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[μ-2-(9-Anthrylmethyl)-2-azapropane-1,3-dithiolato-κ^4S:S']bis[tricarbonyliron(I)]

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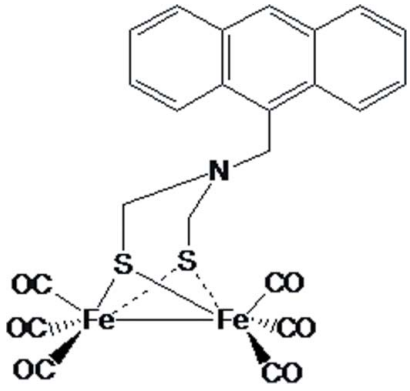
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.085; data-to-parameter ratio = 17.2.

The title compound, $[Fe_2(C_{17}H_{15}NS_2)(CO)_6]$, has been prepared as an azadithiolatoiron model for the active site of iron-only hydrogenase. Each Fe atom is coordinated by two S atoms and three carbonyl groups in a distorted square-pyramidal geometry and the Fe—Fe bond length [2.5040 (8) Å] agrees with values found in other model structures.

Related literature

For general background, see: Cammack (1999); Evans & Pickett (2003); Reihlen *et al.* (1928); Seyferth *et al.* (1980). For related structures, see: Ott *et al.* (2004); Wang *et al.* (2005). For ligand synthesis, see: Lawrence *et al.* (2004).



Experimental

Crystal data

$[Fe_2(C_{17}H_{15}NS_2)(CO)_6]$
M_r = 577.18
Orthorhombic, *Pbcn*
a = 15.234 (6) Å
b = 11.945 (4) Å
c = 25.840 (9) Å
V = 4702 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.45 mm^{-1}
T = 273 (2) K
0.40 × 0.22 × 0.19 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SAINT-Plus*; Bruker, 2001)
T_{min} = 0.598, T_{max} = 0.775
26672 measured reflections
5291 independent reflections
3449 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.085
S = 1.01
5291 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected bond lengths (Å).

Fe1—C1	1.786 (4)	Fe2—C5	1.783 (4)
Fe1—C3	1.791 (3)	Fe2—C4	1.785 (3)
Fe1—C2	1.792 (3)	Fe2—C6	1.797 (4)
Fe1—S2	2.2643 (11)	Fe2—S1	2.2542 (10)
Fe1—S1	2.2649 (11)	Fe2—S2	2.2639 (10)
Fe1—Fe2	2.5040 (8)		

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); 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: HY2063).

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supplementary materials

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[μ-2-(9-Anthrylmethyl)-2-azapropane-1,3-dithiolato-κ^4S:S']bis[tricarbonyliron(I)]

S. Gao and X.-J. Peng

Comment

Hydrogenases are enzymes which catalyze the reduction of protons in numerous microorganisms (Cammack, 1999; Evans & Pickett, 2003). The active site of iron-only hydrogenases, [Fe]H_2ases, resembles many well known iron–sulfur–carbonyl complexes (Reihlen *et al.*, 1928; Seyferth *et al.*, 1980). As a novel hexacarbonyl iron–sulfur complex, the title compound, (I), was prepared to mimic structurally the active site of [Fe]H_2ases. We report here the crystal structure of (I).

In agreement with the other reported models (Ott *et al.*, 2004; Wang *et al.*, 2005), each Fe atom is coordinated in a distorted square-pyramidal geometry and the 2Fe2S unit is in a butterfly framework. The sum of the C—N—C angles around the N atom is 350°, roughly consistent with an sp^3-hybridization of the N atom. The anthrylmethyl moiety is located over the Fe2 side. The angle of C6—Fe2—Fe1 [156.0 (1)°] is enlarged by 9° compared with that of C1—Fe1—Fe2 [146.9 (1)°], thus indicating an interaction between the anthrylmethyl moiety and the $Fe2(CO)_3$ unit. The length of Fe—Fe bond [2.5040 (8) Å] also agrees with those found in the other model structures.

Experimental

The starting compound *N*,*N*′-bis(chloromethyl)-9-anthrylmethylamine was prepared in 62% yield from 9-anthrylmethylamine (Lawrence *et al.*, 2004). $LiEt_3BH$ (1 *M* solution in THF, 2.9 ml, 2.9 mmol) was dropped into the degassed solution of (μ-S_2)$Fe_2(CO)_6$ (0.500 g, 1.45 mmol) in dry THF (30 ml) by syringe at 195 K over 30 min. *N*,*N*′-bis(chloromethyl)-9-anthrylmethylamine (0.882 g, 2.9 mmol) was added to the resulting dark green solution, causing an immediate change in color to red. After stirring for 2 h at 195 K, the reaction mixture was allowed to warm up to room temperature. The solvent was removed *in vacuo* and the resulting dark red solid was purified by column chromatography (silica, 20% dichloromethane in hexane as eluent). The product was obtained as a red solid (yield 58%, 0.485 g). Single crystals of (I) for X-ray analysis were obtained from hexane–dichloromethane (10:1 *v*/*v*,) solution by slow evaporation at room temperature.

Refinement

H atoms attached to C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å(CH) and 0.97 Å(CH_2) and U_{iso}(H) = 1.2U_{eq}(C).

Figures

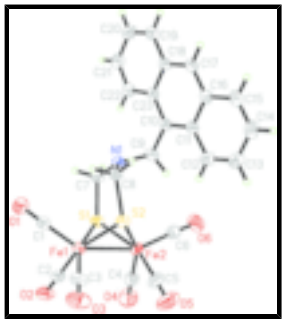


Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

[μ-2-(9-Anthrylmethyl)-2-azapropane-1,3-dithiolato- $\kappa^4S:S'$]bis[tricarbonyliron(I)]

Crystal data

$[Fe_2(C_{17}H_{15}NS_2)(CO)_6]$	F_{000} = 2336
M_r = 577.18	D_x = 1.631 Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2n2ab	Cell parameters from 3797 reflections
a = 15.234 (6) Å	θ = 2.3–21.5º
b = 11.945 (4) Å	μ = 1.45 mm^{-1}
c = 25.840 (9) Å	*T* = 273 (2) K
V = 4702 (3) Å^3	Block, red
Z = 8	0.40 × 0.22 × 0.19 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	5291 independent reflections
Radiation source: fine-focus sealed tube	3449 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.053
T = 273(2) K	θ_{max} = 27.3º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SAINT-Plus; Bruker, 2001)	*h* = −19→18
T_{min} = 0.598, T_{max} = 0.775	*k* = −15→15
26672 measured reflections	*l* = −33→25

Refinement

Refinement on F^2	307 parameters
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$w = 1/[\sigma^2(F_o^2) + (0.0308P)^2 + 1.1601P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.085	$(\Delta/\sigma)_{max}$ = 0.001

S = 1.01	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
5291 reflections	$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.01243 (3)	0.34007 (3)	0.401622 (15)	0.04372 (12)
Fe2	−0.10799 (3)	0.22027 (3)	0.437450 (15)	0.04836 (13)
S1	−0.12743 (5)	0.34232 (6)	0.37191 (3)	0.04503 (18)
S2	0.00238 (5)	0.15340 (6)	0.38759 (3)	0.04378 (17)
O1	0.10661 (18)	0.4136 (2)	0.30884 (10)	0.0954 (9)
O2	−0.01662 (18)	0.55954 (19)	0.44916 (9)	0.0829 (8)
O3	0.16070 (19)	0.2935 (2)	0.47039 (11)	0.1016 (9)
O4	−0.1836 (2)	0.3828 (2)	0.50913 (11)	0.1051 (10)
O5	−0.0141 (2)	0.1204 (3)	0.52462 (11)	0.1190 (11)
O6	−0.2595 (2)	0.0692 (2)	0.43504 (10)	0.1103 (11)
N1	−0.10819 (14)	0.16234 (18)	0.29960 (8)	0.0427 (5)
C1	0.0710 (2)	0.3850 (3)	0.34544 (13)	0.0590 (8)
C2	−0.0057 (2)	0.4742 (3)	0.43081 (11)	0.0559 (8)
C3	0.1030 (2)	0.3116 (3)	0.44377 (13)	0.0625 (9)
C4	−0.1556 (2)	0.3200 (3)	0.48055 (13)	0.0675 (9)
C5	−0.0514 (3)	0.1581 (3)	0.49060 (14)	0.0747 (10)
C6	−0.2004 (3)	0.1270 (3)	0.43469 (12)	0.0690 (10)
C7	−0.13032 (19)	0.2773 (2)	0.30616 (10)	0.0493 (7)
H7A	−0.1892	0.2875	0.2926	0.059*
H7B	−0.0913	0.3204	0.2842	0.059*
C8	−0.02359 (17)	0.1320 (2)	0.31746 (10)	0.0428 (6)
H8A	0.0191	0.1737	0.2974	0.051*
H8B	−0.0149	0.0533	0.3096	0.051*
C9	−0.17766 (17)	0.0783 (2)	0.30591 (11)	0.0481 (7)
H9A	−0.2338	0.1114	0.2970	0.058*
H9B	−0.1802	0.0550	0.3418	0.058*
C10	−0.16135 (16)	−0.0230 (2)	0.27191 (11)	0.0407 (6)
C11	−0.13325 (17)	−0.1252 (2)	0.29368 (11)	0.0433 (7)
C12	−0.1195 (2)	−0.1424 (3)	0.34751 (12)	0.0585 (8)
H12A	−0.1262	−0.0825	0.3702	0.070*
C13	−0.0968 (2)	−0.2441 (3)	0.36658 (13)	0.0716 (10)
H13A	−0.0886	−0.2529	0.4020	0.086*
C14	−0.0855 (2)	−0.3366 (3)	0.33342 (14)	0.0677 (9)
H14A	−0.0710	−0.4061	0.3471	0.081*
C15	−0.09537 (19)	−0.3247 (2)	0.28227 (13)	0.0550 (8)
H15A	−0.0869	−0.3862	0.2608	0.066*
C16	−0.11872 (16)	−0.2194 (2)	0.26002 (11)	0.0413 (6)
C17	−0.12973 (18)	−0.2074 (2)	0.20710 (11)	0.0471 (7)
H17A	−0.1179	−0.2681	0.1856	0.057*
C18	−0.15776 (17)	−0.1080 (2)	0.18520 (11)	0.0434 (7)
C19	−0.1719 (2)	−0.0981 (3)	0.13090 (12)	0.0561 (8)
H19A	−0.1597	−0.1587	0.1095	0.067*

C20	−0.2025 (2)	−0.0029 (3)	0.11016 (12)	0.0638 (9)
H20A	−0.2126	0.0014	0.0747	0.077*
C21	−0.2193 (2)	0.0906 (3)	0.14192 (12)	0.0592 (8)
H21A	−0.2398	0.1565	0.1272	0.071*
C22	−0.20588 (18)	0.0855 (2)	0.19360 (12)	0.0500 (7)
H22A	−0.2171	0.1485	0.2137	0.060*
C23	−0.17492 (16)	−0.0139 (2)	0.21809 (10)	0.0400 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0490 (2)	0.0460 (2)	0.0361 (2)	−0.00432 (19)	−0.00347 (17)	−0.00198 (18)
Fe2	0.0580 (3)	0.0470 (2)	0.0400 (2)	−0.0015 (2)	0.01166 (19)	−0.00189 (19)
S1	0.0487 (4)	0.0398 (4)	0.0466 (4)	0.0050 (3)	−0.0019 (3)	−0.0058 (3)
S2	0.0448 (4)	0.0455 (4)	0.0410 (4)	0.0065 (3)	−0.0015 (3)	−0.0014 (3)
O1	0.101 (2)	0.124 (2)	0.0615 (16)	−0.0508 (18)	0.0168 (14)	−0.0018 (16)
O2	0.136 (2)	0.0519 (14)	0.0603 (15)	0.0105 (15)	−0.0311 (14)	−0.0096 (12)
O3	0.092 (2)	0.118 (2)	0.095 (2)	0.0179 (17)	−0.0492 (17)	−0.0143 (18)
O4	0.137 (3)	0.0893 (19)	0.089 (2)	0.0102 (18)	0.0498 (18)	−0.0313 (16)
O5	0.172 (3)	0.127 (3)	0.0581 (17)	0.020 (2)	−0.0165 (19)	0.0233 (18)
O6	0.118 (2)	0.117 (2)	0.096 (2)	−0.065 (2)	0.0450 (18)	−0.0324 (17)
N1	0.0401 (13)	0.0431 (13)	0.0448 (13)	0.0011 (11)	−0.0019 (10)	−0.0083 (11)
C1	0.061 (2)	0.067 (2)	0.0486 (19)	−0.0214 (17)	−0.0052 (16)	−0.0085 (16)
C2	0.075 (2)	0.0543 (19)	0.0388 (17)	−0.0056 (17)	−0.0162 (15)	0.0053 (15)
C3	0.063 (2)	0.066 (2)	0.059 (2)	−0.0007 (17)	−0.0106 (17)	−0.0135 (17)
C4	0.080 (2)	0.064 (2)	0.059 (2)	−0.0060 (18)	0.0219 (18)	−0.0072 (18)
C5	0.109 (3)	0.070 (2)	0.045 (2)	0.004 (2)	0.009 (2)	0.0062 (18)
C6	0.085 (3)	0.070 (2)	0.052 (2)	−0.016 (2)	0.0289 (18)	−0.0154 (17)
C7	0.0556 (19)	0.0486 (17)	0.0438 (16)	0.0038 (14)	−0.0088 (13)	−0.0057 (14)
C8	0.0374 (15)	0.0492 (16)	0.0417 (16)	−0.0015 (12)	0.0037 (12)	−0.0101 (13)
C9	0.0369 (16)	0.0540 (18)	0.0534 (18)	−0.0015 (13)	0.0023 (13)	−0.0116 (14)
C10	0.0298 (14)	0.0458 (16)	0.0467 (16)	−0.0057 (12)	0.0010 (12)	−0.0065 (13)
C11	0.0353 (15)	0.0473 (17)	0.0473 (17)	−0.0058 (12)	−0.0001 (12)	−0.0029 (13)
C12	0.065 (2)	0.065 (2)	0.0460 (18)	−0.0023 (17)	−0.0070 (15)	−0.0011 (16)
C13	0.087 (3)	0.078 (3)	0.050 (2)	−0.005 (2)	−0.0120 (18)	0.0109 (19)
C14	0.069 (2)	0.058 (2)	0.077 (3)	0.0024 (17)	−0.0117 (18)	0.022 (2)
C15	0.0475 (18)	0.0456 (17)	0.072 (2)	−0.0027 (14)	−0.0038 (15)	0.0011 (16)
C16	0.0286 (14)	0.0425 (15)	0.0528 (17)	−0.0027 (12)	−0.0010 (12)	−0.0010 (13)
C17	0.0456 (17)	0.0421 (16)	0.0536 (18)	−0.0043 (13)	0.0045 (13)	−0.0089 (14)
C18	0.0364 (15)	0.0482 (17)	0.0455 (17)	−0.0087 (13)	−0.0005 (12)	−0.0039 (14)
C19	0.061 (2)	0.0592 (19)	0.0481 (18)	−0.0080 (16)	−0.0021 (15)	−0.0047 (16)
C20	0.065 (2)	0.080 (2)	0.0460 (19)	−0.0072 (18)	−0.0031 (15)	0.0066 (18)
C21	0.0521 (19)	0.063 (2)	0.063 (2)	0.0017 (16)	−0.0031 (15)	0.0135 (17)
C22	0.0406 (17)	0.0497 (17)	0.060 (2)	0.0007 (13)	−0.0001 (14)	0.0006 (15)
C23	0.0286 (14)	0.0448 (16)	0.0468 (16)	−0.0062 (12)	−0.0011 (11)	−0.0003 (13)

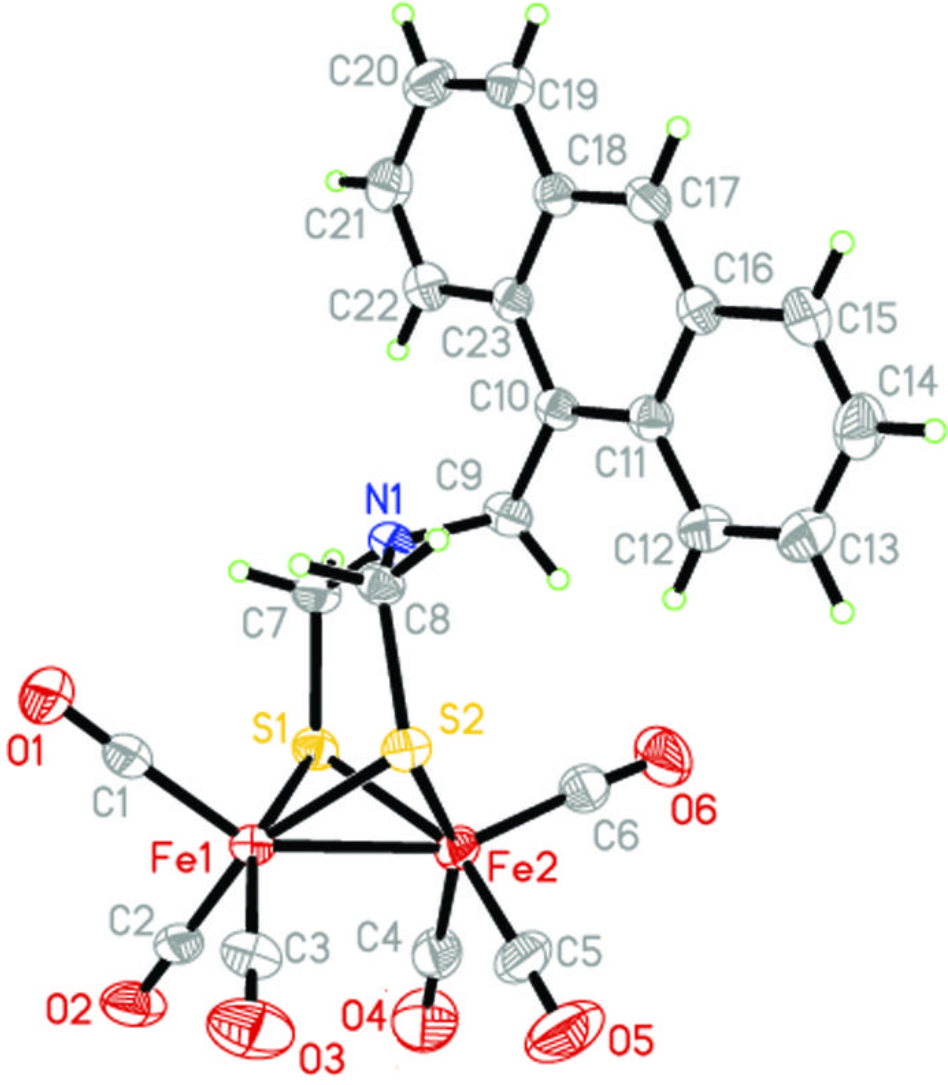
Geometric parameters (Å, °)

Fe1—C1	1.786 (4)	C9—H9A	0.9700

Fe1—C3	1.791 (3)	C9—H9B	0.9700
Fe1—C2	1.792 (3)	C10—C23	1.410 (4)
Fe1—S2	2.2643 (11)	C10—C11	1.410 (4)
Fe1—S1	2.2649 (11)	C11—C12	1.422 (4)
Fe1—Fe2	2.5040 (8)	C11—C16	1.440 (4)
Fe2—C5	1.783 (4)	C12—C13	1.356 (4)
Fe2—C4	1.785 (3)	C12—H12A	0.9300
Fe2—C6	1.797 (4)	C13—C14	1.409 (5)
Fe2—S1	2.2542 (10)	C13—H13A	0.9300
Fe2—S2	2.2639 (10)	C14—C15	1.338 (4)
S1—C7	1.869 (3)	C14—H14A	0.9300
S2—C8	1.872 (3)	C15—C16	1.428 (4)
O1—C1	1.143 (4)	C15—H15A	0.9300
O2—C2	1.137 (3)	C16—C17	1.385 (4)
O3—C3	1.137 (4)	C17—C18	1.383 (4)
O4—C4	1.136 (3)	C17—H17A	0.9300
O5—C5	1.140 (4)	C18—C19	1.424 (4)
O6—C6	1.135 (4)	C18—C23	1.433 (4)
N1—C8	1.416 (3)	C19—C20	1.340 (4)
N1—C7	1.424 (3)	C19—H19A	0.9300
N1—C9	1.468 (3)	C20—C21	1.410 (4)
C7—H7A	0.9700	C20—H20A	0.9300
C7—H7B	0.9700	C21—C22	1.352 (4)
C8—H8A	0.9700	C21—H21A	0.9300
C8—H8B	0.9700	C22—C23	1.426 (4)
C9—C10	1.516 (3)	C22—H22A	0.9300
C1—Fe1—C3	99.59 (16)	S2—C8—H8A	107.8
C1—Fe1—C2	98.65 (15)	N1—C8—H8B	107.8
C3—Fe1—C2	91.86 (14)	S2—C8—H8B	107.8
C1—Fe1—S2	101.50 (11)	H8A—C8—H8B	107.1
C3—Fe1—S2	87.84 (11)	N1—C9—C10	111.3 (2)
C2—Fe1—S2	159.62 (10)	N1—C9—H9A	109.4
C1—Fe1—S1	100.98 (11)	C10—C9—H9A	109.4
C3—Fe1—S1	158.98 (12)	N1—C9—H9B	109.4
C2—Fe1—S1	89.28 (10)	C10—C9—H9B	109.4
S2—Fe1—S1	83.90 (3)	H9A—C9—H9B	108.0
C1—Fe1—Fe2	146.91 (10)	C23—C10—C11	120.3 (2)
C3—Fe1—Fe2	103.36 (12)	C23—C10—C9	119.1 (2)
C2—Fe1—Fe2	104.04 (11)	C11—C10—C9	120.6 (2)
S2—Fe1—Fe2	56.42 (3)	C10—C11—C12	124.1 (3)
S1—Fe1—Fe2	56.15 (3)	C10—C11—C16	118.8 (2)
C5—Fe2—C4	89.64 (17)	C12—C11—C16	117.1 (3)
C5—Fe2—C6	98.69 (18)	C13—C12—C11	121.5 (3)
C4—Fe2—C6	96.92 (15)	C13—C12—H12A	119.2
C5—Fe2—S1	155.70 (13)	C11—C12—H12A	119.2
C4—Fe2—S1	89.06 (12)	C12—C13—C14	120.8 (3)
C6—Fe2—S1	105.56 (12)	C12—C13—H13A	119.6
C5—Fe2—S2	86.13 (12)	C14—C13—H13A	119.6
C4—Fe2—S2	153.17 (11)	C15—C14—C13	120.2 (3)

C6—Fe2—S2	109.91 (10)	C15—C14—H14A	119.9
S1—Fe2—S2	84.16 (3)	C13—C14—H14A	119.9
C5—Fe2—Fe1	99.71 (13)	C14—C15—C16	121.3 (3)
C4—Fe2—Fe1	98.44 (11)	C14—C15—H15A	119.3
C6—Fe2—Fe1	156.02 (10)	C16—C15—H15A	119.3
S1—Fe2—Fe1	56.56 (3)	C17—C16—C15	121.2 (3)
S2—Fe2—Fe1	56.44 (3)	C17—C16—C11	119.8 (2)
C7—S1—Fe2	114.67 (9)	C15—C16—C11	118.9 (3)
C7—S1—Fe1	108.99 (10)	C18—C17—C16	122.0 (3)
Fe2—S1—Fe1	67.30 (3)	C18—C17—H17A	119.0
C8—S2—Fe2	116.24 (9)	C16—C17—H17A	119.0
C8—S2—Fe1	107.69 (9)	C17—C18—C19	121.4 (3)
Fe2—S2—Fe1	67.14 (3)	C17—C18—C23	119.1 (2)
C8—N1—C7	115.1 (2)	C19—C18—C23	119.4 (3)
C8—N1—C9	116.4 (2)	C20—C19—C18	121.1 (3)
C7—N1—C9	118.4 (2)	C20—C19—H19A	119.4
O1—C1—Fe1	178.4 (3)	C18—C19—H19A	119.4
O2—C2—Fe1	179.5 (4)	C19—C20—C21	120.2 (3)
O3—C3—Fe1	179.8 (4)	C19—C20—H20A	119.9
O4—C4—Fe2	177.7 (4)	C21—C20—H20A	119.9
O5—C5—Fe2	178.5 (4)	C22—C21—C20	120.8 (3)
O6—C6—Fe2	177.1 (3)	C22—C21—H21A	119.6
N1—C7—S1	120.22 (19)	C20—C21—H21A	119.6
N1—C7—H7A	107.3	C21—C22—C23	121.7 (3)
S1—C7—H7A	107.3	C21—C22—H22A	119.2
N1—C7—H7B	107.3	C23—C22—H22A	119.2
S1—C7—H7B	107.3	C10—C23—C22	123.4 (2)
H7A—C7—H7B	106.9	C10—C23—C18	119.9 (2)
N1—C8—S2	118.21 (18)	C22—C23—C18	116.8 (2)
N1—C8—H8A	107.8		

Fig. 1


C20
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Fe1
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C5
O2
O4
O3
O5