metal-organic compounds

Pentacarbonyl-1κ^2C,2κ^3C-(μ-pyrazine-2,3-dithiolato-1:2κ^4S,S':S,S')(trimethylphosphane-1κP)diiron(I)(*Fe—Fe*)

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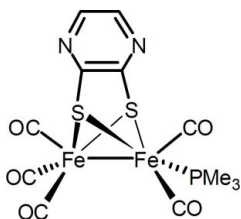Correspondence e-mail: cust_gaoshang@yahoo.cn

In the title compound, [Fe$_2$(C$_4$H$_2$N$_2$S$_2$)(C$_3$H$_9$P)(CO)$_5$], the Fe$_2$S$_2$ core adopts a butterfly conformation. The PMe$_3$ ligand is coordinated in the basal position, roughly *cis* to the Fe—Fe bond. The Fe—Fe distance of 2.4970 (6) Å is relatively short compared to those (*ca* 2.53 Å) found in another monosubstituted diiron compound. A rigid planar dithiolate bridge is featured, with an angle of 2.78 (1)° between the Fe—Fe bond and the normal to the pyrazine-2,3-dithiolate plane.

Related literature

The title compound was prepared as a biomimetic model of the [FeFe]-hydrogenase active site. For general background to hydrogenases and iron–sulfur–carbonyl complexes, see: Cammack (1999); Evans & Pickett (2003); Liu & Xiao (2011); Song *et al.* (2005); Yin *et al.* (2011). For related structures, see: Li *et al.* (2005); Liu & Yin (2010). For the synthesis, see: Durgaprasad *et al.* (2011).

Experimental

Crystal data

[Fe$_2$(C$_4$H$_2$N$_2$S$_2$)(C$_3$H$_9$P)(CO)$_5$]
M_r = 470.02

Orthorhombic, *Pbca*
a = 14.8307 (2) Å
b = 12.1463 (2) Å
c = 19.8806 (3) Å
V = 3581.25 (9) Å^3

Z = 8
Mo $K\alpha$ radiation
μ = 1.97 mm^{-1}
T = 273 K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.828, T_{max} = 0.828

19251 measured reflections
3327 independent reflections
2445 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.070
S = 1.01
3327 reflections

217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected bond lengths (Å).

Fe1—C1	1.803 (4)	Fe2—C4	1.761 (4)
Fe1—C2	1.784 (4)	Fe2—C5	1.771 (4)
Fe1—C3	1.780 (4)	Fe2—S1	2.2859 (9)
Fe1—S1	2.2906 (9)	Fe2—S2	2.2783 (9)
Fe1—S2	2.2893 (9)	Fe2—P1	2.2450 (9)

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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 materials

Pentacarbonyl-1κ^2C,2κ^3C-($^\mu$-pyrazine-2,3-dithiolato-1:2κ^4S,S':S,S')(trimethylphosphane-1κP)diiron(I)(*Fe-Fe*)

S. Gao, C.-A. An, Q. Duan and D.-Y. Jiang

Comment

Hydrogen evolution and uptake in nature is mostly catalyzed by the metalloenzymes called hydrogenases (Evans & Pickett, 2003). Among all types, the [FeFe]-hydrogenases ([FeFe]Hases) are most efficient (Cammack, 1999). The resemblance in structures between the [FeFe]Hase active site and the well known iron-sulfur-carbonyl complexes (Liu & Xiao, 2011; Song *et al.*, 2005; Yin *et al.*, 2011) draws intensive attention to the chemistry of such complexes. The title compound was prepared to mimic structurally the active site of [FeFe]Hases. Herein we report its crystal structure.

In agreement with other reported diiron complexes (Liu & Yin, 2010), the Fe_2S_2 unit in the title compound is in a butterfly conformation and each iron atom is coordinated with a pseudo-square-pyramidal geometry (Fig. 1). The deviation of Fe1 atom from the 2S2C-formed basal plane is 0.362 Å. The Fe—Fe distance of 2.4970 (6) Å in the title compound (Table 1) is enlarged by *ca* 0.03 Å than that found in [Fe_2(μ-$C_4H_2H_2$)(CO)$_6$] (Durgaprasad *et al.*, 2011), indicating the strong electron-donating ability of the PMe$_3$ ligand. The Fe—P distance of 2.2450 (9) Å is in good agreement with those in the phosphane-coordinated diiron compounds (Li *et al.*, 2005). The rigid dithiolate bridge is a special feature for the title compound. The calculated plane of the –SC$_4$H$_2$N$_2$S– bridge is nearly a bisect plane of the molecule. The angle between the Fe—Fe bond and the normal of the pyrazine-2,3-dithiolate plane is 2.78 (1)°.

Experimental

All reactions and operations related to the title compound were carried out under a dry, prepurified nitrogen atmosphere with standard Schlenk techniques. All solvents were dried and distilled prior to use according to standard methods. Me$_3$NO and trimethylphosphane were available commercially and used without further purification. The starting material [Fe_2(μ-C$_4$H$_2$N$_2$)(CO)$_6$] was prepared according to the literature procedure (Durgaprasad *et al.*, 2011). [Fe_2(μ-C$_4$H$_2$N$_2$)(CO)$_6$] (0.42 g, 1.0 mmol) and trimethylphosphane (0.08 g, 1.0 mmol) were reacted in CH$_3$CN (20 ml) in the presence of Me$_3$NO for 20 min at room temperature. The solvent was allowed to evaporate on a rotary evaporator to give a dark-red solid. The crude product was purified by column chromatography on Al$_2$O$_3$ using CH$_2$Cl$_2$/hexane as eluent to give a red solid (yield: 0.04 g, 10%). Recrystallization in a CH$_2$Cl$_2$/pentane solution afforded crystals of the title compound suitable for X-ray study.

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (CH) and 0.96 (CH$_3$) Å and with U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C).
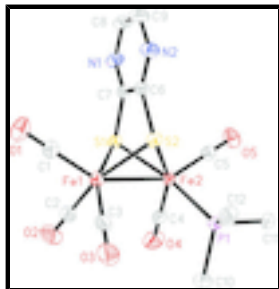
supplementary materials

Figures

Fig. 1. The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

Pentacarbonyl-1κ²C,2κ³C-(μ-pyrazine-2,3-dithiolato- 1:2κ⁴S,S':S,S')(trimethylphosphane- 1κP)diiron(I)(Fe—Fe)

Crystal data

$[Fe_2(C_4H_2N_2S_2)(C_3H_9P)(CO)_5]$	$F(000) = 1888$
$M_r = 470.02$	$D_x = 1.743$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ac 2ab	Cell parameters from 2383 reflections
$a = 14.8307$ (2) Å	$\theta = 2.4–21.5°$
$b = 12.1463$ (2) Å	$\mu = 1.97$ mm^{-1}
$c = 19.8806$ (3) Å	$T = 273$ K
$V = 3581.25$ (9) Å^3	Block, red
$Z = 8$	$0.10 \times 0.10 \times 0.10$ mm

Data collection

Bruker APEX CCD diffractometer	3327 independent reflections
Radiation source: fine-focus sealed tube	2445 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.064$
φ and ω scans	$\theta_{max} = 25.5°$, $\theta_{min} = 2.1°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -17 \rightarrow 17$
$T_{min} = 0.828$, $T_{max} = 0.828$	$k = -12 \rightarrow 14$
19251 measured reflections	$l = -24 \rightarrow 23$

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.034$	$w = 1/[\sigma^2(F_o^2) + (0.0259P)^2 + 0.3172P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.070$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.27$ e Å^{-3}
3327 reflections	$\Delta\rho_{min} = -0.32$ e Å^{-3}

217 parameters

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

	x	*y*	*z*	$U_{iso}*/U_{eq}$
Fe2	0.03732 (3)	0.27229 (3)	0.07013 (2)	0.03067 (13)
Fe1	0.01883 (3)	0.18401 (4)	0.18272 (2)	0.03633 (14)
S2	0.01055 (5)	0.37018 (7)	0.16583 (4)	0.0357 (2)
S1	−0.09264 (5)	0.18655 (6)	0.10298 (4)	0.0365 (2)
P1	0.17667 (5)	0.34273 (7)	0.06048 (4)	0.0347 (2)
C11	0.1950 (2)	0.4175 (3)	−0.01705 (17)	0.0489 (9)
H11A	0.2555	0.4453	−0.0180	0.073*
H11B	0.1532	0.4778	−0.0197	0.073*
H11C	0.1858	0.3690	−0.0546	0.073*
C6	−0.10919 (19)	0.3860 (3)	0.16280 (15)	0.0343 (7)
N2	−0.14764 (17)	0.4745 (2)	0.18771 (14)	0.0444 (7)
C5	−0.0049 (2)	0.3498 (3)	0.00154 (18)	0.0383 (8)
N1	−0.24488 (17)	0.3034 (2)	0.12409 (14)	0.0457 (7)
C10	0.2693 (2)	0.2451 (3)	0.05956 (19)	0.0543 (10)
H10A	0.3253	0.2841	0.0553	0.081*
H10B	0.2623	0.1958	0.0222	0.081*
H10C	0.2693	0.2038	0.1007	0.081*
C7	−0.1565 (2)	0.3014 (3)	0.13199 (15)	0.0353 (8)
C1	−0.0420 (2)	0.1752 (3)	0.2611 (2)	0.0528 (10)
C3	0.1313 (2)	0.1954 (3)	0.21316 (18)	0.0466 (9)
C4	0.0725 (2)	0.1547 (3)	0.02547 (18)	0.0447 (9)
C9	−0.2385 (2)	0.4767 (3)	0.18021 (18)	0.0507 (10)
H9A	−0.2703	0.5367	0.1970	0.061*
C12	0.2126 (2)	0.4416 (3)	0.12345 (18)	0.0530 (10)
H12A	0.2729	0.4654	0.1137	0.080*
H12B	0.2111	0.4078	0.1671	0.080*
H12C	0.1728	0.5039	0.1229	0.080*
C2	0.0344 (2)	0.0406 (3)	0.16750 (17)	0.0478 (9)
C8	−0.2849 (2)	0.3953 (3)	0.14932 (19)	0.0522 (10)
H8A	−0.3471	0.4025	0.1451	0.063*
O5	−0.03314 (16)	0.3954 (2)	−0.04409 (13)	0.0617 (7)
O3	0.20369 (17)	0.2019 (2)	0.23081 (15)	0.0719 (9)
O4	0.09513 (17)	0.0780 (2)	−0.00373 (15)	0.0741 (9)
O2	0.04365 (18)	−0.0509 (2)	0.15663 (15)	0.0756 (9)
O1	−0.0802 (2)	0.1710 (3)	0.31047 (16)	0.0905 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe2	0.0309 (2)	0.0308 (3)	0.0303 (3)	−0.0002 (2)	0.00212 (19)	−0.0006 (2)
Fe1	0.0361 (3)	0.0381 (3)	0.0348 (3)	0.0003 (2)	0.0004 (2)	0.0057 (2)
S2	0.0333 (4)	0.0371 (5)	0.0366 (5)	−0.0017 (4)	0.0008 (3)	−0.0055 (4)
S1	0.0319 (4)	0.0358 (5)	0.0419 (5)	−0.0025 (4)	0.0002 (4)	−0.0044 (4)

P1	0.0294 (4)	0.0340 (5)	0.0406 (5)	0.0023 (4)	0.0032 (4)	0.0025 (4)
C11	0.042 (2)	0.048 (2)	0.057 (3)	−0.0001 (17)	0.0125 (17)	0.0151 (18)
C6	0.0349 (17)	0.0404 (19)	0.0275 (18)	0.0021 (16)	0.0011 (14)	0.0025 (15)
N2	0.0447 (17)	0.0452 (18)	0.0433 (18)	0.0106 (14)	−0.0005 (13)	−0.0074 (14)
C5	0.0347 (18)	0.040 (2)	0.040 (2)	−0.0022 (15)	−0.0006 (16)	−0.0049 (16)
N1	0.0300 (15)	0.059 (2)	0.0480 (19)	0.0030 (14)	−0.0002 (13)	−0.0056 (15)
C10	0.0390 (19)	0.054 (2)	0.070 (3)	0.0136 (17)	0.0019 (18)	0.0046 (19)
C7	0.0343 (18)	0.041 (2)	0.0307 (19)	0.0045 (15)	0.0025 (14)	0.0020 (15)
C1	0.051 (2)	0.057 (2)	0.050 (3)	0.0033 (19)	0.0052 (19)	0.0126 (19)
C3	0.051 (2)	0.042 (2)	0.046 (2)	0.0031 (18)	−0.0053 (18)	0.0098 (17)
C4	0.042 (2)	0.044 (2)	0.048 (2)	−0.0032 (17)	0.0117 (17)	−0.0020 (18)
C9	0.049 (2)	0.059 (3)	0.044 (2)	0.0245 (19)	−0.0006 (17)	−0.0078 (19)
C12	0.043 (2)	0.055 (2)	0.061 (3)	−0.0124 (18)	0.0046 (18)	−0.0097 (19)
C2	0.042 (2)	0.053 (3)	0.048 (2)	−0.0001 (18)	−0.0039 (17)	0.0102 (18)
C8	0.0300 (18)	0.072 (3)	0.054 (2)	0.0123 (19)	0.0010 (17)	−0.004 (2)
O5	0.0699 (18)	0.0627 (18)	0.0526 (18)	0.0014 (14)	−0.0212 (14)	0.0120 (14)
O3	0.0500 (16)	0.082 (2)	0.084 (2)	−0.0072 (14)	−0.0265 (15)	0.0217 (16)
O4	0.0776 (19)	0.0547 (18)	0.090 (2)	0.0011 (15)	0.0267 (16)	−0.0290 (16)
O2	0.083 (2)	0.0428 (18)	0.101 (2)	0.0090 (15)	−0.0070 (17)	−0.0054 (16)
O1	0.101 (2)	0.107 (3)	0.063 (2)	0.011 (2)	0.0383 (18)	0.0209 (18)

Geometric parameters (Å, °)

Fe1—C1	1.803 (4)	C6—N2	1.314 (4)
Fe1—C2	1.784 (4)	C6—C7	1.387 (4)
Fe1—C3	1.780 (4)	N2—C9	1.356 (4)
Fe1—S1	2.2906 (9)	C5—O5	1.143 (4)
Fe1—S2	2.2893 (9)	N1—C7	1.320 (4)
Fe2—C4	1.761 (4)	N1—C8	1.360 (4)
Fe2—C5	1.771 (4)	C10—H10A	0.9600
Fe2—S1	2.2859 (9)	C10—H10B	0.9600
Fe2—S2	2.2783 (9)	C10—H10C	0.9600
Fe2—P1	2.2450 (9)	C1—O1	1.135 (4)
Fe2—Fe1	2.4970 (6)	C3—O3	1.132 (4)
S2—C6	1.787 (3)	C4—O4	1.148 (4)
S1—C7	1.782 (3)	C9—C8	1.352 (5)
P1—C11	1.809 (3)	C9—H9A	0.9300
P1—C10	1.815 (3)	C12—H12A	0.9600
P1—C12	1.815 (3)	C12—H12B	0.9600
C11—H11A	0.9600	C12—H12C	0.9600
C11—H11B	0.9600	C2—O2	1.139 (4)
C11—H11C	0.9600	C8—H8A	0.9300
C4—Fe2—C5	98.48 (16)	C10—P1—Fe2	116.66 (12)
C4—Fe2—P1	89.61 (11)	C12—P1—Fe2	117.62 (11)
C5—Fe2—P1	93.26 (10)	P1—C11—H11A	109.5
C4—Fe2—S2	153.63 (12)	P1—C11—H11B	109.5
C5—Fe2—S2	107.71 (11)	H11A—C11—H11B	109.5
P1—Fe2—S2	91.89 (3)	P1—C11—H11C	109.5
C4—Fe2—S1	91.40 (11)	H11A—C11—H11C	109.5

C5—Fe2—S1	99.45 (10)	H11B—C11—H11C	109.5
P1—Fe2—S1	166.96 (4)	N2—C6—C7	123.6 (3)
S2—Fe2—S1	81.51 (3)	N2—C6—S2	120.4 (2)
C4—Fe2—Fe1	97.83 (11)	C7—C6—S2	116.0 (2)
C5—Fe2—Fe1	151.59 (10)	C6—N2—C9	113.9 (3)
P1—Fe2—Fe1	109.96 (3)	O5—C5—Fe2	176.9 (3)
S2—Fe2—Fe1	57.07 (3)	C7—N1—C8	113.9 (3)
S1—Fe2—Fe1	57.02 (3)	P1—C10—H10A	109.5
C3—Fe1—C2	90.68 (15)	P1—C10—H10B	109.5
C3—Fe1—C1	100.37 (16)	H10A—C10—H10B	109.5
C2—Fe1—C1	98.81 (16)	P1—C10—H10C	109.5
C3—Fe1—S2	91.35 (11)	H10A—C10—H10C	109.5
C2—Fe1—S2	161.26 (11)	H10B—C10—H10C	109.5
C1—Fe1—S2	99.14 (12)	N1—C7—C6	122.7 (3)
C3—Fe1—S1	155.60 (12)	N1—C7—S1	120.3 (2)
C2—Fe1—S1	89.39 (11)	C6—C7—S1	117.0 (2)
C1—Fe1—S1	103.74 (12)	O1—C1—Fe1	179.1 (4)
S2—Fe1—S1	81.17 (3)	O3—C3—Fe1	178.1 (4)
C3—Fe1—Fe2	99.71 (11)	O4—C4—Fe2	179.7 (4)
C2—Fe1—Fe2	104.66 (11)	C8—C9—N2	122.8 (3)
C1—Fe1—Fe2	148.74 (11)	C8—C9—H9A	118.6
S2—Fe1—Fe2	56.65 (2)	N2—C9—H9A	118.6
S1—Fe1—Fe2	56.84 (2)	P1—C12—H12A	109.5
C6—S2—Fe2	101.60 (11)	P1—C12—H12B	109.5
C6—S2—Fe1	99.45 (11)	H12A—C12—H12B	109.5
Fe2—S2—Fe1	66.28 (3)	P1—C12—H12C	109.5
C7—S1—Fe2	100.61 (10)	H12A—C12—H12C	109.5
C7—S1—Fe1	99.80 (11)	H12B—C12—H12C	109.5
Fe2—S1—Fe1	66.13 (3)	O2—C2—Fe1	178.7 (3)
C11—P1—C10	101.87 (16)	C9—C8—N1	123.1 (3)
C11—P1—C12	102.21 (17)	C9—C8—H8A	118.5
C10—P1—C12	102.53 (16)	N1—C8—H8A	118.5
C11—P1—Fe2	113.71 (11)		
C4—Fe2—Fe1—C3	86.09 (15)	C5—Fe2—S1—Fe1	−162.74 (11)
C5—Fe2—Fe1—C3	−149.4 (2)	P1—Fe2—S1—Fe1	4.13 (16)
P1—Fe2—Fe1—C3	−6.35 (12)	S2—Fe2—S1—Fe1	−56.06 (3)
S2—Fe2—Fe1—C3	−85.19 (12)	C3—Fe1—S1—C7	−115.1 (3)
S1—Fe2—Fe1—C3	172.66 (12)	C2—Fe1—S1—C7	154.63 (15)
C4—Fe2—Fe1—C2	−7.18 (15)	C1—Fe1—S1—C7	55.71 (16)
C5—Fe2—Fe1—C2	117.4 (2)	S2—Fe1—S1—C7	−41.61 (10)
P1—Fe2—Fe1—C2	−99.62 (11)	Fe2—Fe1—S1—C7	−97.35 (10)
S2—Fe2—Fe1—C2	−178.46 (11)	C3—Fe1—S1—Fe2	−17.7 (3)
S1—Fe2—Fe1—C2	79.39 (11)	C2—Fe1—S1—Fe2	−108.02 (11)
C4—Fe2—Fe1—C1	−144.6 (3)	C1—Fe1—S1—Fe2	153.05 (12)
C5—Fe2—Fe1—C1	−20.0 (3)	S2—Fe1—S1—Fe2	55.73 (3)
P1—Fe2—Fe1—C1	123.0 (2)	C4—Fe2—P1—C11	85.98 (17)
S2—Fe2—Fe1—C1	44.1 (2)	C5—Fe2—P1—C11	−12.49 (17)
S1—Fe2—Fe1—C1	−58.0 (2)	S2—Fe2—P1—C11	−120.35 (13)
C4—Fe2—Fe1—S2	171.28 (11)	S1—Fe2—P1—C11	−179.51 (18)

C5—Fe2—Fe1—S2	−64.2 (2)	Fe1—Fe2—P1—C11	−175.83 (13)
P1—Fe2—Fe1—S2	78.84 (4)	C4—Fe2—P1—C10	−32.18 (19)
S1—Fe2—Fe1—S2	−102.15 (3)	C5—Fe2—P1—C10	−130.65 (18)
C4—Fe2—Fe1—S1	−86.57 (11)	S2—Fe2—P1—C10	121.49 (14)
C5—Fe2—Fe1—S1	38.0 (2)	S1—Fe2—P1—C10	62.3 (2)
P1—Fe2—Fe1—S1	−179.01 (4)	Fe1—Fe2—P1—C10	66.01 (15)
S2—Fe2—Fe1—S1	102.15 (3)	C4—Fe2—P1—C12	−154.65 (18)
C4—Fe2—S2—C6	−115.1 (3)	C5—Fe2—P1—C12	106.88 (17)
C5—Fe2—S2—C6	57.96 (15)	S2—Fe2—P1—C12	−0.98 (14)
P1—Fe2—S2—C6	151.99 (11)	S1—Fe2—P1—C12	−60.1 (2)
S1—Fe2—S2—C6	−39.31 (11)	Fe1—Fe2—P1—C12	−56.46 (14)
Fe1—Fe2—S2—C6	−95.33 (11)	Fe2—S2—C6—N2	−147.9 (2)
C4—Fe2—S2—Fe1	−19.8 (2)	Fe1—S2—C6—N2	144.6 (2)
C5—Fe2—S2—Fe1	153.29 (10)	Fe2—S2—C6—C7	30.9 (2)
P1—Fe2—S2—Fe1	−112.68 (3)	Fe1—S2—C6—C7	−36.6 (2)
S1—Fe2—S2—Fe1	56.02 (3)	C7—C6—N2—C9	−0.5 (4)
C3—Fe1—S2—C6	−160.66 (15)	S2—C6—N2—C9	178.2 (2)
C2—Fe1—S2—C6	103.2 (4)	C8—N1—C7—C6	−0.5 (5)
C1—Fe1—S2—C6	−59.94 (16)	C8—N1—C7—S1	179.2 (2)
S1—Fe1—S2—C6	42.68 (11)	N2—C6—C7—N1	1.1 (5)
Fe2—Fe1—S2—C6	98.60 (11)	S2—C6—C7—N1	−177.7 (2)
C3—Fe1—S2—Fe2	100.74 (12)	N2—C6—C7—S1	−178.7 (2)
C2—Fe1—S2—Fe2	4.6 (3)	S2—C6—C7—S1	2.6 (3)
C1—Fe1—S2—Fe2	−158.53 (12)	Fe2—S1—C7—N1	145.7 (2)
S1—Fe1—S2—Fe2	−55.92 (3)	Fe1—S1—C7—N1	−146.9 (2)
C4—Fe2—S1—C7	−165.46 (16)	Fe2—S1—C7—C6	−34.5 (2)
C5—Fe2—S1—C7	−66.63 (15)	Fe1—S1—C7—C6	32.8 (2)
P1—Fe2—S1—C7	100.24 (18)	C6—N2—C9—C8	−0.5 (5)
S2—Fe2—S1—C7	40.04 (11)	N2—C9—C8—N1	1.1 (6)
Fe1—Fe2—S1—C7	96.11 (11)	C7—N1—C8—C9	−0.5 (5)
C4—Fe2—S1—Fe1	98.43 (12)		

Fig. 1