STRUCTURAL CHEMISTRY

Volume 77 (2021)

Supporting information for article:

Iron(II)–alkoxide and –aryloxide complexes of a tris(thio-ether)borate ligand: synthesis, molecular structures, and implications on the origin of instability of their iron(II)–catecholate counterpart

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Refinement details:

In compound (3), the aryloxy oxygen atom was found disordered in two positions with a refined site occupancy of 68/32. Geometrical and rigid bond anisotropic displacement restraints were applied to the Fe - O - C_{ipso} moieties. In compound (4), the molecule is located on an inversion centre with a symmetry-unique toluene molecule of solvation disordered in two positions with a 62/38 refined site occupancy ratio. The disordered toluene molecule was treated to idealized phenyl geometry constraints, methyl and C4 equal atomic displacement constraints, methyl geometry restraints and rigid bond anisotropic displacement restraints. In compound (5), the molecule is located on an inversion centre with one *tert*-butyl thioether disordered in two positions with a refined site occupancy ration of 94/6. Equal atomic displacement constraints were applied to the pairs of chemically equivalent atoms. Atoms coincident to both disordered contributions, C1 and C1a, and, C2 and C2a, were constrained to have the same positions. Distances were restrained to be similar between chemically equivalent atoms in the disordered contributions. Chemically equivalent atom pairs between the disordered contributions were constrained with equal atomic displacement parameters.

Preparation and Crystallization of compound (5)

At 45°C, metathesis of [PhTt^{tBu}]CoCl (100 mg, 0.203 mmol) with potassium monoanionic catecholate [0.264 mmol, prepared in situ from the reaction of catechol (29 mg, 0.264 mmol) with potassium hydride (11 mg, 0.264 mmol)] yielded a light green powder. Single crystals suitable for X-ray crystallography were obtained by slow evaporation of a concentrated pentane/diethyl ether solution. ^{1}H NMR (C_6D_6): δ 72.9 (4H, s), 56.3 (2H, s), 15.9 (18H, s), 5.2 (2H, s), −22.5 (2H, s), −33.6 (36H, s).

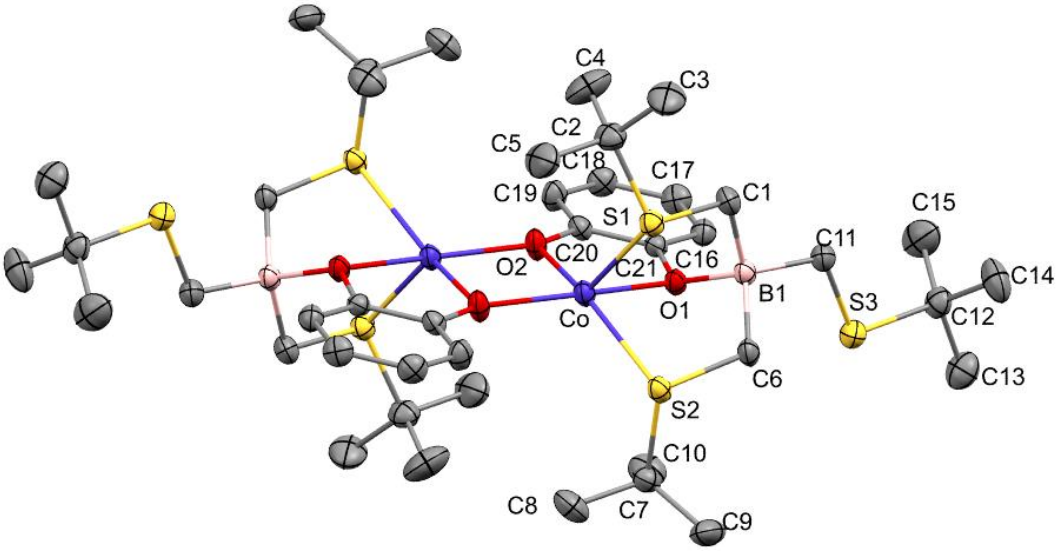

Figure S1 Solid state structure of (5), depicted with 30% probability displacement ellipsoids. Hydrogen atoms and a disordered *tert*-butyl group have been omitted for clarity.

Compound (5), bis[(benzene-1,2-dioxo-κ^1-O1, κ^2-μ_2-O2)-tris(*tert*-butylthiomethyl)borato-κ^1-S,S')]cobalt(II)]

Table S1 Crystal data.

CCDC	2063938
Empirical formula	$C_{42}H_{74}B_2Co_2O_4S_6$
Formula weight	974.85
Temperature/K	200.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	14.409(4)
b/Å	9.494(2)
c/Å	18.745(5)
α/°	90
β/°	90.938(4)
γ/°	90
Volume/Å^3	2564.0(11)
Z	2
ρ_{calc}g/cm^3	1.263
μ/mm^{-1}	0.927
F(000)	1036.0
Crystal size/mm^3	0.14 × 0.091 × 0.076
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.538 to 53.674
Index ranges	$-18 \le h \le 18$, $-12 \le k \le 12$, $-23 \le l \le 23$
Reflections collected	28200

Independent reflections	5489 [R_{int} = 0.0887, R_{sigma} = 0.0704]
Data/restraints/parameters	5489/35/272
Goodness-of-fit on F^2	1.008
Final R indexes [I>=2σ (I)]	R_1 = 0.0466, wR_2 = 0.0923
Final R indexes [all data]	R_1 = 0.0984, wR_2 = 0.1118
Largest diff. peak/hole / e Å^{-3}	0.41/-0.35

Table S2 Fractional atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2×10^3). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Co	10644.6(3)	5293.6(5)	10645.1(2)	35.13(14)
S2	8568.9(6)	2891.4(9)	8691.0(4)	36.5(2)
S3	5720.8(6)	5496.7(10)	8830.8(5)	47.8(3)
O1	8014.3(15)	5617(2)	9377.0(11)	35.8(5)
O2	9482.0(16)	5961(2)	10199.5(11)	43.5(6)
C6	7613(2)	3999(4)	8363.1(17)	39.2(8)
C7	8054(3)	1546(4)	9274.2(18)	44.3(9)
C8	8882(3)	695(4)	9543(2)	62.8(12)
C9	7394(3)	625(4)	8830(2)	73.2(14)
C10	7552(3)	2221(5)	9891(2)	64.9(12)
C11	6676(2)	6425(4)	8437.2(18)	41.9(9)
C12	4684(2)	6589(4)	8648(2)	49.6(10)
C13	3900(3)	5721(5)	8960(2)	68.4(13)
C14	4544(3)	6803(6)	7859(2)	78.6(15)
C15	4769(3)	7994(5)	9029(3)	85.5(16)
C16	7138(2)	7332(4)	10072.0(17)	40.1(8)
C17	7125(3)	8231(4)	10658.2(18)	46.0(9)
C18	7900(3)	8372(4)	11097.8(19)	47.2(9)
C19	8698(3)	7633(4)	10948.3(18)	45.6(9)
C20	8724(2)	6743(3)	10365.8(16)	35.3(8)
C21	7940(2)	6599(3)	9916.3(16)	32.2(7)
B1	7668(3)	5674(4)	8587.3(19)	34.5(9)
S1	9527.5(6)	5582.9(10)	8159.2(5)	37.6(3)
C1	8446(2)	6582(4)	8160.5(18)	44.0(9)
C2	10490(3)	6799(4)	7989(2)	51.4(10)
C3	10388(3)	7331(6)	7226(2)	82.2(17)
C4	10496(4)	8009(5)	8515(3)	91.0(18)
C5	11365(3)	5909(5)	8076(3)	86.2(17)
S1A	9497(8)	6792(15)	8660(6)	37.6(3)
C1A	8446(2)	6582(4)	8160.5(18)	44.0(9)
C2A	10490(3)	6799(4)	7989(2)	51.4(10)

C3A	10340(30)	8140(40)	7560(20)	82.2(17)
C4A	10320(30)	5490(40)	7540(20)	91.0(18)
C5A	11358(11)	6760(70)	8417(16)	86.2(17)

Table S3 Anisotropic displacement parameters ($Å^2×10^3$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Co	38.0(3)	35.0(3)	32.1(2)	-0.9(2)	-9.5(2)	4.8(2)
S2	43.4(5)	33.8(5)	32.2(4)	-2.3(4)	-4.6(4)	5.2(4)
S3	40.2(5)	49.0(6)	53.8(6)	5.7(5)	-5.5(4)	-2.3(5)
O1	39.9(13)	33.5(13)	33.6(12)	-4.4(10)	-10.7(10)	4.3(10)
O2	44.7(15)	46.5(15)	38.7(13)	-9.1(11)	-16.1(11)	14.1(12)
C6	41(2)	41(2)	35.7(19)	0.8(15)	-11.9(16)	4.6(16)
C7	56(2)	37(2)	39(2)	1.9(16)	-1.0(18)	-0.8(18)
C8	83(3)	50(3)	55(3)	13(2)	4(2)	19(2)
C9	98(4)	50(3)	71(3)	8(2)	-19(3)	-28(3)
C10	70(3)	69(3)	57(3)	9(2)	20(2)	4(2)
C11	40(2)	43(2)	42(2)	2.0(17)	-6.6(16)	1.6(17)
C12	36(2)	55(3)	58(2)	-3(2)	1.1(19)	3.1(19)
C13	51(3)	85(3)	69(3)	-9(3)	9(2)	-3(2)
C14	56(3)	109(4)	71(3)	21(3)	-2(2)	29(3)
C15	61(3)	67(3)	129(4)	-19(3)	6(3)	13(3)
C16	37(2)	45(2)	39.0(19)	1.6(16)	-1.8(16)	-0.3(17)
C17	43(2)	50(2)	45(2)	-5.8(18)	10.8(18)	6.3(18)
C18	56(3)	46(2)	40(2)	-9.2(17)	2.2(19)	3.0(19)
C19	49(2)	48(2)	39(2)	-9.3(17)	-10.4(18)	3.8(18)
C20	40(2)	34.7(19)	30.8(17)	3.4(15)	-3.1(15)	5.2(16)
C21	37(2)	28.4(18)	30.8(17)	1.6(14)	-1.0(15)	-0.1(15)
B1	39(2)	34(2)	30(2)	-2.2(16)	-9.2(17)	3.0(18)
S1	39.6(5)	39.5(6)	33.7(5)	0.5(4)	-1.9(4)	0.9(4)
C1	44(2)	44(2)	44(2)	7.9(17)	-8.4(17)	5.2(17)
C2	48(2)	50(2)	56(2)	6.7(19)	8.6(19)	-4.0(19)
C3	79(4)	98(4)	69(3)	35(3)	8(3)	-27(3)
C4	86(4)	84(4)	103(4)	-28(3)	13(3)	-42(3)
C5	44(3)	81(4)	133(5)	20(4)	1(3)	-2(3)
S1A	39.6(5)	39.5(6)	33.7(5)	0.5(4)	-1.9(4)	0.9(4)
C1A	44(2)	44(2)	44(2)	7.9(17)	-8.4(17)	5.2(17)
C2A	48(2)	50(2)	56(2)	6.7(19)	8.6(19)	-4.0(19)
C3A	79(4)	98(4)	69(3)	35(3)	8(3)	-27(3)
C4A	86(4)	84(4)	103(4)	-28(3)	13(3)	-42(3)
C5A	44(3)	81(4)	133(5)	20(4)	1(3)	-2(3)

Table S4 Bond lengths.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co	S2[1]	2.3993(10)	C12	C15	1.517(6)
Co	O1[1]	2.118(2)	C16	C17	1.392(5)
Co	O2[1]	1.987(2)	C16	C21	1.383(4)
Co	O2	1.965(2)	C17	C18	1.384(5)
Co	S1[1]	2.4075(11)	C18	C19	1.379(5)
Co	S1A[1]	2.381(14)	C19	C20	1.382(4)
S2	C6	1.831(3)	C20	C21	1.405(4)
S2	C7	1.845(4)	B1	C1	1.634(5)
S3	C11	1.803(4)	B1	C1A	1.634(5)
S3	C12	1.846(4)	S1	C1	1.824(3)
O1	C21	1.381(4)	S1	C2	1.836(4)
O1	B1	1.555(4)	C2	C3	1.523(5)
O2	C20	1.361(4)	C2	C4	1.513(6)
C6	B1	1.646(5)	C2	C5	1.524(5)
C7	C8	1.520(5)	S1A	C1A	1.778(12)
C7	C9	1.529(5)	S1A	C2A	1.920(12)
C7	C10	1.516(5)	C2A	C3A	1.514(17)
C11	B1	1.618(5)	C2A	C4A	1.517(17)
C12	C13	1.522(5)	C2A	C5A	1.475(17)
C12	C14	1.504(5)			

[1]2-X,1-Y,2-Z

Table S5 Bond angles.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
S2[1]	Co	S1[1]	79.65(4)	C21	C16	C17	119.8(3)
O1[1]	Co	S2[1]	83.10(6)	C18	C17	C16	120.5(3)
O1[1]	Co	S1[1]	89.14(6)	C19	C18	C17	119.8(3)
O1[1]	Co	S1A[1]	76.0(3)	C18	C19	C20	120.3(3)
O2	Co	S2[1]	112.40(7)	O2	C20	C19	123.2(3)
O2[1]	Co	S2[1]	151.66(8)	O2	C20	C21	116.7(3)

O2	Co	O1[1]	153.55(9)	C19	C20	C21	120.1(3)
O2[1]	Co	O1[1]	79.15(8)	O1	C21	C16	124.7(3)
O2	Co	O2[1]	77.77(10)	O1	C21	C20	115.7(3)
O2[1]	Co	S1[1]	121.67(8)	C16	C21	C20	119.4(3)
O2	Co	S1[1]	114.03(8)	O1	B1	C6	102.9(2)
O2[1]	Co	S1A[1]	86.0(3)	O1	B1	C11	116.7(3)
O2	Co	S1A[1]	114.9(3)	O1	B1	C1	105.8(3)
C6	S2	Co[1]	96.20(11)	O1	B1	C1A	105.8(3)
C6	S2	C7	106.78(17)	C11	B1	C6	110.0(3)
C7	S2	Co[1]	112.41(11)	C11	B1	C1	107.1(3)
C11	S3	C12	105.71(17)	C11	B1	C1A	107.1(3)
C21	O1	Co[1]	111.84(18)	C1	B1	C6	114.6(3)
C21	O1	B1	130.2(2)	C1A	B1	C6	114.6(3)
B1	O1	Co[1]	105.92(18)	C1	S1	Co[1]	94.45(11)
Co	O2	Co[1]	102.23(10)	C1	S1	C2	108.69(18)
C20	O2	Co	139.5(2)	C2	S1	Co[1]	117.94(13)
C20	O2	Co[1]	116.49(19)	B1	C1	S1	108.6(2)
B1	C6	S2	115.8(2)	C3	C2	S1	108.1(3)
C8	C7	S2	104.1(3)	C3	C2	C5	110.6(4)
C8	C7	C9	110.8(3)	C4	C2	S1	111.1(3)
C9	C7	S2	109.0(3)	C4	C2	C3	111.1(4)
C10	C7	S2	111.1(3)	C4	C2	C5	110.8(4)
C10	C7	C8	110.7(3)	C5	C2	S1	105.0(3)
C10	C7	C9	111.0(3)	C1A	S1A	C2A	107.0(6)
B1	C11	S3	113.1(2)	B1	C1A	S1A	112.7(5)
C13	C12	S3	103.2(3)	C3A	C2A	S1A	104.2(11)
C14	C12	S3	110.7(3)	C3A	C2A	C4A	111.7(13)
C14	C12	C13	111.2(3)	C4A	C2A	S1A	104.1(11)
C14	C12	C15	110.7(4)	C5A	C2A	S1A	106.2(12)
C15	C12	S3	110.3(3)	C5A	C2A	C3A	114.9(14)
C15	C12	C13	110.5(3)	C5A	C2A	C4A	114.3(13)

[1]2-X,1-Y,2-Z

Table S6 Torsion angles.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
Co[1]	S2	C6	B1	2.7(3)	C6	S2	C7	C9	63.3(3)
Co[1]	S2	C7	C8	-74.2(2)	C6	S2	C7	C10	-59.3(3)
Co[1]	S2	C7	C9	167.6(2)	C6	B1	C1	S1	-46.1(3)
Co[1]	S2	C7	C10	45.0(3)	C6	B1	C1A	S1A	-98.2(6)

Co[1]	O1	C21	C16	-178.0(3)	C7	S2	C6	B1	118.4(3)
Co[1]	O1	C21	C20	-3.8(3)	C11	S3	C12	C13	177.4(2)
Co[1]	O1	B1	C6	63.4(3)	C11	S3	C12	C14	58.3(3)
Co[1]	O1	B1	C11	-176.0(2)	C11	S3	C12	C15	-64.5(3)
Co[1]	O1	B1	C1	-57.1(3)	C11	B1	C1	S1	-168.4(2)
Co[1]	O1	B1	C1A	-57.1(3)	C11	B1	C1A	S1A	139.5(5)
Co	O2	C20	C19	16.7(5)	C12	S3	C11	B1	176.2(2)
Co[1]	O2	C20	C19	178.2(3)	C16	C17	C18	C19	1.0(6)
Co	O2	C20	C21	-162.5(2)	C17	C16	C21	O1	175.8(3)
Co[1]	O2	C20	C21	-1.1(4)	C17	C16	C21	C20	1.8(5)
Co[1]	S1	C1	B1	-38.0(2)	C17	C18	C19	C20	-0.6(6)
Co[1]	S1	C2	C3	-173.6(3)	C18	C19	C20	O2	-178.4(3)
Co[1]	S1	C2	C4	-51.5(3)	C18	C19	C20	C21	0.8(5)
Co[1]	S1	C2	C5	68.4(3)	C19	C20	C21	O1	-175.9(3)
Co[1]	S1A	C1A	B1	26.9(6)	C19	C20	C21	C16	-1.4(5)
S2	C6	B1	O1	-40.8(3)	C21	O1	B1	C6	-158.2(3)
S2	C6	B1	C11	-165.8(2)	C21	O1	B1	C11	-37.7(5)
S2	C6	B1	C1	73.5(3)	C21	O1	B1	C1	81.3(4)
S2	C6	B1	C1A	73.5(3)	C21	O1	B1	C1A	81.3(4)
S3	C11	B1	O1	-65.0(3)	C21	C16	C17	C18	-1.6(5)
S3	C11	B1	C6	51.7(3)	B1	O1	C21	C16	45.5(5)
S3	C11	B1	C1	176.7(2)	B1	O1	C21	C20	-140.3(3)
S3	C11	B1	C1A	176.7(2)	C1	S1	C2	C3	-67.8(3)
O1	B1	C1	S1	66.4(3)	C1	S1	C2	C4	54.3(4)
O1	B1	C1A	S1A	14.4(6)	C1	S1	C2	C5	174.1(3)
O2	C20	C21	O1	3.3(4)	C2	S1	C1	B1	-159.4(2)
O2	C20	C21	C16	177.9(3)	C2A	S1A	C1A	B1	146.3(5)
C6	S2	C7	C8	-178.4(2)					

[1]2-X,1-Y,2-Z

Table S7 Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3).

Atom	*x*	*y*	*z*	U(eq)
H6A	7588.2	3935.87	7836	47
H6B	7024.01	3607.64	8542.46	47
H8A	8667.51	-54.17	9860.04	94
H8B	9310.86	1314.4	9805.85	94
H8C	9200.92	277	9136.91	94
H9A	7150	-132.27	9128.86	110
H9B	7729.66	215.5	8429.49	110
H9C	6878.2	1200.43	8646.29	110
H10A	7308.24	1485.44	10202.98	97
H10B	7037.82	2797.89	9705.85	97

H10C	7985.63	2817.88	10162.9	97
H11A	6567.19	6490.77	7915.48	50
H11B	6697.47	7395.7	8629.86	50
H13A	3308.92	6211.99	8880.99	103
H13B	4010.76	5594.46	9472.98	103
H13C	3876.06	4798.52	8725.88	103
H14A	3952.12	7285.95	7769.65	118
H14B	4535.44	5886.13	7618.32	118
H14C	5052.25	7374.96	7674.2	118
H15A	4187.28	8519.97	8971.05	128
H15B	5278.31	8536.5	8824.54	128
H15C	4895.99	7833.32	9537.84	128
H16	6598.35	7221.9	9779.5	48
H17	6578.99	8752.01	10757.24	55
H18	7882.62	8975.31	11501.61	57
H19	9232.1	7737.33	11247.32	55
H1A	8546.21	7502.32	8397.9	53
H1B	8230.44	6757.77	7664.28	53
H3A	10385.77	6529.33	6896.57	123
H3B	9803.26	7851.43	7172.1	123
H3C	10908.36	7955.38	7117.25	123
H4A	10561.91	7639.14	9001.4	137
H4B	11017.03	8637.37	8414.78	137
H4C	9911.93	8533.42	8469.63	137
H5A	11347.05	5133.42	7731.68	129
H5B	11911.59	6496.3	7991.96	129
H5C	11398.42	5526.24	8561.61	129
H1AA	8189.16	7523.31	8044.87	53
H1AB	8582.49	6101.81	7705.24	53
H3AA	9748.33	8070.73	7296.02	123
H3AB	10319.09	8943.82	7887.06	123
H3AC	10847.2	8257.12	7228.01	123
H4AA	9731.22	5597.06	7272.97	137
H4AB	10827.13	5374.08	7204.97	137
H4AC	10284.12	4666.54	7851.03	137
H5AA	11400.38	5866.31	8674.34	129
H5AB	11889.39	6855.62	8100.38	129
H5AC	11361.28	7542.32	8759.44	129

Table S8 Atomic occupancy.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
S1	0.9417(16)	C1	0.9417(16)	H1A	0.9417(16)
H1B	0.9417(16)	C2	0.9417(16)	C3	0.9417(16)

H3A	0.9417(16)	H3B	0.9417(16)	H3C	0.9417(16)
C4	0.9417(16)	H4A	0.9417(16)	H4B	0.9417(16)
H4C	0.9417(16)	C5	0.9417(16)	H5A	0.9417(16)
H5B	0.9417(16)	H5C	0.9417(16)	S1A	0.0583(16)
C1A	0.0583(16)	H1AA	0.0583(16)	H1AB	0.0583(16)
C2A	0.0583(16)	C3A	0.0583(16)	H3AA	0.0583(16)
H3AB	0.0583(16)	H3AC	0.0583(16)	C4A	0.0583(16)
H4AA	0.0583(16)	H4AB	0.0583(16)	H4AC	0.0583(16)
C5A	0.0583(16)	H5AA	0.0583(16)	H5AB	0.0583(16)
H5AC	0.0583(16)				

Compound (2), (triphenylmethoxo)(phenyltris(*tert*-butylthiomethyl)borato-S,S',S")iron(II)

Table S9 Crystal data.

CCDC	2063936
Empirical formula	$C_{40}H_{53}BFeOS_3$
Formula weight	712.66
Temperature/K	200.15
Crystal system	triclinic
Space group	P-1
a/Å	10.6835(15)
b/Å	12.8042(18)
c/Å	15.795(2)
α/°	77.614(3)
β/°	75.849(3)
γ/°	70.332(3)
Volume/Å^3	1952.1(5)
Z	2
ρ_{calc}g/cm^3	1.212
μ/mm^{-1}	0.576
F(000)	760.0
Crystal size/mm^3	0.337 × 0.284 × 0.202
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.414 to 56.578
Index ranges	$-14 \le h \le 14$, $-17 \le k \le 17$, $-21 \le l \le 21$
Reflections collected	19244
Independent reflections	9591 [R_{int} = 0.0576, R_{sigma} = 0.0983]
Data/restraints/parameters	9591/0/424
Goodness-of-fit on F^2	0.976
Final R indexes [I>=2σ (I)]	R_1 = 0.0550, wR_2 = 0.1093
Final R indexes [all data]	R_1 = 0.0977, wR_2 = 0.1299
Largest diff. peak/hole / e Å^{-3}	0.53/-0.39

Table S10 Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Fe1	1975.1(4)	2477.0(3)	2843.5(2)	25.85(12)
B1	2720(3)	3028(3)	4682(2)	27.0(7)
O1	1004.7(19)	2405.7(16)	2061.5(12)	29.2(4)
S1	966.4(7)	1865.4(6)	4351.7(4)	28.35(17)
S2	1543.0(7)	4359.1(6)	3147.1(4)	26.61(17)
S3	4245.0(7)	1826.1(6)	3142.0(4)	26.64(17)
C1	2472(3)	3238(3)	6387(2)	40.7(8)
C2	2903(4)	3465(3)	7071(2)	48.6(9)
C3	4064(4)	3771(3)	6906(2)	45.6(9)
C4	4789(3)	3854(3)	6048(2)	41.3(8)
C5	4347(3)	3613(2)	5384.6(19)	33.5(7)
C6	3171(3)	3292(2)	5516.3(18)	28.1(6)
C7	1273(3)	2722(3)	5016.9(18)	33.5(7)
C8	2560(3)	4199(2)	3960.6(18)	31.8(7)
C9	3981(3)	1968(2)	4306.1(17)	30.9(7)
C10	-909(3)	2228(3)	4493.8(19)	32.2(7)
C11	-1472(3)	2017(3)	5481(2)	46.4(9)
C12	-1514(3)	3436(3)	4098(2)	42.3(8)
C13	-1147(3)	1421(3)	4017(2)	39.3(8)
C14	2087(3)	5349(2)	2205.2(18)	29.2(6)
C15	1792(4)	6465(2)	2529(2)	43.2(8)
C16	1198(3)	5484(3)	1540.8(19)	38.6(8)
C17	3583(3)	4902(3)	1811(2)	41.3(8)
C18	5197(3)	323(2)	3073.6(18)	27.7(6)
C19	4387(3)	-435(2)	3644.4(19)	35.9(7)
C20	6548(3)	82(3)	3351(2)	39.4(8)
C21	5441(3)	194(3)	2103.7(18)	35.9(7)
C22	1228(3)	2040(2)	1238.5(17)	24.9(6)
C23	1989(3)	73(2)	2053.3(18)	29.8(7)
C24	2761(3)	-1043(3)	2107(2)	37.1(7)
C25	3681(3)	-1443(2)	1383(2)	35.1(7)
C26	3818(3)	-730(2)	602.4(19)	32.2(7)
C27	3039(3)	385(2)	547.2(18)	28.1(6)
C28	2122(3)	816(2)	1274.1(17)	25.0(6)
C29	3209(3)	2810(2)	558.4(18)	29.1(6)
C30	3813(3)	3551(2)	-16.0(19)	33.7(7)
C31	3134(3)	4325(3)	-633.5(19)	35.5(7)
C32	1857(3)	4350(2)	-667.8(19)	34.3(7)
C33	1233(3)	3609(2)	-87.6(18)	30.0(7)
C34	1902(3)	2823(2)	535.9(17)	23.8(6)
C35	-181(3)	1609(3)	345(2)	43.3(8)
C36	-1396(4)	1652(3)	158(3)	54.2(10)

C37	-2582(4)	2162(3)	676(3)	58.2(11)
C38	-2570(3)	2636(3)	1380(3)	52.7(10)
C39	-1334(3)	2605(3)	1561(2)	39.0(8)
C40	-131(3)	2086(2)	1044.2(19)	29.9(7)

Table S11 Anisotropic displacement parameters ($Å^2×10^3$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Fe1	25.9(2)	27.8(2)	25.2(2)	-4.13(18)	-4.82(17)	-9.56(18)
B1	27.1(18)	31.2(18)	24.6(16)	-3.9(14)	-5.6(14)	-10.7(15)
O1	27.6(11)	35.9(12)	25.9(10)	-9.1(9)	-3.3(8)	-10.5(9)
S1	27.5(4)	31.3(4)	26.7(4)	-4.1(3)	-2.2(3)	-11.6(3)
S2	28.5(4)	25.3(4)	27.2(4)	-2.4(3)	-6.3(3)	-9.8(3)
S3	25.8(4)	25.8(4)	27.3(4)	-3.2(3)	-5.5(3)	-6.5(3)
C1	39.0(19)	48(2)	36.4(18)	-13.5(16)	-5.0(15)	-12.1(16)
C2	52(2)	67(2)	29.8(17)	-16.3(17)	-5.6(16)	-17(2)
C3	53(2)	50(2)	40.9(19)	-16.0(17)	-21.6(17)	-9.4(18)
C4	43(2)	37.4(19)	51(2)	-6.6(16)	-18.6(16)	-14.7(16)
C5	38.1(18)	35.3(17)	29.7(16)	-4.9(14)	-8.1(13)	-12.9(15)
C6	32.1(16)	23.7(15)	26.9(15)	-2.5(12)	-8.7(13)	-4.6(13)
C7	40.5(18)	39.3(18)	25.7(15)	-8.1(13)	-6.7(13)	-15.7(15)
C8	37.8(18)	32.9(17)	29.5(15)	-5.9(13)	-10.9(13)	-12.7(14)
C9	35.5(17)	32.0(17)	26.9(15)	-5.1(13)	-12.8(13)	-6.9(14)
C10	25.9(16)	36.7(17)	34.1(16)	-7.0(14)	2.1(13)	-13.9(14)
C11	36.7(19)	62(2)	39.2(19)	-13.6(17)	7.8(15)	-19.0(18)
C12	30.8(18)	39.6(19)	54(2)	-7.7(17)	-5.3(15)	-8.8(15)
C13	35.2(18)	44(2)	44.7(19)	-11.1(16)	-3.4(15)	-19.6(16)
C14	35.1(17)	27.1(16)	27.6(15)	0.6(12)	-8.0(13)	-13.3(14)
C15	61(2)	30.1(18)	47(2)	-3.4(15)	-14.4(17)	-23.2(17)
C16	45(2)	37.3(18)	34.6(17)	2.6(14)	-16.3(15)	-12.9(16)
C17	37.5(19)	56(2)	33.7(17)	-2.2(16)	-5.6(14)	-22.1(17)
C18	28.2(16)	24.1(15)	29.9(15)	-5.8(12)	-7.1(12)	-4.3(13)
C19	48(2)	25.9(16)	35.0(17)	1.0(13)	-9.7(15)	-14.0(15)
C20	32.8(18)	37.0(18)	48.8(19)	-10.6(15)	-13.9(15)	-3.9(15)
C21	34.7(18)	37.4(18)	34.5(17)	-12.6(14)	-1.2(14)	-8.5(15)
C22	23.1(15)	26.9(15)	25.2(14)	-4.5(12)	-6.2(12)	-6.7(12)
C23	31.5(17)	31.5(17)	27.8(15)	-7.6(13)	1.0(13)	-14.0(14)
C24	48(2)	32.8(18)	32.7(17)	0.0(14)	-5.5(15)	-19.7(16)
C25	35.1(18)	24.6(16)	47.4(19)	-8.8(15)	-9.0(15)	-8.1(14)
C26	29.3(17)	34.2(17)	34.7(16)	-11.1(14)	-0.6(13)	-11.4(14)
C27	32.0(16)	28.4(16)	27.2(15)	-3.9(13)	-6.3(12)	-12.7(13)
C28	23.2(15)	28.2(15)	27.5(14)	-5.2(12)	-8.7(12)	-9.4(12)
C29	26.7(16)	26.6(16)	32.3(16)	-2.4(13)	-6.5(13)	-6.4(13)

C30	26.1(16)	35.4(18)	38.9(17)	-8.2(15)	-1.2(14)	-9.9(14)
C31	39.5(19)	33.9(18)	30.9(16)	-3.2(14)	0.7(14)	-14.3(15)
C32	37.9(19)	32.7(17)	29.9(16)	1.1(13)	-10.9(14)	-7.9(15)
C33	26.6(16)	30.5(16)	33.6(16)	-6.4(13)	-8.9(13)	-6.2(13)
C34	25.8(15)	23.9(14)	22.5(14)	-5.6(12)	-3.5(12)	-7.7(12)
C35	41(2)	49(2)	51(2)	-5.3(17)	-22.3(16)	-19.1(17)
C36	54(2)	48(2)	73(3)	0(2)	-35(2)	-21(2)
C37	47(2)	49(2)	89(3)	22(2)	-42(2)	-26(2)
C38	27.6(19)	51(2)	70(3)	13(2)	-7.9(18)	-12.8(17)
C39	29.8(18)	36.3(18)	46.2(19)	6.6(15)	-9.1(15)	-10.1(15)
C40	27.1(16)	29.8(16)	34.6(16)	4.3(13)	-8.8(13)	-14.3(13)

Table S12 Bond lengths.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	O1	1.8295(18)	C14	C17	1.523(4)
Fe1	S1	2.4417(8)	C18	C19	1.520(4)
Fe1	S2	2.4268(9)	C18	C20	1.523(4)
Fe1	S3	2.4141(9)	C18	C21	1.525(4)
B1	C6	1.642(4)	C22	C28	1.534(4)
B1	C7	1.655(4)	C22	C34	1.541(4)
B1	C8	1.663(4)	C22	C40	1.536(4)
B1	C9	1.653(4)	C23	C24	1.385(4)
O1	C22	1.415(3)	C23	C28	1.394(4)
S1	C7	1.822(3)	C24	C25	1.377(4)
S1	C10	1.865(3)	C25	C26	1.376(4)
S2	C8	1.815(3)	C26	C27	1.387(4)
S2	C14	1.850(3)	C27	C28	1.393(4)
S3	C9	1.830(3)	C29	C30	1.377(4)
S3	C18	1.863(3)	C29	C34	1.399(4)
C1	C2	1.389(4)	C30	C31	1.381(4)
C1	C6	1.396(4)	C31	C32	1.369(4)
C2	C3	1.373(5)	C32	C33	1.392(4)
C3	C4	1.389(4)	C33	C34	1.388(4)
C4	C5	1.377(4)	C35	C36	1.381(4)
C5	C6	1.404(4)	C35	C40	1.390(4)
C10	C11	1.528(4)	C36	C37	1.367(5)
C10	C12	1.521(4)	C37	C38	1.381(5)
C10	C13	1.518(4)	C38	C39	1.404(4)
C14	C15	1.527(4)	C39	C40	1.379(4)
C14	C16	1.527(4)			

Table S13 Bond angles.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Fe1	S1	110.51(6)	C16	C14	C15	110.2(2)
O1	Fe1	S2	113.78(6)	C17	C14	S2	111.7(2)
O1	Fe1	S3	141.25(6)	C17	C14	C15	110.5(2)
S2	Fe1	S1	92.36(3)	C17	C14	C16	111.4(2)
S3	Fe1	S1	93.81(3)	C19	C18	S3	111.02(19)
S3	Fe1	S2	94.08(3)	C19	C18	C20	111.8(2)
C6	B1	C7	110.0(2)	C19	C18	C21	110.6(2)
C6	B1	C8	104.9(2)	C20	C18	S3	107.86(19)
C6	B1	C9	105.4(2)	C20	C18	C21	109.5(2)
C7	B1	C8	111.5(2)	C21	C18	S3	105.76(19)
C9	B1	C7	112.4(2)	O1	C22	C28	110.0(2)
C9	B1	C8	112.2(2)	O1	C22	C34	107.3(2)
C22	O1	Fe1	139.39(17)	O1	C22	C40	109.3(2)
C7	S1	Fe1	104.38(10)	C28	C22	C34	111.5(2)
C7	S1	C10	106.06(14)	C28	C22	C40	107.3(2)
C10	S1	Fe1	111.43(10)	C40	C22	C34	111.4(2)
C8	S2	Fe1	105.28(10)	C24	C23	C28	121.2(3)
C8	S2	C14	105.79(13)	C25	C24	C23	120.2(3)
C14	S2	Fe1	115.66(9)	C26	C25	C24	119.7(3)
C9	S3	Fe1	103.16(10)	C25	C26	C27	120.1(3)
C9	S3	C18	105.14(12)	C26	C27	C28	121.4(3)
C18	S3	Fe1	117.00(9)	C23	C28	C22	119.5(2)
C2	C1	C6	123.3(3)	C27	C28	C22	123.1(2)
C3	C2	C1	120.3(3)	C27	C28	C23	117.4(3)
C2	C3	C4	118.8(3)	C30	C29	C34	121.3(3)
C5	C4	C3	119.8(3)	C29	C30	C31	120.2(3)
C4	C5	C6	123.7(3)	C32	C31	C30	119.4(3)
C1	C6	B1	125.6(3)	C31	C32	C33	120.9(3)
C1	C6	C5	114.1(3)	C34	C33	C32	120.5(3)
C5	C6	B1	120.3(2)	C29	C34	C22	119.3(2)
B1	C7	S1	115.79(19)	C33	C34	C22	122.8(2)
B1	C8	S2	115.26(19)	C33	C34	C29	117.7(2)
B1	C9	S3	117.97(19)	C36	C35	C40	121.7(3)
C11	C10	S1	107.6(2)	C37	C36	C35	119.5(4)
C12	C10	S1	110.9(2)	C36	C37	C38	120.4(3)
C12	C10	C11	111.7(3)	C37	C38	C39	119.9(3)
C13	C10	S1	105.3(2)	C40	C39	C38	120.1(3)
C13	C10	C11	110.2(3)	C35	C40	C22	121.0(3)
C13	C10	C12	110.9(3)	C39	C40	C22	120.6(3)
C15	C14	S2	108.2(2)	C39	C40	C35	118.5(3)
C16	C14	S2	104.61(19)				

Table S13 Torsion angles.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Fe1	O1	C22	C28	53.6(3)	C8	S2	C14	C17	60.4(2)
Fe1	O1	C22	C34	-68.0(3)	C9	B1	C6	C1	-119.6(3)
Fe1	O1	C22	C40	171.16(19)	C9	B1	C6	C5	61.0(3)
Fe1	S1	C7	B1	-34.9(2)	C9	B1	C7	S1	-38.3(3)
Fe1	S1	C10	C11	-169.58(18)	C9	B1	C8	S2	86.0(3)
Fe1	S1	C10	C12	-47.1(2)	C9	S3	C18	C19	60.7(2)
Fe1	S1	C10	C13	72.9(2)	C9	S3	C18	C20	-62.2(2)
Fe1	S2	C8	B1	-34.5(2)	C9	S3	C18	C21	-179.30(19)
Fe1	S2	C14	C15	-177.56(17)	C10	S1	C7	B1	-152.7(2)
Fe1	S2	C14	C16	65.0(2)	C14	S2	C8	B1	-157.4(2)
Fe1	S2	C14	C17	-55.7(2)	C18	S3	C9	B1	-157.5(2)
Fe1	S3	C9	B1	-34.4(2)	C23	C24	C25	C26	-0.8(5)
Fe1	S3	C18	C19	-53.0(2)	C24	C23	C28	C22	178.8(3)
Fe1	S3	C18	C20	-175.90(16)	C24	C23	C28	C27	1.4(4)
Fe1	S3	C18	C21	67.0(2)	C24	C25	C26	C27	0.4(4)
O1	C22	C28	C23	35.2(3)	C25	C26	C27	C28	1.0(4)
O1	C22	C28	C27	-147.5(2)	C26	C27	C28	C22	-179.2(2)
O1	C22	C34	C29	66.6(3)	C26	C27	C28	C23	-1.9(4)
O1	C22	C34	C33	-108.6(3)	C28	C22	C34	C29	-54.0(3)
O1	C22	C40	C35	-169.9(3)	C28	C22	C34	C33	130.8(3)
O1	C22	C40	C39	10.2(4)	C28	C22	C40	C35	-50.6(3)
S1	Fe1	O1	C22	-135.4(2)	C28	C22	C40	C39	129.4(3)
S2	Fe1	O1	C22	122.3(2)	C28	C23	C24	C25	-0.1(4)
S3	Fe1	O1	C22	-10.1(3)	C29	C30	C31	C32	0.1(4)
C1	C2	C3	C4	0.2(5)	C30	C29	C34	C22	-175.3(2)
C2	C1	C6	B1	179.7(3)	C30	C29	C34	C33	0.1(4)
C2	C1	C6	C5	-0.9(5)	C30	C31	C32	C33	0.3(4)
C2	C3	C4	C5	-0.9(5)	C31	C32	C33	C34	-0.4(4)
C3	C4	C5	C6	0.7(5)	C32	C33	C34	C22	175.5(2)
C4	C5	C6	B1	179.6(3)	C32	C33	C34	C29	0.2(4)
C4	C5	C6	C1	0.2(4)	C34	C22	C28	C23	154.2(2)
C6	B1	C7	S1	-155.3(2)	C34	C22	C28	C27	-28.5(3)
C6	B1	C8	S2	-160.15(19)	C34	C22	C40	C35	71.7(3)
C6	B1	C9	S3	-153.2(2)	C34	C22	C40	C39	-108.2(3)
C6	C1	C2	C3	0.7(5)	C34	C29	C30	C31	-0.3(4)
C7	B1	C6	C1	1.7(4)	C35	C36	C37	C38	0.4(5)
C7	B1	C6	C5	-177.7(3)	C36	C35	C40	C22	-179.4(3)
C7	B1	C8	S2	-41.2(3)	C36	C35	C40	C39	0.5(5)
C7	B1	C9	S3	87.1(3)	C36	C37	C38	C39	0.5(5)
C7	S1	C10	C11	-56.6(2)	C37	C38	C39	C40	-1.0(5)
C7	S1	C10	C12	65.8(2)	C38	C39	C40	C22	-179.6(3)
C7	S1	C10	C13	-174.1(2)	C38	C39	C40	C35	0.4(4)
C8	B1	C6	C1	121.7(3)	C40	C22	C28	C23	-83.5(3)

C8	B1	C6	C5	-57.7(3)	C40	C22	C28	C27	93.7(3)
C8	B1	C7	S1	88.8(3)	C40	C22	C34	C29	-173.9(2)
C8	B1	C9	S3	-39.6(3)	C40	C22	C34	C33	10.9(4)
C8	S2	C14	C15	-61.5(2)	C40	C35	C36	C37	-0.9(5)
C8	S2	C14	C16	-178.95(19)					

Table S14 Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3).

Atom	***x***	***y***	***z***	**U(eq)**
H1	1659.36	3036.17	6519.72	49
H2	2393.46	3407.54	7653.5	58
H3	4365.33	3924.65	7371.72	55
H4	5587.13	4075.3	5919.39	50
H5	4866.68	3666.71	4804.55	40
H7A	523.09	3432.71	5030.04	40
H7B	1246.06	2325.73	5629.51	40
H8A	3474.64	4225.87	3646.62	38
H8B	2153.29	4846.87	4290.7	38
H9A	3840.34	1266.76	4663.59	37
H9B	4826.78	2027.5	4415.1	37
H11A	-1289.92	2527.95	5784.12	70
H11B	-1036.02	1240.52	5717.88	70
H11C	-2450.55	2149.03	5572.83	70
H12A	-1146.55	3536.04	3463.36	63
H12B	-1285.36	3938.06	4383.01	63
H12C	-2499.86	3612.21	4190.84	63
H13A	-2122.03	1566.71	4068.09	59
H13B	-748.02	648.79	4281.95	59
H13C	-725.35	1526.13	3392.45	59
H15A	2359.85	6365.6	2959.94	65
H15B	836.5	6721.31	2806.67	65
H15C	1991.66	7022.7	2027.4	65
H16A	1405.59	6023.73	1026.82	58
H16B	243.45	5756.37	1816.83	58
H16C	1374.87	4758.28	1352.46	58
H17A	3762.16	4170.71	1631.68	62
H17B	4126.12	4820.15	2253.24	62
H17C	3823.54	5426.97	1295.81	62
H19A	4889.41	-1217.53	3575.29	54
H19B	3513.16	-236.34	3461.94	54
H19C	4237.52	-339.13	4264.14	54
H20A	6387.39	224.15	3959.3	59
H20B	7050.26	570.82	2958.39	59

H20C	7075.15	-703.22	3312.09	59
H21A	5962.01	-582.29	2024.03	54
H21B	5947.5	698.74	1744.85	54
H21C	4569.97	382.39	1919.09	54
H23	1356.86	337.41	2557.04	36
H24	2655.81	-1535.06	2645.01	44
H25	4218.42	-2205.89	1423.12	42
H26	4447.22	-1003.35	100.51	39
H27	3131.95	866.1	1.97	34
H29	3688.78	2279.08	978.11	35
H30	4699.29	3529.11	12.6	40
H31	3550.39	4836.33	-1030.67	43
H32	1388.92	4880.05	-1093.45	41
H33	343.94	3641.46	-118.27	36
H35	640.91	1244.73	-11.83	52
H36	-1406.58	1329.88	-328.29	65
H37	-3420.15	2189.68	552.11	70
H38	-3397.43	2983.93	1741.57	63
H39	-1325.11	2941.35	2039.39	47

Compound (3), (2,6-dimethylphenolato)(phenyltris(*tert*-butylthiomethyl)borato-S,S',S")iron(II)

Table S15 Crystal data.

CCDC	2063937
Empirical formula	$C_{29}H_{47}BFeOS_3$
Formula weight	574.50
Temperature/K	200.15
Crystal system	Monoclinic
Space group	C2/c
a/Å	11.4960(19)
b/Å	15.036(2)
c/Å	36.375(6)
α/°	90
β/°	91.664(2)
γ/°	90
Volume/Å^3	6285.0(18)
Z	8
ρ_{calc}g/cm^3	1.214
μ/mm^{-1}	0.699
F(000)	2464.0
Crystal size/mm^3	0.393 × 0.366 × 0.148
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.462 to 56.55
Index ranges	-15 ≤ h ≤ 15, -20 ≤ k ≤ 20, -48 ≤ l ≤ 48

Reflections collected	42065
Independent reflections	7796 [R_{int} = 0.0258, R_{sigma} = 0.0172]
Data/restraints/parameters	7796/44/337
Goodness-of-fit on F^2	1.119
Final R indexes [I>=2σ (I)]	R_1 = 0.0325, wR_2 = 0.0782
Final R indexes [all data]	R_1 = 0.0338, wR_2 = 0.0791
Largest diff. peak/hole / e Å^{-3}	0.36/-0.33

Table S16 Fractional atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2×10^3). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Fe	7549.0(2)	3045.2(2)	1205.7(2)	28.26(6)
B1	10358.7(13)	2847.8(10)	1540.7(4)	23.7(3)
O1A	6034(3)	3019(10)	1031.5(15)	49.1(16)
O1B	6130(11)	3420(20)	1041(2)	47(3)
S1	9188.3(3)	3699.6(2)	906.1(2)	27.30(8)
S2	8177.1(3)	3549.0(2)	1815.8(2)	26.09(8)
S3	8544.6(3)	1620.1(2)	1276.5(2)	27.50(8)
C1	10422.2(12)	3070.3(10)	1094.7(4)	27.8(3)
C2	9177.3(14)	3498.3(12)	402.9(4)	35.5(3)
C3	8187.8(17)	4071.0(15)	243.3(5)	49.0(4)
C4	8968.7(19)	2522.4(14)	311.9(5)	50.8(5)
C5	10346.0(17)	3817.4(16)	264.2(5)	50.2(5)
C6	9738.0(12)	3672.0(10)	1768.0(4)	28.6(3)
C7	7643.8(13)	4658.3(10)	1955.0(4)	32.1(3)
C8	8224.2(19)	4889.8(13)	2325.8(5)	49.0(5)
C9	7911.7(17)	5363.6(11)	1670.3(5)	42.2(4)
C10	6337.9(16)	4536.8(14)	1995.2(6)	51.0(5)
C11	9696.9(12)	1880.4(9)	1614.6(4)	28.3(3)
C12	7591.8(13)	770.4(10)	1483.6(5)	32.7(3)
C13	6751.2(16)	1206.3(12)	1742.6(6)	44.7(4)
C14	8335.0(17)	77.6(12)	1683.3(7)	51.2(5)
C15	6945.9(18)	352.1(14)	1153.5(6)	54.3(5)
C16	12702.4(12)	2788.5(10)	1514.5(4)	28.4(3)
C17	13810.5(13)	2721.5(11)	1677.1(5)	33.8(3)
C18	13944.8(14)	2594.5(11)	2052.0(5)	36.6(3)
C19	12959.6(15)	2536.5(12)	2262.3(4)	37.3(3)
C20	11858.9(13)	2611.9(11)	2096.8(4)	32.3(3)
C21	11684.4(12)	2747.8(9)	1716.6(4)	24.5(3)
C22	5149.9(16)	4282.9(18)	674.1(5)	56.2(6)
C23	4290.5(18)	4517.5(18)	410.8(6)	58.7(5)
C24	3522.3(18)	3890.4(18)	271.0(6)	60.1(6)
C25	3598.1(18)	3024.5(17)	390.8(5)	54.9(5)
C26	4442.9(17)	2756.6(17)	647.0(5)	52.5(5)

C27	5236.5(15)	3388.9(18)	786.1(5)	52.5(5)
C28	5938(2)	4984(2)	837.3(8)	80.4(8)
C29	4504(3)	1800.6(19)	769.2(7)	78.2(8)

Table S17 Anisotropic displacement parameters ($Å^2×10^3$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Fe	21.71(10)	28.06(11)	34.83(12)	0.48(8)	-2.49(8)	-0.87(8)
B1	20.5(7)	20.5(7)	30.0(7)	-1.2(5)	-0.4(5)	0.1(5)
O1A	26.9(10)	72(5)	47.8(13)	8(2)	-10.8(8)	-0.5(15)
O1B	32(3)	65(8)	41(2)	-2(3)	-10(2)	15(4)
S1	25.15(16)	27.52(17)	29.10(17)	3.59(13)	-1.48(13)	-1.22(13)
S2	24.28(16)	22.49(16)	31.54(17)	-1.09(12)	1.62(12)	1.97(12)
S3	24.76(16)	21.93(16)	35.77(18)	-1.60(13)	0.20(13)	-3.22(12)
C1	22.9(6)	27.8(7)	32.5(7)	1.6(5)	-2.6(5)	-0.7(5)
C2	35.0(8)	43.8(9)	27.4(7)	3.3(6)	-1.1(6)	-0.2(7)
C3	45.2(10)	64.0(12)	37.2(9)	10.8(8)	-7.6(7)	6.9(9)
C4	62.8(12)	50.1(11)	38.9(9)	-8.5(8)	-7.1(8)	-3.1(9)
C5	41.5(10)	72.4(13)	37.1(9)	7.4(9)	7.6(7)	-4.9(9)
C6	22.4(6)	26.4(7)	36.8(7)	-4.2(6)	-1.5(5)	1.3(5)
C7	31.7(7)	26.3(7)	38.2(8)	-4.5(6)	-0.6(6)	8.5(6)
C8	61.7(12)	42.2(10)	42.5(9)	-14.7(8)	-8.1(8)	15.0(9)
C9	48.1(10)	26.5(8)	51.9(10)	2.4(7)	-2.6(8)	6.1(7)
C10	31.7(9)	47.1(10)	74.6(13)	-3.2(9)	7.0(8)	12.7(8)
C11	24.0(6)	23.3(6)	37.2(7)	0.7(5)	-2.9(5)	-0.9(5)
C12	27.2(7)	22.3(7)	48.6(9)	0.2(6)	2.6(6)	-5.8(5)
C13	40.5(9)	37.9(9)	56.6(11)	2.7(8)	15.1(8)	-2.2(7)
C14	41.7(10)	27.5(8)	84.3(15)	15.4(9)	2.7(9)	-1.1(7)
C15	46.7(11)	48.6(11)	67.4(13)	-13.3(9)	0.2(9)	-22.7(9)
C16	25.4(7)	28.7(7)	31.2(7)	-0.3(5)	0.1(5)	0.7(5)
C17	24.1(7)	35.5(8)	41.8(8)	-1.5(6)	1.7(6)	0.4(6)
C18	27.2(7)	38.4(8)	43.6(9)	-4.2(7)	-9.5(6)	2.5(6)
C19	37.9(8)	43.7(9)	29.9(7)	-1.3(6)	-6.3(6)	4.5(7)
C20	28.4(7)	37.0(8)	31.5(7)	-0.5(6)	1.7(6)	3.6(6)
C21	22.2(6)	19.4(6)	31.8(7)	-2.4(5)	-1.4(5)	0.4(5)
C22	29.7(8)	97.8(18)	41.3(10)	-10.6(11)	4.1(7)	3.8(10)
C23	41.2(10)	80.3(16)	54.5(12)	6.0(11)	1.1(9)	10.5(10)
C24	39.9(10)	95.6(18)	44.2(10)	4.9(11)	-12.6(8)	14.3(11)
C25	41.8(10)	82.6(16)	39.9(10)	-6.7(10)	-8.3(8)	6.0(10)
C26	42.4(10)	81.6(15)	33.4(9)	-5.7(9)	0.4(7)	21.2(10)
C27	26.2(8)	101.8(17)	29.6(8)	-1.9(9)	0.1(6)	17.8(9)
C28	48.2(13)	118(2)	75.0(16)	-26.6(16)	4.3(11)	-10.7(14)
C29	96(2)	86.1(19)	51.8(13)	-5.5(12)	-5.7(13)	34.3(16)

Table S18 Bond lengths.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe	O1A	1.837(3)	C7	C8	1.527(2)
Fe	O1B	1.811(6)	C7	C9	1.520(2)
Fe	S1	2.4139(5)	C7	C10	1.524(2)
Fe	S2	2.4344(5)	C12	C13	1.518(2)
Fe	S3	2.4394(5)	C12	C14	1.519(2)
B1	C1	1.660(2)	C12	C15	1.529(2)
B1	C6	1.662(2)	C16	C17	1.393(2)
B1	C11	1.667(2)	C16	C21	1.401(2)
B1	C21	1.642(2)	C17	C18	1.381(2)
O1A	O1B	0.611(16)	C18	C19	1.388(2)
O1A	C27	1.378(5)	C19	C20	1.390(2)
O1B	C27	1.363(9)	C20	C21	1.407(2)
S1	C1	1.8226(14)	C22	C23	1.401(3)
S1	C2	1.8547(16)	C22	C27	1.407(4)
S2	C6	1.8172(15)	C22	C28	1.501(3)
S2	C7	1.8527(15)	C23	C24	1.379(3)
S3	C11	1.8236(15)	C24	C25	1.375(3)
S3	C12	1.8567(15)	C25	C26	1.386(3)
C2	C3	1.528(2)	C26	C27	1.402(3)
C2	C4	1.522(3)	C26	C29	1.506(4)
C2	C5	1.526(2)			

Table S19 Bond angles.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1A	Fe	S1	126.73(18)	B1	C6	S2	114.27(10)
O1A	Fe	S2	125.1(3)	C8	C7	S2	107.89(11)
O1A	Fe	S3	117.1(5)	C9	C7	S2	111.51(11)
O1B	Fe	O1A	19.3(5)	C9	C7	C8	110.52(15)
O1B	Fe	S1	115.6(8)	C9	C7	C10	111.63(14)
O1B	Fe	S2	116.5(4)	C10	C7	S2	104.66(12)
O1B	Fe	S3	136.3(10)	C10	C7	C8	110.43(16)
S1	Fe	S2	94.016(16)	B1	C11	S3	113.87(10)
S1	Fe	S3	92.046(17)	C13	C12	S3	110.39(11)
S2	Fe	S3	92.937(15)	C13	C12	C14	111.03(16)
C1	B1	C6	111.57(11)	C13	C12	C15	111.20(15)
C1	B1	C11	111.50(11)	C14	C12	S3	109.61(11)
C6	B1	C11	111.46(11)	C14	C12	C15	110.31(15)
C21	B1	C1	109.41(11)	C15	C12	S3	104.08(12)
C21	B1	C6	106.35(11)	C17	C16	C21	122.79(14)
C21	B1	C11	106.26(11)	C18	C17	C16	120.28(15)

O1B	O1A	Fe	78.0(8)	C17	C18	C19	118.90(14)
O1B	O1A	C27	75.8(10)	C18	C19	C20	120.22(15)
C27	O1A	Fe	145.2(7)	C19	C20	C21	122.67(14)
O1A	O1B	Fe	82.7(9)	C16	C21	B1	124.84(13)
O1A	O1B	C27	78.5(15)	C16	C21	C20	115.13(13)
C27	O1B	Fe	150.3(11)	C20	C21	B1	120.03(12)
C1	S1	Fe	103.16(5)	C23	C22	C27	118.7(2)
C1	S1	C2	105.64(7)	C23	C22	C28	119.9(3)
C2	S1	Fe	113.33(5)	C27	C22	C28	121.3(2)
C6	S2	Fe	102.25(5)	C24	C23	C22	120.7(2)
C6	S2	C7	105.66(7)	C25	C24	C23	119.78(19)
C7	S2	Fe	115.95(5)	C24	C25	C26	121.7(2)
C11	S3	Fe	102.24(5)	C25	C26	C27	118.8(2)
C11	S3	C12	107.44(7)	C25	C26	C29	120.1(2)
C12	S3	Fe	111.52(5)	C27	C26	C29	121.1(2)
B1	C1	S1	114.62(10)	O1A	C27	C22	127.8(6)
C3	C2	S1	105.48(12)	O1A	C27	C26	111.9(6)
C4	C2	S1	111.62(12)	O1B	C27	O1A	25.8(7)
C4	C2	C3	110.48(15)	O1B	C27	C22	102.2(13)
C4	C2	C5	111.46(16)	O1B	C27	C26	137.4(13)
C5	C2	S1	107.10(12)	C26	C27	C22	120.23(17)
C5	C2	C3	110.48(15)				

Table S20 Torsion angles.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
Fe	O1A	O1B	C27	156.9(4)	C6	B1	C11	S3	92.25(13)
Fe	O1A	C27	O1B	-42.3(9)	C6	B1	C21	C16	-124.38(14)
Fe	O1A	C27	C22	-35.8(17)	C6	B1	C21	C20	55.50(16)
Fe	O1A	C27	C26	144.9(14)	C6	S2	C7	C8	-62.09(14)
Fe	O1B	C27	O1A	52(3)	C6	S2	C7	C9	59.46(13)
Fe	O1B	C27	C22	-123(4)	C6	S2	C7	C10	-179.70(12)
Fe	O1B	C27	C26	62(4)	C7	S2	C6	B1	-164.66(10)
Fe	S1	C1	B1	-40.28(10)	C11	B1	C1	S1	90.48(12)
Fe	S1	C2	C3	71.10(13)	C11	B1	C6	S2	-33.05(15)
Fe	S1	C2	C4	-48.92(14)	C11	B1	C21	C16	116.75(15)
Fe	S1	C2	C5	-171.18(11)	C11	B1	C21	C20	-63.36(16)
Fe	S2	C6	B1	-42.92(11)	C11	S3	C12	C13	80.18(13)
Fe	S2	C7	C8	-174.51(11)	C11	S3	C12	C14	-42.42(14)
Fe	S2	C7	C9	-52.96(13)	C11	S3	C12	C15	-160.41(12)
Fe	S2	C7	C10	67.88(13)	C12	S3	C11	B1	-160.41(10)
Fe	S3	C11	B1	-42.92(10)	C16	C17	C18	C19	-0.1(2)
Fe	S3	C12	C13	-31.09(14)	C17	C16	C21	B1	178.40(13)
Fe	S3	C12	C14	-153.69(12)	C17	C16	C21	C20	-1.5(2)

Fe	S3	C12	C15	88.32(12)	C17	C18	C19	C20	-0.4(3)
O1A	Fe	O1B	C27	-51(3)	C18	C19	C20	C21	0.0(3)
O1A	O1B	C27	C22	-174.8(14)	C19	C20	C21	B1	-178.95(14)
O1A	O1B	C27	C26	9.8(19)	C19	C20	C21	C16	0.9(2)
O1B	Fe	O1A	C27	41.8(10)	C21	B1	C1	S1	-152.27(9)
O1B	O1A	C27	C22	6.5(18)	C21	B1	C6	S2	-148.44(10)
O1B	O1A	C27	C26	-172.9(15)	C21	B1	C11	S3	-152.30(10)
S1	Fe	O1A	O1B	-59.9(18)	C21	C16	C17	C18	1.1(2)
S1	Fe	O1A	C27	-18.1(19)	C22	C23	C24	C25	0.0(3)
S1	Fe	O1B	O1A	129.8(16)	C23	C22	C27	O1A	178.0(4)
S1	Fe	O1B	C27	79(4)	C23	C22	C27	O1B	-179.1(5)
S2	Fe	O1A	O1B	69.2(14)	C23	C22	C27	C26	-2.7(3)
S2	Fe	O1A	C27	111.0(13)	C23	C24	C25	C26	-0.9(3)
S2	Fe	O1B	O1A	-121.2(12)	C24	C25	C26	C27	0.0(3)
S2	Fe	O1B	C27	-172(4)	C24	C25	C26	C29	-179.5(2)
S3	Fe	O1A	O1B	-175.4(14)	C25	C26	C27	O1A	-178.8(4)
S3	Fe	O1A	C27	-133.6(15)	C25	C26	C27	O1B	176.6(6)
S3	Fe	O1B	O1A	5.9(19)	C25	C26	C27	C22	1.8(3)
S3	Fe	O1B	C27	-45(5)	C27	O1A	O1B	Fe	-156.9(4)
C1	B1	C6	S2	92.32(12)	C27	C22	C23	C24	1.8(3)
C1	B1	C11	S3	-33.15(14)	C28	C22	C23	C24	-176.9(2)
C1	B1	C21	C16	-3.75(18)	C28	C22	C27	O1A	-3.4(5)
C1	B1	C21	C20	176.13(13)	C28	C22	C27	O1B	-0.5(5)
C1	S1	C2	C3	-176.67(12)	C28	C22	C27	C26	175.94(19)
C1	S1	C2	C4	63.31(14)	C29	C26	C27	O1A	0.7(4)
C1	S1	C2	C5	-58.95(14)	C29	C26	C27	O1B	-3.8(6)
C2	S1	C1	B1	-159.47(10)	C29	C26	C27	C22	-178.67(19)
C6	B1	C1	S1	-34.87(14)					

Table S21 Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3).

Atom	*x*	*y*	*z*	U(eq)
H1A	10475.68	2502.02	958.77	33
H1B	11143.47	3409.88	1051.66	33
H3A	8160.38	4015.84	-25.31	73
H3B	8321.18	4694.03	311.41	73
H3C	7447.26	3870.43	341.23	73
H4A	8212.22	2338.86	403.55	76
H4B	9584.67	2160.79	428.85	76
H4C	8974.99	2439.06	44.79	76
H5A	10972.1	3451.99	373.11	75
H5B	10466.75	4440.4	334.73	75
H5C	10349.56	3764.85	-4.3	75

H6A	9889.23	4237.79	1638.72	34
H6B	10109.68	3713.22	2016.39	34
H8A	9064.67	4954.33	2296.45	74
H8B	8076.88	4413.83	2502.47	74
H8C	7903.33	5449.8	2416.22	74
H9A	7586	5181.62	1429.99	63
H9B	8756.58	5433.07	1655.22	63
H9C	7565.23	5930.73	1742.25	63
H10A	5986.88	5105.88	2062.41	77
H10B	6196.84	4096.89	2187.63	77
H10C	5990.01	4329.67	1761.43	77
H11A	9360.68	1892.95	1862.02	34
H11B	10284.65	1399.31	1613.08	34
H13A	6256.72	750.11	1850.37	67
H13B	6263.73	1634.48	1605.65	67
H13C	7190.53	1515.68	1938.85	67
H14A	8740.7	353.43	1894.73	77
H14B	8906.97	-163.17	1515.2	77
H14C	7836.94	-404.6	1768.7	77
H15A	6359.24	-64.99	1240.35	81
H15B	7500.85	33.31	1002.14	81
H15C	6563.62	819.92	1006.46	81
H16	12633.64	2865.12	1255.49	34
H17	14476.81	2763.3	1529.59	41
H18	14699.16	2547.58	2163.99	44
H19	13037.69	2445.09	2520.28	45
H20	11197.67	2569.79	2246.52	39
H23	4236.36	5115.37	327.66	70
H24	2942.69	4056.08	92.55	72
H25	3057.75	2599.03	295.57	66
H28A	5842.59	5537.4	697.26	121
H28B	6748.27	4784.37	827.25	121
H28C	5738.85	5088.31	1093.83	121
H29A	5211.5	1525.98	677.23	117
H29B	3820.34	1479.54	671.44	117
H29C	4518.72	1774.07	1038.5	117

Table S22 Atomic occupancy.

Atom	***Occupancy***	**Atom**	***Occupancy***
O1A	0.68(3)	O1B	0.32(3)

Compound (4), cyclo-bis[(phenolato)(phenyl-tris(*t*-butylthiomethyl)borato-κ^1-S,S',κ^1-μ_2-S")iron(II)] di-toluene solvate

Table S23 Crystal data.

CCDC	2063939
Empirical formula	$C_{68}H_{102}B_2Fe_2O_2S_6$
Formula weight	1277.17
Temperature/K	200.15
Crystal system	triclinic
Space group	P-1
a/Å	10.359(3)
b/Å	13.084(4)
c/Å	13.980(4)
α/°	71.048(5)
β/°	87.964(5)
γ/°	82.954(5)
Volume/Å^3	1778.4(9)
Z	1
ρ_{calc}g/cm^3	1.193
μ/mm^{-1}	0.624
F(000)	684.0
Crystal size/mm^3	0.238 × 0.194 × 0.071
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.726 to 56.636
Index ranges	$-12 \leq h \leq 13$, $-17 \leq k \leq 17$, $-18 \leq l \leq 18$
Reflections collected	19673
Independent reflections	8735 [R_{int} = 0.0534, R_{sigma} = 0.0804]
Data/restraints/parameters	8735/180/400
Goodness-of-fit on F^2	1.070
Final R indexes [I>=2σ (I)]	R_1 = 0.0697, wR_2 = 0.1719
Final R indexes [all data]	R_1 = 0.1045, wR_2 = 0.1994
Largest diff. peak/hole / e Å^{-3}	0.93/-0.68

Table S24 Fractional atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2×10^3). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Fe	8949.8(5)	2060.3(4)	5044.0(4)	29.94(16)
S1	11233.4(9)	1884.7(7)	5328.8(7)	28.9(2)
S2	8730.1(8)	292.6(7)	6223.1(7)	28.4(2)
S3	11200.5(9)	-2004.9(7)	6681.3(7)	29.8(2)
O1	7973(3)	3232(2)	5298(2)	49.1(8)
C1	13314(4)	-441(3)	8362(3)	38.4(9)
C2	13992(4)	-772(4)	9264(3)	46.0(10)

C3	13326(5)	-1056(4)	10164(3)	51.4(12)
C4	11994(5)	-997(4)	10145(3)	50.2(11)
C5	11314(4)	-643(4)	9234(3)	38.8(9)
C6	11956(4)	-367(3)	8307(3)	31.3(8)
C7	11618(4)	1295(3)	6664(3)	32.4(8)
C8	11871(4)	3227(3)	4899(3)	37.3(9)
C9	11457(5)	3880(4)	5599(4)	51.9(12)
C10	11330(5)	3790(4)	3852(3)	51.8(12)
C11	13358(4)	2999(4)	4860(4)	60.1(14)
C12	9660(3)	29(3)	7370(3)	30.7(8)
C13	7034(4)	70(3)	6659(3)	32.6(8)
C14	7018(5)	-1137(4)	7198(5)	62.1(14)
C15	6596(5)	711(4)	7362(4)	56.7(13)
C16	6192(5)	440(6)	5731(4)	73.6(19)
C17	11818(4)	-692(3)	6490(3)	28.4(7)
C18	12476(4)	-3120(3)	7368(3)	37.4(9)
C19	13785(4)	-2994(4)	6850(4)	54.8(12)
C20	11982(5)	-4166(3)	7354(4)	51.1(11)
C21	12548(6)	-3115(4)	8455(3)	59.1(13)
C22	8046(5)	3260(4)	6993(4)	52.3(12)
C23	7385(8)	3501(5)	7790(4)	79(2)
C24	6099(9)	3940(5)	7685(6)	90(2)
C25	5465(7)	4121(5)	6793(6)	82(2)
C26	6109(5)	3889(4)	6011(4)	53.0(12)
C27	7403(4)	3448(3)	6094(3)	39.6(9)
B1	11233(4)	39(3)	7205(3)	28.0(8)
C28A	6605(9)	-3043(9)	10238(8)	130(2)
C29A	6224(8)	-3591(10)	9614(8)	131(2)
C30A	7156(11)	-4080(9)	9109(8)	131.0(19)
C31A	8468(10)	-4021(9)	9228(7)	131(2)
C32A	8849(8)	-3473(9)	9852(8)	131(2)
C33A	7918(10)	-2983(9)	10357(7)	130(2)
C34A	8343(14)	-2534(13)	11104(11)	138(3)
C32B	8687(16)	-3485(16)	9708(14)	131(2)
C31B	9286(15)	-2870(17)	10167(14)	131(2)
C30B	8550(20)	-2298(15)	10720(13)	131.0(19)
C29B	7220(20)	-2341(15)	10813(13)	131(2)
C28B	6617(14)	-2956(16)	10354(15)	131(2)
C33B	7352(16)	-3528(15)	9801(15)	131(2)
C34B	6700(20)	-4000(30)	9180(20)	131.0(19)

Table S25 Anisotropic displacement parameters ($Å^2 \times 10^3$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe	27.4(3)	29.3(3)	34.5(3)	-12.2(2)	-2.1(2)	-2.6(2)
S1	28.7(5)	25.8(4)	32.7(5)	-8.8(3)	-0.6(3)	-6.6(3)
S2	22.6(4)	35.2(5)	28.4(4)	-10.5(4)	1.0(3)	-6.3(3)
S3	29.2(5)	27.8(4)	31.4(5)	-8.5(3)	-2.3(3)	-2.5(4)
O1	56(2)	39.0(16)	53.0(19)	-20.2(14)	2.4(15)	4.4(14)
C1	33(2)	48(2)	36(2)	-13.4(18)	-1.3(16)	-8.8(18)
C2	38(2)	58(3)	40(2)	-13(2)	-11.3(18)	-3(2)
C3	52(3)	65(3)	35(2)	-17(2)	-14.6(19)	5(2)
C4	48(3)	69(3)	30(2)	-16(2)	-0.3(18)	5(2)
C5	32(2)	51(2)	32(2)	-14.0(18)	0.3(16)	0.2(18)
C6	31.0(19)	32.6(19)	30.7(18)	-10.8(15)	-2.2(15)	-3.2(15)
C7	34(2)	33.5(19)	32.2(19)	-12.3(15)	-5.0(15)	-6.7(16)
C8	35(2)	25.5(18)	51(2)	-11.4(17)	-0.4(18)	-8.7(16)
C9	67(3)	36(2)	56(3)	-16(2)	-1(2)	-15(2)
C10	66(3)	36(2)	50(3)	-6.2(19)	3(2)	-19(2)
C11	38(3)	50(3)	93(4)	-18(3)	10(3)	-20(2)
C12	25.5(18)	39(2)	28.3(18)	-12.8(15)	-1.7(14)	-2.8(15)
C13	22.0(18)	41(2)	37(2)	-14.3(16)	4.7(14)	-8.9(15)
C14	46(3)	47(3)	93(4)	-18(3)	21(3)	-22(2)
C15	40(3)	68(3)	81(4)	-46(3)	26(2)	-22(2)
C16	26(2)	142(6)	45(3)	-15(3)	-0.2(19)	-22(3)
C17	27.5(18)	26.2(17)	31.6(18)	-9.0(14)	-0.4(14)	-4.2(14)
C18	40(2)	26.1(18)	42(2)	-7.3(16)	-9.7(17)	1.6(16)
C19	35(2)	45(3)	79(4)	-15(2)	-7(2)	7(2)
C20	56(3)	31(2)	61(3)	-8(2)	-12(2)	-1(2)
C21	77(4)	50(3)	43(3)	-7(2)	-22(2)	6(3)
C22	62(3)	37(2)	59(3)	-14(2)	-4(2)	-11(2)
C23	138(7)	56(3)	47(3)	-14(3)	6(4)	-34(4)
C24	124(7)	60(4)	91(5)	-33(4)	62(5)	-21(4)
C25	68(4)	59(4)	116(6)	-28(4)	35(4)	-8(3)
C26	42(3)	44(3)	75(3)	-24(2)	1(2)	-2(2)
C27	40(2)	28.9(19)	52(2)	-15.6(18)	5.7(19)	-5.0(17)
B1	26(2)	31(2)	26.9(19)	-10.0(16)	-0.4(15)	-4.9(16)
C28A	143(4)	123(4)	104(4)	-8(3)	5(3)	-15(4)
C29A	142(4)	124(4)	105(4)	-7(3)	3(3)	-16(4)
C30A	143(4)	124(4)	106(4)	-10(3)	3(3)	-16(4)
C31A	144(4)	125(4)	105(4)	-12(3)	6(3)	-15(4)
C32A	144(4)	125(4)	106(4)	-11(3)	5(3)	-17(4)
C33A	146(4)	123(4)	103(4)	-12(3)	4(3)	-18(4)
C34A	162(6)	128(5)	110(5)	-15(4)	-3(5)	-24(5)
C32B	141(5)	125(5)	107(4)	-9(3)	3(4)	-16(4)
C31B	142(5)	124(4)	107(4)	-10(3)	4(4)	-16(4)
C30B	143(4)	124(4)	106(4)	-10(3)	3(3)	-16(4)
C29B	142(5)	124(4)	106(4)	-8(3)	3(4)	-15(4)

C28B	141(5)	124(5)	106(4)	-7(3)	3(4)	-15(4)
C33B	142(5)	124(5)	106(4)	-8(3)	2(4)	-16(4)
C34B	143(4)	124(4)	106(4)	-10(3)	3(3)	-16(4)

Table S26 Bond lengths.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe	S1	2.3834(12)	C13	C16	1.499(6)
Fe	S2	2.3968(12)	C17	B1	1.649(5)
Fe	S3[1]	2.4475(13)	C18	C19	1.515(6)
Fe	O1	1.857(3)	C18	C20	1.525(6)
S1	C7	1.811(4)	C18	C21	1.526(6)
S1	C8	1.857(4)	C22	C23	1.391(8)
S2	C12	1.812(4)	C22	C27	1.378(6)
S2	C13	1.865(4)	C23	C24	1.377(10)
S3	C17	1.841(4)	C24	C25	1.368(10)
S3	C18	1.872(4)	C25	C26	1.359(8)
O1	C27	1.335(5)	C26	C27	1.386(6)
C1	C2	1.380(5)	C28A	C29A	1.3900
C1	C6	1.401(5)	C28A	C33A	1.3900
C2	C3	1.377(6)	C29A	C30A	1.3900
C3	C4	1.373(7)	C30A	C31A	1.3900
C4	C5	1.390(6)	C31A	C32A	1.3900
C5	C6	1.396(5)	C32A	C33A	1.3900
C6	B1	1.634(5)	C33A	C34A	1.458(14)
C7	B1	1.662(5)	C32B	C31B	1.3900
C8	C9	1.515(6)	C32B	C33B	1.3900
C8	C10	1.502(6)	C31B	C30B	1.3900
C8	C11	1.535(6)	C30B	C29B	1.3900
C12	B1	1.639(5)	C29B	C28B	1.3900
C13	C14	1.514(6)	C28B	C33B	1.3900
C13	C15	1.511(6)	C33B	C34B	1.441(17)

[1]2-X,-Y,1-Z

Table S27 Bond angles.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
S1	Fe	S2	93.03(4)	B1	C17	S3	118.3(2)
S1	Fe	S3[1]	103.51(4)	C19	C18	S3	111.6(3)
S2	Fe	S3[1]	109.35(4)	C19	C18	C20	110.5(4)
O1	Fe	S1	116.06(11)	C19	C18	C21	111.5(4)
O1	Fe	S2	116.61(11)	C20	C18	S3	104.9(3)
O1	Fe	S3[1]	115.48(10)	C20	C18	C21	109.9(4)

C7	S1	Fe	111.05(13)	C21	C18	S3	108.2(3)
C7	S1	C8	106.23(18)	C27	C22	C23	119.6(5)
C8	S1	Fe	111.75(13)	C24	C23	C22	120.6(6)
C12	S2	Fe	111.77(13)	C25	C24	C23	119.5(6)
C12	S2	C13	104.97(17)	C26	C25	C24	120.2(6)
C13	S2	Fe	114.64(13)	C25	C26	C27	121.6(6)
C17	S3	Fe[1]	102.94(12)	O1	C27	C22	123.0(4)
C17	S3	C18	108.29(17)	O1	C27	C26	118.5(4)
C18	S3	Fe[1]	107.77(13)	C22	C27	C26	118.5(4)
C27	O1	Fe	137.2(3)	C6	B1	C7	104.0(3)
C2	C1	C6	123.2(4)	C6	B1	C12	109.3(3)
C3	C2	C1	119.6(4)	C6	B1	C17	111.9(3)
C4	C3	C2	119.1(4)	C12	B1	C7	111.6(3)
C3	C4	C5	121.0(4)	C12	B1	C17	112.2(3)
C4	C5	C6	121.5(4)	C17	B1	C7	107.6(3)
C1	C6	B1	119.9(3)	C29A	C28A	C33A	120.0
C5	C6	C1	115.5(3)	C30A	C29A	C28A	120.0
C5	C6	B1	124.6(3)	C31A	C30A	C29A	120.0
B1	C7	S1	115.1(2)	C30A	C31A	C32A	120.0
C9	C8	S1	111.5(3)	C33A	C32A	C31A	120.0
C9	C8	C11	111.3(4)	C28A	C33A	C34A	120.6(7)
C10	C8	S1	105.4(3)	C32A	C33A	C28A	120.0
C10	C8	C9	111.4(4)	C32A	C33A	C34A	119.0(7)
C10	C8	C11	110.1(4)	C31B	C32B	C33B	120.0
C11	C8	S1	106.9(3)	C32B	C31B	C30B	120.0
B1	C12	S2	114.8(2)	C29B	C30B	C31B	120.0
C14	C13	S2	107.7(3)	C30B	C29B	C28B	120.0
C15	C13	S2	110.5(3)	C33B	C28B	C29B	120.0
C15	C13	C14	110.5(4)	C32B	C33B	C34B	119.7(8)
C16	C13	S2	106.8(3)	C28B	C33B	C32B	120.0
C16	C13	C14	110.6(4)	C28B	C33B	C34B	119.4(8)
C16	C13	C15	110.6(4)				

[1]2-X,-Y,1-Z

Table S28 Torsion angles.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
Fe	S1	C7	B1	62.5(3)	C5	C6	B1	C17	-126.7(4)
Fe	S1	C8	C9	72.6(3)	C6	C1	C2	C3	0.6(7)
Fe	S1	C8	C10	-48.5(3)	C7	S1	C8	C9	-48.7(4)
Fe	S1	C8	C11	-165.6(3)	C7	S1	C8	C10	-169.7(3)
Fe	S2	C12	B1	-61.6(3)	C7	S1	C8	C11	73.2(4)
Fe	S2	C13	C14	167.4(3)	C8	S1	C7	B1	-175.8(3)
Fe	S2	C13	C15	-71.8(3)	C12	S2	C13	C14	-69.5(3)

Fe	S2	C13	C16	48.6(4)	C12	S2	C13	C15	51.3(4)
Fe[1]	S3	C17	B1	141.1(2)	C12	S2	C13	C16	171.7(4)
Fe[1]	S3	C18	C19	58.7(3)	C13	S2	C12	B1	173.6(3)
Fe[1]	S3	C18	C20	-61.0(3)	C17	S3	C18	C19	-52.0(3)
Fe[1]	S3	C18	C21	-178.3(3)	C17	S3	C18	C20	-171.7(3)
Fe	O1	C27	C22	51.3(6)	C17	S3	C18	C21	71.0(3)
Fe	O1	C27	C26	-129.2(4)	C18	S3	C17	B1	-104.9(3)
S1	Fe	O1	C27	-85.7(4)	C22	C23	C24	C25	1.1(9)
S1	C7	B1	C6	168.3(3)	C23	C22	C27	O1	-179.7(4)
S1	C7	B1	C12	-74.0(4)	C23	C22	C27	C26	0.8(7)
S1	C7	B1	C17	49.5(4)	C23	C24	C25	C26	-1.3(9)
S2	Fe	O1	C27	22.4(5)	C24	C25	C26	C27	1.2(9)
S2	C12	B1	C6	-172.5(2)	C25	C26	C27	O1	179.5(5)
S2	C12	B1	C7	73.0(3)	C25	C26	C27	C22	-0.9(7)
S2	C12	B1	C17	-47.8(4)	C27	C22	C23	C24	-0.9(8)
S3[1]	Fe	O1	C27	152.9(4)	C28A	C29A	C30A	C31A	0.0
S3	C17	B1	C6	82.4(3)	C29A	C28A	C33A	C32A	0.0
S3	C17	B1	C7	-164.0(2)	C29A	C28A	C33A	C34A	-172.2(11)
S3	C17	B1	C12	-40.9(4)	C29A	C30A	C31A	C32A	0.0
C1	C2	C3	C4	-0.5(7)	C30A	C31A	C32A	C33A	0.0
C1	C6	B1	C7	-61.6(4)	C31A	C32A	C33A	C28A	0.0
C1	C6	B1	C12	179.1(3)	C31A	C32A	C33A	C34A	172.3(11)
C1	C6	B1	C17	54.3(5)	C33A	C28A	C29A	C30A	0.0
C2	C1	C6	C5	0.5(6)	C32B	C31B	C30B	C29B	0.0
C2	C1	C6	B1	179.7(4)	C31B	C32B	C33B	C28B	0.0
C2	C3	C4	C5	-0.8(8)	C31B	C32B	C33B	C34B	169(2)
C3	C4	C5	C6	2.0(7)	C31B	C30B	C29B	C28B	0.0
C4	C5	C6	C1	-1.8(6)	C30B	C29B	C28B	C33B	0.0
C4	C5	C6	B1	179.1(4)	C29B	C28B	C33B	C32B	0.0
C5	C6	B1	C7	117.5(4)	C29B	C28B	C33B	C34B	-169(2)
C5	C6	B1	C12	-1.8(5)	C33B	C32B	C31B	C30B	0.0

[1]2-X,-Y,1-Z

Table S29 Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3).

Atom	***x***	***y***	***z***	**U(eq)**
H1	13791.57	-255.3	7748.98	46
H2	14913.56	-802.96	9263.69	55
H3	13781.33	-1290.67	10790.65	62
H4	11529.23	-1200.78	10763.57	60
H5	10390.95	-587.24	9243.32	47
H7A	12562.74	1287.61	6754.54	39
H7B	11156.93	1770.29	7023.18	39

H9A	11718.56	4612.72	5310.42	78
H9B	11876.04	3519.59	6260.74	78
H9C	10510.42	3929.23	5679.64	78
H10A	11688.6	4483.45	3558.8	78
H10B	10380.21	3924.9	3884.32	78
H10C	11568.06	3327.7	3429.05	78
H11A	13729.46	3689.06	4584.43	90
H11B	13594.37	2549.11	4425.98	90
H11C	13698.74	2613.87	5543.78	90
H12A	9337.69	584.12	7690.34	37
H12B	9495.96	-689.43	7845.21	37
H14A	6132.24	-1279.97	7424.04	93
H14B	7603.17	-1370.76	7784.63	93
H14C	7308.83	-1540.31	6733.64	93
H15A	5682.04	631.69	7539.76	85
H15B	6692.18	1480.96	7023.49	85
H15C	7131.01	435.37	7977.06	85
H16A	5279.76	384.21	5929.51	110
H16B	6447.55	-19.33	5308.9	110
H16C	6297.87	1198.63	5347.61	110
H17A	12773.36	-835.1	6588.08	34
H17B	11655.19	-240.42	5774.97	34
H19A	14421.38	-3602.3	7216.2	82
H19B	14074.78	-2307.49	6845.26	82
H19C	13704.37	-2992.24	6152.79	82
H20A	12599.59	-4791.96	7715.55	77
H20B	11896.66	-4147.67	6652.74	77
H20C	11132.28	-4231.24	7685.56	77
H21A	13149.11	-3737.58	8846.14	89
H21B	11681.57	-3165.29	8759.31	89
H21C	12860.33	-2438.34	8457.9	89
H22	8936.64	2966.55	7066.52	63
H23	7823.65	3362.56	8412.56	95
H24	5655.21	4115.61	8228.06	108
H25	4573.35	4409	6719.88	99
H26	5660.31	4031.81	5391.31	64
H28A	5968.92	-2708.54	10582.83	156
H29A	5327.55	-3631.89	9532.45	157
H30A	6895.47	-4455.26	8682.42	157
H31A	9104.76	-4355.29	8882.76	157
H32A	9746.16	-3431.94	9933.13	157
H34A	9283.87	-2503.09	11047.26	208
H34B	8135.92	-2997.24	11783.66	208
H34C	7893.74	-1798.3	10982	208
H32B	9189.15	-3876.46	9329.9	157

H31B	10197.92	-2840.65	10103.01	157
H30B	8960.4	-1877.12	11033.67	157
H29B	6714.11	-1949.39	11191.23	157
H28B	5705.32	-2985.18	10418.13	157
H34D	7330.96	-4222.22	8725.77	196
H34E	6015.58	-3463.67	8784.13	196
H34F	6315.25	-4639	9616.34	196

Table S30 Atomic occupancy.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
C28A	0.651(7)	H28A	0.651(7)	C29A	0.651(7)
H29A	0.651(7)	C30A	0.651(7)	H30A	0.651(7)
C31A	0.651(7)	H31A	0.651(7)	C32A	0.651(7)
H32A	0.651(7)	C33A	0.651(7)	C34A	0.651(7)
H34A	0.651(7)	H34B	0.651(7)	H34C	0.651(7)
C32B	0.349(7)	H32B	0.349(7)	C31B	0.349(7)
H31B	0.349(7)	C30B	0.349(7)	H30B	0.349(7)
C29B	0.349(7)	H29B	0.349(7)	C28B	0.349(7)
H28B	0.349(7)	C33B	0.349(7)	C34B	0.349(7)
H34D	0.349(7)	H34E	0.349(7)	H34F	0.349(7)