Electronic Supplementary Information

Hydrogenase biomimics containing non-innocent redox-active ligands: $Fe_2(CO)_4(\mu\text{-edt})(\kappa^2\text{-bpcd})$ with 4,5-bis(diphenylphosphino)-4-cyclopenten-1,3-dione (bpcd) as a potential $[Fe_4\text{-}S_4]_H$ surrogate

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Fig. S1. CVs of $Fe_2(CO)_4(\kappa^2\text{-bpcd})(\mu\text{-edt})$ (**2**) (black), $Fe_2(CO)_4(\kappa^2\text{-dppen})(\mu\text{-edt})$ (**3**) (red) and bpcd (blue) in MeCN (1 mM solution, supporting electrolyte $[NBu_4][PF_6]$, scan rate 0.1 V/s, glassy carbon electrode, potential *vs.* Fc^+/Fc).

Fig. S2. CVs of 4,5-bis(diphenylphosphino)-4-cyclopenten-1,3-dione (bpcd) at various scan rates in acetonitrile (1 mM solution, supporting electrolyte $[NBu_4][PF_6]$, glassy carbon electrode, potential *vs.* Fc^+/Fc) - (a) scanning negative potential window first; (b) scanning positive potential window first.

Fig. S3. CVs of $Fe_2(CO)_4(\kappa^2\text{-bpcd})(\mu\text{-edt})$ (**2**) at various scan rates in acetonitrile (1 mM solution, supporting electrolyte $[NBu_4][PF_6]$, glassy carbon electrode, potential *vs.* Fc^+/Fc) - (a) scanning negative potential window first; (b) scanning positive potential window first.

Fig. S4. CVs of $Fe_2(CO)_4(\kappa^2\text{-bpcd})(\mu\text{-edt})$ (**2**) at various scan rates in acetonitrile with the potential cyclic between –1.45 and –0.25 V (1 mM solution, supporting electrolyte $[NBu_4][PF_6]$, glassy carbon electrode, potential *vs.* Fc^+/Fc).

Fig. S5. (a) IR spectra of $Fe_2(CO)_4(\kappa^2\text{-dppen})(\mu\text{-edt})$ (**3**) in the absence of acid (black) and upon addition of two equivalent of CF_3CO_2H (red) in CH_2Cl_2; (b) Hydride region of the NMR spectrum of $Fe_2(CO)_4(\kappa^2\text{-dppen})(\mu\text{-edt})$ (**3**).

Fig. S6. Plot of electrocatalytic peak current at potential of the second catalytic wave *vs.* equivalents of CF_3CO_2H added for **2** (dark blue diamonds) and **3** (pink squares) [Since for both complexes the potential gap between the two catalytic waves are quite small (the first wave looks like a shoulder of the second wave), we ignore the current for first catalytic wave and plotted the total catalytic current against equivalents of acid].

Fig. S7. DFT-optimized structures of the four different triplet isomers evaluated for the protonation of ^{3}**B**$^{2-}$. The energies are in kcal/mol (ΔG) and are relative to ^{3}**C_μ-H**$^-$.

Atomic coordinates and optimized energies for the reported DFT species.

Table S1. Crystal data and structure refinement for $Fe_2(CO)_4(\kappa^2$-bpcd)(μ-edt) (**2**).

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for $Fe_2(CO)_4(\kappa^2$-bpcd)(μ-edt) (**2**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S3. Bond lengths [Å] and angles [°] for $Fe_2(CO)_4(\kappa^2$-bpcd)(μ-edt) (**2**).

Table S4. Anisotropic displacement parameters (Å^{2}x 10^3) for $Fe_2(CO)_4(\kappa^2$-bpcd)(μ-edt) (**2**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

Table S5. Torsion angles [°] for $Fe_2(CO)_4(\kappa^2$-bpcd)(μ-edt) (**2**).

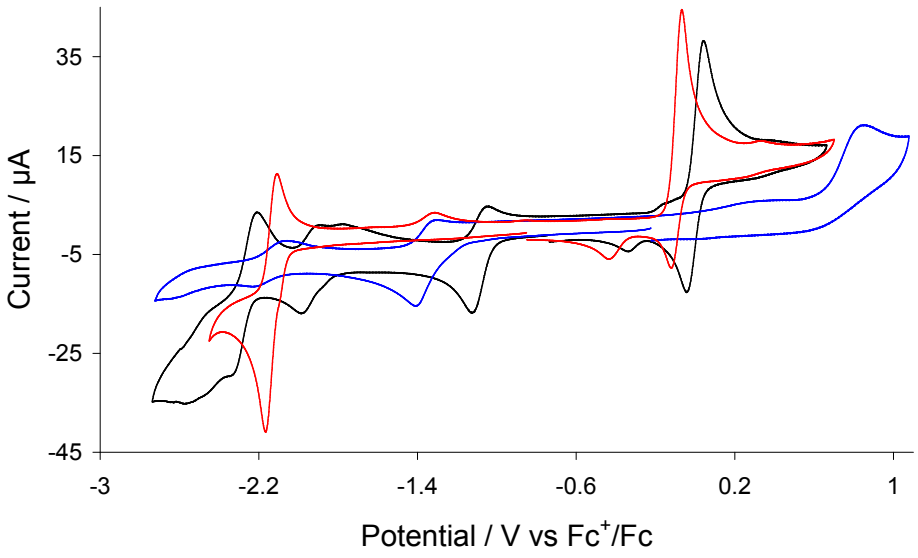
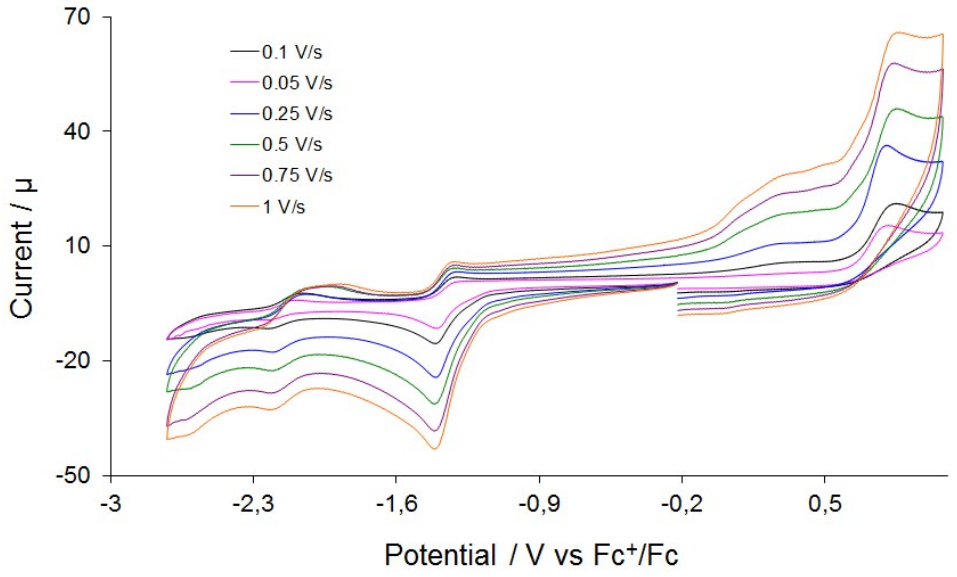
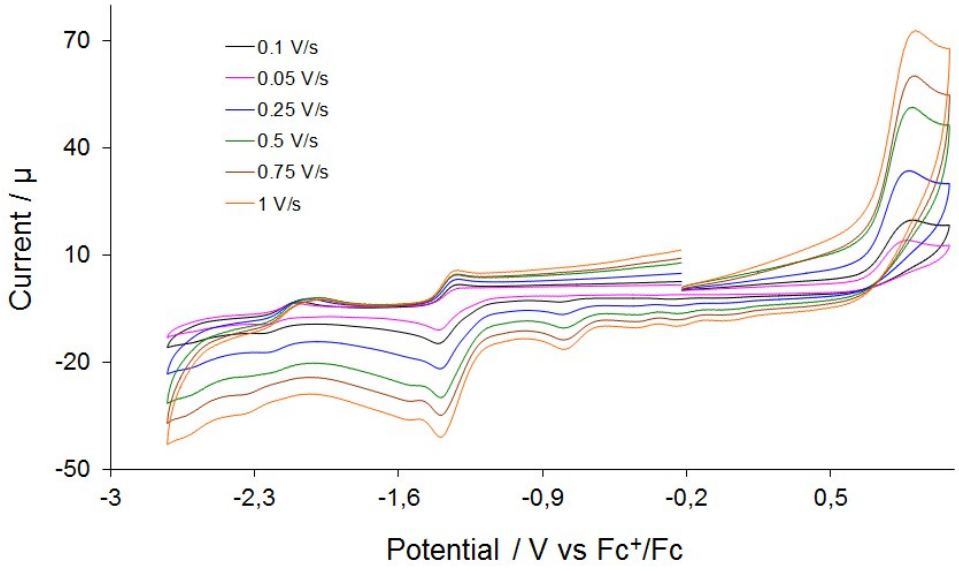


Fig. S1. CVs of $Fe_2(CO)_4(\kappa^2$-bpcd)(µ-edt) (**2**) (black), $Fe_2(CO)_4(\kappa^2$-dppen)(µ-edt) (**3**) (red) and bpcd (blue) in MeCN (1 mM solution, supporting electrolyte $[NBu_4][PF_6]$, scan rate 0.1 V/s, glassy carbon electrode, potential *vs.* Fc^+/Fc).

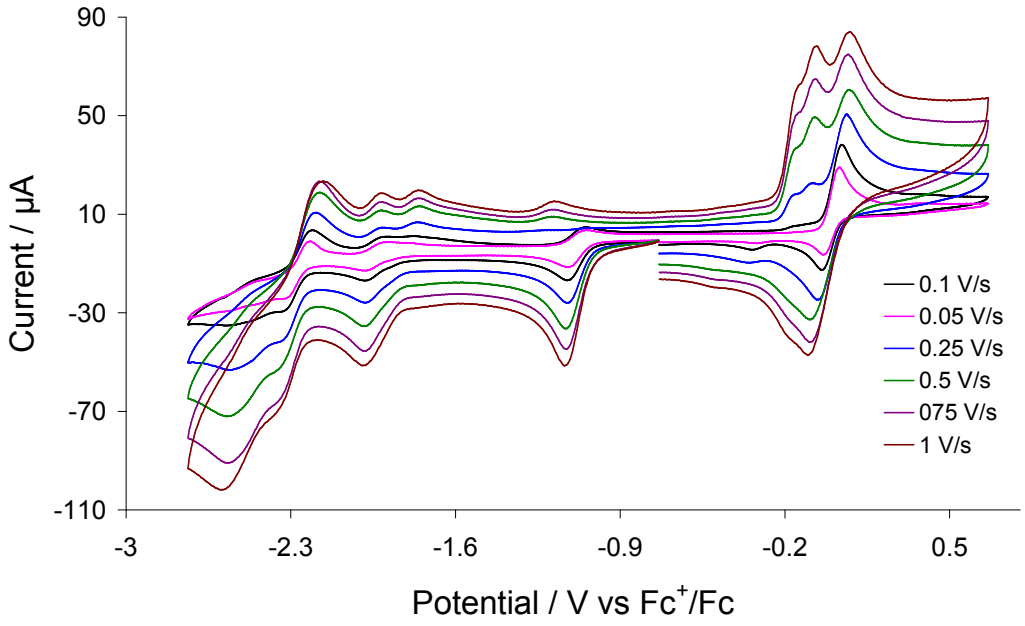


(a)

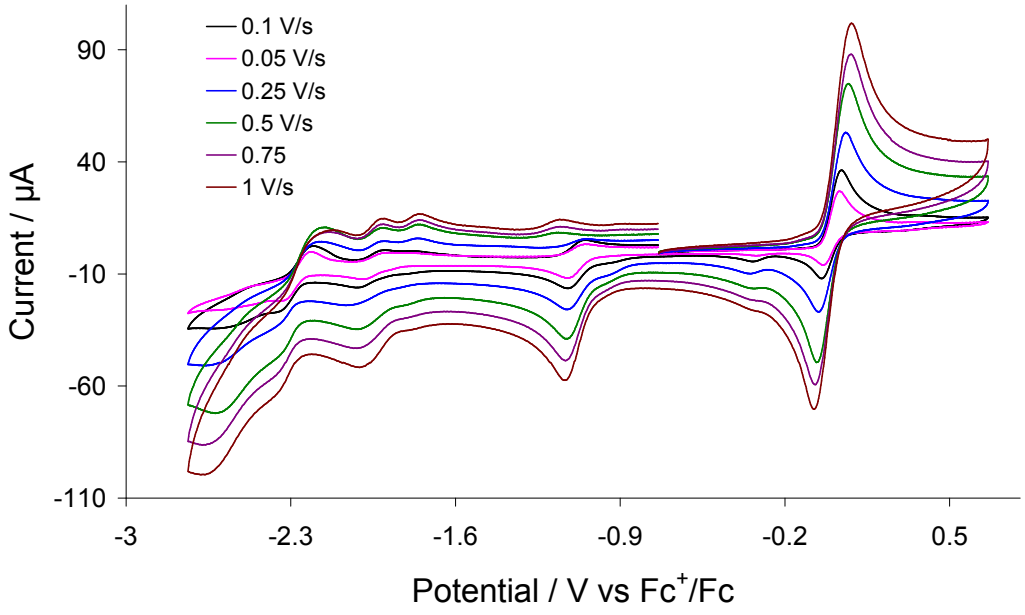


(b)

Fig. S2. CVs of 4,5-bis(diphenylphosphino)-4-cyclopenten-1,3-dione (bpcd) at various scan rates in acetonitrile (1 mM solution, supporting electrolyte $[NBu_4][PF_6]$, glassy carbon electrode, potential *vs.* Fc^+/Fc) - (a) scanning negative potential window first; (b) scanning positive potential window first.



(a)



(b)

Fig. S3. CVs of $Fe_2(CO)_4(\kappa^2\text{-bpcd})(\mu\text{-edt})$ (**2**) at various scan rates in acetonitrile (1 mM solution, supporting electrolyte $[NBu_4][PF_6]$, glassy carbon electrode, potential *vs.* Fc^+/Fc) - (a) scanning negative potential window first; (b) scanning positive potential window first.

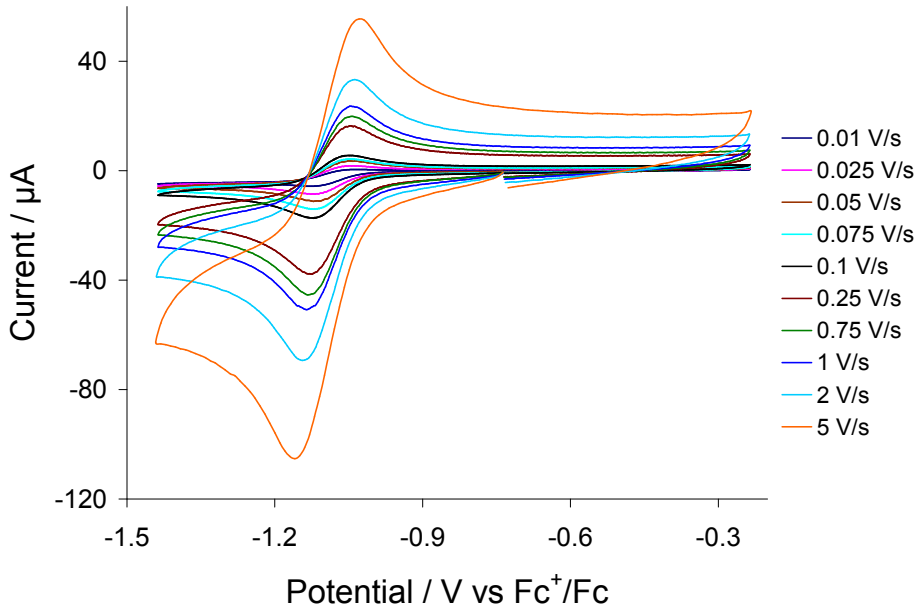
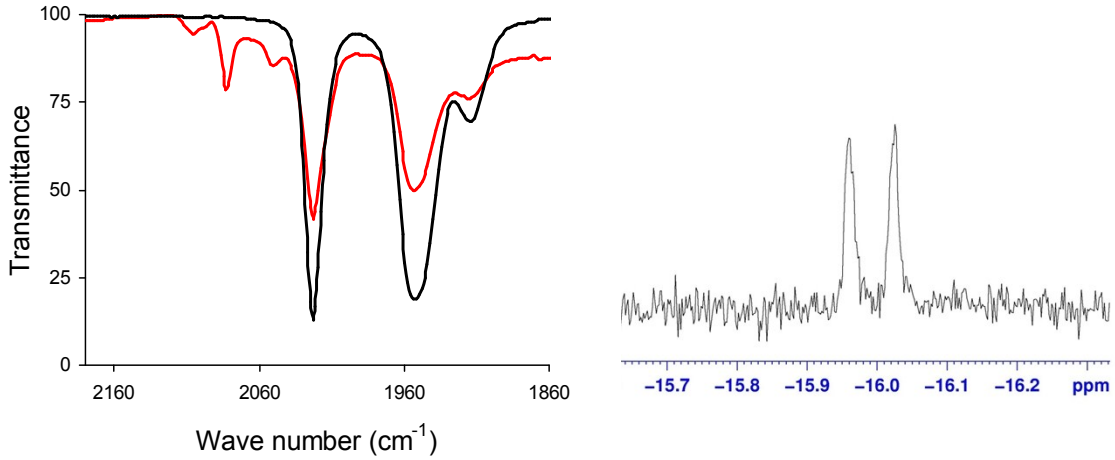
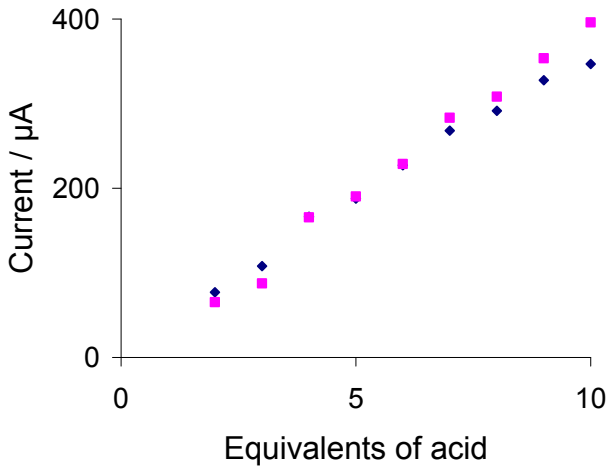


Fig. S4. CVs of $Fe_2(CO)_4(\kappa^2\text{-bpcd})(\mu\text{-edt})$ (**2**) at various scan rates in acetonitrile with the potential cyclic between –1.45 and –0.25 V (1 mM solution, supporting electrolyte $[NBu_4][PF_6]$, glassy carbon electrode, potential *vs*. Fc^+/Fc).



(a) (b)

Fig. S5. (a) IR spectra of $Fe_2(CO)_4(\kappa^2\text{-dppen})(\mu\text{-edt})$ (**3**) in the absence of acid (black) and upon addition of two equivalent of CF_3CO_2H (red) in CH_2Cl_2; (b) Hydride region of the NMR spectrum of $Fe_2(CO)_4(\kappa^2\text{-dppen})(\mu\text{-edt})$ (**3**).



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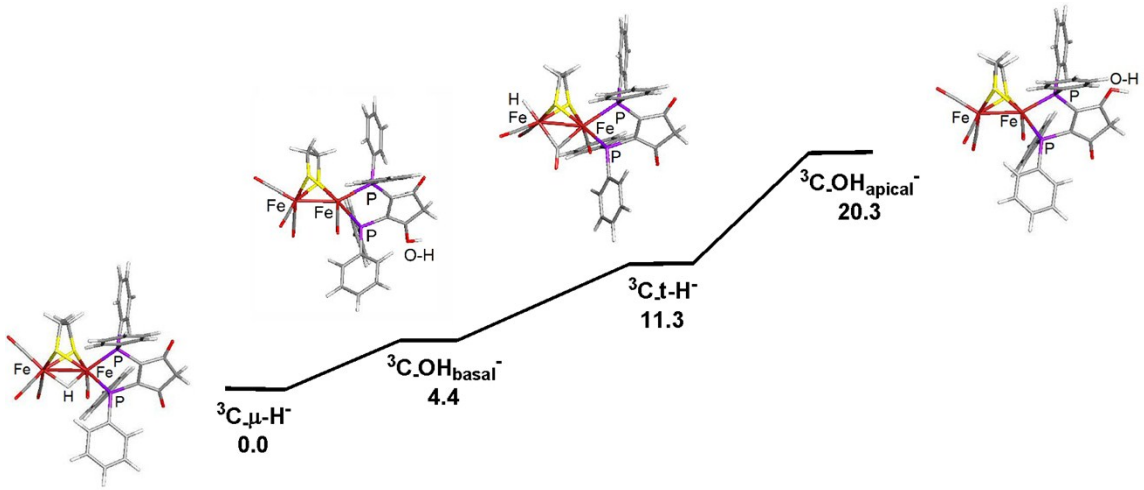

Fig. S7. DFT-optimized structures of the four different triplet isomers evaluated for the protonation of ^{3}**B**$^{2-}$. The energies are in kcal/mol (ΔG) and are relative to ^{3}**C_µ-H**$^-$.

Atomic coordinates and optimized energies for the reported DFT species

Species $^{2}\mathbf{A}^{+}$
SCF Done: E(UB3LYP) = -3527.61606996
Zero-point correction = 0.522562 (Hartree/Particle)
Thermal correction to Energy = 0.569772
Thermal correction to Enthalpy = 0.570716
Thermal correction to Gibbs Free Energy = 0.435898
Sum of electronic and zero-point Energies = -3527.093508
Sum of electronic and thermal Energies = -3527.046298
Sum of electronic and thermal Enthalpies = -3527.045354
Sum of electronic and thermal Free Energies = -3527.180172

Coordinates: $^{2}\mathbf{A}^{+}$

Fe	2.86360000	22.49080000	-2.08730000
Fe	1.98130000	23.56640000	0.18290000
S	0.66980000	22.38560000	-1.31820000
S	3.24110000	21.60630000	0.02520000
C	0.63790000	20.68020000	-0.60550000
C	1.90470000	20.33590000	0.18870000
O	3.01660000	19.98740000	-3.71750000
C	2.97170000	20.95910000	-3.11860000
O	5.69330000	23.36640000	-2.22270000
C	4.60310000	23.02460000	-2.17430000
O	2.08120000	24.33050000	-4.26680000
C	2.37610000	23.62520000	-3.41540000
O	4.36570000	24.79760000	1.45450000
C	3.42430000	24.35110000	0.98300000
P	0.56480000	23.59880000	2.21800000
C	-0.25990000	25.25060000	2.05950000
P	1.13930000	25.78480000	-0.36870000
O	-1.85950000	25.24820000	3.88990000
C	-1.38000000	25.79990000	2.92740000
C	-1.79130000	27.15010000	2.36030000
O	-0.80090000	28.33110000	0.45890000
C	-0.86380000	27.36010000	1.17350000
C	0.00660000	26.12170000	1.04950000
C	1.42340000	23.54080000	3.84010000
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C	3.38390000	22.80630000	5.08440000

C	2.82500000	23.30440000	6.26460000
C	1.56180000	23.90700000	6.23760000
C	0.85610000	24.01990000	5.03700000
C	-0.85710000	22.43980000	2.35030000
C	-0.86760000	21.41820000	3.31390000
C	-1.92760000	20.50600000	3.35820000
C	-2.98480000	20.60740000	2.44910000
C	-2.97890000	21.62390000	1.48620000
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C	0.08030000	26.18410000	-1.81820000
C	-0.99420000	25.33250000	-2.13340000
C	-1.83590000	25.63060000	-3.20810000
H	-2.66370000	24.96500000	-3.44360000
C	-1.60760000	26.77320000	-3.98150000
C	-0.54100000	27.62290000	-3.67050000
C	0.29850000	27.33690000	-2.59120000
C	2.45280000	27.06280000	-0.30610000
C	2.55000000	28.01610000	0.71910000
C	3.61710000	28.92040000	0.73870000
C	4.59040000	28.88440000	-0.26340000
C	4.50050000	27.93500000	-1.28800000
C	3.44330000	27.02360000	-1.30610000
H	2.34400000	19.38770000	-0.14170000
H	1.69250000	20.24660000	1.25910000
H	0.49760000	19.99860000	-1.45090000
H	-0.25300000	20.61890000	0.02750000
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H	-1.92850000	19.72240000	4.11300000
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H	1.80180000	28.07080000	1.50430000
H	1.10590000	28.02070000	-2.34860000
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H	-2.25930000	27.00170000	-4.82200000
H	-1.17290000	24.43130000	-1.55380000
H	-2.84370000	27.14380000	2.04520000
H	-1.68600000	27.94860000	3.10610000

Species **^{1}A**
SCF Done: E(RB3LYP) = -3527.82037091
Zero-point correction = 0.523594 (Hartree/Particle)
Thermal correction to Energy = 0.569702
Thermal correction to Enthalpy = 0.570646
Thermal correction to Gibbs Free Energy = 0.440512
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Sum of electronic and thermal Energies = -3527.250669
Sum of electronic and thermal Enthalpies = -3527.249725
Sum of electronic and thermal Free Energies = -3527.379859

Coordinates: **^{1}A**

Fe	2.92410000	22.57090000	-1.88500000
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C	1.51540000	20.35470000	0.06380000
O	3.15630000	20.22200000	-3.64800000
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O	2.57540000	24.62490000	-3.95720000
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C	-0.22290000	25.23130000	2.11770000
P	1.17660000	25.74560000	-0.26010000
O	-1.79660000	25.10960000	3.97460000
C	-1.35090000	25.69350000	3.01050000
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C	2.95910000	23.14070000	6.13750000
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C	1.03410000	23.98090000	4.92080000
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C	-1.82240000	20.52120000	3.33770000
C	-2.91330000	20.63850000	2.47170000
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C	-1.15770000	25.49830000	-1.82840000
C	-1.99450000	25.76880000	-2.91320000
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C	0.48940000	27.03550000	-2.70870000
C	2.42910000	27.10770000	-0.28420000
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C	3.19590000	29.37680000	0.14430000
C	4.42920000	29.08520000	-0.44730000
C	4.66180000	27.80800000	-0.96530000
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H	1.14170000	20.19610000	1.08150000
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H	-1.47830000	24.77860000	-1.07980000
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Species **^{3}A**
SCF Done: E(UB3LYP) = -3527.81001829
Zero-point correction = 0.520991 (Hartree/Particle)
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Thermal correction to Enthalpy = 0.568971
Thermal correction to Gibbs Free Energy = 0.434579
Sum of electronic and zero-point Energies = -3527.289027
Sum of electronic and thermal Energies = -3527.241992
Sum of electronic and thermal Enthalpies = -3527.241047
Sum of electronic and thermal Free Energies = -3527.375440

Coordinates: **^{3}A**

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O	2.29170000	24.46610000	-4.25530000
C	2.50010000	23.77140000	-3.36840000
O	4.23430000	24.85220000	1.74560000
C	3.33470000	24.43050000	1.17300000

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O	-1.77110000	25.20340000	4.06620000
C	-1.28470000	25.75790000	3.07490000
C	-1.72430000	27.11770000	2.53180000
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C	-0.86560000	27.35660000	1.28920000
C	0.02210000	26.20990000	1.15140000
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C	2.65590000	22.70560000	3.91320000
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C	0.09680000	26.19330000	-1.75720000
C	-1.17120000	25.59350000	-1.84430000
C	-1.97160000	25.78910000	-2.97110000
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C	0.55080000	26.98590000	-2.82260000
C	2.43430000	27.19870000	-0.34510000
C	2.21200000	28.51430000	0.09960000
C	3.22760000	29.46960000	-0.00940000
C	4.46370000	29.13260000	-0.57150000
C	4.68550000	27.83020000	-1.02980000
C	3.67660000	26.86950000	-0.91350000
H	2.12960000	19.51220000	-0.21560000
H	1.46950000	20.34900000	1.19730000
H	0.36710000	20.26510000	-1.55620000
H	-0.40280000	20.86740000	-0.07870000
H	0.20320000	21.05780000	3.71800000
H	-1.58940000	19.35920000	3.67860000

H	-3.64800000	19.73560000	2.32260000
H	-3.88910000	21.84150000	1.00770000
H	-2.09070000	23.53620000	1.03390000
H	3.08040000	22.32350000	2.98730000
H	4.27320000	21.93170000	5.11100000
H	3.33750000	22.80320000	7.25230000
H	1.18000000	24.05200000	7.23960000
H	-0.04220000	24.41600000	5.11240000
H	3.86350000	25.85700000	-1.26430000
H	5.64270000	27.55660000	-1.46970000
H	5.24980000	29.88110000	-0.65300000
H	3.04520000	30.48370000	0.34160000
H	1.24220000	28.79470000	0.49940000
H	1.52280000	27.46870000	-2.77220000
H	0.11060000	27.80220000	-4.76620000
H	-2.13890000	26.73740000	-4.90630000
H	-1.54150000	24.98290000	-1.02460000
H	-2.79390000	27.12040000	2.28180000
H	-1.56920000	27.90980000	3.27680000

Species $^{2}\mathbf{A}^{-}$
SCF Done: E(UB3LYP) = -3527.91748232
Zero-point correction = 0.521606 (Hartree/Particle)
Thermal correction to Energy = 0.567619
Thermal correction to Enthalpy = 0.568564
Thermal correction to Gibbs Free Energy = 0.438557
Sum of electronic and zero-point Energies = -3527.395876
Sum of electronic and thermal Energies = -3527.349863
Sum of electronic and thermal Enthalpies = -3527.348919
Sum of electronic and thermal Free Energies = -3527.478925

Coordinates: $^{2}\mathbf{A}^{-}$

Fe	2.97560000	22.61410000	-1.83010000
Fe	1.95230000	23.70820000	0.28520000
S	0.69680000	22.71990000	-1.37200000
S	2.91910000	21.60920000	0.26500000
C	0.39080000	20.98060000	-0.81950000
C	1.52320000	20.41650000	0.05280000
O	3.29210000	20.22320000	-3.51340000
C	3.13480000	21.15240000	-2.84010000

O	5.76590000	23.38780000	-1.34570000
C	4.65750000	23.09930000	-1.51950000
O	2.72010000	24.56840000	-4.00320000
C	2.80130000	23.81820000	-3.12750000
O	4.30650000	24.79540000	1.63750000
C	3.36210000	24.38420000	1.10850000
P	0.63920000	23.68580000	2.15890000
C	-0.19530000	25.29270000	2.23210000
P	1.14380000	25.84930000	-0.18270000
O	-1.74620000	25.17330000	4.09950000
C	-1.24020000	25.75070000	3.12280000
C	-1.66370000	27.13820000	2.63550000
O	-0.91910000	28.43620000	0.69530000
C	-0.82050000	27.41040000	1.38650000
C	0.04990000	26.26610000	1.20630000
C	1.49720000	23.39230000	3.78330000
C	2.71670000	22.69510000	3.81220000
C	3.36810000	22.44330000	5.02580000
C	2.81110000	22.88910000	6.22750000
C	1.59270000	23.57850000	6.20840000
C	0.93460000	23.82540000	4.99940000
C	-0.74970000	22.45070000	2.25880000
C	-0.62630000	21.25420000	2.98330000
C	-1.66470000	20.31580000	2.99840000
C	-2.84610000	20.56020000	2.29140000
C	-2.98110000	21.75270000	1.57050000
C	-1.94150000	22.68530000	1.55330000
C	0.07090000	26.13200000	-1.67460000
C	-1.25380000	25.66480000	-1.66780000
C	-2.08120000	25.84010000	-2.77840000
H	-3.10710000	25.47540000	-2.74810000
C	-1.59430000	26.48050000	-3.92360000
C	-0.27540000	26.94190000	-3.94420000
C	0.55070000	26.76970000	-2.82800000
C	2.41100000	27.19420000	-0.37120000
C	2.12550000	28.53680000	-0.06060000
C	3.10210000	29.52270000	-0.23590000
C	4.36780000	29.19020000	-0.73320000
C	4.65310000	27.86120000	-1.05850000
C	3.68110000	26.87110000	-0.87630000

H	1.94960000	19.50690000	-0.38790000
H	1.15980000	20.16660000	1.05570000
H	0.26050000	20.38340000	-1.72980000
H	-0.55990000	20.98140000	-0.27590000
H	0.27890000	21.05540000	3.55260000
H	-1.54950000	19.39640000	3.57130000
H	-3.65690000	19.83330000	2.30750000
H	-3.89940000	21.96090000	1.02320000
H	-2.06220000	23.61090000	0.99550000
H	3.16220000	22.34170000	2.88680000
H	4.31490000	21.90500000	5.02350000
H	3.32090000	22.70090000	7.17180000
H	1.14540000	23.92520000	7.13930000
H	-0.02570000	24.33540000	4.99670000
H	3.91530000	25.84020000	-1.12510000
H	5.63230000	27.58550000	-1.44690000
H	5.12500000	29.96210000	-0.86710000
H	2.86630000	30.55680000	0.01280000
H	1.13340000	28.80930000	0.29010000
H	1.57150000	27.13960000	-2.86270000
H	0.11850000	27.43900000	-4.82950000
H	-2.23830000	26.61800000	-4.79120000
H	-1.64550000	25.16890000	-0.78330000
H	-2.73760000	27.17020000	2.40440000
H	-1.48050000	27.89840000	3.40780000

Species $^{1}\mathbf{B}^{2-}$

SCF Done: E(RB3LYP) = -3527.87805019

Zero-point correction = 0.518643 (Hartree/Particle)

Thermal correction to Energy = 0.564830

Thermal correction to Enthalpy = 0.565774

Thermal correction to Gibbs Free Energy = 0.436320

Sum of electronic and zero-point Energies = -3527.359407

Sum of electronic and thermal Energies = -3527.313220

Sum of electronic and thermal Enthalpies = -3527.312276

Sum of electronic and thermal Free Energies = -3527.441730

Coordinates: $^{1}\mathbf{B}^{2-}$

Fe	3.08210000	22.63150000	-1.80100000
Fe	1.98210000	23.78140000	0.33690000

S	0.78180000	22.79430000	-1.36050000
S	2.97090000	21.68060000	0.32770000
C	0.47050000	21.05190000	-0.82140000
C	1.58510000	20.48480000	0.07480000
O	3.60870000	20.15560000	-3.28540000
C	3.34200000	21.11880000	-2.68630000
O	5.76580000	23.64270000	-1.19080000
C	4.68020000	23.27700000	-1.39850000
O	2.88460000	24.31220000	-4.19190000
C	2.93860000	23.67670000	-3.22300000
O	4.20500000	24.98340000	1.80450000
C	3.31160000	24.51750000	1.23150000
P	0.63010000	23.73360000	2.22400000
C	-0.12750000	25.31580000	2.35760000
P	1.10880000	25.94260000	-0.10800000
O	-1.63810000	25.21410000	4.27310000
C	-1.10700000	25.77410000	3.26720000
C	-1.48430000	27.19700000	2.81820000
O	-0.83150000	28.56830000	0.88000000
C	-0.68930000	27.49040000	1.53170000
C	0.12430000	26.35960000	1.29460000
C	1.46670000	23.26820000	3.83030000
C	2.70490000	22.60400000	3.85940000
C	3.31860000	22.27800000	5.07670000
C	2.70190000	22.61050000	6.28670000
C	1.46570000	23.27200000	6.26730000
C	0.84920000	23.59940000	5.05540000
C	-0.74700000	22.45800000	2.21990000
C	-0.65050000	21.20990000	2.85710000
C	-1.70400000	20.28830000	2.80210000
C	-2.87660000	20.60000000	2.10560000
C	-2.98710000	21.84570000	1.47320000
C	-1.93480000	22.76250000	1.53420000
C	0.02920000	26.13680000	-1.63050000
C	-1.36410000	26.03570000	-1.49920000
C	-2.19980000	26.13660000	-2.61510000
H	-3.28020000	26.06370000	-2.48710000
C	-1.65520000	26.34310000	-3.88820000
C	-0.26750000	26.45450000	-4.03000000
C	0.56450000	26.35490000	-2.90950000

C	2.36380000	27.27670000	-0.46600000
C	2.03200000	28.63250000	-0.26700000
C	2.97140000	29.63220000	-0.54020000
C	4.24880000	29.30450000	-1.01670000
C	4.58210000	27.96180000	-1.21880000
C	3.64450000	26.95720000	-0.94520000
H	2.02230000	19.57830000	-0.36350000
H	1.19690000	20.22890000	1.06670000
H	0.36300000	20.45430000	-1.73540000
H	-0.49070000	21.04850000	-0.29560000
H	0.24880000	20.95790000	3.41590000
H	-1.60820000	19.32830000	3.31110000
H	-3.69940000	19.88590000	2.06450000
H	-3.89900000	22.10770000	0.93640000
H	-2.03190000	23.73900000	1.06430000
H	3.19530000	22.33250000	2.92900000
H	4.28170000	21.76680000	5.07130000
H	3.17960000	22.36060000	7.23510000
H	0.97480000	23.53990000	7.20360000
H	-0.11330000	24.11660000	5.04020000
H	3.91560000	25.91690000	-1.10260000
H	5.57140000	27.68660000	-1.58450000
H	4.97730000	30.08920000	-1.22560000
H	2.70050000	30.67630000	-0.37850000
H	1.03340000	28.88510000	0.09730000
H	1.63930000	26.45250000	-3.03940000
H	0.17380000	26.61450000	-5.01400000
H	-2.30570000	26.42180000	-4.76010000
H	-1.78650000	25.90610000	-0.50510000
H	-2.56720000	27.28250000	2.63950000
H	-1.23620000	27.92760000	3.60380000

Species $^{3}\mathbf{B}^{2-}$

SCF Done: E(UB3LYP) = -3527.88049601

Zero-point correction = 0.517925 (Hartree/Particle)

Thermal correction to Energy = 0.564764

Thermal correction to Enthalpy = 0.565708

Thermal correction to Gibbs Free Energy = 0.432273

Sum of electronic and zero-point Energies = -3527.362571

Sum of electronic and thermal Energies = -3527.315732

Sum of electronic and thermal Enthalpies = -3527.314788
Sum of electronic and thermal Free Energies = -3527.448223

Coordinates: $^{3}\mathbf{B}^{2-}$

Fe	2.97560000	22.61410000	-1.83010000
Fe	1.95230000	23.70820000	0.28520000
S	0.69680000	22.71990000	-1.37200000
S	2.91910000	21.60920000	0.26500000
C	0.39080000	20.98060000	-0.81950000
C	1.52320000	20.41650000	0.05280000
O	3.29210000	20.22320000	-3.51340000
C	3.13480000	21.15240000	-2.84010000
O	5.76590000	23.38780000	-1.34570000
C	4.65750000	23.09930000	-1.51950000
O	2.72010000	24.56840000	-4.00320000
C	2.80130000	23.81820000	-3.12750000
O	4.30650000	24.79540000	1.63750000
C	3.36210000	24.38420000	1.10850000
P	0.63920000	23.68580000	2.15890000
C	-0.19530000	25.29270000	2.23210000
P	1.14380000	25.84930000	-0.18270000
O	-1.74620000	25.17330000	4.09950000
C	-1.24020000	25.75070000	3.12280000
C	-1.66370000	27.13820000	2.63550000
O	-0.91910000	28.43620000	0.69530000
C	-0.82050000	27.41040000	1.38650000
C	0.04990000	26.26610000	1.20630000
C	1.49720000	23.39230000	3.78330000
C	2.71670000	22.69510000	3.81220000
C	3.36810000	22.44330000	5.02580000
C	2.81110000	22.88910000	6.22750000
C	1.59270000	23.57850000	6.20840000
C	0.93460000	23.82540000	4.99940000
C	-0.74970000	22.45070000	2.25880000
C	-0.62630000	21.25420000	2.98330000
C	-1.66470000	20.31580000	2.99840000
C	-2.84610000	20.56020000	2.29140000
C	-2.98110000	21.75270000	1.57050000
C	-1.94150000	22.68530000	1.55330000
C	0.07090000	26.13200000	-1.67460000

C	-1.25380000	25.66480000	-1.66780000
C	-2.08120000	25.84010000	-2.77840000
H	-3.10710000	25.47540000	-2.74810000
C	-1.59430000	26.48050000	-3.92360000
C	-0.27540000	26.94190000	-3.94420000
C	0.55070000	26.76970000	-2.82800000
C	2.41100000	27.19420000	-0.37120000
C	2.12550000	28.53680000	-0.06060000
C	3.10210000	29.52270000	-0.23590000
C	4.36780000	29.19020000	-0.73320000
C	4.65310000	27.86120000	-1.05850000
C	3.68110000	26.87110000	-0.87630000
H	1.94960000	19.50690000	-0.38790000
H	1.15980000	20.16660000	1.05570000
H	0.26050000	20.38340000	-1.72980000
H	-0.55990000	20.98140000	-0.27590000
H	0.27890000	21.05540000	3.55260000
H	-1.54950000	19.39640000	3.57130000
H	-3.65690000	19.83330000	2.30750000
H	-3.89940000	21.96090000	1.02320000
H	-2.06220000	23.61090000	0.99550000
H	3.16220000	22.34170000	2.88680000
H	4.31490000	21.90500000	5.02350000
H	3.32090000	22.70090000	7.17180000
H	1.14540000	23.92520000	7.13930000
H	-0.02570000	24.33540000	4.99670000
H	3.91530000	25.84020000	-1.12510000
H	5.63230000	27.58550000	-1.44690000
H	5.12500000	29.96210000	-0.86710000
H	2.86630000	30.55680000	0.01280000
H	1.13340000	28.80930000	0.29010000
H	1.57150000	27.13960000	-2.86270000
H	0.11850000	27.43900000	-4.82950000
H	-2.23830000	26.61800000	-4.79120000
H	-1.64550000	25.16890000	-0.78330000
H	-2.73760000	27.17020000	2.40440000
H	-1.48050000	27.89840000	3.40780000

Species **^{3}C_μ-H^{-}**
SCF Done: E(UB3LYP) = -3528.49490742

Zero-point correction = 0.527415 (Hartree/Particle)
Thermal correction to Energy = 0.574449
Thermal correction to Enthalpy = 0.575393
Thermal correction to Gibbs Free Energy = 0.442383
Sum of electronic and zero-point Energies = -3527.967492
Sum of electronic and thermal Energies = -3527.920458
Sum of electronic and thermal Enthalpies = -3527.919514
Sum of electronic and thermal Free Energies = -3528.052524

Coordinates: **^{3}C_μ-H^{-}**

Fe	3.03310000	22.54610000	-2.04380000
Fe	2.06780000	23.86360000	0.27120000
S	0.75480000	22.73560000	-1.37300000
S	3.13970000	21.76170000	0.19910000
C	0.55010000	21.03250000	-0.68720000
C	1.72030000	20.58300000	0.20960000
O	2.90960000	19.83100000	-3.35540000
C	2.93770000	20.86750000	-2.85120000
O	5.96550000	22.87520000	-2.11210000
C	4.81810000	22.75800000	-2.08800000
O	2.60930000	24.10510000	-4.51400000
C	2.76210000	23.52650000	-3.52810000
O	4.30770000	24.95120000	1.78530000
C	3.38820000	24.54460000	1.21030000
P	0.64600000	23.68700000	2.18390000
C	-0.17450000	25.30430000	2.31130000
P	1.13500000	25.93820000	-0.09670000
O	-1.69520000	25.12400000	4.19960000
C	-1.20970000	25.72980000	3.23000000
C	-1.65700000	27.12340000	2.78570000
O	-1.00120000	28.45730000	0.84120000
C	-0.85420000	27.42710000	1.51890000
C	0.03430000	26.30370000	1.30000000
C	1.48680000	23.32010000	3.80210000
C	2.70600000	22.62080000	3.78740000
C	3.36480000	22.30470000	4.98190000
C	2.81630000	22.68880000	6.20860000
C	1.60000000	23.38210000	6.23300000
C	0.93410000	23.69210000	5.04290000
C	-0.78350000	22.49760000	2.22700000

C	-0.77190000	21.32790000	3.00400000
C	-1.84050000	20.42520000	2.95550000
C	-2.94080000	20.67740000	2.13020000
C	-2.96340000	21.84160000	1.35280000
C	-1.89370000	22.73860000	1.39850000
C	0.07400000	26.15040000	-1.60760000
C	-1.30990000	25.92510000	-1.55170000
C	-2.09850000	26.02760000	-2.70040000
H	-3.17220000	25.85770000	-2.63190000
C	-1.51400000	26.35200000	-3.92930000
C	-0.13540000	26.57520000	-3.99710000
C	0.65110000	26.47630000	-2.84510000
C	2.33710000	27.34430000	-0.30940000
C	1.96050000	28.67950000	-0.07030000
C	2.87670000	29.71760000	-0.26760000
C	4.17440000	29.44670000	-0.71680000
C	4.55140000	28.12530000	-0.97130000
C	3.63970000	27.08280000	-0.76740000
H	2.10270000	19.60440000	-0.10830000
H	1.39560000	20.48820000	1.25190000
H	0.44010000	20.35900000	-1.54540000
H	-0.39190000	21.01570000	-0.13000000
H	0.06830000	21.12250000	3.66330000
H	-1.81310000	19.52750000	3.57220000
H	-3.77470000	19.97770000	2.09600000
H	-3.81450000	22.05270000	0.70670000
H	-1.92230000	23.63560000	0.78450000
H	3.14910000	22.32160000	2.84120000
H	4.31070000	21.76600000	4.94560000
H	3.33140000	22.45080000	7.13880000
H	1.16070000	23.68240000	7.18370000
H	-0.02360000	24.20650000	5.06990000
H	3.94670000	26.06020000	-0.96560000
H	5.55650000	27.89700000	-1.32320000
H	4.88440000	30.25900000	-0.86870000
H	2.56810000	30.74420000	-0.07300000
H	0.94550000	28.90270000	0.24960000
H	1.72020000	26.66220000	-2.91610000
H	0.33480000	26.82380000	-4.94730000
H	-2.12790000	26.43110000	-4.82560000

H	-1.77830000	25.68530000	-0.60040000
H	-2.73800000	27.15390000	2.59100000
H	-1.45210000	27.86900000	3.56710000
H	2.96070000	24.15730000	-0.98620000

Species **UDFT C_μ-H$^-$ singlet <S^2> = 0.5649 after annihilation of spin contaminant**
SCF Done: E(UB3LYP) = -3528.49492181
Zero-point correction = 0.527427 (Hartree/Particle)
Thermal correction to Energy = 0.574448
Thermal correction to Enthalpy = 0.575392
Thermal correction to Gibbs Free Energy = 0.443523
Sum of electronic and zero-point Energies = -3527.967495
Sum of electronic and thermal Energies = -3527.920474
Sum of electronic and thermal Enthalpies = -3527.919530
Sum of electronic and thermal Free Energies = -3528.051398

Coordinates: **UDFT C_μ-H$^-$ singlet**

Fe	3.03140000	22.54610000	-2.04450000
Fe	2.06700000	23.86290000	0.27080000
S	0.75340000	22.73580000	-1.37320000
S	3.13830000	21.76060000	0.19830000
C	0.54830000	21.03250000	-0.68790000
C	1.71880000	20.58210000	0.20820000
O	2.90690000	19.83170000	-3.35730000
C	2.93530000	20.86800000	-2.85250000
O	5.96390000	22.87420000	-2.11330000
C	4.81650000	22.75740000	-2.08890000
O	2.60740000	24.10620000	-4.51390000
C	2.76030000	23.52730000	-3.52830000
O	4.30770000	24.94970000	1.78440000
C	3.38790000	24.54340000	1.20960000
P	0.64530000	23.68640000	2.18320000
C	-0.17630000	25.30330000	2.30920000
P	1.13520000	25.93800000	-0.09720000
O	-1.69820000	25.12250000	4.19640000
C	-1.21230000	25.72860000	3.22730000
C	-1.65900000	27.12240000	2.78310000
O	-1.00040000	28.45770000	0.84040000
C	-0.85440000	27.42690000	1.51760000
C	0.03390000	26.30350000	1.29890000

C	1.48660000	23.32160000	3.80160000
C	2.70590000	22.62250000	3.78750000
C	3.36490000	22.30770000	4.98220000
C	2.81650000	22.69320000	6.20850000
C	1.60010000	23.38630000	6.23230000
C	0.93400000	23.69490000	5.04190000
C	-0.78340000	22.49610000	2.22830000
C	-0.76950000	21.32590000	3.00460000
C	-1.83750000	20.42240000	2.95740000
C	-2.93940000	20.67420000	2.13400000
C	-2.96420000	21.83880000	1.35730000
C	-1.89520000	22.73670000	1.40180000
C	0.07490000	26.15130000	-1.60850000
C	-1.30870000	25.92330000	-1.55360000
C	-2.09690000	26.02670000	-2.70240000
H	-3.17040000	25.85480000	-2.63470000
C	-1.51260000	26.35440000	-3.93040000
C	-0.13430000	26.58020000	-3.99730000
C	0.65190000	26.48050000	-2.84510000
C	2.33810000	27.34350000	-0.30870000
C	1.96250000	28.67870000	-0.06770000
C	2.87930000	29.71640000	-0.26390000
C	4.17670000	29.44520000	-0.71390000
C	4.55270000	28.12390000	-0.97030000
C	3.64040000	27.08180000	-0.76760000
H	2.10100000	19.60370000	-0.11070000
H	1.39440000	20.48650000	1.25040000
H	0.43750000	20.35930000	-1.54620000
H	-0.39340000	21.01600000	-0.13010000
H	0.07200000	21.12090000	3.66230000
H	-1.80840000	19.52440000	3.57350000
H	-3.77280000	19.97380000	2.10080000
H	-3.81660000	22.04970000	0.71290000
H	-1.92560000	23.63420000	0.78850000
H	3.14890000	22.32220000	2.84150000
H	4.31080000	21.76910000	4.94640000
H	3.33180000	22.45630000	7.13890000
H	1.16090000	23.68760000	7.18280000
H	-0.02380000	24.20910000	5.06860000
H	3.94660000	26.05930000	-0.96720000

H	5.55750000	27.89540000	-1.32290000
H	4.88730000	30.25730000	-0.86500000
H	2.57150000	30.74290000	-0.06790000
H	0.94780000	28.90210000	0.25280000
H	1.72070000	26.66840000	-2.91540000
H	0.33590000	26.83140000	-4.94670000
H	-2.12620000	26.43420000	-4.82680000
H	-1.77700000	25.68070000	-0.60300000
H	-2.73970000	27.15300000	2.58670000
H	-1.45550000	27.86760000	3.56520000
H	2.96020000	24.15630000	-0.98660000

Species **^{3}C_t-H$^-$**
SCF Done: E(UB3LYP) = -3528.47927540
Zero-point correction = 0.528193 (Hartree/Particle)
Thermal correction to Energy = 0.574719
Thermal correction to Enthalpy = 0.575663
Thermal correction to Gibbs Free Energy = 0.444792
Sum of electronic and zero-point Energies = -3527.951082
Sum of electronic and thermal Energies = -3527.904557
Sum of electronic and thermal Enthalpies = -3527.903613
Sum of electronic and thermal Free Energies = -3528.034484

Coordinates: **^{3}C_t-H$^-$**

Fe	3.10070000	22.47750000	-1.98830000
Fe	2.20720000	23.91110000	0.16980000
S	0.83620000	22.69310000	-1.36030000
S	3.23740000	21.77740000	0.25170000
C	0.65820000	21.00990000	-0.62720000
C	1.80920000	20.61730000	0.31540000
O	4.10150000	25.27590000	-1.70970000
C	3.46290000	24.34170000	-1.39570000
O	5.89610000	21.75210000	-2.45770000
C	4.80630000	22.07800000	-2.26730000
O	2.48020000	23.04300000	-4.78770000
C	2.73180000	22.86470000	-3.67510000
O	4.32480000	25.02330000	1.85790000
C	3.46770000	24.61100000	1.20170000
P	0.64350000	23.72820000	2.18700000
C	-0.16670000	25.34860000	2.26670000

P	1.12650000	25.97430000	-0.18610000
O	-1.62310000	25.31450000	4.21530000
C	-1.13390000	25.86450000	3.21540000
C	-1.49480000	27.28370000	2.76490000
O	-0.79850000	28.52960000	0.76400000
C	-0.72920000	27.50600000	1.45670000
C	0.03620000	26.29900000	1.21260000
C	1.45490000	23.36830000	3.82020000
C	2.68370000	22.68470000	3.81670000
C	3.33050000	22.36650000	5.01710000
C	2.76030000	22.73270000	6.23930000
C	1.53510000	23.41070000	6.25300000
C	0.88090000	23.72280000	5.05690000
C	-0.79070000	22.54940000	2.19470000
C	-0.80870000	21.38030000	2.97300000
C	-1.88350000	20.48700000	2.89660000
C	-2.95800000	20.74690000	2.04010000
C	-2.94940000	21.90980000	1.26010000
C	-1.87540000	22.79980000	1.33450000
C	0.09460000	26.07680000	-1.72460000
C	-1.27780000	26.36750000	-1.67650000
C	-2.04420000	26.38620000	-2.84630000
H	-3.10680000	26.61790000	-2.78540000
C	-1.45280000	26.11690000	-4.08450000
C	-0.08690000	25.82370000	-4.14470000
C	0.67690000	25.79920000	-2.97430000
C	2.19420000	27.49340000	-0.24930000
C	2.79410000	27.92060000	0.94740000
C	3.63270000	29.03700000	0.96890000
C	3.88800000	29.74790000	-0.20880000
C	3.29280000	29.33270000	-1.40300000
C	2.45330000	28.21390000	-1.42350000
H	2.19630000	19.62300000	0.05890000
H	1.46740000	20.58640000	1.35620000
H	0.61030000	20.32090000	-1.47740000
H	-0.30190000	20.97600000	-0.10130000
H	0.01160000	21.16940000	3.65530000
H	-1.88090000	19.59030000	3.51520000
H	-3.79580000	20.05350000	1.98310000
H	-3.77990000	22.12590000	0.58950000

H	-1.88130000	23.69760000	0.72020000
H	3.14360000	22.39750000	2.87460000
H	4.28310000	21.83930000	4.98910000
H	3.26530000	22.49230000	7.17440000
H	1.07950000	23.69760000	7.20020000
H	-0.07970000	24.23240000	5.07420000
H	1.99080000	27.91940000	-2.36070000
H	3.47640000	29.88050000	-2.32640000
H	4.54110000	30.61940000	-0.19380000
H	4.08380000	29.35100000	1.90910000
H	2.59510000	27.38930000	1.87540000
H	1.73290000	25.55440000	-3.04350000
H	0.38730000	25.59490000	-5.09750000
H	-2.05180000	26.12880000	-4.99410000
H	-1.74960000	26.59420000	-0.72660000
H	-2.57810000	27.39330000	2.61780000
H	-1.19960000	28.02020000	3.52580000
H	2.84880000	21.02870000	-2.44280000

Species **^{3}C_OH_basal^{-}**
SCF Done: E(UB3LYP) = -3528.48427454
Zero-point correction = 0.528543 (Hartree/Particle)
Thermal correction to Energy = 0.577234
Thermal correction to Enthalpy = 0.578178
Thermal correction to Gibbs Free Energy = 0.438798
Sum of electronic and zero-point Energies = -3527.955731
Sum of electronic and thermal Energies = -3527.907040
Sum of electronic and thermal Enthalpies = -3527.906096
Sum of electronic and thermal Free Energies = -3528.045477

Coordinates: **^{3}C_OH_basal^{-}**

Fe	3.15760000	22.08860000	-1.74440000
Fe	1.96320000	23.52540000	0.19750000
S	0.84140000	22.26720000	-1.56210000
S	2.95270000	21.01180000	0.34860000
C	0.34040000	20.71820000	-0.67370000
C	1.52050000	19.93840000	-0.07870000
O	3.37340000	19.66060000	-3.45950000
C	3.30360000	20.60420000	-2.80060000
O	6.01280000	22.48240000	-1.11430000

C	4.89390000	22.34660000	-1.35220000
O	3.15240000	24.18100000	-3.81720000
C	3.14530000	23.36400000	-3.00230000
O	4.45120000	24.79840000	1.24350000
C	3.48530000	24.30640000	0.83080000
P	0.52580000	23.76170000	2.20940000
C	-0.29090000	25.33620000	2.12260000
P	0.99800000	25.95500000	-0.41040000
O	-1.79870000	25.38900000	4.03800000
C	-1.27980000	25.85990000	3.00430000
C	-1.68590000	27.25840000	2.44880000
C	-0.85980000	27.40490000	1.20520000
C	-0.07580000	26.31390000	1.01640000
C	1.42730000	23.57430000	3.82550000
C	2.66860000	22.91720000	3.85510000
C	3.36640000	22.76030000	5.05950000
C	2.83180000	23.26240000	6.24950000
C	1.59200000	23.91450000	6.22900000
C	0.88840000	24.06780000	5.03000000
C	-0.80440000	22.47380000	2.39770000
C	-0.55670000	21.24810000	3.03980000
C	-1.54090000	20.25530000	3.09310000
C	-2.79130000	20.46930000	2.50210000
C	-3.04880000	21.68830000	1.86390000
C	-2.06430000	22.67950000	1.81290000
C	-0.04600000	26.40320000	-1.88110000
C	-0.89580000	25.41340000	-2.40520000
C	-1.71670000	25.68400000	-3.50510000
H	-2.36400000	24.90060000	-3.89680000
C	-1.68980000	26.94540000	-4.10940000
C	-0.84020000	27.93460000	-3.60050000
C	-0.02880000	27.66800000	-2.49310000
C	2.30960000	27.25750000	-0.41390000
C	2.50070000	28.14100000	0.65890000
C	3.56950000	29.04480000	0.65570000
C	4.45980000	29.08260000	-0.42160000
C	4.28040000	28.20170000	-1.49540000
C	3.22100000	27.29120000	-1.48640000
H	1.86640000	19.17360000	-0.78430000
H	1.20710000	19.42570000	0.84060000

H	-0.20440000	20.09430000	-1.39400000
H	-0.36170000	21.02510000	0.10640000
H	0.40800000	21.06850000	3.51010000
H	-1.32930000	19.31440000	3.60050000
H	-3.55930000	19.69790000	2.54510000
H	-4.02250000	21.87340000	1.41140000
H	-2.27450000	23.63290000	1.33250000
H	3.09200000	22.51970000	2.93580000
H	4.32880000	22.24990000	5.06010000
H	3.37550000	23.14630000	7.18680000
H	1.16480000	24.30400000	7.15280000
H	-0.08380000	24.55750000	5.01870000
H	3.10370000	26.60190000	-2.32140000
H	4.97300000	28.21310000	-2.33590000
H	5.29210000	29.78520000	-0.42210000
H	3.70330000	29.72010000	1.49980000
H	1.80870000	28.12170000	1.49710000
H	0.61160000	28.45110000	-2.09740000
H	-0.81210000	28.92150000	-4.06180000
H	-2.32010000	27.15430000	-4.97310000
H	-0.90310000	24.41980000	-1.96360000
H	-2.77160000	27.28000000	2.25950000
H	-1.47040000	28.03220000	3.20200000
O	-0.86560000	28.54020000	0.42030000
H	-1.69220000	29.01880000	0.56640000

Species **^{3}C_OH_apical$^-$**
SCF Done: E(UB3LYP) = -3528.46310510
Zero-point correction = 0.530574 (Hartree/Particle)
Thermal correction to Energy = 0.578428
Thermal correction to Enthalpy = 0.579372
Thermal correction to Gibbs Free Energy = 0.442948
Sum of electronic and zero-point Energies = -3527.932531
Sum of electronic and thermal Energies = -3527.884678
Sum of electronic and thermal Enthalpies = -3527.883733
Sum of electronic and thermal Free Energies = -3528.020157

Coordinates: **^{3}C_OH_apical$^-$**

Fe	2.77430000	22.60700000	-2.31580000
Fe	2.01680000	23.70150000	0.36720000

S	0.65160000	22.65170000	-1.27780000
S	3.33080000	21.79220000	-0.16590000
C	0.66230000	20.91720000	-0.64270000
C	2.00210000	20.51110000	0.00690000
O	2.92640000	19.92500000	-3.65010000
C	2.85860000	20.97160000	-3.16910000
O	5.54290000	23.57940000	-2.68630000
C	4.46120000	23.20760000	-2.53530000
O	1.76810000	24.06080000	-4.67690000
C	2.14440000	23.53180000	-3.72630000
O	4.26580000	24.85000000	1.83470000
C	3.35480000	24.41830000	1.25500000
P	0.54220000	23.63980000	2.28520000
C	-0.29770000	25.25700000	2.27870000
P	1.18140000	25.88010000	-0.08860000
C	-1.32860000	25.70380000	3.03800000
C	-1.74360000	27.07850000	2.60360000
O	-0.92120000	28.44120000	0.73430000
C	-0.81390000	27.38400000	1.38920000
C	0.06030000	26.26670000	1.24600000
C	1.39250000	23.42010000	3.92120000
C	2.56570000	22.64640000	3.94770000
C	3.25370000	22.42490000	5.14610000
C	2.78410000	22.98860000	6.33620000
C	1.62140000	23.76810000	6.31940000
C	0.92590000	23.97940000	5.12420000
C	-0.85620000	22.42690000	2.40690000
C	-0.81230000	21.30090000	3.24650000
C	-1.84230000	20.35250000	3.22970000
C	-2.93490000	20.51090000	2.37140000
C	-2.98730000	21.62820000	1.52800000
C	-1.95780000	22.57210000	1.54290000
C	0.20130000	26.17790000	-1.65030000
C	-1.14070000	25.76600000	-1.70300000
C	-1.90670000	25.95140000	-2.85590000
H	-2.94710000	25.62780000	-2.86910000
C	-1.34390000	26.55620000	-3.98570000
C	-0.00930000	26.96950000	-3.94710000
C	0.75590000	26.77960000	-2.79110000
C	2.46030000	27.22530000	-0.24350000

C	2.16420000	28.56090000	0.08810000
C	3.13860000	29.55490000	-0.05360000
C	4.41450000	29.23870000	-0.53670000
C	4.71240000	27.91660000	-0.88020000
C	3.74090000	26.91960000	-0.73170000
H	2.38680000	19.58480000	-0.43750000
H	1.87770000	20.33430000	1.08160000
H	0.42890000	20.26010000	-1.48860000
H	-0.15800000	20.83510000	0.07870000
H	0.02380000	21.16560000	3.92900000
H	-1.78900000	19.49110000	3.89470000
H	-3.73650000	19.77360000	2.35830000
H	-3.82970000	21.76360000	0.85060000
H	-2.00780000	23.43140000	0.87810000
H	2.95750000	22.23250000	3.02050000
H	4.16440000	21.82770000	5.14180000
H	3.32410000	22.82940000	7.26890000
H	1.25070000	24.21500000	7.24140000
H	0.01480000	24.56910000	5.12840000
H	3.98630000	25.89190000	-0.98980000
H	5.70070000	27.65370000	-1.25560000
H	5.17000000	30.01690000	-0.64420000
H	2.89390000	30.58370000	0.20960000
H	1.16300000	28.81780000	0.42850000
H	1.78950000	27.11730000	-2.77970000
H	0.44340000	27.44110000	-4.81860000
H	-1.94040000	26.70500000	-4.88510000
H	-1.59310000	25.31570000	-0.82250000
H	-2.79760000	27.14870000	2.28760000
H	-1.58840000	27.83440000	3.38920000
O	-1.88850000	25.05160000	4.12630000
H	-2.80960000	25.32980000	4.21960000

Table S1. Crystal data and structure refinement for $Fe_2(CO)_4(\kappa^2$-bpcd)(μ-edt) (**2**).

Identification code	SG3B	
Empirical formula	C71 H54 Cl2 Fe4 O12 P4 S4	
Formula weight	1645.6294	
Temperature	100(2) K	
Wavelength	0.68890 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 8.72050(10) Å	α= 90°.
	b = 30.8866(5) Å	β= 90.9170(10)°.
	c = 25.4645(6) Å	γ = 90°.
Volume	6857.9(2) $Å^3$	
Z	4	
Density (calculated)	1.594 Mg/m^3	
Absorption coefficient	2.516 mm^{-1}	
F(000)	3352	
Crystal size	0.10 x 0.04 x 0.01 mm^3	
Theta range for data collection	1.49 to 29.95°.	
Index ranges	-12<=h<=12, -44<=k<=44, -35<=l<=25	
Reflections collected	84633	
Independent reflections	20913 [R(int) = 0.0416]	
Completeness to theta = 29.95°	95.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.80271	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	20913 / 0 / 1082	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.1063	
R indices (all data)	R1 = 0.0622, wR2 = 0.1148	
Largest diff. peak and hole	1.496 and -1.402 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $Fe_2(CO)_4(\kappa^2$-bpcd)(μ-edt) (**2**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(2)	3122(1)	7293(1)	-757(1)	24(1)
Fe(1)	2088(1)	7650(1)	58(1)	19(1)
S(2)	595(1)	7380(1)	-592(1)	25(1)
S(1)	2953(1)	6967(1)	34(1)	23(1)
C(6)	65(3)	6828(1)	-408(1)	29(1)
C(5)	1253(3)	6623(1)	-45(1)	29(1)
O(4)	3361(2)	6545(1)	-1471(1)	45(1)
C(4)	3222(3)	6830(1)	-1192(1)	30(1)
O(2)	6399(2)	7435(1)	-575(1)	46(1)
C(2)	5119(3)	7380(1)	-645(1)	31(1)
O(3)	2975(4)	7983(1)	-1540(1)	70(1)
C(3)	3013(4)	7714(1)	-1235(1)	40(1)
O(1)	5028(2)	7968(1)	458(1)	33(1)
C(1)	3851(2)	7844(1)	311(1)	23(1)
P(2)	815(1)	7651(1)	793(1)	19(1)
C(8)	-308(2)	8156(1)	802(1)	20(1)
P(1)	1311(1)	8321(1)	-93(1)	20(1)
O(5)	-2172(2)	8091(1)	1493(1)	31(1)
C(9)	-1662(2)	8290(1)	1129(1)	23(1)
C(10)	-2262(3)	8714(1)	899(1)	24(1)
O(6)	-1255(2)	9126(1)	167(1)	31(1)
C(11)	-1214(2)	8813(1)	451(1)	22(1)
C(7)	-74(2)	8445(1)	417(1)	20(1)
C(30)	1923(2)	7646(1)	1407(1)	23(1)
C(31)	3356(3)	7442(1)	1412(1)	27(1)
C(32)	4232(3)	7421(1)	1873(1)	31(1)
C(33)	3676(3)	7597(1)	2331(1)	36(1)
C(34)	2239(3)	7792(1)	2330(1)	37(1)
C(35)	1362(3)	7817(1)	1870(1)	30(1)
C(24)	-685(2)	7255(1)	920(1)	22(1)

C(29)	-552(3)	6946(1)	1316(1)	33(1)
C(28)	-1725(3)	6645(1)	1393(1)	42(1)
C(27)	-3020(3)	6653(1)	1073(1)	38(1)
C(26)	-3167(3)	6957(1)	684(1)	31(1)
C(25)	-2003(2)	7260(1)	604(1)	25(1)
C(18)	172(2)	8452(1)	-679(1)	22(1)
C(23)	-1325(3)	8295(1)	-721(1)	25(1)
C(22)	-2189(3)	8367(1)	-1174(1)	30(1)
C(21)	-1551(3)	8586(1)	-1590(1)	34(1)
C(20)	-67(3)	8744(1)	-1553(1)	32(1)
C(19)	794(3)	8682(1)	-1096(1)	27(1)
C(12)	2726(2)	8756(1)	-44(1)	23(1)
C(13)	2522(3)	9121(1)	270(1)	27(1)
C(14)	3690(3)	9431(1)	311(1)	31(1)
C(15)	5025(3)	9381(1)	41(1)	31(1)
C(16)	5229(3)	9024(1)	-279(1)	29(1)
C(17)	4090(3)	8709(1)	-317(1)	26(1)
Fe(2')	4926(1)	5823(1)	2496(1)	24(1)
Fe(1')	3754(1)	5163(1)	2069(1)	21(1)
S(1')	4616(1)	5735(1)	1618(1)	25(1)
C(5')	2934(3)	6074(1)	1469(1)	32(1)
S(2')	2377(1)	5692(1)	2435(1)	26(1)
C(6')	1805(3)	6068(1)	1915(1)	33(1)
O(4')	5252(2)	6753(1)	2705(1)	49(1)
C(4')	5055(3)	6396(1)	2602(1)	33(1)
O(2')	8199(2)	5645(1)	2381(1)	41(1)
C(2')	6919(3)	5709(1)	2427(1)	28(1)
O(3')	5078(3)	5574(1)	3605(1)	51(1)
C(3')	4983(3)	5671(1)	3172(1)	33(1)
O(1')	6647(2)	4708(1)	1936(1)	39(1)
C(1')	5485(3)	4880(1)	1982(1)	26(1)
P(2')	2414(1)	4815(1)	1473(1)	22(1)
C(8')	1285(2)	4404(1)	1814(1)	23(1)
P(1')	2983(1)	4693(1)	2663(1)	20(1)
O(5')	-513(2)	4092(1)	1184(1)	35(1)
C(9')	-47(3)	4125(1)	1629(1)	26(1)

C(10')	-661(3)	3899(1)	2111(1)	30(1)
O(6')	407(2)	3899(1)	2999(1)	31(1)
C(11')	432(2)	4026(1)	2555(1)	23(1)
C(7')	1553(2)	4347(1)	2330(1)	22(1)
C(30')	3488(3)	4515(1)	981(1)	26(1)
C(31')	4817(3)	4708(1)	790(1)	40(1)
C(32')	5669(4)	4495(1)	415(1)	49(1)
C(33')	5233(4)	4094(1)	233(1)	44(1)
C(34')	3948(4)	3896(1)	430(1)	41(1)
C(35')	3066(3)	4107(1)	799(1)	33(1)
C(24')	960(2)	5102(1)	1086(1)	23(1)
C(29')	1252(3)	5240(1)	581(1)	33(1)
C(28')	181(3)	5489(1)	304(1)	35(1)
C(27')	-1175(3)	5601(1)	534(1)	35(1)
C(26')	-1483(3)	5464(1)	1039(1)	39(1)
C(25')	-418(3)	5218(1)	1317(1)	31(1)
C(18')	1867(2)	4865(1)	3230(1)	23(1)
C(23')	365(3)	5015(1)	3145(1)	26(1)
C(22')	-491(3)	5166(1)	3563(1)	30(1)
C(21')	136(3)	5174(1)	4063(1)	32(1)
C(20')	1618(3)	5027(1)	4150(1)	32(1)
C(19')	2481(3)	4871(1)	3737(1)	27(1)
C(12')	4416(2)	4325(1)	2938(1)	22(1)
C(13')	4202(3)	3882(1)	2984(1)	28(1)
C(14')	5347(3)	3624(1)	3210(1)	37(1)
C(15')	6701(3)	3806(1)	3387(1)	34(1)
C(16')	6939(3)	4246(1)	3340(1)	30(1)
C(17')	5801(3)	4506(1)	3118(1)	27(1)
Cl(1)	2635(1)	3200(1)	1684(1)	82(1)
Cl(2)	1792(2)	2500(1)	2394(1)	101(1)
C(36)	2264(6)	2649(1)	1760(2)	67(1)

Table S3. Bond lengths [Å] and angles [°] for $Fe_2(CO)_4(\kappa^2$-bpcd)(μ-edt) (**2**).

Fe(2)-C(2)	1.781(3)	C(10)-H(63B)	0.87(3)
Fe(2)-C(3)	1.782(3)	O(6)-C(11)	1.208(3)
Fe(2)-C(4)	1.811(3)	C(11)-C(7)	1.514(3)
Fe(2)-S(1)	2.2600(7)	C(30)-C(35)	1.389(4)
Fe(2)-S(2)	2.2651(6)	C(30)-C(31)	1.398(3)
Fe(2)-Fe(1)	2.5289(5)	C(31)-C(32)	1.393(4)
Fe(1)-C(1)	1.762(2)	C(31)-H(30)	0.91(3)
Fe(1)-P(2)	2.1917(7)	C(32)-C(33)	1.381(4)
Fe(1)-P(1)	2.2122(6)	C(32)-H(31)	0.97(3)
Fe(1)-S(1)	2.2414(6)	C(33)-C(34)	1.391(4)
Fe(1)-S(2)	2.2508(6)	C(33)-H(32)	0.97(4)
S(2)-C(6)	1.828(3)	C(34)-C(35)	1.391(4)
S(1)-C(5)	1.833(2)	C(34)-H(33)	0.97(4)
C(6)-C(5)	1.518(4)	C(35)-H(34)	0.99(3)
C(6)-H(6B)	0.96(3)	C(24)-C(29)	1.391(3)
C(6)-H(6A)	0.96(3)	C(24)-C(25)	1.393(3)
C(5)-H(5B)	0.94(3)	C(29)-C(28)	1.399(3)
C(5)-H(5A)	0.93(3)	C(29)-H(29)	0.97(3)
O(4)-C(4)	1.139(3)	C(28)-C(27)	1.382(4)
O(2)-C(2)	1.140(3)	C(28)-H(28)	0.95(4)
O(3)-C(3)	1.139(4)	C(27)-C(26)	1.369(4)
O(1)-C(1)	1.152(3)	C(27)-H(27)	0.88(3)
P(2)-C(24)	1.823(2)	C(26)-C(25)	1.398(3)
P(2)-C(30)	1.824(2)	C(26)-H(26)	0.96(3)
P(2)-C(8)	1.841(2)	C(25)-H(25)	0.97(3)
C(8)-C(7)	1.343(3)	C(18)-C(19)	1.393(3)
C(8)-C(9)	1.514(3)	C(18)-C(23)	1.395(3)
P(1)-C(18)	1.826(2)	C(23)-C(22)	1.385(4)
P(1)-C(12)	1.826(2)	C(23)-H(23)	0.92(3)
P(1)-C(7)	1.829(2)	C(22)-C(21)	1.382(4)
O(5)-C(9)	1.205(3)	C(22)-H(22)	0.96(3)
C(9)-C(10)	1.521(3)	C(21)-C(20)	1.384(4)
C(10)-C(11)	1.504(3)	C(21)-H(21)	0.93(3)
C(10)-H(63A)	0.93(3)	C(20)-C(19)	1.388(4)

C(20)-H(20)	0.91(3)	P(2')-C(30')	1.829(2)
C(19)-H(19)	0.93(3)	P(2')-C(8')	1.835(2)
C(12)-C(17)	1.395(3)	C(8')-C(7')	1.341(4)
C(12)-C(13)	1.396(3)	C(8')-C(9')	1.515(3)
C(13)-C(14)	1.400(3)	P(1')-C(12')	1.821(2)
C(13)-H(13)	0.95(3)	P(1')-C(18')	1.833(2)
C(14)-C(15)	1.370(4)	P(1')-C(7')	1.839(2)
C(14)-H(14)	0.85(3)	O(5')-C(9')	1.202(3)
C(15)-C(16)	1.386(4)	C(9')-C(10')	1.517(4)
C(15)-H(15)	0.92(4)	C(10')-C(11')	1.519(4)
C(16)-C(17)	1.391(3)	C(10')-H(1A')	0.97(4)
C(16)-H(16)	1.03(3)	C(10')-H(1B')	0.81(3)
C(17)-H(17)	0.92(3)	O(6')-C(11')	1.197(3)
Fe(2')-C(2')	1.784(2)	C(11')-C(7')	1.512(3)
Fe(2')-C(3')	1.785(3)	C(30')-C(35')	1.389(4)
Fe(2')-C(4')	1.796(3)	C(30')-C(31')	1.399(4)
Fe(2')-S(2')	2.2625(6)	C(31')-C(32')	1.384(4)
Fe(2')-S(1')	2.2637(8)	C(31')-H(31')	0.94(4)
Fe(2')-Fe(1')	2.5181(5)	C(32')-C(33')	1.375(5)
Fe(1')-C(1')	1.761(2)	C(32')-H(32')	0.91(4)
Fe(1')-P(2')	2.1835(7)	C(33')-C(34')	1.378(5)
Fe(1')-P(1')	2.2076(7)	C(33')-H(33')	0.84(3)
Fe(1')-S(2')	2.2394(6)	C(34')-C(35')	1.387(4)
Fe(1')-S(1')	2.2463(6)	C(34')-H(34')	0.98(4)
S(1')-C(5')	1.835(2)	C(35')-H(35')	0.84(4)
C(5')-C(6')	1.515(4)	C(24')-C(29')	1.383(4)
C(5')-H(5A')	0.97(3)	C(24')-C(25')	1.393(3)
C(5')-H(5B')	0.93(4)	C(29')-C(28')	1.393(4)
S(2')-C(6')	1.824(3)	C(29')-H(29')	0.97(3)
C(6')-H(6A')	0.93(3)	C(28')-C(27')	1.373(4)
C(6')-H(6B')	0.94(3)	C(28')-H(28')	0.94(3)
O(4')-C(4')	1.144(3)	C(27')-C(26')	1.385(5)
O(2')-C(2')	1.141(3)	C(27')-H(27')	0.83(3)
O(3')-C(3')	1.146(4)	C(26')-C(25')	1.385(4)
O(1')-C(1')	1.151(3)	C(26')-H(26')	0.87(4)
P(2')-C(24')	1.823(2)	C(25')-H(25')	0.94(3)

C(18')-C(19')	1.390(4)	C(13')-C(14')	1.393(3)
C(18')-C(23')	1.403(3)	C(13')-H(13')	0.93(3)
C(23')-C(22')	1.390(4)	C(14')-C(15')	1.376(4)
C(23')-H(23')	0.98(3)	C(14')-H(14')	1.02(4)
C(22')-C(21')	1.376(4)	C(15')-C(16')	1.379(4)
C(22')-H(22')	0.96(3)	C(15')-H(15')	1.00(3)
C(21')-C(20')	1.384(4)	C(16')-C(17')	1.390(3)
C(21')-H(21')	0.86(3)	C(16')-H(16')	1.02(3)
C(20')-C(19')	1.389(4)	C(17')-H(17')	0.95(3)
C(20')-H(20')	0.91(4)	Cl(1)-C(36)	1.745(4)
C(19')-H(19')	1.00(3)	Cl(2)-C(36)	1.733(5)
C(12')-C(13')	1.388(3)	C(36)-H(36A)	0.9900
C(12')-C(17')	1.400(3)	C(36)-H(36B)	0.9900

C(2)-Fe(2)-C(3)	92.35(14)	P(2)-Fe(1)-S(2)	109.53(2)
C(2)-Fe(2)-C(4)	99.20(11)	P(1)-Fe(1)-S(2)	92.75(2)
C(3)-Fe(2)-C(4)	99.31(13)	S(1)-Fe(1)-S(2)	79.74(2)
C(2)-Fe(2)-S(1)	90.08(9)	C(1)-Fe(1)-Fe(2)	97.34(8)
C(3)-Fe(2)-S(1)	158.50(9)	P(2)-Fe(1)-Fe(2)	153.34(2)
C(4)-Fe(2)-S(1)	101.38(9)	P(1)-Fe(1)-Fe(2)	112.21(2)
C(2)-Fe(2)-S(2)	154.74(9)	S(1)-Fe(1)-Fe(2)	56.170(19)
C(3)-Fe(2)-S(2)	89.95(10)	S(2)-Fe(1)-Fe(2)	56.213(18)
C(4)-Fe(2)-S(2)	105.24(8)	C(6)-S(2)-Fe(1)	107.58(9)
S(1)-Fe(2)-S(2)	79.05(2)	C(6)-S(2)-Fe(2)	100.86(8)
C(2)-Fe(2)-Fe(1)	99.41(9)	Fe(1)-S(2)-Fe(2)	68.110(19)
C(3)-Fe(2)-Fe(1)	103.09(9)	C(5)-S(1)-Fe(1)	106.13(8)
C(4)-Fe(2)-Fe(1)	150.10(9)	C(5)-S(1)-Fe(2)	103.02(10)
S(1)-Fe(2)-Fe(1)	55.471(17)	Fe(1)-S(1)-Fe(2)	68.36(2)
S(2)-Fe(2)-Fe(1)	55.677(18)	C(5)-C(6)-S(2)	111.95(16)
C(1)-Fe(1)-P(2)	97.93(8)	C(5)-C(6)-H(6B)	109.9(18)
C(1)-Fe(1)-P(1)	90.45(7)	S(2)-C(6)-H(6B)	105.6(18)
P(2)-Fe(1)-P(1)	89.39(2)	C(5)-C(6)-H(6A)	108.0(18)
C(1)-Fe(1)-S(1)	92.17(7)	S(2)-C(6)-H(6A)	109.0(18)
P(2)-Fe(1)-S(1)	101.49(2)	H(6B)-C(6)-H(6A)	112(2)
P(1)-Fe(1)-S(1)	168.33(3)	C(6)-C(5)-S(1)	111.50(17)
C(1)-Fe(1)-S(2)	152.37(8)	C(6)-C(5)-H(5B)	111(2)

S(1)-C(5)-H(5B)	106.0(19)	C(8)-C(7)-P(1)	119.20(16)
C(6)-C(5)-H(5A)	111(2)	C(11)-C(7)-P(1)	129.75(17)
S(1)-C(5)-H(5A)	105(2)	C(35)-C(30)-C(31)	119.4(2)
H(5B)-C(5)-H(5A)	112(3)	C(35)-C(30)-P(2)	122.35(17)
O(4)-C(4)-Fe(2)	176.5(2)	C(31)-C(30)-P(2)	118.20(19)
O(2)-C(2)-Fe(2)	179.8(3)	C(32)-C(31)-C(30)	120.4(2)
O(3)-C(3)-Fe(2)	178.6(3)	C(32)-C(31)-H(30)	123.2(19)
O(1)-C(1)-Fe(1)	177.4(2)	C(30)-C(31)-H(30)	116.4(19)
C(24)-P(2)-C(30)	102.40(11)	C(33)-C(32)-C(31)	119.9(2)
C(24)-P(2)-C(8)	100.52(10)	C(33)-C(32)-H(31)	121.8(19)
C(30)-P(2)-C(8)	105.81(10)	C(31)-C(32)-H(31)	118.3(19)
C(24)-P(2)-Fe(1)	121.63(8)	C(32)-C(33)-C(34)	119.8(3)
C(30)-P(2)-Fe(1)	117.59(8)	C(32)-C(33)-H(32)	120(2)
C(8)-P(2)-Fe(1)	106.70(8)	C(34)-C(33)-H(32)	120(2)
C(7)-C(8)-C(9)	110.27(19)	C(33)-C(34)-C(35)	120.6(3)
C(7)-C(8)-P(2)	117.93(17)	C(33)-C(34)-H(33)	120(2)
C(9)-C(8)-P(2)	131.19(17)	C(35)-C(34)-H(33)	120(2)
C(18)-P(1)-C(12)	104.55(10)	C(30)-C(35)-C(34)	119.8(2)
C(18)-P(1)-C(7)	100.24(10)	C(30)-C(35)-H(34)	118.9(18)
C(12)-P(1)-C(7)	104.57(10)	C(34)-C(35)-H(34)	121.3(18)
C(18)-P(1)-Fe(1)	120.70(7)	C(29)-C(24)-C(25)	119.0(2)
C(12)-P(1)-Fe(1)	118.17(7)	C(29)-C(24)-P(2)	122.39(18)
C(7)-P(1)-Fe(1)	106.05(7)	C(25)-C(24)-P(2)	118.62(18)
O(5)-C(9)-C(8)	125.7(2)	C(24)-C(29)-C(28)	120.3(2)
O(5)-C(9)-C(10)	127.3(2)	C(24)-C(29)-H(29)	120.8(19)
C(8)-C(9)-C(10)	106.9(2)	C(28)-C(29)-H(29)	118.7(19)
C(11)-C(10)-C(9)	104.94(18)	C(27)-C(28)-C(29)	119.8(3)
C(11)-C(10)-H(63A)	112.4(17)	C(27)-C(28)-H(28)	123(2)
C(9)-C(10)-H(63A)	109.1(17)	C(29)-C(28)-H(28)	118(2)
C(11)-C(10)-H(63B)	108(2)	C(26)-C(27)-C(28)	120.4(2)
C(9)-C(10)-H(63B)	114(2)	C(26)-C(27)-H(27)	122(2)
H(63A)-C(10)-H(63B)	109(3)	C(28)-C(27)-H(27)	118(2)
O(6)-C(11)-C(10)	127.3(2)	C(27)-C(26)-C(25)	120.3(2)
O(6)-C(11)-C(7)	125.4(2)	C(27)-C(26)-H(26)	121.0(19)
C(10)-C(11)-C(7)	107.28(18)	C(25)-C(26)-H(26)	118.7(19)
C(8)-C(7)-C(11)	110.56(19)	C(24)-C(25)-C(26)	120.2(2)

C(24)-C(25)-H(25)	118.9(19)	C(16)-C(17)-H(17)	116(2)
C(26)-C(25)-H(25)	120.9(19)	C(12)-C(17)-H(17)	123(2)
C(19)-C(18)-C(23)	119.6(2)	C(2')-Fe(2')-C(3')	91.79(12)
C(19)-C(18)-P(1)	121.49(17)	C(2')-Fe(2')-C(4')	98.62(11)
C(23)-C(18)-P(1)	118.81(18)	C(3')-Fe(2')-C(4')	96.45(13)
C(22)-C(23)-C(18)	120.3(2)	C(2')-Fe(2')-S(2')	156.34(8)
C(22)-C(23)-H(23)	117.4(18)	C(3')-Fe(2')-S(2')	91.79(8)
C(18)-C(23)-H(23)	122.3(18)	C(4')-Fe(2')-S(2')	104.20(8)
C(21)-C(22)-C(23)	119.7(2)	C(2')-Fe(2')-S(1')	88.91(9)
C(21)-C(22)-H(22)	120.8(18)	C(3')-Fe(2')-S(1')	157.33(8)
C(23)-C(22)-H(22)	119.4(18)	C(4')-Fe(2')-S(1')	105.85(10)
C(22)-C(21)-C(20)	120.5(3)	S(2')-Fe(2')-S(1')	79.01(2)
C(22)-C(21)-H(21)	116(2)	C(2')-Fe(2')-Fe(1')	100.85(8)
C(20)-C(21)-H(21)	123(2)	C(3')-Fe(2')-Fe(1')	102.00(8)
C(21)-C(20)-C(19)	120.1(3)	C(4')-Fe(2')-Fe(1')	152.60(8)
C(21)-C(20)-H(20)	119.9(19)	S(2')-Fe(2')-Fe(1')	55.554(18)
C(19)-C(20)-H(20)	119.9(19)	S(1')-Fe(2')-Fe(1')	55.732(18)
C(20)-C(19)-C(18)	119.8(2)	C(1')-Fe(1')-P(2')	96.86(9)
C(20)-C(19)-H(19)	120.7(16)	C(1')-Fe(1')-P(1')	91.81(8)
C(18)-C(19)-H(19)	119.5(16)	P(2')-Fe(1')-P(1')	89.27(2)
C(17)-C(12)-C(13)	119.1(2)	C(1')-Fe(1')-S(2')	151.70(9)
C(17)-C(12)-P(1)	118.13(18)	P(2')-Fe(1')-S(2')	111.29(2)
C(13)-C(12)-P(1)	122.75(18)	P(1')-Fe(1')-S(2')	91.38(2)
C(12)-C(13)-C(14)	119.8(2)	C(1')-Fe(1')-S(1')	91.79(8)
C(12)-C(13)-H(13)	117(2)	P(2')-Fe(1')-S(1')	102.16(3)
C(14)-C(13)-H(13)	123(2)	P(1')-Fe(1')-S(1')	167.51(3)
C(15)-C(14)-C(13)	120.6(3)	S(2')-Fe(1')-S(1')	79.87(2)
C(15)-C(14)-H(14)	123(2)	C(1')-Fe(1')-Fe(2')	96.44(8)
C(13)-C(14)-H(14)	117(2)	P(2')-Fe(1')-Fe(2')	155.05(2)
C(14)-C(15)-C(16)	120.2(2)	P(1')-Fe(1')-Fe(2')	111.30(2)
C(14)-C(15)-H(15)	118(2)	S(2')-Fe(1')-Fe(2')	56.426(18)
C(16)-C(15)-H(15)	122(2)	S(1')-Fe(1')-Fe(2')	56.39(2)
C(15)-C(16)-C(17)	119.9(2)	C(5')-S(1')-Fe(1')	106.30(8)
C(15)-C(16)-H(16)	120.3(18)	C(5')-S(1')-Fe(2')	102.62(11)
C(17)-C(16)-H(16)	119.8(18)	Fe(1')-S(1')-Fe(2')	67.88(2)
C(16)-C(17)-C(12)	120.5(2)	C(6')-C(5')-S(1')	111.46(19)

C(6')-C(5')-H(5A')	112.6(17)	C(9')-C(10')-C(11')	104.93(19)
S(1')-C(5')-H(5A')	107.5(17)	C(9')-C(10')-H(1A')	111(2)
C(6')-C(5')-H(5B')	116(2)	C(11')-C(10')-H(1A')	110(2)
S(1')-C(5')-H(5B')	106(2)	C(9')-C(10')-H(1B')	107(2)
H(5A')-C(5')-H(5B')	102(3)	C(11')-C(10')-H(1B')	110(2)
C(6')-S(2')-Fe(1')	107.79(10)	H(1A')-C(10')-H(1B')	113(3)
C(6')-S(2')-Fe(2')	101.13(8)	O(6')-C(11')-C(7')	126.4(2)
Fe(1')-S(2')-Fe(2')	68.019(19)	O(6')-C(11')-C(10')	126.8(2)
C(5')-C(6')-S(2')	112.19(17)	C(7')-C(11')-C(10')	106.8(2)
C(5')-C(6')-H(6A')	108.6(19)	C(8')-C(7')-C(11')	110.70(19)
S(2')-C(6')-H(6A')	108.1(19)	C(8')-C(7')-P(1')	118.78(16)
C(5')-C(6')-H(6B')	114.3(19)	C(11')-C(7')-P(1')	130.08(18)
S(2')-C(6')-H(6B')	107.0(19)	C(35')-C(30')-C(31')	119.1(2)
H(6A')-C(6')-H(6B')	106(3)	C(35')-C(30')-P(2')	123.6(2)
O(4')-C(4')-Fe(2')	173.2(2)	C(31')-C(30')-P(2')	117.3(2)
O(2')-C(2')-Fe(2')	178.7(2)	C(32')-C(31')-C(30')	119.6(3)
O(3')-C(3')-Fe(2')	177.4(2)	C(32')-C(31')-H(31')	119(2)
O(1')-C(1')-Fe(1')	177.3(2)	C(30')-C(31')-H(31')	121(2)
C(24')-P(2')-C(30')	103.66(11)	C(33')-C(32')-C(31')	120.8(3)
C(24')-P(2')-C(8')	102.67(10)	C(33')-C(32')-H(32')	131(3)
C(30')-P(2')-C(8')	104.89(11)	C(31')-C(32')-H(32')	108(3)
C(24')-P(2')-Fe(1')	119.79(8)	C(32')-C(33')-C(34')	120.0(3)
C(30')-P(2')-Fe(1')	116.83(8)	C(32')-C(33')-H(33')	125(2)
C(8')-P(2')-Fe(1')	107.23(8)	C(34')-C(33')-H(33')	115(2)
C(7')-C(8')-C(9')	110.6(2)	C(33')-C(34')-C(35')	120.0(3)
C(7')-C(8')-P(2')	117.90(17)	C(33')-C(34')-H(34')	123(2)
C(9')-C(8')-P(2')	131.33(19)	C(35')-C(34')-H(34')	117(2)
C(12')-P(1')-C(18')	104.25(11)	C(34')-C(35')-C(30')	120.4(3)
C(12')-P(1')-C(7')	105.74(10)	C(34')-C(35')-H(35')	120(3)
C(18')-P(1')-C(7')	99.62(10)	C(30')-C(35')-H(35')	120(3)
C(12')-P(1')-Fe(1')	117.32(7)	C(29')-C(24')-C(25')	119.1(2)
C(18')-P(1')-Fe(1')	121.38(7)	C(29')-C(24')-P(2')	121.05(18)
C(7')-P(1')-Fe(1')	106.16(8)	C(25')-C(24')-P(2')	119.6(2)
O(5')-C(9')-C(8')	126.0(2)	C(24')-C(29')-C(28')	120.6(2)
O(5')-C(9')-C(10')	127.2(2)	C(24')-C(29')-H(29')	120(2)
C(8')-C(9')-C(10')	106.8(2)	C(28')-C(29')-H(29')	119(2)

C(27')-C(28')-C(29')	119.9(3)	C(20')-C(19')-C(18')	120.2(2)
C(27')-C(28')-H(28')	119.7(18)	C(20')-C(19')-H(19')	119.4(19)
C(29')-C(28')-H(28')	120.4(19)	C(18')-C(19')-H(19')	120.4(19)
C(28')-C(27')-C(26')	120.0(3)	C(13')-C(12')-C(17')	118.8(2)
C(28')-C(27')-H(27')	120(2)	C(13')-C(12')-P(1')	123.74(17)
C(26')-C(27')-H(27')	120(2)	C(17')-C(12')-P(1')	117.48(17)
C(27')-C(26')-C(25')	120.3(3)	C(12')-C(13')-C(14')	120.1(2)
C(27')-C(26')-H(26')	124(2)	C(12')-C(13')-H(13')	120.9(19)
C(25')-C(26')-H(26')	115(2)	C(14')-C(13')-H(13')	119.0(19)
C(26')-C(25')-C(24')	120.1(3)	C(15')-C(14')-C(13')	120.5(2)
C(26')-C(25')-H(25')	120.4(19)	C(15')-C(14')-H(14')	124(2)
C(24')-C(25')-H(25')	119.5(19)	C(13')-C(14')-H(14')	116(2)
C(19')-C(18')-C(23')	118.9(2)	C(14')-C(15')-C(16')	120.2(2)
C(19')-C(18')-P(1')	122.32(17)	C(14')-C(15')-H(15')	121.5(19)
C(23')-C(18')-P(1')	118.72(19)	C(16')-C(15')-H(15')	118.3(19)
C(22')-C(23')-C(18')	120.3(2)	C(15')-C(16')-C(17')	119.7(2)
C(22')-C(23')-H(23')	123.2(17)	C(15')-C(16')-H(16')	116.5(18)
C(18')-C(23')-H(23')	116.5(17)	C(17')-C(16')-H(16')	123.7(18)
C(21')-C(22')-C(23')	120.3(2)	C(16')-C(17')-C(12')	120.7(2)
C(21')-C(22')-H(22')	119.3(18)	C(16')-C(17')-H(17')	120(2)
C(23')-C(22')-H(22')	120.4(18)	C(12')-C(17')-H(17')	119(2)
C(22')-C(21')-C(20')	119.9(3)	Cl(2)-C(36)-Cl(1)	114.1(2)
C(22')-C(21')-H(21')	124(2)	Cl(2)-C(36)-H(36A)	108.7
C(20')-C(21')-H(21')	116(2)	Cl(1)-C(36)-H(36A)	108.7
C(21')-C(20')-C(19')	120.5(3)	Cl(2)-C(36)-H(36B)	108.7
C(21')-C(20')-H(20')	119(2)	Cl(1)-C(36)-H(36B)	108.7
C(19')-C(20')-H(20')	120(2)	H(36A)-C(36)-H(36B)	107.6

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for $Fe_2(CO)_4(\kappa^2\text{-bpcd})(\mu\text{-edt})$ (**2**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(2)	20(1)	26(1)	27(1)	-4(1)	-2(1)	-1(1)
Fe(1)	15(1)	18(1)	23(1)	-1(1)	-4(1)	0(1)
S(2)	19(1)	26(1)	30(1)	-5(1)	-8(1)	1(1)
S(1)	18(1)	20(1)	31(1)	-2(1)	-3(1)	0(1)
C(6)	19(1)	26(1)	42(2)	-10(1)	-3(1)	-5(1)
C(5)	23(1)	21(1)	44(2)	-3(1)	-2(1)	-3(1)
O(4)	39(1)	49(1)	49(1)	-21(1)	-4(1)	-2(1)
C(4)	21(1)	38(1)	32(2)	-5(1)	-4(1)	-2(1)
O(2)	30(1)	67(1)	42(1)	-4(1)	1(1)	-18(1)
C(2)	30(1)	36(1)	28(2)	-3(1)	2(1)	-7(1)
O(3)	102(2)	59(2)	51(2)	18(1)	28(2)	30(1)
C(3)	47(2)	37(1)	35(2)	-3(1)	10(1)	7(1)
O(1)	25(1)	30(1)	45(1)	1(1)	-13(1)	-3(1)
C(1)	22(1)	20(1)	27(1)	1(1)	-5(1)	1(1)
P(2)	16(1)	18(1)	24(1)	1(1)	-4(1)	1(1)
C(8)	16(1)	21(1)	23(1)	-2(1)	-5(1)	0(1)
P(1)	16(1)	19(1)	23(1)	1(1)	-5(1)	-1(1)
O(5)	29(1)	31(1)	33(1)	3(1)	2(1)	4(1)
C(9)	19(1)	23(1)	28(1)	-3(1)	-4(1)	1(1)
C(10)	22(1)	23(1)	28(1)	0(1)	-4(1)	5(1)
O(6)	28(1)	25(1)	38(1)	4(1)	-5(1)	2(1)
C(11)	19(1)	20(1)	26(1)	-1(1)	-7(1)	1(1)
C(7)	17(1)	19(1)	25(1)	-2(1)	-5(1)	0(1)
C(30)	21(1)	21(1)	26(1)	2(1)	-5(1)	0(1)
C(31)	23(1)	28(1)	29(2)	2(1)	-4(1)	5(1)
C(32)	27(1)	35(1)	31(2)	4(1)	-8(1)	7(1)
C(33)	39(1)	39(1)	29(2)	1(1)	-12(1)	9(1)
C(34)	44(1)	40(1)	25(2)	-3(1)	-8(1)	13(1)
C(35)	28(1)	32(1)	31(2)	2(1)	-4(1)	7(1)
C(24)	19(1)	20(1)	29(1)	1(1)	0(1)	0(1)

C(29)	25(1)	28(1)	46(2)	11(1)	-5(1)	-2(1)
C(28)	34(1)	31(1)	60(2)	19(1)	-1(1)	-5(1)
C(27)	25(1)	28(1)	60(2)	3(1)	7(1)	-7(1)
C(26)	19(1)	29(1)	45(2)	-5(1)	0(1)	-3(1)
C(25)	20(1)	25(1)	32(1)	0(1)	-2(1)	-1(1)
C(18)	20(1)	21(1)	26(1)	0(1)	-6(1)	0(1)
C(23)	21(1)	26(1)	28(1)	2(1)	-5(1)	-2(1)
C(22)	23(1)	30(1)	36(2)	2(1)	-12(1)	0(1)
C(21)	34(1)	34(1)	34(2)	6(1)	-16(1)	0(1)
C(20)	35(1)	33(1)	28(2)	8(1)	-7(1)	-3(1)
C(19)	25(1)	26(1)	30(1)	3(1)	-6(1)	-3(1)
C(12)	20(1)	22(1)	26(1)	4(1)	-8(1)	-3(1)
C(13)	24(1)	25(1)	32(2)	1(1)	-6(1)	-4(1)
C(14)	32(1)	25(1)	37(2)	-1(1)	-7(1)	-7(1)
C(15)	24(1)	28(1)	41(2)	8(1)	-10(1)	-9(1)
C(16)	20(1)	32(1)	36(2)	9(1)	-6(1)	-4(1)
C(17)	22(1)	26(1)	31(1)	3(1)	-5(1)	-2(1)
Fe(2')	18(1)	21(1)	34(1)	1(1)	-3(1)	-1(1)
Fe(1')	15(1)	19(1)	28(1)	2(1)	0(1)	-1(1)
S(1')	18(1)	24(1)	33(1)	7(1)	-1(1)	-2(1)
C(5')	24(1)	26(1)	45(2)	11(1)	-7(1)	1(1)
S(2')	18(1)	22(1)	39(1)	0(1)	2(1)	0(1)
C(6')	21(1)	27(1)	51(2)	2(1)	-5(1)	3(1)
O(4')	47(1)	26(1)	75(2)	1(1)	-12(1)	1(1)
C(4')	24(1)	26(1)	47(2)	3(1)	-6(1)	2(1)
O(2')	26(1)	52(1)	45(1)	-5(1)	-8(1)	5(1)
C(2')	26(1)	30(1)	29(1)	0(1)	-6(1)	1(1)
O(3')	66(1)	52(1)	35(1)	-2(1)	-3(1)	-17(1)
C(3')	30(1)	29(1)	42(2)	-4(1)	-1(1)	-6(1)
O(1')	27(1)	39(1)	51(1)	9(1)	7(1)	9(1)
C(1')	23(1)	25(1)	32(1)	6(1)	3(1)	-1(1)
P(2')	19(1)	21(1)	24(1)	1(1)	1(1)	0(1)
C(8')	20(1)	22(1)	27(1)	-1(1)	-1(1)	-1(1)
P(1')	16(1)	20(1)	24(1)	1(1)	-2(1)	-1(1)
O(5')	36(1)	37(1)	32(1)	-3(1)	-6(1)	-6(1)
C(9')	25(1)	23(1)	29(1)	-3(1)	-3(1)	-2(1)

C(10')	24(1)	31(1)	35(2)	4(1)	-5(1)	-8(1)
O(6')	22(1)	35(1)	34(1)	8(1)	-2(1)	-3(1)
C(11')	19(1)	22(1)	29(1)	3(1)	-2(1)	-1(1)
C(7')	18(1)	20(1)	28(1)	1(1)	0(1)	-2(1)
C(30')	27(1)	30(1)	22(1)	2(1)	2(1)	7(1)
C(31')	39(1)	37(1)	43(2)	1(1)	15(1)	1(1)
C(32')	46(2)	53(2)	49(2)	7(2)	22(2)	14(1)
C(33')	46(2)	51(2)	33(2)	-2(1)	6(1)	27(1)
C(34')	43(2)	40(2)	40(2)	-10(1)	-6(1)	17(1)
C(35')	29(1)	36(1)	35(2)	-5(1)	-2(1)	8(1)
C(24')	21(1)	24(1)	26(1)	-1(1)	-2(1)	-1(1)
C(29')	34(1)	34(1)	33(2)	6(1)	6(1)	6(1)
C(28')	44(1)	33(1)	29(2)	7(1)	-4(1)	5(1)
C(27')	34(1)	31(1)	41(2)	1(1)	-13(1)	5(1)
C(26')	23(1)	48(2)	45(2)	3(1)	-1(1)	7(1)
C(25')	23(1)	39(1)	31(2)	5(1)	0(1)	4(1)
C(18')	21(1)	21(1)	26(1)	1(1)	0(1)	-2(1)
C(23')	21(1)	28(1)	29(2)	-1(1)	-1(1)	0(1)
C(22')	22(1)	31(1)	37(2)	-1(1)	2(1)	3(1)
C(21')	34(1)	30(1)	33(2)	-4(1)	8(1)	4(1)
C(20')	37(1)	32(1)	27(2)	-3(1)	-2(1)	3(1)
C(19')	25(1)	26(1)	30(1)	0(1)	-3(1)	1(1)
C(12')	19(1)	22(1)	26(1)	1(1)	0(1)	1(1)
C(13')	20(1)	24(1)	42(2)	1(1)	4(1)	0(1)
C(14')	24(1)	24(1)	62(2)	6(1)	4(1)	4(1)
C(15')	23(1)	32(1)	46(2)	8(1)	2(1)	7(1)
C(16')	21(1)	34(1)	33(2)	2(1)	-3(1)	2(1)
C(17')	22(1)	25(1)	32(2)	1(1)	-6(1)	1(1)
Cl(1)	80(1)	53(1)	111(1)	-22(1)	-11(1)	7(1)
Cl(2)	83(1)	166(2)	55(1)	-5(1)	17(1)	29(1)
C(36)	91(3)	60(2)	49(2)	-7(2)	-14(2)	5(2)

Table S5. Torsion angles [°] for $Fe_2(CO)_4(\kappa^2$-bpcd)(μ-edt) (**2**).

C(2)-Fe(2)-Fe(1)-C(1)	4.12(12)	C(4)-Fe(2)-S(2)-C(6)	49.67(14)
C(3)-Fe(2)-Fe(1)-C(1)	-90.54(13)	S(1)-Fe(2)-S(2)-C(6)	-49.28(10)
C(4)-Fe(2)-Fe(1)-C(1)	131.94(18)	Fe(1)-Fe(2)-S(2)-C(6)	-104.74(10)
S(1)-Fe(2)-Fe(1)-C(1)	87.68(7)	C(2)-Fe(2)-S(2)-Fe(1)	-10.5(2)
S(2)-Fe(2)-Fe(1)-C(1)	-171.34(8)	C(3)-Fe(2)-S(2)-Fe(1)	-105.95(10)
C(2)-Fe(2)-Fe(1)-P(2)	-120.41(10)	C(4)-Fe(2)-S(2)-Fe(1)	154.41(10)
C(3)-Fe(2)-Fe(1)-P(2)	144.93(12)	S(1)-Fe(2)-S(2)-Fe(1)	55.46(2)
C(4)-Fe(2)-Fe(1)-P(2)	7.41(18)	C(1)-Fe(1)-S(1)-C(5)	164.70(13)
S(1)-Fe(2)-Fe(1)-P(2)	-36.85(5)	P(2)-Fe(1)-S(1)-C(5)	66.15(11)
S(2)-Fe(2)-Fe(1)-P(2)	64.13(5)	P(1)-Fe(1)-S(1)-C(5)	-92.46(16)
C(2)-Fe(2)-Fe(1)-P(1)	97.63(9)	S(2)-Fe(1)-S(1)-C(5)	-41.90(11)
C(3)-Fe(2)-Fe(1)-P(1)	2.97(11)	Fe(2)-Fe(1)-S(1)-C(5)	-97.91(11)
C(4)-Fe(2)-Fe(1)-P(1)	-134.55(16)	C(1)-Fe(1)-S(1)-Fe(2)	-97.39(8)
S(1)-Fe(2)-Fe(1)-P(1)	-178.81(3)	P(2)-Fe(1)-S(1)-Fe(2)	164.06(2)
S(2)-Fe(2)-Fe(1)-P(1)	-77.83(3)	P(1)-Fe(1)-S(1)-Fe(2)	5.45(12)
C(2)-Fe(2)-Fe(1)-S(1)	-83.56(9)	S(2)-Fe(1)-S(1)-Fe(2)	56.01(2)
C(3)-Fe(2)-Fe(1)-S(1)	-178.22(11)	C(2)-Fe(2)-S(1)-C(5)	-156.20(12)
C(4)-Fe(2)-Fe(1)-S(1)	44.26(16)	C(3)-Fe(2)-S(1)-C(5)	107.2(3)
S(2)-Fe(2)-Fe(1)-S(1)	100.98(3)	C(4)-Fe(2)-S(1)-C(5)	-56.80(11)
C(2)-Fe(2)-Fe(1)-S(2)	175.46(9)	S(2)-Fe(2)-S(1)-C(5)	46.74(9)
C(3)-Fe(2)-Fe(1)-S(2)	80.80(11)	Fe(1)-Fe(2)-S(1)-C(5)	102.41(9)
C(4)-Fe(2)-Fe(1)-S(2)	-56.72(16)	C(2)-Fe(2)-S(1)-Fe(1)	101.39(9)
S(1)-Fe(2)-Fe(1)-S(2)	-100.98(3)	C(3)-Fe(2)-S(1)-Fe(1)	4.7(3)
C(1)-Fe(1)-S(2)-C(6)	113.71(18)	C(4)-Fe(2)-S(1)-Fe(1)	-159.22(8)
P(2)-Fe(1)-S(2)-C(6)	-59.71(9)	S(2)-Fe(2)-S(1)-Fe(1)	-55.669(19)
P(1)-Fe(1)-S(2)-C(6)	-150.04(9)	Fe(1)-S(2)-C(6)-C(5)	-27.1(2)
S(1)-Fe(1)-S(2)-C(6)	38.95(9)	Fe(2)-S(2)-C(6)-C(5)	43.2(2)
Fe(2)-Fe(1)-S(2)-C(6)	94.92(9)	S(2)-C(6)-C(5)-S(1)	-6.6(3)
C(1)-Fe(1)-S(2)-Fe(2)	18.79(16)	Fe(1)-S(1)-C(5)-C(6)	37.8(2)
P(2)-Fe(1)-S(2)-Fe(2)	-154.63(2)	Fe(2)-S(1)-C(5)-C(6)	-33.1(2)
P(1)-Fe(1)-S(2)-Fe(2)	115.04(2)	C(2)-Fe(2)-C(4)-O(4)	-21(4)
S(1)-Fe(1)-S(2)-Fe(2)	-55.97(2)	C(3)-Fe(2)-C(4)-O(4)	73(4)
C(2)-Fe(2)-S(2)-C(6)	-115.3(2)	S(1)-Fe(2)-C(4)-O(4)	-113(4)
C(3)-Fe(2)-S(2)-C(6)	149.31(14)	S(2)-Fe(2)-C(4)-O(4)	165(4)

Fe(1)-Fe(2)-C(4)-O(4)	-149(4)	Fe(1)-P(2)-C(8)-C(9)	163.44(19)
C(3)-Fe(2)-C(2)-O(2)	-56(100)	C(1)-Fe(1)-P(1)-C(18)	142.25(12)
C(4)-Fe(2)-C(2)-O(2)	44(100)	P(2)-Fe(1)-P(1)-C(18)	-119.82(9)
S(1)-Fe(2)-C(2)-O(2)	145(100)	S(1)-Fe(1)-P(1)-C(18)	39.23(15)
S(2)-Fe(2)-C(2)-O(2)	-151(100)	S(2)-Fe(1)-P(1)-C(18)	-10.30(9)
Fe(1)-Fe(2)-C(2)-O(2)	-160(100)	Fe(2)-Fe(1)-P(1)-C(18)	44.12(9)
C(2)-Fe(2)-C(3)-O(3)	15(12)	C(1)-Fe(1)-P(1)-C(12)	11.76(13)
C(4)-Fe(2)-C(3)-O(3)	-85(12)	P(2)-Fe(1)-P(1)-C(12)	109.69(10)
S(1)-Fe(2)-C(3)-O(3)	111(12)	S(1)-Fe(1)-P(1)-C(12)	-91.26(15)
S(2)-Fe(2)-C(3)-O(3)	169(100)	S(2)-Fe(1)-P(1)-C(12)	-140.79(10)
Fe(1)-Fe(2)-C(3)-O(3)	115(12)	Fe(2)-Fe(1)-P(1)-C(12)	-86.37(10)
P(2)-Fe(1)-C(1)-O(1)	172(98)	C(1)-Fe(1)-P(1)-C(7)	-105.05(11)
P(1)-Fe(1)-C(1)-O(1)	-99(5)	P(2)-Fe(1)-P(1)-C(7)	-7.12(7)
S(1)-Fe(1)-C(1)-O(1)	70(5)	S(1)-Fe(1)-P(1)-C(7)	151.94(13)
S(2)-Fe(1)-C(1)-O(1)	-2(5)	S(2)-Fe(1)-P(1)-C(7)	102.40(7)
Fe(2)-Fe(1)-C(1)-O(1)	14(5)	Fe(2)-Fe(1)-P(1)-C(7)	156.83(7)
C(1)-Fe(1)-P(2)-C(24)	-148.02(11)	C(7)-C(8)-C(9)-O(5)	178.2(2)
P(1)-Fe(1)-P(2)-C(24)	121.61(9)	P(2)-C(8)-C(9)-O(5)	7.6(4)
S(1)-Fe(1)-P(2)-C(24)	-54.16(9)	C(7)-C(8)-C(9)-C(10)	-0.4(3)
S(2)-Fe(1)-P(2)-C(24)	28.91(9)	P(2)-C(8)-C(9)-C(10)	-171.02(18)
Fe(2)-Fe(1)-P(2)-C(24)	-23.61(11)	O(5)-C(9)-C(10)-C(11)	-179.4(2)
C(1)-Fe(1)-P(2)-C(30)	-20.68(11)	C(8)-C(9)-C(10)-C(11)	-0.9(2)
P(1)-Fe(1)-P(2)-C(30)	-111.06(8)	C(9)-C(10)-C(11)-O(6)	-178.3(2)
S(1)-Fe(1)-P(2)-C(30)	73.17(8)	C(9)-C(10)-C(11)-C(7)	1.8(2)
S(2)-Fe(1)-P(2)-C(30)	156.24(8)	C(9)-C(8)-C(7)-C(11)	1.6(2)
Fe(2)-Fe(1)-P(2)-C(30)	103.73(9)	P(2)-C(8)-C(7)-C(11)	173.58(14)
C(1)-Fe(1)-P(2)-C(8)	97.86(10)	C(9)-C(8)-C(7)-P(1)	-171.16(15)
P(1)-Fe(1)-P(2)-C(8)	7.49(7)	P(2)-C(8)-C(7)-P(1)	0.8(2)
S(1)-Fe(1)-P(2)-C(8)	-168.28(7)	O(6)-C(11)-C(7)-C(8)	178.0(2)
S(2)-Fe(1)-P(2)-C(8)	-85.21(7)	C(10)-C(11)-C(7)-C(8)	-2.1(3)
Fe(2)-Fe(1)-P(2)-C(8)	-137.73(8)	O(6)-C(11)-C(7)-P(1)	-10.3(3)
C(24)-P(2)-C(8)-C(7)	-134.35(18)	C(10)-C(11)-C(7)-P(1)	169.60(17)
C(30)-P(2)-C(8)-C(7)	119.41(18)	C(18)-P(1)-C(7)-C(8)	131.51(18)
Fe(1)-P(2)-C(8)-C(7)	-6.57(19)	C(12)-P(1)-C(7)-C(8)	-120.39(18)
C(24)-P(2)-C(8)-C(9)	35.7(2)	Fe(1)-P(1)-C(7)-C(8)	5.23(19)
C(30)-P(2)-C(8)-C(9)	-70.6(2)	C(18)-P(1)-C(7)-C(11)	-39.6(2)

C(12)-P(1)-C(7)-C(11)	68.5(2)	C(19)-C(18)-C(23)-C(22)	0.0(4)
Fe(1)-P(1)-C(7)-C(11)	-165.92(17)	P(1)-C(18)-C(23)-C(22)	-176.14(19)
C(24)-P(2)-C(30)-C(35)	-70.7(2)	C(18)-C(23)-C(22)-C(21)	1.4(4)
C(8)-P(2)-C(30)-C(35)	34.1(2)	C(23)-C(22)-C(21)-C(20)	-1.4(4)
Fe(1)-P(2)-C(30)-C(35)	153.15(18)	C(22)-C(21)-C(20)-C(19)	0.0(4)
C(24)-P(2)-C(30)-C(31)	106.13(19)	C(21)-C(20)-C(19)-C(18)	1.4(4)
C(8)-P(2)-C(30)-C(31)	-149.00(18)	C(23)-C(18)-C(19)-C(20)	-1.4(4)
Fe(1)-P(2)-C(30)-C(31)	-30.0(2)	P(1)-C(18)-C(19)-C(20)	174.6(2)
C(35)-C(30)-C(31)-C(32)	-1.7(4)	C(18)-P(1)-C(12)-C(17)	-86.9(2)
P(2)-C(30)-C(31)-C(32)	-178.6(2)	C(7)-P(1)-C(12)-C(17)	168.24(19)
C(30)-C(31)-C(32)-C(33)	0.9(4)	Fe(1)-P(1)-C(12)-C(17)	50.6(2)
C(31)-C(32)-C(33)-C(34)	0.3(4)	C(18)-P(1)-C(12)-C(13)	95.6(2)
C(32)-C(33)-C(34)-C(35)	-0.9(5)	C(7)-P(1)-C(12)-C(13)	-9.3(2)
C(31)-C(30)-C(35)-C(34)	1.1(4)	Fe(1)-P(1)-C(12)-C(13)	-126.88(18)
P(2)-C(30)-C(35)-C(34)	177.9(2)	C(17)-C(12)-C(13)-C(14)	-1.0(4)
C(33)-C(34)-C(35)-C(30)	0.1(4)	P(1)-C(12)-C(13)-C(14)	176.5(2)
C(30)-P(2)-C(24)-C(29)	-19.1(2)	C(12)-C(13)-C(14)-C(15)	1.0(4)
C(8)-P(2)-C(24)-C(29)	-128.1(2)	C(13)-C(14)-C(15)-C(16)	0.2(4)
Fe(1)-P(2)-C(24)-C(29)	114.7(2)	C(14)-C(15)-C(16)-C(17)	-1.3(4)
C(30)-P(2)-C(24)-C(25)	161.55(19)	C(15)-C(16)-C(17)-C(12)	1.3(4)
C(8)-P(2)-C(24)-C(25)	52.6(2)	C(13)-C(12)-C(17)-C(16)	-0.1(4)
Fe(1)-P(2)-C(24)-C(25)	-64.6(2)	P(1)-C(12)-C(17)-C(16)	-177.71(19)
C(25)-C(24)-C(29)-C(28)	0.3(4)	C(2')-Fe(2')-Fe(1')-C(1')	6.73(12)
P(2)-C(24)-C(29)-C(28)	-179.0(2)	C(3')-Fe(2')-Fe(1')-C(1')	-87.47(12)
C(24)-C(29)-C(28)-C(27)	0.1(5)	C(4')-Fe(2')-Fe(1')-C(1')	141.3(2)
C(29)-C(28)-C(27)-C(26)	-0.4(5)	S(2')-Fe(2')-Fe(1')-C(1')	-171.32(9)
C(28)-C(27)-C(26)-C(25)	0.3(4)	S(1')-Fe(2')-Fe(1')-C(1')	87.86(8)
C(29)-C(24)-C(25)-C(26)	-0.4(4)	C(2')-Fe(2')-Fe(1')-P(2')	-115.12(10)
P(2)-C(24)-C(25)-C(26)	179.00(19)	C(3')-Fe(2')-Fe(1')-P(2')	150.68(10)
C(27)-C(26)-C(25)-C(24)	0.1(4)	C(4')-Fe(2')-Fe(1')-P(2')	19.4(2)
C(12)-P(1)-C(18)-C(19)	28.7(2)	S(2')-Fe(2')-Fe(1')-P(2')	66.83(6)
C(7)-P(1)-C(18)-C(19)	136.8(2)	S(1')-Fe(2')-Fe(1')-P(2')	-33.99(5)
Fe(1)-P(1)-C(18)-C(19)	-107.50(19)	C(2')-Fe(2')-Fe(1')-P(1')	101.21(9)
C(12)-P(1)-C(18)-C(23)	-155.25(19)	C(3')-Fe(2')-Fe(1')-P(1')	7.01(9)
C(7)-P(1)-C(18)-C(23)	-47.1(2)	C(4')-Fe(2')-Fe(1')-P(1')	-124.3(2)
Fe(1)-P(1)-C(18)-C(23)	68.6(2)	S(2')-Fe(2')-Fe(1')-P(1')	-76.84(3)

S(1')-Fe(2')-Fe(1')-P(1')	-177.66(3)	P(1')-Fe(1')-S(2')-Fe(2')	114.84(2)
C(2')-Fe(2')-Fe(1')-S(2')	178.05(9)	S(1')-Fe(1')-S(2')-Fe(2')	-56.20(2)
C(3')-Fe(2')-Fe(1')-S(2')	83.85(9)	C(2')-Fe(2')-S(2')-C(6')	-109.6(2)
C(4')-Fe(2')-Fe(1')-S(2')	-47.4(2)	C(3')-Fe(2')-S(2')-C(6')	151.80(13)
S(1')-Fe(2')-Fe(1')-S(2')	-100.82(3)	C(4')-Fe(2')-S(2')-C(6')	54.68(14)
C(2')-Fe(2')-Fe(1')-S(1')	-81.13(9)	S(1')-Fe(2')-S(2')-C(6')	-49.08(10)
C(3')-Fe(2')-Fe(1')-S(1')	-175.33(9)	Fe(1')-Fe(2')-S(2')-C(6')	-104.86(10)
C(4')-Fe(2')-Fe(1')-S(1')	53.4(2)	C(2')-Fe(2')-S(2')-Fe(1')	-4.8(2)
S(2')-Fe(2')-Fe(1')-S(1')	100.82(3)	C(3')-Fe(2')-S(2')-Fe(1')	-103.34(9)
C(1')-Fe(1')-S(1')-C(5')	166.16(14)	C(4')-Fe(2')-S(2')-Fe(1')	159.54(10)
P(2')-Fe(1')-S(1')-C(5')	68.75(11)	S(1')-Fe(2')-S(2')-Fe(1')	55.78(2)
P(1')-Fe(1')-S(1')-C(5')	-87.15(15)	S(1')-C(5')-C(6')-S(2')	-5.1(3)
S(2')-Fe(1')-S(1')-C(5')	-41.06(11)	Fe(1')-S(2')-C(6')-C(5')	-28.1(2)
Fe(2')-Fe(1')-S(1')-C(5')	-97.29(11)	Fe(2')-S(2')-C(6')-C(5')	42.2(2)
C(1')-Fe(1')-S(1')-Fe(2')	-96.54(9)	C(2')-Fe(2')-C(4')-O(4')	-46(2)
P(2')-Fe(1')-S(1')-Fe(2')	166.04(2)	C(3')-Fe(2')-C(4')-O(4')	47(2)
P(1')-Fe(1')-S(1')-Fe(2')	10.14(11)	S(2')-Fe(2')-C(4')-O(4')	140(2)
S(2')-Fe(1')-S(1')-Fe(2')	56.24(2)	S(1')-Fe(2')-C(4')-O(4')	-137(2)
C(2')-Fe(2')-S(1')-C(5')	-153.39(12)	Fe(1')-Fe(2')-C(4')-O(4')	179(100)
C(3')-Fe(2')-S(1')-C(5')	114.6(2)	C(3')-Fe(2')-C(2')-O(2')	-114(11)
C(4')-Fe(2')-S(1')-C(5')	-54.74(12)	C(4')-Fe(2')-C(2')-O(2')	-17(11)
S(2')-Fe(2')-S(1')-C(5')	47.08(9)	S(2')-Fe(2')-C(2')-O(2')	148(11)
Fe(1')-Fe(2')-S(1')-C(5')	102.68(9)	S(1')-Fe(2')-C(2')-O(2')	89(11)
C(2')-Fe(2')-S(1')-Fe(1')	103.94(8)	Fe(1')-Fe(2')-C(2')-O(2')	144(11)
C(3')-Fe(2')-S(1')-Fe(1')	11.9(2)	C(2')-Fe(2')-C(3')-O(3')	14(5)
C(4')-Fe(2')-S(1')-Fe(1')	-157.41(8)	C(4')-Fe(2')-C(3')-O(3')	-85(5)
S(2')-Fe(2')-S(1')-Fe(1')	-55.601(19)	S(2')-Fe(2')-C(3')-O(3')	171(100)
Fe(1')-S(1')-C(5')-C(6')	36.0(2)	S(1')-Fe(2')-C(3')-O(3')	105(5)
Fe(2')-S(1')-C(5')-C(6')	-34.3(2)	Fe(1')-Fe(2')-C(3')-O(3')	115(5)
C(1')-Fe(1')-S(2')-C(6')	113.55(19)	P(2')-Fe(1')-C(1')-O(1')	164(5)
P(2')-Fe(1')-S(2')-C(6')	-60.29(9)	P(1')-Fe(1')-C(1')-O(1')	-107(5)
P(1')-Fe(1')-S(2')-C(6')	-150.05(9)	S(2')-Fe(1')-C(1')-O(1')	-10(5)
S(1')-Fe(1')-S(2')-C(6')	38.92(9)	S(1')-Fe(1')-C(1')-O(1')	61(5)
Fe(2')-Fe(1')-S(2')-C(6')	95.11(9)	Fe(2')-Fe(1')-C(1')-O(1')	5(5)
C(1')-Fe(1')-S(2')-Fe(2')	18.43(17)	C(1')-Fe(1')-P(2')-C(24')	-144.75(12)
P(2')-Fe(1')-S(2')-Fe(2')	-155.40(3)	P(1')-Fe(1')-P(2')-C(24')	123.51(9)

S(2')-Fe(1')-P(2')-C(24')	32.31(9)	C(7')-C(8')-C(9')-C(10')	3.3(3)
S(1')-Fe(1')-P(2')-C(24')	-51.43(9)	P(2')-C(8')-C(9')-C(10')	-171.17(19)
Fe(2')-Fe(1')-P(2')-C(24')	-22.99(11)	O(5')-C(9')-C(10')-C(11')	175.2(2)
C(1')-Fe(1')-P(2')-C(30')	-18.28(12)	C(8')-C(9')-C(10')-C(11')	-4.7(3)
P(1')-Fe(1')-P(2')-C(30')	-110.02(9)	C(9')-C(10')-C(11')-O(6')	-175.9(2)
S(2')-Fe(1')-P(2')-C(30')	158.78(9)	C(9')-C(10')-C(11')-C(7')	4.5(3)
S(1')-Fe(1')-P(2')-C(30')	75.05(9)	C(9')-C(8')-C(7')-C(11')	-0.4(3)
Fe(2')-Fe(1')-P(2')-C(30')	103.49(10)	P(2')-C(8')-C(7')-C(11')	174.93(15)
C(1')-Fe(1')-P(2')-C(8')	99.00(11)	C(9')-C(8')-C(7')-P(1')	-173.55(15)
P(1')-Fe(1')-P(2')-C(8')	7.26(8)	P(2')-C(8')-C(7')-P(1')	1.8(2)
S(2')-Fe(1')-P(2')-C(8')	-83.94(8)	O(6')-C(11')-C(7')-C(8')	177.7(2)
S(1')-Fe(1')-P(2')-C(8')	-167.67(7)	C(10')-C(11')-C(7')-C(8')	-2.7(3)
Fe(2')-Fe(1')-P(2')-C(8')	-139.23(8)	O(6')-C(11')-C(7')-P(1')	-10.1(4)
C(24')-P(2')-C(8')-C(7')	-134.02(18)	C(10')-C(11')-C(7')-P(1')	169.45(18)
C(30')-P(2')-C(8')-C(7')	117.91(19)	C(12')-P(1')-C(7')-C(8')	-121.17(18)
Fe(1')-P(2')-C(8')-C(7')	-6.95(19)	C(18')-P(1')-C(7')-C(8')	130.94(18)
C(24')-P(2')-C(8')-C(9')	40.2(2)	Fe(1')-P(1')-C(7')-C(8')	4.14(19)
C(30')-P(2')-C(8')-C(9')	-67.9(2)	C(12')-P(1')-C(7')-C(11')	67.2(2)
Fe(1')-P(2')-C(8')-C(9')	167.24(19)	C(18')-P(1')-C(7')-C(11')	-40.7(2)
C(1')-Fe(1')-P(1')-C(12')	14.55(12)	Fe(1')-P(1')-C(7')-C(11')	-167.46(18)
P(2')-Fe(1')-P(1')-C(12')	111.40(9)	C(24')-P(2')-C(30')-C(35')	-86.5(2)
S(2')-Fe(1')-P(1')-C(12')	-137.32(9)	C(8')-P(2')-C(30')-C(35')	20.9(3)
S(1')-Fe(1')-P(1')-C(12')	-92.13(14)	Fe(1')-P(2')-C(30')-C(35')	139.4(2)
Fe(2')-Fe(1')-P(1')-C(12')	-83.08(9)	C(24')-P(2')-C(30')-C(31')	94.5(2)
C(1')-Fe(1')-P(1')-C(18')	144.31(12)	C(8')-P(2')-C(30')-C(31')	-158.1(2)
P(2')-Fe(1')-P(1')-C(18')	-118.84(9)	Fe(1')-P(2')-C(30')-C(31')	-39.6(2)
S(2')-Fe(1')-P(1')-C(18')	-7.56(9)	C(35')-C(30')-C(31')-C(32')	1.3(4)
S(1')-Fe(1')-P(1')-C(18')	37.63(15)	P(2')-C(30')-C(31')-C(32')	-179.7(3)
Fe(2')-Fe(1')-P(1')-C(18')	46.68(9)	C(30')-C(31')-C(32')-C(33')	-0.6(5)
C(1')-Fe(1')-P(1')-C(7')	-103.32(11)	C(31')-C(32')-C(33')-C(34')	-1.1(5)
P(2')-Fe(1')-P(1')-C(7')	-6.48(7)	C(32')-C(33')-C(34')-C(35')	2.1(5)
S(2')-Fe(1')-P(1')-C(7')	104.80(7)	C(33')-C(34')-C(35')-C(30')	-1.5(4)
S(1')-Fe(1')-P(1')-C(7')	149.99(12)	C(31')-C(30')-C(35')-C(34')	-0.2(4)
Fe(2')-Fe(1')-P(1')-C(7')	159.05(7)	P(2')-C(30')-C(35')-C(34')	-179.2(2)
C(7')-C(8')-C(9')-O(5')	-176.6(2)	C(30')-P(2')-C(24')-C(29')	-31.9(2)
P(2')-C(8')-C(9')-O(5')	8.9(4)	C(8')-P(2')-C(24')-C(29')	-141.0(2)

Fe(1')-P(2')-C(24')-C(29')	100.5(2)
C(30')-P(2')-C(24')-C(25')	153.7(2)
C(8')-P(2')-C(24')-C(25')	44.7(2)
Fe(1')-P(2')-C(24')-C(25')	-73.9(2)
C(25')-C(24')-C(29')-C(28')	-0.5(4)
P(2')-C(24')-C(29')-C(28')	-174.9(2)
C(24')-C(29')-C(28')-C(27')	0.4(4)
C(29')-C(28')-C(27')-C(26')	-0.7(4)
C(28')-C(27')-C(26')-C(25')	1.0(5)
C(27')-C(26')-C(25')-C(24')	-1.1(4)
C(29')-C(24')-C(25')-C(26')	0.8(4)
P(2')-C(24')-C(25')-C(26')	175.3(2)
C(12')-P(1')-C(18')-C(19')	26.5(2)
C(7')-P(1')-C(18')-C(19')	135.60(19)
Fe(1')-P(1')-C(18')-C(19')	-108.68(18)
C(12')-P(1')-C(18')-C(23')	-156.77(18)
C(7')-P(1')-C(18')-C(23')	-47.7(2)
Fe(1')-P(1')-C(18')-C(23')	68.04(19)
C(19')-C(18')-C(23')-C(22')	-0.4(3)
P(1')-C(18')-C(23')-C(22')	-177.24(19)
C(18')-C(23')-C(22')-C(21')	1.1(4)
C(23')-C(22')-C(21')-C(20')	-0.9(4)
C(22')-C(21')-C(20')-C(19')	0.1(4)
C(21')-C(20')-C(19')-C(18')	0.6(4)
C(23')-C(18')-C(19')-C(20')	-0.4(3)
P(1')-C(18')-C(19')-C(20')	176.29(19)
C(18')-P(1')-C(12')-C(13')	90.6(2)
C(7')-P(1')-C(12')-C(13')	-13.9(2)
Fe(1')-P(1')-C(12')-C(13')	-132.0(2)
C(18')-P(1')-C(12')-C(17')	-88.7(2)
C(7')-P(1')-C(12')-C(17')	166.7(2)
Fe(1')-P(1')-C(12')-C(17')	48.6(2)
C(17')-C(12')-C(13')-C(14')	0.7(4)
P(1')-C(12')-C(13')-C(14')	-178.7(2)
C(12')-C(13')-C(14')-C(15')	-0.4(4)
C(13')-C(14')-C(15')-C(16')	-0.2(5)
C(14')-C(15')-C(16')-C(17')	0.5(4)
C(15')-C(16')-C(17')-C(12')	-0.2(4)
C(13')-C(12')-C(17')-C(16')	-0.3(4)
P(1')-C(12')-C(17')-C(16')	179.0(2)

Symmetry transformations used to generate equivalent atoms: