**Electronic Supplementary Information (ESI)**

# Models of the iron-only hydrogenase enzyme: Structure, electrochemistry and catalytic activity of $Fe_2(CO)_3$(μ-dithiolate)(μ,$κ^1$,$κ^2$-triphos)

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(i) CVs of oxidation of **1** over a range of scan rates
(ii) CVs of oxidation of **3** over a range of scan rates
(iii) Electrocatalytic performance of **4** on addition of strong acid
(iv) Oxidation response for **3** on addition of strong acid
(v) Computational Details
(vi) Crystallographic data and structure refinement for **1**
(vii) Crystallographic data and structure refinement for **3**

**(i) CVs of oxidation of 1 over a range of scan rates**

**1** undergoes oxidation at $E_{1/2}$ = -0.35 V in a process that was found to be reversible ($i_p^{ox}/i_p^{red}$ *ca*. 1) over all scan rates studied (0.01 – 10 V $s^{-1}$).

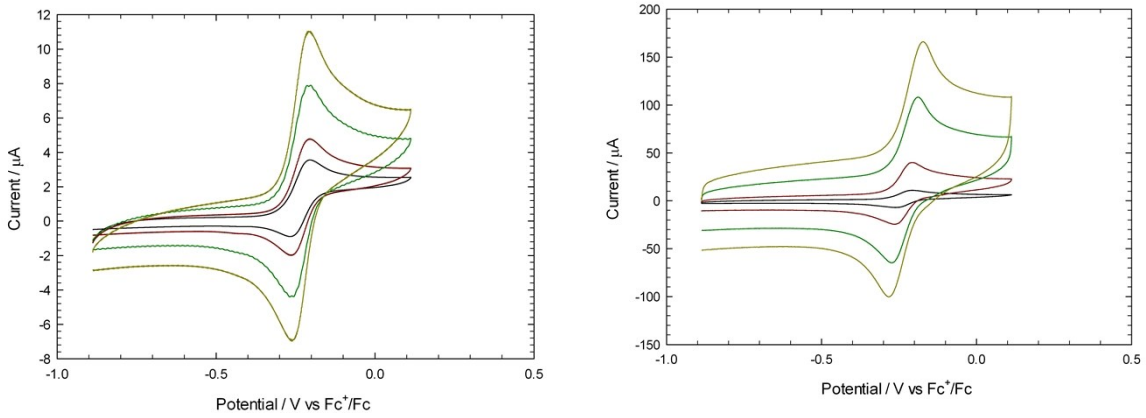


*Fig ESI 1: CV of 0.5 mM complex **1** in 0.1 M $TBAPF_6$/ $CH_2Cl_2$ over range of scan rate. Left: 0.01 V $s^{-1}$ (black); 0.02 V $s^{-1}$ (brown); 0.05 V $s^{-1}$ (dark green); 0.1 V $s^{-1}$ (light green). Right: 0.1 V $s^{-1}$ (black); 1 V $s^{-1}$ (brown); 5 V $s^{-1}$ (dark green); 10 V $s^{-1}$ (light green).*

**(ii) CVs of oxidation of 3 over a range of scan rates**

Oxidation of **3** takes place reversibly at the same potential as for **1** ($E_{1/2}$ = -0.35 V), however a second oxidation couple of similar peak height is observed at $E_{1/2}$ = -0.11 V, suggestive of a further reversible one electron oxidation. The scan rate dependence of the two couples shows the relative peak heights and separations of the two processes do not change significantly with scan rate. The behaviour observed may be attributed to consecutive loss of two electrons from the same orbital; thus the first couple is assigned to the $[FeFe]^{0/+}$ process and the second to $[FeFe]^{+/2+}$.

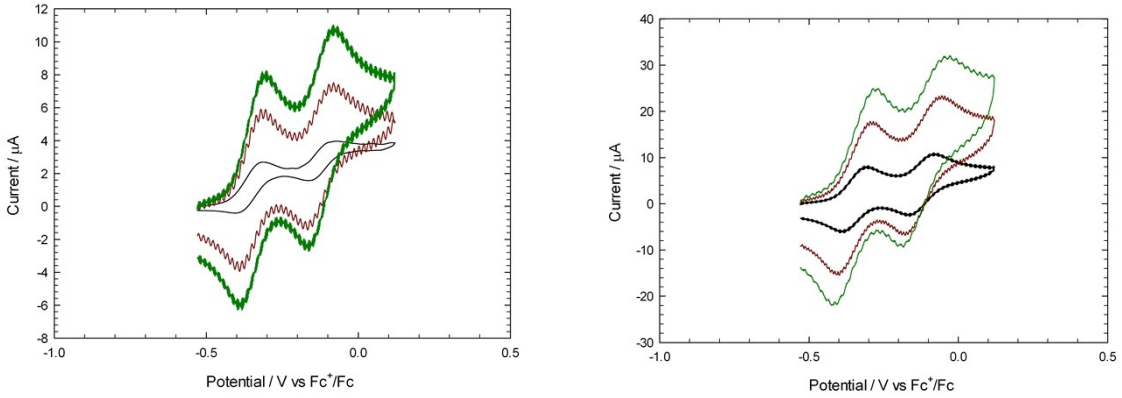


*Fig ESI 2: CV of 0.5 mM complex **3** in 0.1 M $TBAPF_6$/ $CH_2Cl_2$ over range of scan rate. Left: 0.01 V $s^{-1}$ (black); 0.02 V $s^{-1}$ (brown); 0.05 V $s^{-1}$ (dark green); 0.1 V $s^{-1}$ (light green). Right: 0.1 V $s^{-1}$ (black); 1 V $s^{-1}$ (brown); 5 V $s^{-1}$ (dark green); 10 V $s^{-1}$ (light green).*

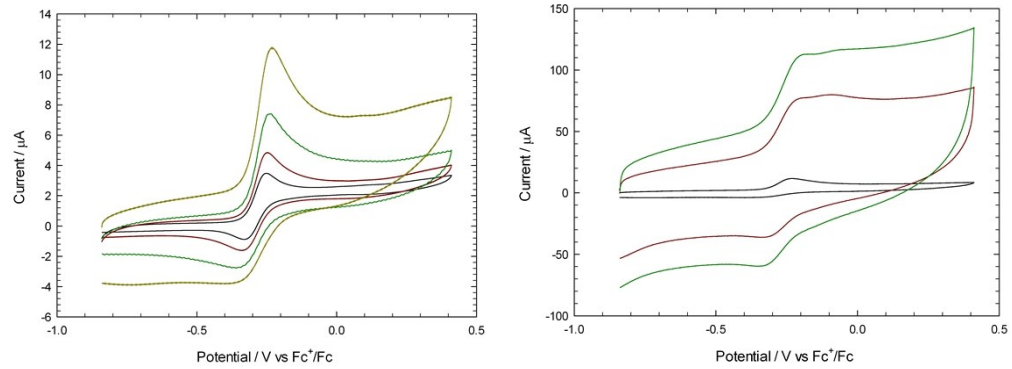


*Fig ESI 3: CV of 0.5 mM complex **3** in 0.1 M $TBAPF_6$/ $CH_3CN$ over range of scan rate. Left: 0.01 V $s^{-1}$ (black); 0.02 V $s^{-1}$ (brown); 0.05 V $s^{-1}$ (dark green); 0.1 V $s^{-1}$ (light green). Right: 0.1 V $s^{-1}$ (black); 1 V $s^{-1}$ (brown); 5 V $s^{-1}$ (dark green); 10 V $s^{-1}$ (light green).*

We find that in $CH_3CN$, **3** instead undergoes a single, irreversible two-electron oxidation at slow scans, which resolves into two consecutive one electron processes as scan rate is increased. This is consistent with further stabilisation of the $\mathbf{3}^{2+}$ species *via* formation of an adduct $[\mathbf{3}(CH_3CN)]^{2+}$ with the coordinating solvent, as isolated

and characterised for similar compounds by Olsen *et al.* (M.T. Olsen, T.B. Rauchfuss, S.R. Wilson, J. Am. Chem. Soc. 132 (2010) 17733-17740.)

**(iii) Electrocatalytic performance of 4 on addition of strong acid**

The performance of open-bridged **4** was investigated in the presence of $HBF_4.Et_2O$ in electrolytes composed of $TBAPF_6$, $TBABF_4$ and $TBAClO_4$. Broadly the same features can be identified as for **1** and hence the reaction mechanism shown in Fig 4 is proposed to also apply for **4**. However it was found that the identity of supporting anion influenced the relative currents observed at potentials **A**, **B** and **C** in a different manner than for **1**.

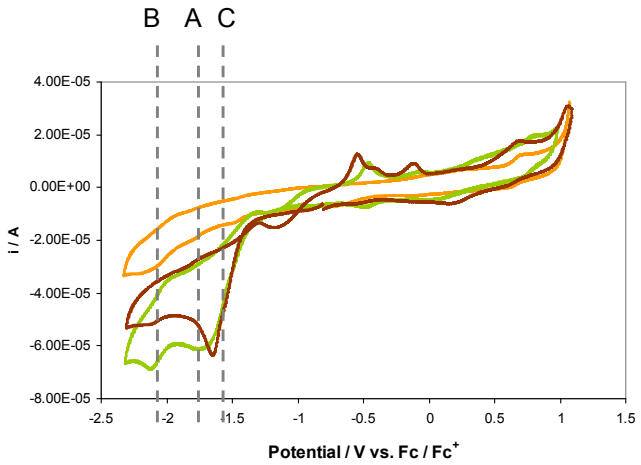


*Fig EC4: CV of 0.5 mM complex **4** with 10 molar equivalent of $HBF_4$-$Et_2O$ (scan rate 0.1 V $s^{-1}$) in 0.1 M $TBAPF_6$ / $CH_2Cl_2$ (orange); 0.1 M $TBABF_4$ / $CH_2Cl_2$ (green) in 0.1 M $TBAClO_4$ / $CH_2Cl_2$ (brown). A, B and C refer to catalytic processes shown in Figure 4 in the main manuscript.*

In $TBAPF_6$ the currents were all very inhibited compared to those for **1**, reaching a maximum after only 4 equivalents of acid were introduced. This indicates that for **4**, $PF_6^-$ plays a retarding role in intramolecular proton transfer leading to $H_2$ elimination. This may be related to the open and flexible nature of the unlinked bridging groups, which may allow closer approach of the anion to the iron centres, where it could occupy a position that blocks the transfer. In the presence of $BF_4^-$ or $ClO_4^-$, currents at potential **C** attributed to reduction of **4(μH)H**$^+$ are enhanced in comparison to those observed for **1(μH)H**$^+$ (Fig 4). This indicates that for **4** these anions facilitate more efficient production of the intermediate **4H** complex after $H_2$ elimination from **4H(μH)H**, suggesting $ClO_4^-$ and $BF_4^-$ may promote the intramolecular proton transfer steps necessary to form **4(μH)-$H_2$**. That this process is accelerated more for **4** than **1**, suggests that optimal positioning of the anions with respect to the pdt or $(SMe)_2$ bridging groups is important.

**(iv) Oxidation response for 3 on addition of strong acid**

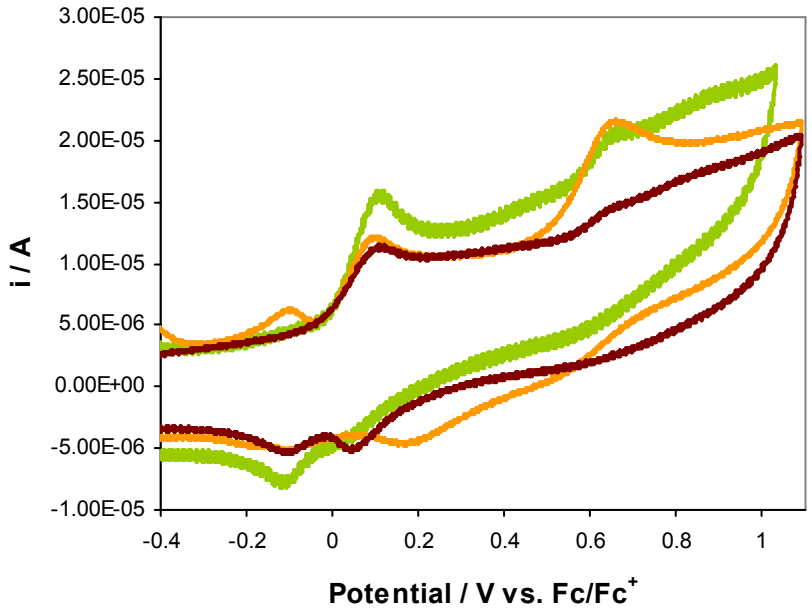


*Fig EC5: CV ofoxidation response of 0.5 mM complex **3** with 10 molar equivalent of $HBF_4$-$Et_2O$ (scan rate 0.1 V $s^{-1}$) in 0.1 M $TBAPF_6$ / $CH_2Cl_2$ (brown); 0.1 M $TBABF_4$ / $CH_2Cl_2$ (green) in 0.1 M $TBAClO_4$ / $CH_2Cl_2$ (orange).*

In excess acid the oxidation peak for protonated **3** is still observed at 0.15 V, the same potential as noted for $\mathbf{3H_N}^+$ in the presence of $TBAPF_6$ and $TBABF_4$. There is only a very small increase in current at 0.75 V, where $\mathbf{3H_{Fe}}^+$ would be expected to undergo oxidation, indicating that this species is not present in solution at high concentration even in excess acid. In TBAClO4 peaks are observed at +0.15 V and at +0.75 V suggesting a mixture of species protonated at nitrogen and iron are present in solution.

**(v) Computational Details**

B3LYP geometries and energies for all optimized structures

**Species A**
HF energy= -3841.81363212
No Imaginary frequency
Zero-point correction = 0.692797 (Hartree/Particle)
Thermal correction to Energy = 0.742326
Thermal correction to Enthalpy = 0.743270
Thermal correction to Gibbs Free Energy = 0.607836
Sum of electronic and zero-point Energies = -3841.120835
Sum of electronic and thermal Energies = -3841.071306
Sum of electronic and thermal Enthalpies = -3841.070362
Sum of electronic and thermal Free Energies = -3841.205796

Coordinates: **A**

| | | | |
|---|---|---|---|
| Fe | -0.03090000 | 6.09640000 | 7.02150000 |
| Fe | -0.61120000 | 7.55000000 | 5.03320000 |
| P | -0.47060000 | 5.00660000 | 8.94120000 |
| P | 0.39550000 | 4.12660000 | 6.03790000 |
| P | -0.61130000 | 6.29820000 | 3.12620000 |
| S | -2.12160000 | 6.05060000 | 5.99580000 |
| S | -0.41340000 | 8.37390000 | 7.21810000 |
| O | 2.76240000 | 6.67270000 | 7.66860000 |
| O | 2.22510000 | 8.17770000 | 4.66390000 |
| O | -1.83000000 | 9.93080000 | 3.83990000 |
| C | 1.66370000 | 6.42570000 | 7.39900000 |
| C | 1.10550000 | 7.91650000 | 4.82160000 |
| C | -1.39850000 | 8.95640000 | 4.29510000 |
| C | -3.46870000 | 6.91730000 | 6.92720000 |
| H | -4.38570000 | 6.72460000 | 6.35570000 |
| H | -3.57440000 | 6.41220000 | 7.89250000 |
| C | -3.29090000 | 8.42000000 | 7.12330000 |
| H | -3.25830000 | 8.92140000 | 6.14860000 |
| H | -4.18440000 | 8.80340000 | 7.64370000 |
| C | -2.06240000 | 8.81000000 | 7.94050000 |
| H | -2.10710000 | 8.35190000 | 8.93690000 |
| H | -2.04110000 | 9.89810000 | 8.07850000 |
| C | -0.09480000 | 3.18580000 | 8.62080000 |
| H | 0.97090000 | 3.05020000 | 8.84830000 |
| H | -0.66160000 | 2.53460000 | 9.29760000 |
| C | -0.36320000 | 2.82570000 | 7.14800000 |
| H | -1.43770000 | 2.86960000 | 6.92740000 |
| H | -0.03490000 | 1.80350000 | 6.92360000 |
| C | -0.37150000 | 3.70050000 | 4.38370000 |
| H | -0.12730000 | 2.64970000 | 4.17460000 |
| H | -1.45970000 | 3.77130000 | 4.49650000 |
| C | 0.12450000 | 4.57200000 | 3.21570000 |
| H | -0.08500000 | 4.06240000 | 2.26730000 |

| | | | |
|---|---|---|---|
| H | 1.21350000 | 4.67750000 | 3.27210000 |
| C | 0.53380000 | 5.38410000 | 10.44680000 |
| C | 1.06000000 | 6.67530000 | 10.61050000 |
| H | 0.89600000 | 7.42390000 | 9.83870000 |
| C | 1.79610000 | 7.00170000 | 11.75370000 |
| H | 2.19930000 | 8.00630000 | 11.86450000 |
| C | 2.02180000 | 6.04050000 | 12.74060000 |
| H | 2.60180000 | 6.29220000 | 13.62640000 |
| C | 1.50100000 | 4.75150000 | 12.58780000 |
| H | 1.67150000 | 3.99880000 | 13.35530000 |
| C | 0.75640000 | 4.42750000 | 11.45270000 |
| H | 0.34230000 | 3.42600000 | 11.35660000 |
| C | -2.17340000 | 4.94540000 | 9.68060000 |
| C | -3.13270000 | 4.01610000 | 9.24400000 |
| H | -2.88190000 | 3.28480000 | 8.48020000 |
| C | -4.42630000 | 4.01930000 | 9.77210000 |
| H | -5.15140000 | 3.28720000 | 9.42160000 |
| C | -4.78800000 | 4.95660000 | 10.74260000 |
| H | -5.79580000 | 4.95990000 | 11.15270000 |
| C | -3.84470000 | 5.88820000 | 11.18380000 |
| H | -4.11270000 | 6.62000000 | 11.94350000 |
| C | -2.55020000 | 5.88190000 | 10.65920000 |
| H | -1.82360000 | 6.60320000 | 11.02600000 |
| C | 2.14170000 | 3.56950000 | 5.75890000 |
| C | 3.07750000 | 4.50010000 | 5.27050000 |
| H | 2.78410000 | 5.53440000 | 5.11710000 |
| C | 4.39250000 | 4.11720000 | 4.99430000 |
| H | 5.09800000 | 4.85660000 | 4.62120000 |
| C | 4.80110000 | 2.79960000 | 5.21110000 |
| H | 5.82770000 | 2.50300000 | 5.00550000 |
| C | 3.88470000 | 1.86530000 | 5.69900000 |
| H | 4.19330000 | 0.83640000 | 5.87430000 |
| C | 2.56700000 | 2.24570000 | 5.96510000 |
| H | 1.87540000 | 1.49420000 | 6.33690000 |
| C | 0.36210000 | 7.04550000 | 1.73600000 |
| C | -0.26940000 | 7.93460000 | 0.84810000 |
| H | -1.33770000 | 8.11770000 | 0.93180000 |
| C | 0.45760000 | 8.58530000 | -0.15020000 |
| H | -0.05220000 | 9.26930000 | -0.82580000 |
| C | 1.83040000 | 8.36030000 | -0.28110000 |
| H | 2.39720000 | 8.86580000 | -1.06030000 |
| C | 2.47070000 | 7.48600000 | 0.59880000 |
| H | 3.54080000 | 7.30780000 | 0.51190000 |
| C | 1.74520000 | 6.83890000 | 1.60230000 |
| H | 2.27690000 | 6.18210000 | 2.28520000 |
| C | -2.23380000 | 5.95820000 | 2.28500000 |
| C | -3.42870000 | 6.49340000 | 2.78650000 |
| H | -3.40370000 | 7.08940000 | 3.69230000 |
| C | -4.64460000 | 6.26090000 | 2.13570000 |
| H | -5.56070000 | 6.68650000 | 2.54060000 |

| | | | |
|---|---|---|---|
| C | -4.68340000 | 5.48790000 | 0.97470000 |
| H | -5.62960000 | 5.30540000 | 0.46880000 |
| C | -3.49780000 | 4.95490000 | 0.45850000 |
| H | -3.51600000 | 4.35980000 | -0.45250000 |
| C | -2.28490000 | 5.19190000 | 1.10590000 |
| H | -1.37060000 | 4.79370000 | 0.67080000 |

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**Species TSAB**
HF energy= -3841.79698330
One imaginary frequency (249*i*)
Zero-point correction = 0.692466 (Hartree/Particle)
Thermal correction to Energy = 0.741659
Thermal correction to Enthalpy = 0.742603
Thermal correction to Gibbs Free Energy = 0.606570
Sum of electronic and zero-point Energies = -3841.104518
Sum of electronic and thermal Energies = -3841.055324
Sum of electronic and thermal Enthalpies = -3841.054380
Sum of electronic and thermal Free Energies = -3841.190413

Coordinates: **TSAB**

| | | | |
|---|---|---|---|
| Fe | 0.01220000 | 6.00850000 | 7.04890000 |
| Fe | -0.58550000 | 7.48930000 | 5.05760000 |
| P | -0.42530000 | 4.91230000 | 8.95240000 |
| P | 0.42970000 | 4.05160000 | 6.04370000 |
| P | -0.59630000 | 6.24100000 | 3.14650000 |
| S | -2.05270000 | 5.99680000 | 6.02630000 |
| S | -0.35820000 | 8.26910000 | 7.22000000 |
| O | 2.81400000 | 6.59120000 | 7.65460000 |
| O | 2.22400000 | 8.21390000 | 4.62520000 |
| O | -1.99290000 | 9.83340000 | 4.01080000 |
| C | 1.71180000 | 6.34040000 | 7.40230000 |
| C | 1.11530000 | 7.92050000 | 4.79540000 |
| C | -1.46930000 | 8.87350000 | 4.39510000 |
| C | -3.45530000 | 6.79180000 | 6.92000000 |
| H | -4.20170000 | 6.95010000 | 6.13230000 |
| H | -3.85300000 | 6.00260000 | 7.56490000 |
| C | -3.30790000 | 8.09920000 | 7.74680000 |
| H | -4.01770000 | 8.82240000 | 7.32650000 |
| H | -3.68070000 | 7.87270000 | 8.75200000 |
| C | -1.95990000 | 8.85140000 | 7.92400000 |
| H | -1.75190000 | 8.96430000 | 8.99490000 |
| H | -2.05870000 | 9.86660000 | 7.52350000 |
| C | -0.05120000 | 3.09300000 | 8.62310000 |
| H | 1.01550000 | 2.95840000 | 8.84690000 |
| H | -0.61370000 | 2.43580000 | 9.29770000 |
| C | -0.32350000 | 2.74180000 | 7.14850000 |
| H | -1.39910000 | 2.78700000 | 6.93240000 |
| H | 0.00430000 | 1.72120000 | 6.91620000 |

| | | | |
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| C | -0.34650000 | 3.63710000 | 4.39020000 |
| H | -0.10340000 | 2.58740000 | 4.17400000 |
| H | -1.43400000 | 3.70730000 | 4.50910000 |
| C | 0.14280000 | 4.51490000 | 3.22350000 |
| H | -0.07120000 | 4.00880000 | 2.27410000 |
| H | 1.23180000 | 4.62120000 | 3.27540000 |
| C | 0.57070000 | 5.27580000 | 10.46740000 |
| C | 1.12670000 | 6.55430000 | 10.62960000 |
| H | 0.98820000 | 7.30150000 | 9.85170000 |
| C | 1.85890000 | 6.86940000 | 11.77850000 |
| H | 2.28560000 | 7.86440000 | 11.88810000 |
| C | 2.05040000 | 5.90870000 | 12.77310000 |
| H | 2.62710000 | 6.15130000 | 13.66350000 |
| C | 1.49940000 | 4.63200000 | 12.62210000 |
| H | 1.64290000 | 3.88000000 | 13.39580000 |
| C | 0.75910000 | 4.31980000 | 11.48110000 |
| H | 0.32110000 | 3.32830000 | 11.38590000 |
| C | -2.13280000 | 4.85740000 | 9.68300000 |
| C | -3.07980000 | 3.89800000 | 9.28690000 |
| H | -2.82010000 | 3.13980000 | 8.55270000 |
| C | -4.37190000 | 3.90280000 | 9.81980000 |
| H | -5.08750000 | 3.14710000 | 9.50130000 |
| C | -4.74300000 | 4.87070000 | 10.75610000 |
| H | -5.74850000 | 4.87410000 | 11.17180000 |
| C | -3.81130000 | 5.83210000 | 11.15740000 |
| H | -4.08640000 | 6.58700000 | 11.89150000 |
| C | -2.51970000 | 5.82550000 | 10.62600000 |
| H | -1.80220000 | 6.57190000 | 10.95950000 |
| C | 2.17410000 | 3.49850000 | 5.74940000 |
| C | 3.10200000 | 4.43330000 | 5.25400000 |
| H | 2.80150000 | 5.46650000 | 5.10580000 |
| C | 4.41580000 | 4.05570000 | 4.96560000 |
| H | 5.11540000 | 4.79800000 | 4.58710000 |
| C | 4.83100000 | 2.73930000 | 5.17740000 |
| H | 5.85680000 | 2.44670000 | 4.96230000 |
| C | 3.92260000 | 1.80110000 | 5.67280000 |
| H | 4.23670000 | 0.77330000 | 5.84450000 |
| C | 2.60570000 | 2.17620000 | 5.95080000 |
| H | 1.92010000 | 1.42220000 | 6.32830000 |
| C | 0.35870000 | 6.99380000 | 1.74670000 |
| C | -0.28310000 | 7.89830000 | 0.88180000 |
| H | -1.34820000 | 8.08850000 | 0.98940000 |
| C | 0.42930000 | 8.55490000 | -0.12300000 |
| H | -0.08830000 | 9.25050000 | -0.78070000 |
| C | 1.79750000 | 8.32090000 | -0.28350000 |
| H | 2.35290000 | 8.83110000 | -1.06780000 |
| C | 2.44800000 | 7.43150000 | 0.57350000 |
| H | 3.51470000 | 7.24620000 | 0.46330000 |
| C | 1.73700000 | 6.77810000 | 1.58340000 |
| H | 2.27630000 | 6.10870000 | 2.24800000 |

| | | | |
|---|---|---|---|
| C | -2.22500000 | 5.89300000 | 2.31910000 |
| C | -3.41960000 | 6.40940000 | 2.84030000 |
| H | -3.38970000 | 6.99930000 | 3.75000000 |
| C | -4.64100000 | 6.16930000 | 2.20280000 |
| H | -5.55670000 | 6.58070000 | 2.62310000 |
| C | -4.68550000 | 5.40720000 | 1.03480000 |
| H | -5.63590000 | 5.21900000 | 0.53880000 |
| C | -3.50050000 | 4.89280000 | 0.49890000 |
| H | -3.52340000 | 4.30640000 | -0.41780000 |
| C | -2.28230000 | 5.13720000 | 1.13360000 |
| H | -1.36890000 | 4.75330000 | 0.68380000 |

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**Species B**
HF energy= -3841.81232981
No Imaginary frequency
Zero-point correction = 0.692653 (Hartree/Particle)
Thermal correction to Energy = 0.742257
Thermal correction to Enthalpy = 0.743201
Thermal correction to Gibbs Free Energy = 0.607063
Sum of electronic and zero-point Energies = -3841.119676
Sum of electronic and thermal Energies = -3841.070073
Sum of electronic and thermal Enthalpies = -3841.069128
Sum of electronic and thermal Free Energies = -3841.205266

Coordinates: **B**

| | | | |
|---|---|---|---|
| Fe | -0.04420000 | 6.04880000 | 7.09410000 |
| Fe | -0.54890000 | 7.48440000 | 5.06240000 |
| P | -0.46940000 | 4.95730000 | 9.02780000 |
| P | 0.36120000 | 4.07330000 | 6.10870000 |
| P | -0.62500000 | 6.19130000 | 3.17720000 |
| S | -2.12970000 | 6.10270000 | 6.05700000 |
| S | -0.29280000 | 8.36800000 | 7.19730000 |
| O | 2.75250000 | 6.55680000 | 7.77880000 |
| O | 2.28320000 | 8.10870000 | 4.63040000 |
| O | -1.82380000 | 9.86580000 | 3.93370000 |
| C | 1.65330000 | 6.33460000 | 7.49050000 |
| C | 1.16600000 | 7.84730000 | 4.79740000 |
| C | -1.35680000 | 8.88960000 | 4.34780000 |
| C | -3.42560000 | 7.09170000 | 6.94120000 |
| H | -3.89420000 | 7.73170000 | 6.18170000 |
| H | -4.18000000 | 6.37000000 | 7.27520000 |
| C | -2.96540000 | 7.92900000 | 8.13150000 |
| H | -3.85290000 | 8.42780000 | 8.55560000 |
| H | -2.57690000 | 7.26790000 | 8.91410000 |
| C | -1.92470000 | 8.99400000 | 7.80420000 |
| H | -1.69930000 | 9.57900000 | 8.70480000 |
| H | -2.30120000 | 9.69340000 | 7.04670000 |
| C | 0.06370000 | 3.17140000 | 8.72680000 |

| | | | |
|---|---|---|---|
| H | 1.15060000 | 3.13770000 | 8.88210000 |
| H | -0.40160000 | 2.49010000 | 9.44950000 |
| C | -0.27030000 | 2.75760000 | 7.28300000 |
| H | -1.35740000 | 2.72270000 | 7.13630000 |
| H | 0.10670000 | 1.75190000 | 7.06380000 |
| C | -0.49610000 | 3.61520000 | 4.50910000 |
| H | -0.30370000 | 2.54770000 | 4.33140000 |
| H | -1.57490000 | 3.73640000 | 4.66410000 |
| C | -0.01440000 | 4.41710000 | 3.28640000 |
| H | -0.31980000 | 3.89700000 | 2.37040000 |
| H | 1.08030000 | 4.44350000 | 3.27500000 |
| C | 0.50500000 | 5.43750000 | 10.51990000 |
| C | 0.85060000 | 6.78820000 | 10.68980000 |
| H | 0.56100000 | 7.51410000 | 9.93300000 |
| C | 1.57920000 | 7.20020000 | 11.80880000 |
| H | 1.84250000 | 8.24980000 | 11.92220000 |
| C | 1.98080000 | 6.26730000 | 12.76720000 |
| H | 2.55610000 | 6.58700000 | 13.63390000 |
| C | 1.64690000 | 4.91920000 | 12.60670000 |
| H | 1.95890000 | 4.18660000 | 13.34870000 |
| C | 0.91010000 | 4.50770000 | 11.49410000 |
| H | 0.64740000 | 3.45700000 | 11.39270000 |
| C | -2.17530000 | 4.70040000 | 9.73110000 |
| C | -3.19240000 | 4.18230000 | 8.90680000 |
| H | -2.99620000 | 3.99170000 | 7.85520000 |
| C | -4.47200000 | 3.94260000 | 9.41100000 |
| H | -5.23960000 | 3.53580000 | 8.75510000 |
| C | -4.77020000 | 4.23540000 | 10.74480000 |
| H | -5.76990000 | 4.05630000 | 11.13560000 |
| C | -3.77680000 | 4.76750000 | 11.56800000 |
| H | -3.99710000 | 5.00730000 | 12.60660000 |
| C | -2.49030000 | 4.99380000 | 11.06850000 |
| H | -1.73090000 | 5.40040000 | 11.72990000 |
| C | 2.10160000 | 3.55590000 | 5.72120000 |
| C | 3.01030000 | 4.52100000 | 5.25010000 |
| H | 2.70320000 | 5.55850000 | 5.16710000 |
| C | 4.31450000 | 4.16640000 | 4.89500000 |
| H | 4.99880000 | 4.93410000 | 4.53970000 |
| C | 4.73890000 | 2.84110000 | 5.00930000 |
| H | 5.75710000 | 2.56600000 | 4.74150000 |
| C | 3.84760000 | 1.87060000 | 5.47260000 |
| H | 4.16670000 | 0.83420000 | 5.56550000 |
| C | 2.54130000 | 2.22400000 | 5.81960000 |
| H | 1.87020000 | 1.44300000 | 6.16730000 |
| C | 0.40120000 | 6.84760000 | 1.77830000 |
| C | -0.16830000 | 7.75180000 | 0.86410000 |
| H | -1.22440000 | 8.00020000 | 0.93300000 |
| C | 0.60480000 | 8.33420000 | -0.14190000 |
| H | 0.14230000 | 9.03070000 | -0.83840000 |
| C | 1.96280000 | 8.02530000 | -0.25380000 |

| | | | |
|---|---|---|---|
| H | 2.56520000 | 8.47730000 | -1.03910000 |
| C | 2.54250000 | 7.13690000 | 0.65360000 |
| H | 3.60100000 | 6.89450000 | 0.58220000 |
| C | 1.77120000 | 6.55800000 | 1.66450000 |
| H | 2.25790000 | 5.88870000 | 2.36910000 |
| C | -2.26470000 | 5.94690000 | 2.33400000 |
| C | -3.43140000 | 6.53550000 | 2.84090000 |
| H | -3.37660000 | 7.12440000 | 3.74970000 |
| C | -4.65920000 | 6.36340000 | 2.19340000 |
| H | -5.55290000 | 6.82930000 | 2.60380000 |
| C | -4.73800000 | 5.59880000 | 1.02890000 |
| H | -5.69340000 | 5.46350000 | 0.52540000 |
| C | -3.58040000 | 5.01290000 | 0.50660000 |
| H | -3.62930000 | 4.42380000 | -0.40730000 |
| C | -2.35610000 | 5.18860000 | 1.15180000 |
| H | -1.46270000 | 4.74880000 | 0.71290000 |

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**Species A_alt**
HF energy= -3841.79355711
No imaginary frequency
Zero-point correction = 0.692796 (Hartree/Particle)
Thermal correction to Energy = 0.742328
Thermal correction to Enthalpy = 0.743272
Thermal correction to Gibbs Free Energy = 0.608161
Sum of electronic and zero-point Energies = -3841.100761
Sum of electronic and thermal Energies = -3841.051229
Sum of electronic and thermal Enthalpies = -3841.050285
Sum of electronic and thermal Free Energies = -3841.185396

Coordinates: **A_alt**

| | | | |
|---|---|---|---|
| Fe | 1.29340000 | 0.45760000 | 0.21000000 |
| Fe | -1.08710000 | -0.01900000 | 0.88080000 |
| P | 3.33840000 | 1.36900000 | 0.19730000 |
| P | 0.82930000 | 1.56940000 | -1.66570000 |
| P | -1.47460000 | -1.29350000 | -0.96050000 |
| S | 0.75000000 | -1.24560000 | 1.68480000 |
| S | 0.12260000 | 1.80650000 | 1.67990000 |
| O | 2.31470000 | -1.78120000 | -1.35690000 |
| O | -3.01920000 | -1.07030000 | 2.81590000 |
| O | -2.88480000 | 2.03720000 | -0.18340000 |
| C | 1.87820000 | -0.87940000 | -0.76460000 |
| C | -2.26070000 | -0.64820000 | 2.04860000 |
| C | -2.17010000 | 1.21310000 | 0.20080000 |
| C | 3.54270000 | 2.12370000 | -1.53770000 |
| H | 3.41510000 | 3.20790000 | -1.43520000 |
| H | 4.55950000 | 1.95380000 | -1.90970000 |
| C | 2.49740000 | 1.57650000 | -2.53470000 |
| H | 2.73600000 | 0.54330000 | -2.81590000 |

| | | | |
|---|---|---|---|
| H | 2.49720000 | 2.17910000 | -3.45140000 |
| C | -0.39490000 | 0.71650000 | -2.81390000 |
| H | -1.32370000 | 1.28890000 | -2.70510000 |
| H | -0.06460000 | 0.86090000 | -3.85290000 |
| C | -0.65510000 | -0.78470000 | -2.58570000 |
| H | 0.28070000 | -1.34670000 | -2.64220000 |
| H | -1.28270000 | -1.14960000 | -3.40920000 |
| C | 1.07910000 | -0.90470000 | 3.47590000 |
| H | 0.78890000 | -1.82040000 | 4.00640000 |
| H | 2.16860000 | -0.80240000 | 3.57330000 |
| C | 0.71060000 | 1.62650000 | 3.42560000 |
| H | 1.79360000 | 1.80430000 | 3.41960000 |
| H | 0.24300000 | 2.45090000 | 3.97720000 |
| C | 3.77730000 | 2.78010000 | 1.31790000 |
| C | 4.65390000 | 2.60540000 | 2.40220000 |
| H | 5.14640000 | 1.64870000 | 2.55410000 |
| C | 4.91220000 | 3.65510000 | 3.28860000 |
| H | 5.59710000 | 3.49870000 | 4.11990000 |
| C | 4.30150000 | 4.89730000 | 3.10640000 |
| H | 4.50620000 | 5.71530000 | 3.79410000 |
| C | 3.42180000 | 5.08080000 | 2.03580000 |
| H | 2.93480000 | 6.04260000 | 1.88640000 |
| C | 3.15570000 | 4.03110000 | 1.15540000 |
| H | 2.44690000 | 4.19090000 | 0.34670000 |
| C | 4.82350000 | 0.27510000 | 0.36930000 |
| C | 4.67680000 | -1.00070000 | 0.93500000 |
| H | 3.69070000 | -1.33880000 | 1.24500000 |
| C | 5.78350000 | -1.84150000 | 1.09220000 |
| H | 5.65010000 | -2.82970000 | 1.52790000 |
| C | 7.04930000 | -1.41860000 | 0.68410000 |
| H | 7.90960000 | -2.07490000 | 0.80110000 |
| C | 7.20970000 | -0.14660000 | 0.12440000 |
| H | 8.19500000 | 0.19200000 | -0.19060000 |
| C | 6.10670000 | 0.69430000 | -0.02730000 |
| H | 6.25330000 | 1.69020000 | -0.44130000 |
| C | 0.30910000 | 3.33360000 | -1.94020000 |
| C | -0.09140000 | 4.16220000 | -0.88060000 |
| H | -0.10170000 | 3.77340000 | 0.13320000 |
| C | -0.48830000 | 5.48290000 | -1.11980000 |
| H | -0.79860000 | 6.10680000 | -0.28390000 |
| C | -0.49590000 | 5.99420000 | -2.41780000 |
| H | -0.80680000 | 7.02080000 | -2.60190000 |
| C | -0.10560000 | 5.17750000 | -3.48370000 |
| H | -0.11150000 | 5.56460000 | -4.50100000 |
| C | 0.29210000 | 3.86140000 | -3.24620000 |
| H | 0.58730000 | 3.24410000 | -4.09270000 |
| C | -3.27960000 | -1.29610000 | -1.42390000 |
| C | -4.17550000 | -2.00740000 | -0.60580000 |
| H | -3.79940000 | -2.57610000 | 0.24140000 |
| C | -5.54500000 | -2.00310000 | -0.86910000 |

| | | | |
|---|---|---|---|
| H | -6.21750000 | -2.56630000 | -0.22500000 |
| C | -6.05110000 | -1.27810000 | -1.95240000 |
| H | -7.12000000 | -1.27090000 | -2.15620000 |
| C | -5.17500000 | -0.56220000 | -2.76830000 |
| H | -5.55620000 | 0.00940000 | -3.61250000 |
| C | -3.80080000 | -0.57160000 | -2.50700000 |
| H | -3.14670000 | 0.00090000 | -3.15910000 |
| C | -1.13670000 | -3.11810000 | -0.93860000 |
| C | -0.95880000 | -3.86010000 | -2.11960000 |
| H | -0.97550000 | -3.36830000 | -3.08850000 |
| C | -0.76710000 | -5.24180000 | -2.07180000 |
| H | -0.62710000 | -5.79770000 | -2.99700000 |
| C | -0.76010000 | -5.90810000 | -0.84320000 |
| H | -0.61140000 | -6.98560000 | -0.80680000 |
| C | -0.94520000 | -5.18370000 | 0.33530000 |
| H | -0.93880000 | -5.69210000 | 1.29750000 |
| C | -1.12780000 | -3.79870000 | 0.28890000 |
| H | -1.24840000 | -3.24120000 | 1.21200000 |
| C | 0.37770000 | 0.29960000 | 4.09720000 |
| H | 0.67640000 | 0.35880000 | 5.15690000 |
| H | -0.70810000 | 0.14670000 | 4.08600000 |

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**Species C**
HF energy= -3841.81352471
No Imaginary frequency
Zero-point correction = 0.692461 (Hartree/Particle)
Thermal correction to Energy = 0.742150
Thermal correction to Enthalpy = 0.743094
Thermal correction to Gibbs Free Energy = 0.607012
Sum of electronic and zero-point Energies = -3841.121064
Sum of electronic and thermal Energies = -3841.071375
Sum of electronic and thermal Enthalpies = -3841.070431
Sum of electronic and thermal Free Energies = -3841.206512

Coordinates: **C**

| | | | |
|---|---|---|---|
| Fe | 1.02150000 | 0.38860000 | 0.75410000 |
| Fe | -1.25560000 | -0.77920000 | 1.00170000 |
| P | 2.59140000 | -0.90400000 | -0.39070000 |
| P | 0.72220000 | 1.47340000 | -1.22520000 |
| P | -2.79780000 | 0.07000000 | -0.42730000 |
| S | 0.62240000 | -1.26850000 | 2.28290000 |
| S | -0.82800000 | 1.42070000 | 1.64880000 |
| O | 2.83640000 | 2.17970000 | 2.15640000 |
| O | -0.41980000 | -2.58570000 | -1.13550000 |
| O | -3.08930000 | -2.42860000 | 2.57160000 |
| C | 2.16960000 | 1.44760000 | 1.55130000 |
| C | -0.69280000 | -1.85780000 | -0.26590000 |
| C | -2.39710000 | -1.71580000 | 1.97070000 |

| | | | |
|---|---|---|---|
| C | 2.24210000 | -0.65060000 | -2.20150000 |
| H | 3.03630000 | -1.04040000 | -2.84950000 |
| H | 1.33830000 | -1.23600000 | -2.40920000 |
| C | 1.98440000 | 0.84150000 | -2.45830000 |
| H | 1.64870000 | 1.00670000 | -3.49060000 |
| H | 2.90240000 | 1.42490000 | -2.31310000 |
| C | -0.84560000 | 1.17940000 | -2.21510000 |
| H | -0.77970000 | 1.80970000 | -3.11300000 |
| H | -0.81040000 | 0.13580000 | -2.55420000 |
| C | -2.16790000 | 1.47830000 | -1.48030000 |
| H | -2.94760000 | 1.76030000 | -2.19920000 |
| H | -2.05870000 | 2.33360000 | -0.80290000 |
| C | 0.47480000 | -0.61330000 | 4.00950000 |
| H | 0.39300000 | -1.49860000 | 4.65220000 |
| H | 1.43140000 | -0.12530000 | 4.24040000 |
| C | -0.66080000 | 1.62650000 | 3.48310000 |
| H | 0.26680000 | 2.18390000 | 3.66610000 |
| H | -1.49570000 | 2.27260000 | 3.78220000 |
| C | 4.36260000 | -0.36830000 | -0.19680000 |
| C | 4.87600000 | -0.20980000 | 1.10220000 |
| H | 4.22860000 | -0.36430000 | 1.96150000 |
| C | 6.20790000 | 0.15200000 | 1.30910000 |
| H | 6.58220000 | 0.26630000 | 2.32450000 |
| C | 7.05150000 | 0.37890000 | 0.21880000 |
| H | 8.08750000 | 0.67040000 | 0.37860000 |
| C | 6.55420000 | 0.23260000 | -1.07720000 |
| H | 7.20160000 | 0.40670000 | -1.93470000 |
| C | 5.22380000 | -0.14410000 | -1.28290000 |
| H | 4.87080000 | -0.26330000 | -2.30370000 |
| C | 2.78940000 | -2.73860000 | -0.22430000 |
| C | 3.15140000 | -3.27500000 | 1.02370000 |
| H | 3.27850000 | -2.62130000 | 1.88090000 |
| C | 3.33860000 | -4.64860000 | 1.18260000 |
| H | 3.61580000 | -5.04290000 | 2.15820000 |
| C | 3.16210000 | -5.51250000 | 0.09890000 |
| H | 3.30420000 | -6.58410000 | 0.22380000 |
| C | 2.79780000 | -4.99220000 | -1.14390000 |
| H | 2.65290000 | -5.65530000 | -1.99460000 |
| C | 2.61270000 | -3.61670000 | -1.30510000 |
| H | 2.32030000 | -3.24220000 | -2.28100000 |
| C | 0.89700000 | 3.31030000 | -1.38250000 |
| C | 0.86780000 | 4.12630000 | -0.24130000 |
| H | 0.73240000 | 3.67460000 | 0.73630000 |
| C | 1.00230000 | 5.51360000 | -0.35420000 |
| H | 0.97620000 | 6.13010000 | 0.54210000 |
| C | 1.17120000 | 6.10430000 | -1.60740000 |
| H | 1.27900000 | 7.18370000 | -1.69420000 |
| C | 1.20240000 | 5.30270000 | -2.75280000 |
| H | 1.33610000 | 5.75490000 | -3.73380000 |
| C | 1.06290000 | 3.91880000 | -2.64050000 |

| | | | |
|---|---|---|---|
| H | 1.09070000 | 3.31280000 | -3.54440000 |
| C | -4.34070000 | 0.83230000 | 0.26640000 |
| C | -4.45700000 | 1.07890000 | 1.64180000 |
| H | -3.63980000 | 0.80420000 | 2.30140000 |
| C | -5.61100000 | 1.67160000 | 2.16250000 |
| H | -5.68690000 | 1.85270000 | 3.23300000 |
| C | -6.66240000 | 2.02570000 | 1.31500000 |
| H | -7.56170000 | 2.48490000 | 1.72100000 |
| C | -6.55870000 | 1.78080000 | -0.05770000 |
| H | -7.37720000 | 2.04630000 | -0.72430000 |
| C | -5.40800000 | 1.18620000 | -0.57730000 |
| H | -5.35050000 | 0.98040000 | -1.64420000 |
| C | -3.50550000 | -1.12150000 | -1.65870000 |
| C | -3.55870000 | -0.88500000 | -3.04150000 |
| H | -3.16820000 | 0.03810000 | -3.46160000 |
| C | -4.11210000 | -1.83290000 | -3.90880000 |
| H | -4.14000000 | -1.63120000 | -4.97810000 |
| C | -4.62560000 | -3.02920000 | -3.40680000 |
| H | -5.05590000 | -3.76630000 | -4.08180000 |
| C | -4.57990000 | -3.27610000 | -2.03150000 |
| H | -4.97410000 | -4.20690000 | -1.62880000 |
| C | -4.02030000 | -2.33500000 | -1.16750000 |
| H | -3.98010000 | -2.54710000 | -0.10210000 |
| C | -0.68850000 | 0.33390000 | 4.29260000 |
| H | -0.66500000 | 0.59480000 | 5.36370000 |
| H | -1.63680000 | -0.18880000 | 4.11620000 |

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**Species TSCD**
HF energy= -3841.79675387
One imaginary frequency (247*i*)
Zero-point correction = 0.692139 (Hartree/Particle)
Thermal correction to Energy = 0.741506
Thermal correction to Enthalpy = 0.742451
Thermal correction to Gibbs Free Energy = 0.605874
Sum of electronic and zero-point Energies = -3841.104615
Sum of electronic and thermal Energies = -3841.055248
Sum of electronic and thermal Enthalpies = -3841.054303
Sum of electronic and thermal Free Energies = -3841.190880

Coordinates: **TSCD**

| | | | |
|---|---|---|---|
| Fe | 1.07880000 | 0.40800000 | 0.70680000 |
| Fe | -1.19920000 | -0.79400000 | 0.96480000 |
| P | 2.63040000 | -0.89310000 | -0.44830000 |
| P | 0.74840000 | 1.47390000 | -1.27250000 |
| P | -2.75550000 | 0.06460000 | -0.44600000 |
| S | 0.67270000 | -1.26460000 | 2.20600000 |
| S | -0.76750000 | 1.37920000 | 1.61870000 |
| O | 2.90440000 | 2.23640000 | 2.04780000 |

| | | | |
|---|---|---|---|
| O | -0.42460000 | -2.66970000 | -1.14170000 |
| O | -2.99310000 | -2.35650000 | 2.66510000 |
| C | 2.23020000 | 1.48730000 | 1.47200000 |
| C | -0.69010000 | -1.91980000 | -0.29080000 |
| C | -2.32040000 | -1.68370000 | 1.99990000 |
| C | 2.26080000 | -0.64860000 | -2.25650000 |
| H | 3.04760000 | -1.04130000 | -2.91180000 |
| H | 1.35440000 | -1.23460000 | -2.45240000 |
| C | 2.00040000 | 0.84250000 | -2.51590000 |
| H | 1.65580000 | 1.00420000 | -3.54590000 |
| H | 2.91980000 | 1.42600000 | -2.37990000 |
| C | -0.82580000 | 1.17830000 | -2.25210000 |
| H | -0.76510000 | 1.81120000 | -3.14860000 |
| H | -0.79140000 | 0.13540000 | -2.59380000 |
| C | -2.14300000 | 1.47400000 | -1.50810000 |
| H | -2.92980000 | 1.75220000 | -2.22080000 |
| H | -2.03070000 | 2.33110000 | -0.83320000 |
| C | 0.35580000 | -0.80980000 | 3.96660000 |
| H | -0.39700000 | -1.53940000 | 4.28350000 |
| H | 1.28240000 | -1.07550000 | 4.48930000 |
| C | -0.49880000 | 1.71790000 | 3.41320000 |
| H | 0.24510000 | 2.52200000 | 3.42340000 |
| H | -1.44150000 | 2.16500000 | 3.75020000 |
| C | 4.40440000 | -0.36000000 | -0.27520000 |
| C | 4.92580000 | -0.18510000 | 1.01850000 |
| H | 4.28200000 | -0.32410000 | 1.88340000 |
| C | 6.26020000 | 0.17440000 | 1.21250000 |
| H | 6.64110000 | 0.30180000 | 2.22390000 |
| C | 7.09800000 | 0.38300000 | 0.11410000 |
| H | 8.13610000 | 0.67290000 | 0.26360000 |
| C | 6.59250000 | 0.22050000 | -1.17700000 |
| H | 7.23550000 | 0.38060000 | -2.04040000 |
| C | 5.25960000 | -0.15430000 | -1.36960000 |
| H | 4.89990000 | -0.28700000 | -2.38640000 |
| C | 2.82950000 | -2.72730000 | -0.27710000 |
| C | 3.21020000 | -3.25780000 | 0.96790000 |
| H | 3.35270000 | -2.59930000 | 1.81910000 |
| C | 3.39900000 | -4.63050000 | 1.13100000 |
| H | 3.69110000 | -5.02020000 | 2.10410000 |
| C | 3.20560000 | -5.49980000 | 0.05440000 |
| H | 3.34920000 | -6.57090000 | 0.18240000 |
| C | 2.82300000 | -4.98550000 | -1.18540000 |
| H | 2.66510000 | -5.65280000 | -2.03050000 |
| C | 2.63620000 | -3.61070000 | -1.35070000 |
| H | 2.32980000 | -3.24110000 | -2.32420000 |
| C | 0.91320000 | 3.31190000 | -1.43390000 |
| C | 0.85110000 | 4.13060000 | -0.29600000 |
| H | 0.70180000 | 3.67920000 | 0.67980000 |
| C | 0.97200000 | 5.51900000 | -0.40950000 |
| H | 0.92060000 | 6.13740000 | 0.48440000 |

| | | | |
|---|---|---|---|
| C | 1.16070000 | 6.10840000 | -1.66050000 |
| H | 1.25870000 | 7.18870000 | -1.74780000 |
| C | 1.22450000 | 5.30430000 | -2.80270000 |
| H | 1.37360000 | 5.75560000 | -3.78190000 |
| C | 1.09780000 | 3.91920000 | -2.68970000 |
| H | 1.14980000 | 3.31160000 | -3.59140000 |
| C | -4.28700000 | 0.83080000 | 0.27050000 |
| C | -4.37690000 | 1.09130000 | 1.64550000 |
| H | -3.54670000 | 0.82430000 | 2.29220000 |
| C | -5.52160000 | 1.68770000 | 2.18230000 |
| H | -5.57700000 | 1.87950000 | 3.25220000 |
| C | -6.58990000 | 2.03170000 | 1.35200000 |
| H | -7.48200000 | 2.49350000 | 1.77080000 |
| C | -6.51240000 | 1.77330000 | -0.01990000 |
| H | -7.34400000 | 2.03110000 | -0.67310000 |
| C | -5.37100000 | 1.17530000 | -0.55570000 |
| H | -5.33330000 | 0.95940000 | -1.62150000 |
| C | -3.48530000 | -1.12570000 | -1.66480000 |
| C | -3.54690000 | -0.89860000 | -3.04860000 |
| H | -3.15130000 | 0.01800000 | -3.47820000 |
| C | -4.11600000 | -1.84770000 | -3.90470000 |
| H | -4.15020000 | -1.65350000 | -4.97520000 |
| C | -4.63710000 | -3.03510000 | -3.38980000 |
| H | -5.07960000 | -3.77300000 | -4.05600000 |
| C | -4.58330000 | -3.27250000 | -2.01300000 |
| H | -4.98350000 | -4.19640000 | -1.60060000 |
| C | -4.00800000 | -2.33050000 | -1.16050000 |
| H | -3.96090000 | -2.53390000 | -0.09340000 |
| C | -0.07750000 | 0.61170000 | 4.41660000 |
| H | 0.74240000 | 1.03150000 | 5.01260000 |
| H | -0.90740000 | 0.47370000 | 5.12100000 |

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**Species D**
HF energy= -3841.81241277
No Imaginary frequency
Zero-point correction = 0.692432 (Hartree/Particle)
Thermal correction to Energy = 0.742135
Thermal correction to Enthalpy = 0.743079
Thermal correction to Gibbs Free Energy = 0.606374
Sum of electronic and zero-point Energies = -3841.119980
Sum of electronic and thermal Energies = -3841.070278
Sum of electronic and thermal Enthalpies = -3841.069334
Sum of electronic and thermal Free Energies = -3841.206038

Coordinates: **D**

| | | | |
|---|---|---|---|
| Fe | 1.09250000 | 0.43930000 | 0.72240000 |
| Fe | -1.17800000 | -0.74760000 | 0.99560000 |
| P | 2.61810000 | -0.88650000 | -0.43870000 |

| | | | |
|---|---|---|---|
| P | 0.74520000 | 1.49550000 | -1.25950000 |
| P | -2.73570000 | 0.08510000 | -0.43070000 |
| S | 0.70230000 | -1.24130000 | 2.24620000 |
| S | -0.76420000 | 1.43590000 | 1.65040000 |
| O | 3.00280000 | 2.31150000 | 1.87910000 |
| O | -0.45710000 | -2.73330000 | -1.03060000 |
| O | -2.98830000 | -2.22130000 | 2.75690000 |
| C | 2.28420000 | 1.53750000 | 1.39860000 |
| C | -0.70480000 | -1.94120000 | -0.21500000 |
| C | -2.30920000 | -1.58300000 | 2.06510000 |
| C | 2.24190000 | -0.63720000 | -2.24430000 |
| H | 3.02170000 | -1.03650000 | -2.90390000 |
| H | 1.32890000 | -1.21420000 | -2.43730000 |
| C | 1.99460000 | 0.85640000 | -2.50090000 |
| H | 1.65170000 | 1.02160000 | -3.53080000 |
| H | 2.91910000 | 1.43160000 | -2.36410000 |
| C | -0.82580000 | 1.21310000 | -2.24730000 |
| H | -0.76110000 | 1.86180000 | -3.13220000 |
| H | -0.79090000 | 0.17630000 | -2.60660000 |
| C | -2.14340000 | 1.49580000 | -1.50170000 |
| H | -2.93570000 | 1.76000000 | -2.21360000 |
| H | -2.04010000 | 2.35800000 | -0.83180000 |
| C | 0.45700000 | -0.65310000 | 3.98490000 |
| H | -0.48490000 | -1.09130000 | 4.33820000 |
| H | 1.26760000 | -1.10970000 | 4.56700000 |
| C | -0.66100000 | 1.61100000 | 3.49410000 |
| H | -0.56640000 | 2.68600000 | 3.69220000 |
| H | -1.63530000 | 1.28920000 | 3.88510000 |
| C | 4.40040000 | -0.38000000 | -0.27330000 |
| C | 4.92920000 | -0.21760000 | 1.01900000 |
| H | 4.28560000 | -0.34750000 | 1.88560000 |
| C | 6.27020000 | 0.11870000 | 1.20890000 |
| H | 6.65710000 | 0.23670000 | 2.21910000 |
| C | 7.10700000 | 0.31660000 | 0.10770000 |
| H | 8.15040000 | 0.58840000 | 0.25410000 |
| C | 6.59390000 | 0.16710000 | -1.18190000 |
| H | 7.23630000 | 0.31930000 | -2.04720000 |
| C | 5.25430000 | -0.18500000 | -1.37050000 |
| H | 4.88850000 | -0.30840000 | -2.38630000 |
| C | 2.79640000 | -2.72350000 | -0.27150000 |
| C | 3.17470000 | -3.26280000 | 0.97040000 |
| H | 3.32270000 | -2.60990000 | 1.82470000 |
| C | 3.35290000 | -4.63780000 | 1.12660000 |
| H | 3.64260000 | -5.03430000 | 2.09770000 |
| C | 3.15230000 | -5.50040000 | 0.04610000 |
| H | 3.28760000 | -6.57320000 | 0.16890000 |
| C | 2.77360000 | -4.97720000 | -1.19110000 |
| H | 2.61050000 | -5.63890000 | -2.03950000 |
| C | 2.59710000 | -3.60020000 | -1.34940000 |
| H | 2.29370000 | -3.22430000 | -2.32150000 |

| | | | |
|---|---|---|---|
| C | 0.91830000 | 3.33310000 | -1.41940000 |
| C | 0.79230000 | 4.15570000 | -0.28940000 |
| H | 0.59220000 | 3.70650000 | 0.67860000 |
| C | 0.91260000 | 5.54420000 | -0.40250000 |
| H | 0.81110000 | 6.16580000 | 0.48500000 |
| C | 1.16490000 | 6.12980000 | -1.64400000 |
| H | 1.26330000 | 7.21010000 | -1.73020000 |
| C | 1.29180000 | 5.32170000 | -2.77800000 |
| H | 1.49010000 | 5.76990000 | -3.74990000 |
| C | 1.16500000 | 3.93640000 | -2.66650000 |
| H | 1.26500000 | 3.32620000 | -3.56220000 |
| C | -4.28160000 | 0.84020000 | 0.26930000 |
| C | -4.37770000 | 1.13270000 | 1.63730000 |
| H | -3.54460000 | 0.89630000 | 2.29120000 |
| C | -5.53200000 | 1.72370000 | 2.15920000 |
| H | -5.59080000 | 1.94070000 | 3.22410000 |
| C | -6.60490000 | 2.03060000 | 1.32050000 |
| H | -7.50460000 | 2.48820000 | 1.72760000 |
| C | -6.52160000 | 1.74090000 | -0.04470000 |
| H | -7.35630000 | 1.96980000 | -0.70470000 |
| C | -5.37020000 | 1.14840000 | -0.56530000 |
| H | -5.32840000 | 0.90880000 | -1.62580000 |
| C | -3.45050000 | -1.12230000 | -1.64220000 |
| C | -3.51000000 | -0.90830000 | -3.02820000 |
| H | -3.12220000 | 0.00820000 | -3.46480000 |
| C | -4.06850000 | -1.86980000 | -3.87750000 |
| H | -4.10140000 | -1.68530000 | -4.94970000 |
| C | -4.58120000 | -3.05690000 | -3.35350000 |
| H | -5.01570000 | -3.80430000 | -4.01430000 |
| C | -4.53000000 | -3.28110000 | -1.97440000 |
| H | -4.92420000 | -4.20450000 | -1.55490000 |
| C | -3.96530000 | -2.32680000 | -1.12880000 |
| H | -3.92030000 | -2.51980000 | -0.05950000 |
| C | 0.46760000 | 0.85860000 | 4.19560000 |
| H | 1.43540000 | 1.26700000 | 3.88210000 |
| H | 0.38290000 | 1.05710000 | 5.27700000 |

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**Species C_alt**
HF energy= - -3841.79222866
No Imaginary frequency
Zero-point correction = 0.692219 (Hartree/Particle)
Thermal correction to Energy = 0.741957
Thermal correction to Enthalpy = 0.742902
Thermal correction to Gibbs Free Energy = 0.606399
Sum of electronic and zero-point Energies = -3841.100009
Sum of electronic and thermal Energies = -3841.050271
Sum of electronic and thermal Enthalpies = -3841.049327
Sum of electronic and thermal Free Energies = -3841.185830

Coordinates: **C_alt**

| | | | |
|---|---|---|---|
| Fe | 1.30090000 | 0.44520000 | 0.52330000 |
| Fe | -1.14180000 | -0.43920000 | 0.89500000 |
| P | 2.93890000 | -0.41140000 | -0.95030000 |
| P | 0.64700000 | 1.65870000 | -1.23010000 |
| P | -1.43560000 | -1.49060000 | -1.07870000 |
| S | 0.81580000 | -1.53230000 | 1.53330000 |
| S | -0.21040000 | 1.35910000 | 1.99840000 |
| O | 3.27310000 | 2.03880000 | 1.95130000 |
| O | -2.98870000 | -1.89440000 | 2.63610000 |
| O | -3.11090000 | 1.57100000 | 0.05990000 |
| C | 2.55300000 | 1.37130000 | 1.32840000 |
| C | -2.25160000 | -1.31480000 | 1.95400000 |
| C | -2.32480000 | 0.77410000 | 0.34840000 |
| C | 2.91810000 | 0.64730000 | -2.51490000 |
| H | 3.93570000 | 0.82120000 | -2.88480000 |
| H | 2.40450000 | 0.04790000 | -3.27630000 |
| C | 2.16280000 | 1.96360000 | -2.29340000 |
| H | 1.89110000 | 2.43010000 | -3.25050000 |
| H | 2.77790000 | 2.68480000 | -1.74010000 |
| C | -0.49730000 | 0.83520000 | -2.48720000 |
| H | -1.50810000 | 1.20480000 | -2.28220000 |
| H | -0.22890000 | 1.19680000 | -3.49090000 |
| C | -0.49600000 | -0.71090000 | -2.49840000 |
| H | 0.51890000 | -1.11720000 | -2.43430000 |
| H | -0.90800000 | -1.06020000 | -3.45460000 |
| C | 1.04300000 | -1.47030000 | 3.37430000 |
| H | 0.87500000 | -2.49290000 | 3.73570000 |
| H | 2.10310000 | -1.23400000 | 3.53230000 |
| C | 0.28730000 | 0.96120000 | 3.73890000 |
| H | 1.31830000 | 1.31550000 | 3.86240000 |
| H | -0.35480000 | 1.58490000 | 4.37270000 |
| C | 4.65650000 | -0.18440000 | -0.29000000 |
| C | 5.21780000 | -1.18900000 | 0.51660000 |
| H | 4.66800000 | -2.11060000 | 0.69530000 |
| C | 6.48260000 | -1.02290000 | 1.08260000 |
| H | 6.90290000 | -1.81340000 | 1.70140000 |
| C | 7.20830000 | 0.14960000 | 0.85240000 |
| H | 8.19500000 | 0.27820000 | 1.29250000 |
| C | 6.65820000 | 1.15550000 | 0.05610000 |
| H | 7.21230000 | 2.07440000 | -0.12550000 |
| C | 5.38990000 | 0.99140000 | -0.50760000 |
| H | 4.97410000 | 1.79700000 | -1.10850000 |
| C | 3.13070000 | -2.10490000 | -1.69280000 |
| C | 2.49310000 | -3.21970000 | -1.13010000 |
| H | 1.85440000 | -3.09330000 | -0.26160000 |
| C | 2.68080000 | -4.49550000 | -1.67500000 |
| H | 2.16940000 | -5.34480000 | -1.22860000 |
| C | 3.50270000 | -4.67220000 | -2.78770000 |

| | | | |
|---|---|---|---|
| H | 3.64490000 | -5.66430000 | -3.21220000 |
| C | 4.14700000 | -3.56780000 | -3.35560000 |
| H | 4.79600000 | -3.69700000 | -4.21990000 |
| C | 3.96760000 | -2.29740000 | -2.80960000 |
| H | 4.49560000 | -1.45520000 | -3.25120000 |
| C | -0.02420000 | 3.37440000 | -1.11180000 |
| C | 0.43810000 | 4.18620000 | -0.06140000 |
| H | 1.11490000 | 3.77050000 | 0.67970000 |
| C | 0.02390000 | 5.51540000 | 0.04690000 |
| H | 0.39020000 | 6.12660000 | 0.86940000 |
| C | -0.86670000 | 6.05200000 | -0.88570000 |
| H | -1.19680000 | 7.08520000 | -0.79630000 |
| C | -1.33540000 | 5.25450000 | -1.93230000 |
| H | -2.03040000 | 5.66360000 | -2.66310000 |
| C | -0.91510000 | 3.92730000 | -2.04690000 |
| H | -1.28950000 | 3.33120000 | -2.87500000 |
| C | -3.20150000 | -1.43670000 | -1.66850000 |
| C | -4.16990000 | -2.08180000 | -0.87770000 |
| H | -3.87080000 | -2.59360000 | 0.03390000 |
| C | -5.51470000 | -2.07940000 | -1.24680000 |
| H | -6.24460000 | -2.58770000 | -0.62000000 |
| C | -5.92280000 | -1.42330000 | -2.41220000 |
| H | -6.97270000 | -1.41490000 | -2.69770000 |
| C | -4.97380000 | -0.77810000 | -3.20510000 |
| H | -5.27920000 | -0.26290000 | -4.11400000 |
| C | -3.62360000 | -0.78740000 | -2.83850000 |
| H | -2.91100000 | -0.27520000 | -3.47870000 |
| C | -1.11120000 | -3.30330000 | -1.30030000 |
| C | -1.09320000 | -3.89840000 | -2.57380000 |
| H | -1.21040000 | -3.28810000 | -3.46630000 |
| C | -0.94640000 | -5.27890000 | -2.71260000 |
| H | -0.93450000 | -5.72310000 | -3.70600000 |
| C | -0.82670000 | -6.08920000 | -1.57870000 |
| H | -0.72280000 | -7.16730000 | -1.68710000 |
| C | -0.84780000 | -5.50950000 | -0.30850000 |
| H | -0.75790000 | -6.13230000 | 0.57950000 |
| C | -0.98670000 | -4.12460000 | -0.16980000 |
| H | -0.98900000 | -3.67640000 | 0.81910000 |
| C | 0.15780000 | -0.50090000 | 4.15490000 |
| H | 0.42830000 | -0.58090000 | 5.22090000 |
| H | -0.89080000 | -0.80980000 | 4.07920000 |

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**Species $A_{ox}$**
HF energy= -3841.64381641
No Imaginary frequency
Zero-point correction = 0.692144 (Hartree/Particle)
Thermal correction to Energy = 0.742872
Thermal correction to Enthalpy = 0.743817

Thermal correction to Gibbs Free Energy = 0.602927
Sum of electronic and zero-point Energies = -3840.951672
Sum of electronic and thermal Energies = -3840.900944
Sum of electronic and thermal Enthalpies = -3840.900000
Sum of electronic and thermal Free Energies = -3841.040889

Coordinates: $\mathbf{A_{ox}}$

| | | | |
|---|---|---|---|
| Fe | 0.02460000 | 6.24970000 | 7.10820000 |
| Fe | -0.49790000 | 7.62550000 | 4.88250000 |
| P | -0.53170000 | 4.95390000 | 9.11700000 |
| P | 0.50300000 | 4.20880000 | 5.98100000 |
| P | -0.59100000 | 6.30070000 | 2.98930000 |
| S | -2.01980000 | 6.24750000 | 6.03730000 |
| S | -0.09690000 | 8.57560000 | 6.98110000 |
| O | 2.82120000 | 6.64320000 | 8.00350000 |
| O | 2.29490000 | 8.33950000 | 4.26680000 |
| O | -1.85300000 | 9.94180000 | 3.63150000 |
| C | 1.74140000 | 6.46650000 | 7.66040000 |
| C | 1.19910000 | 8.06350000 | 4.48070000 |
| C | -1.34700000 | 9.02120000 | 4.09700000 |
| C | -3.25270000 | 7.22560000 | 7.01810000 |
| H | -4.21210000 | 7.05810000 | 6.51460000 |
| H | -3.31540000 | 6.75760000 | 8.00660000 |
| C | -2.97820000 | 8.72160000 | 7.13670000 |
| H | -3.01250000 | 9.19250000 | 6.14770000 |
| H | -3.79920000 | 9.16690000 | 7.72030000 |
| C | -1.67000000 | 9.07860000 | 7.83370000 |
| H | -1.63570000 | 8.65250000 | 8.84450000 |
| H | -1.58210000 | 10.16630000 | 7.93540000 |
| C | -0.10000000 | 3.21040000 | 8.58170000 |
| H | 0.96300000 | 3.07600000 | 8.81940000 |
| H | -0.66140000 | 2.48250000 | 9.18020000 |
| C | -0.34520000 | 2.96480000 | 7.08100000 |
| H | -1.41020000 | 3.06810000 | 6.83890000 |
| H | -0.06160000 | 1.94000000 | 6.81150000 |
| C | -0.25450000 | 3.78350000 | 4.32860000 |
| H | -0.00610000 | 2.73000000 | 4.14200000 |
| H | -1.34450000 | 3.84660000 | 4.43260000 |
| C | 0.24550000 | 4.63720000 | 3.15060000 |
| H | 0.09260000 | 4.08760000 | 2.21450000 |
| H | 1.32570000 | 4.80230000 | 3.23510000 |
| C | 0.43310000 | 5.22350000 | 10.65310000 |
| C | 0.97750000 | 6.49230000 | 10.91130000 |
| H | 0.85090000 | 7.29790000 | 10.19090000 |
| C | 1.68740000 | 6.73040000 | 12.09160000 |
| H | 2.10530000 | 7.71660000 | 12.27980000 |
| C | 1.86540000 | 5.70210000 | 13.01890000 |
| H | 2.42370000 | 5.88510000 | 13.93420000 |
| C | 1.32480000 | 4.43580000 | 12.77160000 |
| H | 1.45860000 | 3.63430000 | 13.49460000 |

| | | | |
|---|---|---|---|
| C | 0.60660000 | 4.19730000 | 11.59980000 |
| H | 0.17700000 | 3.21220000 | 11.43060000 |
| C | -2.27310000 | 4.86980000 | 9.71160000 |
| C | -3.20940000 | 3.98690000 | 9.14770000 |
| H | -2.91540000 | 3.28680000 | 8.37030000 |
| C | -4.53720000 | 3.98890000 | 9.58220000 |
| H | -5.24700000 | 3.29190000 | 9.14210000 |
| C | -4.95040000 | 4.87670000 | 10.57850000 |
| H | -5.98410000 | 4.87610000 | 10.91620000 |
| C | -4.02720000 | 5.76050000 | 11.14410000 |
| H | -4.33750000 | 6.44770000 | 11.92820000 |
| C | -2.69830000 | 5.75870000 | 10.71550000 |
| H | -1.98730000 | 6.43820000 | 11.18010000 |
| C | 2.24800000 | 3.66230000 | 5.79710000 |
| C | 3.20320000 | 4.60110000 | 5.36540000 |
| H | 2.91450000 | 5.63600000 | 5.19810000 |
| C | 4.53060000 | 4.22080000 | 5.15550000 |
| H | 5.25570000 | 4.95980000 | 4.82290000 |
| C | 4.92470000 | 2.90060000 | 5.38550000 |
| H | 5.96010000 | 2.60550000 | 5.23180000 |
| C | 3.98600000 | 1.96010000 | 5.81800000 |
| H | 4.28770000 | 0.93120000 | 6.00030000 |
| C | 2.65570000 | 2.33470000 | 6.01770000 |
| H | 1.94550000 | 1.58030000 | 6.34650000 |
| C | 0.25840000 | 7.05130000 | 1.53340000 |
| C | -0.46590000 | 7.91580000 | 0.69300000 |
| H | -1.52860000 | 8.07530000 | 0.85870000 |
| C | 0.16480000 | 8.56550000 | -0.36920000 |
| H | -0.41090000 | 9.22930000 | -1.01010000 |
| C | 1.52600000 | 8.36080000 | -0.61020000 |
| H | 2.01610000 | 8.86520000 | -1.43960000 |
| C | 2.25420000 | 7.50460000 | 0.21830000 |
| H | 3.31380000 | 7.33810000 | 0.03720000 |
| C | 1.62790000 | 6.85750000 | 1.28630000 |
| H | 2.22380000 | 6.20680000 | 1.92090000 |
| C | -2.24870000 | 5.86060000 | 2.30490000 |
| C | -3.42430000 | 6.41440000 | 2.83340000 |
| H | -3.36930000 | 7.08390000 | 3.68510000 |
| C | -4.66920000 | 6.10960000 | 2.27450000 |
| H | -5.57030000 | 6.55170000 | 2.69370000 |
| C | -4.75450000 | 5.24410000 | 1.18320000 |
| H | -5.72280000 | 5.00600000 | 0.74870000 |
| C | -3.58910000 | 4.69110000 | 0.64250000 |
| H | -3.64660000 | 4.02520000 | -0.21560000 |
| C | -2.34630000 | 5.00090000 | 1.19420000 |
| H | -1.45110000 | 4.58590000 | 0.73610000 |

**Species $C_{ox}$**
HF energy= -3841.63588462
No Imaginary frequency

Zero-point correction = 0.692551 (Hartree/Particle)
Thermal correction to Energy = 0.742942
Thermal correction to Enthalpy = 0.743886
Thermal correction to Gibbs Free Energy = 0.604530
Sum of electronic and zero-point Energies = -3840.943334
Sum of electronic and thermal Energies = -3840.892943
Sum of electronic and thermal Enthalpies = -3840.891999
Sum of electronic and thermal Free Energies = -3841.031354

Coordinates: **$C_{ox}$**

| | | | |
|---|---|---|---|
| Fe | 1.02610000 | 0.38390000 | 0.64630000 |
| Fe | -1.19020000 | -0.89360000 | 1.00720000 |
| P | 2.74180000 | -0.66960000 | -0.58640000 |
| P | 0.60310000 | 1.60730000 | -1.26870000 |
| P | -2.87050000 | -0.13000000 | -0.38150000 |
| S | 0.80320000 | -1.31770000 | 2.18650000 |
| S | -0.86530000 | 1.32250000 | 1.66720000 |
| O | 2.72150000 | 2.28190000 | 2.06470000 |
| O | -0.23830000 | -2.38630000 | -1.35050000 |
| O | -2.57600000 | -3.18570000 | 2.30630000 |
| C | 2.09670000 | 1.52870000 | 1.45970000 |
| C | -0.52140000 | -1.77230000 | -0.41350000 |
| C | -2.06890000 | -2.30420000 | 1.77830000 |
| C | 2.33480000 | -0.29690000 | -2.36470000 |
| H | 3.16240000 | -0.54970000 | -3.03720000 |
| H | 1.50090000 | -0.95820000 | -2.62720000 |
| C | 1.91500000 | 1.17200000 | -2.52450000 |
| H | 1.56400000 | 1.36420000 | -3.54640000 |
| H | 2.76310000 | 1.84310000 | -2.34020000 |
| C | -0.96830000 | 1.14030000 | -2.18150000 |
| H | -0.99620000 | 1.77200000 | -3.07960000 |
| H | -0.84860000 | 0.10770000 | -2.53180000 |
| C | -2.29370000 | 1.32660000 | -1.40260000 |
| H | -3.10030000 | 1.57710000 | -2.10250000 |
| H | -2.22980000 | 2.17260000 | -0.70860000 |
| C | 0.66340000 | -0.72640000 | 3.93550000 |
| H | 0.64610000 | -1.63830000 | 4.54300000 |
| H | 1.59820000 | -0.19790000 | 4.16270000 |
| C | -0.59910000 | 1.46030000 | 3.49860000 |
| H | 0.31360000 | 2.04760000 | 3.65550000 |
| H | -1.44270000 | 2.06750000 | 3.84590000 |
| C | 4.42910000 | 0.02820000 | -0.31170000 |
| C | 4.92590000 | 0.09440000 | 1.00230000 |
| H | 4.30860000 | -0.22890000 | 1.83720000 |
| C | 6.21290000 | 0.57060000 | 1.25480000 |
| H | 6.58110000 | 0.61030000 | 2.27740000 |
| C | 7.02080000 | 1.00090000 | 0.19920000 |
| H | 8.02160000 | 1.37820000 | 0.39590000 |
| C | 6.53770000 | 0.94370000 | -1.10950000 |
| H | 7.16120000 | 1.27290000 | -1.93770000 |

| | | | |
|---|---|---|---|
| C | 5.25350000 | 0.45570000 | -1.36540000 |
| H | 4.91280000 | 0.40770000 | -2.39590000 |
| C | 3.03320000 | -2.48960000 | -0.54430000 |
| C | 3.43330000 | -3.08750000 | 0.66420000 |
| H | 3.54630000 | -2.48780000 | 1.56210000 |
| C | 3.69020000 | -4.45720000 | 0.72770000 |
| H | 4.00040000 | -4.90200000 | 1.67050000 |
| C | 3.54720000 | -5.25260000 | -0.41220000 |
| H | 3.74610000 | -6.32060000 | -0.36170000 |
| C | 3.14950000 | -4.66950000 | -1.61660000 |
| H | 3.03860000 | -5.27960000 | -2.51020000 |
| C | 2.89430000 | -3.29760000 | -1.68500000 |
| H | 2.58900000 | -2.87440000 | -2.63680000 |
| C | 0.56350000 | 3.44510000 | -1.30820000 |
| C | 0.52530000 | 4.20140000 | -0.12650000 |
| H | 0.49650000 | 3.70360000 | 0.83680000 |
| C | 0.51010000 | 5.59820000 | -0.17980000 |
| H | 0.48080000 | 6.17050000 | 0.74460000 |
| C | 0.53290000 | 6.25470000 | -1.41110000 |
| H | 0.52290000 | 7.34160000 | -1.45100000 |
| C | 0.56970000 | 5.51160000 | -2.59540000 |
| H | 0.58970000 | 6.01710000 | -3.55820000 |
| C | 0.58370000 | 4.11810000 | -2.54530000 |
| H | 0.61730000 | 3.55990000 | -3.47890000 |
| C | -4.39510000 | 0.51560000 | 0.42020000 |
| C | -4.46920000 | 0.66190000 | 1.81380000 |
| H | -3.61790000 | 0.39160000 | 2.43230000 |
| C | -5.63130000 | 1.15710000 | 2.41160000 |
| H | -5.67960000 | 1.26150000 | 3.49320000 |
| C | -6.72690000 | 1.51310000 | 1.62270000 |
| H | -7.63140000 | 1.89800000 | 2.08820000 |
| C | -6.66370000 | 1.36590000 | 0.23330000 |
| H | -7.51810000 | 1.63390000 | -0.38410000 |
| C | -5.50790000 | 0.86500000 | -0.36570000 |
| H | -5.48120000 | 0.72980000 | -1.44500000 |
| C | -3.51970000 | -1.34150000 | -1.60940000 |
| C | -3.50550000 | -1.12340000 | -2.99640000 |
| H | -3.10170000 | -0.20510000 | -3.41330000 |
| C | -4.01780000 | -2.08630000 | -3.87190000 |
| H | -3.99920000 | -1.90100000 | -4.94360000 |
| C | -4.55330000 | -3.27500000 | -3.37470000 |
| H | -4.95190000 | -4.02210000 | -4.05710000 |
| C | -4.57840000 | -3.50010000 | -1.99490000 |
| H | -4.99930000 | -4.42080000 | -1.59750000 |
| C | -4.06350000 | -2.54360000 | -1.12050000 |
| H | -4.09700000 | -2.73270000 | -0.05020000 |
| C | -0.54260000 | 0.14590000 | 4.26820000 |
| H | -0.50230000 | 0.38250000 | 5.34280000 |
| H | -1.46940000 | -0.42110000 | 4.10760000 |

(vi) Table 1. Crystal data and structure refinement for str0432 (**1**).

| | | |
|---|---|---|
| Identification code | str0432 | |
| Chemical formula | $C_{41}H_{41}Cl_2Fe_2O_3P_3S_2$ | |
| Formula weight | 921.37 | |
| Temperature | 150(2) K | |
| Radiation, wavelength | MoKα, 0.71073 Å | |
| Crystal system, space group | triclinic, P1bar | |
| Unit cell parameters | a = 9.4439(8) Å | α = 99.7830(10)° |
| | b = 9.6258(9) Å | β = 95.331(2)° |
| | c = 22.437(2) Å | γ = 94.278(2)° |
| Cell volume | 1992.8(3) $Å^3$ | |
| Z | 2 | |
| Calculated density | 1.536 $g/cm^3$ | |
| Absorption coefficient μ | 1.127 $mm^{-1}$ | |
| F(000) | 948 | |
| Crystal colour and size | orange, 0.16 × 0.15 × 0.04 $mm^3$ | |
| Data collection method | Bruker SMART APEX diffractometer<br>ω rotation with narrow frames | |
| θ range for data collection | 1.85 to 28.29° | |
| Index ranges | h −12 to 12, k −12 to 12, l −29 to 28 | |
| Completeness to θ = 26.00° | 98.4 % | |
| Reflections collected | 17384 | |
| Independent reflections | 9087 ($R_{int}$ = 0.0228) | |
| Reflections with $F^2>2\sigma$ | 7520 | |
| Absorption correction | semi-empirical from equivalents | |
| Min. and max. transmission | 0.8403 and 0.9563 | |
| Structure solution | direct methods | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Weighting parameters a, b | 0.0503, 0.9529 | |
| Data / restraints / parameters | 9087 / 0 / 478 | |
| Final R indices [$F^2>2\sigma$] | R1 = 0.0405, wR2 = 0.0950 | |
| R indices (all data) | R1 = 0.0510, wR2 = 0.0998 | |
| Goodness-of-fit on $F^2$ | 1.046 | |
| Largest and mean shift/su | 0.001 and 0.000 | |
| Largest diff. peak and hole | 1.659 and −1.013 e $Å^{-3}$ | |

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å$^2$) for str0432. $U_{eq}$ is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| Fe(1) | 0.13516(3) | 0.76806(3) | 0.319378(14) | 0.01580(9) |
| Fe(2) | 0.08546(4) | 0.89030(3) | 0.229439(14) | 0.01622(9) |
| P(1) | 0.08711(7) | 0.68444(6) | 0.40143(3) | 0.01742(13) |
| P(2) | 0.15237(6) | 0.54995(6) | 0.27423(3) | 0.01711(13) |
| P(3) | 0.03901(6) | 0.73007(6) | 0.14534(3) | 0.01703(13) |
| S(1) | –0.08223(6) | 0.75661(6) | 0.26652(3) | 0.01738(12) |
| S(2) | 0.12665(7) | 1.00513(6) | 0.32849(3) | 0.02051(13) |
| O(1) | 0.43955(19) | 0.8259(2) | 0.35641(9) | 0.0306(4) |
| O(2) | 0.3926(2) | 0.9232(2) | 0.22207(9) | 0.0348(5) |
| O(3) | –0.0007(2) | 1.1229(2) | 0.17081(9) | 0.0398(5) |
| C(1) | 0.3189(3) | 0.8001(2) | 0.34176(11) | 0.0204(5) |
| C(2) | 0.2709(3) | 0.9086(3) | 0.22498(11) | 0.0223(5) |
| C(3) | 0.0273(3) | 1.0285(3) | 0.19386(11) | 0.0230(5) |
| C(4) | –0.2142(3) | 0.8682(3) | 0.29942(12) | 0.0251(5) |
| C(5) | –0.1709(3) | 1.0259(3) | 0.31130(12) | 0.0272(6) |
| C(6) | –0.0390(3) | 1.0665(3) | 0.35590(11) | 0.0266(6) |
| C(7) | 0.1040(3) | 0.4903(2) | 0.38567(11) | 0.0217(5) |
| C(8) | 0.0600(3) | 0.4335(2) | 0.31817(11) | 0.0204(5) |
| C(9) | 0.0676(3) | 0.4818(3) | 0.19608(11) | 0.0206(5) |
| C(10) | 0.1172(3) | 0.5612(3) | 0.14687(11) | 0.0201(5) |
| C(11) | 0.2066(2) | 0.7478(3) | 0.47113(10) | 0.0188(5) |
| C(12) | 0.2650(3) | 0.8881(3) | 0.48240(11) | 0.0242(5) |
| C(13) | 0.3562(3) | 0.9422(3) | 0.53420(11) | 0.0254(5) |
| C(14) | 0.3927(3) | 0.8562(3) | 0.57547(11) | 0.0222(5) |
| C(15) | 0.3343(3) | 0.7169(3) | 0.56554(11) | 0.0248(5) |
| C(16) | 0.2411(3) | 0.6628(3) | 0.51406(11) | 0.0223(5) |
| C(17) | –0.0896(3) | 0.6876(2) | 0.42977(11) | 0.0195(5) |
| C(18) | –0.2103(3) | 0.6263(3) | 0.39049(11) | 0.0217(5) |
| C(19) | –0.3446(3) | 0.6236(3) | 0.41050(12) | 0.0246(5) |
| C(20) | –0.3616(3) | 0.6814(3) | 0.46998(12) | 0.0265(6) |
| C(21) | –0.2434(3) | 0.7427(3) | 0.50926(12) | 0.0272(6) |
| C(22) | –0.1086(3) | 0.7471(3) | 0.48931(11) | 0.0234(5) |
| C(23) | 0.3291(3) | 0.4837(3) | 0.26948(10) | 0.0204(5) |
| C(24) | 0.4356(3) | 0.5627(3) | 0.24687(11) | 0.0241(5) |
| C(25) | 0.5676(3) | 0.5126(3) | 0.23905(12) | 0.0298(6) |
| C(26) | 0.5973(3) | 0.3846(3) | 0.25468(13) | 0.0331(6) |
| C(27) | 0.4947(3) | 0.3053(3) | 0.27820(13) | 0.0334(6) |
| C(28) | 0.3610(3) | 0.3544(3) | 0.28529(11) | 0.0257(5) |
| C(29) | 0.0984(3) | 0.7788(3) | 0.07578(10) | 0.0200(5) |
| C(30) | 0.0038(4) | 0.7926(6) | 0.02752(16) | 0.0719(15) |
| C(31) | 0.0516(4) | 0.8337(7) | –0.02416(19) | 0.0904(19) |
| C(32) | 0.1923(3) | 0.8623(4) | –0.02822(13) | 0.0389(7) |
| C(33) | 0.2881(3) | 0.8487(4) | 0.01921(13) | 0.0395(7) |
| C(34) | 0.2406(3) | 0.8082(4) | 0.07094(13) | 0.0397(8) |
| C(35) | –0.1510(3) | 0.6762(3) | 0.12117(10) | 0.0196(5) |
| C(36) | –0.2490(3) | 0.7756(3) | 0.13237(12) | 0.0254(5) |
| C(37) | –0.3931(3) | 0.7406(3) | 0.11272(13) | 0.0312(6) |
| C(38) | –0.4406(3) | 0.6062(3) | 0.08309(13) | 0.0336(6) |

| | | | | |
|---|---|---|---|---|
| C(39) | –0.3451(3) | 0.5065(3) | 0.07225(13) | 0.0352(7) |
| C(40) | –0.2004(3) | 0.5408(3) | 0.09038(12) | 0.0282(6) |
| C(41) | 0.3661(4) | 0.1912(5) | 0.12401(17) | 0.0640(11) |
| Cl(1) | 0.53156(9) | 0.12141(10) | 0.12418(4) | 0.0513(2) |
| Cl(2) | 0.32746(11) | 0.27003(12) | 0.06063(6) | 0.0759(3) |

Table 3. Bond lengths [Å] and angles [°] for str0432.

| | | | |
|---|---|---|---|
| Fe(1)–C(1) | 1.750(3) | Fe(1)–P(2) | 2.1953(7) |
| Fe(1)–P(1) | 2.2016(7) | Fe(1)–S(1) | 2.2589(7) |
| Fe(1)–S(2) | 2.2644(7) | Fe(1)–Fe(2) | 2.5279(5) |
| Fe(2)–C(3) | 1.760(3) | Fe(2)–C(2) | 1.761(3) |
| Fe(2)–P(3) | 2.2109(7) | Fe(2)–S(1) | 2.2718(7) |
| Fe(2)–S(2) | 2.2918(7) | P(1)–C(11) | 1.827(2) |
| P(1)–C(17) | 1.841(3) | P(1)–C(7) | 1.863(2) |
| P(2)–C(23) | 1.836(2) | P(2)–C(8) | 1.838(2) |
| P(2)–C(9) | 1.848(2) | P(3)–C(29) | 1.828(2) |
| P(3)–C(35) | 1.835(2) | P(3)–C(10) | 1.839(2) |
| S(1)–C(4) | 1.831(2) | S(2)–C(6) | 1.835(3) |
| O(1)–C(1) | 1.153(3) | O(2)–C(2) | 1.156(3) |
| O(3)–C(3) | 1.155(3) | C(4)–C(5) | 1.515(4) |
| C(5)–C(6) | 1.506(4) | C(7)–C(8) | 1.528(3) |
| C(9)–C(10) | 1.534(3) | C(11)–C(12) | 1.392(3) |
| C(11)–C(16) | 1.397(3) | C(12)–C(13) | 1.380(3) |
| C(13)–C(14) | 1.380(4) | C(14)–C(15) | 1.385(4) |
| C(15)–C(16) | 1.385(3) | C(17)–C(22) | 1.394(3) |
| C(17)–C(18) | 1.400(3) | C(18)–C(19) | 1.384(4) |
| C(19)–C(20) | 1.385(4) | C(20)–C(21) | 1.383(4) |
| C(21)–C(22) | 1.388(4) | C(23)–C(28) | 1.397(3) |
| C(23)–C(24) | 1.400(4) | C(24)–C(25) | 1.385(4) |
| C(25)–C(26) | 1.378(4) | C(26)–C(27) | 1.386(4) |
| C(27)–C(28) | 1.394(4) | C(29)–C(30) | 1.369(4) |
| C(29)–C(34) | 1.370(4) | C(30)–C(31) | 1.390(4) |
| C(31)–C(32) | 1.351(5) | C(32)–C(33) | 1.361(4) |
| C(33)–C(34) | 1.387(4) | C(35)–C(36) | 1.388(4) |
| C(35)–C(40) | 1.392(4) | C(36)–C(37) | 1.390(4) |
| C(37)–C(38) | 1.371(4) | C(38)–C(39) | 1.373(4) |
| C(39)–C(40) | 1.388(4) | C(41)–Cl(2) | 1.744(4) |
| C(41)–Cl(1) | 1.747(4) | | |

| | | | |
|---|---|---|---|
| C(1)–Fe(1)–P(2) | 93.26(8) | C(1)–Fe(1)–P(1) | 94.47(8) |
| P(2)–Fe(1)–P(1) | 88.37(3) | C(1)–Fe(1)–S(1) | 162.54(8) |
| P(2)–Fe(1)–S(1) | 88.13(2) | P(1)–Fe(1)–S(1) | 102.97(3) |
| C(1)–Fe(1)–S(2) | 87.99(8) | P(2)–Fe(1)–S(2) | 157.61(3) |
| P(1)–Fe(1)–S(2) | 113.84(3) | S(1)–Fe(1)–S(2) | 84.24(2) |
| C(1)–Fe(1)–Fe(2) | 106.46(8) | P(2)–Fe(1)–Fe(2) | 101.66(2) |
| P(1)–Fe(1)–Fe(2) | 156.05(2) | S(1)–Fe(1)–Fe(2) | 56.328(18) |
| S(2)–Fe(1)–Fe(2) | 56.820(18) | C(3)–Fe(2)–C(2) | 101.97(12) |
| C(3)–Fe(2)–P(3) | 93.47(8) | C(2)–Fe(2)–P(3) | 94.58(8) |
| C(3)–Fe(2)–S(1) | 117.39(9) | C(2)–Fe(2)–S(1) | 140.62(8) |
| P(3)–Fe(2)–S(1) | 84.90(2) | C(3)–Fe(2)–S(2) | 100.30(8) |
| C(2)–Fe(2)–S(2) | 88.60(8) | P(3)–Fe(2)–S(2) | 164.92(3) |
| S(1)–Fe(2)–S(2) | 83.33(2) | C(3)–Fe(2)–Fe(1) | 154.24(8) |
| C(2)–Fe(2)–Fe(1) | 88.00(8) | P(3)–Fe(2)–Fe(1) | 109.52(2) |
| S(1)–Fe(2)–Fe(1) | 55.846(18) | S(2)–Fe(2)–Fe(1) | 55.787(19) |
| C(11)–P(1)–C(17) | 101.93(11) | C(11)–P(1)–C(7) | 103.86(11) |
| C(17)–P(1)–C(7) | 100.77(11) | C(11)–P(1)–Fe(1) | 117.57(8) |
| C(17)–P(1)–Fe(1) | 122.77(8) | C(7)–P(1)–Fe(1) | 107.32(8) |
| C(23)–P(2)–C(8) | 104.10(11) | C(23)–P(2)–C(9) | 100.61(11) |
| C(8)–P(2)–C(9) | 101.86(11) | C(23)–P(2)–Fe(1) | 119.72(8) |
| C(8)–P(2)–Fe(1) | 106.59(8) | C(9)–P(2)–Fe(1) | 121.47(8) |

| | | | |
|---|---|---|---|
| C(29)–P(3)–C(35) | 101.09(11) | C(29)–P(3)–C(10) | 101.80(11) |
| C(35)–P(3)–C(10) | 103.61(11) | C(29)–P(3)–Fe(2) | 116.95(8) |
| C(35)–P(3)–Fe(2) | 115.42(8) | C(10)–P(3)–Fe(2) | 115.78(8) |
| C(4)–S(1)–Fe(1) | 118.18(9) | C(4)–S(1)–Fe(2) | 110.07(9) |
| Fe(1)–S(1)–Fe(2) | 67.83(2) | C(6)–S(2)–Fe(1) | 113.31(9) |
| C(6)–S(2)–Fe(2) | 110.68(9) | Fe(1)–S(2)–Fe(2) | 67.39(2) |
| O(1)–C(1)–Fe(1) | 177.7(2) | O(2)–C(2)–Fe(2) | 178.8(2) |
| O(3)–C(3)–Fe(2) | 175.1(2) | C(5)–C(4)–S(1) | 115.39(18) |
| C(6)–C(5)–C(4) | 112.5(2) | C(5)–C(6)–S(2) | 115.23(17) |
| C(8)–C(7)–P(1) | 109.18(16) | C(7)–C(8)–P(2) | 108.04(16) |
| C(10)–C(9)–P(2) | 115.67(17) | C(9)–C(10)–P(3) | 114.16(16) |
| C(12)–C(11)–C(16) | 118.3(2) | C(12)–C(11)–P(1) | 118.42(18) |
| C(16)–C(11)–P(1) | 123.24(18) | C(13)–C(12)–C(11) | 121.2(2) |
| C(12)–C(13)–C(14) | 120.0(2) | C(13)–C(14)–C(15) | 119.7(2) |
| C(14)–C(15)–C(16) | 120.4(2) | C(15)–C(16)–C(11) | 120.3(2) |
| C(22)–C(17)–C(18) | 118.3(2) | C(22)–C(17)–P(1) | 122.67(19) |
| C(18)–C(17)–P(1) | 119.04(18) | C(19)–C(18)–C(17) | 120.8(2) |
| C(18)–C(19)–C(20) | 120.3(2) | C(21)–C(20)–C(19) | 119.5(2) |
| C(20)–C(21)–C(22) | 120.4(2) | C(21)–C(22)–C(17) | 120.6(2) |
| C(28)–C(23)–C(24) | 118.0(2) | C(28)–C(23)–P(2) | 122.9(2) |
| C(24)–C(23)–P(2) | 119.05(18) | C(25)–C(24)–C(23) | 121.0(2) |
| C(26)–C(25)–C(24) | 120.3(3) | C(25)–C(26)–C(27) | 120.0(3) |
| C(26)–C(27)–C(28) | 119.9(3) | C(27)–C(28)–C(23) | 120.8(3) |
| C(30)–C(29)–C(34) | 117.2(2) | C(30)–C(29)–P(3) | 122.0(2) |
| C(34)–C(29)–P(3) | 120.77(19) | C(29)–C(30)–C(31) | 120.8(3) |
| C(32)–C(31)–C(30) | 121.2(3) | C(31)–C(32)–C(33) | 118.9(3) |
| C(32)–C(33)–C(34) | 120.0(3) | C(29)–C(34)–C(33) | 121.8(3) |
| C(36)–C(35)–C(40) | 118.6(2) | C(36)–C(35)–P(3) | 118.75(19) |
| C(40)–C(35)–P(3) | 122.6(2) | C(35)–C(36)–C(37) | 120.5(2) |
| C(38)–C(37)–C(36) | 120.2(3) | C(37)–C(38)–C(39) | 119.9(3) |
| C(38)–C(39)–C(40) | 120.6(3) | C(39)–C(40)–C(35) | 120.2(3) |
| Cl(2)–C(41)–Cl(1) | 112.1(2) | | |

Table 4. Anisotropic displacement parameters ($Å^2$) for str0432. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Fe(1) | 0.01918(18) | 0.01477(16) | 0.01276(16) | 0.00378(12) | −0.00172(12) | −0.00167(12) |
| Fe(2) | 0.01958(18) | 0.01635(17) | 0.01244(16) | 0.00408(13) | −0.00026(12) | −0.00116(13) |
| P(1) | 0.0217(3) | 0.0163(3) | 0.0136(3) | 0.0043(2) | −0.0016(2) | −0.0021(2) |
| P(2) | 0.0202(3) | 0.0156(3) | 0.0150(3) | 0.0038(2) | −0.0012(2) | −0.0003(2) |
| P(3) | 0.0177(3) | 0.0197(3) | 0.0135(3) | 0.0036(2) | −0.0003(2) | 0.0007(2) |
| S(1) | 0.0189(3) | 0.0181(3) | 0.0150(3) | 0.0044(2) | −0.0001(2) | −0.0003(2) |
| S(2) | 0.0294(3) | 0.0159(3) | 0.0150(3) | 0.0027(2) | −0.0005(2) | −0.0020(2) |
| O(1) | 0.0238(10) | 0.0319(10) | 0.0325(10) | 0.0022(8) | −0.0053(8) | −0.0024(8) |
| O(2) | 0.0251(11) | 0.0463(12) | 0.0343(11) | 0.0128(9) | 0.0051(8) | −0.0040(9) |
| O(3) | 0.0633(15) | 0.0262(10) | 0.0316(11) | 0.0150(9) | −0.0034(10) | 0.0026(10) |
| C(1) | 0.0270(13) | 0.0163(11) | 0.0175(11) | 0.0039(9) | 0.0004(10) | 0.0003(9) |
| C(2) | 0.0290(14) | 0.0213(12) | 0.0152(11) | 0.0026(9) | 0.0000(10) | −0.0026(10) |
| C(3) | 0.0302(14) | 0.0206(12) | 0.0170(11) | 0.0028(10) | −0.0002(10) | −0.0008(10) |
| C(4) | 0.0216(13) | 0.0293(14) | 0.0269(13) | 0.0076(11) | 0.0068(10) | 0.0072(10) |
| C(5) | 0.0343(15) | 0.0268(14) | 0.0243(13) | 0.0072(11) | 0.0104(11) | 0.0114(11) |
| C(6) | 0.0429(16) | 0.0202(12) | 0.0179(12) | 0.0014(10) | 0.0103(11) | 0.0058(11) |
| C(7) | 0.0271(13) | 0.0185(12) | 0.0203(12) | 0.0074(10) | 0.0013(10) | −0.0001(10) |
| C(8) | 0.0250(13) | 0.0165(11) | 0.0190(11) | 0.0032(9) | 0.0016(9) | −0.0017(9) |
| C(9) | 0.0241(13) | 0.0173(12) | 0.0182(11) | 0.0009(9) | −0.0035(9) | −0.0001(9) |
| C(10) | 0.0212(12) | 0.0232(12) | 0.0157(11) | 0.0029(9) | −0.0005(9) | 0.0038(10) |
| C(11) | 0.0194(12) | 0.0215(12) | 0.0147(11) | 0.0039(9) | −0.0007(9) | −0.0010(9) |
| C(12) | 0.0329(14) | 0.0211(12) | 0.0181(12) | 0.0057(10) | −0.0020(10) | −0.0012(10) |
| C(13) | 0.0321(14) | 0.0205(13) | 0.0211(12) | 0.0011(10) | −0.0003(10) | −0.0042(10) |
| C(14) | 0.0216(12) | 0.0282(13) | 0.0147(11) | 0.0016(10) | −0.0015(9) | −0.0023(10) |
| C(15) | 0.0297(14) | 0.0268(13) | 0.0186(12) | 0.0086(10) | −0.0032(10) | 0.0034(11) |
| C(16) | 0.0275(13) | 0.0200(12) | 0.0195(12) | 0.0065(10) | 0.0001(10) | −0.0016(10) |
| C(17) | 0.0238(12) | 0.0172(11) | 0.0186(11) | 0.0080(9) | 0.0006(9) | 0.0007(9) |
| C(18) | 0.0260(13) | 0.0223(12) | 0.0171(11) | 0.0069(10) | 0.0001(10) | −0.0016(10) |
| C(19) | 0.0234(13) | 0.0227(13) | 0.0277(13) | 0.0081(11) | −0.0014(10) | −0.0005(10) |
| C(20) | 0.0253(13) | 0.0253(13) | 0.0322(14) | 0.0100(11) | 0.0076(11) | 0.0073(10) |
| C(21) | 0.0350(15) | 0.0243(13) | 0.0235(13) | 0.0043(10) | 0.0056(11) | 0.0075(11) |
| C(22) | 0.0300(14) | 0.0197(12) | 0.0193(12) | 0.0023(10) | −0.0012(10) | 0.0024(10) |
| C(23) | 0.0231(12) | 0.0214(12) | 0.0154(11) | 0.0015(9) | −0.0025(9) | 0.0028(10) |
| C(24) | 0.0252(13) | 0.0242(13) | 0.0211(12) | 0.0029(10) | −0.0036(10) | 0.0013(10) |
| C(25) | 0.0232(13) | 0.0358(15) | 0.0271(14) | −0.0004(12) | −0.0004(11) | −0.0018(11) |
| C(26) | 0.0283(15) | 0.0365(16) | 0.0306(15) | −0.0036(12) | −0.0052(11) | 0.0094(12) |
| C(27) | 0.0378(16) | 0.0302(15) | 0.0315(15) | 0.0048(12) | −0.0059(12) | 0.0123(12) |
| C(28) | 0.0302(14) | 0.0241(13) | 0.0229(13) | 0.0056(10) | 0.0000(10) | 0.0033(11) |
| C(29) | 0.0230(12) | 0.0218(12) | 0.0157(11) | 0.0039(9) | 0.0034(9) | 0.0028(10) |
| C(30) | 0.0240(17) | 0.162(5) | 0.045(2) | 0.068(3) | 0.0006(14) | 0.000(2) |
| C(31) | 0.038(2) | 0.202(6) | 0.055(2) | 0.089(3) | 0.0029(18) | 0.013(3) |
| C(32) | 0.0383(17) | 0.057(2) | 0.0284(15) | 0.0212(14) | 0.0129(13) | 0.0085(15) |
| C(33) | 0.0270(15) | 0.065(2) | 0.0263(14) | 0.0104(14) | 0.0076(12) | −0.0067(14) |
| C(34) | 0.0226(14) | 0.076(2) | 0.0210(14) | 0.0140(14) | −0.0016(11) | −0.0015(14) |
| C(35) | 0.0200(12) | 0.0253(13) | 0.0133(11) | 0.0052(9) | 0.0002(9) | −0.0017(9) |
| C(36) | 0.0250(13) | 0.0239(13) | 0.0252(13) | 0.0031(10) | −0.0037(10) | 0.0003(10) |
| C(37) | 0.0231(14) | 0.0373(16) | 0.0330(15) | 0.0058(12) | −0.0012(11) | 0.0074(11) |
| C(38) | 0.0222(14) | 0.0424(17) | 0.0337(15) | 0.0068(13) | −0.0052(11) | −0.0036(12) |
| C(39) | 0.0316(15) | 0.0313(15) | 0.0367(16) | −0.0005(13) | −0.0082(12) | −0.0069(12) |
| C(40) | 0.0272(14) | 0.0266(14) | 0.0279(14) | 0.0004(11) | −0.0026(11) | 0.0004(11) |
| C(41) | 0.045(2) | 0.107(4) | 0.041(2) | 0.009(2) | 0.0106(16) | 0.016(2) |
| Cl(1) | 0.0481(5) | 0.0584(5) | 0.0507(5) | 0.0115(4) | 0.0149(4) | 0.0103(4) |
| Cl(2) | 0.0570(6) | 0.0723(7) | 0.0973(9) | 0.0368(6) | −0.0205(6) | −0.0151(5) |

Table 5. Hydrogen coordinates and isotropic displacement parameters (Å²) for str0432.

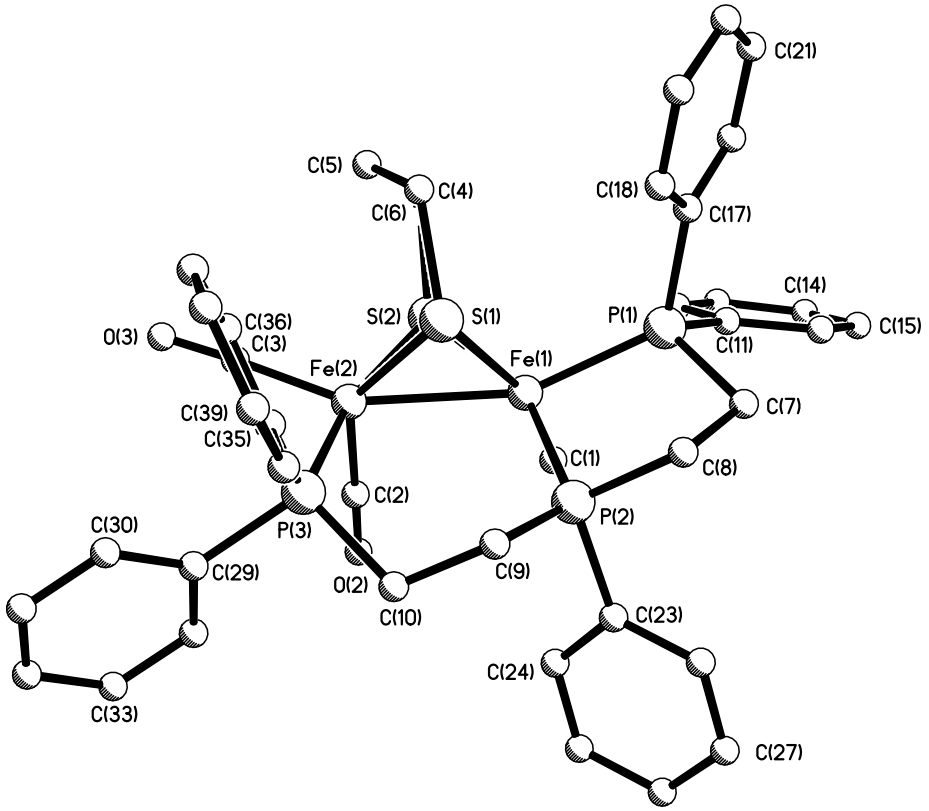
| | x | y | z | U |
|---|---|---|---|---|
| H(4A) | –0.3039 | 0.8493 | 0.2716 | 0.030 |
| H(4B) | –0.2349 | 0.8397 | 0.3383 | 0.030 |
| H(5A) | –0.1530 | 1.0561 | 0.2724 | 0.033 |
| H(5B) | –0.2505 | 1.0768 | 0.3273 | 0.033 |
| H(6A) | –0.0547 | 1.0280 | 0.3932 | 0.032 |
| H(6B) | –0.0263 | 1.1710 | 0.3673 | 0.032 |
| H(7A) | 0.2039 | 0.4717 | 0.3966 | 0.026 |
| H(7B) | 0.0419 | 0.4419 | 0.4105 | 0.026 |
| H(8A) | –0.0447 | 0.4323 | 0.3090 | 0.024 |
| H(8B) | 0.0868 | 0.3356 | 0.3074 | 0.024 |
| H(9A) | 0.0862 | 0.3813 | 0.1850 | 0.025 |
| H(9B) | –0.0369 | 0.4848 | 0.1960 | 0.025 |
| H(10A) | 0.0925 | 0.4994 | 0.1067 | 0.024 |
| H(10B) | 0.2225 | 0.5799 | 0.1535 | 0.024 |
| H(12A) | 0.2416 | 0.9476 | 0.4539 | 0.029 |
| H(13A) | 0.3937 | 1.0386 | 0.5415 | 0.030 |
| H(14A) | 0.4577 | 0.8925 | 0.6105 | 0.027 |
| H(15A) | 0.3584 | 0.6580 | 0.5942 | 0.030 |
| H(16A) | 0.2005 | 0.5675 | 0.5079 | 0.027 |
| H(18A) | –0.1998 | 0.5861 | 0.3496 | 0.026 |
| H(19A) | –0.4255 | 0.5819 | 0.3833 | 0.030 |
| H(20A) | –0.4538 | 0.6790 | 0.4837 | 0.032 |
| H(21A) | –0.2545 | 0.7820 | 0.5502 | 0.033 |
| H(22A) | –0.0284 | 0.7911 | 0.5165 | 0.028 |
| H(24A) | 0.4171 | 0.6520 | 0.2367 | 0.029 |
| H(25A) | 0.6380 | 0.5667 | 0.2228 | 0.036 |
| H(26A) | 0.6881 | 0.3507 | 0.2493 | 0.040 |
| H(27A) | 0.5154 | 0.2176 | 0.2895 | 0.040 |
| H(28A) | 0.2907 | 0.2992 | 0.3011 | 0.031 |
| H(30A) | –0.0957 | 0.7739 | 0.0294 | 0.086 |
| H(31A) | –0.0159 | 0.8419 | –0.0572 | 0.108 |
| H(32A) | 0.2239 | 0.8913 | –0.0636 | 0.047 |
| H(33A) | 0.3875 | 0.8670 | 0.0169 | 0.047 |
| H(34A) | 0.3086 | 0.8007 | 0.1039 | 0.048 |
| H(36A) | –0.2172 | 0.8682 | 0.1536 | 0.030 |
| H(37A) | –0.4590 | 0.8099 | 0.1198 | 0.037 |
| H(38A) | –0.5393 | 0.5822 | 0.0701 | 0.040 |
| H(39A) | –0.3784 | 0.4132 | 0.0522 | 0.042 |
| H(40A) | –0.1349 | 0.4717 | 0.0818 | 0.034 |
| H(41A) | 0.2905 | 0.1144 | 0.1244 | 0.077 |
| H(41B) | 0.3658 | 0.2624 | 0.1614 | 0.077 |

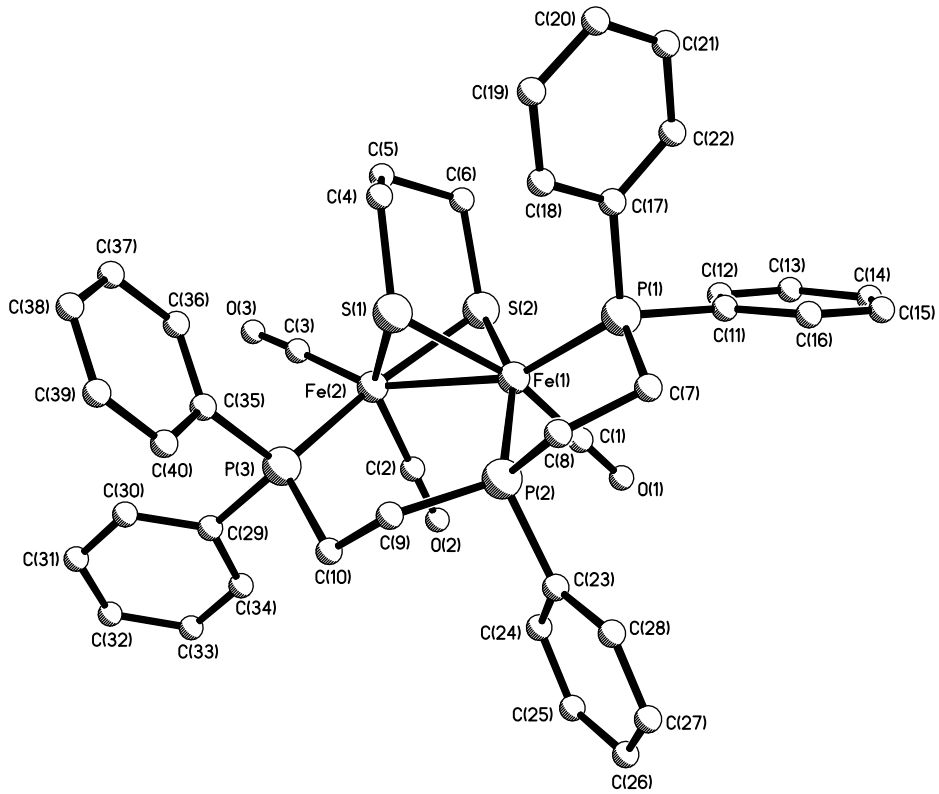
Table 6. Torsion angles [°] for str0432.

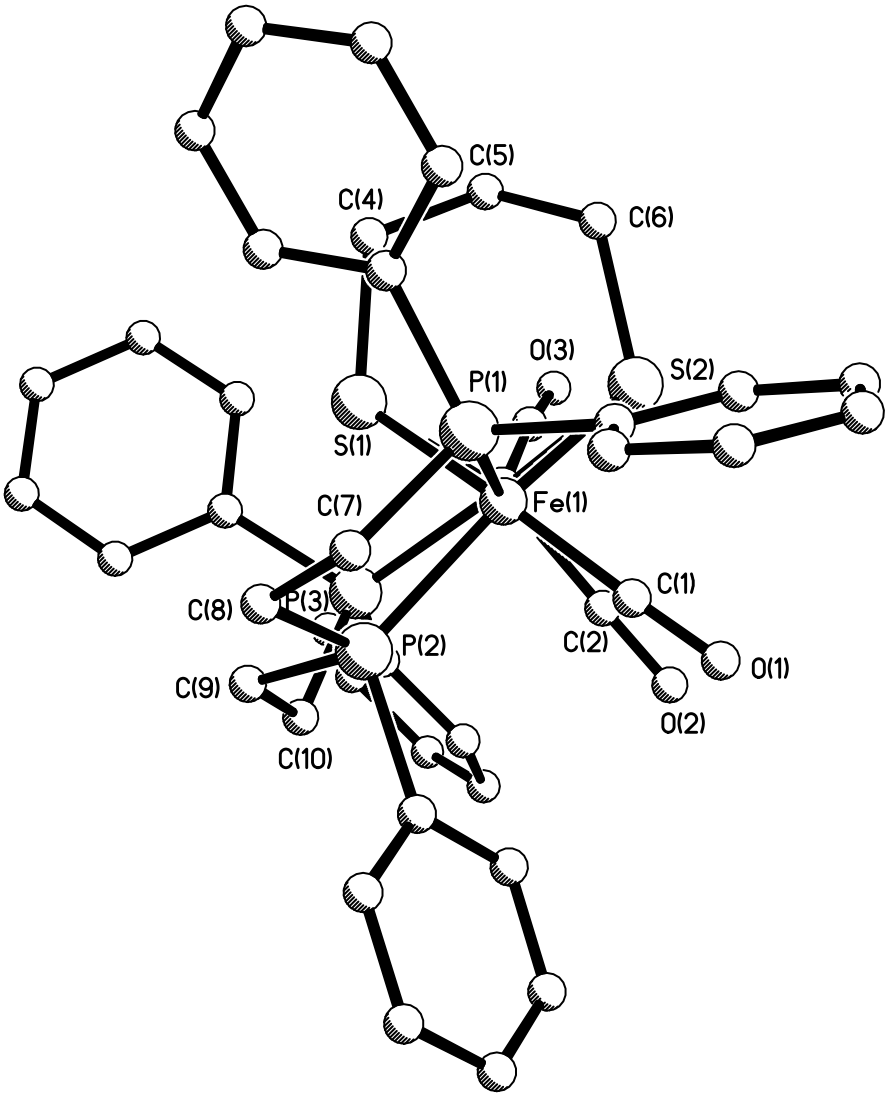
| | | | |
|---|---|---|---|
| C(1)–Fe(1)–Fe(2)–C(3) | −100.5(2) | P(2)–Fe(1)–Fe(2)–C(3) | 162.5(2) |
| P(1)–Fe(1)–Fe(2)–C(3) | 49.4(2) | S(1)–Fe(1)–Fe(2)–C(3) | 82.7(2) |
| S(2)–Fe(1)–Fe(2)–C(3) | −24.2(2) | C(1)–Fe(1)–Fe(2)–C(2) | 13.37(11) |
| P(2)–Fe(1)–Fe(2)–C(2) | −83.61(8) | P(1)–Fe(1)–Fe(2)–C(2) | 163.26(10) |
| S(1)–Fe(1)–Fe(2)–C(2) | −163.39(8) | S(2)–Fe(1)–Fe(2)–C(2) | 89.66(8) |
| C(1)–Fe(1)–Fe(2)–P(3) | 107.52(8) | P(2)–Fe(1)–Fe(2)–P(3) | 10.55(3) |
| P(1)–Fe(1)–Fe(2)–P(3) | −102.58(6) | S(1)–Fe(1)–Fe(2)–P(3) | −69.23(3) |
| S(2)–Fe(1)–Fe(2)–P(3) | −176.18(3) | C(1)–Fe(1)–Fe(2)–S(1) | 176.76(8) |
| P(2)–Fe(1)–Fe(2)–S(1) | 79.78(3) | P(1)–Fe(1)–Fe(2)–S(1) | −33.35(6) |
| S(2)–Fe(1)–Fe(2)–S(1) | −106.94(3) | C(1)–Fe(1)–Fe(2)–S(2) | −76.30(8) |
| P(2)–Fe(1)–Fe(2)–S(2) | −173.27(3) | P(1)–Fe(1)–Fe(2)–S(2) | 73.59(6) |
| S(1)–Fe(1)–Fe(2)–S(2) | 106.94(3) | C(1)–Fe(1)–P(1)–C(11) | 27.65(12) |
| P(2)–Fe(1)–P(1)–C(11) | 120.79(9) | S(1)–Fe(1)–P(1)–C(11) | −151.50(9) |
| S(2)–Fe(1)–P(1)–C(11) | −62.12(10) | Fe(2)–Fe(1)–P(1)–C(11) | −123.50(10) |
| C(1)–Fe(1)–P(1)–C(17) | 155.49(12) | P(2)–Fe(1)–P(1)–C(17) | −111.37(10) |
| S(1)–Fe(1)–P(1)–C(17) | −23.66(10) | S(2)–Fe(1)–P(1)–C(17) | 65.71(10) |
| Fe(2)–Fe(1)–P(1)–C(17) | 4.34(12) | C(1)–Fe(1)–P(1)–C(7) | −88.82(12) |
| P(2)–Fe(1)–P(1)–C(7) | 4.32(9) | S(1)–Fe(1)–P(1)–C(7) | 92.03(9) |
| S(2)–Fe(1)–P(1)–C(7) | −178.59(9) | Fe(2)–Fe(1)–P(1)–C(7) | 120.03(10) |
| C(1)–Fe(1)–P(2)–C(23) | −4.19(12) | P(1)–Fe(1)–P(2)–C(23) | −98.57(9) |
| S(1)–Fe(1)–P(2)–C(23) | 158.39(9) | S(2)–Fe(1)–P(2)–C(23) | 88.44(11) |
| Fe(2)–Fe(1)–P(2)–C(23) | 103.36(9) | C(1)–Fe(1)–P(2)–C(8) | 113.37(12) |
| P(1)–Fe(1)–P(2)–C(8) | 18.99(9) | S(1)–Fe(1)–P(2)–C(8) | −84.05(9) |
| S(2)–Fe(1)–P(2)–C(8) | −154.00(10) | Fe(2)–Fe(1)–P(2)–C(8) | −139.08(8) |
| C(1)–Fe(1)–P(2)–C(9) | −130.92(12) | P(1)–Fe(1)–P(2)–C(9) | 134.70(10) |
| S(1)–Fe(1)–P(2)–C(9) | 31.66(10) | S(2)–Fe(1)–P(2)–C(9) | −38.29(13) |
| Fe(2)–Fe(1)–P(2)–C(9) | −23.37(10) | C(3)–Fe(2)–P(3)–C(29) | 45.92(12) |
| C(2)–Fe(2)–P(3)–C(29) | −56.39(12) | S(1)–Fe(2)–P(3)–C(29) | 163.13(9) |
| S(2)–Fe(2)–P(3)–C(29) | −158.12(12) | Fe(1)–Fe(2)–P(3)–C(29) | −145.89(9) |
| C(3)–Fe(2)–P(3)–C(35) | −72.79(12) | C(2)–Fe(2)–P(3)–C(35) | −175.11(12) |
| S(1)–Fe(2)–P(3)–C(35) | 44.42(9) | S(2)–Fe(2)–P(3)–C(35) | 83.16(14) |
| Fe(1)–Fe(2)–P(3)–C(35) | 95.39(9) | C(3)–Fe(2)–P(3)–C(10) | 165.94(12) |
| C(2)–Fe(2)–P(3)–C(10) | 63.63(12) | S(1)–Fe(2)–P(3)–C(10) | −76.85(9) |
| S(2)–Fe(2)–P(3)–C(10) | −38.10(15) | Fe(1)–Fe(2)–P(3)–C(10) | −25.87(9) |
| C(1)–Fe(1)–S(1)–C(4) | −112.1(3) | P(2)–Fe(1)–S(1)–C(4) | 152.99(10) |
| P(1)–Fe(1)–S(1)–C(4) | 65.10(10) | S(2)–Fe(1)–S(1)–C(4) | −48.08(10) |
| Fe(2)–Fe(1)–S(1)–C(4) | −101.66(10) | C(1)–Fe(1)–S(1)–Fe(2) | −10.4(3) |
| P(2)–Fe(1)–S(1)–Fe(2) | −105.34(2) | P(1)–Fe(1)–S(1)–Fe(2) | 166.76(2) |
| S(2)–Fe(1)–S(1)–Fe(2) | 53.58(2) | C(3)–Fe(2)–S(1)–C(4) | −37.76(13) |
| C(2)–Fe(2)–S(1)–C(4) | 139.96(15) | P(3)–Fe(2)–S(1)–C(4) | −129.03(9) |
| S(2)–Fe(2)–S(1)–C(4) | 60.41(9) | Fe(1)–Fe(2)–S(1)–C(4) | 113.20(9) |
| C(3)–Fe(2)–S(1)–Fe(1) | −150.96(9) | C(2)–Fe(2)–S(1)–Fe(1) | 26.76(13) |
| P(3)–Fe(2)–S(1)–Fe(1) | 117.77(2) | S(2)–Fe(2)–S(1)–Fe(1) | −52.79(2) |
| C(1)–Fe(1)–S(2)–C(6) | −145.08(12) | P(2)–Fe(1)–S(2)–C(6) | 121.25(11) |
| P(1)–Fe(1)–S(2)–C(6) | −51.09(10) | S(1)–Fe(1)–S(2)–C(6) | 50.57(9) |
| Fe(2)–Fe(1)–S(2)–C(6) | 103.72(9) | C(1)–Fe(1)–S(2)–Fe(2) | 111.20(8) |
| P(2)–Fe(1)–S(2)–Fe(2) | 17.53(8) | P(1)–Fe(1)–S(2)–Fe(2) | −154.80(3) |
| S(1)–Fe(1)–S(2)–Fe(2) | −53.14(2) | C(3)–Fe(2)–S(2)–C(6) | 62.04(13) |
| C(2)–Fe(2)–S(2)–C(6) | 163.94(12) | P(3)–Fe(2)–S(2)–C(6) | −93.55(14) |
| S(1)–Fe(2)–S(2)–C(6) | −54.67(9) | Fe(1)–Fe(2)–S(2)–C(6) | −107.52(9) |

| | | | |
|---|---|---|---|
| C(3)–Fe(2)–S(2)–Fe(1) | 169.56(9) | C(2)–Fe(2)–S(2)–Fe(1) | −88.54(8) |
| P(3)–Fe(2)–S(2)–Fe(1) | 13.97(11) | S(1)–Fe(2)–S(2)–Fe(1) | 52.85(2) |
| P(2)–Fe(1)–C(1)–O(1) | 151(6) | P(1)–Fe(1)–C(1)–O(1) | −120(6) |
| S(1)–Fe(1)–C(1)–O(1) | 57(6) | S(2)–Fe(1)–C(1)–O(1) | −7(6) |
| Fe(2)–Fe(1)–C(1)–O(1) | 48(6) | C(3)–Fe(2)–C(2)–O(2) | 29(10) |
| P(3)–Fe(2)–C(2)–O(2) | 123(10) | S(1)–Fe(2)–C(2)–O(2) | −149(10) |
| S(2)–Fe(2)–C(2)–O(2) | −71(10) | Fe(1)–Fe(2)–C(2)–O(2) | −127(10) |
| C(2)–Fe(2)–C(3)–O(3) | −13(3) | P(3)–Fe(2)–C(3)–O(3) | −108(3) |
| S(1)–Fe(2)–C(3)–O(3) | 166(3) | S(2)–Fe(2)–C(3)–O(3) | 78(3) |
| Fe(1)–Fe(2)–C(3)–O(3) | 98(3) | Fe(1)–S(1)–C(4)–C(5) | 59.7(2) |
| Fe(2)–S(1)–C(4)–C(5) | −15.2(2) | S(1)–C(4)–C(5)–C(6) | −61.2(3) |
| C(4)–C(5)–C(6)–S(2) | 68.2(3) | Fe(1)–S(2)–C(6)–C(5) | −70.5(2) |
| Fe(2)–S(2)–C(6)–C(5) | 2.9(2) | C(11)–P(1)–C(7)–C(8) | −157.57(17) |
| C(17)–P(1)–C(7)–C(8) | 97.14(18) | Fe(1)–P(1)–C(7)–C(8) | −32.39(18) |
| P(1)–C(7)–C(8)–P(2) | 48.2(2) | C(23)–P(2)–C(8)–C(7) | 83.58(18) |
| C(9)–P(2)–C(8)–C(7) | −172.14(17) | Fe(1)–P(2)–C(8)–C(7) | −43.88(18) |
| C(23)–P(2)–C(9)–C(10) | −75.29(19) | C(8)–P(2)–C(9)–C(10) | 177.70(18) |
| Fe(1)–P(2)–C(9)–C(10) | 59.6(2) | P(2)–C(9)–C(10)–P(3) | −77.6(2) |
| C(29)–P(3)–C(10)–C(9) | −171.62(17) | C(35)–P(3)–C(10)–C(9) | −66.98(19) |
| Fe(2)–P(3)–C(10)–C(9) | 60.42(19) | C(17)–P(1)–C(11)–C(12) | −101.5(2) |
| C(7)–P(1)–C(11)–C(12) | 154.1(2) | Fe(1)–P(1)–C(11)–C(12) | 35.8(2) |
| C(17)–P(1)–C(11)–C(16) | 77.8(2) | C(7)–P(1)–C(11)–C(16) | −26.6(2) |
| Fe(1)–P(1)–C(11)–C(16) | −144.97(19) | C(16)–C(11)–C(12)–C(13) | 0.8(4) |
| P(1)–C(11)–C(12)–C(13) | −179.9(2) | C(11)–C(12)–C(13)–C(14) | 1.0(4) |
| C(12)–C(13)–C(14)–C(15) | −1.9(4) | C(13)–C(14)–C(15)–C(16) | 0.9(4) |
| C(14)–C(15)–C(16)–C(11) | 0.9(4) | C(12)–C(11)–C(16)–C(15) | −1.8(4) |
| P(1)–C(11)–C(16)–C(15) | 179.0(2) | C(11)–P(1)–C(17)–C(22) | 8.2(2) |
| C(7)–P(1)–C(17)–C(22) | 115.0(2) | Fe(1)–P(1)–C(17)–C(22) | −126.13(18) |
| C(11)–P(1)–C(17)–C(18) | −170.94(19) | C(7)–P(1)–C(17)–C(18) | −64.1(2) |
| Fe(1)–P(1)–C(17)–C(18) | 54.7(2) | C(22)–C(17)–C(18)–C(19) | −0.7(4) |
| P(1)–C(17)–C(18)–C(19) | 178.49(18) | C(17)–C(18)–C(19)–C(20) | −0.2(4) |
| C(18)–C(19)–C(20)–C(21) | 0.4(4) | C(19)–C(20)–C(21)–C(22) | 0.3(4) |
| C(20)–C(21)–C(22)–C(17) | −1.2(4) | C(18)–C(17)–C(22)–C(21) | 1.4(4) |
| P(1)–C(17)–C(22)–C(21) | −177.76(19) | C(8)–P(2)–C(23)–C(28) | 12.4(2) |
| C(9)–P(2)–C(23)–C(28) | −92.8(2) | Fe(1)–P(2)–C(23)–C(28) | 131.25(19) |
| C(8)–P(2)–C(23)–C(24) | −170.14(19) | C(9)–P(2)–C(23)–C(24) | 84.6(2) |
| Fe(1)–P(2)–C(23)–C(24) | −51.3(2) | C(28)–C(23)–C(24)–C(25) | 1.5(4) |
| P(2)–C(23)–C(24)–C(25) | −176.07(19) | C(23)–C(24)–C(25)–C(26) | −1.3(4) |
| C(24)–C(25)–C(26)–C(27) | 0.2(4) | C(25)–C(26)–C(27)–C(28) | 0.8(4) |
| C(26)–C(27)–C(28)–C(23) | −0.6(4) | C(24)–C(23)–C(28)–C(27) | −0.5(4) |
| P(2)–C(23)–C(28)–C(27) | 176.9(2) | C(35)–P(3)–C(29)–C(30) | 11.3(3) |
| C(10)–P(3)–C(29)–C(30) | 117.9(3) | Fe(2)–P(3)–C(29)–C(30) | −114.9(3) |
| C(35)–P(3)–C(29)–C(34) | −171.2(2) | C(10)–P(3)–C(29)–C(34) | −64.6(3) |
| Fe(2)–P(3)–C(29)–C(34) | 62.6(3) | C(34)–C(29)–C(30)–C(31) | 0.5(7) |
| P(3)–C(29)–C(30)–C(31) | 178.1(4) | C(29)–C(30)–C(31)–C(32) | −0.5(9) |
| C(30)–C(31)–C(32)–C(33) | 0.7(8) | C(31)–C(32)–C(33)–C(34) | −0.9(6) |
| C(30)–C(29)–C(34)–C(33) | −0.8(5) | P(3)–C(29)–C(34)–C(33) | −178.4(3) |
| C(32)–C(33)–C(34)–C(29) | 1.0(5) | C(29)–P(3)–C(35)–C(36) | −93.9(2) |
| C(10)–P(3)–C(35)–C(36) | 160.90(19) | Fe(2)–P(3)–C(35)–C(36) | 33.3(2) |
| C(29)–P(3)–C(35)–C(40) | 84.1(2) | C(10)–P(3)–C(35)–C(40) | −21.1(2) |
| Fe(2)–P(3)–C(35)–C(40) | −148.74(19) | C(40)–C(35)–C(36)–C(37) | −0.6(4) |
| P(3)–C(35)–C(36)–C(37) | 177.5(2) | C(35)–C(36)–C(37)–C(38) | 1.4(4) |

| | | | |
|---|---|---|---|
| C(36)–C(37)–C(38)–C(39) | –0.7(4) | C(37)–C(38)–C(39)–C(40) | –0.8(5) |
| C(38)–C(39)–C(40)–C(35) | 1.6(4) | C(36)–C(35)–C(40)–C(39) | –0.9(4) |
| P(3)–C(35)–C(40)–C(39) | –178.9(2) | | |




C(5)
C(4)
C(6)
O(3)
S(2)
P(1)
S(1)
C(7)
Fe(1)
C(1)
C(8)
P(3)
C(2)
P(2)
O(1)
C(9)
O(2)
C(10)

(vii) Table 1. Crystal data and structure refinement for str0735 (**3**).

| | | |
|---|---|---|
| Identification code | str0735 | |
| Chemical formula | $C_{46}H_{44.50}Fe_2NO_{3.25}P_3S_2$ | |
| Formula weight | 932.06 | |
| Temperature | 150(2) K | |
| Radiation, wavelength | MoKα, 0.71073 Å | |
| Crystal system, space group | monoclinic, C2/c | |
| Unit cell parameters | a = 47.771(9) Å | α = 90° |
| | b = 11.747(2) Å | β = 97.984(4)° |
| | c = 15.183(3) Å | γ = 90° |
| Cell volume | 8438(3) Å$^3$ | |
| Z | 8 | |
| Calculated density | 1.467 g/cm$^3$ | |
| Absorption coefficient μ | 0.944 mm$^{-1}$ | |
| F(000) | 3860 | |
| Crystal colour and size | red, 0.14 × 0.13 × 0.09 mm$^3$ | |
| Data collection method | Bruker SMART APEX diffractometer | |
| | ω rotation with narrow frames | |
| θ range for data collection | 2.45 to 28.34° | |
| Index ranges | h −61 to 63, k −15 to 15, l −20 to 20 | |
| Completeness to θ = 26.00° | 99.4 % | |
| Reflections collected | 35672 | |
| Independent reflections | 10136 ($R_{int}$ = 0.0550) | |
| Reflections with $F^2>2\sigma$ | 7618 | |
| Absorption correction | semi-empirical from equivalents | |
| Min. and max. transmission | 0.8792 and 0.9199 | |
| Structure solution | direct methods | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Weighting parameters a, b | 0.0609, 2.3320 | |
| Data / restraints / parameters | 10136 / 0 / 518 | |
| Final R indices [$F^2>2\sigma$] | R1 = 0.0500, wR2 = 0.1107 | |
| R indices (all data) | R1 = 0.0736, wR2 = 0.1203 | |
| Goodness-of-fit on $F^2$ | 1.049 | |
| Largest and mean shift/su | 0.001 and 0.000 | |
| Largest diff. peak and hole | 0.707 and −0.497 e Å$^{-3}$ | |

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for str0735. $U_{eq}$ is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| Fe(1) | 0.092868(8) | 0.18890(3) | 0.49035(2) | 0.01557(10) |
| Fe(2) | 0.139123(8) | 0.28551(3) | 0.46162(3) | 0.01703(10) |
| P(1) | 0.056025(15) | 0.23383(6) | 0.38739(5) | 0.01758(15) |
| P(2) | 0.094368(15) | 0.02960(6) | 0.41550(5) | 0.01703(15) |
| P(3) | 0.165583(15) | 0.16558(6) | 0.39719(5) | 0.01996(16) |
| S(1) | 0.104820(14) | 0.36803(6) | 0.52766(4) | 0.01828(15) |
| S(2) | 0.135642(14) | 0.14610(6) | 0.56169(4) | 0.01764(15) |
| N(1) | 0.14372(5) | 0.3269(2) | 0.67774(15) | 0.0230(5) |
| O(1) | 0.05954(5) | 0.1263(2) | 0.62946(14) | 0.0362(5) |
| O(2) | 0.11626(5) | 0.37997(19) | 0.28922(14) | 0.0332(5) |
| O(3) | 0.18251(5) | 0.45444(19) | 0.51976(16) | 0.0387(6) |
| C(1) | 0.07194(6) | 0.1497(2) | 0.57127(19) | 0.0222(6) |
| C(2) | 0.12483(6) | 0.3423(2) | 0.35745(19) | 0.0220(6) |
| C(3) | 0.16625(6) | 0.3848(3) | 0.49867(19) | 0.0243(6) |
| C(4) | 0.05143(6) | 0.1217(2) | 0.30127(18) | 0.0221(6) |
| C(5) | 0.06068(6) | 0.0065(2) | 0.34296(19) | 0.0227(6) |
| C(6) | 0.11957(6) | 0.0222(2) | 0.33465(18) | 0.0222(6) |
| C(7) | 0.15066(6) | 0.0219(2) | 0.37784(19) | 0.0222(6) |
| C(8) | 0.11705(7) | 0.3812(3) | 0.64706(18) | 0.0262(7) |
| C(9) | 0.14102(6) | 0.2045(2) | 0.67418(18) | 0.0221(6) |
| C(10) | 0.15443(6) | 0.3673(3) | 0.76788(19) | 0.0269(7) |
| C(11) | 0.18349(6) | 0.3212(3) | 0.8008(2) | 0.0268(7) |
| C(12) | 0.18846(7) | 0.2665(3) | 0.8821(2) | 0.0360(8) |
| C(13) | 0.21497(9) | 0.2255(4) | 0.9137(2) | 0.0499(10) |
| C(14) | 0.23697(8) | 0.2400(4) | 0.8652(3) | 0.0521(11) |
| C(15) | 0.23245(8) | 0.2932(3) | 0.7841(3) | 0.0457(9) |
| C(16) | 0.20568(7) | 0.3328(3) | 0.7515(2) | 0.0365(8) |
| C(17) | 0.02234(6) | 0.2303(2) | 0.43347(18) | 0.0204(6) |
| C(18) | 0.01701(6) | 0.3164(3) | 0.4921(2) | 0.0275(7) |
| C(19) | –0.00734(7) | 0.3153(3) | 0.5317(2) | 0.0324(7) |
| C(20) | –0.02690(7) | 0.2284(3) | 0.5129(2) | 0.0325(7) |
| C(21) | –0.02162(7) | 0.1414(3) | 0.4569(2) | 0.0326(7) |
| C(22) | 0.00289(6) | 0.1420(3) | 0.4167(2) | 0.0264(7) |
| C(23) | 0.05115(6) | 0.3649(2) | 0.32049(18) | 0.0206(6) |
| C(24) | 0.05652(6) | 0.4709(2) | 0.35941(19) | 0.0258(6) |
| C(25) | 0.05268(6) | 0.5699(3) | 0.3103(2) | 0.0287(7) |
| C(26) | 0.04329(7) | 0.5662(3) | 0.2208(2) | 0.0357(8) |
| C(27) | 0.03789(9) | 0.4615(3) | 0.1805(2) | 0.0511(11) |
| C(28) | 0.04169(8) | 0.3620(3) | 0.2296(2) | 0.0405(9) |
| C(29) | 0.09996(6) | –0.1073(2) | 0.47225(18) | 0.0192(6) |
| C(30) | 0.09848(6) | –0.1150(2) | 0.56323(19) | 0.0245(6) |
| C(31) | 0.10041(8) | –0.2196(3) | 0.6055(2) | 0.0354(8) |
| C(32) | 0.10444(8) | –0.3172(3) | 0.5585(2) | 0.0389(8) |
| C(33) | 0.10672(7) | –0.3111(2) | 0.4697(2) | 0.0307(7) |
| C(34) | 0.10409(6) | –0.2071(2) | 0.4260(2) | 0.0268(7) |
| C(35) | 0.20089(6) | 0.1296(2) | 0.4542(2) | 0.0248(6) |
| C(36) | 0.20770(7) | 0.1417(4) | 0.5451(2) | 0.0444(9) |
| C(37) | 0.23354(8) | 0.1043(4) | 0.5885(3) | 0.0549(11) |
| C(38) | 0.25308(7) | 0.0584(3) | 0.5413(3) | 0.0460(9) |

| | | | | |
|---|---|---|---|---|
| C(39) | 0.24717(7) | 0.0507(4) | 0.4500(3) | 0.0482(10) |
| C(40) | 0.22114(7) | 0.0836(3) | 0.4077(2) | 0.0417(9) |
| C(41) | 0.17341(6) | 0.2084(2) | 0.28781(19) | 0.0227(6) |
| C(42) | 0.16830(7) | 0.1419(3) | 0.2117(2) | 0.0352(8) |
| C(43) | 0.17407(8) | 0.1832(3) | 0.1304(2) | 0.0417(9) |
| C(44) | 0.18527(7) | 0.2899(3) | 0.1244(2) | 0.0370(8) |
| C(45) | 0.19067(8) | 0.3559(3) | 0.1988(2) | 0.0388(8) |
| C(46) | 0.18475(7) | 0.3165(3) | 0.2799(2) | 0.0327(7) |
| O(4) | –0.0025(12) | –0.126(2) | 0.270(3) | 0.224(14) |

Table 3. Bond lengths [Å] and angles [°] for str0735.

| | | | |
|---|---|---|---|
| Fe(1)–C(1) | 1.750(3) | Fe(1)–P(2) | 2.1957(8) |
| Fe(1)–S(1) | 2.2328(8) | Fe(1)–S(2) | 2.2331(8) |
| Fe(1)–P(1) | 2.2485(9) | Fe(1)–Fe(2) | 2.5746(7) |
| Fe(2)–C(2) | 1.764(3) | Fe(2)–C(3) | 1.775(3) |
| Fe(2)–P(3) | 2.2098(8) | Fe(2)–S(1) | 2.2554(8) |
| Fe(2)–S(2) | 2.2558(8) | P(1)–C(23) | 1.841(3) |
| P(1)–C(17) | 1.842(3) | P(1)–C(4) | 1.847(3) |
| P(2)–C(29) | 1.827(3) | P(2)–C(6) | 1.837(3) |
| P(2)–C(5) | 1.839(3) | P(3)–C(41) | 1.823(3) |
| P(3)–C(35) | 1.835(3) | P(3)–C(7) | 1.840(3) |
| S(1)–C(8) | 1.832(3) | S(2)–C(9) | 1.825(3) |
| N(1)–C(8) | 1.443(4) | N(1)–C(9) | 1.445(4) |
| N(1)–C(10) | 1.471(4) | O(1)–C(1) | 1.163(3) |
| O(2)–C(2) | 1.148(3) | O(3)–C(3) | 1.143(3) |
| C(4)–C(5) | 1.533(4) | C(6)–C(7) | 1.538(4) |
| C(10)–C(11) | 1.509(4) | C(11)–C(12) | 1.383(4) |
| C(11)–C(16) | 1.387(4) | C(12)–C(13) | 1.377(5) |
| C(13)–C(14) | 1.375(6) | C(14)–C(15) | 1.372(6) |
| C(15)–C(16) | 1.386(5) | C(17)–C(22) | 1.393(4) |
| C(17)–C(18) | 1.394(4) | C(18)–C(19) | 1.382(4) |
| C(19)–C(20) | 1.387(4) | C(20)–C(21) | 1.376(5) |
| C(21)–C(22) | 1.393(4) | C(23)–C(24) | 1.387(4) |
| C(23)–C(28) | 1.392(4) | C(24)–C(25) | 1.379(4) |
| C(25)–C(26) | 1.371(4) | C(26)–C(27) | 1.382(5) |
| C(27)–C(28) | 1.384(4) | C(29)–C(34) | 1.394(4) |
| C(29)–C(30) | 1.396(4) | C(30)–C(31) | 1.383(4) |
| C(31)–C(32) | 1.379(5) | C(32)–C(33) | 1.369(5) |
| C(33)–C(34) | 1.388(4) | C(35)–C(36) | 1.380(4) |
| C(35)–C(40) | 1.384(4) | C(36)–C(37) | 1.388(5) |
| C(37)–C(38) | 1.365(5) | C(38)–C(39) | 1.379(5) |
| C(39)–C(40) | 1.374(5) | C(41)–C(42) | 1.388(4) |
| C(41)–C(46) | 1.392(4) | C(42)–C(43) | 1.389(4) |
| C(43)–C(44) | 1.371(5) | C(44)–C(45) | 1.365(5) |
| C(45)–C(46) | 1.381(4) | O(4)–O(4A) | 0.67(9) |

| | | | |
|---|---|---|---|
| C(1)–Fe(1)–P(2) | 101.67(10) | C(1)–Fe(1)–S(1) | 102.74(10) |
| P(2)–Fe(1)–S(1) | 155.37(3) | C(1)–Fe(1)–S(2) | 100.00(10) |
| P(2)–Fe(1)–S(2) | 88.03(3) | S(1)–Fe(1)–S(2) | 84.53(3) |
| C(1)–Fe(1)–P(1) | 94.68(10) | P(2)–Fe(1)–P(1) | 85.35(3) |
| S(1)–Fe(1)–P(1) | 95.91(3) | S(2)–Fe(1)–P(1) | 164.85(3) |
| C(1)–Fe(1)–Fe(2) | 145.32(10) | P(2)–Fe(1)–Fe(2) | 101.39(3) |
| S(1)–Fe(1)–Fe(2) | 55.41(2) | S(2)–Fe(1)–Fe(2) | 55.42(2) |
| P(1)–Fe(1)–Fe(2) | 112.71(3) | C(2)–Fe(2)–C(3) | 102.13(13) |
| C(2)–Fe(2)–P(3) | 91.04(9) | C(3)–Fe(2)–P(3) | 96.99(10) |
| C(2)–Fe(2)–S(1) | 91.22(9) | C(3)–Fe(2)–S(1) | 96.91(9) |
| P(3)–Fe(2)–S(1) | 165.11(3) | C(2)–Fe(2)–S(2) | 145.37(9) |
| C(3)–Fe(2)–S(2) | 112.47(10) | P(3)–Fe(2)–S(2) | 86.30(3) |
| S(1)–Fe(2)–S(2) | 83.49(3) | C(2)–Fe(2)–Fe(1) | 94.83(9) |
| C(3)–Fe(2)–Fe(1) | 147.31(9) | P(3)–Fe(2)–Fe(1) | 110.56(3) |
| S(1)–Fe(2)–Fe(1) | 54.58(2) | S(2)–Fe(2)–Fe(1) | 54.59(2) |
| C(23)–P(1)–C(17) | 100.25(12) | C(23)–P(1)–C(4) | 102.25(13) |
| C(17)–P(1)–C(4) | 103.21(13) | C(23)–P(1)–Fe(1) | 127.35(9) |
| C(17)–P(1)–Fe(1) | 111.80(9) | C(4)–P(1)–Fe(1) | 109.23(9) |

| | | | |
|---|---|---|---|
| C(29)–P(2)–C(6) | 101.95(13) | C(29)–P(2)–C(5) | 102.19(13) |
| C(6)–P(2)–C(5) | 101.13(13) | C(29)–P(2)–Fe(1) | 121.30(9) |
| C(6)–P(2)–Fe(1) | 117.24(9) | C(5)–P(2)–Fe(1) | 110.29(9) |
| C(41)–P(3)–C(35) | 101.64(13) | C(41)–P(3)–C(7) | 103.40(13) |
| C(35)–P(3)–C(7) | 100.06(13) | C(41)–P(3)–Fe(2) | 115.45(10) |
| C(35)–P(3)–Fe(2) | 118.87(10) | C(7)–P(3)–Fe(2) | 115.01(9) |
| C(8)–S(1)–Fe(1) | 111.46(10) | C(8)–S(1)–Fe(2) | 108.95(10) |
| Fe(1)–S(1)–Fe(2) | 70.01(2) | C(9)–S(2)–Fe(1) | 111.69(10) |
| C(9)–S(2)–Fe(2) | 110.09(9) | Fe(1)–S(2)–Fe(2) | 69.99(2) |
| C(8)–N(1)–C(9) | 111.0(2) | C(8)–N(1)–C(10) | 109.6(2) |
| C(9)–N(1)–C(10) | 111.9(2) | O(1)–C(1)–Fe(1) | 175.3(3) |
| O(2)–C(2)–Fe(2) | 178.1(3) | O(3)–C(3)–Fe(2) | 175.2(3) |
| C(5)–C(4)–P(1) | 109.76(18) | C(4)–C(5)–P(2) | 107.17(19) |
| C(7)–C(6)–P(2) | 113.51(19) | C(6)–C(7)–P(3) | 113.30(19) |
| N(1)–C(8)–S(1) | 115.32(19) | N(1)–C(9)–S(2) | 114.16(19) |
| N(1)–C(10)–C(11) | 112.2(2) | C(12)–C(11)–C(16) | 118.6(3) |
| C(12)–C(11)–C(10) | 119.9(3) | C(16)–C(11)–C(10) | 121.5(3) |
| C(13)–C(12)–C(11) | 120.6(3) | C(14)–C(13)–C(12) | 120.3(4) |
| C(15)–C(14)–C(13) | 120.0(4) | C(14)–C(15)–C(16) | 119.7(4) |
| C(15)–C(16)–C(11) | 120.8(3) | C(22)–C(17)–C(18) | 118.7(3) |
| C(22)–C(17)–P(1) | 122.9(2) | C(18)–C(17)–P(1) | 118.2(2) |
| C(19)–C(18)–C(17) | 120.8(3) | C(18)–C(19)–C(20) | 120.0(3) |
| C(21)–C(20)–C(19) | 119.9(3) | C(20)–C(21)–C(22) | 120.3(3) |
| C(17)–C(22)–C(21) | 120.2(3) | C(24)–C(23)–C(28) | 117.4(3) |
| C(24)–C(23)–P(1) | 120.9(2) | C(28)–C(23)–P(1) | 121.7(2) |
| C(25)–C(24)–C(23) | 121.6(3) | C(26)–C(25)–C(24) | 120.6(3) |
| C(25)–C(26)–C(27) | 118.8(3) | C(26)–C(27)–C(28) | 120.7(3) |
| C(27)–C(28)–C(23) | 120.8(3) | C(34)–C(29)–C(30) | 118.3(3) |
| C(34)–C(29)–P(2) | 121.6(2) | C(30)–C(29)–P(2) | 120.0(2) |
| C(31)–C(30)–C(29) | 120.5(3) | C(32)–C(31)–C(30) | 120.2(3) |
| C(33)–C(32)–C(31) | 120.2(3) | C(32)–C(33)–C(34) | 120.2(3) |
| C(33)–C(34)–C(29) | 120.6(3) | C(36)–C(35)–C(40) | 117.7(3) |
| C(36)–C(35)–P(3) | 121.4(2) | C(40)–C(35)–P(3) | 120.7(2) |
| C(35)–C(36)–C(37) | 120.9(3) | C(38)–C(37)–C(36) | 120.2(4) |
| C(37)–C(38)–C(39) | 119.6(3) | C(40)–C(39)–C(38) | 119.9(3) |
| C(39)–C(40)–C(35) | 121.5(3) | C(42)–C(41)–C(46) | 117.8(3) |
| C(42)–C(41)–P(3) | 124.6(2) | C(46)–C(41)–P(3) | 117.5(2) |
| C(41)–C(42)–C(43) | 120.6(3) | C(44)–C(43)–C(42) | 120.4(3) |
| C(45)–C(44)–C(43) | 119.7(3) | C(44)–C(45)–C(46) | 120.5(3) |
| C(45)–C(46)–C(41) | 120.9(3) | | |

Symmetry operations for equivalent atoms
A –x,y,–z+1/2

Table 4. Anisotropic displacement parameters (Å$^2$) for str0735. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Fe(1) | 0.0178(2) | 0.01426(19) | 0.01475(19) | –0.00009(14) | 0.00249(15) | –0.00046(14) |
| Fe(2) | 0.0197(2) | 0.0156(2) | 0.0160(2) | 0.00018(15) | 0.00310(15) | –0.00198(15) |
| P(1) | 0.0194(4) | 0.0175(4) | 0.0156(3) | 0.0001(3) | 0.0017(3) | –0.0006(3) |
| P(2) | 0.0203(4) | 0.0138(3) | 0.0172(3) | –0.0008(3) | 0.0034(3) | –0.0013(3) |
| P(3) | 0.0212(4) | 0.0198(4) | 0.0198(4) | –0.0014(3) | 0.0064(3) | –0.0017(3) |
| S(1) | 0.0226(4) | 0.0149(3) | 0.0168(3) | –0.0003(2) | 0.0007(3) | 0.0011(3) |
| S(2) | 0.0199(3) | 0.0154(3) | 0.0173(3) | 0.0001(2) | 0.0013(3) | –0.0003(2) |
| N(1) | 0.0318(14) | 0.0190(12) | 0.0167(12) | –0.0012(9) | –0.0021(10) | 0.0013(10) |
| O(1) | 0.0387(13) | 0.0433(14) | 0.0298(12) | 0.0099(10) | 0.0160(10) | 0.0019(11) |
| O(2) | 0.0347(13) | 0.0436(14) | 0.0218(11) | 0.0085(10) | 0.0056(10) | 0.0041(10) |
| O(3) | 0.0333(13) | 0.0355(13) | 0.0485(15) | –0.0139(11) | 0.0095(11) | –0.0151(11) |
| C(1) | 0.0226(15) | 0.0214(15) | 0.0222(15) | –0.0003(11) | 0.0024(12) | 0.0033(11) |
| C(2) | 0.0214(15) | 0.0217(15) | 0.0240(15) | 0.0010(12) | 0.0070(12) | –0.0017(11) |
| C(3) | 0.0255(16) | 0.0244(16) | 0.0238(15) | –0.0029(12) | 0.0059(12) | 0.0007(12) |
| C(4) | 0.0259(15) | 0.0236(15) | 0.0157(14) | –0.0017(11) | –0.0011(11) | 0.0002(12) |
| C(5) | 0.0251(15) | 0.0185(14) | 0.0227(15) | –0.0034(11) | –0.0025(12) | –0.0009(11) |
| C(6) | 0.0281(16) | 0.0210(14) | 0.0187(14) | –0.0039(11) | 0.0073(12) | –0.0039(12) |
| C(7) | 0.0258(15) | 0.0181(14) | 0.0242(15) | –0.0007(11) | 0.0091(12) | 0.0011(11) |
| C(8) | 0.0364(17) | 0.0250(16) | 0.0158(14) | –0.0059(11) | –0.0012(12) | 0.0060(13) |
| C(9) | 0.0309(16) | 0.0206(14) | 0.0139(13) | 0.0018(11) | 0.0003(11) | –0.0013(12) |
| C(10) | 0.0291(17) | 0.0302(17) | 0.0210(15) | –0.0041(12) | 0.0018(12) | 0.0022(13) |
| C(11) | 0.0259(16) | 0.0266(16) | 0.0266(16) | –0.0070(13) | –0.0009(13) | –0.0028(12) |
| C(12) | 0.0361(19) | 0.048(2) | 0.0227(17) | –0.0055(15) | –0.0003(14) | 0.0032(16) |
| C(13) | 0.053(2) | 0.066(3) | 0.0280(19) | 0.0001(18) | –0.0055(17) | 0.016(2) |
| C(14) | 0.032(2) | 0.077(3) | 0.044(2) | –0.009(2) | –0.0075(18) | 0.0101(19) |
| C(15) | 0.030(2) | 0.056(2) | 0.052(2) | –0.0065(19) | 0.0103(17) | –0.0017(17) |
| C(16) | 0.0371(19) | 0.0379(19) | 0.0342(19) | 0.0007(15) | 0.0042(15) | –0.0018(15) |
| C(17) | 0.0180(14) | 0.0243(15) | 0.0178(14) | 0.0049(11) | –0.0012(11) | –0.0001(11) |
| C(18) | 0.0225(16) | 0.0323(17) | 0.0286(16) | –0.0037(13) | 0.0063(13) | –0.0033(13) |
| C(19) | 0.0293(17) | 0.0385(19) | 0.0303(17) | –0.0038(14) | 0.0076(14) | 0.0003(14) |
| C(20) | 0.0218(16) | 0.042(2) | 0.0349(18) | 0.0031(15) | 0.0097(13) | –0.0022(14) |
| C(21) | 0.0253(17) | 0.0314(18) | 0.0415(19) | 0.0032(14) | 0.0064(14) | –0.0075(13) |
| C(22) | 0.0241(16) | 0.0272(16) | 0.0273(16) | –0.0030(12) | 0.0013(13) | –0.0029(12) |
| C(23) | 0.0186(14) | 0.0223(14) | 0.0211(14) | 0.0033(11) | 0.0040(11) | 0.0008(11) |
| C(24) | 0.0272(16) | 0.0271(16) | 0.0216(15) | 0.0016(12) | –0.0018(12) | 0.0013(12) |
| C(25) | 0.0304(17) | 0.0216(15) | 0.0327(17) | 0.0008(13) | –0.0003(13) | 0.0005(13) |
| C(26) | 0.046(2) | 0.0279(17) | 0.0306(18) | 0.0122(14) | –0.0047(15) | –0.0016(15) |
| C(27) | 0.090(3) | 0.031(2) | 0.0250(18) | 0.0092(15) | –0.0165(19) | –0.0075(19) |
| C(28) | 0.065(2) | 0.0251(17) | 0.0265(17) | 0.0016(14) | –0.0106(16) | –0.0068(16) |
| C(29) | 0.0185(14) | 0.0150(13) | 0.0242(15) | 0.0019(11) | 0.0030(11) | –0.0028(10) |
| C(30) | 0.0315(17) | 0.0185(14) | 0.0233(15) | –0.0010(11) | 0.0027(12) | –0.0020(12) |
| C(31) | 0.052(2) | 0.0275(17) | 0.0257(17) | 0.0030(13) | 0.0007(15) | –0.0032(15) |
| C(32) | 0.058(2) | 0.0180(16) | 0.039(2) | 0.0078(14) | 0.0000(17) | –0.0014(15) |
| C(33) | 0.0400(19) | 0.0149(15) | 0.0375(18) | –0.0029(13) | 0.0070(15) | 0.0011(13) |
| C(34) | 0.0310(17) | 0.0220(15) | 0.0282(16) | –0.0041(12) | 0.0068(13) | –0.0023(12) |
| C(35) | 0.0215(15) | 0.0243(15) | 0.0290(16) | –0.0005(12) | 0.0052(12) | –0.0011(12) |
| C(36) | 0.0260(18) | 0.072(3) | 0.035(2) | –0.0116(18) | 0.0024(15) | 0.0120(17) |
| C(37) | 0.035(2) | 0.091(3) | 0.036(2) | –0.010(2) | –0.0044(17) | 0.017(2) |
| C(38) | 0.0212(17) | 0.058(2) | 0.057(2) | –0.0069(19) | –0.0017(16) | 0.0053(16) |
| C(39) | 0.0220(18) | 0.072(3) | 0.052(2) | –0.010(2) | 0.0097(16) | 0.0048(17) |
| C(40) | 0.0309(19) | 0.056(2) | 0.039(2) | –0.0044(17) | 0.0090(15) | 0.0052(17) |
| C(41) | 0.0222(15) | 0.0258(15) | 0.0218(15) | 0.0018(12) | 0.0089(12) | –0.0011(12) |
| C(42) | 0.042(2) | 0.0372(19) | 0.0289(17) | –0.0061(14) | 0.0130(15) | –0.0122(15) |
| C(43) | 0.047(2) | 0.056(2) | 0.0238(17) | –0.0091(16) | 0.0108(15) | –0.0124(18) |
| C(44) | 0.0371(19) | 0.050(2) | 0.0267(17) | 0.0095(15) | 0.0125(15) | 0.0009(16) |
| C(45) | 0.055(2) | 0.0270(17) | 0.039(2) | 0.0039(15) | 0.0231(17) | –0.0044(16) |
| C(46) | 0.046(2) | 0.0271(17) | 0.0280(17) | –0.0037(13) | 0.0154(15) | –0.0052(14) |

Table 5. Hydrogen coordinates and isotropic displacement parameters (Å²) for str0735.

| | x | y | z | U |
|---|---|---|---|---|
| H(4A) | 0.0313 | 0.1179 | 0.2744 | 0.027 |
| H(4B) | 0.0629 | 0.1402 | 0.2537 | 0.027 |
| H(5A) | 0.0632 | –0.0495 | 0.2960 | 0.027 |
| H(5B) | 0.0462 | –0.0228 | 0.3780 | 0.027 |
| H(6A) | 0.1158 | –0.0478 | 0.2986 | 0.027 |
| H(6B) | 0.1164 | 0.0881 | 0.2939 | 0.027 |
| H(7A) | 0.1620 | –0.0205 | 0.3390 | 0.027 |
| H(7B) | 0.1521 | –0.0189 | 0.4354 | 0.027 |
| H(8A) | 0.1187 | 0.4631 | 0.6622 | 0.031 |
| H(8B) | 0.1025 | 0.3484 | 0.6800 | 0.031 |
| H(9A) | 0.1249 | 0.1819 | 0.7048 | 0.027 |
| H(9B) | 0.1583 | 0.1703 | 0.7072 | 0.027 |
| H(10A) | 0.1412 | 0.3436 | 0.8092 | 0.032 |
| H(10B) | 0.1551 | 0.4515 | 0.7678 | 0.032 |
| H(12A) | 0.1735 | 0.2572 | 0.9166 | 0.043 |
| H(13A) | 0.2181 | 0.1869 | 0.9692 | 0.060 |
| H(14A) | 0.2553 | 0.2132 | 0.8880 | 0.062 |
| H(15A) | 0.2476 | 0.3029 | 0.7503 | 0.055 |
| H(16A) | 0.2025 | 0.3682 | 0.6947 | 0.044 |
| H(18A) | 0.0303 | 0.3764 | 0.5050 | 0.033 |
| H(19A) | –0.0107 | 0.3742 | 0.5719 | 0.039 |
| H(20A) | –0.0439 | 0.2290 | 0.5387 | 0.039 |
| H(21A) | –0.0347 | 0.0807 | 0.4455 | 0.039 |
| H(22A) | 0.0063 | 0.0819 | 0.3777 | 0.032 |
| H(24A) | 0.0630 | 0.4755 | 0.4214 | 0.031 |
| H(25A) | 0.0566 | 0.6413 | 0.3388 | 0.034 |
| H(26A) | 0.0405 | 0.6344 | 0.1871 | 0.043 |
| H(27A) | 0.0315 | 0.4577 | 0.1185 | 0.061 |
| H(28A) | 0.0378 | 0.2908 | 0.2008 | 0.049 |
| H(30A) | 0.0961 | –0.0479 | 0.5964 | 0.029 |
| H(31A) | 0.0990 | –0.2241 | 0.6672 | 0.042 |
| H(32A) | 0.1056 | –0.3889 | 0.5877 | 0.047 |
| H(33A) | 0.1101 | –0.3782 | 0.4379 | 0.037 |
| H(34A) | 0.1051 | –0.2038 | 0.3640 | 0.032 |
| H(36A) | 0.1945 | 0.1760 | 0.5783 | 0.053 |
| H(37A) | 0.2376 | 0.1108 | 0.6514 | 0.066 |
| H(38A) | 0.2707 | 0.0318 | 0.5712 | 0.055 |
| H(39A) | 0.2611 | 0.0227 | 0.4165 | 0.058 |
| H(40A) | 0.2169 | 0.0746 | 0.3451 | 0.050 |
| H(42A) | 0.1608 | 0.0675 | 0.2153 | 0.042 |
| H(43A) | 0.1702 | 0.1372 | 0.0787 | 0.050 |
| H(44A) | 0.1892 | 0.3177 | 0.0687 | 0.044 |
| H(45A) | 0.1986 | 0.4297 | 0.1948 | 0.047 |
| H(46A) | 0.1885 | 0.3637 | 0.3309 | 0.039 |

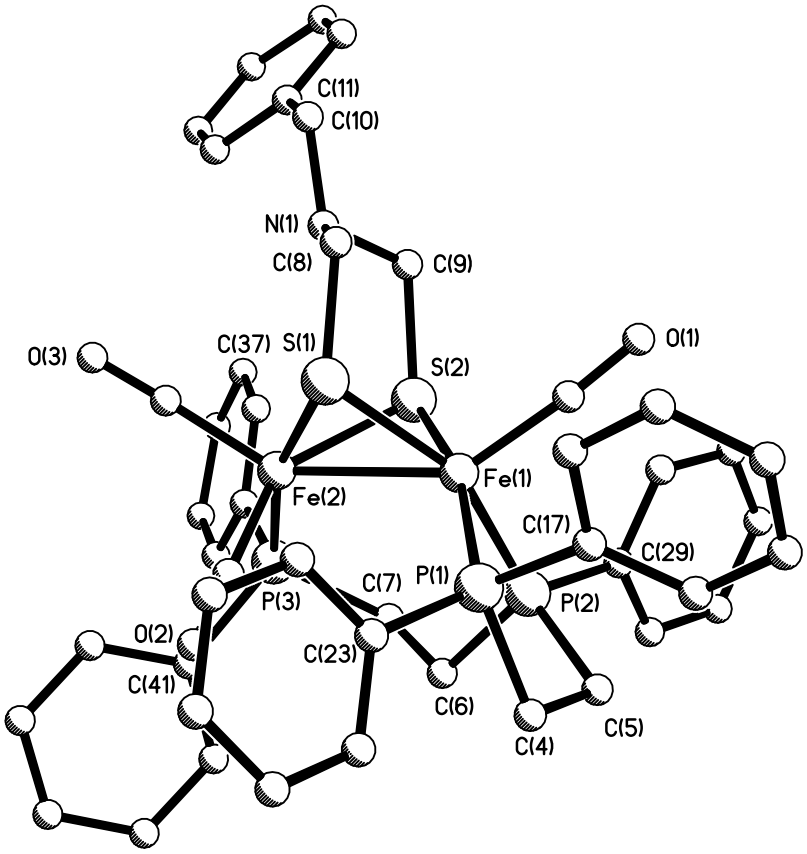
Table 6. Torsion angles [°] for str0735.

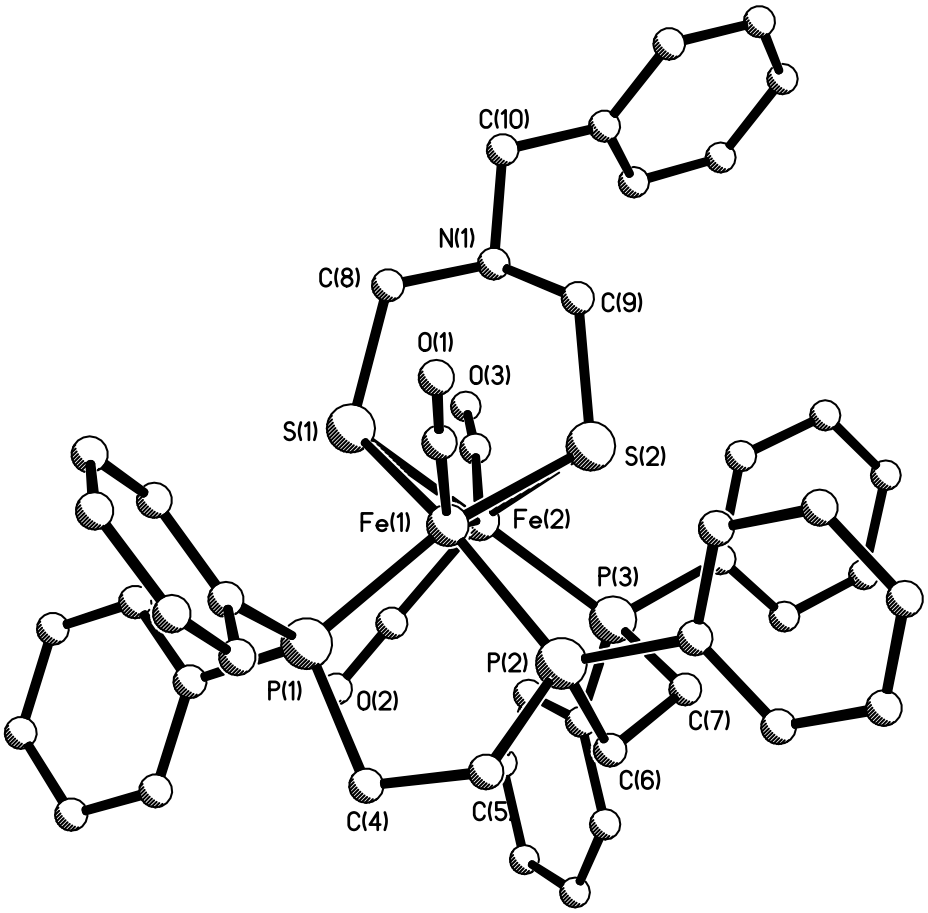
| | | | |
|---|---|---|---|
| C(1)–Fe(1)–Fe(2)–C(2) | −146.35(19) | P(2)–Fe(1)–Fe(2)–C(2) | 82.83(10) |
| S(1)–Fe(1)–Fe(2)–C(2) | −88.07(10) | S(2)–Fe(1)–Fe(2)–C(2) | 162.38(10) |
| P(1)–Fe(1)–Fe(2)–C(2) | −6.86(10) | C(1)–Fe(1)–Fe(2)–C(3) | −24.9(2) |
| P(2)–Fe(1)–Fe(2)–C(3) | −155.68(18) | S(1)–Fe(1)–Fe(2)–C(3) | 33.42(18) |
| S(2)–Fe(1)–Fe(2)–C(3) | −76.14(18) | P(1)–Fe(1)–Fe(2)–C(3) | 114.62(18) |
| C(1)–Fe(1)–Fe(2)–P(3) | 120.72(16) | P(2)–Fe(1)–Fe(2)–P(3) | −10.10(3) |
| S(1)–Fe(1)–Fe(2)–P(3) | 179.00(3) | S(2)–Fe(1)–Fe(2)–P(3) | 69.44(3) |
| P(1)–Fe(1)–Fe(2)–P(3) | −99.80(4) | C(1)–Fe(1)–Fe(2)–S(1) | −58.28(16) |
| P(2)–Fe(1)–Fe(2)–S(1) | 170.90(3) | S(2)–Fe(1)–Fe(2)–S(1) | −109.56(3) |
| P(1)–Fe(1)–Fe(2)–S(1) | 81.20(3) | C(1)–Fe(1)–Fe(2)–S(2) | 51.28(16) |
| P(2)–Fe(1)–Fe(2)–S(2) | −79.54(3) | S(1)–Fe(1)–Fe(2)–S(2) | 109.56(3) |
| P(1)–Fe(1)–Fe(2)–S(2) | −169.24(3) | C(1)–Fe(1)–P(1)–C(23) | 130.71(15) |
| P(2)–Fe(1)–P(1)–C(23) | −127.93(12) | S(1)–Fe(1)–P(1)–C(23) | 27.36(12) |
| S(2)–Fe(1)–P(1)–C(23) | −63.54(18) | Fe(2)–Fe(1)–P(1)–C(23) | −27.52(12) |
| C(1)–Fe(1)–P(1)–C(17) | 7.60(14) | P(2)–Fe(1)–P(1)–C(17) | 108.95(10) |
| S(1)–Fe(1)–P(1)–C(17) | −95.76(10) | S(2)–Fe(1)–P(1)–C(17) | 173.34(14) |
| Fe(2)–Fe(1)–P(1)–C(17) | −150.63(10) | C(1)–Fe(1)–P(1)–C(4) | −106.00(14) |
| P(2)–Fe(1)–P(1)–C(4) | −4.64(10) | S(1)–Fe(1)–P(1)–C(4) | 150.65(10) |
| S(2)–Fe(1)–P(1)–C(4) | 59.75(16) | Fe(2)–Fe(1)–P(1)–C(4) | 95.77(10) |
| C(1)–Fe(1)–P(2)–C(29) | −43.46(14) | S(1)–Fe(1)–P(2)–C(29) | 128.66(12) |
| S(2)–Fe(1)–P(2)–C(29) | 56.35(11) | P(1)–Fe(1)–P(2)–C(29) | −137.29(11) |
| Fe(2)–Fe(1)–P(2)–C(29) | 110.45(10) | C(1)–Fe(1)–P(2)–C(6) | −169.30(14) |
| S(1)–Fe(1)–P(2)–C(6) | 2.82(14) | S(2)–Fe(1)–P(2)–C(6) | −69.49(11) |
| P(1)–Fe(1)–P(2)–C(6) | 96.87(11) | Fe(2)–Fe(1)–P(2)–C(6) | −15.38(11) |
| C(1)–Fe(1)–P(2)–C(5) | 75.76(14) | S(1)–Fe(1)–P(2)–C(5) | −112.12(12) |
| S(2)–Fe(1)–P(2)–C(5) | 175.56(10) | P(1)–Fe(1)–P(2)–C(5) | −18.07(10) |
| Fe(2)–Fe(1)–P(2)–C(5) | −130.33(10) | C(2)–Fe(2)–P(3)–C(41) | 23.81(14) |
| C(3)–Fe(2)–P(3)–C(41) | −78.55(14) | S(1)–Fe(2)–P(3)–C(41) | 122.54(15) |
| S(2)–Fe(2)–P(3)–C(41) | 169.25(11) | Fe(1)–Fe(2)–P(3)–C(41) | 119.36(11) |
| C(2)–Fe(2)–P(3)–C(35) | 144.97(14) | C(3)–Fe(2)–P(3)–C(35) | 42.61(15) |
| S(1)–Fe(2)–P(3)–C(35) | −116.30(16) | S(2)–Fe(2)–P(3)–C(35) | −69.60(11) |
| Fe(1)–Fe(2)–P(3)–C(35) | −119.48(11) | C(2)–Fe(2)–P(3)–C(7) | −96.53(14) |
| C(3)–Fe(2)–P(3)–C(7) | 161.11(14) | S(1)–Fe(2)–P(3)–C(7) | 2.20(18) |
| S(2)–Fe(2)–P(3)–C(7) | 48.90(11) | Fe(1)–Fe(2)–P(3)–C(7) | −0.98(11) |
| C(1)–Fe(1)–S(1)–C(8) | 47.05(14) | P(2)–Fe(1)–S(1)–C(8) | −125.04(13) |
| S(2)–Fe(1)–S(1)–C(8) | −52.00(11) | P(1)–Fe(1)–S(1)–C(8) | 143.22(11) |
| Fe(2)–Fe(1)–S(1)–C(8) | −103.20(11) | C(1)–Fe(1)–S(1)–Fe(2) | 150.25(10) |
| P(2)–Fe(1)–S(1)–Fe(2) | −21.84(8) | S(2)–Fe(1)–S(1)–Fe(2) | 51.20(3) |
| P(1)–Fe(1)–S(1)–Fe(2) | −113.58(3) | C(2)–Fe(2)–S(1)–C(8) | −158.28(14) |
| C(3)–Fe(2)–S(1)–C(8) | −55.90(15) | P(3)–Fe(2)–S(1)–C(8) | 103.02(16) |
| S(2)–Fe(2)–S(1)–C(8) | 56.04(11) | Fe(1)–Fe(2)–S(1)–C(8) | 106.66(11) |
| C(2)–Fe(2)–S(1)–Fe(1) | 95.06(9) | C(3)–Fe(2)–S(1)–Fe(1) | −162.56(10) |
| P(3)–Fe(2)–S(1)–Fe(1) | −3.65(13) | S(2)–Fe(2)–S(1)–Fe(1) | −50.62(2) |
| C(1)–Fe(1)–S(2)–C(9) | −48.81(14) | P(2)–Fe(1)–S(2)–C(9) | −150.31(10) |
| S(1)–Fe(1)–S(2)–C(9) | 53.20(10) | P(1)–Fe(1)–S(2)–C(9) | 145.63(14) |
| Fe(2)–Fe(1)–S(2)–C(9) | 104.40(10) | C(1)–Fe(1)–S(2)–Fe(2) | −153.20(10) |
| P(2)–Fe(1)–S(2)–Fe(2) | 105.29(3) | S(1)–Fe(1)–S(2)–Fe(2) | −51.19(3) |
| P(1)–Fe(1)–S(2)–Fe(2) | 41.23(12) | C(2)–Fe(2)–S(2)–C(9) | −138.66(19) |
| C(3)–Fe(2)–S(2)–C(9) | 38.83(15) | P(3)–Fe(2)–S(2)–C(9) | 134.87(11) |
| S(1)–Fe(2)–S(2)–C(9) | −55.98(11) | Fe(1)–Fe(2)–S(2)–C(9) | −106.60(11) |

| | | | |
|---|---|---|---|
| C(2)–Fe(2)–S(2)–Fe(1) | −32.06(17) | C(3)–Fe(2)–S(2)–Fe(1) | 145.43(10) |
| P(3)–Fe(2)–S(2)–Fe(1) | −118.53(3) | S(1)–Fe(2)–S(2)–Fe(1) | 50.62(3) |
| P(2)–Fe(1)–C(1)–O(1) | 125(3) | S(1)–Fe(1)–C(1)–O(1) | −52(3) |
| S(2)–Fe(1)–C(1)–O(1) | 35(3) | P(1)–Fe(1)–C(1)–O(1) | −149(3) |
| Fe(2)–Fe(1)–C(1)–O(1) | −6(3) | C(3)–Fe(2)–C(2)–O(2) | 40(8) |
| P(3)–Fe(2)–C(2)–O(2) | −57(8) | S(1)–Fe(2)–C(2)–O(2) | 138(8) |
| S(2)–Fe(2)–C(2)–O(2) | −142(8) | Fe(1)–Fe(2)–C(2)–O(2) | −168(8) |
| C(2)–Fe(2)–C(3)–O(3) | 36(3) | P(3)–Fe(2)–C(3)–O(3) | 128(3) |
| S(1)–Fe(2)–C(3)–O(3) | −57(3) | S(2)–Fe(2)–C(3)–O(3) | −143(3) |
| Fe(1)–Fe(2)–C(3)–O(3) | −84(3) | C(23)–P(1)–C(4)–C(5) | 168.5(2) |
| C(17)–P(1)–C(4)–C(5) | −87.7(2) | Fe(1)–P(1)–C(4)–C(5) | 31.4(2) |
| P(1)–C(4)–C(5)–P(2) | −44.9(2) | C(29)–P(2)–C(5)–C(4) | 171.95(19) |
| C(6)–P(2)–C(5)–C(4) | −83.1(2) | Fe(1)–P(2)–C(5)–C(4) | 41.7(2) |
| C(29)–P(2)–C(6)–C(7) | −66.7(2) | C(5)–P(2)–C(6)–C(7) | −171.8(2) |
| Fe(1)–P(2)–C(6)–C(7) | 68.2(2) | P(2)–C(6)–C(7)–P(3) | −87.8(2) |
| C(41)–P(3)–C(7)–C(6) | −78.9(2) | C(35)–P(3)–C(7)–C(6) | 176.5(2) |
| Fe(2)–P(3)–C(7)–C(6) | 47.9(2) | C(9)–N(1)–C(8)–S(1) | −70.0(3) |
| C(10)–N(1)–C(8)–S(1) | 165.9(2) | Fe(1)–S(1)–C(8)–N(1) | 68.5(2) |
| Fe(2)–S(1)–C(8)–N(1) | −6.8(2) | C(8)–N(1)–C(9)–S(2) | 70.4(3) |
| C(10)–N(1)–C(9)–S(2) | −166.8(2) | Fe(1)–S(2)–C(9)–N(1) | −70.3(2) |
| Fe(2)–S(2)–C(9)–N(1) | 5.5(2) | C(8)–N(1)–C(10)–C(11) | −175.1(2) |
| C(9)–N(1)–C(10)–C(11) | 61.3(3) | N(1)–C(10)–C(11)–C(12) | −127.3(3) |
| N(1)–C(10)–C(11)–C(16) | 53.0(4) | C(16)–C(11)–C(12)–C(13) | 0.6(5) |
| C(10)–C(11)–C(12)–C(13) | −179.1(3) | C(11)–C(12)–C(13)–C(14) | 1.0(6) |
| C(12)–C(13)–C(14)–C(15) | −1.6(6) | C(13)–C(14)–C(15)–C(16) | 0.4(6) |
| C(14)–C(15)–C(16)–C(11) | 1.3(6) | C(12)–C(11)–C(16)–C(15) | −1.8(5) |
| C(10)–C(11)–C(16)–C(15) | 177.9(3) | C(23)–P(1)–C(17)–C(22) | 118.6(2) |
| C(4)–P(1)–C(17)–C(22) | 13.3(3) | Fe(1)–P(1)–C(17)–C(22) | −104.0(2) |
| C(23)–P(1)–C(17)–C(18) | −65.6(2) | C(4)–P(1)–C(17)–C(18) | −170.9(2) |
| Fe(1)–P(1)–C(17)–C(18) | 71.9(2) | C(22)–C(17)–C(18)–C(19) | −1.1(4) |
| P(1)–C(17)–C(18)–C(19) | −177.2(2) | C(17)–C(18)–C(19)–C(20) | −0.4(5) |
| C(18)–C(19)–C(20)–C(21) | 2.0(5) | C(19)–C(20)–C(21)–C(22) | −2.0(5) |
| C(18)–C(17)–C(22)–C(21) | 1.1(4) | P(1)–C(17)–C(22)–C(21) | 177.0(2) |
| C(20)–C(21)–C(22)–C(17) | 0.4(5) | C(17)–P(1)–C(23)–C(24) | 82.3(3) |
| C(4)–P(1)–C(23)–C(24) | −171.6(2) | Fe(1)–P(1)–C(23)–C(24) | −45.5(3) |
| C(17)–P(1)–C(23)–C(28) | −97.0(3) | C(4)–P(1)–C(23)–C(28) | 9.1(3) |
| Fe(1)–P(1)–C(23)–C(28) | 135.2(2) | C(28)–C(23)–C(24)–C(25) | 0.0(5) |
| P(1)–C(23)–C(24)–C(25) | −179.3(2) | C(23)–C(24)–C(25)–C(26) | 0.1(5) |
| C(24)–C(25)–C(26)–C(27) | −0.4(5) | C(25)–C(26)–C(27)–C(28) | 0.4(6) |
| C(26)–C(27)–C(28)–C(23) | −0.3(6) | C(24)–C(23)–C(28)–C(27) | 0.0(5) |
| P(1)–C(23)–C(28)–C(27) | 179.4(3) | C(6)–P(2)–C(29)–C(34) | −40.2(3) |
| C(5)–P(2)–C(29)–C(34) | 64.2(3) | Fe(1)–P(2)–C(29)–C(34) | −172.7(2) |
| C(6)–P(2)–C(29)–C(30) | 143.7(2) | C(5)–P(2)–C(29)–C(30) | −112.0(2) |
| Fe(1)–P(2)–C(29)–C(30) | 11.1(3) | C(34)–C(29)–C(30)–C(31) | −1.5(4) |
| P(2)–C(29)–C(30)–C(31) | 174.8(2) | C(29)–C(30)–C(31)–C(32) | 1.4(5) |
| C(30)–C(31)–C(32)–C(33) | 0.4(6) | C(31)–C(32)–C(33)–C(34) | −2.1(5) |
| C(32)–C(33)–C(34)–C(29) | 1.9(5) | C(30)–C(29)–C(34)–C(33) | −0.2(4) |
| P(2)–C(29)–C(34)–C(33) | −176.4(2) | C(41)–P(3)–C(35)–C(36) | 150.5(3) |
| C(7)–P(3)–C(35)–C(36) | −103.4(3) | Fe(2)–P(3)–C(35)–C(36) | 22.6(3) |
| C(41)–P(3)–C(35)–C(40) | −33.0(3) | C(7)–P(3)–C(35)–C(40) | 73.1(3) |
| Fe(2)–P(3)–C(35)–C(40) | −160.9(2) | C(40)–C(35)–C(36)–C(37) | −2.7(6) |
| P(3)–C(35)–C(36)–C(37) | 173.9(3) | C(35)–C(36)–C(37)–C(38) | 2.2(7) |

| | | | |
|---|---|---|---|
| C(36)–C(37)–C(38)–C(39) | 0.9(7) | C(37)–C(38)–C(39)–C(40) | −3.5(6) |
| C(38)–C(39)–C(40)–C(35) | 3.0(6) | C(36)–C(35)–C(40)–C(39) | 0.1(6) |
| P(3)–C(35)–C(40)–C(39) | −176.6(3) | C(35)–P(3)–C(41)–C(42) | 103.8(3) |
| C(7)–P(3)–C(41)–C(42) | 0.4(3) | Fe(2)–P(3)–C(41)–C(42) | −126.1(3) |
| C(35)–P(3)–C(41)–C(46) | −77.7(3) | C(7)–P(3)–C(41)–C(46) | 178.9(2) |
| Fe(2)–P(3)–C(41)–C(46) | 52.4(3) | C(46)–C(41)–C(42)–C(43) | −0.7(5) |
| P(3)–C(41)–C(42)–C(43) | 177.8(3) | C(41)–C(42)–C(43)–C(44) | 0.8(6) |
| C(42)–C(43)–C(44)–C(45) | −0.2(6) | C(43)–C(44)–C(45)–C(46) | −0.5(6) |
| C(44)–C(45)–C(46)–C(41) | 0.6(6) | C(42)–C(41)–C(46)–C(45) | 0.0(5) |
| P(3)–C(41)–C(46)–C(45) | −178.6(3) | | |

Symmetry operations for equivalent atoms

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C(9)
O(1)
O(3)
S(1)
S(2)
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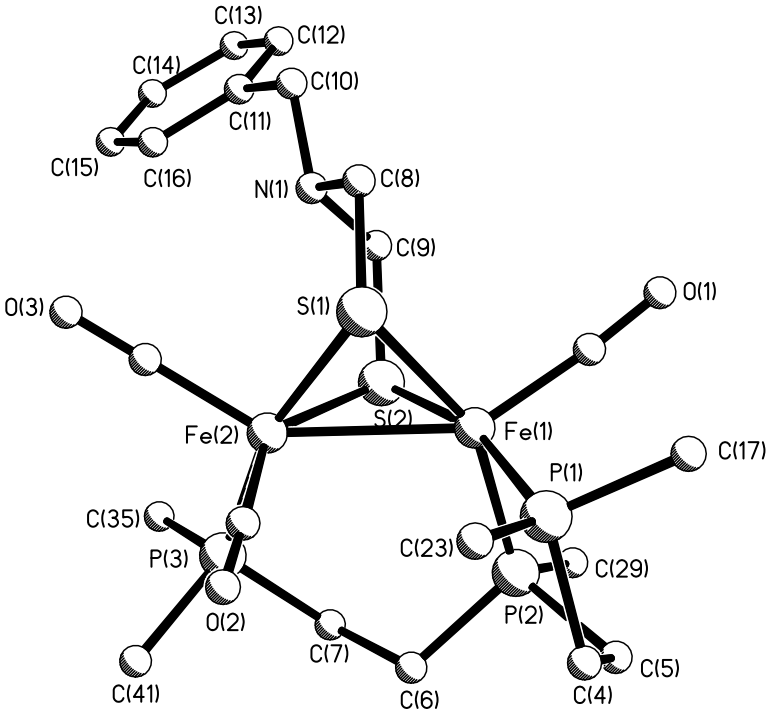
Fe(2)
P(3)
P(2)
P(1)
O(2)
C(7)
C(6)
C(4)
C(5)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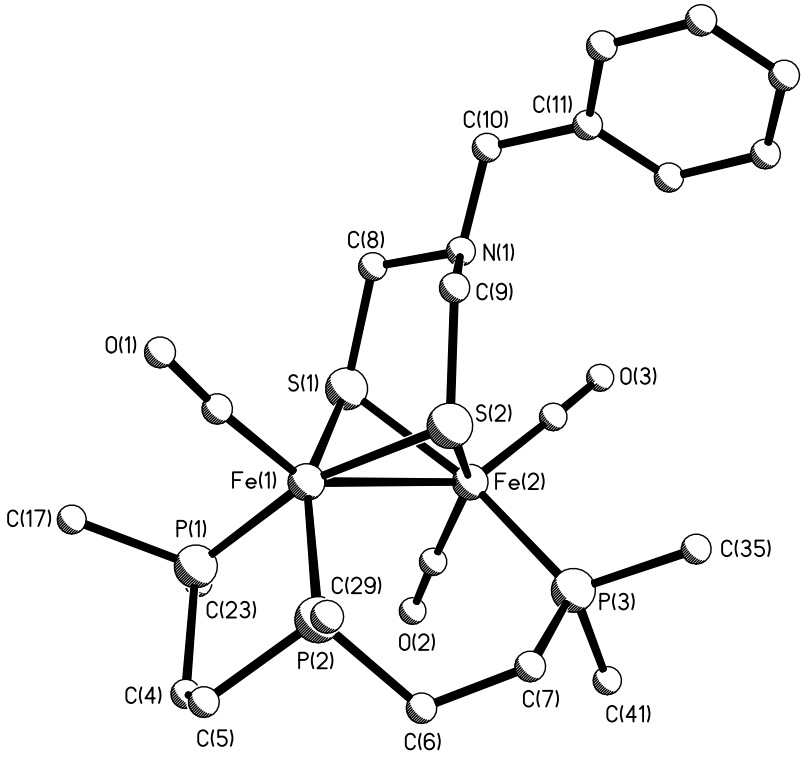
C(16)
N(1)
C(8)
C(9)
O(3)
S(1)
O(1)
S(2)
Fe(2)
Fe(1)
C(17)
P(1)
C(35)
C(23)
P(3)
C(29)
O(2)
P(2)
C(7)
C(5)
C(41)
C(6)
C(4)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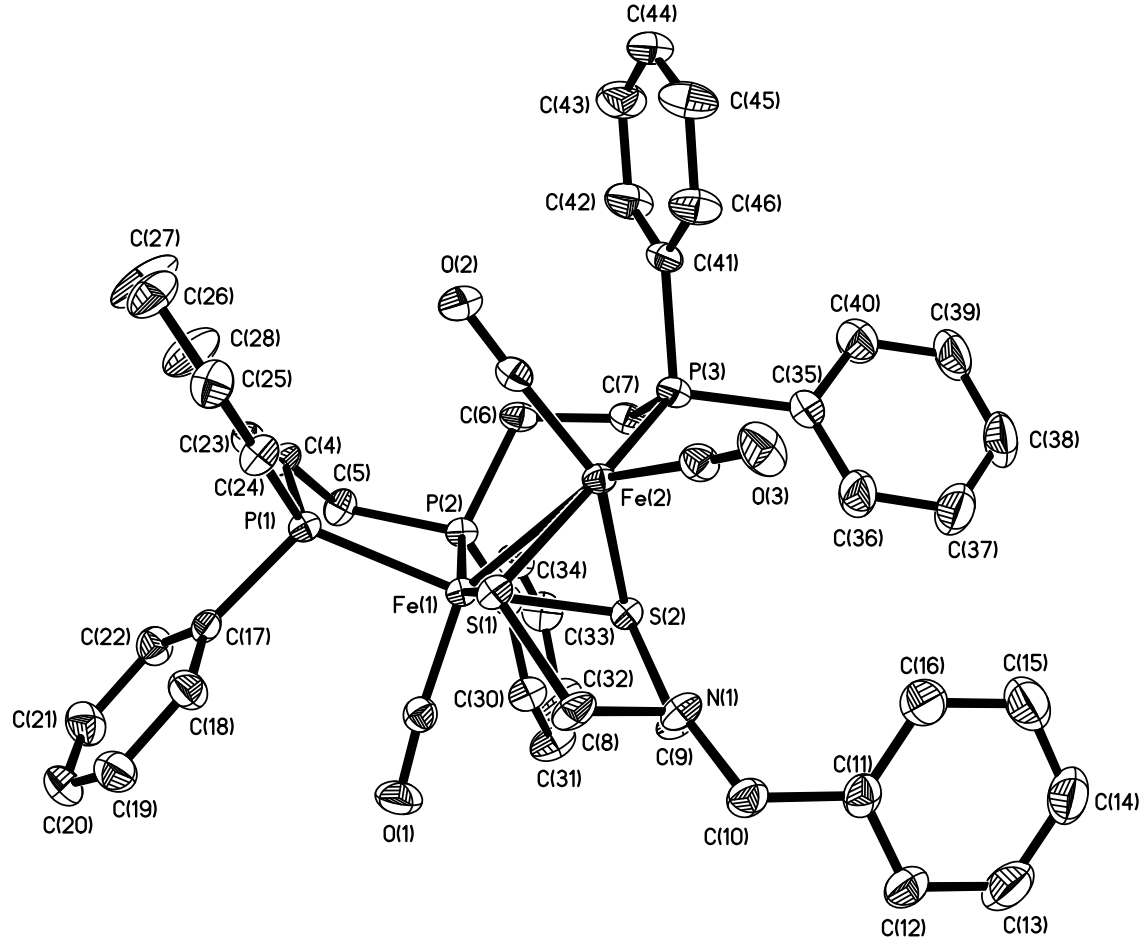
C(11)
C(8)
N(1)
C(9)
O(1)
S(1)
O(3)
S(2)
Fe(1)
Fe(2)
C(17)
P(1)
C(35)
C(29)
C(23)
P(3)
O(2)
P(2)
C(4)
C(7)
C(41)
C(5)
C(6)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C(41)
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O(2)
C(26)
C(40)
C(39)
C(28)
C(25)
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P(3)
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C(6)
C(38)
C(23)
C(4)
C(5)
C(24)
Fe(2)
O(3)
P(2)
P(1)
C(36)
C(37)
C(34)
Fe(1)
S(1)
S(2)
C(22)
C(17)
C(33)
C(16)
C(15)
C(32)
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