Bio-inspired hydrogenase models: The mixed-valence triiron complex $[\text{Fe}_3(\text{CO})_7(\mu-\text{edt})_2]$ and phosphine derivatives $[\text{Fe}_3(\text{CO})_{7-x}(\text{PPh}_3)_x(\mu-\text{edt})_2]$ $(x = 1, 2)$ and $[\text{Fe}_3(\text{CO})_5(\kappa^2\text{-diphosphine})(\mu-\text{edt})_2]$ as proton reduction catalysts

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1 B3LYP geometries and energies for all optimized ground-state minima
2 The complete list of authors for ref. 58
3 Electrochemical and electrocatalytic studies (Figures S1-S5)
4 X-ray crystallography – full tables of bond lengths and angles for 1-4
1 B3LYP geometries and energies for all optimized ground-state minima

Species: \textit{anti-Ru$_3$(CO)$_7$(µ-edt)$_2$}

HF energy = -2828.5021903

No imaginary frequency
Zero-point correction = 0.182216 (Hartree/Particle)
Thermal correction to Energy = 0.212781
Thermal correction to Enthalpy = 0.213725
Thermal correction to Gibbs Free Energy = 0.118210

Sum of electronic and zero-point Energies = -2828.319974
Sum of electronic and thermal Energies = -2828.289410
Sum of electronic and thermal Enthalpies = -2828.288466
Sum of electronic and thermal Free Energies = -2828.383980

Coordinates: \textit{anti-Ru$_3$(CO)$_7$(µ-edt)$_2$}

\begin{tabular}{cccc}
Ru & 0.94970000 & -1.49340000 & 9.96360000 \\
Ru & -0.03570000 & 0.57440000 & 11.54030000 \\
Ru & -1.21390000 & 1.54840000 & 13.82010000 \\
S & 1.60230000 & -1.07030000 & 12.26380000 \\
S & -1.20740000 & -1.50510000 & 11.07620000 \\
S & 0.80230000 & 2.42120000 & 12.78970000 \\
S & -1.95150000 & 1.99410000 & 11.54890000 \\
O & 1.45850000 & -4.50430000 & 9.83880000 \\
O & -0.40030000 & -1.30750000 & 7.20010000 \\
O & 3.74420000 & -0.69110000 & 8.94370000 \\
O & 0.89830000 & 1.89050000 & 8.99910000 \\
O & -2.32690000 & 3.95220000 & 15.40550000 \\
O & 0.43430000 & 0.26010000 & 16.05890000 \\
O & -3.54240000 & -0.39860000 & 14.23860000 \\
C & 0.56680000 & -2.31750000 & 13.16670000 \\
C & -0.82550000 & -2.55060000 & 12.56160000 \\
C & 0.15780000 & 3.89010000 & 11.85240000 \\
C & -1.23170000 & 3.67670000 & 11.23320000 \\
C & 1.27130000 & -3.37280000 & 9.87590000 \\
C & 0.10810000 & -1.36850000 & 8.22340000 \\
C & 2.70170000 & -0.98100000 & 9.31590000 \\
C & 0.59250000 & 1.23400000 & 9.91100000 \\
C & -1.90930000 & 3.06370000 & 14.80850000 \\
C & -0.18600000 & 0.74930000 & 15.22200000 \\
C & -2.67210000 & 0.33830000 & 14.08370000 \\
H & 0.49620000 & -1.95110000 & 14.19530000 \\
H & 1.14740000 & -3.24690000 & 13.17950000 \\
H & -0.94180000 & -3.59120000 & 12.23840000 \\
H & -1.61580000 & -2.33430000 & 13.28710000 \\
H & 0.90300000 & 4.10380000 & 11.07880000 \\
H & 0.15460000 & 4.72520000 & 12.56100000 \\
H & -1.95800000 & 4.39600000 & 11.62630000 \\
H & -1.19680000 & 3.79040000 & 10.14430000
\end{tabular}
Species: syn-Ru₃(CO)₇(μ-edt)₂
HF energy = -2828.507084
No imaginary frequency
Zero-point correction = 0.182886 (Hartree/Particle)
Thermal correction to Energy = 0.213042
Thermal correction to Enthalpy = 0.213986
Thermal correction to Gibbs Free Energy = 0.120402
Sum of electronic and zero-point Energies = -2828.324198
Sum of electronic and thermal Energies = -2828.294042
Sum of electronic and thermal Enthalpies = -2828.293098
Sum of electronic and thermal Free Energies = -2828.386682

Coordinates: syn-Ru₃(CO)₇(μ-edt)₂
Ru    6.46630000  3.76660000  1.21160000  1.21160000
Ru    5.44920000  1.51540000  2.76290000  2.76290000
Ru    7.84320000  0.44080000  1.49320000  1.49320000
S     4.22030000  2.80630000  1.17210000  1.17210000
S     5.85370000  3.72460000  3.57590000  3.57590000
S     5.59170000  0.50560000  1.49820000  1.49820000
S     7.26700000  0.42710000  3.86790000  3.86790000
O     5.57380000  6.63650000  0.71050000  0.71050000
O     9.32540000  4.69820000  1.84420000  1.84420000
O     6.88540000  3.31010000 -1.79720000 -1.79720000
O     3.20760000  0.74840000  4.61200000  4.61200000
O     9.29510000 -2.23740000  1.52290000  1.52290000
O     7.93200000  0.52560000 -1.57700000 -1.57700000
O     10.47930000 1.94430000  1.97370000  1.97370000
C     3.33150000  4.01390000  2.27160000  2.27160000
C     4.15250000  4.47020000  3.48920000  3.48920000
C     5.77300000 -1.77750000  2.84280000  2.84280000
C     6.61720000 -1.30660000  4.03840000  4.03840000
C     5.90610000  5.55420000  0.90360000  0.90360000
C     8.28390000  4.28340000  1.60360000  1.60360000
C     6.76140000  3.41620000 -0.66210000 -0.66210000
C     4.07410000  1.04440000  3.89760000  3.89760000
C     8.74410000 -1.22980000  1.51480000  1.51480000
C     7.88020000  0.56400000 -0.43220000 -0.43220000
C     9.46340000  1.44750000  1.78330000  1.78330000
H     2.41500000  3.50140000  2.58360000  2.58360000
H     3.04370000  4.86540000  1.64530000  1.64530000
H     3.66310000  4.18170000  4.42580000  4.42580000
H     4.27920000  5.55830000  3.49760000  3.49760000
H     4.75010000 -2.01820000  3.15240000  3.15240000
H     6.20360000 -2.67250000  2.38040000  2.38040000
H     6.02690000 -1.30390000  4.96120000  4.96120000
H     7.48270000 -1.95990000  4.19470000  4.19470000
Species: anti-1
HF energy = -2915.3251158
No imaginary frequency
Zero-point correction = 0.184260 (Hartree/Particle)
Thermal correction to Energy = 0.213898
Thermal correction to Enthalpy = 0.214842
Thermal correction to Gibbs Free Energy = 0.123057
Sum of electronic and zero-point Energies = -2915.140856
Sum of electronic and thermal Energies = -2915.111218
Sum of electronic and thermal Enthalpies = -2915.110274
Sum of electronic and thermal Free Energies = -2915.202059

Coordinates: anti-1
S         1.52470000 -0.97940000  12.28900000
S         -1.20290000 -1.40390000  11.10880000
S          0.80000000  2.29120000  12.75310000
S         -1.90510000  1.86930000  11.55730000
O          1.34100000 -4.21370000  10.05720000
O         -0.44590000 -1.14570000   7.44830000
O           3.58120000 -0.52660000   9.18670000
O           0.80710000  1.83420000   9.15330000
O         -2.15380000  3.80970000  15.14420000
O           0.48890000  0.21420000  15.79520000
O         -3.36200000 -0.40770000  14.08320000
C           0.55160000 -2.29800000  13.14930000
C         -0.84070000  2.52380000  12.53740000
C           0.18090000  3.76770000  11.82170000
C         -1.21120000  3.54890000  11.20330000
C           1.16280000 -3.08270000  10.06190000
C           0.06950000 -1.19570000   8.46620000
C           2.53120000 -0.81660000   9.52940000
C           0.51680000  1.15730000  10.05490000
C         -1.75350000  2.89830000  14.57150000
C         -0.14010000  0.70400000  14.96660000
C         -2.49050000  0.32450000  13.92070000
H           0.48540000 -1.99060000  14.19730000
H           1.15220000 -3.21350000  13.11020000
H         -0.94840000 -3.55060000  12.17090000
H         -1.63530000 -2.34980000  13.26950000
H           0.92560000  3.98400000  11.04850000
H           0.17730000  4.60310000  12.52970000
H         -1.93730000  4.27380000  11.58600000
H         -1.17740000  3.64880000  10.11330000
Fe          0.87190000 -1.31450000  10.10000000
Fe         -0.06090000   0.53950000  11.58890000
Fe         -1.12910000  1.46850000  13.67890000

Species: syn-1
HF energy = -2915.3267997
No imaginary frequency
Zero-point correction = 0.184072 (Hartree/Particle)
Thermal correction to Energy = 0.213759
Thermal correction to Enthalpy = 0.214703
Thermal correction to Gibbs Free Energy = 0.122693
Sum of electronic and zero-point Energies = -2915.142727
Sum of electronic and thermal Energies = -2915.113041
Sum of electronic and thermal Enthalpies = -2915.112097
Sum of electronic and thermal Free Energies = -2915.204107

Coordinates: syn-1

S 4.36120000  2.75790000  1.13280000
S 5.96040000  3.65530000  3.48990000
S 5.65260000 -0.37970000  1.44460000
S 7.29680000  0.53490000  3.76450000
O 5.51750000  6.46300000  0.81750000
O 9.20300000  4.61280000  1.87310000
O 6.84970000  3.27320000 -1.65710000
O 3.41260000  0.82140000  4.43300000
O 9.13280000 -2.13920000  1.60300000
O 7.85720000  0.54490000 -1.44280000
O 10.32510000  1.92160000  1.99180000
C 3.41760000  3.89120000  2.25680000
C 4.24270000  4.35250000  3.47450000
C 5.74630000 -1.63640000  2.80480000
C 6.59730000 -1.16560000  4.00070000
C 5.88920000  5.39030000  0.97990000
C 8.16430000  4.20290000  1.61940000
C 6.73110000  3.38580000 -0.52350000
C 4.27590000  1.11540000  3.72540000
C 8.61250000 -1.11780000  1.56430000
C 7.81920000  0.58230000 -0.29880000
C 9.31530000  1.41950000  1.79150000
H 2.52660000  3.33520000  2.56880000
H 3.08290000  4.74490000  1.65770000
H 3.77780000  4.03260000  4.41350000
H 4.33090000  5.44380000  3.50390000
H 4.71170000 -1.83360000  3.10640000
H 6.14710000 -2.55900000  2.37140000
H 6.00200000 -1.12310000  4.91940000
H 7.43740000 -1.84460000  4.18120000
Fe 6.45930000  3.72390000  1.23500000
Fe 5.58380000  1.56160000  2.65070000
Fe 7.80200000  0.46530000  1.50920000
Species: compound 2
HF energy = -3838.2756302
No imaginary frequency
Zero-point correction = 0.452055 (Hartree/Particle)
Thermal correction to Energy = 0.496605
Thermal correction to Enthalpy = 0.497549
Thermal correction to Gibbs Free Energy = 0.371654
Sum of electronic and zero-point Energies = -3837.823575
Sum of electronic and thermal Energies = -3837.779025
Sum of electronic and thermal Enthalpies = -3837.778081
Sum of electronic and thermal Free Energies = -3837.903976

Coordinates: compound 2
Fe      5.53770000  8.05910000  4.66390000
Fe      6.08510000  8.00560000  7.17930000
Fe      5.70620000  7.40350000  9.61730000
P       4.19120000  7.45950000  2.86230000
S       4.02060000  8.61220000  6.33540000
S       5.61790000  6.10970000  5.93520000
S       6.06620000  9.54220000  8.85270000
S       7.67300000  7.04960000  8.48590000
O       5.63190000 10.89210000  3.86040000
O       7.99450000  7.14820000  3.30500000
O       8.18020000  9.53410000  5.90920000
O       2.84260000  8.02100000  9.87400000
O       5.22080000  4.50590000  9.50590000
O       6.56990000  7.64880000 12.42230000
C       5.59820000  9.78290000  4.15400000
C       7.03420000  7.51780000  3.80940000
C       7.26150000  8.89800000  6.24210000
C       3.96500000  7.78410000  9.76740000
C       5.40810000  5.64140000  9.54380000
C       6.24320000  7.55610000 11.32310000
C       3.00340000  7.07250000  6.42680000
H       2.42430000  7.13290000  7.35440000
H       2.29710000  7.10800000  5.58990000
C       3.84780000  5.79280000  6.37500000
C       3.44500000  5.08690000  5.64320000
H       3.86990000  5.29030000  7.34500000
C       7.86300000  9.77550000  9.23820000
H       8.22230000 10.57450000  8.58090000
H       7.91800000 10.13680000 10.27060000
C       8.69040000  8.49160000  9.04870000
H       9.17310000  8.18650000  9.98330000
H       9.47270000  8.63610000  8.29590000
C       5.12960000  7.45010000  1.25910000
C       5.79280000  8.63010000  0.87330000
H       5.74700000  9.51610000  1.50110000
C       6.50670000  8.68830000  0.32330000
| H  | 7.01240000 | 9.61020000 | -0.60210000 |
| C  | 6.57400000 | 7.56730000 | -1.15630000 |
| H  | 7.13620000 | 7.61020000 | -2.08670000 |
| C  | 5.91410000 | 6.39480000 | -0.78760000 |
| H  | 5.95520000 | 5.51810000 | -1.43080000 |
| C  | 5.19310000 | 6.33520000 | 0.40990000  |
| H  | 4.68030000 | 5.41570000 | 0.67390000  |
| C  | 2.76900000 | 8.56370000 | 2.43360000  |
| C  | 2.21370000 | 9.43640000 | 3.38180000  |
| H  | 2.62910000 | 9.48750000 | 4.38410000  |
| C  | 1.12950000 | 10.25270000| 3.04360000  |
| H  | 0.71510000 | 10.92680000| 3.79010000  |
| C  | 0.58880000 | 10.20710000| 1.75820000  |
| H  | -0.25190000| 10.84600000| 1.49550000  |
| C  | 1.13570000 | 9.34120000 | 0.80550000  |
| H  | 0.72310000 | 9.30310000 | -0.20060000 |
| C  | 2.21840000 | 8.52720000 | 1.13790000  |
| H  | 2.64010000 | 7.86550000 | 0.38550000  |
| C  | 3.44320000 | 5.77300000 | 2.94180000  |
| C  | 2.05510000 | 5.57110000 | 2.89300000  |
| H  | 1.38390000 | 6.41720000 | 2.77710000  |
| C  | 1.52210000 | 4.28170000 | 2.99280000  |
| H  | 0.44330000 | 4.14410000 | 2.95970000  |
| C  | 2.36710000 | 3.17960000 | 3.13160000  |
| H  | 1.95130000 | 2.17720000 | 3.20850000  |
| C  | 3.75240000 | 3.36990000 | 3.17660000  |
| H  | 4.41940000 | 2.51820000 | 3.29130000  |
| C  | 4.28720000 | 4.65580000 | 3.09180000  |
| H  | 5.36420000 | 4.78800000 | 3.15650000  |
Species: compound 3
HF energy = -4761.2188321
No imaginary frequency
Zero-point correction = 0.719572 (Hartree/Particle)
Thermal correction to Energy = 0.779074
Thermal correction to Enthalpy = 0.780018
Thermal correction to Gibbs Free Energy = 0.619689
Sum of electronic and zero-point Energies = -4760.499260
Sum of electronic and thermal Energies = -4760.439759
Sum of electronic and thermal Enthalpies = -4760.438814
Sum of electronic and thermal Free Energies = -4760.599143

Coordinates: compound 3
Fe  2.75610000  3.67690000  4.37290000
Fe  3.21950000  6.13190000  4.00850000
Fe  3.20260000  8.34690000  2.69240000
P   2.72560000  1.74900000  5.61780000
P   2.68720000  9.58120000  0.78960000
S   4.82250000  4.66050000  4.68940000
S   2.16380000  5.34120000  5.86630000
S   1.31830000  7.03010000  3.04750000
S   3.95540000  6.32210000  1.81910000
O  -0.03410000  3.58260000  3.49000000
O   3.75580000  2.51920000  1.87940000
O   4.49890000  8.10810000  5.68340000
O   2.07270000 10.36780000  4.51040000
O   6.00750000  9.25830000  2.70420000
C   1.06580000  3.61080000  3.84510000
C   3.36300000  2.97090000  2.87050000
C   3.96000000  7.45690000  4.87760000
C   2.52470000  9.59340000  3.79160000
C   4.90790000  8.93140000  2.69940000
C   4.87980000  4.89930000  6.52600000
H   5.21650000  3.94790000  6.95300000
H   5.65040000  5.65160000  6.72730000
C   3.52650000  5.32650000  7.11900000
H   3.58280000  6.34240000  7.52280000
H   3.21600000  4.65640000  7.92630000
C   1.15750000  6.17610000  1.41620000
H   0.46680000  5.34020000  1.56860000
H   0.67930000  6.88360000  0.72900000
C   2.50330000  5.69550000  0.85680000
H   2.63110000  6.01430000 -0.18180000
H   2.57970000  4.60590000  0.88220000
C   1.42630000  0.53360000  5.07620000
C   0.49920000 -0.05490000  5.94980000
H   0.50700000  0.19870000  7.00580000
C  -0.44510000 -0.97130000  5.47460000
H  -1.15890000 -1.41260000  6.16780000
| Carbon | X-Coordinate | Y-Coordinate | Z-Coordinate |
|--------|--------------|--------------|--------------|
| C      | -0.47170000  | -1.31980000  | 4.12380000   |
| H      | -1.20780000  | -2.03180000  | 3.75570000   |
| C      | 0.45390000   | -0.74740000  | 3.24620000   |
| H      | 0.44500000   | -1.01240000  | 2.19080000   |
| C      | 1.39100000   | 0.17250000   | 3.71680000   |
| H      | 2.10210000   | 0.60710000   | 3.01880000   |
| C      | 4.22350000   | 0.65320000   | 5.62310000   |
| H      | 5.46390000   | 1.14490000   | 5.19030000   |
| C      | 5.54320000   | 2.16850000   | 4.83520000   |
| H      | 6.59740000   | 0.32500000   | 5.20250000   |
| C      | 7.55010000   | 0.72310000   | 4.85900000   |
| H      | 6.50480000   | -0.99490000  | 5.64520000   |
| C      | 7.38600000   | -1.63360000  | 5.65130000   |
| C      | 5.27170000   | -1.49720000  | 6.07490000   |
| H      | 5.18960000   | -2.52750000  | 6.41580000   |
| C      | 4.13980000   | -0.68190000  | 6.06160000   |
| H      | 3.18510000   | -1.08730000  | 6.38850000   |
| C      | 2.36110000   | 1.98140000   | 7.41850000   |
| C      | 3.26170000   | 1.61300000   | 8.43000000   |
| H      | 4.19440000   | 1.11780000   | 8.17530000   |
| C      | 2.97090000   | 1.87780000   | 9.77290000   |
| H      | 3.68390000   | 1.58860000   | 10.54270000  |
| C      | 1.77470000   | 2.50510000   | 10.12420000  |
| H      | 1.54900000   | 2.70900000   | 11.16900000  |
| C      | 0.86920000   | 2.87590000   | 9.12410000   |
| H      | -0.06310000  | 3.37230000   | 9.38550000   |
| C      | 1.16360000   | 2.62610000   | 7.78350000   |
| H      | 0.46340000   | 2.94470000   | 7.01520000   |
| C      | 2.87250000   | 8.70180000   | -0.82510000  |
| C      | 4.11170000   | 8.11110000   | -1.13740000  |
| H      | 4.93930000   | 8.17690000   | -0.43600000  |
| C      | 4.28590000   | 7.42020000   | -2.33690000  |
| H      | 5.25070000   | 6.97060000   | -2.56160000  |
| C      | 3.22160000   | 7.29180000   | -3.23570000  |
| H      | 3.35580000   | 6.74390000   | -4.16600000  |
| C      | 1.98590000   | 7.86420000   | -2.92970000  |
| H      | 1.15090000   | 7.76620000   | -3.62050000  |
| C      | 1.81160000   | 8.56940000   | -1.73430000  |
| H      | 0.84520000   | 9.01410000   | -1.51470000  |
| C      | 1.01500000   | 10.36960000  | 0.67860000   |
| C      | 0.80480000   | 11.46320000  | -0.18340000  |
| H      | 1.62890000   | 11.86000000  | -0.77100000  |
| C      | -0.45590000  | 12.05100000  | -0.28780000  |
| H      | -0.60140000  | 12.89680000  | -0.95690000  |
| C      | -1.52500000  | 11.56050000  | 0.46920000   |
| H      | -2.50660000  | 12.02370000  | 0.39070000   |
| C      | -1.32560000  | 10.48010000  | 1.32930000   |
| H      | -2.14880000  | 10.09500000  | 1.92730000   |
| C      | -0.06350000  | 9.88660000   | 1.43530000   |
HOMO

LUMO
Species: compound 4
2 Complete list of authors for reference 58

(58) Gaussian 09, Revision A.02: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
3 Electrochemical and electrocatalytic studies

a. Oxidation response of 2 over a range of scan rates

Figure S1. CVs of 2 (0.5 mM) in 0.5 M TBAPF$_6$ in dichloromethane (a) at 0.01 (black), 0.02 (brown), 0.05 (dark green) and 0.1 V s$^{-1}$ (light green); b) at 0.1 (black), 1 (brown), 5 (dark green) and 10 V s$^{-1}$ (light green); c) Plot of $i_p$ v$1/2$ against v$1/2$ for the oxidation peak.

The oxidation behavior of the complexes was studied in detail over scan rates of 0.01 – 10 V s$^{-1}$, as shown for 2 in Figure ESI 1 a and b. At all scan rates one oxidation peak occurs, which shifts to higher potentials with increasing scan rate thus indicating quasi-reversibility. The corresponding reduction peak consists of two overlapping processes taking place at a similar potential, which at scan rates above 1 V s$^{-1}$ can be resolved into two components. The first is centered at 0.05 V with a position independent of scan rate and the second, at -0.15 V (at 1 V s$^{-1}$), shifts to more negative potentials at faster scan rates indicating quasi-reversibility. This
would suggest that after the first oxidation the product undergoes chemical or structural change allowing further loss of an electron at a similar potential.

Figure ESI 1c shows a plot of peak current normalized by dividing by square root of scan rate vs. square root of scan rate, which reveals that twice as many electrons are transferred at low scan rates than high; thus we suggest a one electron transfer at fast scan rates that tends to two electrons as the electrochemical timescale is increased. This would suggest that after the first oxidation the product undergoes chemical or structural change allowing further loss of an electron at a similar potential. The rate of this chemical step is likely to be different for complexes with different degrees of substitution and may explain why fewer electrons are involved in oxidation of 3 than the other two complexes.

b. Cyclic voltammetry of 1 in CO-saturated solution

![Cyclic Voltammogram](image)

**Figure S2:** CV at 0.1 Vs\(^{-1}\) of 0.5 mM 1 in 0.1 M TBAPF\(_6\) / dichloromethane in Ar-saturated (black) and CO-saturated (brown) solution.

The CV of 1 was carried out in a CO saturated solution, where the first oxidation and reduction peaks were unchanged in position and magnitude. Additional reduction peaks were observed at -1.87 V and -2.1 V, along with oxidation peaks at -1.7 V (associated with the
reduction at -1.87 V -0.85 V and 0.82 V. Reduction of [Fe₂(CO)₆(µ-edt)] under the same experimental conditions occurs reversibly at -1.9 V vs. Fc/Fc⁺ [20,22] We therefore tentatively assign the reduction response at -1.87 V to this diiron complex, formed as a decomposition product after the reduction of 1. A common decomposition process for these complexes after reduction is the loss of a CO ligand and rapid dimerisation of the remaining products [20,49], which is suppressed in excess CO. The observation that reversibility of the reduction of 1 is not improved in a CO-saturated solution suggests that CO ligand loss is not a major decomposition route in this case and cleavage of iron-sulfur bond(s) and fragmentation of the cluster into di- and mono-iron complexes is most likely.

c. CVs of complexes 4-6 in dichloromethane

![Graph](image)

**Figure S3.** CVs of 0.5 mM 4 (black), 5 (brown) and 6 (green) in CH₂Cl₂ (0.5 mM solution, supporting electrolyte [NBu₄][PF₆], scan rate 0.1 Vs⁻¹, glassy carbon electrode, potential vs Fc⁺/Fc).

d. Electrocatalysis of 4 in MeCN
Figure S4. CVs of 4 in the absence of acid and in the presence of 1 to 10 molar equivalents of HBF₄ as shown in the legend (1 mM solution in acetonitrile, supporting electrolyte [NBu₄][PF₆], scan rate 0.1Vs⁻¹, glassy carbon electrode, potential vs Fc⁺/Fc).

In acetonitrile addition of one molar equivalent of acid to 4 results in two new reduction peaks at $E_p = -1.63$ V and $E_p = -2.26$ V, in addition to the reduction peaks at $E_p = -1.89$ V and $E_p = -2.70$ V associated with 4 in the absence of acid. All the peak currents increase with acid concentration. The shift in reduction to less negative potentials on addition of acid is indicative of protonation of neutral 4 taking place before reduction, i.e. a CE mechanism. Asymmetric diphosphine substitution of these complexes results in sufficient basicity for protonation to take place in MeCN, allowing the electrocatalytic reduction of protons to take place at ca. 0.2 V more positive than the reduction potential of the complex.

e. DigiSim simulation for 1st catalytic process for 2
**Figure S5:** Simulated CVs for 2 (black) and 1 (grey) obtained from DigiSim using the mechanism and parameters given in the text and in ref [23] from main document.

The electrocatalytic response of 1 has been reported previously [23] and rate constants for the protonation steps obtained from simulated results for a very simple ECEC mechanism. A similar mechanism is presented for 2 below (Red text indicates parameters that differ between 1 and 2), and simulated CVs of this mechanism are shown above.

\[
\begin{align*}
    & 
    \begin{array}{c}
    2 \quad E = -1.7 \text{ V} \\
    \quad + e^- \\
    \quad - e^- \\
    \quad K = 10^4 \\
    \quad k_f = 50 \\
    \quad \text{Products}
    \end{array}
    \quad \rightarrow \\
    \begin{array}{c}
    2^- \quad E = -1.6 \text{ V} \\
    \quad + H^+ \\
    \quad - H^+ \\
    \quad K(1) = 10^{10} \\
    \quad k(1) = 10^6 \\
    \quad \text{Products}
    \end{array}
\end{align*}
\]

\[K(2) = 10^{10} \quad + H^+ \quad H^+ \quad - H_2 \quad - H_2\]
\[k(2) = 2 \times 10^4 \quad - H_2 \quad + H_2\]

\[2H^- \quad E = -1.6 \text{ V} \]
Neutral $2$ undergoes reduction at ca. -1.7 V and the resulting $2^-$ species can either undergo further reaction to undefined ‘products’ or protonate to give $2\text{H}$. The rate and equilibrium constants for the non-catalytic route to ‘products’ were obtained by simulating voltammograms for $2$ obtained in the absence of acid and comparing their scan rate dependence with experimental CVs. The equilibrium constant $K(1) = 10^{10}$ for protonation of $2^-$ reflects the difference in pKa of $2^-$ and the strong acid HBF$_4$. $2\text{H}$ then undergoes further reduction to form $2\text{H}^-$ followed by a simultaneous proton addition / hydrogen elimination step. The equilibrium constant $K(2)$ for this step again reflects the difference in pKa of the acid and $2\text{H}^-$ species. The two rate constants $k(1)$ and $k(2)$ for the protonation steps have been varied in the simulation until a fit to the experimental peak currents was obtained. The simulated peak currents are plotted against experimental peak currents for $1$ and $2$ in Figure 6 of the main document.

We have previously reported a value of $k(1)$ of $1 \times 10^5$ mol$^{-1}$ dm$^{-6}$ s$^{-1}$ for complex $1$ compared to $k(1)$ of $1 \times 10^6$ mol$^{-1}$ dm$^{-6}$ s$^{-1}$ found here for $2$. Likewise, the rate constant $k(2)$ for $2$ is found to be greater than for $1$: $2 \times 10^4$ mol$^{-1}$ dm$^{-6}$ s$^{-1}$ compared to $3 \times 10^3$ mol$^{-1}$ dm$^{-6}$ s$^{-1}$. This supports the argument that rate of catalysis increases with basicity of the complex and protonation is the rate limiting step for complex $1$. 
Table 1. Crystal data and structure refinement for str0701 (1).

| Property                                      | Value |
|-----------------------------------------------|-------|
| Identification code                           | str0701 |
| Chemical formula                              | C₁₉H₈Fe₃O₇S₄ |
| Formula weight                                | 547.96 |
| Temperature                                   | 150(2) K |
| Radiation, wavelength                         | MoKα, 0.71073 Å |
| Crystal system, space group                   | triclinic, P1bar |
| Unit cell parameters                          | a = 6.4228(14) Å, α = 77.541(3)°, b = 8.2906(18) Å, β = 83.384(3)°, c = 18.331(4) Å, γ = 68.854(3)° |
| Cell volume                                   | 888.2(3) Å³ |
| Z                                             | 2 |
| Calculated density                            | 2.049 g/cm³ |
| Absorption coefficient μ                       | 2.918 mm⁻¹ |
| F(000)                                        | 544 |
| Crystal colour and size                       | red, 0.14 × 0.14 × 0.03 mm³ |
| Data collection method                        | Bruker SMART APEX diffractometer |
| ω rotation with narrow frames                  | |
| θ range for data collection                   | 1.14 to 28.28° |
| Index ranges                                  | h = −8 to 8, k = −10 to 10, l = −23 to 24 |
| Completeness to θ = 26.00°                    | 95.7% |
| Reflections collected                         | 7497 |
| Independent reflections                       | 3970 (Rint = 0.0333) |
| Reflections with F²>2σ                        | 3453 |
| Absorption correction                         | semi-empirical from equivalents |
| Min. and max. transmission                    | 0.6855 and 0.9176 |
| Structure solution                            | Patterson synthesis |
| Refinement method                             | Full-matrix least-squares on F² |
| Weighting parameters a, b                      | 0.0957, 0.3371 |
| Data / restraints / parameters                | 3970 / 0 / 226 |
| Final R indices [F²>2σ]                        | R₁ = 0.0417, wR₂ = 0.1248 |
| R indices (all data)                          | R₁ = 0.0480, wR₂ = 0.1411 |
| Goodness-of-fit on F²                          | 1.051 |
| Largest and mean shift/su                     | 0.000 and 0.000 |
| Largest diff. peak and hole                   | 1.362 and −0.649 e Å⁻³ |
Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å\(^2\)) for str0701. \(U_{eq}\) is defined as one third of the trace of the orthogonalized \(U^{ij}\) tensor.

|      | x         | y         | z         | \(U_{eq}\) |
|------|-----------|-----------|-----------|-------------|
| Fe(1)| 0.49104(9)| 0.18472(7)| 0.12332(3)| 0.01900(16) |
| Fe(2)| 0.45340(8)| 0.05416(6)| 0.26069(3)| 0.01601(16) |
| Fe(3)| 0.52323(8)| -0.20844(6)| 0.37009(3)| 0.01768(16)|
| S(1) | 0.77282(15)| 0.07540(12)| 0.20364(5)| 0.0191(2)   |
| S(2) | 0.47024(15)| -0.08479(11)| 0.16718(5)| 0.0188(2)   |
| S(3) | 0.52767(15)| 0.05756(12)| 0.37525(5)| 0.0196(2)   |
| S(4) | 0.19084(15)| -0.04207(12)| 0.32264(5)| 0.0202(2)   |
| O(1) | 0.7607(6)| 0.0944(5)| -0.01223(18)| 0.0445(9)   |
| O(2) | 0.5150(6)| 0.5388(4)| 0.1039(2)| 0.0459(9)   |
| O(3) | 0.0485(5)| 0.3139(5)| 0.0581(2)| 0.0441(9)   |
| O(4) | 0.1328(5)| 0.4110(4)| 0.24480(18)| 0.0341(7)   |
| O(5) | 1.0014(5)| -0.3758(4)| 0.3984(2)| 0.0407(8)   |
| O(6) | 0.5304(6)| -0.4978(4)| 0.30040(19)| 0.0393(8)   |
| O(7) | 0.3501(6)| -0.3226(4)| 0.51996(17)| 0.0389(8)   |
| C(1) | 0.6539(7)| 0.1340(5)| 0.0398(2)| 0.0274(9)   |
| C(2) | 0.5048(7)| 0.4029(5)| 0.1128(2)| 0.0269(8)   |
| C(3) | 0.2184(7)| 0.2630(5)| 0.0841(2)| 0.0287(9)   |
| C(4) | 0.2685(7)| 0.2742(5)| 0.2432(2)| 0.0234(8)   |
| C(5) | 0.8171(7)| -0.3069(5)| 0.3850(2)| 0.0254(8)   |
| C(6) | 0.5271(7)| -0.3852(5)| 0.3266(2)| 0.0232(8)   |
| C(7) | 0.4207(7)| -0.2793(5)| 0.4623(2)| 0.0265(8)   |
| C(8) | 0.9194(6)| -0.1438(5)| 0.1826(2)| 0.0222(8)   |
| C(9) | 0.7642(6)| -0.2232(5)| 0.1587(2)| 0.0232(8)   |
| C(10)| 0.2491(6)| 0.1588(5)| 0.4170(2)| 0.0257(8)   |
| C(11)| 0.0713(6)| 0.1072(5)| 0.3892(2)| 0.0265(8)   |
Table 3. Bond lengths [Å] and angles [°] for str0701.

| Bond                  | Length       | Bond                  | Length       |
|-----------------------|--------------|-----------------------|--------------|
| Fe(1)–C(1)            | 1.790(4)     | Fe(1)–C(3)            | 1.809(4)     |
| Fe(1)–C(2)            | 1.810(4)     | Fe(1)–S(2)            | 2.2521(11)   |
| Fe(1)–S(1)            | 2.2627(11)   | Fe(1)–Fe(2)           | 2.5385(8)    |
| Fe(2)–C(4)            | 1.765(4)     | Fe(2)–S(3)            | 2.2146(11)   |
| Fe(2)–S(4)            | 2.2155(11)   | Fe(2)–S(2)            | 2.2353(11)   |
| Fe(2)–S(1)            | 2.2406(11)   | Fe(2)–Fe(3)           | 2.5655(8)    |
| Fe(3)–C(5)            | 1.793(4)     | Fe(3)–C(7)            | 1.797(4)     |
| Fe(3)–C(6)            | 1.805(4)     | Fe(3)–S(4)            | 2.2367(11)   |
| Fe(3)–S(3)            | 2.2381(11)   | S(1)–C(8)             | 1.823(4)     |
| S(2)–C(9)             | 1.831(4)     | S(3)–C(10)            | 1.836(4)     |
| S(4)–C(11)            | 1.833(4)     | O(1)–C(1)             | 1.145(5)     |
| O(2)–C(2)             | 1.129(5)     | O(3)–C(3)             | 1.139(5)     |
| O(4)–C(4)             | 1.158(5)     | O(5)–C(5)             | 1.143(5)     |
| O(6)–C(6)             | 1.131(5)     | O(7)–C(7)             | 1.138(5)     |
| C(8)–C(9)             | 1.522(5)     | C(10)–C(11)           | 1.527(6)     |
|                       |              |                       |              |
| C(1)–Fe(1)–C(3)       | 97.48(19)    | C(1)–Fe(1)–C(2)       | 95.69(19)    |
| C(3)–Fe(1)–C(2)       | 94.20(18)    | C(1)–Fe(1)–S(2)       | 96.68(14)    |
| C(3)–Fe(1)–S(2)       | 91.48(13)    | C(2)–Fe(1)–S(2)       | 165.59(14)   |
| C(1)–Fe(1)–S(1)       | 98.11(13)    | C(3)–Fe(1)–S(1)       | 163.24(14)   |
| C(2)–Fe(1)–S(1)       | 90.35(13)    | S(2)–Fe(1)–S(1)       | 80.63(4)     |
| C(1)–Fe(1)–Fe(2)      | 141.34(13)   | C(3)–Fe(1)–Fe(2)      | 108.13(14)   |
| C(2)–Fe(1)–Fe(2)      | 110.37(14)   | S(2)–Fe(1)–Fe(2)      | 55.24(3)     |
| S(1)–Fe(1)–Fe(2)      | 55.28(3)     | C(4)–Fe(2)–S(3)       | 95.38(13)    |
| C(4)–Fe(2)–S(4)       | 92.57(14)    | S(3)–Fe(2)–S(4)       | 81.76(4)     |
| C(4)–Fe(2)–S(2)       | 112.05(13)   | S(3)–Fe(2)–S(2)       | 152.18(4)    |
| S(4)–Fe(2)–S(2)       | 92.09(4)     | C(4)–Fe(2)–S(1)       | 102.59(14)   |
| S(3)–Fe(2)–S(1)       | 97.52(4)     | S(4)–Fe(2)–S(1)       | 164.81(4)    |
| S(2)–Fe(2)–S(1)       | 81.48(4)     | C(4)–Fe(2)–Fe(1)      | 70.99(13)    |
| S(3)–Fe(2)–Fe(1)      | 144.18(4)    | S(4)–Fe(2)–Fe(1)      | 130.32(3)    |
| S(2)–Fe(2)–Fe(1)      | 55.86(3)     | S(1)–Fe(2)–Fe(1)      | 56.10(3)     |
| C(4)–Fe(2)–Fe(3)      | 136.25(13)   | S(3)–Fe(2)–Fe(3)      | 55.25(3)     |
| S(4)–Fe(2)–Fe(3)      | 55.20(3)     | S(2)–Fe(2)–Fe(3)      | 99.13(4)     |
| S(1)–Fe(2)–Fe(3)      | 112.03(3)    | Fe(1)–Fe(2)–Fe(3)     | 151.74(3)    |
| C(5)–Fe(3)–C(7)       | 98.79(19)    | C(5)–Fe(3)–C(6)       | 91.75(18)    |
| C(7)–Fe(3)–C(6)       | 99.36(18)    | C(5)–Fe(3)–S(4)       | 163.63(13)   |
| C(7)–Fe(3)–S(4)       | 96.95(14)    | C(6)–Fe(3)–S(4)       | 90.11(13)    |
| C(5)–Fe(3)–S(3)       | 91.32(13)    | C(7)–Fe(3)–S(3)       | 102.86(13)   |
| C(6)–Fe(3)–S(3)       | 156.81(13)   | S(4)–Fe(3)–S(3)       | 80.78(4)     |
| C(5)–Fe(3)–Fe(2)      | 109.39(13)   | C(7)–Fe(3)–Fe(2)      | 143.02(13)   |
| C(6)–Fe(3)–Fe(2)      | 103.11(12)   | S(4)–Fe(3)–Fe(2)      | 54.43(3)     |
| S(3)–Fe(3)–Fe(2)      | 54.39(3)     | C(8)–S(1)–Fe(2)       | 103.01(12)   |
| C(8)–S(1)–Fe(1)       | 102.13(15)   | Fe(2)–S(1)–Fe(1)      | 68.62(3)     |
| C(9)–S(2)–Fe(2)       | 104.89(13)   | C(9)–S(2)–Fe(1)       | 100.80(13)   |
| Fe(2)–S(2)–Fe(1)      | 69.90(3)     | C(10)–S(3)–Fe(2)      | 102.78(13)   |
| C(10)–S(3)–Fe(3)      | 101.56(14)   | Fe(2)–S(3)–Fe(3)      | 70.36(3)     |
| C(11)–S(4)–Fe(2)      | 103.06(14)   | C(11)–S(4)–Fe(3)      | 102.08(13)   |
| Fe(2)–S(4)–Fe(3)      | 70.37(4)     | O(1)–C(1)–Fe(1)       | 177.2(4)     |
| O(2)–C(2)–Fe(1)       | 177.8(4)     | O(3)–C(3)–Fe(1)       | 178.5(4)     |
| Bond                  | Angle (°) | Bond                  | Angle (°) | Bond                  | Angle (°) |
|----------------------|-----------|----------------------|-----------|----------------------|-----------|
| O(4)–C(4)–Fe(2)      | 167.6(4)  | O(5)–C(5)–Fe(3)      | 175.9(4)  |
| O(6)–C(6)–Fe(3)      | 178.9(4)  | O(7)–C(7)–Fe(3)      | 178.2(4)  |
| C(9)–C(8)–S(1)       | 112.9(3)  | C(8)–C(9)–S(2)       | 111.9(3)  |
| C(11)–C(10)–S(3)     | 112.3(3)  | C(10)–C(11)–S(4)     | 111.6(3)  |
Table 4. Anisotropic displacement parameters (Å\(^2\)) for str0701. The anisotropic displacement factor exponent takes the form: 
\[-2\pi^2 h^2 a^* a U_{11} + \ldots + 2hka^* b^* U_{12}\]

|     | U\(^{11}\)   | U\(^{22}\)   | U\(^{33}\)   | U\(^{23}\)   | U\(^{13}\)   | U\(^{12}\)   |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Fe(1)| 0.0196(3)    | 0.0183(3)    | 0.0180(3)    | 0.0016(2)    | 0.0059(2)    | 0.0066(2)    |
| Fe(2)| 0.0148(3)    | 0.0148(3)    | 0.0170(3)    | -0.00056(19) | -0.00403(19) | -0.0039(2)   |
| Fe(3)| 0.0176(3)    | 0.0148(3)    | 0.0188(3)    | 0.0002(2)    | -0.0046(2)   | -0.0041(2)   |
| S(1) | 0.0160(4)    | 0.0198(4)    | 0.0215(4)    | -0.0003(3)   | -0.0052(3)   | -0.0067(3)   |
| S(2) | 0.0176(4)    | 0.0181(4)    | 0.0210(4)    | -0.0023(3)   | -0.0040(3)   | -0.0064(3)   |
| S(3) | 0.0214(5)    | 0.0180(4)    | 0.0196(5)    | -0.0033(3)   | -0.0050(3)   | -0.0058(3)   |
| S(4) | 0.0161(4)    | 0.0234(5)    | 0.0209(5)    | -0.0015(4)   | -0.0037(3)   | -0.0071(4)   |
| O(1) | 0.041(2)     | 0.058(2)     | 0.0244(17)   | -0.0049(15)  | -0.0017(14)  | -0.0079(17)  |
| O(2) | 0.057(2)     | 0.0263(17)   | 0.057(2)     | 0.0012(15)   | -0.0111(18)  | -0.0209(16)  |
| O(3) | 0.0269(17)   | 0.046(2)     | 0.052(2)     | 0.0073(16)   | -0.0249(15)  | -0.0067(15)  |
| O(4) | 0.0322(17)   | 0.0225(15)   | 0.0338(17)   | 0.0001(12)   | -0.0049(13)  | 0.0049(13)   |
| O(5) | 0.0249(17)   | 0.0305(17)   | 0.061(2)     | 0.0013(15)   | -0.0086(15)  | -0.0061(13)  |
| O(6) | 0.057(2)     | 0.0285(16)   | 0.0367(18)   | -0.0090(13)  | -0.0053(15)  | -0.0180(16)  |
| O(7) | 0.053(2)     | 0.0259(16)   | 0.0260(16)   | 0.0004(12)   | 0.0087(14)   | 0.0060(15)   |
| C(1) | 0.026(2)     | 0.029(2)     | 0.023(2)     | 0.0057(16)   | -0.0091(16)  | -0.0077(17)  |
| C(2) | 0.028(2)     | 0.0226(19)   | 0.028(2)     | 0.0009(16)   | -0.0099(16)  | -0.0061(16)  |
| C(3) | 0.032(2)     | 0.0220(19)   | 0.028(2)     | 0.0007(16)   | -0.0016(17)  | -0.0066(17)  |
| C(4) | 0.025(2)     | 0.0221(18)   | 0.0186(18)   | 0.0004(14)   | -0.0063(14)  | -0.0039(16)  |
| C(5) | 0.029(2)     | 0.0194(18)   | 0.026(2)     | -0.0015(15)  | -0.0022(16)  | -0.0088(16)  |
| C(6) | 0.0232(19)   | 0.0183(18)   | 0.0241(19)   | 0.0006(15)   | -0.0036(15)  | -0.0042(15)  |
| C(7) | 0.033(2)     | 0.0164(17)   | 0.026(2)     | -0.0039(15)  | -0.0040(16)  | -0.0029(16)  |
| C(8) | 0.0166(18)   | 0.0224(18)   | 0.0233(19)   | -0.0038(15)  | 0.0005(14)   | -0.0022(14)  |
| C(9) | 0.0186(18)   | 0.0204(18)   | 0.0261(19)   | -0.0050(15)  | -0.0023(14)  | -0.0008(14)  |
| C(10)| 0.022(2)     | 0.0244(19)   | 0.028(2)     | -0.0093(16)  | -0.0036(15)  | -0.0013(15)  |
| C(11)| 0.0165(18)   | 0.028(2)     | 0.026(2)     | -0.0045(16)  | -0.0026(14)  | 0.0028(15)   |
Table 5. Hydrogen coordinates and isotropic displacement parameters (Å$^2$) for str0701.

|   | x      | y      | z      | U    |
|---|--------|--------|--------|------|
| H(8A) | 1.0340 | −0.1372 | 0.1422 | 0.027 |
| H(8B) | 0.9973 | −0.2224 | 0.2275 | 0.027 |
| H(9A) | 0.7873 | −0.3410 | 0.1900 | 0.028 |
| H(9B) | 0.8022 | −0.2382 | 0.1061 | 0.028 |
| H(10A) | 0.2540 | 0.1223 | 0.4721 | 0.031 |
| H(10B) | 0.2075 | 0.2885 | 0.4049 | 0.031 |
| H(11A) | −0.0456 | 0.2146 | 0.3648 | 0.032 |
| H(11B) | −0.0002 | 0.0490 | 0.4323 | 0.032 |
Table 6. Torsion angles [°] for str0701.

| Bond                  | Value 1 | Value 2 | Value 3 |
|-----------------------|---------|---------|---------|
| C(1)–Fe(1)–Fe(2)–C(4)| 174.4(3)|         |         |
| C(2)–Fe(1)–Fe(2)–C(4)| 45.1(2) |         |         |
| S(1)–Fe(1)–Fe(2)–C(4)| 120.62(14)|       |         |
| C(3)–Fe(1)–Fe(2)–S(3)| −128.76(15)|     |         |
| S(2)–Fe(1)–Fe(2)–S(3)| 152.44(7)|       |         |
| C(1)–Fe(1)–Fe(2)–S(4)| −108.9(2)|         |         |
| C(2)–Fe(1)–Fe(2)–S(4)| 121.75(14)|       |         |
| S(1)–Fe(1)–Fe(2)–S(4)| −162.69(5)|     |         |
| C(3)–Fe(1)–Fe(2)–S(4)| 78.81(14)|       |         |
| S(2)–Fe(1)–Fe(2)–S(4)| −103.87(4)|     |         |
| C(4)–Fe(2)–Fe(3)–C(5)| −133.1(2)|         |         |
| S(4)–Fe(2)–Fe(3)–C(5)| 177.18(15)|     |         |
| C(S)–Fe(2)–Fe(3)–C(5)| 6.57(15)|       |         |
| C(4)–Fe(2)–Fe(3)–C(7)| 4.3(3)|       |         |
| S(4)–Fe(2)–Fe(3)–C(7)| −45.4(2)|         |         |
| S(1)–Fe(2)–Fe(3)–C(7)| 144.0(2)|       |         |
| C(4)–Fe(2)–Fe(3)–C(6)| 130.2(2)|       |         |
| S(4)–Fe(2)–Fe(3)–C(6)| 80.56(13)|       |         |
| C(1)–Fe(2)–Fe(3)–C(6)| −90.05(13)|     |         |
| S(1)–Fe(2)–Fe(3)–C(6)| 49.69(19)|       |         |
| S(2)–Fe(2)–Fe(3)–C(6)| −86.17(4)|       |         |
| Fe(1)–Fe(2)–Fe(3)–S(3)| −111.81(6)|     |         |
| S(4)–Fe(2)–Fe(3)–S(3)| −105.65(5)|     |         |
| S(1)–Fe(2)–Fe(3)–S(3)| 83.74(4)|       |         |
| C(4)–Fe(2)–S(1)–C(8)| −154.59(19)|     |         |
| S(4)–Fe(2)–S(1)–C(8)| 21.9(2)|       |         |
| C(1)–Fe(2)–S(1)–C(8)| −98.12(13)|     |         |
| Fe(1)–Fe(2)–S(1)–C(8)| 52.86(13)|       |         |
| C(4)–Fe(2)–S(1)–Fe(1)| −56.48(13)|     |         |
| S(4)–Fe(2)–S(1)–Fe(1)| 120.04(15)|     |         |
| Fe(3)–Fe(2)–S(1)–Fe(1)| 150.80(3)|       |         |
| C(3)–Fe(1)–S(1)–C(8)| 108.3(5)|       |         |
| S(2)–Fe(1)–S(1)–C(8)| 45.45(13)|       |         |
| C(1)–Fe(1)–S(1)–C(8)| −149.42(14)|     |         |
| C(2)–Fe(1)–S(1)–C(8)| 114.78(14)|     |         |
| C(4)–Fe(2)–S(2)–C(9)| 141.7(2)|       |         |
| S(4)–Fe(2)–S(2)–C(9)| −124.70(14)|     |         |
| Fe(1)–Fe(2)–S(2)–C(9)| 96.04(14)|       |         |
| Fe(3)–Fe(2)–S(2)–C(9)| 45.63(15)|       |         |
| S(4)–Fe(2)–S(2)–Fe(1)| 139.26(4)|       |         |
| Fe(3)–Fe(2)–S(2)–Fe(1)| −165.67(3)|     |         |
| C(3)–Fe(1)–S(2)–C(9)| 146.91(19)|     |         |
| S(1)–Fe(1)–S(2)–C(9)| −47.96(13)|     |         |
| Bond                        | Value 1  | Value 2  | Value 3  |
|-----------------------------|----------|----------|----------|
| C(1)–Fe(1)–S(2)–Fe(2)      | 151.14(13)|         | -111.16(14)|
| C(2)–Fe(1)–S(2)–Fe(2)      | 2.1(5)    |          | 53.97(3)  |
| C(4)–Fe(2)–S(3)–C(10)      | 46.98(19) |          | -44.85(14)|
| S(2)–Fe(2)–S(3)–C(10)      | -123.57(16)|        | 150.47(14)|
| Fe(1)–Fe(2)–S(3)–C(10)     | 111.59(15)|         | -97.88(14)|
| C(4)–Fe(2)–S(3)–Fe(3)      | 144.86(14)|         | 53.03(3)  |
| S(2)–Fe(2)–S(3)–Fe(3)      | -25.68(9) |          | -111.65(4)|
| Fe(1)–Fe(2)–S(3)–Fe(3)     | -150.52(5)|        | 99.60(14) |
| C(4)–Fe(2)–S(3)–Fe(3)      | 113.07(13)|         | -147.60(14)|
| S(2)–Fe(2)–S(3)–Fe(3)      | 144.86(14)|         | 133.62(19)|
| Fe(1)–Fe(2)–S(3)–Fe(3)     | -112.86(13)|       | 53.03(3)  |
| C(4)–Fe(2)–S(3)–Fe(3)      | -106.10(13)|       | 52.48(3)  |
| S(2)–Fe(2)–S(3)–Fe(3)      | 93.5(3)   |          | 99.60(14) |
| C(4)–Fe(2)–S(3)–Fe(3)      | -19(8)    |          | 62(8)     |
| C(4)–Fe(2)–S(3)–Fe(3)      | 20(8)     |          | 20(10)    |
| C(4)–Fe(2)–S(3)–Fe(3)      | -78(10)   |          | 169(10)   |
| C(4)–Fe(2)–S(3)–Fe(3)      | 118(10)   |          | 171(10)   |
| C(4)–Fe(2)–S(3)–Fe(3)      | -38(17)   |          | 59(17)    |
| C(4)–Fe(2)–S(3)–Fe(3)      | -135(17)  |          | 164(17)   |
| C(4)–Fe(2)–S(3)–Fe(3)      | 172(17)   |          | -42.6(18) |
| C(4)–Fe(2)–S(3)–Fe(3)      | 39.3(18)  |          | 132.6(17) |
| C(4)–Fe(2)–S(3)–Fe(3)      | -141.6(17)|          | 171.4(18) |
| C(4)–Fe(2)–S(3)–Fe(3)      | 0.5(19)   |          | 17(5)     |
| C(4)–Fe(2)–S(3)–Fe(3)      | -83(5)    |          | -180(100)|
| C(4)–Fe(2)–S(3)–Fe(3)      | 120(5)    |          | 172(5)    |
| C(4)–Fe(2)–S(3)–Fe(3)      | 65(20)    |          | -34(20)   |
| C(4)–Fe(2)–S(3)–Fe(3)      | -131(20)  |          | 162(19)   |
| C(4)–Fe(2)–S(3)–Fe(3)      | 175(100)  |          | -172(11)  |
| C(4)–Fe(2)–S(3)–Fe(3)      | -79(11)   |          | 13(11)    |
| C(4)–Fe(2)–S(3)–Fe(3)      | 95(11)    |          | 48(11)    |
| C(4)–Fe(2)–S(3)–Fe(3)      | 38.3(3)   |          | -32.2(3)  |
| C(4)–Fe(2)–S(3)–Fe(3)      | -5.9(4)   |          | -29.2(3)  |
| C(4)–Fe(2)–S(3)–Fe(3)      | 41.6(3)   |          | 35.0(3)   |
| C(4)–Fe(2)–S(3)–Fe(3)      | -37.3(3)  |          | 0.4(4)    |
| C(4)–Fe(2)–S(3)–Fe(3)      | -35.6(3)  |          | 36.8(3)   |
Table 1. Crystal data and structure refinement for str0734 (2).

| Identification code  | str0734          |
|----------------------|------------------|
| Chemical formula     | C_{28}H_{23}Fe_{3}O_{6}PS_{4} |
| Formula weight       | 782.22           |
| Temperature          | 150(2) K         |
| Radiation, wavelength| MoKα, 0.71073 Å  |
| Crystal system, space group | triclinic, P1bar |
| Unit cell parameters |                  |
| a = 8.799(5) Å      | α = 90.571(7)°  |
| b = 11.268(6) Å     | β = 90.498(14)° |
| c = 16.543(9) Å     | γ = 109.469(8)° |
| Cell volume          | 1546.2(14) Å³    |
| Z                    | 2                |
| Calculated density   | 1.680 g/cm³      |
| Absorption coefficient μ | 1.751 mm⁻¹     |
| F(000)               | 792              |
| Crystal colour and size | orange, 0.26 × 0.10 × 0.03 mm³ |
| Data collection method | Bruker SMART APEX diffractometer |
| θ range for data collection | 1.92 to 28.50° |
| Index ranges         | h −11 to 11, k −14 to 14, l −21 to 20 |
| Completeness to θ = 26.00° | 96.0% |
| Reflections collected | 12859           |
| Independent reflections | 6918 (R_{int} = 0.0526) |
| Reflections with F^2 > 2σ | 5013          |
| Absorption correction | semi-empirical from equivalents |
| Min. and max. transmission | 0.6588 and 0.9493 |
| Structure solution   | direct methods   |
| Refinement method    | Full-matrix least-squares on F^2 |
| Weighting parameters a, b | 0.1153, 23.3869 |
| Data / restraints / parameters | 6918 / 0 / 379 |
| Final R indices [F^2 > 2σ] | R1 = 0.0943, wR2 = 0.2600 |
| R indices (all data)  | R1 = 0.1181, wR2 = 0.2787 |
| Goodness-of-fit on F^2 | 1.052          |
| Largest and mean shift/su | 0.000 and 0.000 |
| Largest diff. peak and hole | 1.045 and −1.726 e Å⁻³ |
Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å$^2$) for str0734. $U_{eq}$ is defined as one third of the trace of the orthogonalized $U^i$ tensor.

|       | x         | y         | z         | $U_{eq}$  |
|-------|-----------|-----------|-----------|-----------|
| Fe(1) | 0.96236(15)| 0.75489(12)| 0.27600(7)| 0.0210(3) |
| Fe(2) | 1.02441(15)| 0.75027(12)| 0.42629(7)| 0.0210(3) |
| Fe(3) | 0.93980(15)| 0.73262(13)| 0.57610(8)| 0.0254(3) |
| P(1)  | 0.7852(3)  | 0.7072(2)  | 0.17239(14)| 0.0234(5) |
| S(1)  | 0.8304(3)  | 0.8181(2)  | 0.37425(13)| 0.0247(5) |
| S(2)  | 0.8856(3)  | 0.5792(2)  | 0.35165(14)| 0.0249(5) |
| S(3)  | 1.1034(3)  | 0.9050(2)  | 0.51675(14)| 0.0265(5) |
| S(4)  | 1.1145(3)  | 0.6519(2)  | 0.51945(13)| 0.0252(5) |
| O(1)  | 1.1288(11) | 0.1074(7)  | 0.2324(5)  | 0.051(2)  |
| O(2)  | 1.1775(9)  | 0.6511(8)  | 0.1886(5)  | 0.046(2)  |
| O(3)  | 1.3416(9)  | 0.8435(8)  | 0.3554(5)  | 0.046(2)  |
| O(4)  | 0.6838(9)  | 0.8454(8)  | 0.5909(5)  | 0.048(2)  |
| O(5)  | 0.7057(10)| 0.4828(8)  | 0.6058(6)  | 0.053(2)  |
| O(6)  | 1.0825(12)| 0.7830(11)| 0.7384(5)  | 0.066(3)  |
| C(1)  | 1.0612(12)| 0.9142(10)| 0.2481(6)  | 0.033(2)  |
| C(2)  | 1.0952(11)| 0.6934(9)  | 0.2214(5)  | 0.029(2)  |
| C(3)  | 1.2091(13)| 0.8051(10)| 0.3751(6)  | 0.033(2)  |
| C(4)  | 0.7839(11)| 0.8025(10)| 0.5833(6)  | 0.029(2)  |
| C(5)  | 0.7970(14)| 0.5782(12)| 0.5936(8)  | 0.045(3)  |
| C(6)  | 1.0224(13)| 0.7631(12)| 0.6756(7)  | 0.043(3)  |
| C(7)  | 0.6460(11)| 0.6819(9)  | 0.3840(6)  | 0.027(19)|
| C(8)  | 0.6787(11)| 0.5582(9)  | 0.3792(6)  | 0.029(2)  |
| C(9)  | 1.3020(13)| 0.9020(11)| 0.5491(7)  | 0.039(2)  |
| C(10)| 1.3055(11)| 0.7679(10)| 0.5492(6)  | 0.031(2)  |
| C(11)| 0.8862(12)| 0.7166(10)| 0.0744(5)  | 0.029(2)  |
| C(12)| 0.9900(13)| 0.8332(12)| 0.0517(7)  | 0.040(3)  |
| C(13)| 1.0745(16)| 0.8483(17)| -0.0200(8)| 0.061(4)  |
| C(14)| 1.0556(18)| 0.7458(18)| -0.0684(7)| 0.067(5)  |
| C(15)| 0.953(2)  | 0.6311(17)| -0.0485(7)| 0.063(4)  |
| C(16)| 0.8671(16)| 0.6160(13)| 0.0221(6)  | 0.046(3)  |
| C(17)| 0.6568(12)| 0.8028(10)| 0.1519(6)  | 0.032(2)  |
| C(18)| 0.6422(13)| 0.8918(9)  | 0.2064(6)  | 0.034(2)  |
| C(19)| 0.5397(13)| 0.9589(10)| 0.1874(7)  | 0.037(2)  |
| C(20)| 0.4560(14)| 0.9401(11)| 0.1160(7)  | 0.043(3)  |
| C(21)| 0.4742(14)| 0.8554(13)| 0.0609(8)  | 0.050(3)  |
| C(22)| 0.5721(13)| 0.7841(11)| 0.0772(7)  | 0.038(2)  |
| C(23)| 0.6428(12)| 0.5460(9)  | 0.1753(6)  | 0.029(2)  |
| C(24)| 0.4776(12)| 0.5208(11)| 0.1821(7)  | 0.038(2)  |
| C(25)| 0.3736(15)| 0.3982(12)| 0.1939(8)  | 0.048(3)  |
| C(26)| 0.4326(14)| 0.3013(12)| 0.1973(9)  | 0.051(3)  |
| C(27)| 0.5994(16)| 0.3236(11)| 0.1884(8)  | 0.048(3)  |
| C(28)| 0.7001(13)| 0.4448(10)| 0.1807(7)  | 0.036(2)  |
| Bond Lengths [Å] and Angles [°] for str0734. |
|---------------------------------------------|
| Fe(1)–C(1) 1.782(11) | Fe(1)–C(2) 1.791(8) |
| Fe(1)–P(1) 2.244(3)  | Fe(1)–S(1) 2.249(3)  |
| Fe(1)–S(2) 2.261(3)  | Fe(1)–Fe(2) 2.546(2) |
| Fe(2)–C(3) 1.762(11) | Fe(2)–S(4) 2.198(3)  |
| Fe(2)–S(3) 2.210(3)  | Fe(2)–S(2) 2.256(3)  |
| Fe(2)–S(1) 2.258(3)  | Fe(2)–Fe(3) 2.584(2) |
| Fe(3)–C(6) 1.776(12) | Fe(3)–C(4) 1.799(10) |
| Fe(3)–C(5) 1.802(13) | Fe(3)–S(3) 2.238(3)  |
| Fe(3)–S(4) 2.238(3)  | Fe(3)–C(23) 1.832(10) |
| P(1)–C(17) 1.834(10) | P(1)–C(11) 1.842(9)  |
| S(1)–C(7) 1.834(10)  | S(2)–C(8) 1.819(10)  |
| S(3)–C(9) 1.834(11) | S(4)–C(10) 1.812(10) |
| O(1)–C(1) 1.149(13)  | O(2)–C(2) 1.130(11)  |
| O(3)–C(3) 1.151(13) | O(4)–C(4) 1.145(12)  |
| O(5)–C(5) 1.128(14) | O(6)–C(6) 1.147(14)  |
| C(7)–C(8) 1.516(13) | C(9)–C(10) 1.522(15) |
| C(11)–C(16) 1.383(15) | C(11)–C(12) 1.384(16) |
| C(12)–C(13) 1.388(16) | C(13)–C(14) 1.36(2)  |
| C(14)–C(15) 1.35(2)  | C(15)–C(16) 1.377(18) |
| C(17)–C(18) 1.381(14) | C(17)–C(22) 1.386(14) |
| C(18)–C(19) 1.392(13) | C(19)–C(20) 1.363(16) |
| C(20)–C(21) 1.363(18) | C(21)–C(22) 1.386(14) |
| C(23)–C(24) 1.391(14) | C(23)–C(28) 1.395(14) |
| C(24)–C(25) 1.396(17) | C(25)–C(26) 1.357(17) |
| C(26)–C(27) 1.414(17) | C(27)–C(28) 1.366(16) |

| Bond Angles [°] for str0734. |
|--------------------------------|
| C(1)–Fe(1)–C(2) 95.1(5) | C(1)–Fe(1)–P(1) 95.9(3) |
| C(2)–Fe(1)–P(1) 90.9(3)  | C(1)–Fe(1)–S(1) 103.41(10) |
| C(2)–Fe(1)–S(1) 164.0(3) | P(1)–Fe(1)–S(1) 89.4(3)  |
| C(1)–Fe(1)–S(2) 159.9(3) | C(2)–Fe(1)–S(2) 89.3(4)  |
| C(1)–Fe(1)–Fe(2) 103.66(10) | C(2)–Fe(1)–Fe(2) 108.3(3) |
| P(1)–Fe(1)–Fe(2) 104.5(3) | C(2)–Fe(1)–Fe(2) 108.3(3) |
| C(1)–Fe(1)–Fe(3) 150.27(9) | C(2)–Fe(1)–Fe(2) 108.3(3) |
| S(2)–Fe(2)–S(1) 55.59(7)  | S(1)–Fe(1)–Fe(2) 55.77(7)  |
| C(3)–Fe(2)–S(3) 92.3(4)  | C(3)–Fe(2)–S(4) 94.4(3)  |
| C(3)–Fe(2)–S(2) 102.1(4) | S(4)–Fe(2)–S(3) 81.83(10) |
| S(3)–Fe(2)–S(2) 165.54(10) | S(4)–Fe(2)–S(3) 81.83(10) |
| S(4)–Fe(2)–S(1) 151.29(10) | S(3)–Fe(2)–S(1) 93.42(10) |
| S(2)–Fe(2)–S(1) 80.33(9)  | C(3)–Fe(2)–S(1) 114.1(3)  |
| S(4)–Fe(2)–Fe(1) 144.25(9) | C(3)–Fe(2)–S(1) 114.1(3)  |
| S(2)–Fe(2)–Fe(1) 55.80(7)  | S(3)–Fe(2)–Fe(1) 72.1(3)  |
| C(3)–Fe(2)–Fe(3) 135.1(3) | S(3)–Fe(2)–Fe(1) 72.1(3)  |
| S(3)–Fe(2)–Fe(3) 54.98(8)  | S(4)–Fe(2)–Fe(3) 55.10(7)  |
| S(1)–Fe(2)–Fe(3) 99.15(8)  | S(2)–Fe(2)–Fe(3) 55.10(7)  |
| C(6)–Fe(3)–C(4) 100.1(5) | S(1)–Fe(2)–Fe(3) 55.10(7)  |
| C(4)–Fe(3)–C(5) 91.3(5)  | C(6)–Fe(3)–C(5) 97.7(6)  |
| C(4)–Fe(3)–S(3) 90.9(3)  | C(6)–Fe(3)–C(5) 97.7(6)  |
| C(6)–Fe(3)–S(4) 100.0(4) | C(6)–Fe(3)–C(5) 97.7(6)  |
| C(5)–Fe(3)–S(4) 91.9(4)  | C(6)–Fe(3)–C(5) 97.7(6)  |
| C(6)–Fe(3)–Fe(2) 141.5(4) | C(6)–Fe(3)–C(5) 97.7(6)  |
| C(5)–Fe(3)–Fe(2) 109.5(4) | C(6)–Fe(3)–C(5) 97.7(6)  |
| S(4)–Fe(3)–Fe(2) 53.65(7) | C(23)–P(1)–C(17) 103.8(5) |
| C(23)–P(1)–C(11) 104.6(5) | C(17)–P(1)–C(11) 100.5(4) |
| Bond                      | Angle (°)   | Bond                      | Angle (°)   | Bond                      | Angle (°)   |
|---------------------------|-------------|---------------------------|-------------|---------------------------|-------------|
| C(23)–P(1)–Fe(1)         | 113.4(3)    | C(17)–P(1)–Fe(1)         | 120.9(3)    | Fe(1)–S(1)–Fe(2)         | 68.79(8)    |
| C(11)–P(1)–Fe(1)         | 111.8(3)    | C(7)–S(1)–Fe(1)          | 102.5(3)    | Fe(1)–S(2)–Fe(2)         | 104.8(3)    |
| C(7)–S(1)–Fe(2)          | 103.6(3)    | Fe(1)–S(1)–Fe(2)         | 68.79(8)    | C(8)–S(2)–Fe(1)          | 104.8(3)    |
| C(8)–S(2)–Fe(2)          | 101.8(3)    | C(9)–S(3)–Fe(2)          | 103.0(4)    | C(9)–S(3)–Fe(3)          | 71.05(9)    |
| Fe(2)–S(2)–Fe(1)         | 68.61(9)    | Fe(2)–S(3)–Fe(3)         | 71.05(9)    | C(10)–S(4)–Fe(3)         | 101.3(3)    |
| C(9)–S(3)–Fe(3)          | 101.3(4)    | Fe(2)–S(4)–Fe(3)         | 71.26(8)    | Fe(2)–S(4)–Fe(3)         | 177.6(10)   |
| C(10)–S(4)–Fe(2)         | 102.7(4)    | O(1)–C(1)–Fe(1)          | 177.4(9)    | O(4)–C(4)–Fe(3)          | 177.4(9)    |
| Fe(2)–S(4)–Fe(3)         | 71.26(8)    | O(3)–C(3)–Fe(2)          | 167.7(9)    | O(4)–C(4)–Fe(3)          | 178.3(11)   |
| O(2)–C(2)–Fe(1)          | 177.6(9)    | O(5)–C(5)–Fe(3)          | 178.3(11)   | O(5)–C(5)–Fe(3)          | 178.3(11)   |
| O(6)–C(6)–Fe(3)          | 176.8(10)   | C(8)–C(7)–S(1)           | 112.2(6)    | C(7)–C(8)–S(2)           | 110.8(7)    |
| C(7)–C(8)–S(2)           | 112.4(6)    | O(5)–C(5)–Fe(3)          | 178.3(11)   | C(9)–C(10)–S(4)          | 113.1(7)    |
| C(9)–C(10)–S(4)          | 113.1(7)    | C(16)–C(11)–C(12)        | 117.6(10)   | C(16)–C(11)–P(1)         | 125.0(9)    |
| C(16)–C(11)–P(1)         | 125.0(9)    | C(12)–C(11)–P(1)         | 117.5(7)    | C(11)–C(12)–C(13)        | 121.3(12)   |
| C(11)–C(12)–C(13)        | 121.3(12)   | C(14)–C(13)–C(12)        | 119.0(14)   | C(15)–C(14)–C(13)        | 121.0(12)   |
| C(15)–C(14)–C(13)        | 121.0(12)   | C(14)–C(15)–C(16)        | 120.2(13)   | C(15)–C(16)–C(11)        | 120.9(13)   |
| C(15)–C(16)–C(11)        | 120.9(13)   | C(18)–C(17)–C(22)        | 119.8(9)    | C(18)–C(17)–P(1)         | 122.1(8)    |
| C(18)–C(17)–P(1)         | 122.1(8)    | C(22)–C(17)–P(1)         | 118.1(8)    | C(17)–C(18)–C(19)        | 118.9(10)   |
| C(17)–C(18)–C(19)        | 118.9(10)   | C(20)–C(19)–C(18)        | 121.6(10)   | C(19)–C(20)–C(21)        | 119.7(10)   |
| C(19)–C(20)–C(21)        | 119.7(10)   | C(20)–C(21)–C(22)        | 121.2(12)   | C(21)–C(22)–C(17)        | 118.8(11)   |
| C(21)–C(22)–C(17)        | 118.8(11)   | C(24)–C(23)–C(28)        | 117.7(10)   | C(24)–C(23)–P(1)         | 122.0(8)    |
| C(24)–C(23)–P(1)         | 122.0(8)    | C(28)–C(23)–P(1)         | 119.9(8)    | C(23)–C(24)–C(25)        | 120.8(11)   |
| C(23)–C(24)–C(25)        | 120.8(11)   | C(26)–C(25)–C(24)        | 120.2(11)   | C(25)–C(26)–C(27)        | 120.3(11)   |
| C(25)–C(26)–C(27)        | 120.3(11)   | C(28)–C(27)–C(26)        | 118.6(11)   | C(27)–C(28)–C(23)        | 122.3(10)   |
Table 4. Anisotropic displacement parameters (Å\(^2\)) for str0734. The anisotropic displacement factor exponent takes the form: \(-2\pi^2[h^2a^*2U^{11} + ... + 2hka*b*U^{12}]\)

|      | \(U^{11}\)   | \(U^{12}\)   | \(U^{13}\)   | \(U^{23}\)   | \(U^{12}\)   |
|------|-------------|-------------|-------------|-------------|-------------|
| Fe(1) | 0.0218(6)   | 0.0277(7)   | 0.0169(6)   | 0.0010(5)   | 0.0005(5)   |
| Fe(2) | 0.0193(6)   | 0.0294(7)   | 0.0168(6)   | -0.0007(5)  | 0.0010(5)   |
| Fe(3) | 0.0225(7)   | 0.0376(8)   | 0.0194(6)   | 0.0001(5)   | 0.0010(5)   |
| P(1)  | 0.0231(11)  | 0.0298(12)  | 0.0213(11)  | -0.0005(9)  | 0.0010(5)   |
| S(1)  | 0.0238(11)  | 0.0319(12)  | 0.0224(11)  | -0.0032(8)  | 0.0015(8)   |
| S(2)  | 0.0271(11)  | 0.0268(11)  | 0.0236(11)  | 0.0014(8)   | 0.0013(9)   |
| S(3)  | 0.0223(11)  | 0.0314(12)  | 0.0262(11)  | -0.0028(9)  | 0.0015(8)   |
| S(4)  | 0.0250(11)  | 0.0363(12)  | 0.0224(11)  | 0.0024(9)   | 0.0006(8)   |
| O(1)  | 0.057(5)    | 0.035(4)    | 0.050(5)    | 0.011(4)    | 0.011(4)    |
| O(2)  | 0.038(4)    | 0.067(5)    | 0.047(5)    | -0.011(4)   | 0.000(4)    |
| O(3)  | 0.025(4)    | 0.069(6)    | 0.041(4)    | 0.007(4)    | 0.006(3)    |
| O(4)  | 0.034(4)    | 0.065(5)    | 0.053(5)    | -0.002(4)   | 0.010(4)    |
| O(5)  | 0.042(5)    | 0.050(5)    | 0.059(6)    | 0.006(4)    | 0.026(4)    |
| O(6)  | 0.067(6)    | 0.129(9)    | 0.019(4)    | -0.008(5)   | 0.009(4)    |
| C(1)  | 0.029(5)    | 0.036(6)    | 0.037(5)    | 0.001(4)    | -0.005(4)   |
| C(2)  | 0.031(5)    | 0.034(5)    | 0.020(4)    | -0.004(4)   | 0.004(4)    |
| C(3)  | 0.043(6)    | 0.036(5)    | 0.025(5)    | 0.008(4)    | 0.005(4)    |
| C(4)  | 0.019(4)    | 0.044(6)    | 0.024(5)    | 0.009(4)    | 0.001(3)    |
| C(5)  | 0.031(6)    | 0.052(7)    | 0.055(7)    | -0.002(6)   | 0.004(5)    |
| C(6)  | 0.029(5)    | 0.067(8)    | 0.034(6)    | -0.002(5)   | -0.002(4)   |
| C(7)  | 0.024(4)    | 0.036(5)    | 0.027(5)    | 0.005(4)    | 0.001(4)    |
| C(8)  | 0.023(4)    | 0.031(5)    | 0.028(5)    | 0.002(4)    | -0.002(4)   |
| C(9)  | 0.031(5)    | 0.047(6)    | 0.039(6)    | -0.006(5)   | -0.010(4)   |
| C(10) | 0.025(5)    | 0.047(6)    | 0.021(4)    | -0.010(4)   | -0.001(4)   |
| C(11) | 0.033(5)    | 0.049(6)    | 0.019(4)    | -0.001(4)   | 0.002(4)    |
| C(12) | 0.033(6)    | 0.056(7)    | 0.032(6)    | 0.000(5)    | 0.011(4)    |
| C(13) | 0.041(7)    | 0.106(12)   | 0.042(7)    | 0.023(8)    | 0.013(6)    |
| C(14) | 0.068(9)    | 0.131(15)   | 0.021(6)    | 0.025(8)    | 0.013(6)    |
| C(15) | 0.088(11)   | 0.098(12)   | 0.024(6)    | -0.010(7)   | 0.000(6)    |
| C(16) | 0.060(8)    | 0.065(8)    | 0.023(5)    | -0.006(5)   | -0.003(5)   |
| C(17) | 0.025(5)    | 0.038(5)    | 0.034(5)    | 0.002(4)    | -0.002(4)   |
| C(18) | 0.043(6)    | 0.035(5)    | 0.033(5)    | 0.006(4)    | 0.006(4)    |
| C(19) | 0.042(6)    | 0.044(6)    | 0.036(6)    | 0.013(5)    | 0.004(5)    |
| C(20) | 0.042(6)    | 0.049(7)    | 0.050(7)    | 0.010(5)    | 0.007(5)    |
| C(21) | 0.038(6)    | 0.065(8)    | 0.055(8)    | 0.016(6)    | -0.004(5)   |
| C(22) | 0.037(6)    | 0.047(6)    | 0.038(6)    | 0.009(5)    | -0.002(5)   |
| C(23) | 0.032(5)    | 0.035(5)    | 0.021(4)    | 0.000(4)    | -0.001(4)   |
| C(24) | 0.025(5)    | 0.052(6)    | 0.037(6)    | 0.002(5)    | 0.003(4)    |
| C(25) | 0.036(6)    | 0.056(7)    | 0.055(8)    | 0.011(6)    | -0.005(5)   |
| C(26) | 0.033(6)    | 0.039(6)    | 0.074(9)    | 0.010(6)    | -0.001(6)   |
| C(27) | 0.057(8)    | 0.033(6)    | 0.052(7)    | -0.004(5)   | 0.006(6)    |
| C(28) | 0.030(5)    | 0.034(5)    | 0.040(6)    | -0.011(4)   | 0.000(4)    |
Table 5. Hydrogen coordinates and isotropic displacement parameters (Å²) for str0734.

| x    | y    | z    | U    |
|------|------|------|------|
| H(7A)| 0.5953 | 0.6878 | 0.4364 | 0.032 |
| H(7B)| 0.5690 | 0.6838 | 0.3404 | 0.032 |
| H(8A)| 0.6046 | 0.5024 | 0.3387 | 0.035 |
| H(8B)| 0.6562 | 0.5165 | 0.4323 | 0.035 |
| H(9A)| 1.3852 | 0.9536 | 0.5121 | 0.047 |
| H(9B)| 1.3273 | 0.9391 | 0.6042 | 0.047 |
| H(10A)| 1.3352 | 0.7483 | 0.6041 | 0.037 |
| H(10B)| 1.3898 | 0.7619 | 0.5117 | 0.037 |
| H(12A)| 1.0036 | 0.9043 | 0.0860 | 0.048 |
| H(13A)| 1.1446 | 0.9289 | −0.0351 | 0.074 |
| H(14A)| 1.1154 | 0.7550 | −0.1168 | 0.080 |
| H(15A)| 0.9401 | 0.5607 | −0.0833 | 0.076 |
| H(16A)| 0.7938 | 0.5355 | 0.0351 | 0.055 |
| H(18A)| 0.7010 | 0.9070 | 0.2561 | 0.041 |
| H(19A)| 0.5278 | 1.0193 | 0.2251 | 0.044 |
| H(20A)| 0.3853 | 0.9859 | 0.1048 | 0.051 |
| H(21A)| 0.4189 | 0.8450 | 0.0103 | 0.060 |
| H(22A)| 0.5820 | 0.7238 | 0.0389 | 0.045 |
| H(24A)| 0.4350 | 0.5877 | 0.1786 | 0.045 |
| H(25A)| 0.2613 | 0.3825 | 0.1996 | 0.058 |
| H(26A)| 0.3614 | 0.2182 | 0.2057 | 0.061 |
| H(27A)| 0.6407 | 0.2557 | 0.1877 | 0.058 |
| H(28A)| 0.8130 | 0.4608 | 0.1790 | 0.043 |
Table 6. Torsion angles [°] for str0734.

| Bond                              | Torsion Angle [°] |
|-----------------------------------|-------------------|
| C(1)–Fe(1)–Fe(2)–C(3)             | 57.6(5)           |
| P(1)–Fe(1)–Fe(2)–C(3)             | 170.6(4)          |
| S(2)–Fe(1)–Fe(2)–C(3)             | 119.1(4)          |
| C(2)–Fe(1)–Fe(2)–S(4)             | -29.0(4)          |
| S(1)–Fe(1)–Fe(2)–S(4)             | 150.0(17)         |
| S(1)–Fe(1)–Fe(2)–S(3)             | 19.8(4)           |
| P(1)–Fe(1)–Fe(2)–S(3)             | -111.97(19)       |
| S(2)–Fe(1)–Fe(2)–S(3)             | -163.50(13)       |
| C(2)–Fe(1)–Fe(2)–S(2)             | -76.2(3)          |
| S(1)–Fe(1)–Fe(2)–S(2)             | 102.80(11)        |
| P(1)–Fe(1)–Fe(2)–S(2)             | -179.0(3)         |
| S(2)–Fe(1)–Fe(2)–S(1)             | -102.80(11)       |
| C(2)–Fe(1)–Fe(2)–Fe(3)            | -150.3(4)         |
| S(1)–Fe(1)–Fe(2)–Fe(3)            | 28.72(15)         |
| C(3)–Fe(2)–Fe(3)–C(6)             | -0.7(8)           |
| S(3)–Fe(2)–Fe(3)–C(6)             | -51.4(7)          |
| S(1)–Fe(2)–Fe(3)–C(6)             | -139.2(7)         |
| C(3)–Fe(2)–Fe(3)–C(4)             | 129.8(6)          |
| S(3)–Fe(2)–Fe(3)–C(4)             | 79.2(4)           |
| S(1)–Fe(2)–Fe(3)–C(4)             | -8.6(4)           |
| C(3)–Fe(2)–Fe(3)–C(5)             | -132.9(6)         |
| S(3)–Fe(2)–Fe(3)–C(5)             | 176.4(4)          |
| S(1)–Fe(2)–Fe(3)–C(5)             | 88.6(4)           |
| C(3)–Fe(2)–Fe(3)–S(3)             | 50.7(5)           |
| S(2)–Fe(2)–Fe(3)–S(3)             | -171.05(11)       |
| Fe(1)–Fe(2)–Fe(3)–S(3)            | -111.39(16)       |
| S(3)–Fe(2)–Fe(3)–S(4)             | -106.11(12)       |
| S(1)–Fe(2)–Fe(3)–S(4)             | 166.13(11)        |
| C(1)–Fe(1)–P(1)–C(23)             | -177.8(5)         |
| S(1)–Fe(1)–P(1)–C(23)             | -85.9(4)          |
| Fe(2)–Fe(1)–P(1)–C(23)            | -44.4(4)          |
| C(2)–Fe(1)–P(1)–C(17)             | -148.9(5)         |
| C(2)–Fe(1)–P(1)–C(17)             | 121.5(4)          |
| S(1)–Fe(1)–P(1)–C(11)             | 64.2(5)           |
| S(1)–Fe(1)–P(1)–C(11)             | 156.2(4)          |
| Fe(2)–Fe(1)–P(1)–C(11)            | -162.3(4)         |
| C(2)–Fe(1)–S(1)–C(7)              | -96.5(12)         |
| S(2)–Fe(1)–S(1)–C(7)              | -45.3(3)          |
| C(1)–Fe(1)–S(1)–Fe(2)             | -107.3(3)         |
| P(1)–Fe(1)–S(1)–Fe(2)             | 156.56(9)         |
| C(3)–Fe(2)–S(1)–C(7)              | 142.5(5)          |
| S(3)–Fe(2)–S(1)–C(7)              | -123.4(3)         |
| Fe(1)–Fe(2)–S(1)–C(7)             | 98.4(3)           |
| C(3)–Fe(2)–S(1)–Fe(1)             | 44.1(4)           |
| S(3)–Fe(2)–S(1)–Fe(1)             | 138.23(9)         |
| S(3)–Fe(2)–S(1)–Fe(1)             | -166.71(7)        |
| S(4)–Fe(2)–S(2)–C(8)              | 104.2(3)          |
| S(1)–Fe(2)–S(2)–C(8)              | -46.8(3)          |
| Fe(3)–Fe(2)–S(2)–C(8)             | 49.1(3)           |
| S(4)–Fe(2)–S(2)–Fe(1)             | -154.39(9)        |
| Bond                     | Angle (°)  |
|-------------------------|------------|
| S(1)–Fe(2)–S(2)–Fe(1)  | 54.56(8)   |
| C(1)–Fe(1)–S(2)–C(8)   | 106.5(10)  |
| P(1)–Fe(1)–S(2)–C(8)   | −59.3(3)   |
| Fe(2)–Fe(1)–S(2)–C(8)  | 97.2(3)    |
| C(2)–Fe(1)–S(2)–Fe(2)  | 112.8(3)   |
| S(1)–Fe(1)–S(2)–Fe(2)  | −54.85(8)  |
| S(4)–Fe(2)–S(3)–C(9)   | 44.9(4)    |
| S(1)–Fe(2)–S(3)–C(9)   | −163.5(4)  |
| Fe(2)–Fe(1)–S(2)–C(8)  | 9.3(10)    |
| C(2)–Fe(2)–S(3)–Fe(3)  | 5.0(5)     |
| S(1)–Fe(2)–S(3)–Fe(3)  | 98.78(9)   |
| Fe(3)–Fe(2)–S(3)–Fe(3) | 97.7(4)    |
| S(5)–Fe(3)–S(3)–C(9)   | 50.5(5)    |
| Fe(2)–Fe(3)–S(3)–C(9)  | 52.64(9)   |
| C(6)–Fe(3)–S(3)–C(9)   | −111.9(13) |
| Fe(2)–Fe(3)–S(3)–Fe(2) | −100.1(4)  |
| C(4)–Fe(3)–S(3)–Fe(2)  | −109.2(3)  |
| S(4)–Fe(3)–S(3)–Fe(2)  | 51.71(8)   |
| S(3)–Fe(3)–S(3)–C(10)  | −45.2(3)   |
| S(1)–Fe(2)–S(3)–C(10)  | −127.3(4)  |
| Fe(3)–Fe(2)–S(4)–C(10) | −97.8(3)   |
| S(3)–Fe(2)–S(4)–Fe(3)  | 52.64(9)   |
| S(1)–Fe(2)–S(4)–Fe(3)  | −29.5(2)   |
| C(6)–Fe(3)–S(4)–C(10)  | −49.2(5)   |
| C(5)–Fe(3)–S(4)–C(10)  | −147.3(5)  |
| Fe(2)–Fe(3)–S(4)–C(10) | 99.7(4)    |
| C(4)–Fe(3)–S(4)–C(10)  | 14.3(9)    |
| S(3)–Fe(3)–S(4)–Fe(2)  | −52.02(8)  |
| P(1)–Fe(1)–C(1)–O(1)   | −176.100   |
| S(2)–Fe(1)–C(1)–O(1)   | 18.25      |
| C(1)–Fe(1)–C(2)–O(2)   | 158.22     |
| S(1)–Fe(1)–C(2)–O(2)   | 48.23      |
| S(2)–Fe(1)–C(2)–O(2)   | 51.22      |
| S(3)–Fe(2)–C(3)–O(3)   | 44.5       |
| S(1)–Fe(2)–C(3)–O(3)   | 139.4      |
| Fe(3)–Fe(2)–C(3)–O(3)  | 5.0        |
| C(5)–Fe(3)–C(4)–O(4)   | 63.21      |
| S(4)–Fe(3)–C(4)–O(4)   | 161.21     |
| C(6)–Fe(3)–C(5)–O(5)   | 62.44      |
| S(3)–Fe(3)–C(5)–O(5)   | −135.43    |
| Fe(2)–Fe(3)–C(5)–O(5)  | −145.44    |
| C(5)–Fe(3)–C(6)–O(6)   | 117.23     |
| S(4)–Fe(3)–C(6)–O(6)   | 23.23      |
| Fe(1)–S(1)–C(7)–C(8)   | 41.0(7)    |
| S(1)–C(7)–C(8)–S(2)    | −7.8(9)    |
| Fe(1)–S(2)–C(8)–C(7)   | −28.7(7)   |
| Fe(3)–S(3)–C(9)–C(10)  | 36.8(6)    |
| Fe(2)–S(4)–C(10)–C(9)  | 36.1(8)    |
| C(23)–P(1)–C(11)–C(16) | −7.0(10)   |
| Fe(1)–P(1)–C(11)–C(16) | 116.0(9)   |
| C(17)–P(1)–C(11)–C(12) | 66.1(9)    |
| C(16)–C(11)–C(12)–C(13) | −1.3(16)   |
| C(11)–C(12)–C(13)–C(14) | −0.6(19)   |
| C(13)–C(14)–C(15)–C(16) | −1(2)      |
C(12)–C(11)–C(16)–C(15) 2.2(17)  P(1)–C(11)–C(16)–C(15) −177.2(10)
C(23)–P(1)–C(17)–C(18) 116.5(9)  C(11)–P(1)–C(17)–C(18) −135.5(9)
Fe(1)–P(1)–C(17)–C(18) −12.1(10)  C(23)–P(1)–C(17)–C(22) −64.0(9)
C(11)–P(1)–C(17)–C(22) 44.0(9)  Fe(1)–P(1)–C(17)–C(22) 167.4(7)
C(22)–C(17)–C(18)–C(19) 1.9(16)  P(1)–C(17)–C(18)–C(19) −178.6(8)
C(17)–C(18)–C(19)–C(20) −1.0(17)  C(18)–C(19)–C(20)–C(21) −1.1(18)
C(19)–C(20)–C(21)–C(22) 2.4(19)  C(20)–C(21)–C(22)–C(17) −1.5(18)
C(18)–C(17)–C(22)–C(21) 0.7(16)  P(1)–C(17)–C(22)–C(21) 179.8(9)
C(17)–P(1)–C(23)–C(24) −15.1(10)  C(11)–P(1)–C(23)–C(24) −120.0(9)
Fe(1)–P(1)–C(23)–C(24) 118.0(8)  C(17)–P(1)–C(23)–C(28) 172.7(8)
C(11)–P(1)–C(23)–C(28) 67.8(9)  Fe(1)–P(1)–C(23)–C(28) −54.2(9)
C(28)–C(23)–C(24)–C(25) 0.1(16)  P(1)–C(23)–C(24)–C(25) −172.3(9)
C(23)–C(24)–C(25)–C(26) −1.4(19)  C(24)–C(25)–C(26)–C(27) 0(2)
C(25)–C(26)–C(27)–C(28) 3(2)  C(26)–C(27)–C(28)–C(23) −4.9(18)
C(24)–C(23)–C(28)–C(27) 3.1(16)  P(1)–C(23)–C(28)–C(27) 175.7(9)
Table 1. Crystal data and structure refinement for str0732 (3).

| Identification code   | str0732       |
|-----------------------|---------------|
| Chemical formula      | C\(_{50}\)H\(_{38}\)Fe\(_3\)O\(_{5.50}\)P\(_2\)S\(_4\) |
| Formula weight        | 1084.53       |
| Temperature           | 150(2) K      |
| Radiation, wavelength | MoK\(\alpha\), 0.71073 Å |
| Crystal system, space group | orthorhombic, C2/c |
| Unit cell parameters  | \(a = 25.520(16) \text{ Å}\) \(\alpha = 90^\circ\) \(\beta = 94.720(10)^\circ\) \(\gamma = 90^\circ\) |
| Cell volume           | 10360(11) Å\(^3\) |
| Z                     | 8             |
| Calculated density    | 1.391 g/cm\(^3\) |
| Absorption coefficient \(\mu\) | 1.096 mm\(^{-1}\) |
| F(000)                | 4432          |
| Crystal colour and size | red, 0.22 × 0.10 × 0.05 mm\(^3\) |
| Data collection method | Bruker SMART APEX diffractometer |
| \(\theta\) range for data collection | 2.22 to 28.31° |
| Index ranges          | \(h = -32 \text{ to 33, } k = -17 \text{ to 17, } l = -39 \text{ to 39}\) |
| Completeness to \(\theta = 26.00^\circ\) | 99.1 % |
| Reflections collected | 41674         |
| Independent reflections | 12131 (R\(_{int}\) = 0.2646) |
| Reflections with \(\text{Fo}^2>2\sigma\) | 5012          |
| Absorption correction | semi-empirical from equivalents |
| Min. and max. transmission | 0.7945 and 0.9472 |
| Structure solution    | direct methods |
| Refinement method     | Full-matrix least-squares on \(\text{Fo}^2\) |
| Weighting parameters a, b | 0.0984, 0.0000 |
| Data / restraints / parameters | 12131 / 0 / 581 |
| Final R indices \([\text{Fo}^2>2\sigma]\) | R1 = 0.1027, wR2 = 0.2069 |
| R indices (all data)  | R1 = 0.2394, wR2 = 0.2551 |
| Goodness-of-fit on \(\text{Fo}^2\) | 0.960 |
| Extinction coefficient | 0.0092(4) |
| Largest and mean shift/su | 0.000 and 0.000 |
| Largest diff. peak and hole | 1.051 and −0.631 e Å\(^{-3}\) |
Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å$^2$) for str0732. $U_{eq}$ is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

|        | x          | y          | z          | $U_{eq}$ |
|--------|------------|------------|------------|----------|
| Fe(1)  | 0.12442(4) | 0.27778(9) | 0.14586(4) | 0.0394(4) |
| Fe(2)  | 0.14810(4) | 0.45862(9) | 0.13345(4) | 0.0406(4) |
| Fe(3)  | 0.13819(4) | 0.61971(9) | 0.08961(4) | 0.0398(4) |
| P(1)   | 0.12235(8) | 0.13768(16)| 0.18617(7) | 0.0377(5) |
| P(2)   | 0.10912(8) | 0.70490(17)| 0.19108(7) | 0.0442(6) |
| S(1)   | 0.20526(8) | 0.34334(17)| 0.15897(8) | 0.0461(6) |
| S(2)   | 0.10574(8) | 0.40396(17)| 0.19108(7) | 0.0442(6) |
| S(3)   | 0.07318(8) | 0.50690(17)| 0.09584(8) | 0.0445(6) |
| S(4)   | 0.17740(8) | 0.48029(16)| 0.06520(8) | 0.0440(6) |
| O(1)   | 0.0127(2)  | 0.2662(5)  | 0.1141(2)  | 0.0544(16)|
| O(2)   | 0.1603(3)  | 0.1924(5)  | 0.0649(2)  | 0.0628(18)|
| O(3)   | 0.2041(3)  | 0.7025(5)  | 0.1522(2)  | 0.0561(17)|
| O(4)   | 0.0904(2)  | 0.7525(5)  | 0.1522(2)  | 0.0561(17)|
| O(5)   | 0.2423(2)  | 0.7139(5)  | 0.0954(2)  | 0.0561(17)|
| C(1)   | 0.0565(4)  | 0.2713(6)  | 0.1274(3)  | 0.043(2)  |
| C(2)   | 0.1450(3)  | 0.2239(7)  | 0.0964(3)  | 0.047(2)  |
| C(3)   | 0.1800(4)  | 0.5544(7)  | 0.1641(3)  | 0.055(2)  |
| C(4)   | 0.1093(3)  | 0.7025(7)  | 0.1270(3)  | 0.045(2)  |
| C(5)   | 0.2009(3)  | 0.6811(6)  | 0.0933(3)  | 0.043(2)  |
| C(6)   | 0.2109(3)  | 0.3650(7)  | 0.2187(3)  | 0.052(2)  |
| C(7)   | 0.1596(4)  | 0.4017(7)  | 0.2356(3)  | 0.054(2)  |
| C(8)   | 0.0714(3)  | 0.4398(7)  | 0.0421(3)  | 0.050(2)  |
| C(9)   | 0.1260(3)  | 0.4232(7)  | 0.0271(3)  | 0.046(2)  |
| C(10)  | 0.0660(3)  | 0.0579(6)  | 0.1687(3)  | 0.041(2)  |
| C(11)  | 0.0307(4)  | 0.0231(8)  | 0.1978(3)  | 0.065(3)  |
| C(12)  | −0.0088(5) | −0.0383(9) | 0.1840(4)  | 0.096(5)  |
| C(13)  | −0.0164(4) | −0.0667(8) | 0.1395(4)  | 0.070(3)  |
| C(14)  | 0.0181(4)  | −0.0336(7) | 0.1100(3)  | 0.052(2)  |
| C(15)  | 0.0592(4)  | 0.0284(7)  | 0.1252(3)  | 0.055(2)  |
| C(16)  | 0.1767(3)  | 0.0497(6)  | 0.1827(3)  | 0.040(2)  |
| C(17)  | 0.2258(3)  | 0.0849(7)  | 0.1753(3)  | 0.048(2)  |
| C(18)  | 0.2677(4)  | 0.0172(8)  | 0.1709(3)  | 0.061(3)  |
| C(19)  | 0.2586(4)  | −0.0837(8) | 0.1724(3)  | 0.059(3)  |
| C(20)  | 0.2093(4)  | −0.1190(7) | 0.1805(3)  | 0.054(3)  |
| C(21)  | 0.1683(4)  | −0.0519(7) | 0.1855(3)  | 0.051(2)  |
| C(22)  | 0.1181(3)  | 0.1554(6)  | 0.2452(3)  | 0.044(2)  |
| C(23)  | 0.1569(4)  | 0.1231(7)  | 0.2772(3)  | 0.056(2)  |
| C(24)  | 0.1540(5)  | 0.1450(9)  | 0.3226(4)  | 0.080(3)  |
| C(25)  | 0.1117(5)  | 0.2008(9)  | 0.3351(4)  | 0.077(3)  |
| C(26)  | 0.0723(4)  | 0.2300(8)  | 0.3046(4)  | 0.065(3)  |
| C(27)  | 0.0767(4)  | 0.2090(7)  | 0.2598(3)  | 0.054(2)  |
| C(28)  | 0.1143(3)  | 0.6397(6)  | −0.0241(3) | 0.042(2)  |
| C(29)  | 0.1650(3)  | 0.6144(6)  | −0.0365(3) | 0.041(2)  |
| C(30)  | 0.1697(4)  | 0.5595(7)  | −0.0740(3) | 0.054(2)  |
| C(31)  | 0.1249(3)  | 0.5302(7)  | −0.1011(3) | 0.053(2)  |
| C(32)  | 0.0758(3)  | 0.5557(7)  | −0.0889(3) | 0.057(3)  |
| C(33)  | 0.0707(3)  | 0.6108(7)  | −0.0515(3) | 0.045(2)  |
| C(34)  | 0.0408(3)  | 0.7497(6)  | 0.0246(3)  | 0.042(2)  |
| C(35)  | 0.0242(4)  | 0.8252(7)  | −0.0048(3) | 0.054(2)  |
|   |   |   |   |   |
|---|---|---|---|---|
| C(36) | -0.0264(4) | 0.8604(7) | -0.0083(3) | 0.056(3) |
| C(37) | -0.0628(4) | 0.8196(7) | 0.0186(3) | 0.054(2) |
| C(38) | -0.0476(3) | 0.7446(7) | 0.0484(3) | 0.048(2) |
| C(39) | 0.0036(3) | 0.7100(7) | 0.0523(3) | 0.047(2) |
| C(40) | 0.1445(3) | 0.8207(6) | 0.0207(3) | 0.042(2) |
| C(41) | 0.1551(3) | 0.8822(7) | 0.0582(3) | 0.051(2) |
| C(42) | 0.1821(4) | 0.9711(7) | 0.0537(4) | 0.058(3) |
| C(43) | 0.2004(4) | 0.9973(7) | 0.0146(4) | 0.056(3) |
| C(44) | 0.1918(4) | 0.9388(7) | -0.0221(4) | 0.059(3) |
| C(45) | 0.1641(3) | 0.8489(7) | -0.0191(3) | 0.054(2) |
| C(46) | 0.2049(13) | 0.203(3) | -0.0754(13) | 0.138(14) |
| C(47) | 0.1634(4) | 0.1235(10) | -0.1074(4) | 0.089(4) |
| C(48) | 0.1943(5) | 0.3085(10) | -0.0743(6) | 0.086(4) |
| C(49) | 0.1998(6) | 0.2672(15) | -0.0425(7) | 0.118(6) |
| C(50) | 0.1530(6) | 0.2277(14) | -0.1371(8) | 0.180(10) |
| O(6) | 0.076(2) | 0.344(4) | -0.2145(18) | 0.34(3) |
| C(51) | 0.029(3) | 0.395(6) | -0.218(2) | 0.32(4) |
Table 3. Bond lengths [Å] and angles [°] for str0732.

| Bond                  | Length [Å] | Bond                  | Length [Å] |
|-----------------------|------------|-----------------------|------------|
| Fe(1)–C(1)            | 1.778(9)   | Fe(1)–C(2)            | 1.779(11)  |
| Fe(1)–S(1)            | 2.249(3)   | Fe(1)–P(1)            | 2.250(3)   |
| Fe(1)–S(2)            | 2.257(3)   | Fe(1)–Fe(2)           | 2.547(2)   |
| Fe(2)–C(3)            | 1.751(10)  | Fe(2)–S(1)            | 2.226(3)   |
| Fe(2)–S(3)            | 2.239(3)   | Fe(2)–S(2)            | 2.248(3)   |
| Fe(2)–S(4)            | 2.269(3)   | Fe(2)–Fe(3)           | 2.546(2)   |
| Fe(3)–C(4)            | 1.790(11)  | Fe(3)–C(5)            | 1.797(9)   |
| Fe(3)–P(2)            | 2.251(3)   | Fe(3)–S(3)            | 2.270(3)   |
| Fe(3)–S(4)            | 2.281(3)   | P(1)–C(22)            | 1.810(9)   |
| P(1)–C(16)            | 1.835(9)   | P(1)–C(10)            | 1.837(8)   |
| P(2)–C(28)            | 1.828(9)   | P(2)–C(40)            | 1.829(8)   |
| P(2)–C(34)            | 1.840(8)   | S(1)–C(6)             | 1.822(9)   |
| S(2)–C(7)             | 1.844(9)   | S(3)–C(8)             | 1.855(9)   |
| S(4)–C(9)             | 1.840(8)   | O(1)–C(1)             | 1.115(9)   |
| O(2)–C(2)             | 1.139(10)  | O(3)–C(3)             | 1.173(10)  |
| O(4)–C(4)             | 1.151(10)  | O(5)–C(5)             | 1.141(9)   |
| C(6)–C(7)             | 1.526(13)  | C(8)–C(9)             | 1.516(12)  |
| C(10)–C(15)           | 1.372(11)  | C(10)–C(11)           | 1.391(12)  |
| C(11)–C(12)           | 1.344(14)  | C(12)–C(13)           | 1.396(15)  |
| C(13)–C(14)           | 1.377(13)  | C(14)–C(15)           | 1.390(12)  |
| C(16)–C(17)           | 1.374(12)  | C(16)–C(21)           | 1.390(12)  |
| C(17)–C(18)           | 1.422(12)  | C(18)–C(19)           | 1.381(14)  |
| C(19)–C(20)           | 1.386(13)  | C(20)–C(21)           | 1.399(12)  |
| C(22)–C(27)           | 1.381(12)  | C(22)–C(23)           | 1.397(12)  |
| C(23)–C(24)           | 1.411(13)  | C(24)–C(25)           | 1.392(15)  |
| C(25)–C(26)           | 1.365(15)  | C(26)–C(27)           | 1.397(13)  |
| C(28)–C(33)           | 1.387(11)  | C(28)–C(29)           | 1.416(11)  |
| C(29)–C(30)           | 1.366(12)  | C(30)–C(31)           | 1.408(12)  |
| C(31)–C(32)           | 1.377(12)  | C(32)–C(33)           | 1.368(12)  |
| C(34)–C(35)           | 1.394(12)  | C(34)–C(39)           | 1.419(11)  |
| C(35)–C(36)           | 1.372(12)  | C(36)–C(37)           | 1.397(13)  |
| C(37)–C(38)           | 1.386(13)  | C(38)–C(39)           | 1.385(12)  |
| C(40)–C(45)           | 1.390(12)  | C(40)–C(41)           | 1.413(12)  |
| C(41)–C(42)           | 1.396(12)  | C(42)–C(43)           | 1.352(13)  |
| C(43)–C(44)           | 1.364(13)  | C(44)–C(45)           | 1.410(13)  |
| C(46)–C(49)           | 1.33(4)    | C(46)–C(48)           | 1.45(4)    |
| C(46)–C(47)           | 1.74(4)    | C(47)–C(50)           | 1.68(2)    |
| C(48)–C(49)           | 1.107(19)  | O(6)–C(51)            | 1.37(8)    |

Angular Data:

| Bond                  | Angle [°] |
|-----------------------|-----------|
| C(1)–Fe(1)–C(2)      | 93.7(4)   |
| C(1)–Fe(1)–S(1)      | 88.7(3)   |
| C(1)–Fe(1)–P(1)      | 97.6(3)   |
| C(1)–Fe(1)–S(2)      | 88.8(3)   |
| S(1)–Fe(1)–S(2)      | 80.42(9)  |
| C(1)–Fe(1)–Fe(2)     | 103.7(3)  |
| S(1)–Fe(1)–Fe(2)     | 54.86(7)  |
| S(2)–Fe(1)–Fe(2)     | 55.39(7)  |
| C(3)–Fe(2)–S(3)      | 113.2(3)  |
| C(3)–Fe(2)–S(2)      | 93.8(3)   |
| S(3)–Fe(2)–S(2)      | 92.48(10) |
| S(2)–Fe(2)–S(4)      | 98.56(10) |
| S(2)–Fe(2)–Fe(3)     | 164.03(10) |
| S(1)–Fe(2)–Fe(3)     | 144.12(8) |

C(1)–Fe(1)–C(2)      158.5(3)
C(1)–Fe(1)–S(1)      93.6(3)
C(1)–Fe(1)–P(1)      107.27(9)
C(1)–Fe(1)–S(2)      155.2(3)
C(1)–Fe(1)–Fe(2)     100.2(3)
S(1)–Fe(1)–S(2)      106.85(10)
C(1)–Fe(1)–Fe(2)     100.2(3)
S(1)–Fe(1)–Fe(2)     154.11(8)
S(2)–Fe(1)–Fe(2)     94.0(3)
C(3)–Fe(2)–S(3)      152.48(10)
C(3)–Fe(2)–S(2)      81.14(10)
C(3)–Fe(2)–S(4)      102.2(3)
S(3)–Fe(2)–S(4)      80.39(10)
C(3)–Fe(2)–Fe(3)     70.6(3)
S(3)–Fe(2)–Fe(3)     56.21(7)
| Bond                  | Angle (°)         |
|----------------------|------------------|
| S(2)–Fe(2)–Fe(3)     | 130.48(8)        |
| C(3)–Fe(2)–Fe(1)     | 137.3(3)         |
| S(3)–Fe(2)–Fe(1)     | 98.63(8)         |
| S(4)–Fe(2)–Fe(1)     | 110.91(8)        |
| C(4)–Fe(3)–C(5)      | 94.9(4)          |
| C(5)–Fe(3)–P(2)      | 92.7(3)          |
| C(5)–Fe(3)–S(3)      | 163.1(3)         |
| C(4)–Fe(3)–S(4)      | 158.9(3)         |
| P(2)–Fe(3)–S(4)      | 106.18(10)       |
| C(4)–Fe(3)–Fe(2)     | 103.5(3)         |
| C(5)–Fe(3)–C(10)     | 118.7(6)         |
| C(9)–C(10)–C(11)     | 118.0(8)         |
| C(11)–C(10)–P(1)     | 123.2(7)         |
| C(11)–C(12)–C(13)    | 120.6(10)        |
| C(13)–C(14)–C(15)    | 119.2(9)         |
| C(17)–C(16)–C(21)    | 119.8(8)         |
| C(21)–C(16)–P(1)     | 120.9(7)         |
| C(19)–C(18)–C(17)    | 119.9(9)         |
| C(19)–C(20)–C(21)    | 119.6(9)         |
| C(27)–C(22)–C(23)    | 117.4(9)         |
| C(23)–C(22)–P(1)     | 123.0(7)         |
| C(25)–C(24)–C(23)    | 118.7(10)        |
| C(25)–C(26)–C(27)    | 118.7(10)        |
| C(33)–C(28)–C(29)    | 118.7(8)         |
| C(29)–C(28)–P(2)     | 118.66(3)        |
| C(29)–C(30)–C(31)    | 120.7(8)         |
| C(33)–C(32)–C(31)    | 120.5(8)         |
| C(35)–C(34)–C(39)    | 117.9(8)         |
| C(39)–C(34)–P(2)     | 121.0(6)         |
| C(35)–C(36)–C(37)    | 118.9(9)         |
| C(39)–C(38)–C(37)    | 120.8(8)         |
| C(45)–C(40)–C(41)    | 118.3(8)         |
| C(41)–C(40)–P(2)     | 117.5(7)         |
| C(43)–C(42)–C(41)    | 121.2(9)         |
| C(43)–C(44)–C(45)    | 119.5(9)         |
| C(49)–C(46)–C(48)    | 46.6(16)         |
| C(48)–C(46)–C(47)    | 121(2)           |
| C(49)–C(48)–C(46)    | 61.1(18)         |
| Atom | $U^{11}$ | $U^{12}$ | $U^{13}$ | $U^{14}$ | $U^{15}$ |
|------|----------|----------|----------|----------|----------|
| Fe(1) | 0.0420(7) | 0.0407(7) | 0.0348(7) | 0.0011(6) | -0.0011(5) |
| Fe(2) | 0.0442(7) | 0.0406(8) | 0.0358(8) | 0.0028(6) | -0.0042(5) |
| Fe(3) | 0.0417(7) | 0.0402(7) | 0.0368(8) | 0.0021(6) | -0.0002(5) |
| P(1)  | 0.0504(12) | 0.0400(13) | 0.0323(13) | 0.0021(10) | 0.0010(9) |
| P(2)  | 0.0407(12) | 0.0440(14) | 0.0340(13) | 0.0016(10) | -0.0020(10) |
| S(1)  | 0.0466(12) | 0.0471(14) | 0.0431(14) | 0.0028(11) | -0.0054(10) |
| S(2)  | 0.0512(13) | 0.0471(14) | 0.0333(13) | 0.0012(10) | -0.0025(10) |
| S(3)  | 0.0458(12) | 0.0455(14) | 0.0408(14) | 0.0056(10) | -0.0039(10) |
| S(4)  | 0.0470(12) | 0.0413(13) | 0.0430(14) | 0.0027(10) | -0.0006(10) |
| O(1)  | 0.0444(4) | 0.0574(5) | 0.0604(5) | 0.0093 | -0.0083 |
| O(2)  | 0.0845(5) | 0.0584(5) | 0.0484 | -0.0034 | 0.0134 |
| O(3)  | 0.0755(5) | 0.0504(5) | 0.0484 | 0.0023 | -0.0143 |
| O(4)  | 0.0564(5) | 0.0665(5) | 0.0494 | -0.0113 | 0.0103 |
| O(5)  | 0.0544(5) | 0.0574(5) | 0.0564 | -0.0083 | -0.0033 |
| O(6)  | 0.0556(5) | 0.0375(5) | 0.0365 | 0.0024 | -0.0034 |
| O(7)  | 0.0455(5) | 0.0435(5) | 0.0516 | 0.0105 | -0.0044 |
| O(8)  | 0.0736(6) | 0.0546(5) | 0.0386 | 0.0065 | 0.0005 |
| O(9)  | 0.0354(5) | 0.0546(5) | 0.0436 | 0.0055 | -0.0104 |
| O(10) | 0.0495(5) | 0.0405(5) | 0.0395 | -0.0024 | -0.0024 |
| O(11) | 0.0515(5) | 0.0536(6) | 0.0496 | 0.0125 | -0.0124 |
| O(12) | 0.0636(6) | 0.0616(7) | 0.0366 | 0.0050 | -0.0044 |
| O(13) | 0.0555(5) | 0.0536(5) | 0.0406 | 0.0034 | -0.0054 |
| O(14) | 0.0606(5) | 0.0425(5) | 0.0365 | 0.0024 | -0.0014 |
| O(15) | 0.0475(5) | 0.0415(5) | 0.0335 | 0.0004 | 0.0004 |
| O(16) | 0.0707(7) | 0.0798(5) | 0.0496 | -0.0215 | 0.0175 |
| O(17) | 0.1111(10) | 0.1011(10) | 0.0859 | -0.0458 | 0.0668 |
| O(18) | 0.0636(6) | 0.0699(7) | 0.0778 | -0.0156 | 0.0106 |
| O(19) | 0.0616(6) | 0.0516(6) | 0.0416 | -0.0034 | -0.0105 |
| O(20) | 0.0666(6) | 0.0446(6) | 0.0547 | 0.0035 | 0.0055 |
| O(21) | 0.0555(5) | 0.0365(5) | 0.0295 | 0.0024 | -0.0034 |
| O(22) | 0.0596(5) | 0.0506(5) | 0.0355 | 0.0144 | 0.0034 |
| O(23) | 0.0566(6) | 0.0838(5) | 0.0456 | 0.0185 | 0.0025 |
| O(24) | 0.0647(6) | 0.0567(6) | 0.0547 | 0.0005 | -0.0075 |
| O(25) | 0.0727(7) | 0.0436(6) | 0.0436 | -0.0044 | -0.0165 |
| O(26) | 0.0586(5) | 0.0466(5) | 0.0476 | 0.0045 | -0.0094 |
| O(27) | 0.0495(5) | 0.0425(5) | 0.0436 | 0.0024 | 0.0044 |
| O(28) | 0.0636(5) | 0.0627(6) | 0.0416 | -0.0045 | -0.0105 |
| O(29) | 0.0878(5) | 0.1051(9) | 0.0447 | 0.0076 | -0.0136 |
| O(30) | 0.0879(9) | 0.0981(10) | 0.0477 | -0.0176 | 0.0126 |
| O(31) | 0.0596(5) | 0.0808(8) | 0.0557 | -0.0076 | 0.0095 |
| O(32) | 0.0586(5) | 0.0606(6) | 0.0436 | -0.0075 | 0.0095 |
| O(33) | 0.0545(5) | 0.0425(5) | 0.0395 | 0.0034 | 0.0054 |
| O(34) | 0.0395(5) | 0.0495(5) | 0.0375 | 0.0034 | 0.0064 |
| O(35) | 0.0505(5) | 0.0586(6) | 0.0557 | -0.0045 | 0.0155 |
| O(36) | 0.0546(5) | 0.0757(6) | 0.0295 | -0.0145 | 0.0004 |
| O(37) | 0.0455(5) | 0.0757(6) | 0.0496 | -0.0155 | -0.0054 |
| O(38) | 0.0455(5) | 0.0586(6) | 0.0335 | 0.0024 | 0.0064 |

Table 4. Anisotropic displacement parameters ($\AA^2$) for str0732. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^2U^{11} + \ldots + 2hka*b*U^{12}]$.
| C(34) | 0.046(5) | 0.045(5) | 0.033(5) | −0.004(4) | −0.002(4) | −0.004(4) |
|-------|----------|----------|----------|-----------|-----------|-----------|
| C(35) | 0.056(6) | 0.071(7) | 0.034(5) | 0.010(5)  | −0.004(4) | −0.007(5) |
| C(36) | 0.067(7) | 0.058(7) | 0.041(6) | 0.002(5)  | −0.010(5) | 0.018(5)  |
| C(37) | 0.052(6) | 0.058(6) | 0.049(6) | −0.006(5) | −0.013(5) | 0.002(4)  |
| C(38) | 0.040(5) | 0.061(6) | 0.043(6) | 0.002(5)  | 0.002(4)  | −0.002(4) |
| C(39) | 0.058(6) | 0.048(6) | 0.032(5) | 0.003(4)  | −0.010(4) | −0.006(4) |
| C(40) | 0.049(5) | 0.032(5) | 0.043(6) | 0.003(4)  | −0.001(4) | −0.003(4) |
| C(41) | 0.054(5) | 0.046(6) | 0.049(6) | 0.006(5)  | −0.008(4) | 0.007(4)  |
| C(42) | 0.066(6) | 0.037(6) | 0.068(7) | −0.001(5) | −0.009(5) | −0.008(4) |
| C(43) | 0.058(6) | 0.045(6) | 0.068(7) | 0.004(5)  | 0.009(5)  | −0.006(4) |
| C(44) | 0.053(6) | 0.062(7) | 0.063(7) | 0.001(6)  | 0.009(5)  | −0.003(5) |
| C(46) | 0.10(2)  | 0.18(4)  | 0.12(3)  | −0.04(3)  | −0.02(2)  | 0.03(2)   |
| C(47) | 0.067(7) | 0.119(11)| 0.079(9) | 0.003(8)  | 0.002(6)  | 0.008(7)  |
| C(48) | 0.073(8) | 0.076(10)| 0.111(12)| 0.014(9)  | 0.011(8)  | −0.006(7) |
| C(49) | 0.086(10)| 0.112(14)| 0.161(18)| 0.037(13) | 0.038(11) | −0.008(9) |
| C(50) | 0.075(10)| 0.159(17)| 0.32(3)  | 0.053(18) | 0.094(14) | 0.018(10) |
Table 5. Hydrogen coordinates and isotropic displacement parameters (Å$^2$) for str0732.

|     | x     | y     | z     | U    |
|-----|-------|-------|-------|------|
| H(6A)| 0.2215| 0.3025| 0.2342| 0.062|
| H(6B)| 0.2388| 0.4147| 0.2260| 0.062|
| H(7A)| 0.1649| 0.4693| 0.2480| 0.065|
| H(7B)| 0.1498| 0.3578| 0.2599| 0.065|
| H(8A)| 0.0540| 0.3749| 0.0452| 0.060|
| H(8B)| 0.0503| 0.4784| 0.0192| 0.060|
| H(9A)| 0.1277| 0.4516| -0.0029| 0.056|
| H(9B)| 0.1327| 0.3511| 0.0253| 0.056|
| H(11A)| 0.0347| 0.0430| 0.2281| 0.078|
| H(12A)| -0.0317| -0.0626| 0.2047| 0.115|
| H(13A)| -0.0451| -0.1084| 0.1297| 0.083|
| H(14A)| 0.0138| -0.0530| 0.0797| 0.062|
| H(15A)| 0.0831| 0.0508| 0.1049| 0.066|
| H(17A)| 0.2316| 0.1543| 0.1732| 0.058|
| H(18A)| 0.3020| 0.0413| 0.1669| 0.073|
| H(19A)| 0.2862| -0.1289| 0.1680| 0.070|
| H(20A)| 0.2033| -0.1883| 0.1825| 0.065|
| H(21A)| 0.1345| -0.0761| 0.1910| 0.062|
| H(23A)| 0.1858| 0.0857| 0.2683| 0.067|
| H(24A)| 0.1803| 0.1222| 0.3443| 0.096|
| H(25A)| 0.1103| 0.2189| 0.3653| 0.092|
| H(26A)| 0.0423| 0.2639| 0.3137| 0.077|
| H(27A)| 0.0502| 0.2327| 0.2384| 0.064|
| H(29A)| 0.1955| 0.6356| -0.0189| 0.050|
| H(30A)| 0.2036| 0.5408| -0.0818| 0.065|
| H(31A)| 0.1284| 0.4935| -0.1275| 0.063|
| H(32A)| 0.0453| 0.5347| -0.1066| 0.068|
| H(33A)| 0.0366| 0.6297| -0.0441| 0.054|
| H(35A)| 0.0489| 0.8534| -0.0230| 0.065|
| H(36A)| -0.0366| 0.9118| -0.0288| 0.067|
| H(37A)| -0.0980| 0.8433| 0.0166| 0.065|
| H(38A)| -0.0727| 0.7166| 0.0663| 0.058|
| H(39A)| 0.0139| 0.6600| 0.0733| 0.056|
| H(41A)| 0.1440| 0.8631| 0.0862| 0.061|
| H(42A)| 0.1878| 1.0140| 0.0786| 0.069|
| H(43A)| 0.2195| 1.0574| 0.0127| 0.068|
| H(44A)| 0.2044| 0.9584| -0.0495| 0.071|
| H(45A)| 0.1587| 0.8073| -0.0444| 0.064|
Table 6. Torsion angles [°] for str0732.

| Bond Sequence                  | Torsion Angle [°] |
|--------------------------------|-------------------|
| C(1)–Fe(1)–Fe(2)–C(3)          | 130.4(6)          |
| S(1)–Fe(1)–Fe(2)–C(3)          | −52.1(5)          |
| S(2)–Fe(1)–Fe(2)–C(3)          | 51.7(5)           |
| C(2)–Fe(1)–Fe(2)–S(1)          | −81.1(3)          |
| S(2)–Fe(1)–Fe(2)–S(1)          | 103.8(11)         |
| C(2)–Fe(1)–Fe(2)–S(1)          | 88.0(3)           |
| P(1)–Fe(1)–Fe(2)–S(1)          | −139.14(18)       |
| C(1)–Fe(1)–Fe(2)–S(2)          | 78.7(3)           |
| S(1)–Fe(1)–Fe(2)–S(2)          | −103.80(11)       |
| C(1)–Fe(1)–Fe(2)–S(4)          | −91.4(3)          |
| S(1)–Fe(1)–Fe(2)–S(4)          | 86.14(11)         |
| S(2)–Fe(2)–Fe(3)–C(3)          | 44.2(4)           |
| S(4)–Fe(2)–Fe(3)–C(3)          | −176.0(3)         |
| S(4)–Fe(2)–Fe(3)–C(5)          | −178.1(3)         |
| S(4)–Fe(2)–Fe(3)–C(5)          | −76.2(3)          |
| C(3)–Fe(2)–Fe(3)–P(2)          | 178.1(4)          |
| S(3)–Fe(2)–Fe(3)–P(2)          | −44.14(18)        |
| S(4)–Fe(2)–Fe(3)–P(2)          | 57.77(18)         |
| C(3)–Fe(2)–Fe(3)–S(3)          | −137.7(4)         |
| C(3)–Fe(2)–Fe(3)–S(3)          | −59.83(12)        |
| Fe(1)–Fe(2)–Fe(3)–S(3)         | 31.37(15)         |
| S(1)–Fe(2)–Fe(3)–S(4)          | 51.68(15)         |
| S(2)–Fe(2)–Fe(3)–S(4)          | −161.74(12)       |
| C(1)–Fe(1)–P(1)–C(22)          | −99.8(4)          |
| S(1)–Fe(1)–P(1)–C(22)          | 75.0(3)           |
| Fe(2)–Fe(1)–P(1)–C(22)         | 32.7(4)           |
| C(2)–Fe(1)–P(1)–C(16)          | 42.3(4)           |
| S(2)–Fe(1)–P(1)–C(16)          | −133.7(3)         |
| C(1)–Fe(1)–P(1)–C(10)          | 20.3(4)           |
| S(1)–Fe(1)–P(1)–C(10)          | −164.9(3)         |
| Fe(2)–Fe(1)–P(1)–C(10)         | 152.8(3)          |
| C(5)–Fe(3)–P(2)–C(28)          | 98.1(4)           |
| C(4)–Fe(3)–P(2)–C(40)          | 74.1(4)           |
| S(3)–Fe(3)–P(2)–C(40)          | 166.5(3)          |
| Fe(2)–Fe(3)–P(2)–C(40)         | −157.8(3)         |
| C(5)–Fe(3)–P(2)–C(34)          | −138.8(4)         |
| S(4)–Fe(3)–P(2)–C(34)          | 131.2(3)          |
| C(3)–Fe(2)–S(1)–C(6)           | 47.8(4)           |
| S(2)–Fe(2)–S(1)–C(6)           | −45.4(3)          |
| Fe(3)–Fe(2)–S(1)–C(6)          | 109.5(3)          |
| C(3)–Fe(2)–S(1)–Fe(1)          | 147.5(3)          |
| S(2)–Fe(2)–S(1)–Fe(1)          | 54.33(8)          |
| Fe(3)–Fe(2)–S(1)–Fe(1)         | −150.76(13)       |
| C(2)–Fe(1)–S(1)–C(6)           | −157.4(4)         |

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| Bond | Distance (Å) | Bond | Distance (Å) |
|------|-------------|------|-------------|
| S(2)–Fe(1)–S(1)–C(6) | 45.0(3) | Fe(2)–Fe(1)–S(1)–C(6) | 99.2(3) |
| C(1)–Fe(1)–S(1)–Fe(2) | 67.8 | C(2)–Fe(1)–S(1)–Fe(2) | 103.4(3) |
| P(1)–Fe(1)–S(1)–Fe(2) | −158.95(9) | S(2)–Fe(1)–S(1)–Fe(2) | −54.15(8) |
| C(3)–Fe(2)–S(2)–C(7) | −46.6(5) | S(1)–Fe(2)–S(2)–C(7) | 46.9(3) |
| S(3)–Fe(2)–S(2)–C(7) | −160.1(3) | S(4)–Fe(2)–S(2)–C(7) | 137.1(4) |
| Fe(3)–Fe(2)–S(2)–Fe(1) | −114.1(3) | Fe(1)–Fe(2)–S(2)–C(7) | 101.2(3) |
| C(3)–Fe(2)–S(2)–Fe(1) | −147.7(3) | S(1)–Fe(2)–S(2)–Fe(1) | −54.33(8) |
| S(3)–Fe(2)–S(2)–Fe(1) | 98.76(9) | S(4)–Fe(2)–S(2)–Fe(1) | 35.9(4) |
| Fe(3)–Fe(2)–S(2)–Fe(1) | 144.74(9) | C(1)–Fe(1)–S(2)–C(7) | 155.7(4) |
| C(2)–Fe(1)–S(2)–C(7) | −108.2(7) | S(1)–Fe(1)–S(2)–C(7) | −43.9(3) |
| P(1)–Fe(1)–S(2)–C(7) | 62.3(3) | Fe(2)–Fe(1)–S(2)–C(7) | −96.6(3) |
| C(1)–Fe(1)–S(2)–Fe(2) | −107.7(3) | C(2)–Fe(1)–S(2)–Fe(2) | −11.6(7) |
| S(1)–Fe(1)–S(2)–Fe(2) | 53.65(8) | P(1)–Fe(1)–S(2)–Fe(2) | 158.92(8) |
| Fe(1)–Fe(1)–S(3)–C(8) | 141.7(4) | S(1)–Fe(2)–S(3)–C(8) | −47.6(4) |
| C(5)–Fe(3)–S(3)–C(8) | −95.3(10) | S(4)–Fe(2)–S(3)–C(8) | 42.5(3) |
| S(4)–Fe(3)–S(3)–C(8) | −46.1(3) | Fe(1)–Fe(2)–S(3)–C(8) | −67.4(3) |
| C(4)–Fe(3)–S(3)–Fe(2) | −105.5(3) | S(1)–Fe(2)–S(3)–Fe(2) | −145.7(2) |
| P(2)–Fe(3)–S(3)–Fe(2) | 159.79(9) | S(4)–Fe(3)–S(3)–Fe(2) | 55.54(8) |
| C(3)–Fe(2)–S(4)–C(9) | −155.7(5) | S(1)–Fe(2)–S(4)–C(9) | 108.3(3) |
| S(3)–Fe(2)–S(4)–C(9) | −43.8(3) | S(2)–Fe(2)–S(4)–C(9) | 20.6(5) |
| S(3)–Fe(2)–S(4)–C(9) | −99.4(3) | S(3)–Fe(2)–S(4)–Fe(3) | −152.29(8) |
| C(3)–Fe(2)–S(4)–Fe(3) | −56.3(3) | S(1)–Fe(2)–S(4)–Fe(3) | −152.29(8) |
| S(3)–Fe(2)–S(4)–Fe(3) | 55.56(8) | S(2)–Fe(2)–S(4)–Fe(3) | 120.0(4) |
| Fe(1)–Fe(2)–S(4)–Fe(3) | 151.20(7) | C(4)–Fe(3)–S(4)–C(9) | 110.7(8) |
| C(5)–Fe(3)–S(4)–C(9) | −147.6(4) | P(2)–Fe(3)–S(4)–C(9) | −54.9(3) |
| S(3)–Fe(3)–S(4)–C(9) | 45.2(3) | Fe(2)–Fe(3)–S(4)–C(9) | 99.8(3) |
| C(4)–Fe(3)–S(4)–Fe(2) | 10.9(7) | C(5)–Fe(3)–S(4)–Fe(2) | 112.6(3) |
| P(2)–Fe(3)–S(4)–Fe(2) | −154.75(8) | S(3)–Fe(3)–S(4)–Fe(2) | −54.65(7) |
| C(2)–Fe(1)–C(1)–O(1) | −7(23) | S(1)–Fe(1)–C(1)–O(1) | 88(23) |
| P(1)–Fe(1)–C(1)–O(1) | −105(23) | S(2)–Fe(1)–C(1)–O(1) | 148(23) |
| Fe(2)–Fe(1)–C(1)–O(1) | 94(23) | C(1)–Fe(1)–C(2)–O(2) | 143(14) |
| S(1)–Fe(1)–C(2)–O(2) | −16(14) | P(1)–Fe(1)–C(2)–O(2) | −123(14) |
| S(2)–Fe(1)–C(2)–O(2) | 48(15) | Fe(2)–Fe(1)–C(2)–O(2) | 38(14) |
| S(1)–Fe(2)–C(3)–O(3) | −29(4) | S(3)–Fe(2)–C(3)–O(3) | 147(4) |
| S(2)–Fe(2)–C(3)–O(3) | 53(4) | S(4)–Fe(2)–C(3)–O(3) | −128(4) |
| Fe(3)–Fe(2)–C(3)–O(3) | −176(5) | Fe(1)–Fe(2)–C(3)–O(3) | 12(5) |
| C(5)–Fe(3)–C(4)–O(4) | −117(15) | P(2)–Fe(3)–C(4)–O(4) | 149(15) |
| S(3)–Fe(3)–C(4)–O(4) | 47(15) | S(4)–Fe(3)–C(4)–O(4) | −17(15) |
| Fe(2)–Fe(3)–C(4)–O(4) | −8(15) | C(4)–Fe(3)–C(5)–O(5) | 145(10) |
| P(2)–Fe(3)–C(5)–O(5) | −121(10) | S(3)–Fe(3)–C(5)–O(5) | 33(10) |
| S(4)–Fe(3)–C(5)–O(5) | −15(10) | Fe(2)–Fe(3)–C(5)–O(5) | 39(10) |
| Fe(2)–S(1)–C(6)–C(7) | 33.1(7) | Fe(1)–S(1)–C(6)–C(7) | −38.5(7) |
| S(1)–C(6)–C(7)–S(2) | 4.4(9) | Fe(2)–S(2)–C(7)–S(6) | −39.4(7) |
| Fe(1)–S(2)–C(7)–C(6) | 31.4(7) | Fe(2)–S(3)–C(8)–S(4) | −30.8(7) |
| Fe(3)–S(3)–C(8)–C(9) | 38.8(7) | S(3)–C(8)–C(9)–S(4) | −30.8(7) |
| Fe(2)–S(4)–C(9)–C(8) | 36.4(7) | Fe(3)–S(4)–C(9)–C(8) | −34.0(7) |
| C(22)–P(1)–C(10)–C(15) | −178.2(7) | C(16)–P(1)–C(10)–C(15) | −70.1(7) |
| Bond/Angle | Distance/Angle |
|------------|---------------|
| Fe(1)–P(1)–C(10)–C(15) | 55.7(8) |
| C(16)–P(1)–C(10)–C(11) | 107.7(9) |
| C(15)–C(10)–C(11)–C(12) | 0.4(16) |
| C(10)–C(11)–C(12)–C(13) | −2(2) |
| C(12)–C(13)–C(14)–C(15) | −0.9(16) |
| P(1)–C(10)–C(15)–C(14) | 178.6(7) |
| C(22)–P(1)–C(16)–C(17) | −98.3(7) |
| Fe(1)–P(1)–C(16)–C(17) | 30.8(8) |
| C(10)–P(1)–C(16)–C(21) | 84.4(7) |
| C(16)–P(1)–C(22)–C(27) | 172.4(7) |
| C(34)–P(2)–C(28)–C(33) | 120.9(7) |
| Fe(3)–P(2)–C(28)–C(29) | 66.3(7) |
| C(33)–C(28)–C(29)–C(30) | −2.4(12) |
| C(28)–C(29)–C(30)–C(31) | 1.9(13) |
| C(30)–C(31)–C(32)–C(33) | 1.7(15) |
| C(29)–C(28)–C(33)–C(32) | 2.6(13) |
| C(28)–P(2)–C(34)–C(35) | −70.0(8) |
| Fe(3)–P(2)–C(34)–C(35) | 161.4(6) |
| C(40)–P(2)–C(34)–C(39) | −141.8(7) |
| C(39)–C(34)–C(35)–C(36) | −1.3(13) |
| C(34)–C(35)–C(36)–C(37) | 0.4(14) |
| C(36)–C(37)–C(38)–C(39) | 0.9(14) |
| C(35)–C(34)–C(39)–C(38) | 2.1(12) |
| C(28)–P(2)–C(40)–C(45) | 6.1(8) |
| Fe(3)–P(2)–C(40)–C(45) | 131.7(7) |
| P(2)–C(2)–C(3)–C(4) | −178.8(7) |
| C(49)–C(46)–C(47)–C(50) | 85.5(5) |
| C(47)–C(46)–C(48)–C(49) | 126.3(4) |
Table 1. Crystal data and structure refinement for str0889 (4).

| Identification code | str0889 |
|---------------------|---------|
| Chemical formula    | C_{35}H_{30}Fe_{3}O_{5}P_{2}S_{4} |
| Formula weight      | 888.32 |
| Temperature         | 150(2) K |
| Radiation, wavelength| MoKα, 0.71073 Å |
| Crystal system, space group | orthorhombic, Pnma |
| Unit cell parameters| a = 23.939(7) Å, α = 90°  
b = 17.775(5) Å, β = 90°  
c = 8.513(2) Å, γ = 90° |
| Cell volume         | 3622.4(18) Å³ |
| Z                   | 4 |
| Calculated density  | 1.629 g/cm³ |
| Absorption coefficient μ | 1.546 mm⁻¹ |
| F(000)              | 1808 |
| Crystal colour and size | orange, 0.40 × 0.34 × 0.03 mm³ |
| Data collection method | Bruker SMART 1K CCD diffractometer |
| θ range for data collection | ω rotation with narrow frames |
| Index ranges        | h −30 to 31, k −23 to 23, l −11 to 10 |
| Completeness to θ = 26.00° | 99.6 % |
| Reflections collected | 28927 |
| Independent reflections | 4433 (R_{int} = 0.0695) |
| Reflections with F²>2σ | 2997 |
| Absorption correction | semi-empirical from equivalents |
| Min. and max. transmission | 0.5767 and 0.9551 |
| Structure solution  | direct methods |
| Refinement method   | Full-matrix least-squares on F² |
| Weighting parameters a, b | 0.0514, 0.0000 |
| Data / restraints / parameters | 4433 / 0 / 235 |
| Final R indices [F²>2σ] | R₁ = 0.0396, wR₂ = 0.0854 |
| R indices (all data) | R₁ = 0.0661, wR₂ = 0.0903 |
| Goodness-of-fit on F² | 0.906 |
| Largest and mean shift/su | 0.001 and 0.000 |
| Largest diff. peak and hole | 1.430 and −0.608 e Å⁻³ |
Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å$^2$) for str0889. $U_{eq}$ is defined as one third of the trace of the orthogonalized $U^0$ tensor.

| Atom | x          | y          | z          | $U_{eq}$     |
|------|------------|------------|------------|--------------|
| Fe(1)| 0.15503(2) | 0.2500     | 0.59365(6) | 0.01868(13)  |
| Fe(2)| 0.25908(2) | 0.2500     | 0.52604(6) | 0.01954(13)  |
| Fe(3)| 0.36290(2) | 0.2500     | 0.58924(7) | 0.03029(16)  |
| P(1) | 0.10398(3) | 0.16421(4) | 0.46965(8) | 0.02208(16)  |
| S(1) | 0.21782(3) | 0.16739(4) | 0.68991(7) | 0.02195(15)  |
| S(2) | 0.31925(3) | 0.16841(4) | 0.42807(8) | 0.03068(18)  |
| C(1) | 0.11999(15)| 0.2500     | 0.7598(5)  | 0.0255(9)    |
| C(2) | 0.21393(14)| 0.2500     | 0.3608(5)  | 0.0221(8)    |
| C(3) | 0.36755(12)| 0.1787(2)  | 0.7368(4)  | 0.0389(8)    |
| C(4) | 0.43235(19)| 0.2500     | 0.5080(5)  | 0.0485(13)   |
| O(1) | 0.08707(12)| 0.2500     | 0.8762(3)  | 0.0425(8)    |
| O(2) | 0.19911(10)| 0.2500     | 0.2319(3)  | 0.0246(6)    |
| O(3) | 0.37049(9) | 0.13483(15)| 0.8352(3)  | 0.0570(7)    |
| O(4) | 0.47546(13)| 0.2500     | 0.4516(4)  | 0.0816(14)   |
| C(5) | 0.23246(11)| 0.20701(15)| 0.8834(3)  | 0.0289(6)    |
| C(6) | 0.33451(13)| 0.20760(18)| 0.2349(3)  | 0.0407(8)    |
| C(7) | 0.44611(11)| 0.21312(15)| 0.3820(3)  | 0.0267(6)    |
| C(8) | 0.13317(11)| 0.11023(15)| 0.3069(3)  | 0.0249(6)    |
| C(9) | 0.18200(12)| 0.06805(16)| 0.3319(3)  | 0.0330(7)    |
| C(10)| 0.20534(13)| 0.02725(18)| 0.2092(4)  | 0.0415(8)    |
| C(11)| 0.18149(14)| 0.02861(18)| 0.0624(4)  | 0.0441(8)    |
| C(12)| 0.13430(13)| 0.07173(17)| 0.0348(4)  | 0.0391(8)    |
| C(13)| 0.11035(11)| 0.11240(16)| 0.1569(3)  | 0.0307(7)    |
| C(14)| 0.06892(11)| 0.09328(15)| 0.5902(3)  | 0.0263(6)    |
| C(15)| 0.08770(14)| 0.01996(17)| 0.6018(4)  | 0.0467(9)    |
| C(16)| 0.06150(17)| -0.03110(19)| 0.7023(4)  | 0.0597(11)   |
| C(17)| 0.01652(14)| -0.0098(2) | 0.7876(4)  | 0.0480(9)    |
| C(18)| -0.00350(13)| 0.0626(2) | 0.7764(4)  | 0.0499(9)    |
| C(19)| 0.02277(12)| 0.11379(19)| 0.6794(4)  | 0.0424(8)    |
Table 3. Bond lengths [Å] and angles [°] for str0889.

| Bond  | Length  | Bond  | Length  |
|-------|---------|-------|---------|
| Fe(1)–C(1) | 1.750(4) | Fe(1)–P(1) | 2.2211(8) |
| Fe(1)–P(1A) | 2.2211(8) | Fe(1)–S(1A) | 2.2554(8) |
| Fe(1)–S(1) | 2.2554(8) | Fe(1)–C(2) | 1.774(4) |
| Fe(2)–S(2A) | 2.2075(9) | Fe(2)–S(2) | 2.2075(9) |
| Fe(2)–S(1) | 2.2533(8) | Fe(2)–S(1A) | 2.2533(8) |
| Fe(2)–Fe(3) | 2.5430(10) | Fe(2)–C(3A) | 1.787(3) |
| Fe(3)–C(3) | 1.787(3) | Fe(3)–C(4) | 1.800(5) |
| Fe(3)–S(2) | 2.2534(9) | Fe(3)–S(2A) | 2.2534(9) |
| C(8)–P(1) | 1.824(3) | C(7)–P(1) | 1.825(3) |
| P(1)–C(8) | 1.825(3) | P(1)–C(7) | 1.825(3) |
| S(1)–C(5) | 1.825(3) | S(2)–C(6) | 1.823(3) |
| Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|----------------------|--------------|----------------------|--------------|
| C(14)–P(1)–Fe(1)    | 117.32(9)    | C(5)–S(1)–Fe(2)     | 102.89(9)    |
| C(5)–S(1)–Fe(1)     | 101.81(9)    | Fe(2)–S(1)–Fe(1)    | 69.08(3)     |
| C(6)–S(2)–Fe(2)     | 102.74(10)   | C(6)–S(2)–Fe(3)     | 102.15(11)   |
| Fe(2)–S(2)–Fe(3)    | 69.50(3)     | O(1)–C(1)–Fe(1)     |              |
| O(2)–C(2)–Fe(2)     | 160.4(3)     | O(2)–C(2)–Fe(1)     | 126.7(3)     |
| Fe(2)–C(2)–Fe(1)    | 72.96(14)    | O(3)–C(3)–Fe(3)     | 177.7(3)     |
| O(4)–C(4)–Fe(3)     | 177.6(4)     | C(5A)–C(5)–S(1)     | 112.69(9)    |
| C(6A)–C(6)–S(2)     | 112.46(10)   | C(7A)–C(7)–P(1)     | 118.44(9)    |
| C(13)–C(8)–C(9)     | 118.8(3)     | C(13)–C(8)–P(1)     | 122.2(2)     |
| C(9)–C(8)–P(1)      | 119.0(2)     | C(10)–C(9)–C(8)     | 119.9(3)     |
| C(11)–C(10)–C(9)    | 120.5(3)     | C(10)–C(11)–C(12)   | 120.2(3)     |
| C(11)–C(12)–C(13)   | 119.9(3)     | C(12)–C(13)–C(8)    | 120.7(3)     |
| C(15)–C(14)–C(19)   | 117.8(3)     | C(15)–C(14)–P(1)    | 122.7(2)     |
| C(19)–C(14)–P(1)    | 119.4(2)     | C(14)–C(15)–C(16)   | 120.7(3)     |
| C(17)–C(16)–C(15)   | 120.3(3)     | C(16)–C(17)–C(18)   | 120.1(3)     |
| C(17)–C(18)–C(19)   | 119.9(3)     | C(18)–C(19)–C(14)   | 121.1(3)     |

Symmetry operations for equivalent atoms

A: \(x, -y + 1/2, z\)
Table 4. Anisotropic displacement parameters (Å²) for str0889. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\hbar^2a^*U_11+...+2hka^*b^*U_{12}]$

|       | $U_1$  | $U_2$  | $U_3$  | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|-------|--------|--------|--------|---------|---------|---------|
| Fe(1) | 0.0165(3) | 0.0242(3) | 0.0153(3) | 0.0000 | 0.0001(2) | 0.0000 |
| Fe(2) | 0.0172(3) | 0.0253(3) | 0.0161(3) | 0.0000 | 0.0015(2) | 0.0000 |
| Fe(3) | 0.0177(3) | 0.0497(4) | 0.0235(3) | 0.0000 | 0.0015(2) | 0.0000 |
| P(1)  | 0.0197(3) | 0.0268(4) | 0.0197(3) | 0.0000 | -0.0005(3) | -0.0020(3) |
| S(1)  | 0.0213(3) | 0.0260(3) | 0.0186(3) | 0.0001(3) | 0.0004(3) | 0.0013(3) |
| S(2)  | 0.0279(4) | 0.0387(4) | 0.0255(4) | -0.0048(3) | 0.0040(3) | 0.0076(3) |
| C(1)  | 0.0195(19) | 0.030(2) | 0.027(2) | 0.0000 | -0.0042(17) | 0.0000 |
| C(2)  | 0.0172(19) | 0.024(2) | 0.025(2) | 0.0000 | 0.0013(16) | 0.0000 |
| C(3)  | 0.0270(16) | 0.058(2) | 0.0318(17) | 0.0009(16) | -0.0006(14) | 0.0110(15) |
| C(4)  | 0.029(2) | 0.087(4) | 0.030(3) | 0.0000 | -0.002(2) | 0.0000 |
| O(1)  | 0.0346(17) | 0.067(2) | 0.0255(16) | 0.0000 | 0.0127(14) | 0.0000 |
| O(2)  | 0.0257(14) | 0.0329(16) | 0.0152(14) | 0.0000 | 0.0019(11) | 0.0000 |
| O(3)  | 0.0516(15) | 0.0725(17) | 0.0468(16) | 0.0156(14) | -0.0012(12) | 0.0203(13) |
| O(4)  | 0.0271(19) | 0.173(4) | 0.045(2) | 0.0000 | 0.0116(17) | 0.0000 |
| C(5)  | 0.0279(15) | 0.0410(17) | 0.0177(14) | 0.0053(12) | -0.0030(12) | 0.0006(13) |
| C(6)  | 0.0359(17) | 0.065(2) | 0.0215(15) | -0.0037(14) | 0.0085(13) | 0.0119(16) |
| C(7)  | 0.0210(13) | 0.0370(15) | 0.0219(14) | -0.0005(11) | -0.0026(11) | -0.0018(11) |
| C(8)  | 0.0275(14) | 0.0238(15) | 0.0233(14) | -0.0044(11) | -0.0005(12) | -0.0072(12) |
| C(9)  | 0.0355(17) | 0.0306(17) | 0.0328(17) | -0.0060(13) | 0.0009(13) | 0.0011(13) |
| C(10) | 0.0423(19) | 0.0354(18) | 0.047(2) | -0.0075(15) | 0.0052(16) | 0.0042(15) |
| C(11) | 0.056(2) | 0.0379(19) | 0.039(2) | -0.0158(15) | 0.0171(16) | -0.0099(16) |
| C(12) | 0.0447(19) | 0.048(2) | 0.0243(16) | -0.0081(14) | 0.0063(14) | -0.0183(16) |
| C(13) | 0.0294(15) | 0.0358(17) | 0.0269(16) | -0.0027(13) | 0.0030(12) | -0.0114(13) |
| C(14) | 0.0243(14) | 0.0304(15) | 0.0241(14) | -0.0004(12) | -0.0036(12) | -0.0071(12) |
| C(15) | 0.060(2) | 0.0305(18) | 0.050(2) | 0.0002(15) | 0.0212(17) | -0.0031(16) |
| C(16) | 0.087(3) | 0.0268(19) | 0.066(3) | 0.0011(17) | 0.026(2) | -0.0106(19) |
| C(17) | 0.046(2) | 0.053(2) | 0.045(2) | 0.0093(17) | -0.0035(17) | -0.0261(18) |
| C(18) | 0.0259(16) | 0.073(3) | 0.051(2) | 0.0240(19) | 0.0087(15) | -0.0014(17) |
| C(19) | 0.0303(16) | 0.049(2) | 0.047(2) | 0.0166(16) | 0.0079(15) | 0.0069(15) |
Table 5. Hydrogen coordinates and isotropic displacement parameters (Å²) for str0889.

|        | x     | y     | z     | U     |
|--------|-------|-------|-------|-------|
| H(5A)  | 0.2040| 0.1888| 0.9587| 0.035 |
| H(5B)  | 0.2694| 0.1888| 0.9196| 0.035 |
| H(6A)  | 0.3715| 0.1894| 0.1997| 0.049 |
| H(6B)  | 0.3063| 0.1894| 0.1589| 0.049 |
| H(7A)  | 0.0144| 0.1858| 0.3375| 0.032 |
| H(9A)  | 0.1991| 0.0674| 0.4327| 0.040 |
| H(10A) | 0.2380| −0.0018| 0.2268| 0.050 |
| H(11A) | 0.1974| −0.0001| −0.0204| 0.053 |
| H(12A) | 0.1183| 0.0735| −0.0673| 0.047 |
| H(13A) | 0.0780| 0.1420| 0.1376| 0.037 |
| H(15A) | 0.1188| 0.0041| 0.5408| 0.056 |
| H(16A) | 0.0753| −0.0810| 0.7108| 0.072 |
| H(17A) | −0.0013| −0.0448| 0.8554| 0.058 |
| H(18A) | −0.0354| 0.0773| 0.8354| 0.060 |
| H(19A) | 0.0091| 0.1639| 0.6736| 0.051 |
Table 6. Torsion angles [°] for str0889.

| Bond | Angle [°] | Bond | Angle [°] |
|------|----------|------|----------|
| C(1)–Fe(1)–Fe(2)–C(2) | 180.0 | P(1)–Fe(1)–Fe(2)–C(2) | 49.47(3) |
| P(1A)–Fe(1)–Fe(2)–C(2) | −49.47(3) | S(1A)–Fe(1)–Fe(2)–C(2) | −127.75(2) |
| S(1)–Fe(1)–Fe(2)–C(2) | 127.75(2) | C(1)–Fe(1)–Fe(2)–S(2A) | −108.61(4) |
| P(1)–Fe(1)–Fe(2)–S(2A) | 120.86(5) | P(1A)–Fe(1)–Fe(2)–S(2A) | 21.92(5) |
| S(1A)–Fe(1)–Fe(2)–S(2A) | −56.36(5) | S(1)–Fe(1)–Fe(2)–S(2A) | −160.86(5) |
| C(2)–Fe(1)–Fe(2)–S(2A) | 71.39(4) | C(1)–Fe(1)–Fe(2)–S(2A) | 108.61(4) |
| P(1)–Fe(1)–Fe(2)–S(2A) | −21.92(5) | P(1A)–Fe(1)–Fe(2)–S(2A) | −120.86(5) |
| S(1A)–Fe(1)–Fe(2)–S(2A) | −79.28(4) | S(1)–Fe(1)–Fe(2)–S(2A) | 56.36(5) |
| S(1)–Fe(1)–Fe(2)–C(2) | 127.75(2) | S(1A)–Fe(1)–Fe(2)–C(2) | 108.61(4) |
| C(2)–Fe(1)–Fe(2)–C(2) | −108.61(4) | P(1)–Fe(1)–Fe(2)–C(2) | −21.92(5) |
| P(1A)–Fe(1)–Fe(2)–C(2) | 120.86(5) | P(1A)–Fe(1)–Fe(2)–C(2) | 49.47(3) |
| S(1)–Fe(1)–Fe(2)–C(2) | −56.36(5) | S(1A)–Fe(1)–Fe(2)–C(2) | −160.86(5) |
| C(2)–Fe(1)–Fe(2)–C(2) | 71.39(4) | C(1)–Fe(1)–Fe(2)–C(2) | 108.61(4) |
| P(1)–Fe(1)–Fe(2)–C(2) | −21.92(5) | P(1A)–Fe(1)–Fe(2)–C(2) | −120.86(5) |
| S(1A)–Fe(1)–Fe(2)–C(2) | −79.28(4) | S(1)–Fe(1)–Fe(2)–C(2) | 56.36(5) |
| S(1)–Fe(1)–Fe(2)–C(2) | 127.75(2) | S(1A)–Fe(1)–Fe(2)–C(2) | 108.61(4) |
| C(2)–Fe(1)–Fe(2)–C(2) | −108.61(4) | P(1)–Fe(1)–Fe(2)–C(2) | −21.92(5) |
| P(1A)–Fe(1)–Fe(2)–C(2) | 120.86(5) | P(1A)–Fe(1)–Fe(2)–C(2) | 49.47(3) |
| S(1)–Fe(1)–Fe(2)–C(2) | −56.36(5) | S(1A)–Fe(1)–Fe(2)–C(2) | −160.86(5) |
| C(2)–Fe(1)–Fe(2)–C(2) | 71.39(4) | C(1)–Fe(1)–Fe(2)–C(2) | 108.61(4) |
| P(1)–Fe(1)–Fe(2)–C(2) | −21.92(5) | P(1A)–Fe(1)–Fe(2)–C(2) | −120.86(5) |
| S(1A)–Fe(1)–Fe(2)–C(2) | −79.28(4) | S(1)–Fe(1)–Fe(2)–C(2) | 56.36(5) |
| Bond                  | Angle (deg) |
|-----------------------|-------------|
| C(2)–Fe(1)–S(1)–Fe(2) | 31.79(6)    |
| S(2A)–Fe(2)–S(2)–C(6) | -44.22(11) |
| S(1A)–Fe(2)–S(2)–C(6) | -127.31(14) |
| Fe(1)–Fe(2)–S(2)–C(6) | 110.74(11) |
| S(2A)–Fe(2)–S(2)–Fe(3) | 54.16(3)    |
| S(1A)–Fe(2)–S(2)–Fe(3) | -28.93(10)  |
| S(3A)–Fe(3)–S(2)–C(6) | 113.4(3)    |
| C(4)–Fe(3)–S(2)–C(6)  | -53.36(14)  |
| Fe(2)–Fe(3)–S(2)–C(6) | 99.23(10)   |
| C(3)–Fe(3)–S(2)–Fe(2) | 104.90(10)  |
| S(2A)–Fe(3)–S(2)–Fe(2) | -52.99(3)   |
| S(1A)–Fe(3)–S(2)–Fe(2) | -127.31(14) |
| Fe(1)–Fe(3)–S(2)–C(6) | -98.38(11)  |
| C(3A)–Fe(3)–S(2)–C(6) | 110.74(11)  |
| C(4)–Fe(3)–S(2)–C(6)  | -52.99(10)  |
| Fe(2)–Fe(3)–S(2)–C(6) | 113.4(3)    |
| Fe(1)–Fe(3)–S(2)–C(6) | -44.22(11)  |

Symmetry operations for equivalent atoms

A $x,-y+1/2,z$
