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Pentacarbonyl-1 κ^2 C,2 κ^3 C-(4-iodophenyl isocyanide-1 κ C)(μ -propane-1,3-dithiolato-1:2 κ^4 S,S':S,S')iron(I)(Fe—Fe)

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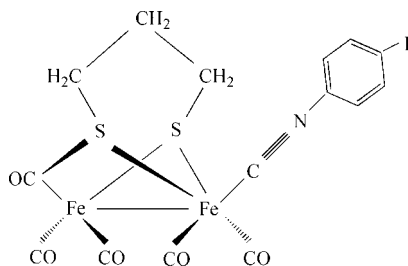
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C—C}) = 0.009$ Å; R factor = 0.051; wR factor = 0.110; data-to-parameter ratio = 13.8.

In the title compound, $[\text{Fe}_2(\text{C}_7\text{H}_4\text{IN})(\text{C}_3\text{H}_6\text{S}_2)(\text{CO})_5]$, the Fe—Fe distance of 2.5156 (11) Å compares well with that in related model structures. The phenyl isocyanide ligand is in the basal position and *trans* to the S atoms of the propanedithiolate ligand due to steric hindrance. The crystal structure features C—H \cdots O interactions.

Related literature

The title compound was prepared as a model for the iron-only hydrogenase ([Fe] H_2 ase) active site. Iron-only hydrogenase in micro-organisms can catalyse the reversible reduction of protons to hydrogen, see: Cammack (1999); Frey (2002); Nicolet *et al.* (2000). For the active site of [Fe] H_2 ase, see: Nicolet *et al.* (1999); Peters *et al.* (1998). For an analogous structure, see: Lyon *et al.* (1999). For the preparation of the starting material $[\text{Fe}_2(\text{S}_2\text{C}_3\text{H}_6)(\text{CO})_6]$, see: Winter *et al.* (1982).



Experimental

Crystal data

| | |
|---|-----------------------------------|
| $[\text{Fe}_2(\text{C}_7\text{H}_4\text{IN})(\text{C}_3\text{H}_6\text{S}_2)(\text{CO})_5]$ | $V = 2001.47$ (15) Å ³ |
| $M_r = 586.96$ | $Z = 4$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation |
| $a = 7.7290$ (3) Å | $\mu = 3.23$ mm ⁻¹ |
| $b = 11.7215$ (5) Å | $T = 293$ K |
| $c = 22.3974$ (10) Å | $0.15 \times 0.14 \times 0.12$ mm |
| $\beta = 99.466$ (1)° | |

Data collection

| | |
|--|--|
| Bruker Smart APEX CCD area-detector diffractometer | 5430 measured reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2000) | 3254 independent reflections |
| $T_{\min} = 0.630$, $T_{\max} = 0.680$ | 2913 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.018$ |

Refinement

| | |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.051$ | 219 restraints |
| $wR(F^2) = 0.110$ | H-atom parameters constrained |
| $S = 1.09$ | $\Delta\rho_{\text{max}} = 0.78$ e Å ⁻³ |
| 3254 reflections | $\Delta\rho_{\text{min}} = -0.64$ e Å ⁻³ |
| 235 parameters | |

Table 1

Selected bond lengths (Å).

| | | | |
|--------|-------------|--------|-------------|
| Fe1—C2 | 1.785 (7) | S1—Fe2 | 2.2590 (16) |
| Fe1—C1 | 1.805 (6) | Fe2—C8 | 1.785 (6) |
| Fe1—C3 | 1.812 (6) | Fe2—C7 | 1.797 (6) |
| Fe1—S1 | 2.2656 (17) | Fe2—C9 | 1.867 (6) |
| Fe1—S2 | 2.2692 (15) | Fe2—S2 | 2.2689 (14) |

Table 2

Hydrogen-bond geometry (Å, °).

| $D\cdots H\cdots A$ | $D\cdots H$ | $H\cdots A$ | $D\cdots A$ | $D\cdots H\cdots A$ |
|------------------------------------|-------------|-------------|-------------|---------------------|
| C12—H12A \cdots O2 ⁱ | 0.93 | 2.57 | 3.423 (9) | 153 |
| C15—H15A \cdots O5 ⁱⁱ | 0.93 | 2.55 | 3.464 (8) | 168 |

 Symmetry codes: (i) $x, y + 1, z$; (ii) $-x + 1, -y + 1, -z + 2$.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2032).

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supporting information

Acta Cryst. (2011). E67, m1753–m1754 [https://doi.org/10.1107/S1600536811047088]

Pentacarbonyl-1 κ^2 C,2 κ^3 C-(4-iodophenyl isocyanide-1 κ C)(μ -propane-1,3-dithiolato-1:2 κ^4 S,S':S,S')iron(I)(Fe—Fe)

Jinli Zhu, Yanfeng Tang, Guo -Min Jiang, Miao Wang and Ping Hua

S1. Comment

The iron-only Hydrogenases ([Fe]H₂ase) in microorganisms can catalyze the reversible reduction of protons to hydrogen according to the reaction: 2H⁺+2 e⁻=H₂. (Cammack *et al.* 1999, Nicolet *et al.* 2000, Frey *et al.* 2002) The active site of [Fe]H₂ase is consisted of a 2Fe₂S linked to a [4Fe₄S] cluster by a bridged cysteine sulfur (Peters *et al.* 1998, Nicolet *et al.* 1999). In the 2Fe₂S unit, the two iron atoms are coordinated by CO and CN⁻ ligands. We have prepared the title complex as a structural model for the iron-only hydrogenases active site. Herein we report its crystal structure.

The molecular structure of the title complex is shown in Fig.1 and selected bond distances are listed in Table 1. The crystal packing diagram reveals that molecules of the title compound form layers in the yz plane (Fig. 2) and the intermolecular interactions present in the structure are listed in Table 2. The Fe—Fe distance of 2.5157 (14) Å compares well with that in the (μ -PDT) Fe₂(CO)₆ analogous structure (Lyon *et al.*, 1999). The phenyl isocyanide ligand is in the basal position and *trans* to the sulfur atoms of the propanedithiolate ligand due to the steric hindrance. The Fe—CN distance of 1.87 Å is longer than Fe—CO distance of 1.79–1.81 Å, suggesting the strong electron σ -donating of the isocyanide ligand with iron center. The π - π conjugation between CN triple bond and phenyl ring is somewhat interrupted in the solid state, as the angle of C(9) N(1) C(10) is 169.8 (9)°, indicating a slight distorting from linearity.

S2. Experimental

A solution of Fe₂(S₂C₃H₆)(CO)₆ (Winter *et al.* 1982) (1.5 g, 3.88 mmol) in 100 ml MeCN was treated with a solution of Me₃NO.2H₂O (433 mg, 3.9 mmol) in 30 ml of MeCN followed by a solution of *p*-benzylisocyanide (895 mg, 3.9 mmol) in 30 ml of MeCN at ambient temperature. After 2 h at this temperature, the solvent was removed in vacuo, and the resulting red residue was purified on silica gel to give title compound as a red solid (1.94 g, 85% yield). Single crystals of the title compound for X-ray analysis were grown by slow evaporation. A near saturated solution of the title compound was prepared in a CH₂Cl₂ -hexane (1:5 v/v) solution. The solution was then being left in a glass tube that has a perforated cap at ambient temperature. After one week, some of the crystals grow on the side of the tube.

S3. Refinement

Carbon-bound H atoms were positioned geometrically, with C—H = 0.97 Å for methylene and 0.93 Å for aromatic, and refined using a riding model, with U_{iso} (H) = 1.2 U_{eq} (C). The hydroxyl H atom was positioned geometrically and freely refined.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

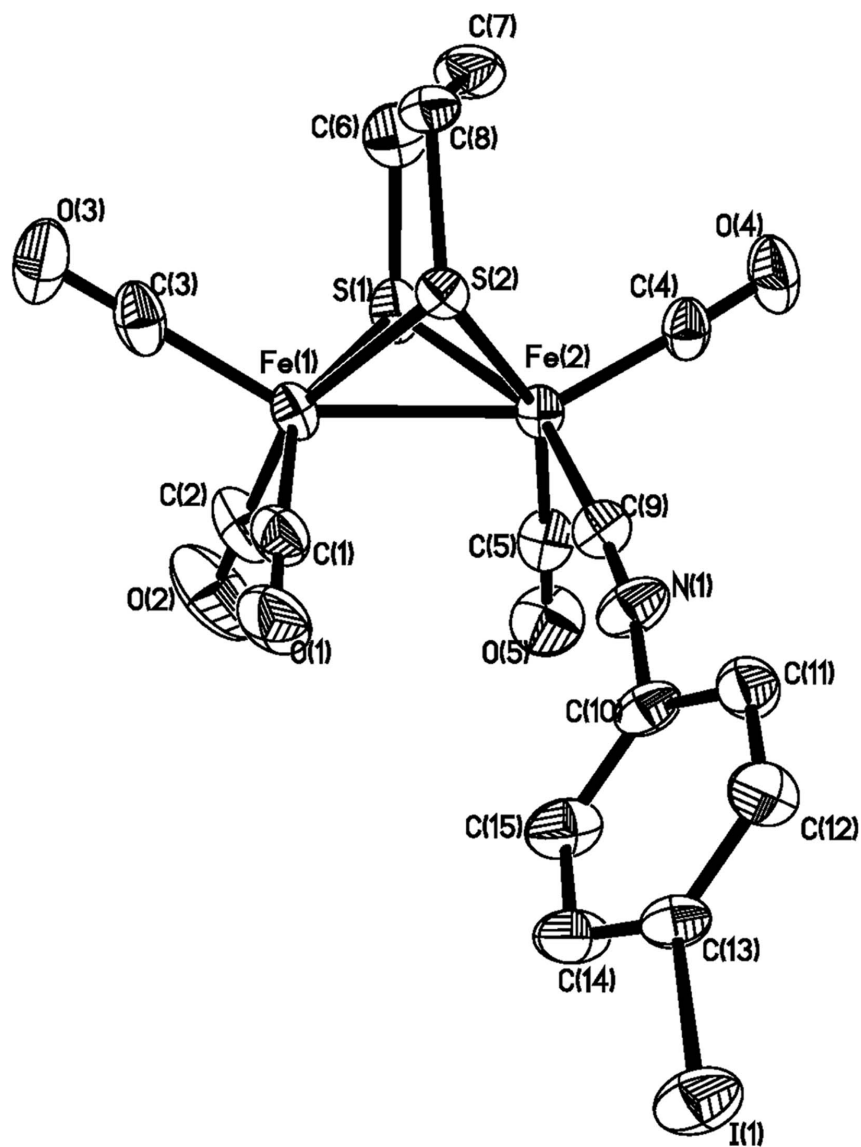


Figure 1

View of the title compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

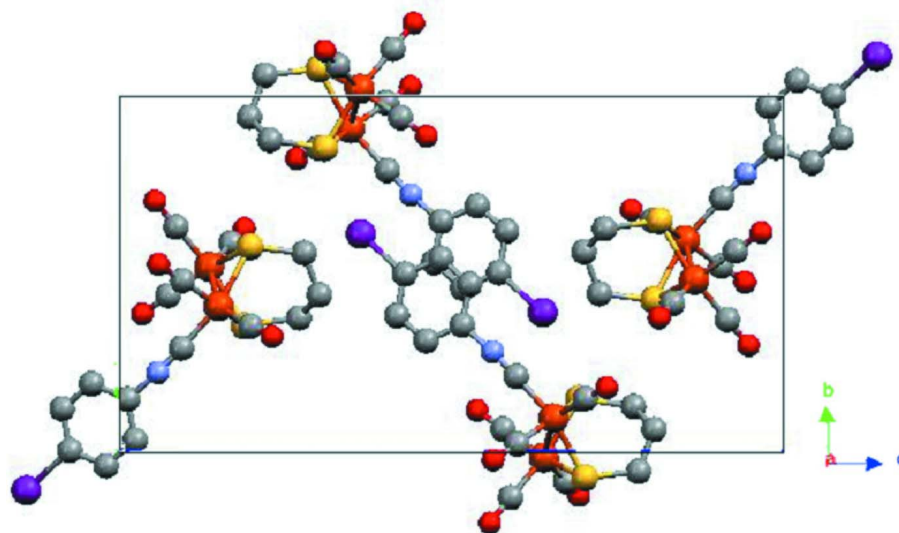


Figure 2

A packing diagram for the title compound viewed along the [001] axis (H atoms are omitted for clarity)

Pentacarbonyl-1 κ^2 C,2 κ^3 C-(4-iodophenyl isocyanide-1 κ C)(μ -propane-1,3-dithiolato-1:2 κ^4 S,S': S,S')iron(I) (Fe—Fe)

Crystal data

[Fe₂(C₇H₄IN)(C₃H₆S₂)(CO)₅]

$M_r = 586.96$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 7.7290$ (3) Å

$b = 11.7215$ (5) Å

$c = 22.3974$ (10) Å

$\beta = 99.466$ (1)°

$V = 2001.47$ (15) Å³

$Z = 4$

$F(000) = 1136$

$D_x = 1.948$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

$\mu = 3.23$ mm⁻¹

$T = 293$ K

Cuboid, red

$0.15 \times 0.14 \times 0.12$ mm

Data collection

Bruker Smart APEX CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2000)

$T_{\min} = 0.630$, $T_{\max} = 0.680$

5430 measured reflections

3254 independent reflections

2913 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$

$\theta_{\text{max}} = 24.5^\circ$, $\theta_{\text{min}} = 1.8^\circ$

$h = -6 \rightarrow 9$

$k = -13 \rightarrow 10$

$l = -22 \rightarrow 25$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.051$

$wR(F^2) = 0.110$

$S = 1.09$

3254 reflections

235 parameters

219 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0001P)^2 + 16.8715P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$

$$\Delta\rho_{\max} = 0.78 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\min} = -0.64 \text{ e } \text{Å}^{-3}$$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|--------------|---------------|----------------------------------|
| N1 | 0.3432 (6) | 0.7795 (5) | 0.9391 (2) | 0.0648 (15) |
| I1 | 0.13693 (6) | 1.11048 (4) | 1.135787 (19) | 0.07267 (14) |
| Fe1 | 0.09353 (10) | 0.48170 (7) | 0.86223 (4) | 0.0473 (2) |
| S1 | 0.28437 (19) | 0.42518 (11) | 0.80138 (7) | 0.0531 (4) |
| O1 | -0.0108 (7) | 0.6147 (5) | 0.9623 (2) | 0.0910 (16) |
| C1 | 0.0272 (8) | 0.5622 (5) | 0.9234 (3) | 0.0599 (14) |
| Fe2 | 0.36277 (9) | 0.59245 (6) | 0.84823 (3) | 0.04142 (18) |
| S2 | 0.08546 (16) | 0.64796 (11) | 0.80994 (6) | 0.0403 (3) |
| O2 | 0.2466 (8) | 0.2970 (5) | 0.9430 (3) | 0.124 (2) |
| C2 | 0.1834 (9) | 0.3696 (6) | 0.9117 (3) | 0.0699 (14) |
| O3 | -0.2423 (6) | 0.3742 (5) | 0.8099 (2) | 0.0927 (17) |
| C3 | -0.1125 (8) | 0.4154 (5) | 0.8299 (3) | 0.0605 (13) |
| O4 | 0.6000 (6) | 0.6782 (4) | 0.7683 (2) | 0.0833 (14) |
| C4 | 0.1905 (9) | 0.4428 (5) | 0.7209 (3) | 0.0649 (14) |
| H4A | 0.2723 | 0.4100 | 0.6972 | 0.078* |
| H4B | 0.0839 | 0.3978 | 0.7129 | 0.078* |
| O5 | 0.6200 (6) | 0.4745 (5) | 0.9381 (2) | 0.0909 (17) |
| C5 | 0.1472 (9) | 0.5607 (6) | 0.6976 (3) | 0.0666 (15) |
| H5A | 0.2554 | 0.6040 | 0.7012 | 0.080* |
| H5B | 0.0990 | 0.5555 | 0.6549 | 0.080* |
| C6 | 0.0215 (8) | 0.6253 (5) | 0.7284 (2) | 0.0564 (14) |
| H6A | -0.0898 | 0.5852 | 0.7217 | 0.068* |
| H6B | 0.0024 | 0.6993 | 0.7091 | 0.068* |
| C7 | 0.5080 (8) | 0.6483 (5) | 0.8004 (3) | 0.0553 (13) |
| C8 | 0.5211 (8) | 0.5203 (5) | 0.9022 (3) | 0.0580 (14) |
| C9 | 0.3564 (7) | 0.7105 (5) | 0.9038 (3) | 0.0524 (12) |
| C10 | 0.3002 (8) | 0.8540 (5) | 0.9841 (2) | 0.0542 (12) |
| C11 | 0.2862 (8) | 0.9692 (5) | 0.9732 (3) | 0.0573 (12) |
| H11A | 0.3087 | 0.9986 | 0.9366 | 0.069* |
| C12 | 0.2389 (8) | 1.0414 (5) | 1.0164 (3) | 0.0576 (13) |
| H12A | 0.2269 | 1.1193 | 1.0087 | 0.069* |
| C13 | 0.2097 (7) | 0.9983 (5) | 1.0706 (2) | 0.0512 (12) |

| | | | | |
|------|------------|------------|------------|-------------|
| C14 | 0.2235 (9) | 0.8808 (5) | 1.0821 (3) | 0.0616 (13) |
| C15 | 0.2705 (8) | 0.8104 (5) | 1.0382 (3) | 0.0614 (13) |
| H15A | 0.2822 | 0.7324 | 1.0455 | 0.074* |
| H14A | 0.1991 | 0.8516 | 1.1182 | 0.074* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|------------|-------------|------------|-------------|
| N1 | 0.057 (3) | 0.073 (3) | 0.062 (3) | 0.007 (3) | 0.004 (2) | -0.029 (3) |
| I1 | 0.0759 (3) | 0.0804 (3) | 0.0617 (2) | 0.0098 (2) | 0.0113 (2) | -0.0295 (2) |
| Fe1 | 0.0490 (4) | 0.0437 (4) | 0.0540 (4) | -0.0003 (3) | 0.0224 (3) | 0.0047 (3) |
| S1 | 0.0550 (7) | 0.0342 (7) | 0.0756 (9) | 0.0039 (6) | 0.0268 (7) | -0.0082 (6) |
| O1 | 0.118 (3) | 0.100 (4) | 0.067 (3) | -0.016 (3) | 0.051 (2) | -0.017 (3) |
| C1 | 0.058 (3) | 0.064 (3) | 0.062 (3) | 0.002 (2) | 0.024 (2) | 0.004 (2) |
| Fe2 | 0.0412 (4) | 0.0367 (4) | 0.0491 (4) | 0.0025 (3) | 0.0154 (3) | -0.0058 (3) |
| S2 | 0.0453 (6) | 0.0367 (6) | 0.0408 (6) | 0.0046 (5) | 0.0126 (5) | -0.0034 (5) |
| O2 | 0.130 (4) | 0.111 (4) | 0.138 (4) | 0.038 (3) | 0.048 (3) | 0.072 (3) |
| C2 | 0.071 (3) | 0.065 (3) | 0.078 (3) | 0.007 (2) | 0.026 (2) | 0.019 (2) |
| O3 | 0.071 (3) | 0.095 (4) | 0.117 (4) | -0.030 (3) | 0.033 (3) | -0.032 (3) |
| C3 | 0.061 (2) | 0.058 (3) | 0.069 (3) | -0.005 (2) | 0.029 (2) | -0.007 (2) |
| O4 | 0.082 (3) | 0.079 (3) | 0.100 (3) | -0.022 (3) | 0.050 (2) | -0.004 (3) |
| C4 | 0.075 (3) | 0.063 (3) | 0.061 (3) | -0.002 (2) | 0.023 (2) | -0.020 (2) |
| O5 | 0.077 (3) | 0.089 (3) | 0.101 (4) | 0.022 (3) | -0.002 (3) | 0.013 (3) |
| C5 | 0.074 (3) | 0.075 (3) | 0.052 (3) | -0.002 (3) | 0.016 (2) | -0.012 (3) |
| C6 | 0.064 (3) | 0.061 (3) | 0.045 (2) | -0.004 (3) | 0.010 (2) | -0.008 (2) |
| C7 | 0.059 (2) | 0.050 (2) | 0.062 (2) | -0.005 (2) | 0.022 (2) | -0.011 (2) |
| C8 | 0.055 (3) | 0.052 (3) | 0.069 (3) | 0.006 (2) | 0.018 (2) | -0.005 (2) |
| C9 | 0.054 (2) | 0.051 (2) | 0.054 (2) | 0.006 (2) | 0.013 (2) | -0.007 (2) |
| C10 | 0.062 (2) | 0.053 (2) | 0.046 (2) | 0.006 (2) | 0.006 (2) | -0.013 (2) |
| C11 | 0.071 (2) | 0.053 (2) | 0.049 (2) | 0.000 (2) | 0.013 (2) | -0.007 (2) |
| C12 | 0.073 (3) | 0.049 (2) | 0.050 (2) | 0.005 (2) | 0.010 (2) | -0.004 (2) |
| C13 | 0.061 (2) | 0.050 (2) | 0.041 (2) | 0.008 (2) | 0.005 (2) | -0.009 (2) |
| C14 | 0.081 (3) | 0.055 (2) | 0.047 (2) | 0.004 (2) | 0.004 (2) | -0.004 (2) |
| C15 | 0.078 (2) | 0.049 (2) | 0.055 (2) | 0.007 (2) | 0.002 (2) | -0.007 (2) |

Geometric parameters (Å, °)

| | | | |
|---------|-------------|---------|-----------|
| N1—C9 | 1.148 (7) | C4—C5 | 1.495 (9) |
| N1—C10 | 1.413 (7) | C4—H4A | 0.9700 |
| I1—C13 | 2.109 (5) | C4—H4B | 0.9700 |
| Fe1—C2 | 1.785 (7) | O5—C8 | 1.148 (7) |
| Fe1—C1 | 1.805 (6) | C5—C6 | 1.488 (9) |
| Fe1—C3 | 1.812 (6) | C5—H5A | 0.9700 |
| Fe1—S1 | 2.2656 (17) | C5—H5B | 0.9700 |
| Fe1—S2 | 2.2692 (15) | C6—H6A | 0.9700 |
| Fe1—Fe2 | 2.5156 (11) | C6—H6B | 0.9700 |
| S1—C4 | 1.841 (6) | C10—C15 | 1.370 (8) |
| S1—Fe2 | 2.2590 (16) | C10—C11 | 1.373 (8) |

| | | | |
|------------|-------------|--------------|-----------|
| O1—C1 | 1.144 (7) | C11—C12 | 1.380 (8) |
| Fe2—C8 | 1.785 (6) | C11—H11A | 0.9300 |
| Fe2—C7 | 1.797 (6) | C12—C13 | 1.369 (8) |
| Fe2—C9 | 1.867 (6) | C12—H12A | 0.9300 |
| Fe2—S2 | 2.2689 (14) | C13—C14 | 1.401 (8) |
| S2—C6 | 1.831 (5) | C14—C15 | 1.376 (8) |
| O2—C2 | 1.157 (8) | C14—H14A | 0.9272 |
| O3—C3 | 1.137 (7) | C15—H15A | 0.9300 |
| O4—C7 | 1.146 (7) | | |
| | | | |
| C9—N1—C10 | 170.0 (6) | C5—C4—S1 | 118.4 (4) |
| C2—Fe1—C1 | 92.5 (3) | C5—C4—H4A | 107.7 |
| C2—Fe1—C3 | 99.2 (3) | S1—C4—H4A | 107.7 |
| C1—Fe1—C3 | 100.8 (3) | C5—C4—H4B | 107.7 |
| C2—Fe1—S1 | 86.2 (2) | S1—C4—H4B | 107.7 |
| C1—Fe1—S1 | 154.6 (2) | H4A—C4—H4B | 107.1 |
| C3—Fe1—S1 | 104.5 (2) | C6—C5—C4 | 115.8 (6) |
| C2—Fe1—S2 | 158.1 (2) | C6—C5—H5A | 108.3 |
| C1—Fe1—S2 | 87.5 (2) | C4—C5—H5A | 108.3 |
| C3—Fe1—S2 | 102.4 (2) | C6—C5—H5B | 108.3 |
| S1—Fe1—S2 | 84.61 (5) | C4—C5—H5B | 108.3 |
| C2—Fe1—Fe2 | 102.2 (2) | H5A—C5—H5B | 107.4 |
| C1—Fe1—Fe2 | 99.7 (2) | C5—C6—S2 | 116.5 (4) |
| C3—Fe1—Fe2 | 149.5 (2) | C5—C6—H6A | 108.2 |
| S1—Fe1—Fe2 | 56.10 (4) | S2—C6—H6A | 108.2 |
| S2—Fe1—Fe2 | 56.33 (4) | C5—C6—H6B | 108.2 |
| C4—S1—Fe2 | 112.9 (2) | S2—C6—H6B | 108.2 |
| C4—S1—Fe1 | 111.4 (2) | H6A—C6—H6B | 107.3 |
| Fe2—S1—Fe1 | 67.56 (5) | O4—C7—Fe2 | 176.2 (5) |
| O1—C1—Fe1 | 178.2 (6) | O5—C8—Fe2 | 178.0 (6) |
| C8—Fe2—C7 | 98.6 (3) | N1—C9—Fe2 | 175.5 (6) |
| C8—Fe2—C9 | 89.5 (3) | C15—C10—C11 | 120.3 (5) |
| C7—Fe2—C9 | 102.4 (3) | C15—C10—N1 | 119.6 (5) |
| C8—Fe2—S1 | 90.3 (2) | C11—C10—N1 | 120.1 (5) |
| C7—Fe2—S1 | 100.69 (19) | C10—C11—C12 | 120.0 (6) |
| C9—Fe2—S1 | 156.70 (19) | C10—C11—H11A | 120.0 |
| C8—Fe2—S2 | 153.1 (2) | C12—C11—H11A | 120.0 |
| C7—Fe2—S2 | 108.30 (19) | C13—C12—C11 | 119.8 (6) |
| C9—Fe2—S2 | 84.98 (17) | C13—C12—H12A | 120.1 |
| S1—Fe2—S2 | 84.77 (5) | C11—C12—H12A | 120.1 |
| C8—Fe2—Fe1 | 99.2 (2) | C12—C13—C14 | 120.5 (5) |
| C7—Fe2—Fe1 | 150.77 (19) | C12—C13—I1 | 119.0 (4) |
| C9—Fe2—Fe1 | 100.75 (18) | C14—C13—I1 | 120.5 (4) |
| S1—Fe2—Fe1 | 56.35 (5) | C15—C14—C13 | 118.7 (6) |
| S2—Fe2—Fe1 | 56.34 (4) | C15—C14—H14A | 121.2 |
| C6—S2—Fe1 | 111.7 (2) | C13—C14—H14A | 120.1 |
| C6—S2—Fe2 | 114.7 (2) | C10—C15—C14 | 120.7 (6) |
| Fe1—S2—Fe2 | 67.33 (4) | C10—C15—H15A | 119.7 |

| | | | |
|-----------|-----------|--------------|-------|
| O2—C2—Fe1 | 177.7 (7) | C14—C15—H15A | 119.7 |
| O3—C3—Fe1 | 179.5 (6) | | |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|--------------------------------------|-------------|---------------|-----------------------|-------------------------|
| C12—H12 <i>A</i> ...O2 ⁱ | 0.93 | 2.57 | 3.423 (9) | 153 |
| C15—H15 <i>A</i> ...O5 ⁱⁱ | 0.93 | 2.55 | 3.464 (8) | 168 |

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, -y+1, -z+2$.