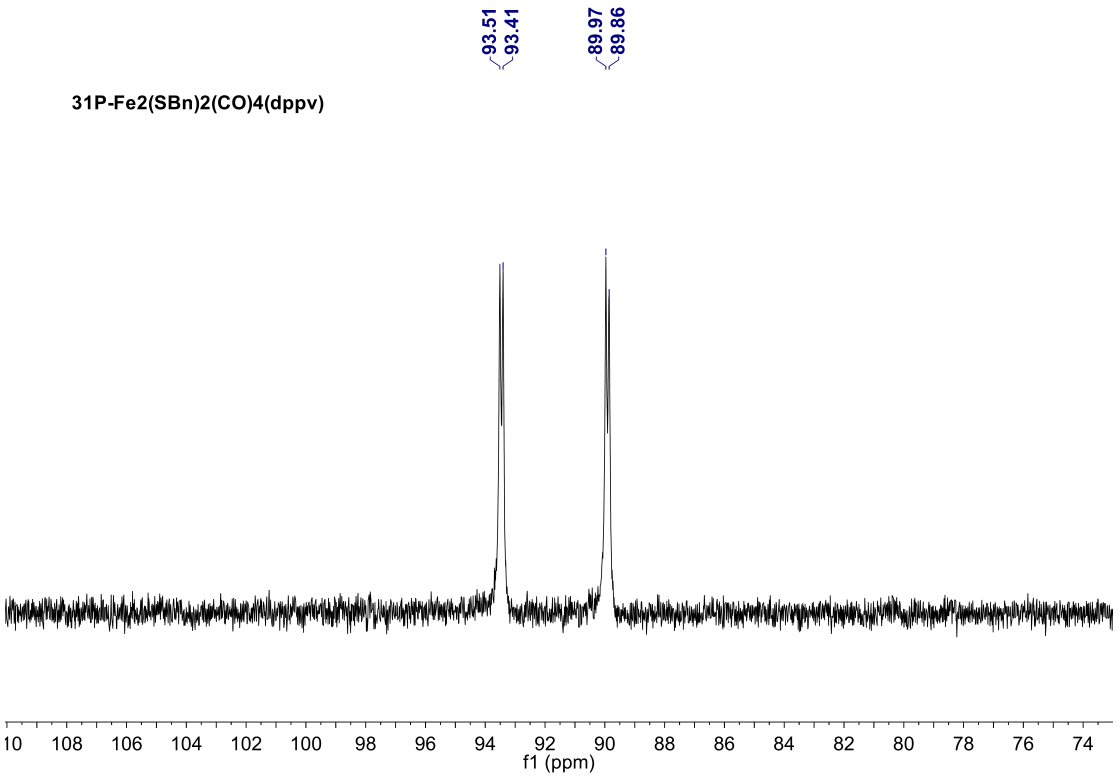


Figure S16. 202 MHz ^{31}P NMR spectrum of $Fe_2(SBn)_2(CO)_4(dppv)$ in CD_2Cl_2 solution.

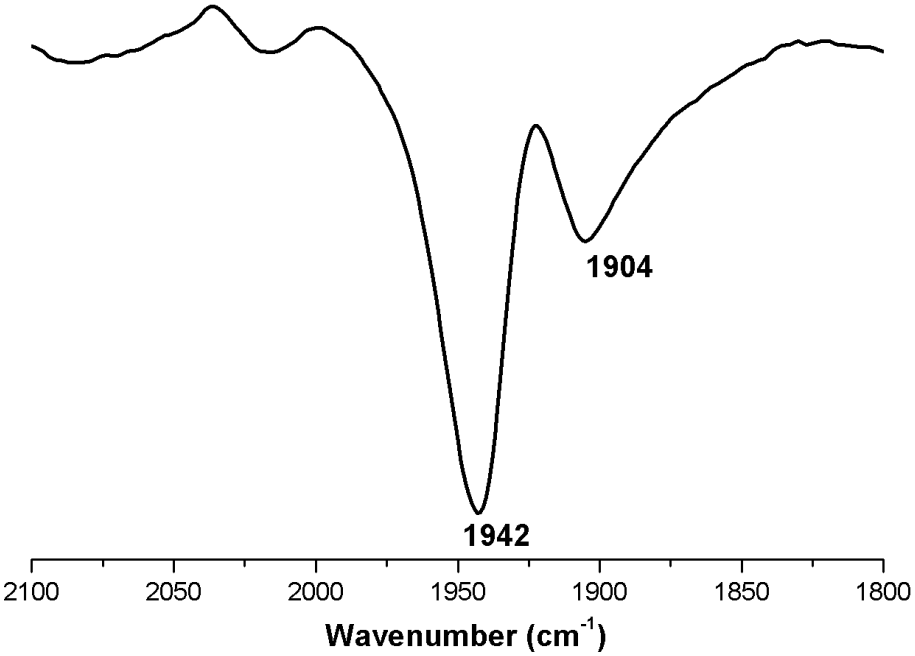


Figure S17. FT-IR spectrum of $[Fe_2(SBn)_2(CO)_2(dppv)_2]BF_4$ ([**3**]BF_4) in CH_2Cl_2 solution. *Assignments:* ν_{CO} = 1942, 1904 cm^{-1}.

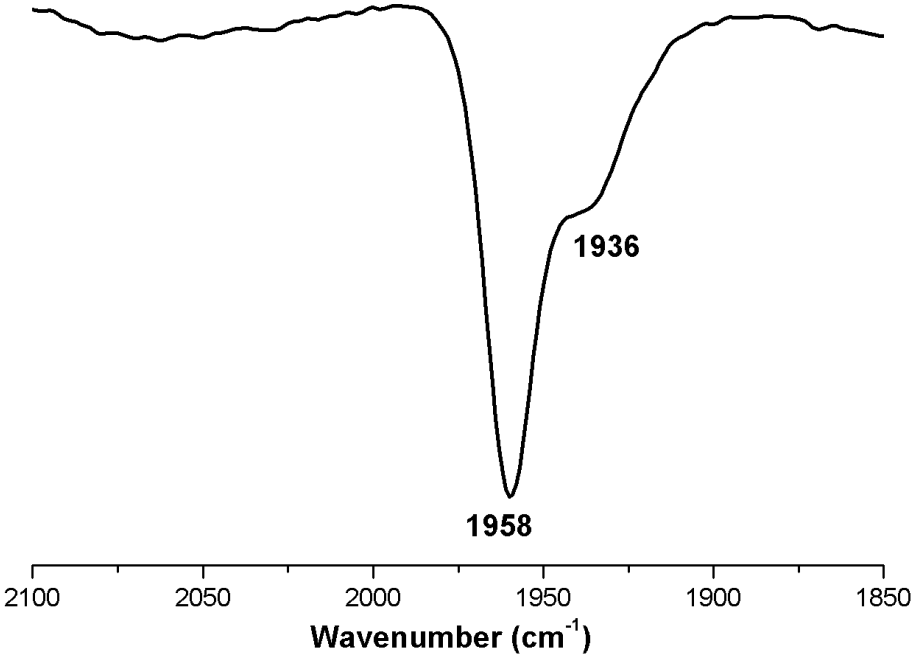


Figure S18. FT-IR spectrum of $[Fe_2(SBn)(S)(CO)_2(dppv)_2]BF_4$ ([**4**]BF_4) in CH_2Cl_2 solution. *Assignments:* ν_{CO} = 1958, 1936 cm^{-1}.

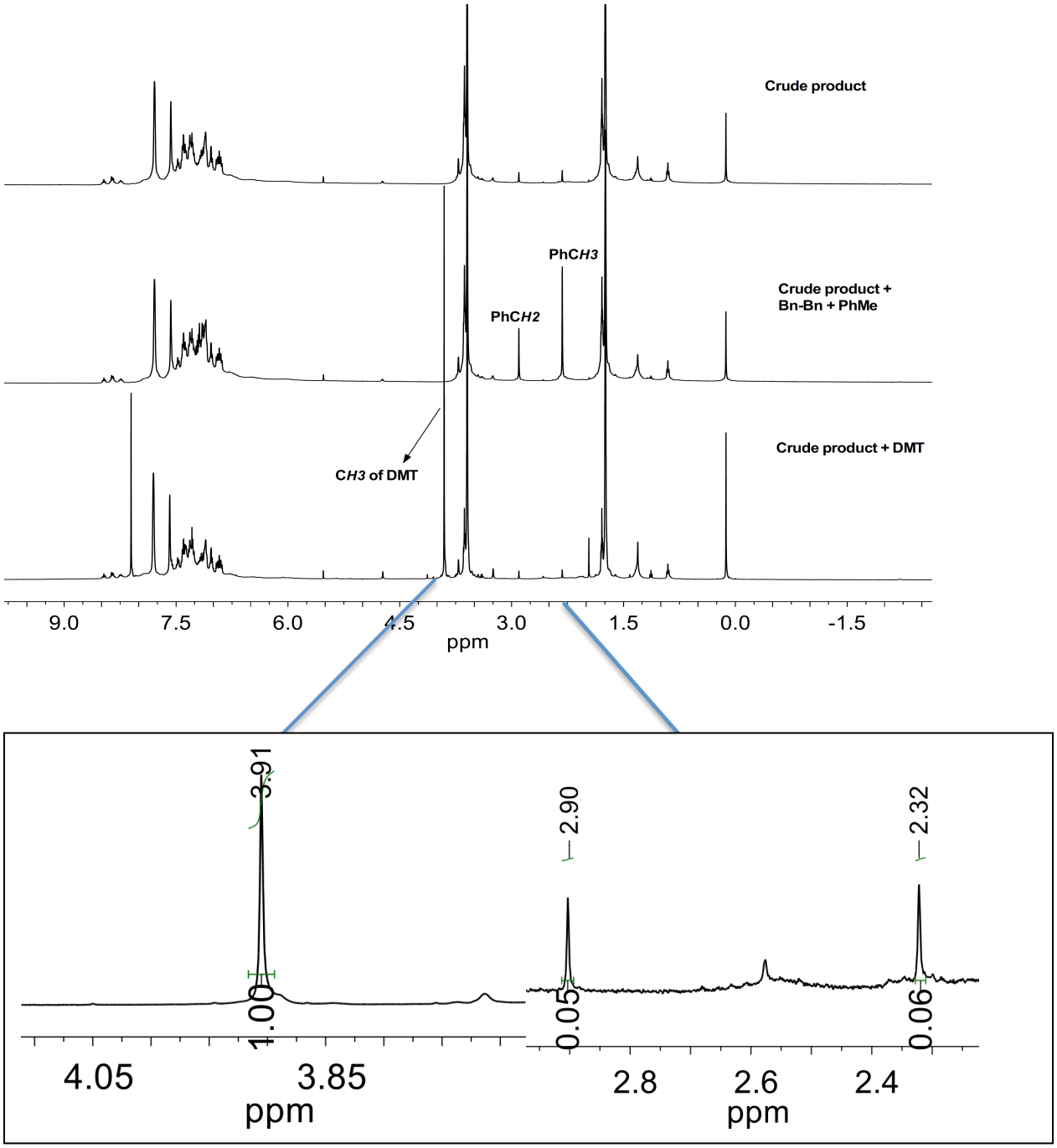


Figure S19. ^{1}H NMR spectrum of 7 mg of crude $[Fe_2(SBn)(S)(CO)_2(dppv)_2]BAr^F{}_4$ ([3]BAr_4F) and 1 mg DMT (dimethyl terephthalate) in (d_8-THF solution) followed by the addition of dibenzyl and toluene to confirm assignments.

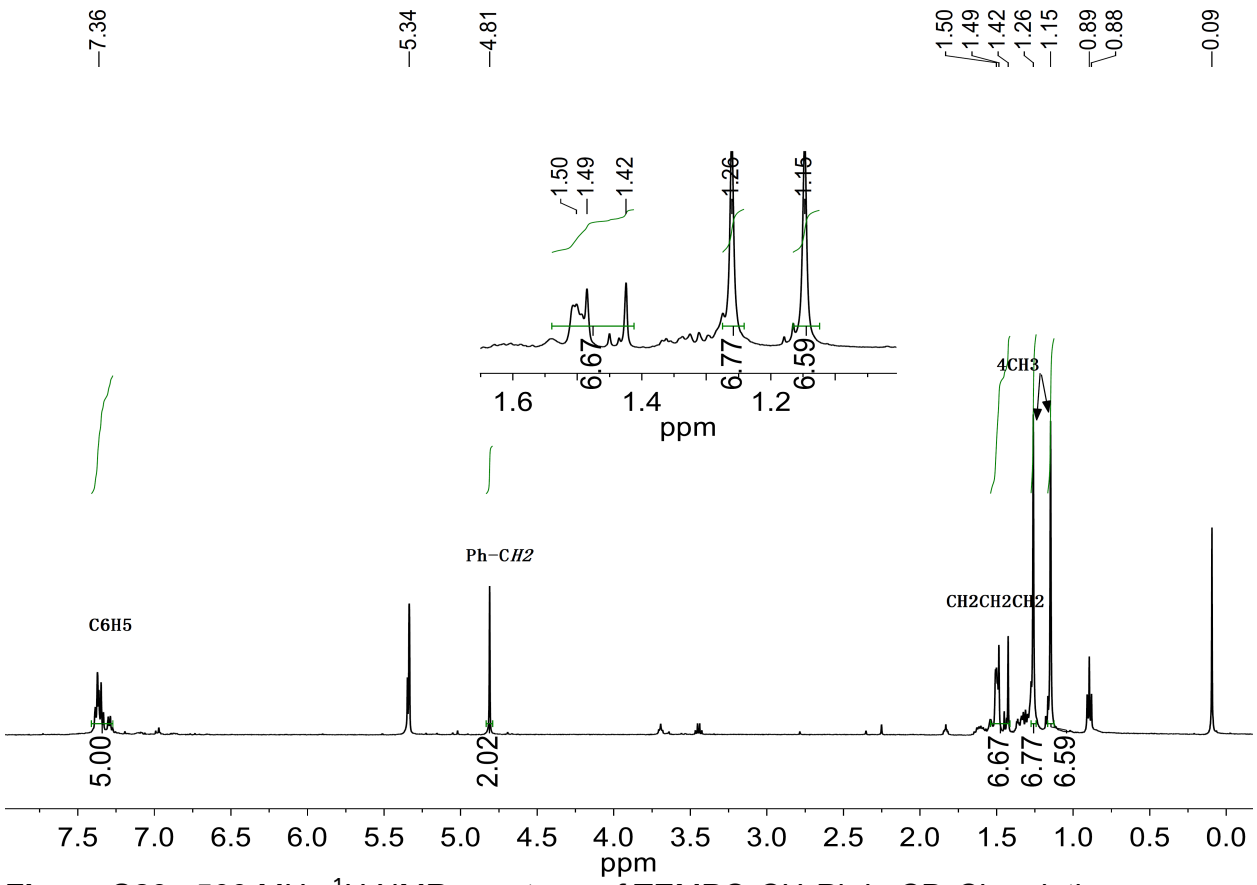


Figure S20. 500 MHz ^{1}H NMR spectrum of TEMPO-CH_2Ph in CD_2Cl_2 solution. *Assignments*: δ = 7.27-7.38 (m, 5H, C_6H_5), 4.81 (s, 2H, PhCH_2), 1.42-1.59 (m, 6H, $CH_2CH_2CH_2$), 1.15, 1.26 (2s, 12H, 4CH_3).

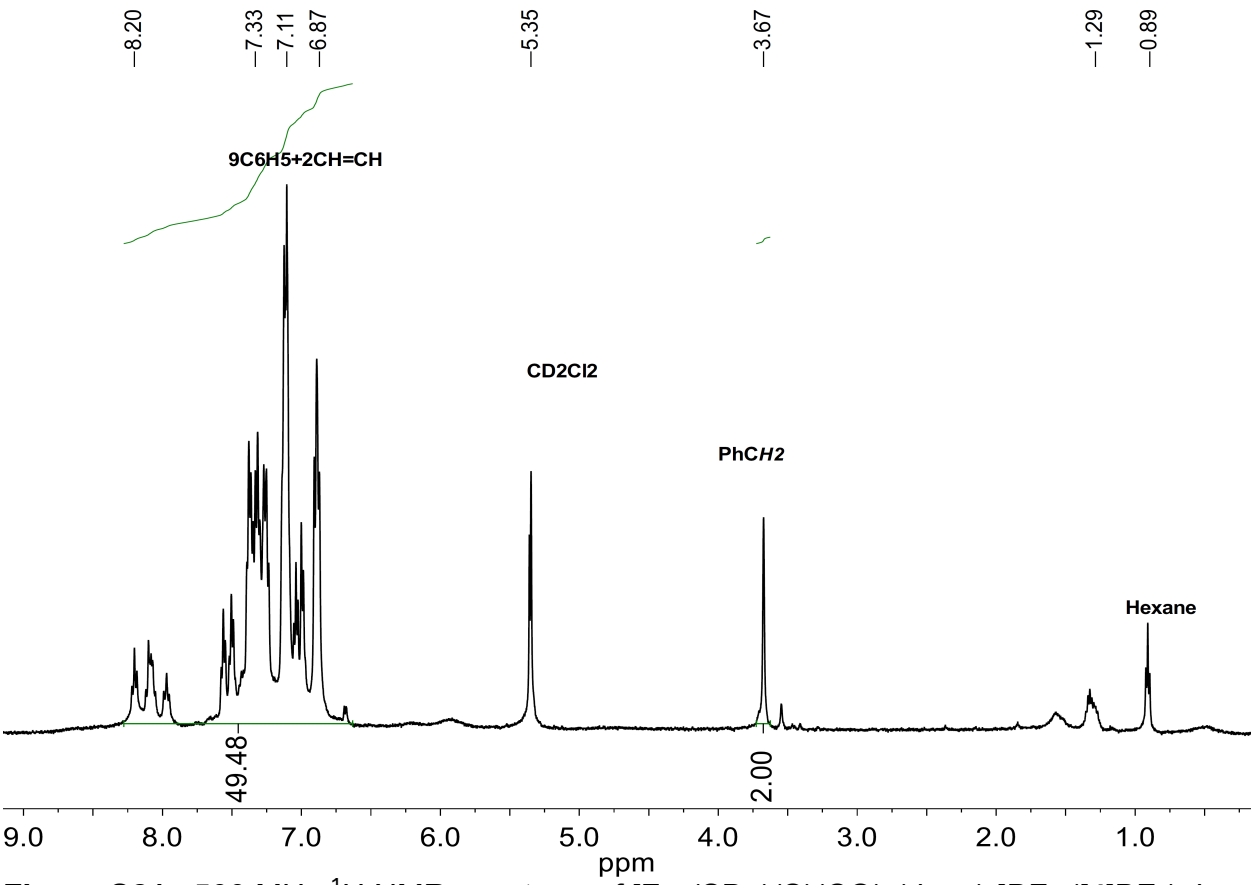


Figure S21. 500 MHz ^{1}H NMR spectrum of $[Fe_2(SBn)(S)(CO)_2(dppv)_2]BF_4$ ([**4**]BF_4) in CD_2Cl_2 solution at 20 ºC.
Assignments: δ = 8.20-6.87, (m, 49H, 9C6H5, 2CH=CH); 3.67(s, 2H, CH2).

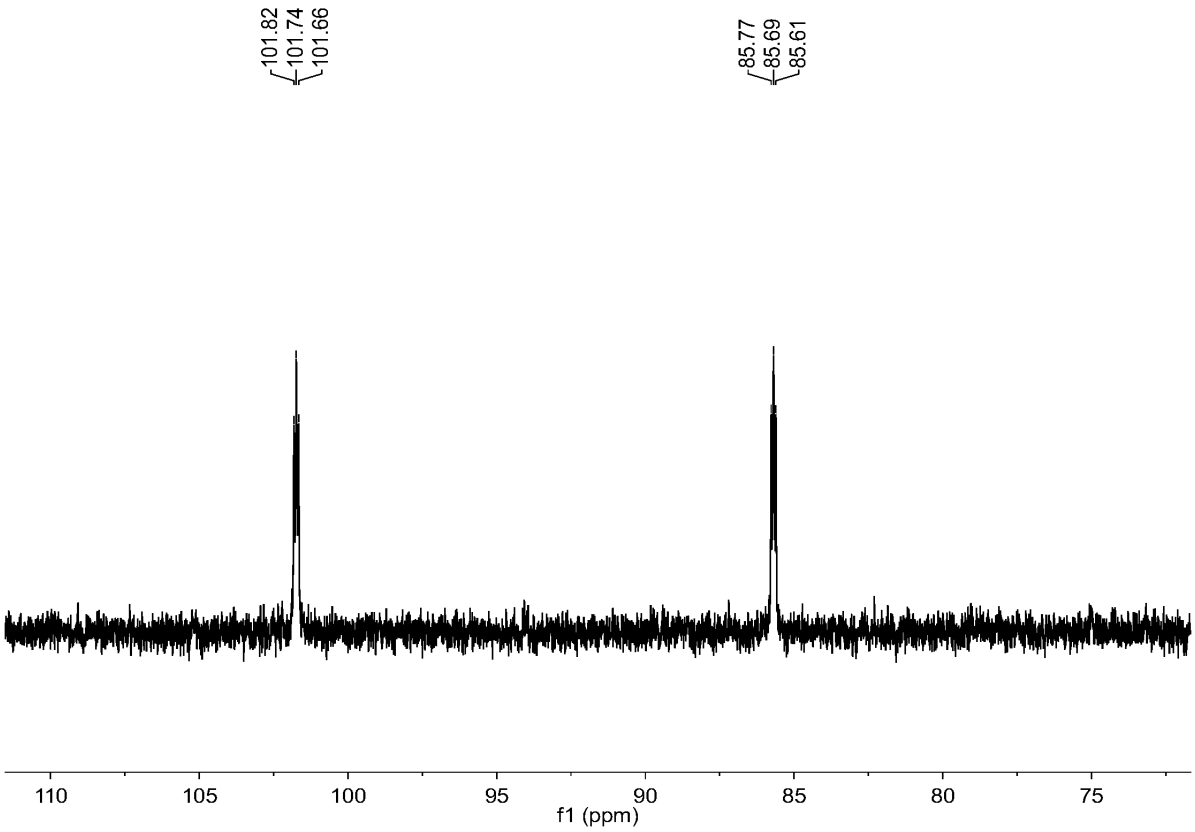


Figure S22. 202 MHz ^{31}P NMR spectrum of $[Fe_2(SBn)(S)(CO)_2(dppv)_2]BF_4$ ([**4**]BF_4) in CD_2Cl_2 solution at 20 ºC. *Assignments:* δ = 101.7 (t, $J_{p\text{-}p}$ = 20 Hz), 85.6 (t, $J_{p\text{-}p}$ = 20 Hz).

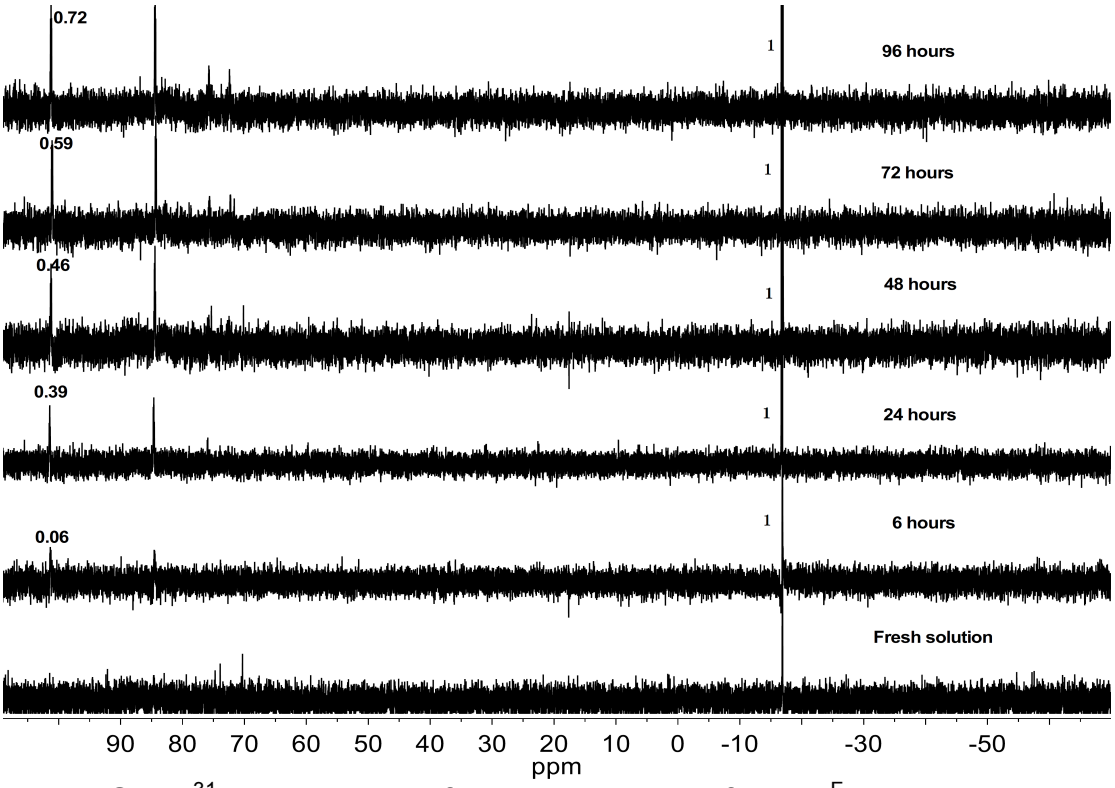


Figure S23. ^{31}P NMR spectra for the conversion of [**3**]BAr^F_4 (8 mg) in d_6-benzene (0.6 mL) to [**4**]BAr^F_4 in presence of $OP(OPh)_3$ (2 mg).

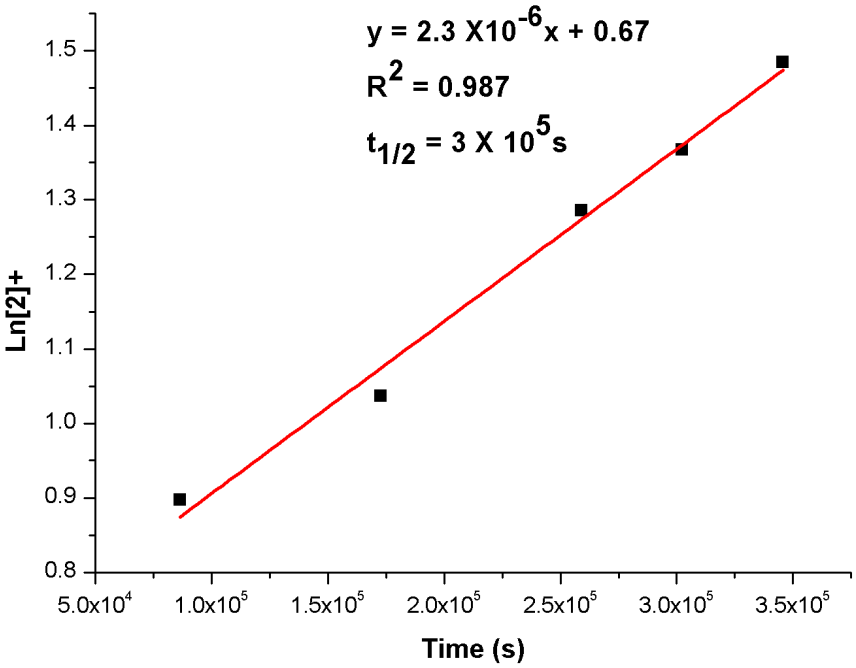


Figure S24. Time course for the appearance of $[Fe_2(SBn)(S)(CO)_2(dppv)_2]BAr^F{}_4$ from the decomposition of a C_6D_6 solution of $[Fe_2(SBn)_2(CO)_2(dppv)_2]BAr^F{}_4$.

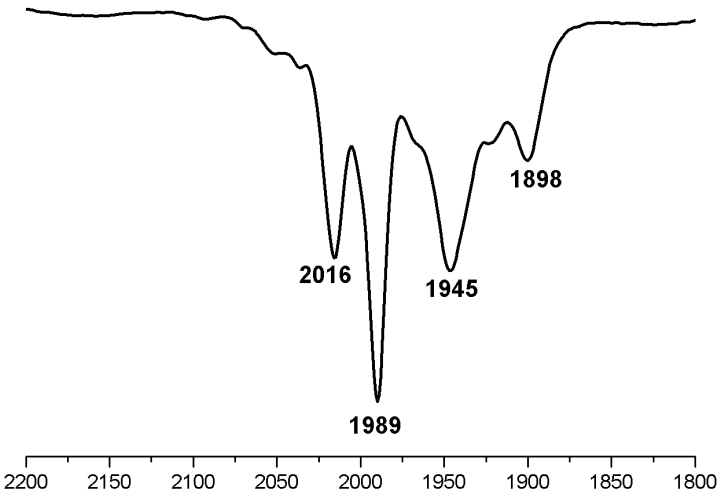


Figure S25. FT-IR spectrum of $[Fe_2(SBn)(S)(CO)_4(dppv)_2]BF_4$ ([**5**]BF_4) in CH_2Cl_2 solution. *Assignments:* ν_{CO} = 2016, 1989, 1945, 1898 cm^{-1}.

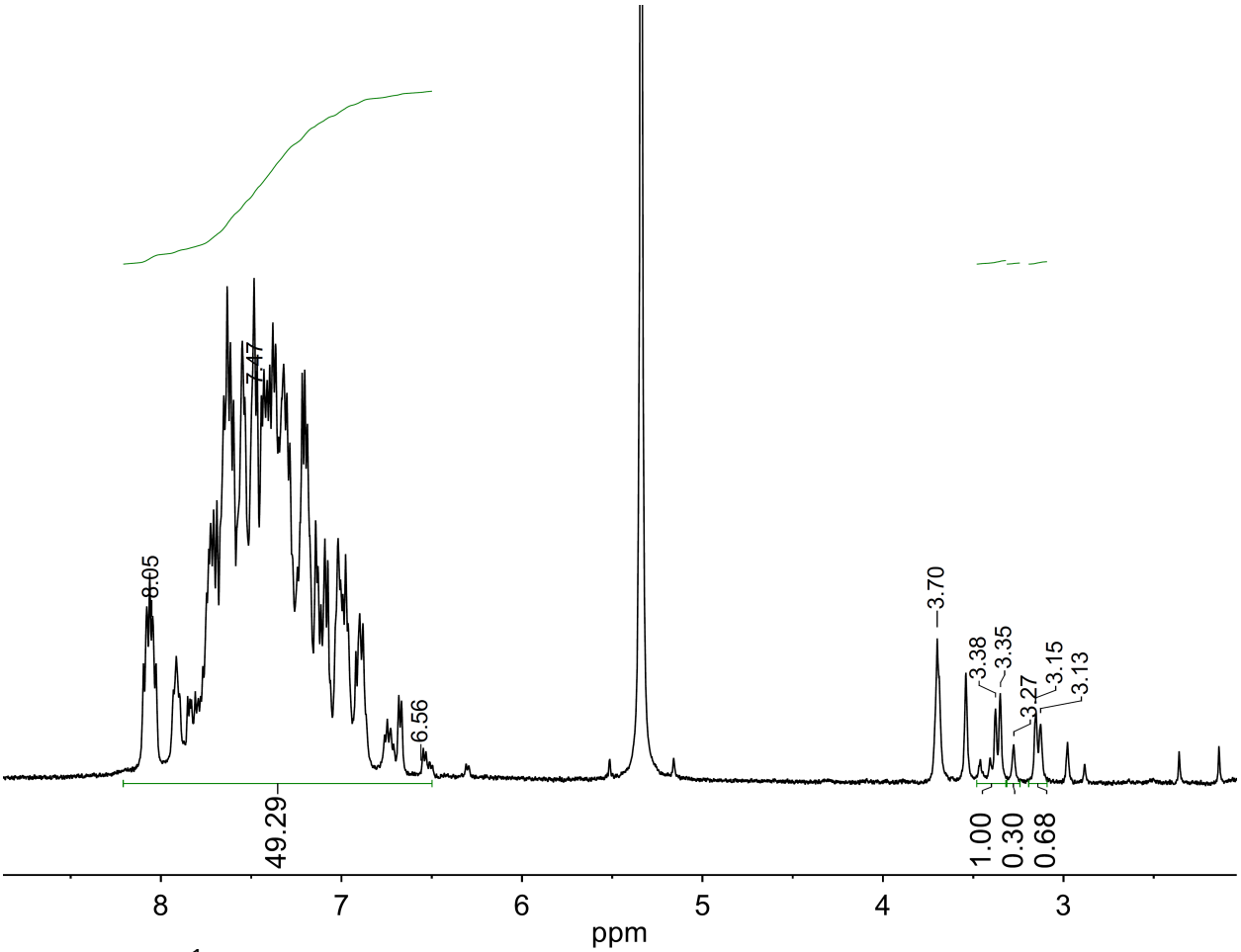


Figure S26. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2) of $[Fe_2(SBn)(S)(CO)_4(dppv)_2]BF_4$ ([**5**]BF_4) at 20 ºC.
Assignments: δ 8.05-6.56, (m, 49H, $9C_6H_5$, PC*H*=C*H*P); 3.38, 3.35, 3.27, 3.15, 3.13 (2H, CH_2).

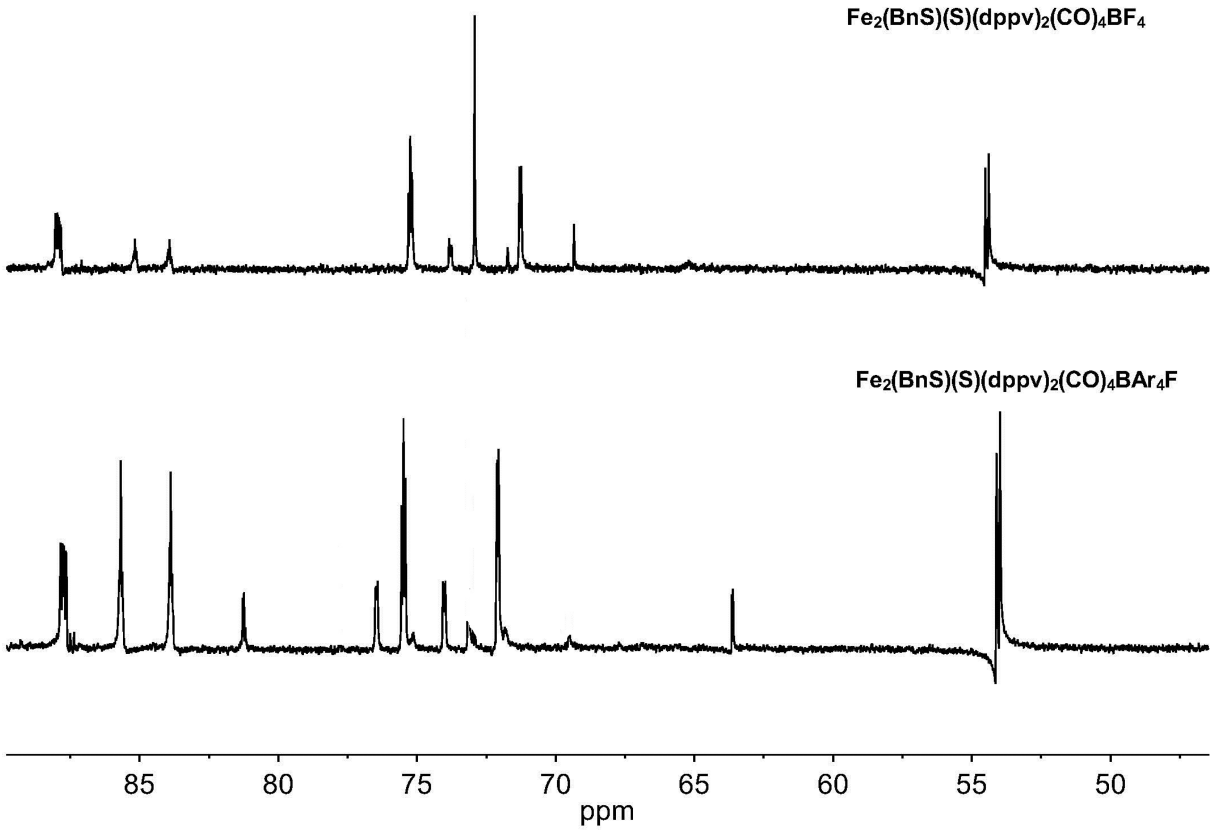
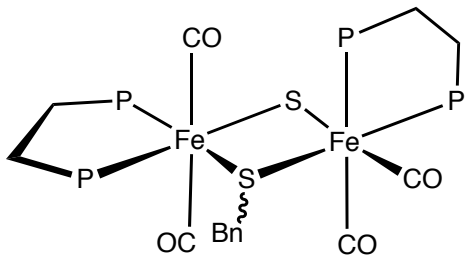


Figure S27. *Top:* 202 MHz ^{31}P NMR spectrum of [**5**]BF_4 in CD_2Cl_2 solution at 20 ºC. *Assignments:* δ = 88.6, 85.6, 84.9, 75.89. 74.42. 72.30, 71.82, 55.03. Signals at δ =73.5 and 69.9 are for $[Fe_2(SBn)_2(\mu\text{-}Cl)(CO)_2(dppv)_2]BF_4$ and $[Fe_2(SBn)_2(\mu\text{-}OH)(CO)_2(dppv)_2]BF_4$).
Bottom: 202 MHz ^{31}P NMR spectrum of [**4**]$BAr^F{}_4$ in d_6-benzene solution at 20 ºC.
Below: one of four possible dibasal/apical-basal isomers. Other isomeric possibilities include many bis(apical-basal) isomers and an all-basal isomer.



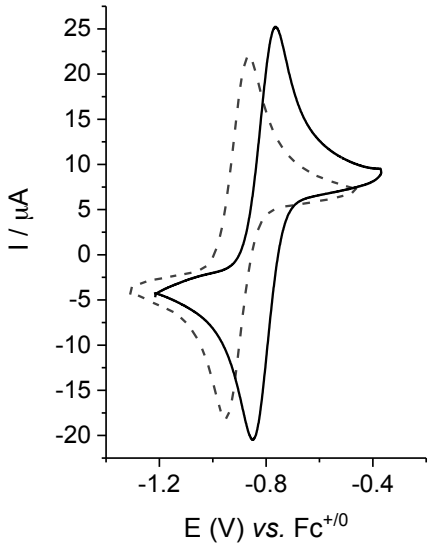


Figure S28. Cyclic voltammograms of [**1**]^0 (dash) and [**3**]^0 (solid). *Conditions:* 2.7 mM complex, 0.3 M $TBAPF_6$ in CH_2Cl_2 with scan rate of 100 mV/s.

Compound	$E_{1/2}$ (V) vs $Fc^{+/0}$	ΔE_p	i_{pa}/i_{pc}
[3]^0 (R = Bn)	-0.81	79	1
[2]^0 (R = Ph)	-0.85	79	1
[1]^0 (R = Me)	-0.9	86	1
[2]$^+$	-0.81	78	1
[3]$^+$	-1.1	77	0.95

II. X-ray Crystallography

Table S1. Crystal data and structure refinement for [**3**]^0 and [**3**]BF_4, [**4**]$BF_4 \cdot 2CH_2Cl_2$, and [**5**]$BF_4 \cdot CH_2Cl_2$.

Identification code	$[1]^0$	$[1]BF_4$	
Empirical formula	$C_{69}H_{60}Cl_2Fe_2O_2P_4S_2$	$C_{68}H_{58}BF_4Fe_2O_2P_4S_2$	
Formula weight	1291.77	1293.65	
Temperature	100(2) K	100(2) K	
Wavelength	0.71073 Å	0.71073 Å	
Crystal system	Triclinic	Monoclinic	
Space group	P-1	$P2_1$	
Unit cell dimensions	a = 12.7351(4) Å α= 86.3827(6)°	a = 12.6009(3) Å α= 90°	
	b = 13.0341(4) Å β= 74.4047(6)°	b = 18.6756(4) Å β= 109.0281(4)°	
	c = 20.9862(6) Å γ = 61.9885(5)°	c = 13.4119(3) Å γ = 90°	
Volume	2954.02(16) Å^3	2983.75(12) Å^3	
Z	2	2	
Density (calculated)	1.452 Mg/m^3	1.440 Mg/m^3	
Absorption coefficient	0.808 mm^{-1}	0.723 mm^{-1}	
F(000)	1336	1334	
Crystal size	0.306 x 0.161 x 0.062 mm^3	0.330 x 0.125 x 0.096 mm^3	
Theta range for data collection	2.309 to 28.349°	2.709 to 28.342°	
Index ranges	-16≤h≤17, -17≤k≤17, -28≤l≤28	-16≤h≤16, -24≤k≤24, -17≤l≤17	
Reflections collected	203271	96860	
Independent reflections	14711 [R(int) = 0.0545]	14832 [R(int) = 0.0313]	
Completeness to theta = 25.242°	99.9 %	99.8 %	
Absorption correction	Numerical	Numerical	
Max. and min. transmission	0.9602 and 0.8458	0.9561 and 0.8400	
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	
Data / restraints / parameters	14711 / 0 / 730	14832 / 188 / 779	
Goodness-of-fit on F^2	1.044	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0286, wR2 = 0.0640	R1 = 0.0218, wR2 = 0.0534	
R indices (all data)	R1 = 0.0374, wR2 = 0.0677	R1 = 0.0231, wR2 = 0.0540	
Absolute structure parameter	n/a	-0.007(2)	
Extinction coefficient	n/a	n/a	
Largest diff. peak and hole	0.402 and -0.380 e.Å^{-3}	0.425 and -0.390 e.Å^{-3}	

Identification code	[**2**]$BF_4 \cdot 2CH_2Cl_2$	[**3**]$BF_4 \cdot CH_2Cl_2$
Empirical formula	$C_{63}H_{55}BCl_4F_4Fe_2O_2P_4S_2$	$C_{64}H_{53}BCl_2F_4Fe_2O_4P_4S_2$
Formula weight	1372.38	1343.47
Temperature	100(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/n$
Unit cell dimensions	a = 10.3348(2) Å α= 90°	a = 11.9296(4) Å α= 90°
	b = 27.0056(6) Å β= 103.1233(6)°	b = 24.6134(7) Å β= 101.8542(6)°
	c = 22.3320(5) Å γ = 90°	c = 20.8732(6) Å γ = 90°
Volume	6070.0(2) $Å^3$	5998.2(3) $Å^3$
Z	4	4
Density (calculated)	1.502 Mg/m^3	1.488 Mg/m^3
Absorption coefficient	0.885 mm^{-1}	0.810 mm^{-1}
F(000)	2808	2752
Crystal size	0.465 x 0.109 x 0.076 mm^3	0.24 x 0.142 x 0.11 mm^3
Theta range for data collection	2.405 to 25.384°	2.405 to 28.336°
Index ranges	-11≤h≤12, -32≤k≤32, -26≤l≤26	-15≤h≤15, -32≤k≤32, -27≤l≤27
Reflections collected	73393	112208
Independent reflections	11140 [R(int) = 0.0394]	14912 [R(int) = 0.0370]
Completeness to theta = 25.242°	99.9 %	99.9 %
Absorption correction	Numerical	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.8523	0.94807 and 0.89941
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	11140 / 120 / 795	14912 / 113 / 780
Goodness-of-fit on F^2	1.070	1.083
Final R indices [I>2sigma(I)]	R1 = 0.0370, wR2 = 0.0984	R1 = 0.0307, wR2 = 0.0739
R indices (all data)	R1 = 0.0441, wR2 = 0.1028	R1 = 0.0366, wR2 = 0.0775
Extinction coefficient	n/a	n/a
Largest diff. peak and hole	0.654 and -0.980 $e.Å^{-3}$	0.718 and -0.892 $e.Å^{-3}$

Intensity data for [**3**]^0 were collected on a Bruker D8 Venture kappa diffractometer equipped with a Photon 100 CMOS detector. An Iμs microfocus source provided the Mo Kα radiation (λ = 0.71073 Å) that was monochromated with multilayer mirrors. The sample was mounted on a 0.3 mm loop with the minimal amount of Paratone-N oil. Data was collected as a series of φ and/or ω scans. Data were collected at 100 K using a cold stream of N_2. The collection, cell refinement, and integration of intensity data were carried out with the APEX3 software (1). A face-indexed absorption correction was performed numerically with SADABS (2). The structure was solved with intrinsic phasing methods using SHELXS (3) and refined with the full-matrix least-squares program SHELXL (3). All H atoms were included as riding idealized contributors.

Intensity data for [**3**]BF_4 were collected on a Bruker D8 Venture kappa diffractometer equipped with a Photon 100 CMOS detector. An Iμs microfocus source provided the Mo Kα radiation (λ = 0.71073 Å) that was monochromated with multilayer mirrors. The sample was mounted on a 0.3 mm loop with the minimal amount of Paratone-N oil. Data were collected as a series of φ and/or ω scans. Data were collected at 100 K using a cold stream of N_2. The collection, cell refinement, and integration of intensity data were carried out with the APEX3 software (1). A face-indexed absorption correction was performed numerically with SADABS (2). The structure was solved with direct methods using SHELXS (3) and refined with the full-matrix least-squares program SHELXL (3). One phenyl ring was found to be disordered over two orientations. The disordered phenyl rings were constrained to be perfect hexagons. Similar displacement amplitudes (esd 0.005) were imposed on disordered sites overlapping by less than the sum of van der Waals radii. Similarity restraints (esd 0.01 Å) were also imposed on the C---C bond distances connecting the disordered phenyl rings to the ligand phosphorus atom. The site occupancy ratio of the two phenyl ring orientations was allowed to freely refine; at convergence the ratio was 0.69(2):0.31(2). All H atoms were included as riding idealized contributors. On the basis of 7189 unmerged Friedel opposites, the fractional contribution of the racemic twin was negligible (4,5). The absolute structure parameter y was calculated using PLATON (6). The resulting value was y = -0.012(2) indicating that the absolute structure has probably been determined correctly.

Intensity data for [**4**]BF_4 were collected on a Bruker D8 Venture kappa diffractometer equipped with a Photon 100 CMOS detector. An Iμs microfocus source provided the Mo Kα radiation (λ = 0.71073 Å) that was monochromated with multilayer mirrors. The sample was mounted on a 0.3 mm loop with the minimal amount of Paratone-N oil. Data was collected as a series of φ and/or ω scans. Data was collected at 100 K using a cold stream of N_2. The collection, cell refinement, and integration of intensity data was carried out with the APEX3 software (1). A face-indexed absorption correction was performed numerically with SADABS (2). The structure was solved with intrinsic phasing methods using SHELXT (7) and refined with the full-matrix least-squares program SHELXL (3). Both of the dichloromethane solvate molecules were modeled as disordered over two orientations. Similar displacement amplitudes (esd 0.005) were imposed on disordered sites overlapping by less than the sum of van der Waals radii. The 1,2 and 1,3 distances of the minor disordered components were restrained (esd 0.01, 0.02 Å) to be similar to the major disordered components. The site occupancy ratio of the disordered sites was allowed to freely refine. At convergence, the ratios were 0.821(7):0.179(7) for the solvate molecule containing C62 and 0.551(4):0.449(4) for the solvate molecule containing C63. All H atoms were included as riding idealized contributors.

Intensity data for [**5**]BF_4 were collected on a Bruker D8 Venture kappa diffractometer equipped with a Photon 100 CMOS detector. An Iμs microfocus source provided the Mo Kα radiation (λ =

0.71073 Å) that was monochromated with multilayer mirrors. The sample was mounted on a 0.3 mm loop with the minimal amount of Paratone-N oil. Data were collected as a series of φ and/or ω scans. Data was collected at 100 K using a cold stream of N_2. The collection, cell refinement, and integration of intensity data were carried out with the APEX3 software .[1] A semi-empirical absorption correction was performed with SADABS. The structure was solved with intrinsic methods using SHELXT and refined with the full-matrix least-squares program SHELXL. One Cl atom on the dichloromethane solvate molecule was disordered over 2 orientations. The disordered C---Cl bond distances and Cl-C-Cl bond angles were restrained to be similar (esd 0.01 Å and 0.02° respectively). The displacement parameters for the 2 Cl positions were constrained to be equivalent. The disordered BF_4 had disordered rotation about the B1-F1 bond. F 2, 3, and 4 were disordered over 2 orientations. All B---F bond distances and F-B-F bond angles were restrained to be similar (esd 0.02 Å and 0.04° respectively). Similar displacement amplitudes (esd 0.01) were imposed on F disordered sites overlapping by less than the sum of van der Waals radii. All H atoms were included as riding idealized contributors.

References

(1) Bruker (2016). APEX3. Bruker AXS, Inc., Madison, Wisconsin, USA.

III. Selected DFT-Calculated Bond Distances

Table S2. Main geometrical parameters of $[Fe_2(SCH_2Ph)_2(CO)_{6-x}(PMe_3)_x]]^{0/+}$ and $[Fe_2(adt)(CO)_{6-x}(PMe_3)_x]]^{0/+}$ (x = 0 or 4). Selected distances in Å. For cationic forms, both rotated and unrotated isomers are presented, together with their relative in-solvent (CH_2Cl_2) energies (in kcal/mol).

	$[Fe_2(adt)(CO)_6]^0$	**$[Fe_2(adt)(CO)_2(PMe_3)_4]]^0$**	**$[Fe_2(SCH_2Ph)_2(CO)_6]^0$**	**$[Fe_2(SCH_2Ph)_2(CO)_2(PMe_3)_4]^0$**
Fe-Fe	2.552	2.661	2.546	2.668
Fe-S_{avg}	2.295	2.302	2.297	2.307
S-C	1.907 – 1.906	1.901 – 1.895	1.892 – 1.885	1.879 – 1.872

	$[Fe_2(adt)(CO)_6]^+$ rotated	**$[Fe_2(adt)(CO)_2(PMe_3)_4]]^+$ rotated**	**$[Fe_2(SCH_2Ph)_2(CO)_6]^+$ rotated**	**$[Fe_2(SCH_2Ph)_2(CO)_2(PMe_3)_4]^+$ rotated**
Fe-Fe	2.617	2.688	2.632	2.657
Fe-S_{avg}	2.288	2.305	2.287	2.308
S-C	1.971 – 1.961	1.920 – 1.915	1.905 – 1.900	1.884 – 1.877
	$[Fe_2(adt)(CO)_6]^+$ unrotated	**$[Fe_2(adt)(CO)_2(PMe_3)_4]]^+$ unrotated**	**$[Fe_2(SCH_2Ph)_2(CO)_6]^+$ unrotated**	**$[Fe_2(SCH_2Ph)_2(CO)_2(PMe_3)_4]^+$ unrotated**
Fe-Fe	2.667	-	2.648	2.834
Fe-S_{avg}	2.269	-	2.275	2.301
S-C	1.975 – 1.972	-	1.922 – 1.902	1.885 – 1.872
ΔE (unrot-rot)	-0.8	-	-0.2	+2.7

Notes:

Both 4-substituted species ($Fe_2(adt)(CO)_2(PMe_3)_4$ and $Fe_2(SCH_2Ph)_2(CO)_2(PMe_3)_4$) feature PMe_3 ligands in bis-(apical-basal) disposition.

In $Fe_2(SCH_2Ph)_2(CO)_6$ and $Fe_2(SCH_2Ph)_2(CO)_2(PMe_3)_4$ the two benzyl groups are in anti disposition.

Rotated isomer of cationic forms appears to be definitely stable only in substituted (with some donor L replacing CO) derivatives. Indeed, rotated $[Fe_2(SCH_2Ph)_2(CO)_2(PMe_3)_4]^+$ is ca 3 kcal/mol more stable that the unrotated isomer and unrotated $[Fe_2(adt)(CO)_2(PMe_3)_4]]^+$ has not even been found as stable structure at the BP86/TZVP level.

In contrast, in all-CO H_{ox}-like species, rotated and unrotated isomers are predicted to be nearly isoenergetic (independently of the nature of $(SR)_2$).

IV. DFT Results vs Level of Theory

Table S3. Calculated redox potentials for the couple $[\mathbf{3}]^{+/0}$ referred to the Fc/Fc^{+} couple (V).

	Exp	BP86, ΔE_{solv}	BP86, ΔG_{solv}	BP86-D3 ΔE_{solv}	BP86-D3 ΔG_{solv}	B3LYP ΔE_{solv}	B3LYP ΔG_{solv}
$[\mathbf{3}]^{+/0}$	-0.81	-0.800	-0.727	-0.853	-0.785	-1.299	-1.231

Table S4. Calculated S-C homolysis energies at various levels of theory.

Complex	BP86		BP86-D3		B97-D		M06-L	
	$Fe^{I}Fe^{I}$	$Fe^{II}Fe^{I}$	$Fe^{I}Fe^{I}$	$Fe^{II}Fe^{I}$	$Fe^{I}Fe^{I}$	$Fe^{II}Fe^{I}$	$Fe^{I}Fe^{I}$	$Fe^{II}Fe^{I}$
$[Fe_2(SCH_2Ph)_2(CO)_6]^z$	23.7	7.4	35.4	18.1	29.6	11.0	25.1	18.1
$[Fe_2(SCH_2Ph)_2(CO)_4(PMe_3)_2]^z$	13.7	2.7	30.2	10.7	22.2	6.7	23.1	13.8
$[Fe_2(SCH_2Ph)_2(CO)_2(PMe_3)_4]^z$	5.2	-2.5	18.8	8.8	14.3	-1.9	12.9	9.0
$[Fe_2(SCH_2Ph)_2(CO)_2(dppv)_2]^z$	1.2	-8.9	22.1	8.3	16.0	-2.0	10.5	3.4

V. XYZ Coordinates of DFT-Optimized Geometries (Gas Phase) BP86/TZVP

$Fe_2(SBn)_2(CO)_2(dppv)_2$

C	-1.241778	-4.519625	2.861659
C	-0.168220	-5.122903	2.188128
C	0.309399	-6.365261	2.641759
C	-0.276950	-6.985254	3.748390
C	-1.348724	-6.379954	4.411828
C	-1.830474	-5.146744	3.965274
P	0.697249	-4.296824	0.750278
C	0.050320	-2.546048	0.883338
C	0.625656	-1.589073	1.737570
C	0.117393	-0.287878	1.794405
C	-0.977241	0.074474	1.003896
C	-1.559352	-0.871538	0.156100
C	-1.046017	-2.170217	0.091749
Fe	1.004915	-5.157585	-1.306102
S	0.989945	-6.222811	-3.328871
C	1.056024	-5.042901	-4.818342
C	1.843984	-5.637435	-5.949354
C	1.196480	-6.213654	-7.054715
C	1.930803	-6.759840	-8.111433
C	3.328278	-6.741151	-8.080850
C	3.986322	-6.163229	-6.988941
C	3.250602	-5.614128	-5.936371
Fe	-1.074882	-6.426007	-2.363677
P	-1.838978	-7.953574	-3.793693
C	-1.103439	-9.664731	-3.812599
C	-1.791274	-10.764972	-3.271923
C	-1.191233	-12.027471	-3.222340
C	0.102255	-12.210669	-3.717626
C	0.796466	-11.120828	-4.255396
C	0.205431	-9.855602	-4.294388
C	-3.616712	-8.311471	-3.415946
C	-4.139857	-7.723192	-2.336837
P	-3.011472	-6.715821	-1.249715
C	-3.246023	-7.794327	0.270131
C	-4.108197	-7.476156	1.329894
C	-4.328367	-8.390804	2.365931

C	-3.700173	-9.637600	2.351615
C	-2.848188	-9.966362	1.292701
C	-2.617401	-9.050895	0.263845
C	-2.051554	-7.599330	-5.626475
C	-2.612173	-6.362033	-5.989961
C	-2.885633	-6.069548	-7.328893
C	-2.603405	-7.007672	-8.326844
C	-2.048941	-8.241375	-7.974644
C	-1.774853	-8.536803	-6.634388
C	-4.111284	-5.256837	-0.893491
C	-5.154672	-4.907096	-1.765112
C	-5.942005	-3.778339	-1.516603
C	-5.696540	-2.984417	-0.393447
C	-4.648298	-3.316024	0.471130
C	-3.854715	-4.437415	0.217791
S	0.223939	-7.225599	-0.640136
C	1.314024	-8.745396	-1.018443
C	1.793656	-9.381755	0.253319
C	0.964712	-10.264205	0.969349
C	1.391789	-10.853678	2.160314
C	2.666201	-10.573771	2.666254
C	3.503616	-9.701158	1.965061
C	3.071464	-9.112935	0.772443
P	3.200933	-4.932320	-0.947285
C	4.105393	-3.535803	-1.817813
C	3.720270	-2.210929	-1.547241
C	4.345296	-1.142914	-2.194758
C	5.358579	-1.378985	-3.129406
C	5.746448	-2.691983	-3.406445
C	5.128238	-3.763171	-2.752375
C	0.785062	-3.591287	-2.042063
O	0.653943	-2.556819	-2.577413
C	2.374788	-4.117588	1.536779
C	3.459835	-4.398485	0.808496
C	4.466657	-6.293978	-1.155990
C	5.515295	-6.511676	-0.245417
C	6.456374	-7.521102	-0.470101
C	6.371334	-8.324454	-1.611459
C	5.334037	-8.115068	-2.524480

C	4.385738	-7.111791	-2.296798
H	0.667449	-9.427993	-1.582129
H	2.142196	-8.434683	-1.663842
H	3.736248	-8.439677	0.231210
H	4.504136	-9.480933	2.343057
H	3.003050	-11.034330	3.596844
H	0.729341	-11.537619	2.695061
H	-0.031446	-10.485605	0.584360
H	1.513370	-4.113997	-4.461093
H	0.022557	-4.832855	-5.113134
H	3.768754	-5.145054	-5.096204
H	5.077377	-6.132775	-6.963559
H	3.901851	-7.163684	-8.907861
H	1.407104	-7.196955	-8.963910
H	0.105580	-6.226407	-7.089447
H	-4.200640	-8.954407	-4.081707
H	2.450807	-3.799563	2.580900
H	4.466644	-4.264327	1.213519
H	-5.179618	-7.870530	-2.028579
H	2.923936	-2.006404	-0.829889
H	4.031546	-0.121778	-1.971424
H	5.842353	-0.543754	-3.638899
H	6.538709	-2.889232	-4.131079
H	5.458394	-4.780537	-2.964647
H	5.608546	-5.901024	0.651614
H	7.258126	-7.678650	0.253604
H	7.106435	-9.111853	-1.784999
H	5.251906	-8.739247	-3.415783
H	3.567976	-6.967522	-3.006137
H	1.479413	-1.848445	2.363793
H	0.581961	0.444557	2.457535
H	-1.369808	1.092470	1.043767
H	-2.407560	-0.599557	-0.474160
H	-1.492213	-2.892620	-0.593405
H	1.139814	-6.851867	2.130803
H	0.106017	-7.949025	4.086685
H	-1.803863	-6.866031	5.276703
H	-2.662689	-4.662636	4.479911
H	-1.606282	-3.543760	2.538970

H	-5.351534	-5.512360	-2.651218
H	-6.749503	-3.521137	-2.204671
H	-6.314273	-2.107096	-0.194843
H	-4.441156	-2.694351	1.343681
H	-3.035775	-4.681234	0.897040
H	-4.622292	-6.516281	1.349805
H	-5.002979	-8.124790	3.182228
H	-3.875698	-10.352855	3.157280
H	-2.360833	-10.942615	1.268529
H	-1.952085	-9.316277	-0.559185
H	-2.803057	-10.638574	-2.882318
H	-1.740448	-12.869746	-2.796430
H	0.569427	-13.196189	-3.679005
H	1.810893	-11.253900	-4.635945
H	0.768817	-9.007877	-4.689682
H	-1.344164	-9.505014	-6.378567
H	-1.828869	-8.983307	-8.745257
H	-2.818026	-6.778302	-9.372169
H	-3.319472	-5.102850	-7.590805
H	-2.841759	-5.620844	-5.224766
C	-1.732750	-4.960462	-3.041865
O	-2.176771	-3.961300	-3.475352

$[Fe_2(SBn)_2(CO)_2(dppv)_2]^+$

C	-1.237885	-4.648750	2.807746
C	0.006637	-5.140962	2.374889
C	0.643690	-6.122543	3.150183
C	0.051772	-6.602426	4.323264
C	-1.184729	-6.105012	4.742616
C	-1.828855	-5.124332	3.978971
C	0.622129	-4.641018	1.096315
S	1.174650	-2.840681	1.289876
Fe	3.418654	-2.303664	1.328308
C	4.857188	-1.374193	0.955406
O	5.789930	-0.744943	0.648357
S	3.456248	-3.424001	-0.646085
Fe	1.775308	-1.883993	-0.742862
P	2.059141	-1.263232	-2.911132
C	3.607026	-0.468776	-3.566837

C	5.126872	-3.179225	-1.511812
C	5.425666	-4.190002	-2.583343
C	5.714980	-3.765168	-3.889840
C	6.069390	-4.686478	-4.880045
C	6.137190	-6.049548	-4.579835
C	5.851111	-6.485880	-3.280785
C	5.503261	-5.563551	-2.292209
P	-0.361219	-1.212235	-1.108420
C	-1.549550	-2.456468	-1.812888
C	2.219563	-0.309634	-0.078888
O	2.352098	0.826240	0.197891
C	-1.359820	-0.316756	0.163913
C	-0.288511	0.050701	-2.461232
P	4.513712	-3.817016	2.593454
C	6.373555	-3.694219	2.590071
P	3.092227	-1.129157	3.285878
C	4.234163	0.290503	3.684853
C	4.104845	-3.466062	4.356880
C	4.304525	-5.670598	2.487193
C	1.460675	-0.493601	3.917143
C	3.487018	-2.317704	4.646373
C	1.629670	-2.541672	-4.198084
C	0.789282	0.037973	-3.250905
H	-0.120949	-4.617598	0.289089
H	1.472854	-5.253342	0.780389
H	1.604722	-6.523384	2.825107
H	0.558367	-7.372639	4.906554
H	-1.648556	-6.483299	5.654989
H	-2.800270	-4.737982	4.292866
H	-1.744220	-3.881757	2.219018
H	5.848626	-3.264185	-0.688689
H	5.168766	-2.157159	-1.902160
H	5.298492	-5.912636	-1.277856
H	5.913865	-7.547355	-3.034759
H	6.418321	-6.768433	-5.350975
H	6.297215	-4.336434	-5.887963
H	5.667987	-2.701531	-4.130673
H	0.923179	0.727896	-4.088155
H	3.207534	-2.057098	5.671172

H	4.382216	-4.174740	5.140441
H	-1.124671	0.740758	-2.605910
C	7.003577	-2.620519	3.241445
C	8.394343	-2.495737	3.206890
C	9.169505	-3.430853	2.514385
C	8.547362	-4.493807	1.854186
C	7.156339	-4.629487	1.893481
H	6.413530	-1.875447	3.777818
H	8.872468	-1.661995	3.723494
H	10.255690	-3.331572	2.490325
H	9.144377	-5.229130	1.312248
H	6.687348	-5.478461	1.394460
C	4.647989	-6.483120	3.583647
C	4.551730	-7.873584	3.494156
C	4.125310	-8.477173	2.306194
C	3.801331	-7.679879	1.206914
C	3.887985	-6.285503	1.297732
H	5.014478	-6.045606	4.512137
H	4.818671	-8.487137	4.356027
H	4.053666	-9.563529	2.238919
H	3.474124	-8.139205	0.272797
H	3.632697	-5.667497	0.435548
C	4.898294	0.372704	4.921079
C	5.723744	1.462572	5.211489
C	5.890183	2.487837	4.276745
C	5.228565	2.416197	3.048112
C	4.409341	1.323747	2.749540
H	4.781444	-0.412036	5.668227
H	6.234615	1.508697	6.174661
H	6.531708	3.340049	4.505666
H	5.351613	3.212079	2.311879
H	3.903031	1.284144	1.785600
C	0.517443	-1.415383	4.404208
C	-0.662124	-0.962644	4.998430
C	-0.917724	0.407978	5.100273
C	0.004920	1.326084	4.592749
C	1.190445	0.880077	4.002079
H	0.704719	-2.488027	4.334163
H	-1.378719	-1.687334	5.387637

H	-1.833323	0.760227	5.577392
H	-0.188193	2.397654	4.667842
H	1.914971	1.607285	3.635679
C	-1.149593	1.059168	0.354796
C	-1.947947	1.771993	1.253100
C	-2.952411	1.118914	1.972576
C	-3.145417	-0.255749	1.806939
C	-2.350605	-0.973247	0.909916
H	-0.368879	1.580846	-0.200862
H	-1.787141	2.842850	1.384707
H	-3.583624	1.680702	2.662391
H	-3.925300	-0.771825	2.368763
H	-2.527361	-2.039429	0.765809
C	-2.879029	-2.110851	-2.115666
C	-3.728562	-3.047726	-2.707689
C	-3.261283	-4.333656	-3.003975
C	-1.938552	-4.678243	-2.715496
C	-1.083778	-3.741487	-2.125388
H	-3.257209	-1.114687	-1.880673
H	-4.759042	-2.772552	-2.938374
H	-3.928965	-5.063722	-3.463927
H	-1.566932	-5.676214	-2.952127
H	-0.043469	-4.003751	-1.922838
C	0.759422	-2.244884	-5.261799
C	0.447873	-3.219846	-6.213757
C	0.995994	-4.501488	-6.113207
C	1.855293	-4.805789	-5.053498
C	2.165613	-3.835325	-4.097141
H	0.312137	-1.255379	-5.351266
H	-0.229025	-2.974997	-7.034027
H	0.751056	-5.261105	-6.857138
H	2.287981	-5.803368	-4.964476
H	2.828955	-4.093761	-3.272169
C	3.929907	-0.544782	-4.931970
C	5.048612	0.131945	-5.427272
C	5.857735	0.880205	-4.566585
C	5.543560	0.953348	-3.206631
C	4.423879	0.282290	-2.706558
H	3.312113	-1.135468	-5.609669

H	5.289521	0.069493	-6.489760
H	6.731902	1.404224	-4.955679
H	6.172186	1.530433	-2.527077
H	4.191499	0.347779	-1.644687

$Fe_2(SBn)(S)(CO)_2(dppv)_2$

C	0.041262	-6.611311	3.354852
C	0.858128	-6.710581	2.219372
C	1.733389	-7.803479	2.099382
C	1.785289	-8.779653	3.096424
C	0.964687	-8.678224	4.224662
C	0.095559	-7.591844	4.352165
P	0.928422	-5.376855	0.909357
C	-0.327997	-4.146088	1.514597
C	0.026697	-2.946333	2.150876
C	-0.958232	-2.034141	2.544031
C	-2.306744	-2.311830	2.307252
C	-2.666610	-3.501606	1.665881
C	-1.684893	-4.409649	1.263975
Fe	1.088596	-5.737730	-1.299729
S	1.139561	-6.347327	-3.490082
C	0.918467	-4.859770	-4.625971
C	1.401380	-5.122723	-6.029761
C	0.628042	-4.723199	-7.131207
C	1.094522	-4.894121	-8.438227
C	2.342076	-5.479561	-8.669829
C	3.118621	-5.892862	-7.581816
C	2.653621	-5.713985	-6.276854
Fe	-0.763652	-7.236784	-2.566928
C	-1.850081	-5.873572	-2.340195
O	-2.616224	-5.004382	-2.135442
P	-1.635292	-7.995858	-4.480260
C	-0.733790	-9.372634	-5.350908
C	-1.261831	-10.671577	-5.433568
C	-0.538442	-11.693374	-6.056964
C	0.719235	-11.430500	-6.605956
C	1.255220	-10.140647	-6.520353
C	0.539988	-9.119573	-5.891449
C	-3.270654	-8.778876	-4.084744

C	-3.530995	-9.023149	-2.796320
P	-2.165693	-8.651655	-1.590295
C	-1.703860	-10.419507	-1.190811
C	-2.576057	-11.243123	-0.458245
C	-2.274906	-12.593837	-0.263583
C	-1.102506	-13.136032	-0.800446
C	-0.235720	-12.322175	-1.534938
C	-0.534000	-10.970435	-1.733130
C	-2.172417	-6.904539	-5.902879
C	-2.808459	-5.685034	-5.615196
C	-3.318494	-4.891898	-6.647579
C	-3.199098	-5.304714	-7.978532
C	-2.567704	-6.516788	-8.270943
C	-2.057528	-7.313093	-7.240909
C	-3.104298	-8.130821	-0.079057
C	-4.315052	-7.430881	-0.210636
C	-5.018672	-7.016578	0.924196
C	-4.514934	-7.288871	2.199918
C	-3.297461	-7.964000	2.335465
C	-2.589494	-8.377802	1.204101
S	0.775301	-7.961833	-1.107444
P	3.225519	-5.216749	-1.124518
C	3.872046	-3.809713	-2.157684
C	3.578728	-2.485803	-1.789106
C	3.990867	-1.418950	-2.591756
C	4.688712	-1.660527	-3.779321
C	4.975693	-2.975469	-4.158037
C	4.572505	-4.043966	-3.351955
C	0.551686	-4.084894	-1.596500
O	0.174297	-2.996692	-1.804974
C	2.537857	-4.626664	1.462621
C	3.547847	-4.581248	0.587267
C	4.597318	-6.471188	-1.303853
C	5.936095	-6.109599	-1.065319
C	6.952484	-7.061781	-1.164249
C	6.644231	-8.383165	-1.508619
C	5.317603	-8.744530	-1.754329
C	4.294718	-7.794271	-1.650828
H	1.515274	-4.060533	-4.164792

H	-0.132647	-4.549965	-4.615602
H	3.260948	-6.045739	-5.433075
H	4.093888	-6.354510	-7.750331
H	2.706474	-5.615783	-9.689718
H	0.475347	-4.573006	-9.277936
H	-0.351688	-4.272016	-6.961291
H	-3.971776	-9.013881	-4.891191
H	2.661965	-4.325613	2.507537
H	4.541996	-4.214287	0.859932
H	-4.456087	-9.499081	-2.457202
H	3.021025	-2.285900	-0.872573
H	3.758843	-0.395975	-2.290108
H	5.004637	-0.827296	-4.409332
H	5.515013	-3.173237	-5.086011
H	4.815866	-5.065289	-3.647738
H	6.191017	-5.077616	-0.816569
H	7.987515	-6.771116	-0.974118
H	7.439641	-9.126857	-1.586898
H	5.070524	-9.772225	-2.027314
H	3.253566	-8.076359	-1.830160
H	1.074993	-2.708606	2.334778
H	-0.667022	-1.102461	3.032853
H	-3.074573	-1.598086	2.611303
H	-3.715245	-3.721275	1.460423
H	-1.976883	-5.322391	0.742370
H	2.370605	-7.894505	1.219517
H	2.467024	-9.625079	2.987594
H	1.007200	-9.441783	5.003748
H	-0.541703	-7.499590	5.234184
H	-0.640222	-5.767020	3.465189
H	-4.711144	-7.204339	-1.202287
H	-5.962857	-6.480993	0.808912
H	-5.066346	-6.969995	3.086249
H	-2.889406	-8.167884	3.326360
H	-1.636863	-8.897521	1.317809
H	-3.488365	-10.828576	-0.026208
H	-2.957832	-13.222578	0.311146
H	-0.866606	-14.190671	-0.646067
H	0.682311	-12.736887	-1.954959

H	0.147814	-10.330823	-2.294808
H	-2.238881	-10.894244	-5.002154
H	-0.963417	-12.697456	-6.112390
H	1.282240	-12.227704	-7.094703
H	2.239852	-9.925971	-6.939480
H	0.978380	-8.122615	-5.817532
H	-1.564715	-8.254720	-7.483426
H	-2.466533	-6.847599	-9.306340
H	-3.597105	-4.684333	-8.783667
H	-3.809552	-3.947169	-6.406845
H	-2.911873	-5.350565	-4.583210

$[Fe_2(SBn)(S)(CO)_2(dppv)_2]^+$

C	4.165406	-7.798196	-1.673017
C	4.526020	-6.480615	-1.363510
C	5.884394	-6.157153	-1.184785
C	6.862290	-7.145380	-1.310386
C	6.496725	-8.460626	-1.618415
C	5.150373	-8.783357	-1.802450
P	3.231844	-5.165155	-1.147979
C	3.615398	-4.501326	0.534108
C	2.662895	-4.563228	1.470169
P	1.057047	-5.366495	1.030310
Fe	1.100488	-5.743251	-1.200258
C	0.562580	-4.081867	-1.467691
O	0.133761	-3.017156	-1.665052
C	1.061776	-6.726147	2.300475
C	0.223323	-6.699186	3.424407
C	0.321888	-7.701501	4.395693
C	1.255135	-8.731145	4.253359
C	2.096502	-8.757851	3.135931
C	2.001108	-7.762187	2.162574
C	-0.230987	-4.180786	1.627244
C	0.098780	-2.955101	2.226667
C	-0.910446	-2.069415	2.616922
C	-2.252554	-2.398898	2.411946
C	-2.585792	-3.616504	1.809698
C	-1.582080	-4.501316	1.410920
S	1.095257	-6.342356	-3.392808

Fe	-0.806597	-7.263780	-2.535959
S	0.530148	-7.837228	-0.904645
C	0.932403	-4.868307	-4.545116
C	1.449924	-5.141350	-5.936675
C	0.772391	-4.601939	-7.041311
C	1.277187	-4.754845	-8.335588
C	2.463645	-5.461824	-8.549535
C	3.141612	-6.014482	-7.458334
C	2.640949	-5.851926	-6.163784
C	-1.917546	-5.931172	-2.412610
O	-2.634433	-5.026452	-2.221672
P	-1.645122	-7.954595	-4.509182
C	-2.074295	-6.842193	-5.936222
C	-2.764448	-5.643521	-5.685574
C	-3.219831	-4.858379	-6.748199
C	-2.991410	-5.259639	-8.068286
C	-2.305248	-6.449939	-8.321661
C	-1.847170	-7.239790	-7.263140
P	-2.307523	-8.679996	-1.623953
C	-3.268858	-8.118021	-0.150763
C	-4.476370	-7.421227	-0.319788
C	-5.202518	-6.994202	0.795988
C	-4.723866	-7.250423	2.084172
C	-3.510046	-7.924833	2.255367
C	-2.779047	-8.353486	1.144872
C	-0.703306	-9.353327	-5.282306
C	-1.252037	-10.643914	-5.360869
C	-0.521586	-11.685092	-5.941503
C	0.760484	-11.449366	-6.443366
C	1.313629	-10.166747	-6.362047
C	0.591350	-9.123609	-5.779574
C	-3.301236	-8.702384	-4.166772
C	-3.612741	-8.982567	-2.897782
C	-1.847166	-10.433529	-1.212917
C	-2.764336	-11.254168	-0.532542
C	-2.472350	-12.602978	-0.318485
C	-1.268246	-13.143360	-0.782136
C	-0.357475	-12.331232	-1.462798
C	-0.644748	-10.980671	-1.682594

C	3.815969	-3.794822	-2.249540
C	3.522321	-2.463597	-1.906612
C	3.913363	-1.418188	-2.746393
C	4.589978	-1.691362	-3.939529
C	4.880454	-3.013632	-4.287684
C	4.498332	-4.062883	-3.446920
H	1.526127	-4.076227	-4.066399
H	-0.114287	-4.544941	-4.566663
H	3.177133	-6.286854	-5.318188
H	4.069013	-6.568391	-7.615149
H	2.858024	-5.581932	-9.559709
H	0.738626	-4.321484	-9.179934
H	-0.157622	-4.051377	-6.885341
H	-3.975843	-8.900399	-5.004614
H	2.838200	-4.243775	2.501561
H	4.612073	-4.098974	0.736420
H	-4.558311	-9.451316	-2.610112
H	2.989548	-2.238124	-0.981088
H	3.686657	-0.388075	-2.467730
H	4.891708	-0.874180	-4.596277
H	5.407972	-3.232349	-5.217046
H	4.747118	-5.089409	-3.717701
H	6.185982	-5.132226	-0.962512
H	7.912787	-6.887007	-1.168251
H	7.263243	-9.231006	-1.716425
H	4.860652	-9.806472	-2.047160
H	3.112252	-8.050392	-1.810694
H	1.140934	-2.677185	2.386681
H	-0.643463	-1.118135	3.079885
H	-3.037785	-1.704474	2.714366
H	-3.630680	-3.876835	1.636600
H	-1.853491	-5.442374	0.929090
H	2.661793	-7.792256	1.294739
H	2.830525	-9.556803	3.020802
H	1.332812	-9.508843	5.014676
H	-0.328621	-7.668932	5.271452
H	-0.501581	-5.894147	3.549823
H	-4.859153	-7.213387	-1.320675
H	-6.146946	-6.465917	0.655801

H	-5.296611	-6.926414	2.954405
H	-3.129856	-8.123658	3.258154
H	-1.835493	-8.882642	1.286966
H	-3.701501	-10.840549	-0.157008
H	-3.187607	-13.231875	0.213957
H	-1.041313	-14.196946	-0.611660
H	0.583734	-12.747395	-1.825052
H	0.069817	-10.348104	-2.209498
H	-2.249339	-10.845305	-4.968161
H	-0.960381	-12.682333	-6.001079
H	1.328261	-12.263044	-6.897312
H	2.314429	-9.974942	-6.751920
H	1.037972	-8.129533	-5.719643
H	-1.315914	-8.167014	-7.475690
H	-2.123074	-6.771132	-9.348227
H	-3.351029	-4.647276	-8.896643
H	-3.759234	-3.932831	-6.540568
H	-2.965420	-5.319233	-4.665271

$Fe_2(SBn)_2(CO)_2(PMe_3)_4$

C	6.025117	-2.909864	-4.286412
C	5.111377	-3.522128	-3.425573
C	4.296937	-2.756679	-2.570731
C	4.425685	-1.358427	-2.612835
C	5.336652	-0.741181	-3.477147
C	6.143666	-1.515551	-4.314816
C	3.293302	-3.404557	-1.650736
S	4.055746	-4.791387	-0.633082
Fe	2.579646	-6.236625	0.361444
P	2.106806	-7.411627	-1.482126
Fe	4.258386	-4.622924	1.673700
P	2.914419	-2.943275	2.316772
C	4.405355	-4.961630	3.361848
O	4.568479	-5.188872	4.508561
P	6.230747	-3.564749	1.539004
S	4.552263	-6.895154	1.349130
P	1.605016	-7.590609	1.859163
C	1.182864	-5.223593	0.265738
O	0.224305	-4.532002	0.195154

H	5.418348	0.347555	-3.489568
H	2.834697	-2.666457	-0.989521
H	3.801042	-0.742225	-1.961296
H	6.861740	-1.038578	-4.984594
H	6.651276	-3.523553	-4.937149
H	5.040284	-4.610944	-3.391615
H	2.487537	-3.877399	-2.227281
C	0.534766	-8.427799	-1.584110
C	1.830149	-6.403870	-3.032449
C	3.320862	-8.663098	-2.161337
H	0.441836	-8.891635	-2.576848
H	0.527683	-9.223147	-0.828127
H	-0.331345	-7.774147	-1.412690
H	2.934080	-9.118633	-3.084541
H	4.271110	-8.161270	-2.384391
H	3.509874	-9.451009	-1.420358
H	1.572724	-7.053311	-3.881023
H	1.007741	-5.695781	-2.861413
H	2.736356	-5.836896	-3.279443
C	-0.255927	-7.698857	1.869706
C	2.069703	-9.398922	1.789851
C	1.896760	-7.290163	3.672646
C	7.142685	-3.229879	3.131206
C	7.593547	-4.368187	0.555265
C	6.291994	-1.875538	0.743202
H	-0.598925	-8.378789	2.662591
H	-0.675727	-6.701065	2.049241
H	-0.626833	-8.059008	0.903660
H	1.392107	-8.062856	4.271368
H	2.971677	-7.306229	3.884216
H	1.503781	-6.305599	3.948877
H	1.522859	-9.971520	2.552647
H	1.849911	-9.821573	0.801490
H	3.148121	-9.486152	1.974218
H	8.100265	-2.722916	2.940902
H	6.529578	-2.606434	3.793772
H	7.335969	-4.180178	3.645907
H	8.493117	-3.735614	0.562149
H	7.837084	-5.350475	0.979769

H	7.255090	-4.498919	-0.480856
H	7.314712	-1.471311	0.767447
H	5.965544	-1.957963	-0.301636
H	5.621635	-1.177800	1.260625
C	3.662421	-1.763796	3.564477
C	2.121319	-1.686946	1.182662
C	1.405598	-3.430101	3.303301
H	2.903770	-1.058065	3.932303
H	4.058989	-2.336656	4.412478
H	4.486050	-1.193823	3.116027
H	0.871970	-2.538830	3.666890
H	0.733006	-4.025076	2.675961
H	1.724894	-4.034286	4.161710
H	1.593133	-0.930137	1.780352
H	2.886617	-1.184283	0.578269
H	1.398431	-2.184475	0.524934
C	5.903783	-7.452223	0.174175
C	7.146299	-7.996324	0.851169
H	5.455332	-8.239096	-0.446685
H	6.146523	-6.612176	-0.491310
C	8.054490	-8.751814	0.085869
C	9.219827	-9.271329	0.653331
C	9.506114	-9.042294	2.003896
C	8.611718	-8.297895	2.777074
C	7.441736	-7.781989	2.206495
H	7.848243	-8.930454	-0.972636
H	9.904927	-9.858411	0.037978
H	10.417514	-9.445729	2.448399
H	8.821634	-8.121407	3.834541
H	6.732515	-7.223253	2.820727

$[Fe_2(SBn)_2(CO)_2(PMe_3)_4]^+$

C	4.910098	-4.361868	-4.160945
C	4.190901	-4.746396	-3.016829
C	3.279365	-5.811160	-3.125046
C	3.082785	-6.460681	-4.346190
C	3.799413	-6.063395	-5.480106
C	4.717483	-5.014208	-5.382703
C	4.473586	-4.073547	-1.695915

S	2.960119	-3.789797	-0.623011
Fe	1.605550	-1.931139	-0.575814
P	-0.532150	-1.071272	-0.583812
C	-1.731433	-1.569978	0.747784
Fe	3.385559	-2.601444	1.279838
P	4.372682	-4.246729	2.459576
C	3.431322	-5.083656	3.821472
S	1.117322	-2.918391	1.498357
C	0.396061	-4.622992	1.144216
C	0.059523	-5.424581	2.374620
C	0.396527	-6.788063	2.419377
C	0.037099	-7.580332	3.514278
C	-0.659348	-7.017422	4.587037
C	-0.998511	-5.660388	4.554833
C	-0.645086	-4.871946	3.457234
P	3.277431	-1.080410	3.013795
C	1.802217	0.055328	3.075421
C	2.485082	-0.508886	-0.021825
O	2.950112	0.571999	0.080506
C	3.202058	-1.690167	4.771964
C	4.676798	0.133035	3.095063
P	2.067923	-1.230587	-2.691573
C	1.541163	-2.370605	-4.057243
C	1.390557	0.408618	-3.258153
C	3.852019	-0.907709	-3.081981
C	-0.667853	0.774416	-0.420103
C	-1.590596	-1.455249	-2.070030
C	4.929255	-5.732283	1.491441
C	5.977160	-3.801644	3.287278
H	-0.511844	-4.410731	0.559954
H	1.089583	-5.166001	0.490157
H	0.933261	-7.237403	1.580077
H	0.299901	-8.639313	3.526763
H	-0.941739	-7.633481	5.441830
H	-1.548894	-5.216468	5.386104
H	-0.915837	-3.814438	3.439968
H	5.092030	-4.730426	-1.068753
H	5.032121	-3.140049	-1.823910
H	2.715956	-6.129459	-2.245936

H	2.371809	-7.286161	-4.411449
H	3.647346	-6.573593	-6.432223
H	5.290169	-4.703413	-6.257890
H	5.644815	-3.555543	-4.093444
H	3.928139	-0.408308	-4.057692
H	4.290633	-0.261579	-2.311747
H	4.410413	-1.845470	-3.127413
H	1.807454	-1.942578	-5.033821
H	2.042012	-3.338794	-3.936054
H	0.456768	-2.531340	-4.017375
H	1.735046	0.603657	-4.282962
H	0.296115	0.434435	-3.250286
H	1.773071	1.203066	-2.604027
H	4.526956	0.834120	3.927381
H	5.629758	-0.393210	3.233546
H	4.723708	0.693459	2.152992
H	1.818483	0.618240	4.018752
H	1.829561	0.759249	2.237747
H	0.881223	-0.539287	3.027168
H	3.170547	-0.827993	5.452614
H	2.289559	-2.283661	4.911531
H	4.072009	-2.303870	5.030974
H	6.392423	-4.675228	3.808380
H	6.697016	-3.462616	2.531067
H	5.838228	-2.992211	4.013754
H	5.323731	-6.494170	2.178114
H	4.088510	-6.151308	0.926303
H	5.725778	-5.448503	0.792644
H	4.072744	-5.832148	4.308080
H	3.094044	-4.359507	4.568834
H	2.547507	-5.580570	3.403176
H	-2.684291	-1.045335	0.591240
H	-1.913964	-2.651251	0.720691
H	-1.329530	-1.311392	1.733390
H	-1.716271	1.088292	-0.519574
H	-0.302255	1.062983	0.573998
H	-0.060126	1.291949	-1.168311
H	-2.583903	-0.999096	-1.956018
H	-1.140203	-1.086946	-2.998231

H	-1.708335	-2.544035	-2.152663
C	4.928253	-1.989609	0.750007
O	5.955700	-1.586425	0.362072

$Fe_2(SBn)(S)(CO)_2(PMe_3)_4$

C	5.471184	-1.915236	-4.147852
C	4.735427	-2.796860	-3.353012
C	3.775277	-2.320614	-2.441949
C	3.576441	-0.932307	-2.356680
C	4.311537	-0.046530	-3.151146
C	5.262894	-0.534754	-4.050525
C	2.936620	-3.264662	-1.618619
S	3.941583	-4.621396	-0.784171
Fe	2.636639	-6.224480	0.184920
P	2.383576	-7.397142	-1.684943
Fe	4.442487	-4.580789	1.484902
P	3.282618	-2.847099	2.347734
C	4.804590	-5.032620	3.117586
O	5.082066	-5.336586	4.220533
P	6.444744	-3.676791	1.124817
S	4.641771	-6.770997	1.028528
P	1.796945	-7.693133	1.640536
C	1.149876	-5.308602	0.135811
O	0.169332	-4.650915	0.133800
H	4.137521	1.027965	-3.067523
H	2.342011	-2.722690	-0.879828
H	2.824225	-0.541720	-1.667833
H	5.836869	0.153823	-4.673026
H	6.209866	-2.307492	-4.849583
H	4.913974	-3.871315	-3.423658
H	2.234202	-3.810967	-2.263545
C	0.980282	-8.611588	-1.905943
C	2.146036	-6.426579	-3.259646
C	3.845974	-8.448481	-2.154244
H	1.017169	-9.071291	-2.904644
H	1.032416	-9.407445	-1.152036
H	0.022974	-8.085460	-1.791758
H	3.696142	-8.945702	-3.124497
H	4.731469	-7.801739	-2.195779

H	4.020586	-9.199902	-1.374270
H	2.075816	-7.097201	-4.128433
H	1.223864	-5.834258	-3.189679
H	2.994089	-5.745000	-3.398664
C	-0.040625	-8.010604	1.592248
C	2.468974	-9.431223	1.627889
C	1.997655	-7.283224	3.442029
C	7.584485	-3.462720	2.580421
C	7.511900	-4.696662	-0.005235
C	6.584713	-2.000647	0.322302
H	-0.336654	-8.725498	2.373215
H	-0.573061	-7.063404	1.748303
H	-0.334665	-8.407408	0.613261
H	1.542159	-8.063176	4.069770
H	3.065259	-7.195871	3.672990
H	1.514660	-6.320712	3.650658
H	2.018051	-10.031933	2.431054
H	2.265032	-9.915524	0.664082
H	3.555836	-9.378153	1.770723
H	8.559798	-3.068644	2.259925
H	7.139990	-2.773581	3.309782
H	7.728959	-4.432334	3.073882
H	8.489138	-4.219375	-0.170403
H	7.647064	-5.690086	0.441043
H	6.988350	-4.823509	-0.961002
H	7.637486	-1.730719	0.152037
H	6.052073	-2.011857	-0.636956
H	6.123228	-1.239493	0.965370
C	4.192717	-1.854558	3.644297
C	2.551458	-1.434775	1.365362
C	1.776727	-3.322660	3.338633
H	3.519839	-1.138472	4.137763
H	4.611546	-2.531474	4.400275
H	5.018682	-1.299895	3.179420
H	1.308133	-2.439720	3.798597
H	1.053781	-3.816319	2.677495
H	2.074429	-4.026675	4.125868
H	2.214175	-0.639226	2.045999
H	3.297531	-1.025686	0.672980

H	1.685737	-1.790631	0.792192

$[Fe_2(SBn)(S)(CO)_2(PMe_3)_4]^+$

C	5.375767	-1.913484	-4.000742
C	4.643912	-2.798139	-3.205602
C	3.660793	-2.324998	-2.318939
C	3.425287	-0.941531	-2.260149
C	4.155011	-0.054168	-3.057493
C	5.135137	-0.537214	-3.927952
C	2.815046	-3.269332	-1.501953
S	3.813886	-4.613884	-0.645354
Fe	2.538368	-6.296043	0.213268
P	2.455109	-7.420973	-1.687126
Fe	4.502938	-4.547562	1.570141
P	3.515387	-2.689060	2.432788
C	5.011610	-4.925199	3.195821
O	5.349585	-5.193338	4.280420
P	6.477042	-3.684868	1.033779
S	4.379315	-6.720371	1.315283
P	1.565198	-7.813590	1.592415
C	0.995730	-5.492798	-0.022816
O	-0.010584	-4.902770	-0.126783
H	3.951902	1.016331	-3.001187
H	2.203434	-2.730665	-0.773076
H	2.647011	-0.554132	-1.599484
H	5.704347	0.152712	-4.552346
H	6.132047	-2.299787	-4.686188
H	4.843299	-3.870067	-3.268354
H	2.127273	-3.831596	-2.148794
C	1.200314	-8.764845	-1.943360
C	2.176486	-6.430862	-3.230788
C	4.051971	-8.287264	-2.056583
H	1.345523	-9.220576	-2.933211
H	1.301141	-9.547860	-1.182092
H	0.187701	-8.344456	-1.894445
H	4.001524	-8.796943	-3.029555
H	4.858841	-7.544268	-2.068861
H	4.268354	-9.016947	-1.267251
H	2.195060	-7.091786	-4.108649

H	1.200218	-5.931180	-3.184804
H	2.962343	-5.674409	-3.339228
C	-0.225349	-8.222525	1.320845
C	2.348545	-9.486872	1.754015
C	1.521956	-7.242620	3.356427
C	7.701136	-3.483186	2.409293
C	7.395558	-4.783521	-0.141421
C	6.551703	-2.035853	0.192676
H	-0.575421	-8.908377	2.104384
H	-0.822514	-7.302810	1.356749
H	-0.377361	-8.695740	0.344338
H	1.000333	-7.979695	3.982898
H	2.546912	-7.108378	3.721448
H	0.994013	-6.282718	3.417515
H	1.831726	-10.075479	2.524305
H	2.298796	-10.028850	0.801363
H	3.402032	-9.363570	2.033780
H	8.647441	-3.091430	2.010879
H	7.320593	-2.791225	3.170593
H	7.886713	-4.453593	2.886215
H	8.375450	-4.348936	-0.385681
H	7.532276	-5.768488	0.321504
H	6.802423	-4.902586	-1.055494
H	7.588436	-1.805802	-0.091433
H	5.923221	-2.045928	-0.706419
H	6.193118	-1.249670	0.869554
C	4.460027	-1.785020	3.754095
C	2.912844	-1.253133	1.416111
C	1.962865	-3.154299	3.340525
H	3.816573	-1.037343	4.237550
H	4.822799	-2.487172	4.514635
H	5.322919	-1.268346	3.313671
H	1.493074	-2.266662	3.787675
H	1.257378	-3.620150	2.640653
H	2.202322	-3.874017	4.133115
H	2.644479	-0.420900	2.081876
H	3.685440	-0.920002	0.713654
H	2.019863	-1.542188	0.849301

$Fe_2(SBn)(S)(CO)_6$

C	7.387370	2.369300	-0.930447
C	7.274201	1.063815	-1.414291
C	6.547616	0.097596	-0.699559
C	5.935933	0.468339	0.510152
C	6.047954	1.772667	0.994176
C	6.774020	2.727043	0.274194
C	6.415916	-1.304693	-1.215402
S	4.787400	-1.488530	-2.159200
Fe	4.301715	-3.647657	-2.748852
C	3.324852	-4.080822	-1.320622
O	2.695459	-4.357537	-0.391092
Fe	4.956895	-1.753412	-4.438088
C	4.731168	-0.044494	-4.911402
O	4.584266	1.058108	-5.224267
C	4.834607	-2.439229	-6.084066
O	4.756116	-2.871010	-7.152990
C	6.748298	-1.828537	-4.439204
O	7.905475	-1.880745	-4.451653
S	2.907141	-2.567584	-4.113646
C	3.935377	-5.115684	-3.704879
O	3.688267	-6.068085	-4.310399
C	5.891093	-4.276125	-2.199388
O	6.911399	-4.690792	-1.842947
H	5.571825	2.044430	1.937799
H	7.251566	-1.590996	-1.861947
H	5.369233	-0.274584	1.076523
H	6.864132	3.746215	0.653339
H	7.959244	3.108535	-1.493635
H	7.761647	0.788352	-2.352075
H	6.341638	-2.026064	-0.391294

$[Fe_2(SBn)(S)(CO)_6]^+$

C	7.387370	2.369300	-0.930447
C	7.274201	1.063815	-1.414291
C	6.547616	0.097596	-0.699559
C	5.935933	0.468339	0.510152
C	6.047954	1.772667	0.994176
C	6.774020	2.727043	0.274194

C	6.415916	-1.304693	-1.215402
S	4.787400	-1.488530	-2.159200
Fe	4.301715	-3.647657	-2.748852
C	3.324852	-4.080822	-1.320622
O	2.695459	-4.357537	-0.391092
Fe	4.956895	-1.753412	-4.438088
C	4.731168	-0.044494	-4.911402
O	4.584266	1.058108	-5.224267
C	4.834607	-2.439229	-6.084066
O	4.756116	-2.871010	-7.152990
C	6.748298	-1.828537	-4.439204
O	7.905475	-1.880745	-4.451653
S	2.907141	-2.567584	-4.113646
C	3.935377	-5.115684	-3.704879
O	3.688267	-6.068085	-4.310399
C	5.891093	-4.276125	-2.199388
O	6.911399	-4.690792	-1.842947
H	5.571825	2.044430	1.937799
H	7.251566	-1.590996	-1.861947
H	5.369233	-0.274584	1.076523
H	6.864132	3.746215	0.653339
H	7.959244	3.108535	-1.493635
H	7.434597	-11.103610	-8.716635
H	6.552967	-11.182023	-6.383493
H	5.364470	-9.218035	-5.436236
H	7.761647	0.788352	-2.352075
H	6.341638	-2.026064	-0.391294

$Fe_2(SBn)(S)(CO)_4(PMe_3)_2$

C	-0.214285	-2.566551	-6.369136
P	0.558639	-7.437815	-8.920856
S	2.971808	-7.064423	-6.754080
Fe	1.998439	-5.223148	-5.788765
Fe	2.041112	-5.780908	-8.400512
C	3.111022	-6.044262	-9.766300
O	3.831511	-6.150678	-10.677917
S	3.022928	-4.062376	-7.367828
C	0.980022	-4.625747	-9.208177
O	0.294545	-3.859754	-9.761022

C	2.955145	-5.264229	-4.310457
O	3.589713	-5.320026	-3.331800
C	0.587938	-6.187087	-5.304598
O	-0.334707	-6.826803	-4.977615
P	0.991128	-3.309172	-5.175488
C	2.131935	-1.896890	-4.810198
C	-1.213961	-7.190256	-8.423658
C	0.388556	-7.701085	-10.750650
C	0.897839	-9.159103	-8.321219
C	-0.006363	-3.412626	-3.613532
H	-1.843929	-8.005742	-8.807949
H	-1.290224	-7.159788	-7.330242
H	-1.573683	-6.235310	-8.827589
H	0.139542	-9.850884	-8.714868
H	1.894787	-9.470918	-8.656239
H	0.885926	-9.183208	-7.224971
H	-0.355059	-8.480431	-10.968593
H	0.079154	-6.762602	-11.229136
H	1.358804	-7.996344	-11.169937
H	1.561892	-1.001550	-4.525000
H	2.805630	-2.177667	-3.990564
H	2.735594	-1.685667	-5.701407
H	-0.432704	-2.433630	-3.352839
H	-0.819731	-4.138859	-3.739139
H	0.637525	-3.756156	-2.793500
H	-0.657534	-1.650476	-5.952818
H	0.306387	-2.331812	-7.305377
H	-1.009409	-3.291081	-6.585328
C	4.842755	-6.835116	-6.637027
H	5.045938	-6.740119	-5.563158
H	5.084201	-5.886895	-7.132099
C	5.564122	-8.013034	-7.220296
C	6.068642	-7.980378	-8.530927
C	6.736658	-9.085371	-9.065912
C	6.910768	-10.241829	-8.299268
C	6.414361	-10.286177	-6.991577
C	5.748603	-9.180920	-6.458355
H	5.940057	-7.080823	-9.134773
H	7.126066	-9.040280	-10.084586

H	7.434597	-11.103610	-8.716635
H	6.552967	-11.182023	-6.383493
H	5.364470	-9.218035	-5.436236

$[Fe_2(SBn)(S)(CO)_4(PMe_3)_2]^+$

Fe	3.551888	-9.760747	-7.307373
Fe	4.749006	-7.177261	-7.404401
P	6.502975	-6.734351	-8.794974
H	8.273231	-8.048939	-7.736416
C	2.607667	-12.975970	-6.464232
P	2.947731	-11.288780	-5.799705
C	4.258373	-11.545532	-4.526093
S	3.169438	-7.970670	-5.958194
C	3.658060	-6.215904	-8.427072
O	2.930401	-5.644839	-9.125458
S	5.646732	-9.131205	-7.109620
C	5.192520	-5.838772	-6.361827
O	5.514034	-4.986356	-5.648333
C	8.171974	-7.004826	-8.056078
C	6.573096	-4.987811	-9.393705
C	6.500140	-7.737927	-10.343780
C	1.942045	-9.693577	-8.069177
O	0.918211	-9.614285	-8.606065
C	4.149116	-10.975099	-8.457939
O	4.537249	-11.750552	-9.224197
C	1.430271	-10.906123	-4.819710
H	1.229380	-11.723458	-4.113222
H	1.575434	-9.974812	-4.259260
H	0.567748	-10.793722	-5.488969
H	3.930652	-12.297747	-3.794404
H	5.180351	-11.884899	-5.013322
H	4.458656	-10.595423	-4.016392
H	2.315809	-13.645676	-5.643213
H	1.791978	-12.933224	-7.197349
H	3.501740	-13.380079	-6.954656
H	8.950148	-6.769983	-8.795151
H	8.296531	-6.354190	-7.181032
H	7.446682	-4.851419	-10.045681
H	5.665040	-4.742514	-9.958491

H	6.653897	-4.300640	-8.541683
H	7.331435	-7.430969	-10.993393
H	6.605798	-8.799459	-10.089550
H	5.552559	-7.594919	-10.878717
C	1.456496	-7.183176	-6.099238
C	1.402487	-5.884092	-5.349029
H	1.198760	-7.060096	-7.155856
H	0.787200	-7.936189	-5.659309
C	1.228766	-4.674696	-6.040835
C	1.150119	-3.465041	-5.345145
C	1.254417	-3.449807	-3.951790
C	1.428955	-4.650042	-3.253408
C	1.498604	-5.858586	-3.946626
H	1.130611	-4.681036	-7.128247
H	1.000499	-2.533858	-5.893295
H	1.191771	-2.506098	-3.408402
H	1.501231	-4.643387	-2.165001
H	1.626296	-6.791726	-3.392806

B97-D/TZVP:

$Fe_2(SBn)_2(CO)_2(dppv)_2$

C	-1.184907	-4.565045	2.823208
C	-0.113673	-5.121917	2.106791
C	0.364339	-6.392458	2.474240
C	-0.238641	-7.102748	3.513968
C	-1.318252	-6.550041	4.209760
C	-1.782595	-5.276528	3.868919
P	0.702089	-4.232631	0.679929
C	-0.023942	-2.526269	0.841410
C	0.473170	-1.556682	1.728500
C	-0.142764	-0.305649	1.823994
C	-1.269175	-0.015480	1.046480
C	-1.773083	-0.979345	0.168646
C	-1.150815	-2.225473	0.061075
Fe	0.949385	-5.054436	-1.385328
S	0.885335	-6.155917	-3.380713
C	0.919801	-5.040173	-4.903167
C	1.854304	-5.674180	-5.890170
C	1.385207	-6.630250	-6.805552

C	2.273801	-7.298420	-7.651933
C	3.645176	-7.023360	-7.593634
C	4.120422	-6.067501	-6.688465
C	3.230820	-5.398663	-5.843765
Fe	-1.145830	-6.302281	-2.358800
P	-1.888529	-7.844081	-3.750032
C	-1.008439	-9.475386	-3.719332
C	-1.473896	-10.540319	-2.929547
C	-0.706309	-11.700152	-2.782476
C	0.534242	-11.810569	-3.418307
C	1.000994	-10.754648	-4.210122
C	0.239855	-9.593971	-4.359083
C	-3.641473	-8.286056	-3.333085
C	-4.151772	-7.714304	-2.239023
P	-3.008273	-6.672267	-1.187348
C	-3.091840	-7.764162	0.332523
C	-3.967155	-7.529654	1.404159
C	-4.049127	-8.439528	2.463847
C	-3.262766	-9.593732	2.465426
C	-2.398545	-9.840427	1.394319
C	-2.315074	-8.935584	0.335395
C	-2.047586	-7.517148	-5.585320
C	-2.349165	-6.213275	-6.009677
C	-2.485283	-5.922813	-7.370333
C	-2.327523	-6.931836	-8.325115
C	-2.049104	-8.237858	-7.909784
C	-1.913702	-8.530613	-6.549213
C	-4.084187	-5.226444	-0.758998
C	-5.129214	-4.816828	-1.600626
C	-5.852269	-3.655395	-1.312536
C	-5.538086	-2.891986	-0.184459
C	-4.488725	-3.289584	0.650970
C	-3.760864	-4.443552	0.359678
S	0.211743	-7.117280	-0.699047
C	1.321001	-8.595355	-1.146920
C	1.624953	-9.359985	0.105486
C	0.910108	-10.523627	0.429817
C	1.154719	-11.208039	1.623362
C	2.117577	-10.735553	2.521128

C	2.840313	-9.578202	2.207095
C	2.592757	-8.898601	1.013516
P	3.141330	-4.925385	-1.079976
C	4.054995	-3.566907	-1.989071
C	3.676956	-2.239679	-1.719550
C	4.277844	-1.178881	-2.399063
C	5.257971	-1.426414	-3.366739
C	5.638237	-2.742860	-3.640835
C	5.047827	-3.808015	-2.951677
C	0.731186	-3.481020	-2.113337
O	0.595214	-2.446941	-2.639811
C	2.410809	-4.044184	1.411638
C	3.467573	-4.384675	0.667078
C	4.276043	-6.378056	-1.335604
C	5.150621	-6.861308	-0.348821
C	5.955210	-7.978437	-0.597333
C	5.905658	-8.622426	-1.836797
C	5.043953	-8.143221	-2.828674
C	4.231683	-7.034984	-2.579514
H	0.768165	-9.205132	-1.859779
H	2.221012	-8.214608	-1.629387
H	3.155308	-8.000397	0.772724
H	3.599185	-9.207343	2.895258
H	2.310370	-11.268299	3.450756
H	0.591382	-12.111059	1.855681
H	0.161839	-10.893544	-0.268472
H	1.251997	-4.047007	-4.594469
H	-0.102085	-4.976939	-5.280817
H	3.602433	-4.659171	-5.135664
H	5.185024	-5.842175	-6.640965
H	4.336822	-7.544719	-8.253410
H	1.894033	-8.035218	-8.358367
H	0.321206	-6.850081	-6.850547
H	-4.206966	-8.964726	-3.972939
H	2.520908	-3.692178	2.438064
H	4.489120	-4.276131	1.033843
H	-5.170616	-7.893854	-1.892820
H	2.902611	-2.033639	-0.984015
H	3.970214	-0.158406	-2.178986

H	5.720001	-0.599183	-3.902207
H	6.402533	-2.946623	-4.389378
H	5.367504	-4.824099	-3.166954
H	5.201728	-6.383369	0.626100
H	6.617952	-8.348346	0.183238
H	6.530736	-9.493352	-2.025236
H	4.991735	-8.634851	-3.798625
H	3.548973	-6.692902	-3.352851
H	1.338938	-1.766390	2.351272
H	0.256261	0.441106	2.508483
H	-1.748602	0.959050	1.123295
H	-2.647712	-0.766158	-0.442276
H	-1.536778	-2.963966	-0.637543
H	1.199610	-6.838139	1.945226
H	0.130950	-8.094918	3.765082
H	-1.794038	-7.108093	5.014170
H	-2.613430	-4.832530	4.415220
H	-1.551540	-3.573480	2.570496
H	-5.372942	-5.393241	-2.491116
H	-6.658679	-3.344959	-1.975080
H	-6.102733	-1.988343	0.038309
H	-4.223190	-2.691791	1.520811
H	-2.938108	-4.739121	1.005631
H	-4.590474	-6.640570	1.419069
H	-4.729080	-8.238886	3.290551
H	-3.323040	-10.297015	3.294582
H	-1.769043	-10.726777	1.389010
H	-1.636898	-9.138024	-0.487225
H	-2.431389	-10.461916	-2.418197
H	-1.077515	-12.516925	-2.165088
H	1.134352	-12.709611	-3.293880
H	1.969055	-10.827195	-4.702983
H	0.625032	-8.771665	-4.956873
H	-1.688400	-9.548096	-6.241085
H	-1.932867	-9.032545	-8.645083
H	-2.423412	-6.703033	-9.384951
H	-2.706013	-4.903578	-7.681822
H	-2.470718	-5.419755	-5.279111
C	-1.821428	-4.817518	-2.981781

O	-2.276637	-3.810387	-3.374770

$[Fe_2(SBn)_2(CO)_2(dppv)_2]^+$

C	-0.945841	-4.256368	3.211096
C	0.110979	-4.924943	2.565882
C	0.755691	-5.973448	3.236378
C	0.362591	-6.340567	4.527961
C	-0.679029	-5.662652	5.166702
C	-1.337113	-4.621080	4.499888
C	0.558090	-4.481615	1.196341
S	1.175409	-2.705962	1.332233
Fe	3.429372	-2.273785	1.348646
C	4.916705	-1.422143	0.978249
O	5.878319	-0.845395	0.668043
S	3.418189	-3.394924	-0.623153
Fe	1.802548	-1.791241	-0.702191
P	2.057086	-1.173597	-2.858318
C	3.662626	-0.494733	-3.463807
C	5.142257	-3.271062	-1.391266
C	5.304792	-4.079100	-2.643946
C	5.683559	-3.449231	-3.838556
C	5.817991	-4.186097	-5.018070
C	5.575401	-5.562324	-5.018120
C	5.205745	-6.201730	-3.828216
C	5.076606	-5.465617	-2.648913
P	-0.340547	-1.288891	-1.142724
C	-1.271395	-2.633018	-2.009699
C	2.204799	-0.187284	-0.058522
O	2.334034	0.939244	0.232452
C	-1.488772	-0.694643	0.163656
C	-0.295450	0.098961	-2.376393
P	4.362001	-3.824871	2.658753
C	6.214183	-3.708141	2.719969
P	3.097029	-1.057955	3.259613
C	4.339489	0.258729	3.674171
C	3.842554	-3.462101	4.396380
C	4.120174	-5.666415	2.495509
C	1.488160	-0.263760	3.746410
C	3.297687	-2.269904	4.647604

C	1.556226	-2.425621	-4.143195
C	0.804406	0.168657	-3.133399
H	-0.278964	-4.438634	0.491929
H	1.340006	-5.121764	0.783171
H	1.565300	-6.507576	2.749478
H	0.873113	-7.158079	5.033163
H	-0.981437	-5.946330	6.172722
H	-2.155548	-4.094611	4.987656
H	-1.441129	-3.429317	2.706443
H	5.788890	-3.637850	-0.586182
H	5.371659	-2.220738	-1.564192
H	4.785253	-5.963785	-1.725501
H	5.025428	-7.275023	-3.820749
H	5.676187	-6.135774	-5.937332
H	6.107472	-3.682463	-5.938081
H	5.854452	-2.376135	-3.848120
H	0.950278	0.911357	-3.917100
H	2.962981	-1.987326	5.645620
H	3.996091	-4.193983	5.187460
H	-1.137969	0.783528	-2.473016
C	6.819241	-2.637627	3.398331
C	8.201710	-2.457125	3.330275
C	8.990842	-3.336106	2.580781
C	8.391502	-4.400133	1.900294
C	7.008157	-4.590037	1.969376
H	6.216137	-1.931634	3.963428
H	8.660683	-1.624611	3.859468
H	10.067728	-3.191479	2.526310
H	9.000341	-5.088442	1.317522
H	6.553980	-5.429390	1.446990
C	4.368794	-6.509347	3.593878
C	4.223558	-7.892600	3.471809
C	3.848413	-8.458361	2.248593
C	3.630947	-7.630092	1.145433
C	3.766569	-6.243243	1.268163
H	4.690763	-6.103683	4.548560
H	4.412261	-8.529715	4.333454
H	3.736137	-9.536517	2.156786
H	3.348270	-8.058743	0.185929

H	3.583066	-5.607656	0.408204
C	4.962904	0.318713	4.931582
C	5.890846	1.325754	5.210728
C	6.196535	2.288585	4.244227
C	5.570465	2.239895	2.995444
C	4.649573	1.229453	2.708452
H	4.739694	-0.418617	5.697593
H	6.370531	1.358094	6.186866
H	6.917857	3.072587	4.464404
H	5.802906	2.984355	2.236986
H	4.176656	1.200269	1.732006
C	0.449572	-1.077911	4.231434
C	-0.730203	-0.500751	4.702332
C	-0.887748	0.887734	4.689904
C	0.130541	1.698261	4.181598
C	1.314524	1.127918	3.706635
H	0.557154	-2.159346	4.251006
H	-1.524448	-1.140519	5.081635
H	-1.804071	1.336053	5.068124
H	0.011730	2.779936	4.164352
H	2.106130	1.771851	3.333592
C	-1.396759	0.632644	0.611618
C	-2.270720	1.095412	1.596434
C	-3.222233	0.236307	2.153068
C	-3.294408	-1.093897	1.730765
C	-2.430588	-1.561912	0.738342
H	-0.647711	1.304115	0.195635
H	-2.200952	2.126055	1.935124
H	-3.901860	0.601035	2.920194
H	-4.030538	-1.767621	2.165182
H	-2.507370	-2.591373	0.397093
C	-2.558908	-2.415724	-2.527135
C	-3.208191	-3.433687	-3.228097
C	-2.578573	-4.669991	-3.415202
C	-1.297036	-4.887227	-2.902866
C	-0.643065	-3.870425	-2.203658
H	-3.057516	-1.460188	-2.375240
H	-4.205631	-3.263456	-3.628129
H	-3.088228	-5.460819	-3.961711

H	-0.798803	-5.841621	-3.057360
H	0.368555	-4.026056	-1.832722
C	0.484318	-2.193750	-5.021292
C	0.089051	-3.181578	-5.926921
C	0.759379	-4.406925	-5.969481
C	1.827840	-4.641847	-5.098561
C	2.219303	-3.661386	-4.185581
H	-0.062935	-1.256387	-4.990662
H	-0.748761	-2.991989	-6.594448
H	0.447241	-5.175195	-6.673858
H	2.362019	-5.588762	-5.119342
H	3.036574	-3.871347	-3.506721
C	3.971090	-0.476769	-4.833838
C	5.199511	0.031058	-5.263799
C	6.128160	0.511485	-4.332889
C	5.822522	0.494433	-2.968615
C	4.591159	-0.003288	-2.534663
H	3.267176	-0.878291	-5.559321
H	5.436665	0.040932	-6.325553
H	7.089036	0.893124	-4.671264
H	6.542090	0.855964	-2.237423
H	4.363816	-0.029073	-1.473681

$Fe_2(SBn)(S)(CO)_2(dppv)_2$

C	0.026741	-6.792778	3.290243
C	0.894792	-6.777718	2.190550
C	1.829744	-7.816192	2.036977
C	1.882534	-8.859057	2.962505
C	1.005548	-8.876791	4.053857
C	0.083125	-7.840543	4.217018
P	0.912601	-5.394562	0.937936
C	-0.417186	-4.249527	1.528524
C	-0.151278	-3.026615	2.162077
C	-1.201735	-2.171891	2.511170
C	-2.523090	-2.534213	2.234784
C	-2.791396	-3.751771	1.600159
C	-1.745743	-4.602344	1.239030
Fe	1.061276	-5.730451	-1.254629
S	1.169664	-6.371348	-3.436937

C	1.014370	-4.890139	-4.583948
C	1.490401	-5.225855	-5.973645
C	0.680171	-4.973941	-7.088724
C	1.131127	-5.259079	-8.381688
C	2.399171	-5.811523	-8.580712
C	3.213062	-6.080608	-7.473389
C	2.762158	-5.789770	-6.184770
Fe	-0.789404	-7.159656	-2.526250
C	-1.867981	-5.787552	-2.283848
O	-2.646313	-4.938096	-2.062378
P	-1.644356	-7.885018	-4.438017
C	-0.721982	-9.278825	-5.242635
C	-1.198828	-10.599086	-5.213141
C	-0.430823	-11.639843	-5.744662
C	0.818425	-11.373011	-6.311898
C	1.298607	-10.057571	-6.343631
C	0.538887	-9.015966	-5.809421
C	-3.312106	-8.623513	-4.068325
C	-3.586208	-8.870188	-2.783643
P	-2.196124	-8.556667	-1.584398
C	-1.738102	-10.331347	-1.244076
C	-2.550178	-11.149133	-0.441205
C	-2.248804	-12.504995	-0.286010
C	-1.139864	-13.056044	-0.937359
C	-0.334282	-12.245446	-1.743167
C	-0.630097	-10.888546	-1.898659
C	-2.078537	-6.772158	-5.870523
C	-2.644622	-5.516091	-5.596732
C	-3.059602	-4.687062	-6.642651
C	-2.908240	-5.098244	-7.971379
C	-2.342077	-6.345514	-8.248666
C	-1.931927	-7.180270	-7.205416
C	-3.042733	-8.023709	-0.035200
C	-4.229720	-7.276194	-0.099939
C	-4.837735	-6.821175	1.073021
C	-4.264528	-7.105691	2.316371
C	-3.069606	-7.829171	2.380991
C	-2.451123	-8.278725	1.212571
S	0.694601	-7.947589	-1.040149

P	3.181560	-5.212273	-1.090465
C	3.757761	-3.823450	-2.177671
C	3.398990	-2.503623	-1.857666
C	3.698410	-1.459154	-2.734606
C	4.343629	-1.722668	-3.947906
C	4.697212	-3.035452	-4.274959
C	4.412705	-4.080168	-3.391969
C	0.506437	-4.082262	-1.564386
O	0.112100	-3.005264	-1.777545
C	2.504750	-4.591959	1.488955
C	3.514655	-4.550844	0.613625
C	4.534707	-6.470758	-1.318040
C	5.883451	-6.117840	-1.132247
C	6.890494	-7.069311	-1.307966
C	6.560413	-8.379667	-1.676278
C	5.221546	-8.730459	-1.869183
C	4.208958	-7.781092	-1.691185
H	1.644404	-4.112541	-4.136966
H	-0.021980	-4.543337	-4.581633
H	3.390138	-6.015366	-5.326808
H	4.200409	-6.518647	-7.614501
H	2.750722	-6.035341	-9.586533
H	0.480986	-5.057689	-9.231231
H	-0.315672	-4.562950	-6.944152
H	-4.003819	-8.840154	-4.883439
H	2.617437	-4.269412	2.525045
H	4.502349	-4.166384	0.871548
H	-4.519572	-9.322163	-2.445710
H	2.867011	-2.294331	-0.931957
H	3.415926	-0.440601	-2.474824
H	4.564884	-0.909985	-4.637340
H	5.188660	-3.249991	-5.221974
H	4.703327	-5.096455	-3.645533
H	6.148798	-5.095395	-0.869496
H	7.932476	-6.788683	-1.162070
H	7.346174	-9.120147	-1.817425
H	4.956909	-9.744877	-2.163009
H	3.166037	-8.053557	-1.839319
H	0.871716	-2.725611	2.374057

H	-0.984686	-1.220953	2.994960
H	-3.338751	-1.864928	2.503529
H	-3.813893	-4.040358	1.368960
H	-1.964461	-5.532174	0.720377
H	2.505853	-7.815579	1.186000
H	2.603849	-9.662868	2.826198
H	1.044451	-9.693630	4.772620
H	-0.597182	-7.844876	5.067606
H	-0.704213	-5.998522	3.419609
H	-4.672641	-7.036375	-1.064545
H	-5.759045	-6.244003	1.013992
H	-4.737834	-6.751285	3.230053
H	-2.603269	-8.034493	3.340811
H	-1.508016	-8.817481	1.265765
H	-3.408850	-10.726301	0.076168
H	-2.878806	-13.129427	0.345494
H	-0.905193	-14.112210	-0.814777
H	0.531016	-12.666536	-2.252037
H	0.001633	-10.255947	-2.515769
H	-2.160646	-10.822678	-4.757218
H	-0.811298	-12.659283	-5.709753
H	1.416024	-12.183774	-6.724961
H	2.271241	-9.838821	-6.780875
H	0.931114	-8.002175	-5.831822
H	-1.487059	-8.145004	-7.434193
H	-2.211480	-6.670745	-9.279392
H	-3.226335	-4.447993	-8.784379
H	-3.496174	-3.715872	-6.416569
H	-2.762018	-5.179386	-4.571028

$[Fe_2(SBn)(S)(CO)_2(dppv)_2]^+$

C	4.056498	-7.814090	-1.697818
C	4.449907	-6.536937	-1.278143
C	5.808680	-6.276202	-1.020879
C	6.756450	-7.290597	-1.169343
C	6.357701	-8.568908	-1.578575
C	5.010492	-8.825876	-1.846671
P	3.203232	-5.177426	-1.091150
C	3.559693	-4.471836	0.585568

C	2.585583	-4.518571	1.499806
P	0.998590	-5.347055	1.021866
Fe	1.077028	-5.697229	-1.197177
C	0.547442	-4.032028	-1.489718
O	0.118464	-2.975151	-1.706072
C	0.988110	-6.778314	2.203679
C	0.037404	-6.900502	3.225708
C	0.056680	-8.018970	4.066424
C	1.018881	-9.016594	3.891646
C	1.976863	-8.889869	2.878155
C	1.963996	-7.776627	2.037692
C	-0.353732	-4.234066	1.590077
C	-0.109457	-3.002929	2.216835
C	-1.179589	-2.174874	2.568408
C	-2.492801	-2.569410	2.296868
C	-2.737251	-3.793575	1.665780
C	-1.674082	-4.621501	1.304447
S	1.121092	-6.312929	-3.385449
Fe	-0.815235	-7.164850	-2.507637
S	0.510471	-7.787309	-0.897444
C	1.041173	-4.841478	-4.554660
C	1.499288	-5.233744	-5.936612
C	0.682112	-5.006341	-7.051616
C	1.107309	-5.368072	-8.334122
C	2.355290	-5.967982	-8.519341
C	3.180182	-6.200030	-7.411864
C	2.755495	-5.834519	-6.133797
C	-1.917215	-5.833373	-2.299948
O	-2.631949	-4.947521	-2.043763
P	-1.660593	-7.805027	-4.475494
C	-2.092330	-6.656673	-5.862576
C	-2.567280	-5.368873	-5.568627
C	-3.002634	-4.529142	-6.597253
C	-2.962573	-4.965006	-7.925630
C	-2.485634	-6.245382	-8.222187
C	-2.055263	-7.091628	-7.197473
P	-2.275970	-8.612536	-1.616785
C	-3.153715	-8.042648	-0.105587
C	-4.336318	-7.293836	-0.210213

C	-4.955171	-6.803509	0.942725
C	-4.395668	-7.052037	2.199698
C	-3.208214	-7.783411	2.302396
C	-2.580705	-8.273226	1.155979
C	-0.643228	-9.144693	-5.241482
C	-0.962013	-10.496054	-5.033675
C	-0.126790	-11.498014	-5.536962
C	1.029473	-11.158987	-6.245058
C	1.348781	-9.811288	-6.453747
C	0.521746	-8.805571	-5.952316
C	-3.297502	-8.611801	-4.141824
C	-3.596312	-8.919588	-2.876463
C	-1.757419	-10.349070	-1.224992
C	-2.606721	-11.186749	-0.480786
C	-2.257880	-12.522716	-0.267878
C	-1.065752	-13.030364	-0.796716
C	-0.222998	-12.198874	-1.539930
C	-0.566385	-10.861997	-1.757450
C	3.799167	-3.870027	-2.250502
C	3.429068	-2.533297	-2.025279
C	3.761552	-1.548752	-2.957687
C	4.455372	-1.891722	-4.123910
C	4.829684	-3.219924	-4.348135
C	4.508270	-4.207157	-3.413080
H	1.712789	-4.098629	-4.109273
H	0.025522	-4.439366	-4.558193
H	3.392997	-6.031061	-5.275944
H	4.156235	-6.662974	-7.546287
H	2.684527	-6.252870	-9.516593
H	0.455989	-5.185696	-9.186193
H	-0.296895	-4.554837	-6.917193
H	-3.959824	-8.821364	-4.982338
H	2.727047	-4.171954	2.523835
H	4.544927	-4.055485	0.795932
H	-4.523604	-9.413168	-2.584521
H	2.872137	-2.261438	-1.131046
H	3.472882	-0.515435	-2.776534
H	4.704641	-1.125064	-4.854344
H	5.368500	-3.491165	-5.253376

H	4.814891	-5.236009	-3.583383
H	6.132322	-5.281353	-0.721959
H	7.805638	-7.083337	-0.967340
H	7.097566	-9.358330	-1.693523
H	4.695479	-9.814364	-2.175045
H	3.009777	-8.015846	-1.908725
H	0.906271	-2.677117	2.426743
H	-0.984684	-1.220451	3.053013
H	-3.322737	-1.921529	2.571280
H	-3.754205	-4.106185	1.443217
H	-1.873906	-5.565680	0.803794
H	2.699356	-7.695385	1.239829
H	2.729433	-9.662821	2.736940
H	1.026593	-9.887337	4.544221
H	-0.681665	-8.107258	4.861308
H	-0.721741	-6.134909	3.362918
H	-4.773822	-7.086569	-1.184893
H	-5.875752	-6.229805	0.857490
H	-4.878709	-6.670148	3.096259
H	-2.759244	-7.968181	3.274530
H	-1.648491	-8.826261	1.241297
H	-3.529598	-10.797169	-0.056315
H	-2.916538	-13.166456	0.311781
H	-0.796614	-14.071286	-0.629484
H	0.705580	-12.588117	-1.952409
H	0.089999	-10.218262	-2.336039
H	-1.851924	-10.772851	-4.474398
H	-0.384107	-12.542725	-5.374271
H	1.677184	-11.940643	-6.637081
H	2.243829	-9.538315	-7.008848
H	0.784471	-7.765006	-6.121921
H	-1.679802	-8.081971	-7.441287
H	-2.444915	-6.589169	-9.253798
H	-3.299567	-4.309067	-8.725424
H	-3.368831	-3.532978	-6.357416
H	-2.601703	-5.011336	-4.545167

$Fe_2(SBn)_2(CO)_2(PMe_3)_4$

C	6.513651	-2.360620	-3.479543
C	5.570428	-3.251799	-2.964689

C	4.368078	-2.786100	-2.403580
C	4.128727	-1.403789	-2.396827
C	5.070492	-0.507914	-2.914136
C	6.269855	-0.982423	-3.452163
C	3.351655	-3.747406	-1.842606
S	4.108603	-5.032836	-0.706690
Fe	2.537073	-6.319441	0.359545
P	2.072317	-7.694635	-1.332020
Fe	4.278395	-4.795163	1.611537
P	2.994288	-3.059550	2.120180
C	4.381281	-5.057535	3.316743
O	4.503836	-5.202922	4.477515
P	6.263309	-3.767216	1.460444
S	4.461878	-7.104600	1.387566
P	1.414921	-7.401521	1.946207
C	1.226176	-5.236038	0.065366
O	0.330535	-4.497989	-0.151760
H	4.866772	0.561508	-2.894375
H	2.539360	-3.224451	-1.341341
H	3.194234	-1.024807	-1.987358
H	7.006443	-0.286649	-3.849464
H	7.441901	-2.741396	-3.902483
H	5.771524	-4.321386	-2.968138
H	2.908598	-4.338385	-2.651396
C	0.288497	-8.218637	-1.541628
C	2.365271	-7.022570	-3.050744
C	2.932494	-9.347760	-1.521842
H	0.146189	-8.763682	-2.482926
H	-0.022919	-8.860060	-0.711703
H	-0.339041	-7.321263	-1.540908
H	2.436853	-9.958354	-2.287089
H	3.968388	-9.170101	-1.826121
H	2.936231	-9.883611	-0.569048
H	2.163180	-7.785042	-3.813126
H	1.702202	-6.167059	-3.214005
H	3.403339	-6.685021	-3.128163
C	-0.434785	-7.179987	1.990958
C	1.560346	-9.266089	1.938379
C	1.831977	-7.106240	3.735603

C	7.141123	-3.390307	3.060704
C	7.628292	-4.621758	0.531000
C	6.327933	-2.107152	0.604640
H	-0.883457	-7.811231	2.767134
H	-0.664250	-6.130098	2.198359
H	-0.861749	-7.433639	1.017043
H	1.205986	-7.739534	4.376100
H	2.885936	-7.340283	3.902683
H	1.670186	-6.057048	3.982404
H	1.027550	-9.703998	2.791583
H	1.155088	-9.681898	1.012178
H	2.624291	-9.514699	2.004050
H	8.107574	-2.905328	2.874583
H	6.519200	-2.741223	3.683198
H	7.300673	-4.329505	3.600200
H	8.485266	-3.948562	0.402381
H	7.941758	-5.513163	1.078290
H	7.248615	-4.928302	-0.447075
H	7.329645	-1.668057	0.692827
H	6.087712	-2.248639	-0.452178
H	5.594933	-1.417502	1.031106
C	3.738954	-1.872398	3.366754
C	2.363984	-1.830885	0.868633
C	1.410168	-3.412989	3.044491
H	3.002366	-1.117778	3.667906
H	4.057702	-2.437678	4.247987
H	4.611457	-1.367655	2.943480
H	0.869349	-2.480529	3.251167
H	0.781911	-4.079972	2.452997
H	1.665504	-3.893986	3.993468
H	1.939707	-0.962812	1.387115
H	3.187678	-1.508479	0.227811
H	1.582552	-2.298078	0.263679
C	5.673223	-7.838373	0.151699
C	7.100251	-7.965054	0.632741
H	5.266599	-8.837590	-0.044574
H	5.630813	-7.267875	-0.781130
C	8.142818	-7.907377	-0.306235
C	9.476564	-8.039281	0.088117

C	9.792331	-8.229687	1.437542
C	8.762255	-8.291206	2.381488
C	7.427973	-8.163428	1.982461
H	7.904462	-7.736754	-1.355900
H	10.269683	-7.983383	-0.656011
H	10.830589	-8.324931	1.750449
H	8.997108	-8.436116	3.434946
H	6.632244	-8.193088	2.723481

$[Fe_2(SBn)_2(CO)_2(PMe_3)_4]^+$

C	4.920364	-4.312712	-4.159724
C	4.176660	-4.707660	-3.036878
C	3.188763	-5.693506	-3.198604
C	2.932676	-6.245917	-4.455916
C	3.668282	-5.831567	-5.571746
C	4.669030	-4.868252	-5.418257
C	4.490320	-4.115977	-1.681984
S	2.983772	-3.816342	-0.610738
Fe	1.633720	-1.947211	-0.564924
P	-0.532937	-1.161770	-0.608860
C	-1.749556	-1.699359	0.695014
Fe	3.416618	-2.617071	1.285575
P	4.366725	-4.247216	2.486551
C	3.388412	-5.084591	3.820853
S	1.150025	-2.921743	1.537273
C	0.418007	-4.619594	1.173094
C	0.071947	-5.401989	2.412958
C	0.446927	-6.751503	2.505423
C	0.112603	-7.510652	3.631229
C	-0.598961	-6.926425	4.682705
C	-0.981519	-5.582669	4.598088
C	-0.650440	-4.827585	3.470805
P	3.282468	-1.077485	2.994086
C	1.841282	0.108198	2.988592
C	2.479287	-0.480591	-0.070161
O	2.954657	0.591996	0.004987
C	3.103767	-1.700439	4.739429
C	4.719613	0.084254	3.124503

P	2.098657	-1.286618	-2.683688
C	1.558531	-2.419477	-4.048823
C	1.438646	0.366032	-3.232815
C	3.895022	-0.997360	-3.045746
C	-0.677743	0.679422	-0.404546
C	-1.556767	-1.532517	-2.123505
C	4.938835	-5.724368	1.515404
C	5.951543	-3.789194	3.344207
H	-0.477783	-4.408712	0.577366
H	1.112157	-5.173698	0.536341
H	1.004367	-7.211155	1.689606
H	0.407500	-8.556766	3.686403
H	-0.858779	-7.514675	5.560216
H	-1.542805	-5.125194	5.410576
H	-0.946289	-3.781759	3.410578
H	5.074931	-4.830359	-1.093416
H	5.084548	-3.203395	-1.759271
H	2.606945	-6.017392	-2.338120
H	2.160958	-7.005593	-4.564551
H	3.468671	-6.262975	-6.550164
H	5.258160	-4.550450	-6.276140
H	5.715213	-3.575949	-4.049667
H	3.994251	-0.384436	-3.947981
H	4.362040	-0.483448	-2.201630
H	4.391964	-1.948900	-3.216554
H	1.815962	-1.982384	-5.020438
H	2.062019	-3.382498	-3.936992
H	0.477606	-2.577277	-3.994446
H	1.780471	0.566342	-4.254050
H	0.348533	0.403736	-3.216538
H	1.835592	1.138753	-2.566941
H	4.569008	0.788825	3.949787
H	5.641265	-0.482513	3.288217
H	4.810147	0.634100	2.182930
H	1.806477	0.630925	3.950582
H	1.958046	0.837646	2.186408
H	0.910916	-0.449586	2.846038
H	3.052862	-0.847779	5.425703
H	2.174223	-2.273601	4.811076

H	3.942845	-2.334983	5.031975
H	6.361302	-4.656636	3.873636
H	6.672779	-3.448904	2.594257
H	5.789595	-2.977560	4.057939
H	5.295430	-6.503610	2.198406
H	4.111780	-6.109112	0.912955
H	5.760110	-5.429292	0.856115
H	4.019935	-5.825800	4.324503
H	3.019592	-4.365596	4.551741
H	2.527782	-5.584058	3.371115
H	-2.697396	-1.172294	0.537397
H	-1.927894	-2.776344	0.635888
H	-1.357476	-1.465221	1.687404
H	-1.721309	0.994901	-0.516786
H	-0.329171	0.931796	0.602344
H	-0.051663	1.209264	-1.122947
H	-2.558666	-1.102440	-2.011897
H	-1.099478	-1.133971	-3.030932
H	-1.644483	-2.619357	-2.228993
C	4.954356	-2.005225	0.737725
O	5.971003	-1.602927	0.331708

$Fe_2(SBn)(S)(CO)_2(PMe_3)_4$

C	5.471184	-1.915236	-4.147852
C	4.735427	-2.796860	-3.353012
C	3.775277	-2.320614	-2.441949
C	3.576441	-0.932307	-2.356680
C	4.311537	-0.046530	-3.151146
C	5.262894	-0.534754	-4.050525
C	2.936620	-3.264662	-1.618619
S	3.941583	-4.621396	-0.784171
Fe	2.636639	-6.224480	0.184920
P	2.383576	-7.397142	-1.684943
Fe	4.442487	-4.580789	1.484902
P	3.282618	-2.847099	2.347734
C	4.804590	-5.032620	3.117586
O	5.082066	-5.336586	4.220533
P	6.444744	-3.676791	1.124817
S	4.641771	-6.770997	1.028528

P	1.796945	-7.693133	1.640536
C	1.149876	-5.308602	0.135811
O	0.169332	-4.650915	0.133800
H	4.137521	1.027965	-3.067523
H	2.342011	-2.722690	-0.879828
H	2.824225	-0.541720	-1.667833
H	5.836869	0.153823	-4.673026
H	6.209866	-2.307492	-4.849583
H	4.913974	-3.871315	-3.423658
H	2.234202	-3.810967	-2.263545
C	0.980282	-8.611588	-1.905943
C	2.146036	-6.426579	-3.259646
C	3.845974	-8.448481	-2.154244
H	1.017169	-9.071291	-2.904644
H	1.032416	-9.407445	-1.152036
H	0.022974	-8.085460	-1.791758
H	3.696142	-8.945702	-3.124497
H	4.731469	-7.801739	-2.195779
H	4.020586	-9.199902	-1.374270
H	2.075816	-7.097201	-4.128433
H	1.223864	-5.834258	-3.189679
H	2.994089	-5.745000	-3.398664
C	-0.040625	-8.010604	1.592248
C	2.468974	-9.431223	1.627889
C	1.997655	-7.283224	3.442029
C	7.584485	-3.462720	2.580421
C	7.511900	-4.696662	-0.005235
C	6.584713	-2.000647	0.322302
H	-0.336654	-8.725498	2.373215
H	-0.573061	-7.063404	1.748303
H	-0.334665	-8.407408	0.613261
H	1.542159	-8.063176	4.069770
H	3.065259	-7.195871	3.672990
H	1.514660	-6.320712	3.650658
H	2.018051	-10.031933	2.431054
H	2.265032	-9.915524	0.664082
H	3.555836	-9.378153	1.770723
H	8.559798	-3.068644	2.259925
H	7.139990	-2.773581	3.309782

H	7.728959	-4.432334	3.073882
H	8.489138	-4.219375	-0.170403
H	7.647064	-5.690086	0.441043
H	6.988350	-4.823509	-0.961002
H	7.637486	-1.730719	0.152037
H	6.052073	-2.011857	-0.636956
H	6.123228	-1.239493	0.965370
C	4.192717	-1.854558	3.644297
C	2.551458	-1.434775	1.365362
C	1.776727	-3.322660	3.338633
H	3.519839	-1.138472	4.137763
H	4.611546	-2.531474	4.400275
H	5.018682	-1.299895	3.179420
H	1.308133	-2.439720	3.798597
H	1.053781	-3.816319	2.677495
H	2.074429	-4.026675	4.125868
H	2.214175	-0.639226	2.045999
H	3.297531	-1.025686	0.672980
H	1.685737	-1.790631	0.792192

$[Fe_2(SBn)(S)(CO)_2(PMe_3)_4]^+$

C	4.920364	-4.312712	-4.159724
C	4.176660	-4.707660	-3.036878
C	3.188763	-5.693506	-3.198604
C	2.932676	-6.245917	-4.455916
C	3.668282	-5.831567	-5.571746
C	4.669030	-4.868252	-5.418257
C	4.490320	-4.115977	-1.681984
S	2.983772	-3.816342	-0.610738
Fe	1.633720	-1.947211	-0.564924
P	-0.532937	-1.161770	-0.608860
C	-1.749556	-1.699359	0.695014
Fe	3.416618	-2.617071	1.285575
P	4.366725	-4.247216	2.486551
C	3.388412	-5.084591	3.820853
S	1.150025	-2.921743	1.537273
C	0.418007	-4.619594	1.173094
C	0.071947	-5.401989	2.412958
C	0.446927	-6.751503	2.505423

C	0.112603	-7.510652	3.631229
C	-0.598961	-6.926425	4.682705
C	-0.981519	-5.582669	4.598088
C	-0.650440	-4.827585	3.470805
P	3.282468	-1.077485	2.994086
C	1.841282	0.108198	2.988592
C	2.479287	-0.480591	-0.070161
O	2.954657	0.591996	0.004987
C	3.103767	-1.700439	4.739429
C	4.719613	0.084254	3.124503
P	2.098657	-1.286618	-2.683688
C	1.558531	-2.419477	-4.048823
C	1.438646	0.366032	-3.232815
C	3.895022	-0.997360	-3.045746
C	-0.677743	0.679422	-0.404546
C	-1.556767	-1.532517	-2.123505
C	4.938835	-5.724368	1.515404
C	5.951543	-3.789194	3.344207
H	-0.477783	-4.408712	0.577366
H	1.112157	-5.173698	0.536341
H	1.004367	-7.211155	1.689606
H	0.407500	-8.556766	3.686403
H	-0.858779	-7.514675	5.560216
H	-1.542805	-5.125194	5.410576
H	-0.946289	-3.781759	3.410578
H	5.074931	-4.830359	-1.093416
H	5.084548	-3.203395	-1.759271
H	2.606945	-6.017392	-2.338120
H	2.160958	-7.005593	-4.564551
H	3.468671	-6.262975	-6.550164
H	5.258160	-4.550450	-6.276140
H	5.715213	-3.575949	-4.049667
H	3.994251	-0.384436	-3.947981
H	4.362040	-0.483448	-2.201630
H	4.391964	-1.948900	-3.216554
H	1.815962	-1.982384	-5.020438
H	2.062019	-3.382498	-3.936992
H	0.477606	-2.577277	-3.994446
H	1.780471	0.566342	-4.254050

H	0.348533	0.403736	-3.216538
H	1.835592	1.138753	-2.566941
H	4.569008	0.788825	3.949787
H	5.641265	-0.482513	3.288217
H	4.810147	0.634100	2.182930
H	1.806477	0.630925	3.950582
H	1.958046	0.837646	2.186408
H	0.910916	-0.449586	2.846038
H	3.052862	-0.847779	5.425703
H	2.174223	-2.273601	4.811076
H	3.942845	-2.334983	5.031975
H	6.361302	-4.656636	3.873636
H	6.672779	-3.448904	2.594257
H	5.789595	-2.977560	4.057939
H	5.295430	-6.503610	2.198406
H	4.111780	-6.109112	0.912955
H	5.760110	-5.429292	0.856115
H	4.019935	-5.825800	4.324503
H	3.019592	-4.365596	4.551741
H	2.527782	-5.584058	3.371115
H	-2.697396	-1.172294	0.537397
H	-1.927894	-2.776344	0.635888
H	-1.357476	-1.465221	1.687404
H	-1.721309	0.994901	-0.516786
H	-0.329171	0.931796	0.602344
H	-0.051663	1.209264	-1.122947
H	-2.558666	-1.102440	-2.011897
H	-1.099478	-1.133971	-3.030932
H	-1.644483	-2.619357	-2.228993
C	4.954356	-2.005225	0.737725
O	5.971003	-1.602927	0.331708

$Fe_2(SBn)(S)(CO)_4(PMe_3)_2$

C	6.840313	2.391478	-1.779323
C	6.743056	1.017279	-2.021261
C	6.226733	0.167070	-1.039946
C	5.808420	0.678673	0.198134
C	5.899922	2.060535	0.427729
C	6.414984	2.911741	-0.551770

C	5.238308	-0.233298	1.245910
S	3.359004	-0.198435	1.155353
Fe	2.490156	-1.889298	-0.125350
S	0.639806	-1.184823	0.920416
Fe	2.145817	-1.625216	2.525301
P	3.715828	-2.999343	3.444469
C	2.029386	-0.440234	3.836102
O	1.929175	0.351866	4.678884
C	0.937251	-2.729633	3.172866
O	0.136079	-3.445051	3.621634
C	2.667578	-1.118911	-1.712090
O	2.800136	-0.634421	-2.759402
P	1.227450	-3.544168	-0.944796
C	3.937671	-2.898586	-0.115511
O	4.901643	-3.560561	-0.091384
H	6.484828	3.980752	-0.358488
H	5.592648	-1.253552	1.113177
H	5.560924	2.466306	1.380069
H	7.242954	3.054256	-2.543063
H	7.068131	0.607740	-2.975943
H	6.147558	-0.901912	-1.230970
H	5.493272	0.111766	2.253606
C	2.069316	-4.616454	-2.205124
C	0.578813	-4.778306	0.273793
C	-0.297090	-3.011032	-1.852239
H	-0.004475	-5.553063	-0.238177
H	1.419061	-5.238984	0.801680
H	-0.048825	-4.257733	1.001357
H	1.386302	-5.388344	-2.578571
H	2.401321	-3.989101	-3.039142
H	2.948255	-5.088934	-1.755466
H	-0.825563	-3.881404	-2.258497
H	-0.946655	-2.465513	-1.162174
H	-0.006978	-2.339678	-2.666565
C	3.526120	-3.084605	5.293522
C	3.530796	-4.790266	2.973620
C	5.563533	-2.815838	3.304275
H	4.197199	-3.836504	5.725630
H	3.752775	-2.101669	5.719045

H	2.489174	-3.334351	5.537952
H	6.038630	-3.536903	3.980426
H	5.880642	-3.027180	2.280767
H	5.870553	-1.804544	3.581364
H	4.213300	-5.416068	3.561049
H	2.498617	-5.103180	3.155221
H	3.758901	-4.903630	1.910323

$[Fe_2(SBn)(S)(CO)_4(PMe_3)_2]^+$

Fe	3.352764	-9.842953	-7.410583
Fe	4.585468	-7.212669	-7.348560
P	6.382582	-6.652599	-8.629076
H	8.131761	-7.903679	-7.483397
C	2.820435	-13.127922	-6.480810
P	2.934848	-11.391385	-5.870121
C	4.250454	-11.431048	-4.575953
S	3.037338	-8.123783	-5.918681
C	3.472670	-6.404592	-8.465759
O	2.730698	-5.967706	-9.237816
S	5.467492	-9.211224	-7.216763
C	4.847359	-5.794194	-6.321053
O	5.079569	-4.896573	-5.635554
C	8.006446	-6.857946	-7.777358
C	6.377060	-4.889172	-9.177388
C	6.525100	-7.620176	-10.193427
C	1.673987	-9.770599	-8.034824
O	0.602745	-9.675872	-8.455336
C	3.886590	-11.010120	-8.652308
O	4.233140	-11.759585	-9.457115
C	1.367933	-11.139945	-4.926025
H	1.237808	-11.949326	-4.198648
H	1.417024	-10.181734	-4.401372
H	0.518318	-11.129411	-5.615315
H	4.001675	-12.177607	-3.812681
H	5.206430	-11.678416	-5.045616
H	4.324304	-10.438426	-4.122957
H	2.621702	-13.799542	-5.637706
H	2.009803	-13.211016	-7.211358
H	3.761627	-13.412721	-6.960148

H	8.820350	-6.561230	-8.448236
H	8.023226	-6.230888	-6.880490
H	7.273687	-4.676967	-9.769695
H	5.486730	-4.696734	-9.783677
H	6.356886	-4.234793	-8.300579
H	7.376755	-7.259866	-10.781288
H	6.661966	-8.676836	-9.947219
H	5.604570	-7.506438	-10.774417
C	1.370636	-7.243035	-6.023652
C	1.499728	-5.885720	-5.396651
H	1.062950	-7.192005	-7.069401
H	0.676558	-7.890628	-5.475729
C	1.495285	-4.730328	-6.192445
C	1.653109	-3.470671	-5.608180
C	1.828898	-3.355849	-4.226185
C	1.834341	-4.504136	-3.425558
C	1.670033	-5.761078	-4.007736
H	1.348682	-4.815247	-7.266835
H	1.634213	-2.579121	-6.231349
H	1.952486	-2.375435	-3.771487
H	1.960593	-4.416933	-2.348541
H	1.677396	-6.654608	-3.384761

$Fe_2(SBn)(S)(CO)_6$

C	7.435792	2.165242	-1.276454
C	7.282122	0.799270	-1.524296
C	6.519811	-0.000024	-0.657964
C	5.909882	0.595773	0.457905
C	6.064536	1.960822	0.707380
C	6.826299	2.749769	-0.161328
C	6.308852	-1.457685	-0.949328
S	4.684539	-1.653740	-1.891309
Fe	4.331901	-3.754967	-2.764835
C	3.289554	-4.425526	-1.462455
O	2.614748	-4.842431	-0.626356
Fe	4.922293	-1.611732	-4.190392
C	4.651148	0.157903	-4.393129
O	4.472834	1.288912	-4.516660
C	4.862441	-2.045011	-5.932960

O	4.821014	-2.316488	-7.051788
C	6.720930	-1.674464	-4.145711
O	7.873931	-1.737409	-4.115187
S	2.902701	-2.563126	-4.019194
C	4.125168	-5.087485	-3.956165
O	3.985593	-5.936524	-4.721878
C	5.939866	-4.351932	-2.204660
O	6.974300	-4.717951	-1.847477
H	5.591596	2.409144	1.578972
H	7.126823	-1.891039	-1.526716
H	5.311405	-0.016348	1.131319
H	6.945681	3.814189	0.030962
H	8.031755	2.773975	-1.953580
H	7.762517	0.347683	-2.389440
H	6.171784	-2.040982	-0.032435

$[Fe_2(SBn)(S)(CO)_6]^+$

Fe	5.842841	-1.889786	-3.974522
Fe	3.900385	-3.715301	-2.847789
C	5.377360	0.956351	-0.260200
H	9.223180	1.259586	-0.723192
C	8.145041	1.175073	-0.606705
C	6.600957	-2.112739	-5.621992
C	3.665357	-5.315965	-3.706968
C	4.516481	-4.522609	-1.316474
C	6.206743	-0.124374	-3.925716
O	6.394502	1.003276	-3.935982
S	4.035663	-2.758356	-4.822948
S	4.511869	-1.637098	-2.108304
C	5.493937	-1.547603	-0.488035
C	6.153131	-0.203143	-0.440706
C	7.541401	-0.084238	-0.617433
C	7.365998	2.324429	-0.435319
C	5.981711	2.212985	-0.257015
C	7.338436	-2.427350	-3.095187
O	8.235784	-2.876898	-2.541509
O	7.080002	-2.229221	-6.652358
C	2.198556	-3.576027	-2.343322
O	1.099630	-3.460010	-2.043771

O	4.937334	-5.003540	-0.367127
O	3.511857	-6.316475	-4.236122
H	6.204217	-2.375489	-0.444419
H	8.154246	-0.975865	-0.725771
H	7.837612	3.304443	-0.427226
H	5.377330	3.104539	-0.107713
H	4.301122	0.869625	-0.117435
H	4.728729	-1.676428	0.285461