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4,5-Diferrocenyl-1,2-dithiol-3-one

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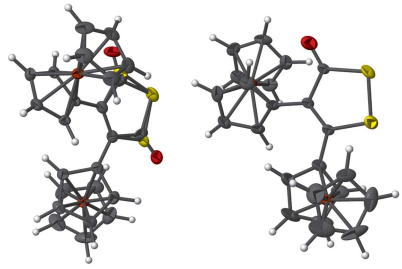
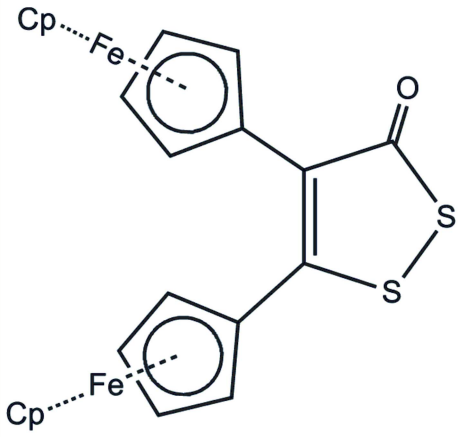
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Fe_2(C_5H_5)_2(C_{13}H_8OS_2)]$, crystallizes with two molecules in the asymmetric unit. Each molecule comprises a pair of ferrocenyl units bridged by a dithiol-3-one moiety. The dihedral angles between the dithiol-3-one ring and the substituted cyclopentadienyl rings are in the range 32.4 (3)–39.3 (3)°. One of the dithiol-3-one rings was refined as being disordered over two sets of sites while the same kind of disorder in the other molecule was negligible. The molecular packing is dominated by C—H···O hydrogen bonds and C—H···π interactions.

3D view



Chemical scheme



Structure description

Background to the chemistry of ferrocenes and their potential applications was compiled by Togni & Hayashi (1995). 1,2-Dithiole-3-one derivatives are of current interest since they have a broad spectrum of biological activities (He *et al.*, 2004) and may be useful synthons for many sulfur-containing heterocycles (Konstantinova *et al.*, 2007). An analogue of these compounds is *Oltipraz* (4-methyl-5-(2-pyrazinyl)-1,2-dithiole-3-thione) that has been clinically tested as a preventive agent against various types of cancer (Iida *et al.*, 2004).

Each of the two molecules *A* and *B* in the asymmetric unit of the title compound is constituted by a pair of ferrocenyl units bridged by a dithiol-3-one ring (Fig. 1). The cyclopentadienyl (Cp) rings are almost parallel, making dihedral angles of 1.3 (3) and 1.7 (2)° for molecule *A* containing Fe1 and Fe2, and 1.7 (2) and 2.7 (3)° for molecule *B* containing Fe3 and Fe4, respectively. The dihedral angles between the dithiol-3-one ring and the substituted cyclopentadienyl rings are 39.3 (3) and 32.6 (2)° for molecule *A* and 37.6 (2) and 32.4 (2)° for molecule *B*. The cyclopentadienyl rings of the ferrocenyl moieties in both molecules adopt eclipsed conformations. All bond lengths and angles for two crystallographically independent molecules are similar (Table 1).

In the crystal structure (Fig. 2), molecules *B* are linked *via* weak C—H···O hydrogen bonds between the Cp rings and the O atoms of the 1,2-dithiole-3-one moieties (Table 2) with a graph-set motif $C_1^1(8)$ forming a chain parallel to the *a* axis. Molecules *A* and *B*, on

Table 1
Selected geometric parameters (Å, °).

C5—C6	1.474 (5)	C29—C30	1.466 (5)
C5—Fe1	2.048 (4)	C29—Fe3	2.052 (4)
C6—C7	1.357 (6)	C30—C31	1.361 (5)
C7—C8	1.465 (5)	C31—C33	1.471 (5)
C7—S1	1.756 (5)	C31—S4	1.748 (4)
C8—Fe2	2.055 (4)	C33—Fe4	2.037 (4)
S2—S1	1.983 (6)	S4—S5	2.0259 (15)
C18—O1	1.25 (3)	C32—O3	1.182 (5)
C4—C5—C6—C7	37.8 (6)	C25—C29—C30—C31	144.0 (4)
C6—C7—C8—C9	33.9 (6)	C30—C31—C33—C34	147.4 (4)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C36S—H36···O3^{i}	1.00	2.36	3.354 (6)	170

Symmetry code: (i) $x+1, y, z$.

the other hand, show intermolecular interactions of the type C—H···π, with C1—H1···*Cg*10 and C43—H43···*Cg*6 distances of 3.04 and 3.12 Å, respectively, where *Cg*10 and *Cg*6 are the centroids of the rings C38–C42 and C20–24. These interactions form slabs lying parallel to the *ac* plane.

Synthesis and crystallization

A mixture of sodium sulfide (10 mmol) and sulfur (5 mmol) in ethanol (80 ml) was added to 1,2-diferrocenylcyclopropenone (5 mmol) and stirred at 353 K for 4 h. The solvents were removed *in vacuo*, and the residues purified by column chromatography with alumina and a mixture of hexane:diethyl ether (ratio 1:1 *v*/*v*) as eluent. Red crystals of 4,5-diferrocenyl-1,2-dithiol-3-one, suitable for single-crystal diffraction analysis, were obtained by slow evaporation of a saturated dichloromethane/hexane (ratio 1:1 *v*/*v*) solution. Yield (75%), mp. 468-470 K.

^{1}H NMR (300 MHz, $CDCl_3$) δ: 4.24 (5 H, *s*, C_5H_5), δ: 4.05 (5 H, *s*, C_5H_5), δ: 4.04 (4 H, *s*, C_5H_4), δ: 4.22 (2 H, *m*, C_5H_4), δ: 4.17 (2 H, *s*, C_5H_4) p.p.m., ^{13}C NMR (75 MHz, $CDCl_3$) δ: 79.45, 81.45 (2C_{ipso} Fc), δ: 69.60 (C_5H_5), δ: 70.61 (C_5H_5), δ: 4.60, 69.55, 69.03, 67.96 (4C_5H_4), 136.15, 164.69, (2 C), 169.25 (C═O) p.p.m., MS: *m*/*z* 486 $[M]^+$. Analysis calculated for

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Fe_2(C_5H_5)_2(C_{13}H_8OS_2)]$
M_r	486.19
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	130
a, *b*, *c* (Å)	9.8525 (4), 10.6407 (6), 19.2720 (9)
α, β, γ (°)	98.867 (4), 95.255 (4), 105.512 (4)
V (Å^3)	1904.76 (17)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	1.75
Crystal size (mm)	0.16 × 0.13 × 0.06
Data collection	
Diffractometer	Agilent Xcalibur Atlas Gemini
Absorption correction	Analytical (*CrysAlis RED*; Agilent, 2013)
T_{min}, T_{max}	0.856, 0.937
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19834, 7772, 5624
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.046, 0.110, 1.02
No. of reflections	7772
No. of parameters	515
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.91, −0.51

Computer programs: *CrysAlis PRO* and *CrysAlis RED* (Agilent, 2013), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008).

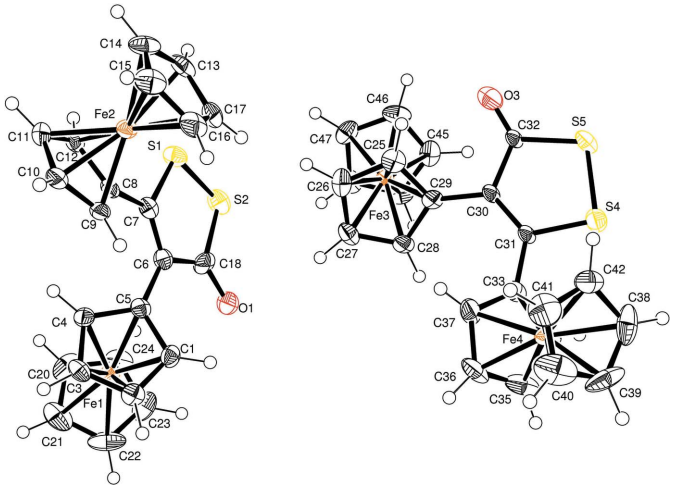


Figure 1
The molecular structures of the two entities in the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level. Only the major component of disorder is shown for molecule *A*.

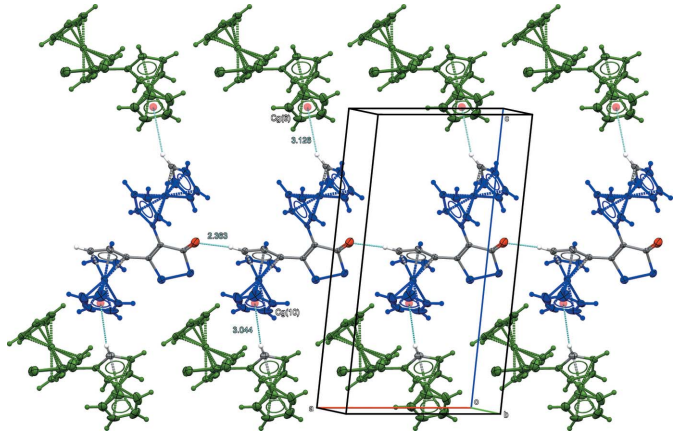


Figure 2
The molecular packing of the title compound showing intermolecular contacts of the type C—H···O forming graph set motifs $C_1^1(8)$ along the *a* axis, as well as C—H···π interactions parallel to the *ac* plane. Molecule *A* is green, molecule *B* is blue.

$C_{23}H_{18}Fe_2OS_2$: C, 56.90, H, 3.68, S, 12.85, Found C, 56.70, H, 3.90, S, 13.05%.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Atoms C18, O1 and S1 of molecule *A* were refined as being disordered over two sets of sites with occupancies of 0.56: 0.44 using restraints so that the bond lengths and angles of the two components are comparable. Remaining electron densities close to the same type of atoms were also found for molecule *B* but to a much lesser extend (preliminary refinement of the occupancies about 0.93:0.07). For the final model this type of disorder was neglected.

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full crystallographic data

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Crystal data

$[Fe_2(C_5H_5)_2(C_{13}H_8OS_2)]$
M_r = 486.19
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.8525 (4) Å
b = 10.6407 (6) Å
c = 19.2720 (9) Å
α = 98.867 (4)°
β = 95.255 (4)°
γ = 105.512 (4)°
V = 1904.76 (17) Å^3
Z = 4
$F(000)$ = 992
D_x = 1.695 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4380 reflections
θ = 3.5–29.5°
μ = 1.75 mm^{-1}
T = 130 K
Block, dark red
0.16 × 0.13 × 0.06 mm

Data collection

Agilent Xcalibur Atlas Gemini diffractometer
Graphite monochromator
Detector resolution: 10.4685 pixels mm^{-1}
ω scans
Absorption correction: analytical (*CrysAlis RED*; Agilent, 2013)
T_{min} = 0.856, T_{max} = 0.937
19834 measured reflections
7772 independent reflections
5624 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 26.4°, θ_{min} = 3.5°
h = −12→12
k = −13→13
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.110
S = 1.02
7772 reflections
515 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2 + 2.1419P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.7650 (4)	−0.2765 (4)	0.8413 (2)	0.0277 (9)	
H1	0.717766	−0.361755	0.807503	0.033*	
C2	0.9125 (4)	−0.2109 (4)	0.8546 (2)	0.0283 (9)	
H2	0.987812	−0.242726	0.83218	0.034*	
C3	0.9362 (4)	−0.0949 (4)	0.9059 (2)	0.0264 (9)	
H3	1.030954	−0.030483	0.925819	0.032*	
C4	0.8038 (4)	−0.0858 (4)	0.9250 (2)	0.0252 (9)	
H4	0.788102	−0.013583	0.960429	0.03*	
C5	0.6954 (4)	−0.1981 (4)	0.8841 (2)	0.0246 (9)	
C6	0.5408 (4)	−0.2258 (4)	0.8849 (2)	0.0259 (9)	
C7	0.4686 (4)	−0.1333 (4)	0.8899 (2)	0.0248 (9)	
C8	0.5258 (4)	0.0088 (4)	0.8901 (2)	0.0242 (9)	
C9	0.6355 (4)	0.0713 (4)	0.8529 (2)	0.0241 (9)	
H9	0.688804	0.024483	0.821315	0.029*	
C10	0.6565 (4)	0.2088 (4)	0.8676 (2)	0.0294 (9)	
H10	0.727351	0.276738	0.848641	0.035*	
C11	0.5580 (4)	0.2346 (4)	0.9140 (2)	0.0334 (10)	
H11	0.547666	0.323862	0.933131	0.04*	
C12	0.4767 (4)	0.1116 (4)	0.9277 (2)	0.0263 (9)	
H12	0.399114	0.098759	0.958204	0.032*	
C13	0.2404 (4)	0.0579 (5)	0.7823 (2)	0.0341 (10)	
H13	0.159834	0.019829	0.807937	0.041*	
C14	0.3016 (5)	0.1943 (5)	0.7819 (2)	0.0375 (11)	
H14	0.272346	0.269719	0.807527	0.045*	
C15	0.4120 (5)	0.2050 (5)	0.7387 (2)	0.0381 (11)	
H15	0.474338	0.289612	0.728965	0.046*	
C16	0.4199 (5)	0.0770 (5)	0.7127 (2)	0.0378 (11)	
H16	0.488598	0.054851	0.681139	0.045*	
C17	0.3151 (4)	−0.0157 (5)	0.7394 (2)	0.0362 (11)	
H17	0.295695	−0.114355	0.729435	0.043*	
C20	0.8309 (6)	−0.2611 (5)	1.0507 (2)	0.0427 (12)	
H20	0.808591	−0.192404	1.085689	0.051*	
C21	0.9678 (5)	−0.2604 (5)	1.0344 (3)	0.0482 (14)	
H21	1.059139	−0.19195	1.055888	0.058*	
C22	0.9523 (5)	−0.3730 (5)	0.9829 (3)	0.0500 (14)	
H22	1.031113	−0.399257	0.960867	0.06*	
C23	0.8068 (5)	−0.4429 (5)	0.9671 (3)	0.0432 (12)	
H23	0.764202	−0.527807	0.932351	0.052*	
C24	0.7318 (5)	−0.3733 (5)	1.0099 (2)	0.0400 (11)	
H24	0.626754	−0.39954	1.010682	0.048*	
Fe1	0.83868 (6)	−0.25721 (6)	0.94571 (3)	0.02384 (14)	
Fe2	0.45226 (6)	0.11315 (6)	0.82134 (3)	0.02371 (14)	
S2	0.26696 (11)	−0.37118 (12)	0.89084 (6)	0.0378 (3)	
C18	0.449 (3)	−0.364 (2)	0.8800 (13)	0.037 (6)	0.566 (9)
O1	0.4857 (6)	−0.4677 (9)	0.8665 (4)	0.0383 (17)	0.566 (9)

S1	0.2859 (4)	−0.1795 (5)	0.8963 (3)	0.0314 (14)	0.566 (9)
C18P	0.316 (3)	−0.188 (3)	0.8948 (15)	0.037 (6)	0.434 (9)
O1P	0.2338 (10)	−0.1248 (10)	0.9115 (5)	0.046 (2)	0.434 (9)
S1P	0.4606 (8)	−0.3903 (8)	0.8827 (5)	0.033 (2)	0.434 (9)
C25	0.0640 (4)	−0.4890 (4)	0.6256 (2)	0.0303 (10)	
H25	0.00186	−0.439769	0.60492	0.036*	
C26	0.1588 (4)	−0.4436 (4)	0.6905 (2)	0.0328 (10)	
H26	0.175421	−0.356539	0.723145	0.039*	
C27	0.2257 (4)	−0.5430 (4)	0.7008 (2)	0.0312 (10)	
H27	0.297464	−0.53827	0.742071	0.037*	
C28	0.1719 (4)	−0.6507 (4)	0.6437 (2)	0.0277 (9)	
H28	0.199384	−0.73527	0.637466	0.033*	
C29	0.0714 (4)	−0.6183 (4)	0.5959 (2)	0.0240 (9)	
C30	−0.0088 (4)	−0.7010 (4)	0.52902 (18)	0.0218 (5)	
C31	0.0423 (4)	−0.7819 (4)	0.48323 (18)	0.0218 (5)	
C32	−0.1611 (4)	−0.6994 (4)	0.51047 (19)	0.0218 (5)	
C33	0.1864 (4)	−0.7976 (4)	0.4869 (2)	0.0288 (9)	
C34	0.2209 (4)	−0.9175 (5)	0.4626 (2)	0.0351 (11)	
H34	0.151723	−1.004898	0.440025	0.042*	
C35	0.3703 (5)	−0.8902 (6)	0.4755 (3)	0.0468 (14)	
H35	0.4252	−0.955266	0.463279	0.056*	
C36	0.4291 (5)	−0.7560 (6)	0.5073 (2)	0.0517 (15)	
H36	0.532815	−0.709774	0.521739	0.062*	
C37	0.3161 (4)	−0.6955 (5)	0.5143 (2)	0.0418 (12)	
H37	0.325846	−0.600954	0.535199	0.05*	
C38	0.2421 (6)	−0.8212 (5)	0.3059 (2)	0.0507 (14)	
H38	0.165484	−0.902267	0.281206	0.061*	
C39	0.3910 (7)	−0.8058 (7)	0.3170 (3)	0.0611 (18)	
H39	0.438232	−0.876079	0.302569	0.073*	
C40	0.4575 (6)	−0.6801 (7)	0.3507 (3)	0.0631 (17)	
H40	0.562468	−0.643238	0.365739	0.076*	
C41	0.3600 (6)	−0.6110 (5)	0.3620 (3)	0.0523 (14)	
H41	0.381509	−0.51599	0.385577	0.063*	
C42	0.2260 (5)	−0.6961 (5)	0.3344 (2)	0.0389 (11)	
H42	0.134159	−0.672852	0.334469	0.047*	
C43	−0.0265 (4)	−0.6703 (5)	0.7900 (2)	0.0336 (10)	
H43	0.04719	−0.658521	0.831638	0.04*	
C44	−0.0753 (4)	−0.7821 (4)	0.7351 (2)	0.0347 (10)	
H44	−0.041558	−0.863285	0.730826	0.042*	
C45	−0.1783 (4)	−0.7603 (4)	0.6870 (2)	0.0354 (11)	
H45	−0.231137	−0.822922	0.642765	0.042*	
C46	−0.1940 (4)	−0.6329 (5)	0.7123 (2)	0.0352 (11)	
H46	−0.26021	−0.590069	0.689252	0.042*	
C47	−0.1000 (4)	−0.5783 (4)	0.7762 (2)	0.0346 (10)	
H47	−0.087676	−0.489549	0.806351	0.041*	
Fe3	0.01045 (5)	−0.61637 (5)	0.69496 (3)	0.02121 (14)	
Fe4	0.31671 (6)	−0.77061 (6)	0.41095 (3)	0.02489 (15)	
O3	−0.2167 (3)	−0.6240 (4)	0.53877 (17)	0.0477 (9)	

S4	−0.07427 (11)	−0.88197 (12)	0.40941 (6)	0.0358 (3)
S5	−0.24512 (10)	−0.81968 (11)	0.43199 (6)	0.0323 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.035 (2)	0.028 (2)	0.020 (2)	0.0103 (18)	0.0017 (17)	0.0019 (17)
C2	0.029 (2)	0.037 (3)	0.022 (2)	0.0097 (18)	0.0093 (17)	0.0097 (19)
C3	0.0230 (19)	0.031 (2)	0.026 (2)	0.0046 (16)	−0.0021 (17)	0.0138 (18)
C4	0.028 (2)	0.023 (2)	0.026 (2)	0.0112 (16)	0.0008 (17)	0.0059 (17)
C5	0.027 (2)	0.030 (2)	0.0192 (19)	0.0106 (17)	−0.0003 (16)	0.0079 (17)
C6	0.028 (2)	0.028 (2)	0.021 (2)	0.0068 (17)	0.0011 (17)	0.0052 (17)
C7	0.0229 (19)	0.030 (2)	0.020 (2)	0.0038 (16)	0.0029 (16)	0.0071 (17)
C8	0.0201 (18)	0.032 (2)	0.020 (2)	0.0088 (16)	−0.0035 (16)	0.0035 (17)
C9	0.0223 (19)	0.030 (2)	0.021 (2)	0.0123 (16)	−0.0005 (16)	0.0030 (17)
C10	0.0201 (19)	0.030 (2)	0.035 (2)	0.0054 (16)	−0.0003 (18)	0.0041 (19)
C11	0.030 (2)	0.033 (3)	0.031 (2)	0.0089 (18)	−0.0028 (19)	−0.0066 (19)
C12	0.0240 (19)	0.034 (2)	0.018 (2)	0.0077 (17)	0.0001 (16)	0.0011 (17)
C13	0.024 (2)	0.054 (3)	0.025 (2)	0.0128 (19)	−0.0040 (18)	0.012 (2)
C14	0.041 (2)	0.052 (3)	0.035 (2)	0.031 (2)	0.008 (2)	0.023 (2)
C15	0.043 (3)	0.049 (3)	0.032 (2)	0.019 (2)	0.008 (2)	0.023 (2)
C16	0.041 (2)	0.058 (3)	0.020 (2)	0.022 (2)	0.0011 (19)	0.012 (2)
C17	0.039 (2)	0.043 (3)	0.023 (2)	0.013 (2)	−0.0102 (19)	0.002 (2)
C20	0.078 (4)	0.044 (3)	0.019 (2)	0.034 (3)	0.010 (2)	0.015 (2)
C21	0.044 (3)	0.050 (3)	0.052 (3)	0.010 (2)	−0.011 (2)	0.032 (3)
C22	0.049 (3)	0.060 (4)	0.071 (4)	0.039 (3)	0.031 (3)	0.046 (3)
C23	0.067 (3)	0.023 (3)	0.040 (3)	0.010 (2)	0.016 (2)	0.009 (2)
C24	0.040 (3)	0.050 (3)	0.039 (3)	0.018 (2)	0.012 (2)	0.023 (2)
Fe1	0.0270 (3)	0.0243 (3)	0.0221 (3)	0.0099 (2)	0.0033 (2)	0.0056 (2)
Fe2	0.0247 (3)	0.0275 (3)	0.0217 (3)	0.0112 (2)	0.0033 (2)	0.0059 (2)
S2	0.0268 (5)	0.0408 (7)	0.0401 (7)	−0.0004 (5)	0.0029 (5)	0.0091 (5)
C18	0.047 (9)	0.049 (10)	0.018 (5)	0.025 (6)	0.006 (5)	−0.002 (5)
O1	0.035 (3)	0.023 (4)	0.052 (4)	0.005 (3)	−0.001 (3)	0.002 (3)
S1	0.0215 (18)	0.033 (2)	0.0409 (17)	0.0053 (15)	0.0072 (14)	0.0124 (14)
C18P	0.047 (9)	0.049 (10)	0.018 (5)	0.025 (6)	0.006 (5)	−0.002 (5)
O1P	0.031 (4)	0.047 (6)	0.069 (6)	0.023 (4)	0.011 (4)	0.015 (5)
S1P	0.024 (2)	0.025 (3)	0.044 (2)	−0.002 (2)	0.0001 (17)	0.004 (2)
C25	0.033 (2)	0.035 (3)	0.027 (2)	0.0073 (18)	0.0118 (18)	0.0153 (19)
C26	0.034 (2)	0.031 (2)	0.025 (2)	−0.0053 (18)	0.0078 (19)	0.0041 (19)
C27	0.022 (2)	0.046 (3)	0.023 (2)	0.0059 (18)	0.0014 (17)	0.008 (2)
C28	0.0223 (19)	0.044 (3)	0.021 (2)	0.0147 (18)	0.0094 (17)	0.0064 (19)
C29	0.0193 (18)	0.036 (2)	0.0201 (19)	0.0089 (16)	0.0126 (16)	0.0081 (18)
C30	0.0198 (11)	0.0356 (14)	0.0118 (10)	0.0103 (9)	0.0013 (9)	0.0063 (9)
C31	0.0198 (11)	0.0356 (14)	0.0118 (10)	0.0103 (9)	0.0013 (9)	0.0063 (9)
C32	0.0198 (11)	0.0356 (14)	0.0118 (10)	0.0103 (9)	0.0013 (9)	0.0063 (9)
C33	0.023 (2)	0.048 (3)	0.018 (2)	0.0121 (18)	0.0062 (17)	0.0104 (19)
C34	0.034 (2)	0.048 (3)	0.036 (2)	0.018 (2)	0.013 (2)	0.027 (2)
C35	0.036 (3)	0.088 (4)	0.038 (3)	0.036 (3)	0.018 (2)	0.037 (3)

C36	0.022 (2)	0.113 (5)	0.021 (2)	0.023 (3)	0.0027 (19)	0.010 (3)
C37	0.024 (2)	0.070 (4)	0.024 (2)	0.009 (2)	0.0053 (18)	−0.007 (2)
C38	0.090 (4)	0.036 (3)	0.017 (2)	0.003 (3)	0.002 (2)	0.007 (2)
C39	0.103 (5)	0.086 (5)	0.038 (3)	0.078 (4)	0.043 (3)	0.033 (3)
C40	0.049 (3)	0.094 (5)	0.065 (4)	0.026 (3)	0.033 (3)	0.050 (4)
C41	0.066 (3)	0.033 (3)	0.061 (4)	0.013 (3)	0.003 (3)	0.019 (3)
C42	0.045 (3)	0.062 (3)	0.025 (2)	0.032 (2)	0.013 (2)	0.018 (2)
C43	0.031 (2)	0.050 (3)	0.023 (2)	0.007 (2)	0.0134 (18)	0.018 (2)
C44	0.035 (2)	0.028 (2)	0.048 (3)	0.0095 (19)	0.017 (2)	0.019 (2)
C45	0.030 (2)	0.038 (3)	0.031 (2)	−0.0026 (19)	0.0128 (19)	0.003 (2)
C46	0.025 (2)	0.052 (3)	0.042 (3)	0.018 (2)	0.020 (2)	0.026 (2)
C47	0.037 (2)	0.033 (3)	0.035 (2)	0.0073 (19)	0.020 (2)	0.004 (2)
Fe3	0.0230 (3)	0.0241 (3)	0.0175 (3)	0.0067 (2)	0.0058 (2)	0.0050 (2)
Fe4	0.0263 (3)	0.0316 (3)	0.0211 (3)	0.0128 (2)	0.0091 (2)	0.0063 (3)
O3	0.0367 (17)	0.066 (2)	0.0414 (19)	0.0227 (16)	−0.0037 (15)	0.0030 (17)
S4	0.0283 (5)	0.0486 (7)	0.0276 (6)	0.0101 (5)	0.0025 (5)	0.0011 (5)
S5	0.0214 (5)	0.0456 (7)	0.0278 (6)	0.0062 (4)	−0.0025 (4)	0.0104 (5)

Geometric parameters (Å, º)

C1—C2	1.414 (6)	C18—O1	1.25 (3)
C1—C5	1.430 (5)	C18P—O1P	1.22 (3)
C1—Fe1	2.036 (4)	C25—C26	1.425 (6)
C1—H1	1	C25—C29	1.430 (6)
C2—C3	1.408 (6)	C25—Fe3	2.050 (4)
C2—Fe1	2.041 (4)	C25—H25	1
C2—H2	1	C26—C27	1.416 (6)
C3—C4	1.412 (5)	C26—Fe3	2.039 (4)
C3—Fe1	2.037 (4)	C26—H26	1
C3—H3	1	C27—C28	1.409 (6)
C4—C5	1.436 (5)	C27—Fe3	2.041 (4)
C4—Fe1	2.035 (4)	C27—H27	1
C4—H4	1	C28—C29	1.436 (5)
C5—C6	1.474 (5)	C28—Fe3	2.031 (4)
C5—Fe1	2.048 (4)	C28—H28	1
C6—C7	1.357 (6)	C29—C30	1.466 (5)
C6—C18	1.49 (2)	C29—Fe3	2.052 (4)
C6—S1P	1.708 (8)	C30—C31	1.361 (5)
C7—C8	1.465 (5)	C30—C32	1.516 (5)
C7—C18P	1.48 (2)	C31—C33	1.471 (5)
C7—S1	1.756 (5)	C31—S4	1.748 (4)
C8—C9	1.425 (5)	C32—O3	1.182 (5)
C8—C12	1.434 (5)	C32—S5	1.794 (4)
C8—Fe2	2.055 (4)	C33—C34	1.428 (6)
C9—C10	1.401 (6)	C33—C37	1.431 (6)
C9—Fe2	2.034 (4)	C33—Fe4	2.037 (4)
C9—H9	1	C34—C35	1.413 (6)
C10—C11	1.430 (6)	C34—Fe4	2.046 (4)

C10—Fe2	2.044 (4)	C34—H34	1
C10—H10	1	C35—C36	1.405 (8)
C11—C12	1.417 (6)	C35—Fe4	2.043 (4)
C11—Fe2	2.042 (4)	C35—H35	1
C11—H11	1	C36—C37	1.434 (7)
C12—Fe2	2.044 (4)	C36—Fe4	2.036 (4)
C12—H12	1	C36—H36	1
C13—C14	1.416 (6)	C37—Fe4	2.029 (4)
C13—C17	1.435 (6)	C37—H37	1
C13—Fe2	2.047 (4)	C38—C42	1.415 (7)
C13—H13	1	C38—C39	1.424 (8)
C14—C15	1.420 (6)	C38—Fe4	2.026 (4)
C14—Fe2	2.051 (4)	C38—H38	1
C14—H14	1	C39—C40	1.350 (8)
C15—C16	1.402 (6)	C39—Fe4	2.033 (5)
C15—Fe2	2.055 (4)	C39—H39	1
C15—H15	1	C40—C41	1.371 (8)
C16—C17	1.419 (6)	C40—Fe4	2.031 (5)
C16—Fe2	2.049 (4)	C40—H40	1
C16—H16	1	C41—C42	1.388 (7)
C17—Fe2	2.037 (4)	C41—Fe4	2.033 (5)
C17—H17	1	C41—H41	1
C20—C24	1.394 (7)	C42—Fe4	2.025 (4)
C20—C21	1.410 (7)	C42—H42	1
C20—Fe1	2.037 (4)	C43—C47	1.406 (6)
C20—H20	1	C43—C44	1.407 (6)
C21—C22	1.398 (7)	C43—Fe3	2.037 (4)
C21—Fe1	2.045 (4)	C43—H43	1
C21—H21	1	C44—C45	1.401 (6)
C22—C23	1.408 (7)	C44—Fe3	2.041 (4)
C22—Fe1	2.036 (4)	C44—H44	1
C22—H22	1	C45—C46	1.421 (6)
C23—C24	1.410 (6)	C45—Fe3	2.044 (4)
C23—Fe1	2.029 (4)	C45—H45	1
C23—H23	1	C46—C47	1.412 (6)
C24—Fe1	2.044 (4)	C46—Fe3	2.038 (4)
C24—H24	1	C46—H46	1
S2—C18	1.80 (3)	C47—Fe3	2.038 (4)
S2—C18P	1.87 (3)	C47—H47	1
S2—S1	1.983 (6)	S4—S5	2.0259 (15)
S2—S1P	1.989 (9)		

C2—C1—C5	107.7 (4)	O1P—C18P—C7	127 (3)
C2—C1—Fe1	69.9 (2)	O1P—C18P—S2	120.9 (19)
C5—C1—Fe1	69.9 (2)	C7—C18P—S2	111.5 (16)
C2—C1—H1	126.2	C6—S1P—S2	95.8 (5)
C5—C1—H1	126.2	C26—C25—C29	108.1 (4)
Fe1—C1—H1	126.2	C26—C25—Fe3	69.2 (2)

C3—C2—C1	108.7 (4)	C29—C25—Fe3	69.7 (2)
C3—C2—Fe1	69.7 (2)	C26—C25—H25	126
C1—C2—Fe1	69.5 (2)	C29—C25—H25	126
C3—C2—H2	125.6	Fe3—C25—H25	126
C1—C2—H2	125.6	C27—C26—C25	108.1 (4)
Fe1—C2—H2	125.6	C27—C26—Fe3	69.7 (2)
C2—C3—C4	108.5 (3)	C25—C26—Fe3	70.0 (2)
C2—C3—Fe1	70.0 (2)	C27—C26—H26	125.9
C4—C3—Fe1	69.6 (2)	C25—C26—H26	125.9
C2—C3—H3	125.8	Fe3—C26—H26	125.9
C4—C3—H3	125.8	C28—C27—C26	108.4 (4)
Fe1—C3—H3	125.8	C28—C27—Fe3	69.4 (2)
C3—C4—C5	107.7 (4)	C26—C27—Fe3	69.6 (2)
C3—C4—Fe1	69.8 (2)	C28—C27—H27	125.8
C5—C4—Fe1	69.9 (2)	C26—C27—H27	125.8
C3—C4—H4	126.1	Fe3—C27—H27	125.8
C5—C4—H4	126.1	C27—C28—C29	108.5 (4)
Fe1—C4—H4	126.1	C27—C28—Fe3	70.1 (2)
C1—C5—C4	107.4 (3)	C29—C28—Fe3	70.2 (2)
C1—C5—C6	126.3 (4)	C27—C28—H28	125.8
C4—C5—C6	126.3 (4)	C29—C28—H28	125.8
C1—C5—Fe1	69.1 (2)	Fe3—C28—H28	125.8
C4—C5—Fe1	68.9 (2)	C25—C29—C28	107.0 (3)
C6—C5—Fe1	128.4 (3)	C25—C29—C30	126.0 (3)
C7—C6—C5	125.3 (4)	C28—C29—C30	127.0 (4)
C7—C6—C18	113.7 (11)	C25—C29—Fe3	69.5 (2)
C5—C6—C18	121.0 (11)	C28—C29—Fe3	68.6 (2)
C7—C6—S1P	122.7 (4)	C30—C29—Fe3	127.0 (3)
C5—C6—S1P	111.9 (4)	C31—C30—C29	124.8 (3)
C6—C7—C8	127.1 (3)	C31—C30—C32	117.5 (3)
C6—C7—C18P	113.6 (13)	C29—C30—C32	117.7 (3)
C8—C7—C18P	119.2 (13)	C30—C31—C33	128.4 (3)
C6—C7—S1	120.3 (4)	C30—C31—S4	117.9 (3)
C8—C7—S1	112.6 (3)	C33—C31—S4	113.7 (3)
C9—C8—C12	107.1 (3)	O3—C32—C30	126.5 (4)
C9—C8—C7	127.7 (4)	O3—C32—S5	122.8 (3)
C12—C8—C7	125.1 (3)	C30—C32—S5	110.5 (3)
C9—C8—Fe2	68.8 (2)	C34—C33—C37	108.3 (4)
C12—C8—Fe2	69.1 (2)	C34—C33—C31	125.6 (4)
C7—C8—Fe2	125.9 (3)	C37—C33—C31	126.1 (4)
C10—C9—C8	109.1 (4)	C34—C33—Fe4	69.9 (2)
C10—C9—Fe2	70.3 (2)	C37—C33—Fe4	69.1 (2)
C8—C9—Fe2	70.4 (2)	C31—C33—Fe4	126.0 (3)
C10—C9—H9	125.5	C35—C34—C33	107.7 (4)
C8—C9—H9	125.5	C35—C34—Fe4	69.7 (3)
Fe2—C9—H9	125.5	C33—C34—Fe4	69.2 (2)
C9—C10—C11	107.8 (4)	C35—C34—H34	126.1
C9—C10—Fe2	69.5 (2)	C33—C34—H34	126.1

C11—C10—Fe2	69.5 (2)	Fe4—C34—H34	126.1
C9—C10—H10	126.1	C36—C35—C34	108.7 (4)
C11—C10—H10	126.1	C36—C35—Fe4	69.6 (3)
Fe2—C10—H10	126.1	C34—C35—Fe4	69.9 (2)
C12—C11—C10	108.2 (4)	C36—C35—H35	125.7
C12—C11—Fe2	69.8 (2)	C34—C35—H35	125.7
C10—C11—Fe2	69.6 (2)	Fe4—C35—H35	125.7
C12—C11—H11	125.9	C35—C36—C37	108.7 (4)
C10—C11—H11	125.9	C35—C36—Fe4	70.1 (3)
Fe2—C11—H11	125.9	C37—C36—Fe4	69.1 (2)
C11—C12—C8	107.8 (3)	C35—C36—H36	125.6
C11—C12—Fe2	69.6 (2)	C37—C36—H36	125.6
C8—C12—Fe2	69.9 (2)	Fe4—C36—H36	125.6
C11—C12—H12	126.1	C33—C37—C36	106.6 (5)
C8—C12—H12	126.1	C33—C37—Fe4	69.7 (2)
Fe2—C12—H12	126.1	C36—C37—Fe4	69.6 (3)
C14—C13—C17	107.6 (4)	C33—C37—H37	126.7
C14—C13—Fe2	69.9 (2)	C36—C37—H37	126.7
C17—C13—Fe2	69.1 (2)	Fe4—C37—H37	126.7
C14—C13—H13	126.2	C42—C38—C39	105.5 (5)
C17—C13—H13	126.2	C42—C38—Fe4	69.5 (2)
Fe2—C13—H13	126.2	C39—C38—Fe4	69.7 (3)
C13—C14—C15	108.0 (4)	C42—C38—H38	127.2
C13—C14—Fe2	69.6 (2)	C39—C38—H38	127.2
C15—C14—Fe2	69.9 (2)	Fe4—C38—H38	127.2
C13—C14—H14	126	C40—C39—C38	108.4 (5)
C15—C14—H14	126	C40—C39—Fe4	70.5 (3)
Fe2—C14—H14	126	C38—C39—Fe4	69.2 (3)
C16—C15—C14	108.4 (4)	C40—C39—H39	125.8
C16—C15—Fe2	69.8 (2)	C38—C39—H39	125.8
C14—C15—Fe2	69.6 (2)	Fe4—C39—H39	125.8
C16—C15—H15	125.8	C39—C40—C41	110.0 (5)
C14—C15—H15	125.8	C39—C40—Fe4	70.7 (3)
Fe2—C15—H15	125.8	C41—C40—Fe4	70.4 (3)
C15—C16—C17	108.5 (4)	C39—C40—H40	125
C15—C16—Fe2	70.2 (2)	C41—C40—H40	125
C17—C16—Fe2	69.2 (2)	Fe4—C40—H40	125
C15—C16—H16	125.8	C40—C41—C42	107.9 (5)
C17—C16—H16	125.8	C40—C41—Fe4	70.2 (3)
Fe2—C16—H16	125.8	C42—C41—Fe4	69.7 (3)
C16—C17—C13	107.5 (4)	C40—C41—H41	126.1
C16—C17—Fe2	70.1 (2)	C42—C41—H41	126.1
C13—C17—Fe2	69.8 (2)	Fe4—C41—H41	126.1
C16—C17—H17	126.2	C41—C42—C38	108.1 (4)
C13—C17—H17	126.2	C41—C42—Fe4	70.3 (3)
Fe2—C17—H17	126.2	C38—C42—Fe4	69.6 (2)
C24—C20—C21	108.8 (4)	C41—C42—H42	125.9
C24—C20—Fe1	70.3 (3)	C38—C42—H42	125.9

C21—C20—Fe1	70.1 (3)	Fe4—C42—H42	125.9
C24—C20—H20	125.6	C47—C43—C44	108.0 (4)
C21—C20—H20	125.6	C47—C43—Fe3	69.8 (2)
Fe1—C20—H20	125.6	C44—C43—Fe3	69.9 (2)
C22—C21—C20	107.4 (4)	C47—C43—H43	126
C22—C21—Fe1	69.6 (3)	C44—C43—H43	126
C20—C21—Fe1	69.5 (2)	Fe3—C43—H43	126
C22—C21—H21	126.3	C45—C44—C43	108.6 (4)
C20—C21—H21	126.3	C45—C44—Fe3	70.1 (2)
Fe1—C21—H21	126.3	C43—C44—Fe3	69.7 (2)
C21—C22—C23	108.3 (4)	C45—C44—H44	125.7
C21—C22—Fe1	70.3 (3)	C43—C44—H44	125.7
C23—C22—Fe1	69.4 (3)	Fe3—C44—H44	125.7
C21—C22—H22	125.9	C44—C45—C46	107.7 (4)
C23—C22—H22	125.9	C44—C45—Fe3	69.8 (2)
Fe1—C22—H22	125.9	C46—C45—Fe3	69.4 (2)
C22—C23—C24	107.9 (5)	C44—C45—H45	126.1
C22—C23—Fe1	70.0 (3)	C46—C45—H45	126.1
C24—C23—Fe1	70.3 (3)	Fe3—C45—H45	126.1
C22—C23—H23	126	C47—C46—C45	107.7 (4)
C24—C23—H23	126	C47—C46—Fe3	69.8 (2)
Fe1—C23—H23	126	C45—C46—Fe3	69.9 (2)
C20—C24—C23	107.5 (4)	C47—C46—H46	126.2
C20—C24—Fe1	69.8 (3)	C45—C46—H46	126.2
C23—C24—Fe1	69.2 (3)	Fe3—C46—H46	126.2
C20—C24—H24	126.2	C43—C47—C46	108.1 (4)
C23—C24—H24	126.2	C43—C47—Fe3	69.8 (2)
Fe1—C24—H24	126.2	C46—C47—Fe3	69.7 (2)
C23—Fe1—C4	161.96 (18)	C43—C47—H47	126
C23—Fe1—C1	107.29 (18)	C46—C47—H47	126
C4—Fe1—C1	69.13 (16)	Fe3—C47—H47	126
C23—Fe1—C22	40.5 (2)	C28—Fe3—C43	122.97 (17)
C4—Fe1—C22	156.2 (2)	C28—Fe3—C46	157.75 (18)
C1—Fe1—C22	123.4 (2)	C43—Fe3—C46	68.09 (17)
C23—Fe1—C3	156.13 (18)	C28—Fe3—C47	159.62 (17)
C4—Fe1—C3	40.58 (15)	C43—Fe3—C47	40.37 (17)
C1—Fe1—C3	68.53 (16)	C46—Fe3—C47	40.55 (17)
C22—Fe1—C3	120.75 (18)	C28—Fe3—C26	68.51 (18)
C23—Fe1—C20	67.58 (19)	C43—Fe3—C26	120.59 (18)
C4—Fe1—C20	108.75 (18)	C46—Fe3—C26	125.21 (19)
C1—Fe1—C20	158.06 (19)	C47—Fe3—C26	107.64 (18)
C22—Fe1—C20	67.5 (2)	C28—Fe3—C27	40.49 (16)
C3—Fe1—C20	124.96 (19)	C43—Fe3—C27	106.40 (16)
C23—Fe1—C2	121.21 (18)	C46—Fe3—C27	161.05 (19)
C4—Fe1—C2	68.31 (17)	C47—Fe3—C27	123.67 (18)
C1—Fe1—C2	40.58 (16)	C26—Fe3—C27	40.63 (17)
C22—Fe1—C2	106.97 (18)	C28—Fe3—C44	106.95 (18)
C3—Fe1—C2	40.39 (16)	C43—Fe3—C44	40.37 (18)

C20—Fe1—C2	160.6 (2)	C46—Fe3—C44	67.93 (17)
C23—Fe1—C24	40.51 (18)	C47—Fe3—C44	67.83 (18)
C4—Fe1—C24	125.38 (17)	C26—Fe3—C44	155.64 (18)
C1—Fe1—C24	122.32 (18)	C27—Fe3—C44	120.43 (17)
C22—Fe1—C24	67.92 (18)	C28—Fe3—C45	121.42 (18)
C3—Fe1—C24	161.50 (19)	C43—Fe3—C45	67.92 (17)
C20—Fe1—C24	39.94 (19)	C46—Fe3—C45	40.75 (18)
C2—Fe1—C24	157.27 (19)	C47—Fe3—C45	68.16 (17)
C23—Fe1—C21	67.9 (2)	C26—Fe3—C45	162.63 (19)
C4—Fe1—C21	121.7 (2)	C27—Fe3—C45	155.85 (19)
C1—Fe1—C21	159.5 (2)	C44—Fe3—C45	40.10 (17)
C22—Fe1—C21	40.1 (2)	C28—Fe3—C25	68.74 (17)
C3—Fe1—C21	107.40 (17)	C43—Fe3—C25	156.72 (19)
C20—Fe1—C21	40.42 (19)	C46—Fe3—C25	109.03 (17)
C2—Fe1—C21	123.47 (18)	C47—Fe3—C25	122.29 (18)
C24—Fe1—C21	67.80 (19)	C26—Fe3—C25	40.77 (16)
C23—Fe1—C5	124.66 (19)	C27—Fe3—C25	68.43 (16)
C4—Fe1—C5	41.20 (15)	C44—Fe3—C25	161.95 (18)
C1—Fe1—C5	40.99 (15)	C45—Fe3—C25	126.01 (17)
C22—Fe1—C5	160.8 (2)	C28—Fe3—C29	41.19 (15)
C3—Fe1—C5	68.55 (15)	C43—Fe3—C29	160.50 (18)
C20—Fe1—C5	123.00 (18)	C46—Fe3—C29	122.54 (16)
C2—Fe1—C5	68.33 (16)	C47—Fe3—C29	157.92 (17)
C24—Fe1—C5	108.79 (17)	C26—Fe3—C29	68.75 (16)
C21—Fe1—C5	158.0 (2)	C27—Fe3—C29	68.67 (15)
C9—Fe2—C17	117.78 (18)	C44—Fe3—C29	124.55 (18)
C9—Fe2—C11	68.25 (17)	C45—Fe3—C29	108.41 (16)
C17—Fe2—C11	169.18 (18)	C25—Fe3—C29	40.80 (16)
C9—Fe2—C10	40.19 (16)	C42—Fe4—C38	40.90 (19)
C17—Fe2—C10	149.26 (18)	C42—Fe4—C37	119.2 (2)
C11—Fe2—C10	40.96 (16)	C38—Fe4—C37	155.9 (2)
C9—Fe2—C12	68.65 (15)	C42—Fe4—C40	66.7 (2)
C17—Fe2—C12	131.11 (17)	C38—Fe4—C40	67.4 (2)
C11—Fe2—C12	40.59 (16)	C37—Fe4—C40	123.1 (3)
C10—Fe2—C12	68.69 (16)	C42—Fe4—C39	67.71 (19)
C9—Fe2—C13	152.24 (18)	C38—Fe4—C39	41.1 (2)
C17—Fe2—C13	41.14 (17)	C37—Fe4—C39	159.4 (2)
C11—Fe2—C13	129.68 (18)	C40—Fe4—C39	38.8 (2)
C10—Fe2—C13	167.12 (18)	C42—Fe4—C41	40.0 (2)
C12—Fe2—C13	109.75 (16)	C38—Fe4—C41	68.0 (2)
C9—Fe2—C16	107.79 (17)	C37—Fe4—C41	105.4 (2)
C17—Fe2—C16	40.63 (18)	C40—Fe4—C41	39.4 (2)
C11—Fe2—C16	148.70 (19)	C39—Fe4—C41	66.5 (2)
C10—Fe2—C16	115.62 (18)	C42—Fe4—C36	153.7 (2)
C12—Fe2—C16	169.28 (18)	C38—Fe4—C36	162.5 (2)
C13—Fe2—C16	68.36 (18)	C37—Fe4—C36	41.31 (19)
C9—Fe2—C14	165.74 (17)	C40—Fe4—C36	106.6 (2)
C17—Fe2—C14	68.49 (19)	C39—Fe4—C36	124.1 (2)

C11—Fe2—C14	107.91 (19)	C41—Fe4—C36	118.5 (2)
C10—Fe2—C14	128.07 (18)	C42—Fe4—C33	108.87 (16)
C12—Fe2—C14	118.05 (17)	C38—Fe4—C33	122.4 (2)
C13—Fe2—C14	40.43 (18)	C37—Fe4—C33	41.23 (17)
C16—Fe2—C14	67.89 (18)	C40—Fe4—C33	161.0 (3)
C9—Fe2—C15	127.67 (17)	C39—Fe4—C33	158.8 (3)
C17—Fe2—C15	68.02 (19)	C41—Fe4—C33	125.3 (2)
C11—Fe2—C15	116.4 (2)	C36—Fe4—C33	68.66 (16)
C10—Fe2—C15	106.58 (18)	C42—Fe4—C35	165.2 (2)
C12—Fe2—C15	150.17 (19)	C38—Fe4—C35	127.3 (2)
C13—Fe2—C15	68.03 (18)	C37—Fe4—C35	69.0 (2)
C16—Fe2—C15	39.95 (18)	C40—Fe4—C35	120.7 (2)
C14—Fe2—C15	40.48 (17)	C39—Fe4—C35	109.2 (2)
C9—Fe2—C8	40.77 (15)	C41—Fe4—C35	153.5 (2)
C17—Fe2—C8	109.65 (17)	C36—Fe4—C35	40.3 (2)
C11—Fe2—C8	68.42 (17)	C33—Fe4—C35	68.42 (17)
C10—Fe2—C8	68.34 (16)	C42—Fe4—C34	128.16 (18)
C12—Fe2—C8	40.94 (15)	C38—Fe4—C34	110.24 (19)
C13—Fe2—C8	119.47 (16)	C37—Fe4—C34	69.3 (2)
C16—Fe2—C8	129.93 (18)	C40—Fe4—C34	156.2 (2)
C14—Fe2—C8	152.11 (16)	C39—Fe4—C34	123.5 (2)
C15—Fe2—C8	166.75 (17)	C41—Fe4—C34	163.8 (2)
C18—S2—S1	97.4 (7)	C36—Fe4—C34	68.2 (2)
C18P—S2—S1P	96.4 (7)	C33—Fe4—C34	40.94 (17)
O1—C18—C6	126 (2)	C35—Fe4—C34	40.41 (17)
O1—C18—S2	121.1 (17)	C31—S4—S5	96.09 (13)
C6—C18—S2	112.8 (15)	C32—S5—S4	97.94 (13)
C7—S1—S2	95.5 (3)		

C5—C1—C2—C3	1.2 (4)	C6—C7—C18P—O1P	167 (2)
Fe1—C1—C2—C3	−58.8 (3)	C8—C7—C18P—O1P	−14 (3)
C5—C1—C2—Fe1	60.0 (3)	C6—C7—C18P—S2	−1.1 (19)
C1—C2—C3—C4	−0.4 (4)	C8—C7—C18P—S2	178.3 (8)
Fe1—C2—C3—C4	−59.1 (3)	S1P—S2—C18P—O1P	−168 (2)
C1—C2—C3—Fe1	58.7 (3)	S1P—S2—C18P—C7	0.6 (18)
C2—C3—C4—C5	−0.5 (4)	C7—C6—S1P—S2	−0.7 (6)
Fe1—C3—C4—C5	−59.9 (3)	C5—C6—S1P—S2	176.6 (3)
C2—C3—C4—Fe1	59.3 (3)	C29—C25—C26—C27	0.5 (4)
C2—C1—C5—C4	−1.5 (4)	Fe3—C25—C26—C27	59.5 (3)
Fe1—C1—C5—C4	58.5 (3)	C29—C25—C26—Fe3	−59.0 (3)
C2—C1—C5—C6	177.1 (4)	C25—C26—C27—C28	−1.0 (4)
Fe1—C1—C5—C6	−122.9 (4)	Fe3—C26—C27—C28	58.7 (3)
C2—C1—C5—Fe1	−60.0 (3)	C25—C26—C27—Fe3	−59.7 (3)
C3—C4—C5—C1	1.2 (4)	C26—C27—C28—C29	1.1 (4)
Fe1—C4—C5—C1	−58.5 (3)	Fe3—C27—C28—C29	60.0 (2)
C3—C4—C5—C6	−177.4 (3)	C26—C27—C28—Fe3	−58.9 (3)
Fe1—C4—C5—C6	122.8 (4)	C26—C25—C29—C28	0.2 (4)
C3—C4—C5—Fe1	59.8 (3)	Fe3—C25—C29—C28	−58.6 (2)

C1—C5—C6—C7	−140.5 (4)	C26—C25—C29—C30	−179.8 (3)
C4—C5—C6—C7	37.8 (6)	Fe3—C25—C29—C30	121.5 (4)
Fe1—C5—C6—C7	128.5 (4)	C26—C25—C29—Fe3	58.7 (3)
C1—C5—C6—C18	39.5 (12)	C27—C28—C29—C25	−0.8 (4)
C4—C5—C6—C18	−142.1 (11)	Fe3—C28—C29—C25	59.2 (2)
Fe1—C5—C6—C18	−51.4 (12)	C27—C28—C29—C30	179.2 (3)
C1—C5—C6—S1P	42.3 (6)	Fe3—C28—C29—C30	−120.9 (4)
C4—C5—C6—S1P	−139.4 (5)	C27—C28—C29—Fe3	−59.9 (3)
Fe1—C5—C6—S1P	−48.7 (5)	C25—C29—C30—C31	144.0 (4)
C5—C6—C7—C8	4.9 (7)	C28—C29—C30—C31	−35.9 (6)
C18—C6—C7—C8	−175.1 (11)	Fe3—C29—C30—C31	−125.7 (4)
S1P—C6—C7—C8	−178.1 (5)	C25—C29—C30—C32	−37.9 (5)
C5—C6—C7—C18P	−175.6 (13)	C28—C29—C30—C32	142.2 (4)
S1P—C6—C7—C18P	1.3 (13)	Fe3—C29—C30—C32	52.5 (5)
C5—C6—C7—S1	−175.6 (4)	C29—C30—C31—C33	−4.8 (6)
C18—C6—C7—S1	4.3 (11)	C32—C30—C31—C33	177.0 (4)
C6—C7—C8—C9	33.9 (6)	C29—C30—C31—S4	175.4 (3)
C18P—C7—C8—C9	−145.5 (13)	C32—C30—C31—S4	−2.8 (5)
S1—C7—C8—C9	−145.6 (4)	C31—C30—C32—O3	−169.7 (4)
C6—C7—C8—C12	−147.9 (4)	C29—C30—C32—O3	12.0 (6)
C18P—C7—C8—C12	32.7 (14)	C31—C30—C32—S5	4.4 (4)
S1—C7—C8—C12	32.6 (5)	C29—C30—C32—S5	−173.9 (3)
C6—C7—C8—Fe2	123.7 (4)	C30—C31—C33—C34	147.4 (4)
C18P—C7—C8—Fe2	−55.7 (14)	S4—C31—C33—C34	−32.8 (5)
S1—C7—C8—Fe2	−55.8 (4)	C30—C31—C33—C37	−33.7 (6)
C12—C8—C9—C10	1.1 (4)	S4—C31—C33—C37	146.1 (4)
C7—C8—C9—C10	179.6 (3)	C30—C31—C33—Fe4	−122.7 (4)
Fe2—C8—C9—C10	59.8 (3)	S4—C31—C33—Fe4	57.1 (4)
C12—C8—C9—Fe2	−58.7 (2)	C37—C33—C34—C35	0.7 (5)
C7—C8—C9—Fe2	119.7 (4)	C31—C33—C34—C35	179.7 (4)
C8—C9—C10—C11	−0.8 (4)	Fe4—C33—C34—C35	59.2 (3)
Fe2—C9—C10—C11	59.2 (3)	C37—C33—C34—Fe4	−58.6 (3)
C8—C9—C10—Fe2	−59.9 (3)	C31—C33—C34—Fe4	120.5 (4)
C9—C10—C11—C12	0.1 (4)	C33—C34—C35—C36	0.0 (5)
Fe2—C10—C11—C12	59.3 (3)	Fe4—C34—C35—C36	58.9 (3)
C9—C10—C11—Fe2	−59.2 (3)	C33—C34—C35—Fe4	−58.9 (3)
C10—C11—C12—C8	0.6 (4)	C34—C35—C36—C37	−0.7 (5)
Fe2—C11—C12—C8	59.7 (3)	Fe4—C35—C36—C37	58.4 (3)
C10—C11—C12—Fe2	−59.2 (3)	C34—C35—C36—Fe4	−59.2 (3)
C9—C8—C12—C11	−1.0 (4)	C34—C33—C37—C36	−1.1 (5)
C7—C8—C12—C11	−179.5 (3)	C31—C33—C37—C36	179.9 (4)
Fe2—C8—C12—C11	−59.6 (3)	Fe4—C33—C37—C36	−60.1 (3)
C9—C8—C12—Fe2	58.5 (2)	C34—C33—C37—Fe4	59.1 (3)
C7—C8—C12—Fe2	−120.0 (4)	C31—C33—C37—Fe4	−120.0 (4)
C17—C13—C14—C15	0.6 (5)	C35—C36—C37—C33	1.1 (5)
Fe2—C13—C14—C15	59.6 (3)	Fe4—C36—C37—C33	60.2 (3)
C17—C13—C14—Fe2	−59.0 (3)	C35—C36—C37—Fe4	−59.1 (3)
C13—C14—C15—C16	−0.2 (5)	C42—C38—C39—C40	0.8 (5)

Fe2—C14—C15—C16	59.2 (3)	Fe4—C38—C39—C40	−59.9 (4)
C13—C14—C15—Fe2	−59.4 (3)	C42—C38—C39—Fe4	60.6 (3)
C14—C15—C16—C17	−0.2 (5)	C38—C39—C40—C41	−0.5 (6)
Fe2—C15—C16—C17	58.8 (3)	Fe4—C39—C40—C41	−59.5 (4)
C14—C15—C16—Fe2	−59.1 (3)	C38—C39—C40—Fe4	59.1 (3)
C15—C16—C17—C13	0.6 (4)	C39—C40—C41—C42	0.0 (6)
Fe2—C16—C17—C13	60.1 (3)	Fe4—C40—C41—C42	−59.7 (3)
C15—C16—C17—Fe2	−59.5 (3)	C39—C40—C41—Fe4	59.7 (4)
C14—C13—C17—C16	−0.7 (4)	C40—C41—C42—C38	0.5 (5)
Fe2—C13—C17—C16	−60.3 (3)	Fe4—C41—C42—C38	−59.5 (3)
C14—C13—C17—Fe2	59.6 (3)	C40—C41—C42—Fe4	60.1 (4)
C24—C20—C21—C22	0.3 (5)	C39—C38—C42—C41	−0.8 (5)
Fe1—C20—C21—C22	−59.6 (3)	Fe4—C38—C42—C41	60.0 (3)
C24—C20—C21—Fe1	59.8 (3)	C39—C38—C42—Fe4	−60.8 (3)
C20—C21—C22—C23	0.2 (5)	C47—C43—C44—C45	0.3 (4)
Fe1—C21—C22—C23	−59.3 (3)	Fe3—C43—C44—C45	−59.5 (3)
C20—C21—C22—Fe1	59.5 (3)	C47—C43—C44—Fe3	59.7 (3)
C21—C22—C23—C24	−0.5 (5)	C43—C44—C45—C46	0.0 (4)
Fe1—C22—C23—C24	−60.4 (3)	Fe3—C44—C45—C46	−59.3 (3)
C21—C22—C23—Fe1	59.8 (3)	C43—C44—C45—Fe3	59.2 (3)
C21—C20—C24—C23	−0.6 (5)	C44—C45—C46—C47	−0.2 (4)
Fe1—C20—C24—C23	59.1 (3)	Fe3—C45—C46—C47	−59.8 (3)
C21—C20—C24—Fe1	−59.7 (3)	C44—C45—C46—Fe3	59.5 (3)
C22—C23—C24—C20	0.7 (5)	C44—C43—C47—C46	−0.4 (4)
Fe1—C23—C24—C20	−59.5 (3)	Fe3—C43—C47—C46	59.4 (3)
C22—C23—C24—Fe1	60.2 (3)	C44—C43—C47—Fe3	−59.8 (3)
C7—C6—C18—O1	170.8 (17)	C45—C46—C47—C43	0.4 (4)
C5—C6—C18—O1	−9 (3)	Fe3—C46—C47—C43	−59.4 (3)
C7—C6—C18—S2	−5.7 (16)	C45—C46—C47—Fe3	59.8 (3)
C5—C6—C18—S2	174.2 (7)	C30—C31—S4—S5	0.0 (3)
S1—S2—C18—O1	−172.3 (17)	C33—C31—S4—S5	−179.8 (3)
S1—S2—C18—C6	4.4 (15)	O3—C32—S5—S4	170.7 (3)
C6—C7—S1—S2	−1.0 (4)	C30—C32—S5—S4	−3.7 (3)
C8—C7—S1—S2	178.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C36S—H36···O3^{i}	1.00	2.36	3.354 (6)	170

Symmetry code: (i) *x*+1, *y*, *z*.