Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(μ-9-anthrylmethylthiolato)-bis[tricarbonyliron(I)](*Fe*—*Fe*)

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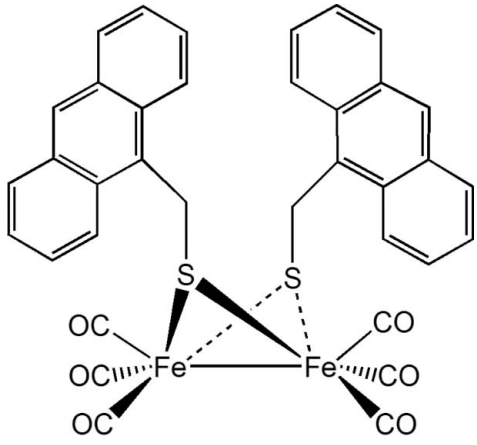
Received 16 May 2007; accepted 23 May 2007

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.008 Å; R factor = 0.045; wR factor = 0.102; data-to-parameter ratio = 13.5.

The title compound, $[Fe_2(C_{15}H_{11}S)_2(CO)_6]$, has been prepared as a structural model for the iron hydrogenase active site. The asymmetric unit consists of two molecules. The Fe_2S_2 units in both molecules exhibit a butterfly conformation.

Related literature

For related literature, see: Lan *et al.* (2003); Li & Rauchfuss (2002); Lyon *et al.* (1999); Ott *et al.* (2003); Peters *et al.* (1998).



Experimental

Crystal data

$[Fe_2(C_{30}H_{22}S_2)(CO)_6]$
M_r = 726.36
Triclinic, $P\overline{1}$
a = 11.471 (4) Å
b = 16.990 (6) Å
c = 17.698 (6) Å
α = 70.218 (4)°
β = 88.973 (4)°
γ = 86.239 (5)°
V = 3239 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.07 mm^{-1}
T = 273 (2) K
0.45 × 0.29 × 0.10 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.645, T_{max} = 0.904
16289 measured reflections
11208 independent reflections
7705 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.102
S = 1.01
11208 reflections
829 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—C2	1.794 (4)	Fe3—C38	1.783 (4)
Fe1—C1	1.795 (4)	Fe3—C39	1.784 (4)
Fe1—C3	1.796 (4)	Fe3—C37	1.802 (5)
Fe1—S2	2.2517 (11)	Fe3—S3	2.2560 (12)
Fe1—S1	2.2745 (12)	Fe3—S4	2.2659 (11)
Fe1—Fe2	2.5148 (9)	Fe3—Fe4	2.5092 (9)
Fe2—C4	1.781 (4)	Fe4—C40	1.777 (5)
Fe2—C5	1.788 (4)	Fe4—C41	1.788 (4)
Fe2—C6	1.805 (4)	Fe4—C42	1.804 (4)
Fe2—S2	2.2634 (11)	Fe4—S3	2.2502 (12)
Fe2—S1	2.2743 (11)	Fe4—S4	2.2780 (13)
C1—Fe1—Fe2	152.62 (12)	Fe2—S1—Fe1	67.13 (3)
C6—Fe2—Fe1	149.27 (12)	Fe1—S2—Fe2	67.69 (3)
C37—Fe3—Fe4	145.68 (13)	Fe4—S3—Fe3	67.67 (3)
C42—Fe4—Fe3	152.71 (13)	Fe3—S4—Fe4	67.04 (3)

Data collection: *SMART APEX2* (Bruker, 2005); 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, 1997); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Ministry of Education of China and the National Natural Science Foundation of China (project Nos. 20128005, 20376010 and 20472012).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2028).

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  doi:10.1107/S160053680702524X

supplementary materials

Acta Cryst. (2007). E**63**, m1996 [**doi:10.1107/S160053680702524X**]

Bis(*μ*-9-anthrylmethylthiolato)bis[tricarbonyliron(I)](*Fe-Fe*)

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Comment

Since the crystal structure of iron hydrogenases ([Fe]H_2ases) was solved (Peters *et al.*, 1998), the classical organometallic diiron dithiolate complexes again became hot research topics for chemists alover due to their structural resemblance of the active site of the [Fe]H_2ases (H-Cluster). Title compound (I) was prepared with the ambitious aim of helping to solve the mystery of the chemical reactivity of the H-Cluster. Here we report the crystal structure of (I).

There are two molecules in the asymmetric unit, with essentially identical geometries. Including the Fe—Fe bond each Fe atom is hexacoordinated and exhibits a heavily distorted octahedral geometry. The bond lengths (Fe—Fe, Fe—S and Fe—C) and angles (C—Fe—Fe and Fe—S—Fe) in each molecule are indistinguishable from those in the other and are within the expected range (Lyon *et al.*, 1999, Li *et al.*, 2002, Ott *et al.*, 2003). The C atoms of the anthracene rings in each molecule are almost coplanar, the planes formed have r.m.s. deviations from the mean plane of only 0.038 Å for A (C8–C21), 0.030 Å for B (C23–C36), 0.022 Å for C (C44–C57), and 0.057 Å for D (C59–C72), respectively. The dihedral angles between the anthracene planes in each molecule are 59.449° for A/B and 78.175° for C/D.

Selected bond distances and angles are summarized in Table 1, *ORTEP* representations of both crystallographically independent molecules are depicted in Figures 1 and 2.

Experimental

The starting compound 9-bromomethylanthracene was prepared from 9-hydroxymethylanthracene according to the literature procedure (Lan *et al.*, 2003). Super hydride ($LiEt_3BH$, 1 *M* solution in THF, 3 ml, 3 mmol) was added to a degassed solution of [(μ-S_2)$Fe_2(CO)_6$] (516 mg, 1.5 mmol) in dry THF (35 ml) at −78 °C over 30 min. 9-Bromomethylanthracene (813 mg, 3 mmol) was added to the dark emerald green solution, causing an immediate change in color to red. The reaction mixture was allowed to warm to room temperature and stirred for an additional hour. The solvent was removed on a rotary evaporator. The crude product was purified by column chromatography with silica using CH_2Cl_2/hexanes (1:10) as the eluent to give compound (I) as a red solid (893 mg, 82%). A single-crystal of (I) was obtained by slow evaporation of the dichloromethane/hexane (5:1, *v/v*) solution at room temperature.

Refinement

One of the anthracene moieties (C59 to C71) shows large anistropic displacement parameters due to pronounced thermal motion (back and forth rocking of the anthracene around the S3—C58 bond). Restraining the anisotropic displacement parameters of atoms closer than 1.7 Å to each other to have similar U^{ij} components did not significantely improve the quality of the model and was thus omitted in the final refinement cycles. The H atoms attached to C were placed in geometrically calculated positions (C—H = 0.93–0.97 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

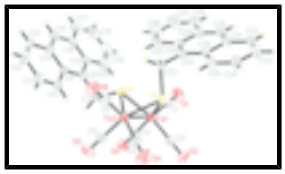

Fig. 1. The molecular structure of the first molecule in the asymmetric unit of (I), with displacement ellipsoids drawn at 30% probability level.

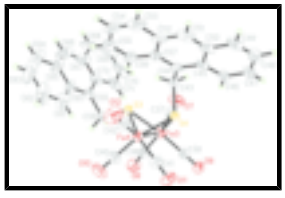

Fig. 2. The molecular structure of the second molecule in the asymmetric unit of (I), with displacement ellipsoids drawn at 30% probability level.

Bis(μ-9-anthrylmethylthiolato)bis[tricarbonyliron(I)](Fe—Fe)

Crystal data

$[Fe_2(C_{30}H_{22}S_2)(CO)_6]$	$Z = 4$
$M_r = 726.36$	$F_{000} = 1480$
Triclinic, $P\bar{1}$	$D_x = 1.490$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 11.471$ (4) Å	Cell parameters from 3698 reflections
$b = 16.990$ (6) Å	$\theta = 2.3$–22.7º
$c = 17.698$ (6) Å	$\mu = 1.07$ mm^{-1}
$\alpha = 70.218$ (4)º	$T = 273$ (2) K
$\beta = 88.973$ (4)º	Block, red
$\gamma = 86.239$ (5)º	0.45 × 0.29 × 0.10 mm
$V = 3239$ (2) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	11208 independent reflections
Radiation source: fine-focus sealed tube	7705 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.024$
$T = 273$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -13 \rightarrow 13$
$T_{min} = 0.645$, $T_{max} = 0.904$	$k = -12 \rightarrow 20$
16289 measured reflections	$l = -20 \rightarrow 21$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.102$	$\Delta\rho_{max} = 0.34$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -0.27$ e Å^{-3}
11208 reflections	Extinction correction: none
829 parameters	

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)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.56624 (4)	0.30124 (3)	0.08483 (3)	0.04097 (14)
Fe2	0.71838 (4)	0.18116 (3)	0.12968 (3)	0.04349 (14)
Fe3	0.44492 (4)	0.86636 (3)	0.44222 (3)	0.04723 (15)
Fe4	0.37153 (4)	0.73358 (3)	0.53846 (3)	0.04643 (15)
S1	0.56929 (7)	0.18750 (6)	0.04441 (5)	0.0410 (2)
S2	0.74699 (7)	0.30516 (5)	0.03247 (5)	0.0403 (2)
S3	0.30760 (8)	0.79305 (6)	0.41106 (5)	0.0460 (2)
S4	0.31290 (7)	0.86388 (6)	0.53965 (5)	0.0462 (2)
C1	0.4843 (3)	0.3829 (2)	0.0091 (2)	0.0516 (9)
C2	0.4504 (3)	0.2546 (3)	0.1509 (2)	0.0532 (10)
C3	0.6040 (3)	0.3621 (2)	0.1453 (2)	0.0500 (9)
C4	0.6514 (3)	0.0976 (3)	0.2038 (2)	0.0655 (12)
C5	0.7848 (3)	0.2103 (3)	0.2062 (2)	0.0554 (10)
C6	0.8363 (3)	0.1186 (2)	0.1049 (2)	0.0500 (9)
C7	0.8453 (3)	0.3749 (2)	0.0567 (2)	0.0482 (9)
H7A	0.8024	0.4266	0.0551	0.058*
H7B	0.8775	0.3480	0.1103	0.058*
C8	0.9419 (3)	0.3934 (2)	−0.0040 (2)	0.0434 (8)
C9	1.0409 (3)	0.3361 (2)	0.0082 (2)	0.0459 (9)
C10	1.0527 (3)	0.2596 (3)	0.0741 (2)	0.0570 (10)
H10A	0.9937	0.2469	0.1122	0.068*
C11	1.1469 (3)	0.2045 (3)	0.0833 (3)	0.0733 (13)
H11A	1.1513	0.1549	0.1270	0.088*
C12	1.2373 (4)	0.2223 (3)	0.0271 (3)	0.0802 (14)
H12A	1.3005	0.1835	0.0328	0.096*
C13	1.2341 (3)	0.2946 (3)	−0.0350 (3)	0.0713 (13)

H13A	1.2965	0.3064	−0.0704	0.086*
C14	1.1358 (3)	0.3534 (3)	−0.0471 (2)	0.0547 (10)
C15	1.1282 (4)	0.4271 (3)	−0.1120 (2)	0.0666 (12)
H15A	1.1909	0.4396	−0.1472	0.080*
C16	1.0316 (4)	0.4830 (3)	−0.1266 (2)	0.0631 (12)
C17	1.0251 (5)	0.5572 (3)	−0.1945 (3)	0.0905 (16)
H17A	1.0878	0.5692	−0.2297	0.109*
C18	0.9300 (7)	0.6107 (4)	−0.2091 (3)	0.112 (2)
H18A	0.9283	0.6595	−0.2537	0.134*
C19	0.8336 (6)	0.5938 (3)	−0.1581 (4)	0.1052 (19)
H19A	0.7680	0.6311	−0.1696	0.126*
C20	0.8342 (4)	0.5229 (3)	−0.0913 (3)	0.0755 (13)
H20A	0.7690	0.5124	−0.0582	0.091*
C21	0.9339 (3)	0.4653 (2)	−0.0721 (2)	0.0534 (10)
C22	0.6230 (3)	0.2023 (2)	−0.05877 (18)	0.0437 (8)
H22A	0.6881	0.2381	−0.0699	0.052*
H22B	0.6513	0.1484	−0.0618	0.052*
C23	0.5296 (3)	0.2407 (2)	−0.12195 (19)	0.0427 (8)
C24	0.5369 (3)	0.3243 (2)	−0.1743 (2)	0.0513 (10)
C25	0.6283 (4)	0.3762 (3)	−0.1727 (2)	0.0687 (12)
H25A	0.6865	0.3557	−0.1338	0.082*
C26	0.6331 (5)	0.4550 (3)	−0.2265 (3)	0.0916 (16)
H26A	0.6946	0.4872	−0.2243	0.110*
C27	0.5455 (6)	0.4879 (3)	−0.2854 (3)	0.1047 (19)
H27A	0.5494	0.5420	−0.3218	0.126*
C28	0.4570 (5)	0.4427 (3)	−0.2896 (3)	0.0902 (16)
H28A	0.4000	0.4658	−0.3290	0.108*
C29	0.4474 (4)	0.3593 (3)	−0.2350 (2)	0.0618 (11)
C30	0.3580 (4)	0.3110 (3)	−0.2407 (2)	0.0667 (12)
H30A	0.3006	0.3345	−0.2797	0.080*
C31	0.3504 (3)	0.2281 (3)	−0.1904 (2)	0.0535 (10)
C32	0.2575 (3)	0.1790 (3)	−0.1969 (3)	0.0699 (12)
H32A	0.1998	0.2027	−0.2356	0.084*
C33	0.2518 (4)	0.0997 (3)	−0.1485 (3)	0.0803 (14)
H33A	0.1897	0.0690	−0.1530	0.096*
C34	0.3397 (4)	0.0625 (3)	−0.0907 (3)	0.0731 (12)
H34A	0.3364	0.0067	−0.0583	0.088*
C35	0.4287 (3)	0.1067 (2)	−0.0818 (2)	0.0567 (10)
H35A	0.4851	0.0806	−0.0427	0.068*
C36	0.4394 (3)	0.1921 (2)	−0.1301 (2)	0.0459 (9)
C37	0.4056 (4)	0.9648 (3)	0.3649 (3)	0.0666 (12)
C38	0.5612 (4)	0.8249 (3)	0.3958 (2)	0.0640 (11)
C39	0.5495 (3)	0.8992 (2)	0.4969 (3)	0.0607 (11)
C40	0.4635 (4)	0.6573 (3)	0.5143 (2)	0.0688 (12)
C41	0.4593 (3)	0.7249 (3)	0.6237 (2)	0.0597 (11)
C42	0.2565 (4)	0.6679 (3)	0.5887 (2)	0.0681 (12)
C43	0.1693 (3)	0.9094 (2)	0.4939 (2)	0.0505 (9)
H43A	0.1722	0.9697	0.4706	0.061*
H43B	0.1539	0.8882	0.4508	0.061*

C44	0.0708 (3)	0.8894 (2)	0.5531 (2)	0.0483 (9)
C45	0.0546 (3)	0.9341 (3)	0.6074 (2)	0.0530 (10)
C46	0.1298 (4)	0.9949 (3)	0.6119 (2)	0.0630 (11)
H46A	0.1954	1.0049	0.5792	0.076*
C47	0.1097 (4)	1.0394 (3)	0.6627 (3)	0.0837 (15)
H47A	0.1617	1.0786	0.6642	0.100*
C48	0.0123 (5)	1.0268 (4)	0.7123 (3)	0.0991 (19)
H48A	−0.0017	1.0585	0.7457	0.119*
C49	−0.0619 (4)	0.9686 (4)	0.7121 (3)	0.0848 (17)
H49A	−0.1259	0.9599	0.7463	0.102*
C50	−0.0444 (4)	0.9199 (3)	0.6604 (2)	0.0681 (13)
C51	−0.1196 (4)	0.8617 (4)	0.6573 (3)	0.0841 (17)
H51A	−0.1828	0.8520	0.6922	0.101*
C52	−0.1074 (3)	0.8164 (3)	0.6056 (3)	0.0733 (14)
C53	−0.1882 (5)	0.7581 (4)	0.6017 (4)	0.109 (2)
H53A	−0.2529	0.7495	0.6352	0.131*
C54	−0.1737 (5)	0.7150 (4)	0.5507 (5)	0.126 (3)
H54A	−0.2278	0.6767	0.5505	0.151*
C55	−0.0771 (5)	0.7267 (3)	0.4970 (4)	0.111 (2)
H55A	−0.0684	0.6968	0.4617	0.133*
C56	0.0019 (4)	0.7823 (3)	0.4984 (3)	0.0812 (14)
H56A	0.0649	0.7900	0.4634	0.097*
C57	−0.0082 (3)	0.8298 (3)	0.5521 (2)	0.0595 (11)
C58	0.3526 (3)	0.7409 (2)	0.3382 (2)	0.0553 (10)
H58A	0.4122	0.7714	0.3027	0.066*
H58B	0.3842	0.6842	0.3660	0.066*
C59	0.2460 (3)	0.7397 (3)	0.2910 (2)	0.0621 (11)
C60	0.1765 (4)	0.6703 (4)	0.3161 (3)	0.0821 (14)
C61	0.1979 (5)	0.6009 (4)	0.3877 (4)	0.1090 (19)
H61A	0.2609	0.6009	0.4201	0.131*
C62	0.1293 (8)	0.5344 (5)	0.4107 (5)	0.165 (3)
H62A	0.1460	0.4896	0.4576	0.199*
C63	0.0338 (11)	0.5341 (8)	0.3630 (8)	0.208 (6)
H63A	−0.0133	0.4888	0.3795	0.250*
C64	0.0079 (9)	0.5959 (8)	0.2951 (7)	0.178 (5)
H64A	−0.0550	0.5926	0.2641	0.214*
C65	0.0768 (5)	0.6684 (6)	0.2689 (5)	0.119 (2)
C66	0.0527 (5)	0.7352 (7)	0.2007 (5)	0.139 (4)
H66A	−0.0088	0.7323	0.1684	0.167*
C67	0.1138 (5)	0.8065 (5)	0.1768 (3)	0.109 (2)
C68	0.0829 (8)	0.8789 (7)	0.1093 (5)	0.168 (5)
H68A	0.0193	0.8774	0.0781	0.201*
C69	0.1395 (9)	0.9478 (7)	0.0887 (5)	0.171 (6)
H69A	0.1160	0.9933	0.0439	0.205*
C70	0.2379 (6)	0.9524 (4)	0.1357 (3)	0.129 (3)
H70A	0.2773	1.0014	0.1220	0.155*
C71	0.2737 (5)	0.8844 (4)	0.2008 (3)	0.0930 (18)
H71A	0.3387	0.8874	0.2302	0.112*
C72	0.2140 (4)	0.8105 (4)	0.2239 (3)	0.0746 (14)

O1	0.4307 (3)	0.43621 (19)	−0.03723 (18)	0.0804 (9)
O2	0.3786 (2)	0.2228 (2)	0.19443 (17)	0.0766 (9)
O3	0.6322 (3)	0.39878 (19)	0.18440 (17)	0.0751 (8)
O4	0.6111 (3)	0.0426 (2)	0.2508 (2)	0.1122 (13)
O5	0.8250 (3)	0.23076 (19)	0.25447 (17)	0.0798 (9)
O6	0.9113 (2)	0.07995 (19)	0.08964 (17)	0.0758 (9)
O7	0.3758 (3)	1.0255 (2)	0.3152 (2)	0.1025 (12)
O8	0.6386 (3)	0.7966 (2)	0.3698 (2)	0.1035 (12)
O9	0.6178 (3)	0.9199 (2)	0.5311 (2)	0.0962 (11)
O10	0.5247 (3)	0.6095 (2)	0.4982 (2)	0.1114 (13)
O11	0.5177 (3)	0.7201 (2)	0.67673 (17)	0.0894 (10)
O12	0.1870 (3)	0.6244 (2)	0.6217 (2)	0.1164 (14)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0363 (3)	0.0441 (3)	0.0424 (3)	0.0005 (2)	0.0025 (2)	−0.0152 (2)
Fe2	0.0388 (3)	0.0451 (3)	0.0420 (3)	0.0010 (2)	−0.0001 (2)	−0.0094 (2)
Fe3	0.0474 (3)	0.0471 (3)	0.0470 (3)	−0.0075 (3)	0.0075 (2)	−0.0152 (3)
Fe4	0.0535 (3)	0.0473 (3)	0.0363 (3)	−0.0061 (3)	−0.0004 (2)	−0.0107 (2)
S1	0.0366 (4)	0.0424 (5)	0.0440 (5)	−0.0038 (4)	0.0028 (4)	−0.0145 (4)
S2	0.0352 (4)	0.0431 (5)	0.0434 (5)	−0.0047 (4)	0.0024 (4)	−0.0152 (4)
S3	0.0519 (5)	0.0518 (6)	0.0368 (5)	−0.0036 (5)	−0.0003 (4)	−0.0183 (4)
S4	0.0455 (5)	0.0545 (6)	0.0423 (5)	−0.0027 (5)	0.0017 (4)	−0.0211 (5)
C1	0.048 (2)	0.047 (2)	0.060 (2)	0.0003 (19)	−0.0002 (19)	−0.018 (2)
C2	0.047 (2)	0.066 (3)	0.050 (2)	0.003 (2)	0.0013 (18)	−0.025 (2)
C3	0.048 (2)	0.057 (3)	0.049 (2)	0.0027 (19)	0.0053 (18)	−0.023 (2)
C4	0.045 (2)	0.073 (3)	0.061 (3)	0.001 (2)	0.0050 (19)	−0.001 (2)
C5	0.058 (2)	0.057 (3)	0.043 (2)	0.002 (2)	−0.0007 (19)	−0.008 (2)
C6	0.047 (2)	0.043 (2)	0.056 (2)	−0.0029 (19)	−0.0017 (18)	−0.0114 (19)
C7	0.0431 (19)	0.051 (2)	0.057 (2)	−0.0094 (18)	0.0038 (17)	−0.0249 (19)
C8	0.0415 (19)	0.049 (2)	0.048 (2)	−0.0111 (18)	0.0019 (16)	−0.0258 (19)
C9	0.0408 (19)	0.053 (2)	0.050 (2)	−0.0131 (18)	0.0043 (16)	−0.023 (2)
C10	0.039 (2)	0.065 (3)	0.066 (3)	−0.008 (2)	0.0034 (18)	−0.020 (2)
C11	0.053 (3)	0.072 (3)	0.088 (3)	−0.001 (2)	−0.004 (2)	−0.019 (3)
C12	0.055 (3)	0.082 (4)	0.113 (4)	0.001 (3)	0.000 (3)	−0.046 (3)
C13	0.045 (2)	0.096 (4)	0.094 (4)	−0.018 (3)	0.020 (2)	−0.057 (3)
C14	0.049 (2)	0.069 (3)	0.058 (2)	−0.021 (2)	0.0078 (19)	−0.034 (2)
C15	0.073 (3)	0.083 (3)	0.054 (3)	−0.031 (3)	0.018 (2)	−0.032 (3)
C16	0.094 (3)	0.053 (3)	0.041 (2)	−0.035 (3)	−0.005 (2)	−0.009 (2)
C17	0.135 (5)	0.076 (4)	0.063 (3)	−0.041 (4)	0.001 (3)	−0.020 (3)
C18	0.183 (7)	0.070 (4)	0.072 (4)	−0.035 (5)	−0.038 (4)	−0.004 (3)
C19	0.137 (5)	0.055 (4)	0.121 (5)	0.003 (4)	−0.052 (4)	−0.026 (4)
C20	0.090 (3)	0.051 (3)	0.087 (3)	−0.002 (3)	−0.021 (3)	−0.025 (3)
C21	0.066 (2)	0.045 (2)	0.055 (2)	−0.019 (2)	−0.005 (2)	−0.021 (2)
C22	0.0431 (19)	0.046 (2)	0.046 (2)	−0.0005 (17)	0.0029 (16)	−0.0215 (18)
C23	0.050 (2)	0.040 (2)	0.042 (2)	0.0026 (18)	0.0051 (16)	−0.0192 (17)
C24	0.071 (3)	0.048 (2)	0.038 (2)	0.001 (2)	0.0071 (19)	−0.0198 (19)

C25	0.103 (3)	0.056 (3)	0.049 (2)	−0.018 (3)	0.000 (2)	−0.018 (2)
C26	0.150 (5)	0.063 (3)	0.066 (3)	−0.039 (3)	0.007 (3)	−0.022 (3)
C27	0.185 (6)	0.051 (3)	0.068 (3)	−0.017 (4)	−0.012 (4)	−0.004 (3)
C28	0.145 (5)	0.055 (3)	0.061 (3)	0.010 (3)	−0.018 (3)	−0.008 (3)
C29	0.085 (3)	0.051 (3)	0.049 (2)	0.012 (2)	−0.001 (2)	−0.019 (2)
C30	0.070 (3)	0.079 (3)	0.053 (2)	0.016 (3)	−0.013 (2)	−0.028 (2)
C31	0.054 (2)	0.062 (3)	0.048 (2)	0.006 (2)	−0.0054 (18)	−0.025 (2)
C32	0.053 (2)	0.095 (4)	0.065 (3)	0.003 (3)	−0.013 (2)	−0.032 (3)
C33	0.064 (3)	0.095 (4)	0.089 (3)	−0.025 (3)	−0.005 (3)	−0.038 (3)
C34	0.072 (3)	0.067 (3)	0.082 (3)	−0.018 (3)	−0.010 (3)	−0.024 (3)
C35	0.055 (2)	0.053 (3)	0.061 (2)	−0.004 (2)	−0.0081 (19)	−0.019 (2)
C36	0.043 (2)	0.050 (2)	0.045 (2)	0.0072 (18)	−0.0023 (16)	−0.0192 (19)
C37	0.061 (3)	0.064 (3)	0.070 (3)	−0.013 (2)	0.018 (2)	−0.016 (2)
C38	0.058 (2)	0.080 (3)	0.062 (3)	−0.010 (2)	0.005 (2)	−0.033 (2)
C39	0.052 (2)	0.050 (3)	0.086 (3)	−0.006 (2)	0.008 (2)	−0.031 (2)
C40	0.093 (3)	0.059 (3)	0.049 (2)	0.007 (3)	−0.010 (2)	−0.014 (2)
C41	0.063 (3)	0.061 (3)	0.049 (2)	−0.008 (2)	0.004 (2)	−0.010 (2)
C42	0.074 (3)	0.061 (3)	0.059 (3)	−0.017 (2)	−0.003 (2)	−0.004 (2)
C43	0.051 (2)	0.054 (2)	0.044 (2)	0.0002 (19)	−0.0009 (17)	−0.0127 (18)
C44	0.041 (2)	0.051 (2)	0.041 (2)	0.0050 (18)	−0.0025 (16)	−0.0017 (18)
C45	0.050 (2)	0.060 (3)	0.035 (2)	0.019 (2)	−0.0023 (17)	−0.0018 (19)
C46	0.066 (3)	0.068 (3)	0.053 (2)	0.011 (2)	0.001 (2)	−0.022 (2)
C47	0.085 (3)	0.100 (4)	0.075 (3)	0.023 (3)	−0.011 (3)	−0.047 (3)
C48	0.105 (4)	0.126 (5)	0.065 (3)	0.048 (4)	−0.016 (3)	−0.041 (4)
C49	0.075 (3)	0.115 (5)	0.049 (3)	0.043 (3)	0.009 (2)	−0.016 (3)
C50	0.052 (2)	0.082 (3)	0.046 (2)	0.021 (3)	0.004 (2)	0.004 (2)
C51	0.052 (3)	0.094 (4)	0.070 (3)	0.019 (3)	0.014 (2)	0.015 (3)
C52	0.037 (2)	0.069 (3)	0.085 (3)	0.003 (2)	−0.004 (2)	0.012 (3)
C53	0.054 (3)	0.082 (5)	0.150 (6)	−0.007 (3)	−0.007 (3)	0.014 (4)
C54	0.069 (4)	0.077 (5)	0.206 (8)	−0.022 (4)	−0.036 (5)	−0.010 (5)
C55	0.078 (4)	0.088 (4)	0.163 (6)	−0.008 (3)	−0.029 (4)	−0.037 (4)
C56	0.056 (3)	0.073 (3)	0.109 (4)	−0.006 (3)	−0.019 (3)	−0.022 (3)
C57	0.050 (2)	0.052 (3)	0.065 (3)	0.004 (2)	−0.010 (2)	−0.004 (2)
C58	0.065 (2)	0.064 (3)	0.044 (2)	0.008 (2)	−0.0052 (18)	−0.029 (2)
C59	0.064 (3)	0.090 (3)	0.049 (2)	0.012 (3)	−0.008 (2)	−0.047 (2)
C60	0.083 (3)	0.113 (4)	0.080 (3)	−0.017 (3)	0.006 (3)	−0.069 (3)
C61	0.135 (5)	0.106 (5)	0.107 (5)	−0.039 (4)	0.017 (4)	−0.059 (4)
C62	0.217 (9)	0.125 (6)	0.183 (8)	−0.079 (6)	0.042 (7)	−0.080 (6)
C63	0.204 (11)	0.249 (15)	0.265 (15)	−0.132 (11)	0.066 (12)	−0.190 (12)
C64	0.123 (6)	0.290 (16)	0.219 (11)	−0.077 (9)	0.029 (8)	−0.202 (11)
C65	0.085 (4)	0.207 (8)	0.126 (5)	−0.029 (5)	0.010 (4)	−0.132 (6)
C66	0.070 (4)	0.290 (13)	0.112 (6)	0.022 (6)	−0.024 (4)	−0.145 (8)
C67	0.078 (4)	0.197 (8)	0.068 (4)	0.060 (4)	−0.018 (3)	−0.079 (5)
C68	0.128 (7)	0.300 (14)	0.066 (6)	0.134 (9)	−0.031 (5)	−0.075 (7)
C69	0.189 (11)	0.225 (12)	0.058 (4)	0.150 (9)	0.005 (5)	−0.024 (6)
C70	0.190 (7)	0.114 (5)	0.069 (4)	0.077 (5)	0.026 (4)	−0.029 (4)
C71	0.126 (5)	0.096 (4)	0.054 (3)	0.045 (4)	0.006 (3)	−0.032 (3)
C72	0.074 (3)	0.114 (4)	0.046 (3)	0.035 (3)	−0.007 (2)	−0.048 (3)
O1	0.085 (2)	0.060 (2)	0.083 (2)	0.0111 (17)	−0.0246 (17)	−0.0093 (17)

O2	0.0613 (17)	0.099 (2)	0.0689 (19)	−0.0230 (18)	0.0235 (15)	−0.0260 (17)
O3	0.090 (2)	0.082 (2)	0.0690 (19)	−0.0119 (18)	0.0029 (16)	−0.0458 (18)
O4	0.085 (2)	0.102 (3)	0.103 (3)	−0.019 (2)	0.017 (2)	0.027 (2)
O5	0.103 (2)	0.081 (2)	0.0537 (18)	−0.0003 (19)	−0.0225 (17)	−0.0210 (17)
O6	0.0639 (18)	0.077 (2)	0.090 (2)	0.0180 (17)	0.0015 (16)	−0.0376 (18)
O7	0.089 (2)	0.076 (3)	0.104 (3)	0.005 (2)	0.018 (2)	0.017 (2)
O8	0.070 (2)	0.158 (4)	0.109 (3)	0.005 (2)	0.0222 (19)	−0.082 (3)
O9	0.073 (2)	0.085 (2)	0.151 (3)	−0.0081 (19)	−0.025 (2)	−0.064 (2)
O10	0.145 (3)	0.092 (3)	0.093 (3)	0.054 (3)	−0.015 (2)	−0.037 (2)
O11	0.091 (2)	0.115 (3)	0.0603 (19)	−0.014 (2)	−0.0231 (17)	−0.0236 (19)
O12	0.103 (3)	0.110 (3)	0.109 (3)	−0.058 (2)	0.012 (2)	0.007 (2)

Geometric parameters (Å, °)

Fe1—C2	1.794 (4)	C29—C30	1.381 (6)
Fe1—C1	1.795 (4)	C30—C31	1.396 (6)
Fe1—C3	1.796 (4)	C30—H30A	0.9300
Fe1—S2	2.2517 (11)	C31—C32	1.424 (5)
Fe1—S1	2.2745 (12)	C31—C36	1.439 (5)
Fe1—Fe2	2.5148 (9)	C32—C33	1.335 (6)
Fe2—C4	1.781 (4)	C32—H32A	0.9300
Fe2—C5	1.788 (4)	C33—C34	1.406 (6)
Fe2—C6	1.805 (4)	C33—H33A	0.9300
Fe2—S2	2.2634 (11)	C34—C35	1.349 (5)
Fe2—S1	2.2743 (11)	C34—H34A	0.9300
Fe3—C38	1.783 (4)	C35—C36	1.424 (5)
Fe3—C39	1.784 (4)	C35—H35A	0.9300
Fe3—C37	1.802 (5)	C37—O7	1.142 (5)
Fe3—S3	2.2560 (12)	C38—O8	1.145 (4)
Fe3—S4	2.2659 (11)	C39—O9	1.140 (4)
Fe3—Fe4	2.5092 (9)	C40—O10	1.143 (5)
Fe4—C40	1.777 (5)	C41—O11	1.140 (4)
Fe4—C41	1.788 (4)	C42—O12	1.136 (5)
Fe4—C42	1.804 (4)	C43—C44	1.503 (4)
Fe4—S3	2.2502 (12)	C43—H43A	0.9700
Fe4—S4	2.2780 (13)	C43—H43B	0.9700
S1—C22	1.857 (3)	C44—C57	1.406 (5)
S2—C7	1.843 (3)	C44—C45	1.416 (5)
S3—C58	1.845 (3)	C45—C46	1.411 (5)
S4—C43	1.850 (3)	C45—C50	1.440 (5)
C1—O1	1.145 (4)	C46—C47	1.365 (6)
C2—O2	1.148 (4)	C46—H46A	0.9300
C3—O3	1.140 (4)	C47—C48	1.391 (6)
C4—O4	1.138 (5)	C47—H47A	0.9300
C5—O5	1.141 (4)	C48—C49	1.347 (7)
C6—O6	1.132 (4)	C48—H48A	0.9300
C7—C8	1.502 (4)	C49—C50	1.430 (6)
C7—H7A	0.9700	C49—H49A	0.9300
C7—H7B	0.9700	C50—C51	1.370 (6)

C8—C21	1.395 (5)	C51—C52	1.381 (7)
C8—C9	1.416 (5)	C51—H51A	0.9300
C9—C10	1.422 (5)	C52—C53	1.420 (7)
C9—C14	1.429 (5)	C52—C57	1.446 (6)
C10—C11	1.357 (5)	C53—C54	1.341 (8)
C10—H10A	0.9300	C53—H53A	0.9300
C11—C12	1.400 (6)	C54—C55	1.426 (8)
C11—H11A	0.9300	C54—H54A	0.9300
C12—C13	1.341 (6)	C55—C56	1.357 (6)
C12—H12A	0.9300	C55—H55A	0.9300
C13—C14	1.424 (5)	C56—C57	1.439 (6)
C13—H13A	0.9300	C56—H56A	0.9300
C14—C15	1.382 (5)	C58—C59	1.498 (5)
C15—C16	1.380 (6)	C58—H58A	0.9700
C15—H15A	0.9300	C58—H58B	0.9700
C16—C17	1.416 (6)	C59—C60	1.407 (6)
C16—C21	1.445 (5)	C59—C72	1.409 (6)
C17—C18	1.343 (7)	C60—C61	1.420 (7)
C17—H17A	0.9300	C60—C65	1.436 (7)
C18—C19	1.397 (8)	C61—C62	1.362 (8)
C18—H18A	0.9300	C61—H61A	0.9300
C19—C20	1.373 (6)	C62—C63	1.397 (12)
C19—H19A	0.9300	C62—H62A	0.9300
C20—C21	1.422 (5)	C63—C64	1.324 (14)
C20—H20A	0.9300	C63—H63A	0.9300
C22—C23	1.510 (4)	C64—C65	1.445 (12)
C22—H22A	0.9700	C64—H64A	0.9300
C22—H22B	0.9700	C65—C66	1.367 (10)
C23—C36	1.404 (5)	C66—C67	1.375 (10)
C23—C24	1.416 (5)	C66—H66A	0.9300
C24—C25	1.421 (5)	C67—C68	1.425 (10)
C24—C29	1.446 (5)	C67—C72	1.451 (7)
C25—C26	1.358 (6)	C68—C69	1.314 (14)
C25—H25A	0.9300	C68—H68A	0.9300
C26—C27	1.407 (7)	C69—C70	1.436 (12)
C26—H26A	0.9300	C69—H69A	0.9300
C27—C28	1.331 (7)	C70—C71	1.373 (7)
C27—H27A	0.9300	C70—H70A	0.9300
C28—C29	1.428 (6)	C71—C72	1.402 (7)
C28—H28A	0.9300	C71—H71A	0.9300
C2—Fe1—C1	100.16 (16)	C26—C25—C24	121.8 (4)
C2—Fe1—C3	92.67 (17)	C26—C25—H25A	119.1
C1—Fe1—C3	97.63 (17)	C24—C25—H25A	119.1
C2—Fe1—S2	155.19 (12)	C25—C26—C27	120.3 (5)
C1—Fe1—S2	103.31 (12)	C25—C26—H26A	119.9
C3—Fe1—S2	92.11 (11)	C27—C26—H26A	119.9
C2—Fe1—S1	86.37 (13)	C28—C27—C26	120.8 (5)
C1—Fe1—S1	105.34 (13)	C28—C27—H27A	119.6
C3—Fe1—S1	156.82 (12)	C26—C27—H27A	119.6

S2—Fe1—S1	79.80 (4)	C27—C28—C29	121.6 (5)
C2—Fe1—Fe2	98.82 (12)	C27—C28—H28A	119.2
C1—Fe1—Fe2	152.62 (12)	C29—C28—H28A	119.2
C3—Fe1—Fe2	101.02 (11)	C30—C29—C28	121.9 (4)
S2—Fe1—Fe2	56.37 (3)	C30—C29—C24	119.6 (4)
S1—Fe1—Fe2	56.43 (3)	C28—C29—C24	118.4 (4)
C4—Fe2—C5	90.72 (19)	C29—C30—C31	122.7 (4)
C4—Fe2—C6	97.14 (18)	C29—C30—H30A	118.7
C5—Fe2—C6	101.29 (17)	C31—C30—H30A	118.7
C4—Fe2—S2	162.42 (12)	C30—C31—C32	122.0 (4)
C5—Fe2—S2	93.68 (13)	C30—C31—C36	118.4 (4)
C6—Fe2—S2	98.66 (12)	C32—C31—C36	119.6 (4)
C4—Fe2—S1	88.73 (13)	C33—C32—C31	121.2 (4)
C5—Fe2—S1	152.53 (12)	C33—C32—H32A	119.4
C6—Fe2—S1	106.03 (12)	C31—C32—H32A	119.4
S2—Fe2—S1	79.55 (4)	C32—C33—C34	120.1 (4)
C4—Fe2—Fe1	106.62 (13)	C32—C33—H33A	120.0
C5—Fe2—Fe1	97.68 (12)	C34—C33—H33A	120.0
C6—Fe2—Fe1	149.27 (12)	C35—C34—C33	120.8 (4)
S2—Fe2—Fe1	55.93 (3)	C35—C34—H34A	119.6
S1—Fe2—Fe1	56.44 (3)	C33—C34—H34A	119.6
C38—Fe3—C39	89.57 (18)	C34—C35—C36	122.3 (4)
C38—Fe3—C37	101.71 (19)	C34—C35—H35A	118.8
C39—Fe3—C37	100.1 (2)	C36—C35—H35A	118.8
C38—Fe3—S3	94.55 (14)	C23—C36—C35	124.2 (3)
C39—Fe3—S3	161.87 (14)	C23—C36—C31	120.0 (3)
C37—Fe3—S3	96.31 (14)	C35—C36—C31	115.9 (3)
C38—Fe3—S4	155.51 (14)	O7—C37—Fe3	176.6 (4)
C39—Fe3—S4	88.66 (13)	O8—C38—Fe3	176.4 (4)
C37—Fe3—S4	102.64 (13)	O9—C39—Fe3	178.8 (4)
S3—Fe3—S4	80.29 (4)	O10—C40—Fe4	178.3 (5)
C38—Fe3—Fe4	100.53 (14)	O11—C41—Fe4	178.1 (4)
C39—Fe3—Fe4	105.84 (14)	O12—C42—Fe4	177.6 (4)
C37—Fe3—Fe4	145.68 (13)	C44—C43—S4	112.9 (2)
S3—Fe3—Fe4	56.05 (3)	C44—C43—H43A	109.0
S4—Fe3—Fe4	56.71 (3)	S4—C43—H43A	109.0
C40—Fe4—C41	91.94 (19)	C44—C43—H43B	109.0
C40—Fe4—C42	98.8 (2)	S4—C43—H43B	109.0
C41—Fe4—C42	99.21 (18)	H43A—C43—H43B	107.8
C40—Fe4—S3	92.62 (13)	C57—C44—C45	120.1 (3)
C41—Fe4—S3	155.07 (13)	C57—C44—C43	120.5 (4)
C42—Fe4—S3	104.28 (13)	C45—C44—C43	119.3 (3)
C40—Fe4—S4	156.18 (15)	C46—C45—C44	123.5 (3)
C41—Fe4—S4	85.87 (14)	C46—C45—C50	116.6 (4)
C42—Fe4—S4	104.95 (15)	C44—C45—C50	119.9 (4)
S3—Fe4—S4	80.15 (4)	C47—C46—C45	122.3 (4)
C40—Fe4—Fe3	100.89 (15)	C47—C46—H46A	118.9
C41—Fe4—Fe3	98.80 (13)	C45—C46—H46A	118.9
C42—Fe4—Fe3	152.71 (13)	C46—C47—C48	120.7 (5)

S3—Fe4—Fe3	56.27 (3)	C46—C47—H47A	119.6
S4—Fe4—Fe3	56.25 (3)	C48—C47—H47A	119.6
C22—S1—Fe2	111.55 (11)	C49—C48—C47	120.0 (5)
C22—S1—Fe1	116.60 (12)	C49—C48—H48A	120.0
Fe2—S1—Fe1	67.13 (3)	C47—C48—H48A	120.0
C7—S2—Fe1	116.02 (11)	C48—C49—C50	121.5 (5)
C7—S2—Fe2	116.99 (12)	C48—C49—H49A	119.3
Fe1—S2—Fe2	67.69 (3)	C50—C49—H49A	119.3
C58—S3—Fe4	117.90 (12)	C51—C50—C49	122.9 (5)
C58—S3—Fe3	115.48 (13)	C51—C50—C45	118.2 (5)
Fe4—S3—Fe3	67.67 (3)	C49—C50—C45	118.9 (5)
C43—S4—Fe3	109.89 (11)	C50—C51—C52	124.0 (4)
C43—S4—Fe4	117.34 (13)	C50—C51—H51A	118.0
Fe3—S4—Fe4	67.04 (3)	C52—C51—H51A	118.0
O1—C1—Fe1	177.6 (4)	C51—C52—C53	123.2 (5)
O2—C2—Fe1	177.9 (4)	C51—C52—C57	118.4 (4)
O3—C3—Fe1	177.2 (3)	C53—C52—C57	118.4 (5)
O4—C4—Fe2	178.1 (4)	C54—C53—C52	121.7 (6)
O5—C5—Fe2	178.1 (4)	C54—C53—H53A	119.2
O6—C6—Fe2	179.1 (3)	C52—C53—H53A	119.2
C8—C7—S2	108.4 (2)	C53—C54—C55	121.5 (6)
C8—C7—H7A	110.0	C53—C54—H54A	119.3
S2—C7—H7A	110.0	C55—C54—H54A	119.3
C8—C7—H7B	110.0	C56—C55—C54	118.7 (6)
S2—C7—H7B	110.0	C56—C55—H55A	120.6
H7A—C7—H7B	108.4	C54—C55—H55A	120.6
C21—C8—C9	120.3 (3)	C55—C56—C57	122.4 (5)
C21—C8—C7	120.7 (3)	C55—C56—H56A	118.8
C9—C8—C7	119.0 (3)	C57—C56—H56A	118.8
C8—C9—C10	123.5 (3)	C44—C57—C56	123.4 (4)
C8—C9—C14	120.2 (3)	C44—C57—C52	119.4 (4)
C10—C9—C14	116.3 (3)	C56—C57—C52	117.2 (4)
C11—C10—C9	122.4 (4)	C59—C58—S3	107.1 (2)
C11—C10—H10A	118.8	C59—C58—H58A	110.3
C9—C10—H10A	118.8	S3—C58—H58A	110.3
C10—C11—C12	120.0 (4)	C59—C58—H58B	110.3
C10—C11—H11A	120.0	S3—C58—H58B	110.3
C12—C11—H11A	120.0	H58A—C58—H58B	108.5
C13—C12—C11	120.9 (4)	C60—C59—C72	121.0 (4)
C13—C12—H12A	119.6	C60—C59—C58	120.1 (4)
C11—C12—H12A	119.6	C72—C59—C58	118.9 (4)
C12—C13—C14	120.6 (4)	C59—C60—C61	123.4 (5)
C12—C13—H13A	119.7	C59—C60—C65	119.6 (6)
C14—C13—H13A	119.7	C61—C60—C65	116.9 (6)
C15—C14—C13	122.0 (4)	C62—C61—C60	122.3 (7)
C15—C14—C9	118.3 (4)	C62—C61—H61A	118.9
C13—C14—C9	119.8 (4)	C60—C61—H61A	118.9
C16—C15—C14	122.8 (4)	C61—C62—C63	119.4 (9)
C16—C15—H15A	118.6	C61—C62—H62A	120.3

C14—C15—H15A	118.6	C63—C62—H62A	120.3
C15—C16—C17	121.6 (5)	C64—C63—C62	122.3 (13)
C15—C16—C21	119.5 (4)	C64—C63—H63A	118.8
C17—C16—C21	118.9 (5)	C62—C63—H63A	118.8
C18—C17—C16	121.3 (6)	C63—C64—C65	120.3 (11)
C18—C17—H17A	119.4	C63—C64—H64A	119.8
C16—C17—H17A	119.4	C65—C64—H64A	119.8
C17—C18—C19	120.6 (6)	C66—C65—C60	118.2 (7)
C17—C18—H18A	119.7	C66—C65—C64	123.1 (8)
C19—C18—H18A	119.7	C60—C65—C64	118.7 (8)
C20—C19—C18	121.0 (6)	C65—C66—C67	124.0 (7)
C20—C19—H19A	119.5	C65—C66—H66A	118.0
C18—C19—H19A	119.5	C67—C66—H66A	118.0
C19—C20—C21	120.5 (5)	C66—C67—C68	124.0 (8)
C19—C20—H20A	119.7	C66—C67—C72	118.9 (6)
C21—C20—H20A	119.7	C68—C67—C72	117.0 (8)
C8—C21—C20	123.6 (4)	C69—C68—C67	123.5 (11)
C8—C21—C16	118.8 (4)	C69—C68—H68A	118.2
C20—C21—C16	117.6 (4)	C67—C68—H68A	118.2
C23—C22—S1	112.6 (2)	C68—C69—C70	119.7 (10)
C23—C22—H22A	109.1	C68—C69—H69A	120.2
S1—C22—H22A	109.1	C70—C69—H69A	120.2
C23—C22—H22B	109.1	C71—C70—C69	119.9 (8)
S1—C22—H22B	109.1	C71—C70—H70A	120.1
H22A—C22—H22B	107.8	C69—C70—H70A	120.1
C36—C23—C24	120.9 (3)	C70—C71—C72	121.2 (6)
C36—C23—C22	119.6 (3)	C70—C71—H71A	119.4
C24—C23—C22	119.5 (3)	C72—C71—H71A	119.4
C23—C24—C25	124.4 (3)	C71—C72—C59	123.3 (4)
C23—C24—C29	118.5 (4)	C71—C72—C67	118.7 (6)
C25—C24—C29	117.1 (4)	C59—C72—C67	118.0 (6)
C2—Fe1—Fe2—C4	2.68 (19)	C8—C9—C14—C13	−179.0 (3)
C1—Fe1—Fe2—C4	−130.8 (3)	C10—C9—C14—C13	1.0 (5)
C3—Fe1—Fe2—C4	97.17 (19)	C13—C14—C15—C16	177.1 (4)
S2—Fe1—Fe2—C4	−177.68 (16)	C9—C14—C15—C16	−2.1 (6)
S1—Fe1—Fe2—C4	−76.96 (16)	C14—C15—C16—C17	−178.5 (4)
C2—Fe1—Fe2—C5	−90.39 (17)	C14—C15—C16—C21	0.7 (6)
C1—Fe1—Fe2—C5	136.2 (3)	C15—C16—C17—C18	178.9 (4)
C3—Fe1—Fe2—C5	4.10 (17)	C21—C16—C17—C18	−0.3 (7)
S2—Fe1—Fe2—C5	89.26 (13)	C16—C17—C18—C19	−1.1 (8)
S1—Fe1—Fe2—C5	−170.03 (13)	C17—C18—C19—C20	1.0 (9)
C2—Fe1—Fe2—C6	141.8 (3)	C18—C19—C20—C21	0.5 (7)
C1—Fe1—Fe2—C6	8.3 (4)	C9—C8—C21—C20	175.7 (3)
C3—Fe1—Fe2—C6	−123.7 (3)	C7—C8—C21—C20	−3.2 (5)
S2—Fe1—Fe2—C6	−38.6 (2)	C9—C8—C21—C16	−4.5 (5)
S1—Fe1—Fe2—C6	62.1 (2)	C7—C8—C21—C16	176.6 (3)
C2—Fe1—Fe2—S2	−179.64 (12)	C19—C20—C21—C8	178.0 (4)
C1—Fe1—Fe2—S2	46.9 (3)	C19—C20—C21—C16	−1.8 (6)
C3—Fe1—Fe2—S2	−85.16 (12)	C15—C16—C21—C8	2.7 (5)

S1—Fe1—Fe2—S2	100.72 (5)	C17—C16—C21—C8	−178.1 (3)
C2—Fe1—Fe2—S1	79.64 (12)	C15—C16—C21—C20	−177.5 (3)
C1—Fe1—Fe2—S1	−53.8 (3)	C17—C16—C21—C20	1.7 (5)
C3—Fe1—Fe2—S1	174.13 (12)	Fe2—S1—C22—C23	−156.9 (2)
S2—Fe1—Fe2—S1	−100.72 (5)	Fe1—S1—C22—C23	−82.5 (3)
C38—Fe3—Fe4—C40	−2.55 (19)	S1—C22—C23—C36	−73.4 (4)
C39—Fe3—Fe4—C40	−95.12 (19)	S1—C22—C23—C24	109.1 (3)
C37—Fe3—Fe4—C40	127.1 (3)	C36—C23—C24—C25	−176.8 (3)
S3—Fe3—Fe4—C40	85.84 (14)	C22—C23—C24—C25	0.7 (5)
S4—Fe3—Fe4—C40	−172.69 (14)	C36—C23—C24—C29	1.7 (5)
C38—Fe3—Fe4—C41	91.15 (18)	C22—C23—C24—C29	179.2 (3)
C39—Fe3—Fe4—C41	−1.42 (18)	C23—C24—C25—C26	177.5 (4)
C37—Fe3—Fe4—C41	−139.2 (3)	C29—C24—C25—C26	−1.0 (6)
S3—Fe3—Fe4—C41	179.55 (13)	C24—C25—C26—C27	0.8 (7)
S4—Fe3—Fe4—C41	−78.99 (13)	C25—C26—C27—C28	−0.2 (8)
C38—Fe3—Fe4—C42	−138.1 (3)	C26—C27—C28—C29	−0.1 (8)
C39—Fe3—Fe4—C42	129.4 (3)	C27—C28—C29—C30	−177.7 (5)
C37—Fe3—Fe4—C42	−8.4 (4)	C27—C28—C29—C24	−0.1 (7)
S3—Fe3—Fe4—C42	−49.7 (3)	C23—C24—C29—C30	−0.2 (5)
S4—Fe3—Fe4—C42	51.8 (3)	C25—C24—C29—C30	178.3 (4)
C38—Fe3—Fe4—S3	−88.40 (13)	C23—C24—C29—C28	−177.9 (3)
C39—Fe3—Fe4—S3	179.03 (13)	C25—C24—C29—C28	0.7 (5)
C37—Fe3—Fe4—S3	41.3 (3)	C28—C29—C30—C31	176.9 (4)
S4—Fe3—Fe4—S3	101.46 (5)	C24—C29—C30—C31	−0.7 (6)
C38—Fe3—Fe4—S4	170.14 (13)	C29—C30—C31—C32	179.9 (4)
C39—Fe3—Fe4—S4	77.57 (13)	C29—C30—C31—C36	0.1 (6)
C37—Fe3—Fe4—S4	−60.2 (3)	C30—C31—C32—C33	179.6 (4)
S3—Fe3—Fe4—S4	−101.46 (5)	C36—C31—C32—C33	−0.6 (6)
C4—Fe2—S1—C22	−138.18 (19)	C31—C32—C33—C34	−1.2 (7)
C5—Fe2—S1—C22	132.7 (3)	C32—C33—C34—C35	1.9 (7)
C6—Fe2—S1—C22	−41.11 (17)	C33—C34—C35—C36	−0.6 (7)
S2—Fe2—S1—C22	54.99 (13)	C24—C23—C36—C35	177.6 (3)
Fe1—Fe2—S1—C22	110.85 (13)	C22—C23—C36—C35	0.1 (5)
C4—Fe2—S1—Fe1	110.97 (14)	C24—C23—C36—C31	−2.2 (5)
C5—Fe2—S1—Fe1	21.8 (3)	C22—C23—C36—C31	−179.7 (3)
C6—Fe2—S1—Fe1	−151.96 (12)	C34—C35—C36—C23	179.0 (4)
S2—Fe2—S1—Fe1	−55.86 (4)	C34—C35—C36—C31	−1.1 (6)
C2—Fe1—S1—C22	153.35 (16)	C30—C31—C36—C23	1.3 (5)
C1—Fe1—S1—C22	53.80 (17)	C32—C31—C36—C23	−178.4 (3)
C3—Fe1—S1—C22	−118.3 (3)	C30—C31—C36—C35	−178.5 (3)
S2—Fe1—S1—C22	−47.33 (12)	C32—C31—C36—C35	1.7 (5)
Fe2—Fe1—S1—C22	−103.56 (12)	C38—Fe3—C37—O7	107 (7)
C2—Fe1—S1—Fe2	−103.09 (12)	C39—Fe3—C37—O7	−161 (7)
C1—Fe1—S1—Fe2	157.37 (12)	S3—Fe3—C37—O7	11 (7)
C3—Fe1—S1—Fe2	−14.8 (3)	S4—Fe3—C37—O7	−70 (7)
S2—Fe1—S1—Fe2	56.23 (4)	Fe4—Fe3—C37—O7	−22 (7)
C2—Fe1—S2—C7	−109.4 (3)	C39—Fe3—C38—O8	44 (7)
C1—Fe1—S2—C7	89.98 (18)	C37—Fe3—C38—O8	144 (7)
C3—Fe1—S2—C7	−8.38 (18)	S3—Fe3—C38—O8	−118 (7)

S1—Fe1—S2—C7	−166.51 (14)	S4—Fe3—C38—O8	−42 (7)
Fe2—Fe1—S2—C7	−110.22 (14)	Fe4—Fe3—C38—O8	−62 (7)
C2—Fe1—S2—Fe2	0.8 (3)	C38—Fe3—C39—O9	12 (21)
C1—Fe1—S2—Fe2	−159.81 (13)	C37—Fe3—C39—O9	−89 (21)
C3—Fe1—S2—Fe2	101.84 (12)	S3—Fe3—C39—O9	116 (21)
S1—Fe1—S2—Fe2	−56.29 (4)	S4—Fe3—C39—O9	168 (100)
C4—Fe2—S2—C7	116.2 (5)	Fe4—Fe3—C39—O9	113 (21)
C5—Fe2—S2—C7	12.07 (17)	C41—Fe4—C40—O10	−71 (13)
C6—Fe2—S2—C7	−89.95 (17)	C42—Fe4—C40—O10	−171 (100)
S1—Fe2—S2—C7	165.22 (13)	S3—Fe4—C40—O10	84 (13)
Fe1—Fe2—S2—C7	108.85 (13)	S4—Fe4—C40—O10	13 (14)
C4—Fe2—S2—Fe1	7.4 (5)	Fe3—Fe4—C40—O10	28 (13)
C5—Fe2—S2—Fe1	−96.79 (12)	C40—Fe4—C41—O11	63 (12)
C6—Fe2—S2—Fe1	161.19 (12)	C42—Fe4—C41—O11	162 (12)
S1—Fe2—S2—Fe1	56.36 (4)	S3—Fe4—C41—O11	−37 (13)
C40—Fe4—S3—C58	6.6 (2)	S4—Fe4—C41—O11	−93 (12)
C41—Fe4—S3—C58	106.9 (3)	Fe3—Fe4—C41—O11	−38 (12)
C42—Fe4—S3—C58	−93.1 (2)	C40—Fe4—C42—O12	44 (11)
S4—Fe4—S3—C58	163.79 (15)	C41—Fe4—C42—O12	−49 (11)
Fe3—Fe4—S3—C58	107.99 (15)	S3—Fe4—C42—O12	139 (11)
C40—Fe4—S3—Fe3	−101.35 (15)	S4—Fe4—C42—O12	−138 (11)
C41—Fe4—S3—Fe3	−1.1 (3)	Fe3—Fe4—C42—O12	180 (100)
C42—Fe4—S3—Fe3	158.86 (15)	Fe3—S4—C43—C44	164.5 (2)
S4—Fe4—S3—Fe3	55.80 (4)	Fe4—S4—C43—C44	90.8 (3)
C38—Fe3—S3—C58	−11.74 (19)	S4—C43—C44—C57	−105.8 (3)
C39—Fe3—S3—C58	−114.4 (4)	S4—C43—C44—C45	77.4 (4)
C37—Fe3—S3—C58	90.60 (19)	C57—C44—C45—C46	−179.9 (3)
S4—Fe3—S3—C58	−167.60 (14)	C43—C44—C45—C46	−3.1 (5)
Fe4—Fe3—S3—C58	−111.38 (14)	C57—C44—C45—C50	−1.3 (5)
C38—Fe3—S3—Fe4	99.64 (14)	C43—C44—C45—C50	175.5 (3)
C39—Fe3—S3—Fe4	−3.0 (4)	C44—C45—C46—C47	177.5 (4)
C37—Fe3—S3—Fe4	−158.02 (13)	C50—C45—C46—C47	−1.2 (6)
S4—Fe3—S3—Fe4	−56.22 (4)	C45—C46—C47—C48	−0.4 (7)
C38—Fe3—S4—C43	−136.1 (3)	C46—C47—C48—C49	1.7 (7)
C39—Fe3—S4—C43	137.85 (19)	C47—C48—C49—C50	−1.3 (7)
C37—Fe3—S4—C43	37.8 (2)	C48—C49—C50—C51	−178.4 (4)
S3—Fe3—S4—C43	−56.59 (14)	C48—C49—C50—C45	−0.3 (6)
Fe4—Fe3—S4—C43	−112.16 (14)	C46—C45—C50—C51	179.7 (3)
C38—Fe3—S4—Fe4	−24.0 (3)	C44—C45—C50—C51	1.0 (5)
C39—Fe3—S4—Fe4	−109.99 (13)	C46—C45—C50—C49	1.5 (5)
C37—Fe3—S4—Fe4	149.92 (15)	C44—C45—C50—C49	−177.2 (3)
S3—Fe3—S4—Fe4	55.57 (3)	C49—C50—C51—C52	177.1 (4)
C40—Fe4—S4—C43	119.4 (3)	C45—C50—C51—C52	−1.0 (6)
C41—Fe4—S4—C43	−155.19 (17)	C50—C51—C52—C53	−178.1 (4)
C42—Fe4—S4—C43	−56.75 (19)	C50—C51—C52—C57	1.2 (6)
S3—Fe4—S4—C43	45.53 (13)	C51—C52—C53—C54	−179.9 (5)
Fe3—Fe4—S4—C43	101.36 (13)	C57—C52—C53—C54	0.8 (8)
C40—Fe4—S4—Fe3	18.0 (3)	C52—C53—C54—C55	−1.0 (10)
C41—Fe4—S4—Fe3	103.46 (12)	C53—C54—C55—C56	0.6 (9)

C42—Fe4—S4—Fe3	−158.10 (14)	C54—C55—C56—C57	0.0 (7)
S3—Fe4—S4—Fe3	−55.82 (4)	C45—C44—C57—C56	179.5 (3)
C2—Fe1—C1—O1	62 (8)	C43—C44—C57—C56	2.7 (5)
C3—Fe1—C1—O1	−32 (8)	C45—C44—C57—C52	1.5 (5)
S2—Fe1—C1—O1	−126 (8)	C43—C44—C57—C52	−175.2 (3)
S1—Fe1—C1—O1	151 (8)	C55—C56—C57—C44	−178.2 (4)
Fe2—Fe1—C1—O1	−165 (8)	C55—C56—C57—C52	−0.2 (6)
C1—Fe1—C2—O2	169 (10)	C51—C52—C57—C44	−1.4 (6)
C3—Fe1—C2—O2	−92 (10)	C53—C52—C57—C44	177.9 (4)
S2—Fe1—C2—O2	8(11)	C51—C52—C57—C56	−179.5 (4)
S1—Fe1—C2—O2	64 (10)	C53—C52—C57—C56	−0.2 (6)
Fe2—Fe1—C2—O2	9(10)	Fe4—S3—C58—C59	134.7 (3)
C2—Fe1—C3—O3	113 (7)	Fe3—S3—C58—C59	−148.2 (3)
C1—Fe1—C3—O3	−146 (7)	S3—C58—C59—C60	−92.3 (4)
S2—Fe1—C3—O3	−43 (7)	S3—C58—C59—C72	84.7 (4)
S1—Fe1—C3—O3	26 (8)	C72—C59—C60—C61	−173.5 (4)
Fe2—Fe1—C3—O3	13 (8)	C58—C59—C60—C61	3.4 (7)
C5—Fe2—C4—O4	−98 (14)	C72—C59—C60—C65	5.2 (6)
C6—Fe2—C4—O4	3(14)	C58—C59—C60—C65	−177.8 (4)
S2—Fe2—C4—O4	157 (13)	C59—C60—C61—C62	−179.9 (5)
S1—Fe2—C4—O4	109 (14)	C65—C60—C61—C62	1.3 (8)
Fe1—Fe2—C4—O4	163 (14)	C60—C61—C62—C63	−0.6 (12)
C4—Fe2—C5—O5	−108 (11)	C61—C62—C63—C64	1.0 (18)
C6—Fe2—C5—O5	155 (11)	C62—C63—C64—C65	−2(2)
S2—Fe2—C5—O5	55 (11)	C59—C60—C65—C66	−0.3 (8)
S1—Fe2—C5—O5	−19 (12)	C61—C60—C65—C66	178.6 (5)
Fe1—Fe2—C5—O5	−1(11)	C59—C60—C65—C64	178.9 (6)
C4—Fe2—C6—O6	−122 (26)	C61—C60—C65—C64	−2.2 (8)
C5—Fe2—C6—O6	−30 (26)	C63—C64—C65—C66	−178.2 (11)
S2—Fe2—C6—O6	66 (26)	C63—C64—C65—C60	2.7 (15)
S1—Fe2—C6—O6	147 (26)	C60—C65—C66—C67	−4.1 (10)
Fe1—Fe2—C6—O6	97 (26)	C64—C65—C66—C67	176.8 (7)
Fe1—S2—C7—C8	−160.2 (2)	C65—C66—C67—C68	−174.6 (6)
Fe2—S2—C7—C8	122.8 (2)	C65—C66—C67—C72	3.3 (9)
S2—C7—C8—C21	94.4 (3)	C66—C67—C68—C69	177.5 (9)
S2—C7—C8—C9	−84.5 (3)	C72—C67—C68—C69	−0.5 (12)
C21—C8—C9—C10	−176.9 (3)	C67—C68—C69—C70	−0.2 (16)
C7—C8—C9—C10	2.1 (5)	C68—C69—C70—C71	1.3 (13)
C21—C8—C9—C14	3.1 (5)	C69—C70—C71—C72	−1.6 (8)
C7—C8—C9—C14	−178.0 (3)	C70—C71—C72—C59	−178.8 (4)
C8—C9—C10—C11	178.1 (4)	C70—C71—C72—C67	0.9 (6)
C14—C9—C10—C11	−1.8 (5)	C60—C59—C72—C71	173.7 (4)
C9—C10—C11—C12	0.4 (6)	C58—C59—C72—C71	−3.3 (6)
C10—C11—C12—C13	2.0 (7)	C60—C59—C72—C67	−6.0 (6)
C11—C12—C13—C14	−2.8 (7)	C58—C59—C72—C67	177.0 (3)
C12—C13—C14—C15	−177.9 (4)	C66—C67—C72—C71	−177.9 (5)
C12—C13—C14—C9	1.3 (6)	C68—C67—C72—C71	0.2 (7)
C8—C9—C14—C15	0.3 (5)	C66—C67—C72—C59	1.8 (7)
C10—C9—C14—C15	−179.8 (3)	C68—C67—C72—C59	179.8 (5)

Fig. 1

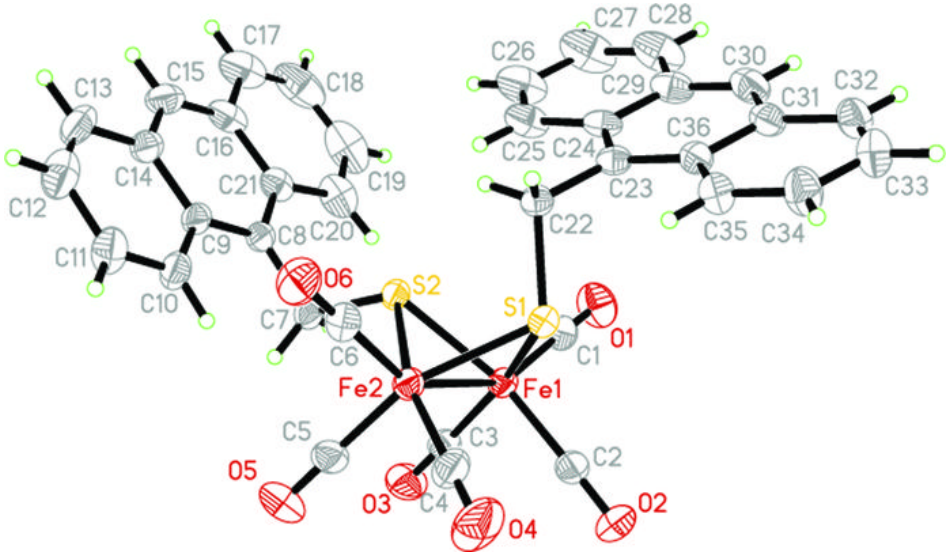
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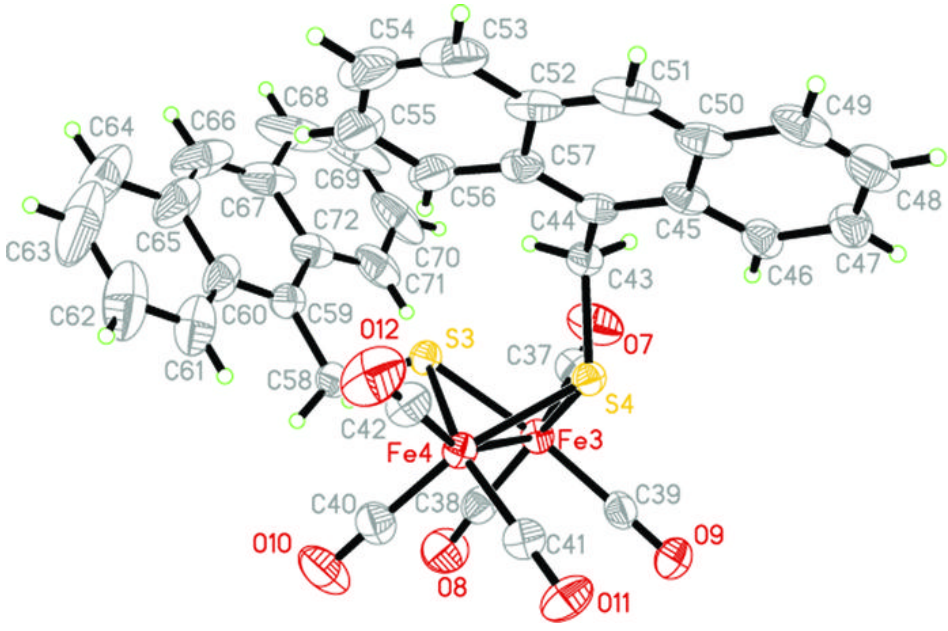
Fig. 2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