Table S-I-1. Atomic Coordinates and B_{iso}/B_{eq} for 6

atom	x	y	z	B_{eq}
Fe(1)	0.7089(1)	0.0984(1)	0.4057(1)	2.81(4)
Fe(2)	0.6996(1)	0.10901(10)	0.5856(1)	2.81(4)
Cl()	0.0721(4)	0.0387(3)	0.7110(5)	11.7(2)
S()	0.5374(2)	0.1294(2)	0.4701(3)	3.79(8)
O(2)	0.8397(5)	0.0463(6)	0.5128(9)	6.0(3)
O(3)	0.8085(6)	0.2232(6)	0.3620(9)	6.0(3)
O(4)	0.7990(7)	0.2353(5)	0.6277(7)	5.5(3)
C(1)	0.6359(6)	0.1601(6)	0.4866(10)	3.1(3)
C(2)	0.6337(6)	0.2467(7)	0.4738(9)	3.1(3)
C(3)	0.6250(7)	0.2777(7)	0.384(1)	3.8(3)
C(4)	0.6151(8)	0.3536(8)	0.372(1)	5.7(5)
C(5)	0.6126(8)	0.3994(8)	0.447(2)	6.5(5)
C(6)	0.6210(9)	0.3741(9)	0.536(1)	5.0(4)
C(7)	0.6322(7)	0.2934(7)	0.552(1)	4.1(3)
C(10)	0.7784(7)	0.0716(7)	0.505(1)	3.7(3)
C(11)	0.7664(8)	0.1770(8)	0.3811(10)	3.4(3)
C(12)	0.7584(8)	0.1871(8)	0.6054(10)	3.6(3)
C(13)	0.634(1)	0.0660(9)	0.296(1)	5.0(4)
C(14)	0.6352(8)	0.0083(8)	0.3638(10)	3.5(3)
C(15)	0.7095(8)	-0.0180(8)	0.368(1)	4.1(4)
C(16)	0.752(1)	0.023(1)	0.301(1)	6.4(5)
C(17)	0.704(1)	0.0745(10)	0.262(1)	5.5(5)
C(18)	0.671(1)	0.1040(10)	0.730(1)	5.9(5)
C(19)	0.6073(9)	0.0855(8)	0.678(1)	4.6(4)

Table S-I-1. (continued)

atom	x	y	z	B_{eq}
C(20)	0.6235(8)	0.0199(8)	0.6254(10)	3.5(4)
C(21)	0.6970(10)	-0.0014(9)	0.650(1)	4.6(4)
C(22)	0.7297(10)	0.051(1)	0.713(1)	5.9(5)
C(23)	0.4768(6)	0.2045(6)	0.515(1)	4.0(3)
C(24)	0.3949(6)	0.1785(7)	0.512(1)	4.1(3)
C(25)	0.0000	0.0000	0.639(2)	11(1)
H(1)	0.6232	0.2429	0.3281	4.5047
H(2)	0.6109	0.3778	0.3058	7.5629
H(3)	0.6002	0.4518	0.4358	6.5750
H(4)	0.6222	0.4110	0.5894	6.3560
H(5)	0.6356	0.2730	0.6157	4.8880
H(6)	0.5886	0.0943	0.2753	5.3393
H(7)	0.5917	-0.0097	0.4029	4.5307
H(8)	0.7281	-0.0590	0.4132	5.5153
H(9)	0.8081	0.0156	0.2902	7.9219
H(10)	0.7211	0.1071	0.2114	5.0342
H(11)	0.6724	0.1471	0.7741	7.4741
H(12)	0.5568	0.1129	0.6782	5.3101
H(13)	0.5907	-0.0079	0.5817	4.1906
H(14)	0.7234	-0.0469	0.6217	5.0342
H(15)	0.7783	0.0485	0.7462	7.6136
H(16)	0.4834	0.2507	0.4802	4.6502
H(17)	0.4904	0.2167	0.5821	4.6502
H(18)	0.3820	0.1662	0.4463	4.8688
H(19)	0.3607	0.2148	0.5348	4.8688
H(20)	0.3890	0.1322	0.5483	6.5750
H(21)	0.0210	-0.0390	0.5950	4.0000

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table S-I-2. Atomic Coordinates and B_{iso}/B_{eq} for 7

atom	x	y	z	B_{eq}
Fe((1))	0.7539(1)	0.90980(10)	0.2010(2)	3.56(3)
Fe((2))	0.8895(1)	0.73263(10)	0.2664(2)	3.52(3)
S()	0.6261(2)	0.7020(2)	0.2483(3)	3.96(6)
O((2))	1.0001(6)	0.9304(5)	0.2883(9)	5.5(2)
O((3))	0.7993(7)	0.9196(6)	-0.1313(9)	6.4(2)
O((4))	0.9858(6)	0.6503(6)	-0.0450(10)	6.0(2)
C((10))	0.9186(9)	0.8807(7)	0.265(1)	4.1(2)
C((11))	0.7800(10)	0.9099(8)	-0.001(1)	5.0(3)
C((12))	0.9422(8)	0.6836(7)	0.077(1)	4.5(2)
C((13))	0.6374(9)	1.0634(8)	0.197(1)	4.8(3)
C((14))	0.5864(8)	0.9900(8)	0.258(1)	4.6(2)
C((15))	0.661(1)	0.9680(8)	0.413(1)	5.0(3)
C((16))	0.7534(10)	1.0267(9)	0.439(1)	5.6(3)
C((17))	0.7403(9)	1.0882(8)	0.308(1)	5.3(3)
C((18))	0.8627(10)	0.7130(10)	0.511(1)	5.5(3)
C((19))	0.9612(9)	0.7661(9)	0.534(1)	5.0(3)
C((20))	1.0443(9)	0.6942(9)	0.443(1)	5.1(3)
C((21))	0.9953(10)	0.5933(8)	0.360(1)	5.1(3)
C((22))	0.8831(9)	0.6057(8)	0.402(1)	4.8(3)
C((23))	0.4806(8)	0.7110(7)	0.129(1)	3.6(2)
C((24))	0.3928(9)	0.7859(8)	0.202(1)	4.5(3)
C((25))	0.2766(10)	0.7907(8)	0.125(1)	5.2(3)
C((26))	0.2480(9)	0.7205(9)	-0.035(2)	5.3(3)
C((27))	0.3310(10)	0.6463(8)	-0.109(1)	5.0(3)

Table S-I-2. (continued)

atom	x	y	z	B_{eq}
C((28))	0.4489(8)	0.6381(7)	-0.031(1)	3.8(2)
C((1))	0.7226(7)	0.7457(6)	0.1349(10)	2.9(2)
C((2))	0.6955(7)	0.6853(6)	-0.0499(10)	3.1(2)
C((3))	0.6242(8)	0.7393(7)	-0.175(1)	4.1(2)
C((4))	0.5908(10)	0.680(1)	-0.340(1)	5.7(3)
C((5))	0.629(1)	0.565(1)	-0.384(1)	6.3(3)
C((6))	0.6986(9)	0.5080(8)	-0.264(1)	5.5(3)
C((7))	0.7335(7)	0.5684(7)	-0.098(1)	3.9(2)
H(1)	0.5875	0.8179	-0.1360	6.3850
H(2)	0.5320	0.7080	-0.4129	6.3850
H(3)	0.6152	0.5258	-0.5103	6.3850
H(4)	0.7256	0.4321	-0.3056	6.3850
H(5)	0.7783	0.5338	-0.0211	6.3850
H(6)	0.6093	1.0802	0.0902	6.3850
H(7)	0.5279	0.9610	0.2119	6.3850
H(8)	0.6434	0.9234	0.4786	6.3850
H(9)	0.8006	1.0307	0.5126	6.3850
H(10)	0.7925	1.1298	0.2890	6.3850
H(11)	0.7993	0.7447	0.5506	6.3850
H(12)	0.9658	0.8313	0.5942	6.3850
H(13)	1.1153	0.7142	0.4350	6.3850
H(14)	1.0412	0.5279	0.2906	6.3850
H(15)	0.8306	0.5549	0.3609	6.3850
H(16)	0.4155	0.8238	0.3057	6.3850
H(17)	0.2196	0.8395	0.1703	6.3850
H(18)	0.1738	0.7301	-0.0768	6.3850
H(19)	0.3169	0.6010	-0.2105	6.3850
H(20)	0.5136	0.5872	-0.0923	6.3850

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table S-I-3. Atomic Coordinates and B_{iso}/B_{eq} for 15

atom	x	y	z	B_{eq}
Fe(1)	0.8910(3)	0.2069(1)	0.8650(1)	3.29(6)
Fe(2)	1.0560(3)	0.1902(1)	0.7507(1)	3.00(5)
S()	1.2448(5)	0.1454(2)	0.9043(2)	3.43(10)
O(2)	0.733(1)	0.2069(8)	0.7163(6)	5.8(3)
O(3)	0.796(1)	0.3928(8)	0.8593(7)	5.5(4)
O(4)	1.061(1)	0.3708(7)	0.6889(6)	5.2(3)
C(1)	1.115(2)	0.2269(9)	0.8598(7)	2.9(4)
C(2)	1.186(2)	0.3184(9)	0.8767(7)	2.5(3)
C(3)	1.311(2)	0.349(1)	0.8385(9)	4.0(4)
C(4)	1.377(2)	0.430(1)	0.8563(8)	3.7(4)
C(5)	1.328(2)	0.4839(10)	0.9135(8)	3.6(4)
C(6)	1.208(2)	0.4547(9)	0.9530(8)	3.5(4)
C(7)	1.138(2)	0.3741(9)	0.9360(7)	3.1(4)
C(8)	1.409(2)	0.573(1)	0.9305(9)	5.5(5)
C(10)	0.843(2)	0.205(1)	0.7580(8)	3.6(4)
C(11)	0.842(2)	0.320(1)	0.8608(8)	3.3(4)
C(12)	1.060(2)	0.2990(10)	0.7169(7)	3.2(4)
C(13)	0.742(3)	0.093(2)	0.874(1)	7.3(7)
C(14)	0.681(3)	0.163(2)	0.907(2)	7.4(7)
C(15)	0.776(3)	0.193(1)	0.968(1)	6.6(6)
C(16)	0.903(2)	0.133(1)	0.9716(10)	5.7(5)
C(17)	0.889(2)	0.075(1)	0.910(1)	5.6(6)
C(18)	1.004(2)	0.060(1)	0.7037(9)	4.7(5)
C(19)	1.041(2)	0.120(1)	0.6460(8)	4.6(5)

Table S-I-3. (continued)

atom	x	y	z	B_{eq}
C(20)	1.190(2)	0.149(1)	0.6598(9)	4.6(5)
C(21)	1.253(2)	0.111(1)	0.7275(8)	4.0(4)
C(22)	1.134(2)	0.055(1)	0.7541(8)	4.2(4)
C(23)	1.308(2)	0.1896(10)	0.9978(7)	4.1(4)
C(24)	1.404(2)	0.1182(9)	1.0395(7)	3.3(4)
C(25)	1.474(2)	0.152(1)	1.1146(8)	4.4(4)
C(26)	1.585(2)	0.086(1)	1.1515(9)	4.9(5)
H(1)	1.3519	0.3126	0.7992	6.1648
H(2)	1.4618	0.4494	0.8278	4.2031
H(3)	1.1701	0.4906	0.9936	4.5307
H(4)	1.0554	0.3546	0.9642	3.7404
H(5)	1.3642	0.6188	0.8981	5.4433
H(6)	1.5137	0.5678	0.9198	5.4433
H(7)	1.3990	0.5889	0.9823	6.1648
H(8)	0.7007	0.0599	0.8302	8.1479
H(9)	0.5821	0.1881	0.8906	7.9261
H(10)	0.7549	0.2402	1.0021	7.0717
H(11)	0.9825	0.1355	1.0113	6.4077
H(12)	0.9557	0.0267	0.8986	6.1648
H(13)	0.9051	0.0250	0.7071	4.7489
H(14)	0.9735	0.1436	0.6115	5.4433
H(15)	1.2434	0.1879	0.6257	4.8910
H(16)	1.3540	0.0997	0.7562	5.4433
H(17)	1.1144	0.0115	0.7973	5.4433

Table S-I-3. (continued)

atom	x	y	z	B_{eq}
H(18)	1.3671	0.2426	0.9916	5.0821
H(19)	1.2221	0.2042	1.0271	5.9628
H(20)	1.4829	0.1010	1.0076	4.0115
H(21)	1.3406	0.0684	1.0490	4.8709
H(22)	1.5232	0.2067	1.1065	5.4433
H(23)	1.3939	0.1606	1.1495	4.8709
H(24)	1.6673	0.0776	1.1179	5.6430
H(25)	1.6262	0.1110	1.1987	5.6430
H(26)	1.5379	0.0313	1.1608	5.6430

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table S-I-4. Atomic Coordinates and B_{iso}/B_{eq} for 17

atom	x	y	z	B_{eq}
Fe(1)	0.0882(2)	0.04022(6)	0.69567(6)	3.27(3)
Fe(2)	0.1711(2)	-0.05696(7)	0.81722(6)	3.24(3)
O(2)	-0.1209(9)	0.0670(4)	0.8517(4)	6.0(2)
O(3)	-0.2606(9)	-0.0253(4)	0.6291(5)	7.6(2)
O(4)	-0.1307(9)	-0.1780(4)	0.8221(4)	6.1(2)
C(1)	0.239(1)	-0.0655(4)	0.6944(4)	3.1(2)
C(2)	0.212(1)	-0.1368(5)	0.6370(5)	3.3(2)
C(3)	0.360(1)	-0.1614(6)	0.5857(6)	5.3(3)
C(4)	0.350(2)	-0.2268(6)	0.5300(6)	6.5(3)
C(5)	0.190(2)	-0.2739(6)	0.5247(6)	5.9(3)
C(6)	0.039(1)	-0.2541(5)	0.5742(6)	4.9(3)
C(7)	0.047(1)	-0.1852(5)	0.6298(5)	3.9(2)
C(10)	-0.008(1)	0.0327(5)	0.8099(5)	3.8(2)
C(11)	-0.115(1)	-0.0032(5)	0.6563(5)	4.2(2)
C(12)	-0.014(1)	-0.1290(5)	0.8161(5)	3.8(2)
C(13)	0.278(2)	0.0988(6)	0.6102(8)	6.5(3)
C(14)	0.322(2)	0.1245(7)	0.6910(9)	6.8(3)
C(15)	0.168(2)	0.1662(6)	0.7255(6)	6.1(3)
C(16)	0.024(2)	0.1643(5)	0.6630(9)	6.4(3)
C(17)	0.095(2)	0.1211(7)	0.5921(7)	7.0(4)
C(18)	0.330(2)	-0.1328(6)	0.8968(8)	6.9(3)
C(19)	0.449(2)	-0.089(1)	0.8492(8)	8.9(5)
C(20)	0.428(2)	-0.004(1)	0.866(1)	9.2(5)
C(21)	0.285(2)	0.0001(8)	0.9277(8)	7.2(4)

Table S-I-4. (continued)

atom	x	y	z	B_{eq}
C(22)	0.229(2)	-0.0775(8)	0.9462(6)	6.1(3)
H(1)	0.3670	-0.0259	0.6869	5.1603
H(2)	0.4810	-0.1290	0.5876	6.1790
H(3)	0.4585	-0.2402	0.4940	7.5505
H(4)	0.1856	-0.3212	0.4871	7.0220
H(5)	-0.0771	-0.2877	0.5713	6.2856
H(6)	-0.0659	-0.1683	0.6629	4.7657
H(7)	0.3617	0.0680	0.5717	7.6720
H(8)	0.4495	0.1161	0.7200	8.0564
H(9)	0.1593	0.1923	0.7816	7.2794
H(10)	-0.1023	0.1901	0.6669	6.1790
H(11)	0.0303	0.1120	0.5370	7.7490
H(12)	0.3188	-0.1941	0.8987	8.0878
H(13)	0.5405	-0.1132	0.8096	9.6728
H(14)	0.4961	0.0441	0.8433	10.8156
H(15)	0.2338	0.0514	0.9557	8.0610
H(16)	0.1304	-0.0930	0.9896	7.4590

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table S-II-1. Anisotropic Displacement Parameters for 6

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	0.041(1)	0.031(1)	0.0343(10)	0.0009(9)	0.0015(10)	-0.001(1)
Fe(2)	0.040(1)	0.032(1)	0.0348(10)	-0.007(1)	0.001(1)	-0.002(1)
Cl()	0.179(6)	0.117(5)	0.149(6)	0.046(5)	-0.028(5)	-0.019(5)
S()	0.035(2)	0.033(2)	0.076(3)	-0.001(1)	-0.005(2)	-0.003(2)
O(2)	0.042(5)	0.119(8)	0.068(7)	0.032(6)	0.003(6)	0.005(8)
O(3)	0.055(7)	0.066(7)	0.106(9)	-0.019(6)	0.019(7)	0.015(7)
O(4)	0.081(8)	0.048(6)	0.078(8)	-0.024(6)	-0.036(6)	-0.004(6)
C(1)	0.029(6)	0.041(7)	0.047(8)	0.001(5)	0.001(7)	-0.003(7)
C(2)	0.028(6)	0.037(7)	0.05(1)	-0.005(6)	-0.002(6)	-0.002(6)
C(3)	0.041(8)	0.034(8)	0.07(1)	0.004(6)	-0.002(7)	0.009(7)
C(4)	0.052(10)	0.035(9)	0.13(2)	0.002(7)	0.00(1)	0.001(10)
C(5)	0.030(8)	0.027(8)	0.19(2)	0.012(7)	0.00(1)	0.03(1)
C(6)	0.046(10)	0.039(9)	0.11(1)	0.006(8)	0.011(9)	-0.024(9)
C(7)	0.036(7)	0.048(8)	0.07(1)	-0.012(7)	0.005(7)	-0.024(8)
C(10)	0.047(8)	0.054(8)	0.039(8)	-0.006(6)	0.007(9)	-0.008(9)
C(11)	0.045(8)	0.038(8)	0.047(10)	0.006(7)	0.015(7)	0.001(7)
C(12)	0.052(9)	0.053(9)	0.031(8)	-0.003(8)	-0.009(7)	-0.004(7)
C(13)	0.09(1)	0.05(1)	0.05(1)	0.019(10)	-0.040(10)	-0.026(9)
C(14)	0.061(10)	0.039(8)	0.034(8)	0.000(7)	-0.003(7)	-0.016(7)
C(15)	0.048(9)	0.041(8)	0.07(1)	0.007(7)	0.003(8)	-0.013(8)
C(16)	0.08(1)	0.08(1)	0.08(1)	0.01(1)	0.02(1)	-0.05(1)
C(17)	0.10(2)	0.05(1)	0.06(1)	-0.01(1)	0.01(1)	-0.003(9)
C(18)	0.12(2)	0.05(1)	0.047(10)	-0.03(1)	0.02(1)	-0.011(9)
C(19)	0.055(10)	0.039(9)	0.08(1)	0.003(8)	0.025(9)	0.004(8)

Table S-II-1. (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(20)	0.044(8)	0.040(9)	0.048(10)	-0.010(7)	0.002(7)	0.009(7)
C(21)	0.07(1)	0.06(1)	0.048(10)	-0.013(9)	0.008(9)	0.022(8)
C(22)	0.06(1)	0.09(1)	0.07(1)	0.00(1)	-0.03(1)	0.04(1)
C(23)	0.035(7)	0.041(7)	0.08(1)	0.002(5)	0.005(8)	-0.012(8)
C(24)	0.031(6)	0.061(8)	0.064(9)	0.002(6)	-0.008(9)	0.011(8)
C(25)	0.16(3)	0.24(4)	0.03(1)	0.08(3)	0.0000	0.0000

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table S-II-2. Anisotropic Displacement Parameters for 7

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe((1))	0.0554(9)	0.0315(7)	0.0405(8)	-0.0024(6)	0.0001(6)	0.0022(6)
Fe((2))	0.0454(9)	0.0355(7)	0.0427(8)	0.0011(6)	-0.0029(6)	0.0030(6)
S()	0.056(2)	0.053(1)	0.041(1)	-0.007(1)	0.003(1)	0.014(1)
O((2))	0.065(5)	0.052(4)	0.087(5)	-0.021(4)	0.004(4)	0.002(4)
O((3))	0.124(7)	0.067(5)	0.055(5)	-0.023(4)	0.016(5)	0.009(4)
O((4))	0.067(5)	0.071(5)	0.077(5)	-0.016(4)	0.019(4)	-0.018(4)
C((10))	0.070(7)	0.043(5)	0.039(5)	-0.013(5)	0.009(5)	-0.004(4)
C((11))	0.098(9)	0.035(5)	0.047(6)	-0.014(5)	-0.013(6)	0.007(5)
C((12))	0.054(7)	0.038(5)	0.061(7)	-0.005(5)	-0.004(5)	-0.010(5)
C((13))	0.070(7)	0.038(5)	0.067(7)	-0.002(5)	0.002(6)	0.008(5)
C((14))	0.059(7)	0.040(5)	0.059(6)	0.009(5)	0.009(5)	-0.006(5)
C((15))	0.091(9)	0.042(6)	0.051(6)	0.011(6)	0.024(6)	0.000(5)
C((16))	0.064(8)	0.061(7)	0.061(7)	0.006(6)	-0.004(6)	-0.015(6)
C((17))	0.067(8)	0.039(5)	0.090(8)	-0.014(5)	0.009(6)	0.000(5)
C((18))	0.070(8)	0.081(8)	0.049(6)	0.007(6)	-0.009(6)	0.026(6)
C((19))	0.058(7)	0.070(7)	0.050(6)	-0.007(6)	-0.010(5)	0.008(5)
C((20))	0.047(6)	0.059(6)	0.074(7)	-0.001(5)	-0.010(5)	0.012(6)
C((21))	0.068(8)	0.044(6)	0.064(7)	0.020(5)	-0.004(6)	0.011(5)
C((22))	0.073(8)	0.052(6)	0.051(6)	-0.006(5)	-0.006(6)	0.013(5)
C((23))	0.046(6)	0.037(5)	0.052(6)	-0.002(4)	0.008(5)	0.013(4)
C((24))	0.052(7)	0.054(6)	0.068(7)	-0.007(5)	0.012(5)	0.015(5)
C((25))	0.065(8)	0.056(6)	0.077(7)	0.004(5)	0.026(6)	0.014(6)
C((26))	0.043(6)	0.066(7)	0.096(9)	-0.013(5)	0.004(6)	0.027(6)
C((27))	0.065(8)	0.056(6)	0.071(7)	-0.029(6)	-0.004(6)	0.018(5)

Table S-II-2. (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C((28))	0.054(7)	0.045(5)	0.051(6)	-0.009(5)	0.018(5)	0.010(4)
C((1))	0.044(5)	0.031(4)	0.033(5)	0.007(4)	0.014(4)	0.007(3)
C((2))	0.045(5)	0.035(5)	0.033(5)	-0.007(4)	-0.001(4)	0.003(4)
C((3))	0.067(7)	0.053(6)	0.036(5)	-0.017(5)	0.001(5)	0.009(4)
C((4))	0.079(8)	0.096(9)	0.043(6)	-0.033(7)	-0.009(5)	0.015(6)
C((5))	0.094(9)	0.103(10).	0.038(6)	-0.050(8)	0.004(6)	-0.016(6)
C((6))	0.073(8)	0.055(6)	0.065(7)	-0.019(6)	0.013(6)	-0.026(5)
C((7))	0.045(6)	0.039(5)	0.059(6)	-0.006(4)	0.006(5)	0.001(4)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table S-II-3. Anisotropic Displacement Parameters for 15

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	0.045(2)	0.038(1)	0.042(1)	-0.005(1)	-0.003(1)	0.000(1)
Fe(2)	0.053(2)	0.029(1)	0.030(1)	0.000(1)	-0.012(1)	0.001(1)
S()	0.055(3)	0.039(2)	0.034(2)	0.004(2)	-0.014(2)	0.001(2)
O(2)	0.074(9)	0.069(8)	0.074(8)	0.005(8)	-0.031(7)	-0.008(7)
O(3)	0.07(1)	0.049(7)	0.091(9)	0.006(8)	0.003(7)	0.005(7)
O(4)	0.11(1)	0.032(6)	0.056(7)	-0.006(7)	-0.010(7)	0.021(6)
C(1)	0.06(1)	0.028(8)	0.026(8)	0.001(8)	0.006(7)	0.005(6)
C(2)	0.032(9)	0.035(8)	0.029(7)	0.004(9)	-0.003(6)	0.003(7)
C(3)	0.04(1)	0.05(1)	0.06(1)	-0.01(1)	-0.010(9)	-0.010(9)
C(4)	0.04(1)	0.07(1)	0.034(9)	0.00(1)	-0.004(7)	0.007(9)
C(5)	0.05(1)	0.040(9)	0.041(10)	-0.02(1)	-0.029(8)	0.004(8)
C(6)	0.07(1)	0.028(8)	0.034(9)	0.01(1)	-0.015(9)	-0.009(7)
C(7)	0.06(1)	0.032(8)	0.023(8)	-0.012(9)	-0.004(7)	-0.001(6)
C(8)	0.08(2)	0.040(9)	0.08(1)	-0.02(1)	-0.05(1)	0.012(9)
C(10)	0.036(10)	0.05(1)	0.049(9)	0.01(1)	-0.016(8)	-0.006(8)
C(11)	0.04(1)	0.046(10)	0.043(9)	0.00(1)	0.007(7)	0.001(8)
C(12)	0.05(1)	0.036(9)	0.039(8)	0.009(10)	-0.005(7)	-0.002(8)
C(13)	0.08(2)	0.09(2)	0.11(2)	-0.05(2)	-0.01(1)	-0.01(1)
C(14)	0.05(1)	0.10(2)	0.13(2)	0.02(2)	0.01(1)	0.04(2)
C(15)	0.10(2)	0.07(1)	0.09(1)	0.01(2)	0.01(1)	-0.01(1)
C(16)	0.07(2)	0.09(1)	0.05(1)	0.00(1)	0.000(10)	0.01(1)
C(17)	0.06(2)	0.05(1)	0.10(2)	-0.02(1)	0.02(1)	0.00(1)
C(18)	0.08(1)	0.05(1)	0.05(1)	0.00(1)	-0.02(1)	-0.022(9)
C(19)	0.08(2)	0.05(1)	0.04(1)	0.00(1)	-0.026(9)	-0.006(8)

Table S-II-3. (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(20)	0.09(2)	0.05(1)	0.04(1)	-0.01(1)	0.009(10)	-0.002(8)
C(21)	0.06(1)	0.06(1)	0.035(9)	0.01(1)	0.004(8)	-0.012(8)
C(22)	0.07(1)	0.04(1)	0.042(10)	0.01(1)	-0.001(9)	-0.008(8)
C(23)	0.07(1)	0.054(10)	0.026(7)	0.00(1)	-0.014(8)	-0.005(8)
C(24)	0.05(1)	0.044(9)	0.028(8)	-0.011(9)	-0.001(7)	0.014(7)
C(25)	0.06(1)	0.07(1)	0.039(9)	-0.03(1)	-0.002(8)	0.011(8)
C(26)	0.07(1)	0.06(1)	0.06(1)	-0.01(1)	-0.028(10)	0.016(9)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table S-II-4. Anisotropic Displacement Parameters for 17

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	0.0503(8)	0.0375(6)	0.0363(6)	-0.0028(6)	-0.0010(5)	0.0049(6)
Fe(2)	0.0450(7)	0.0446(7)	0.0336(6)	0.0036(6)	-0.0021(5)	0.0030(6)
O(2)	0.086(5)	0.078(5)	0.065(4)	0.036(4)	0.024(4)	-0.004(3)
O(3)	0.062(5)	0.108(6)	0.120(6)	-0.010(4)	-0.030(4)	0.001(5)
O(4)	0.075(5)	0.071(5)	0.085(5)	-0.020(4)	0.023(4)	0.019(4)
C(1)	0.049(5)	0.038(5)	0.030(4)	-0.001(4)	0.005(3)	-0.002(4)
C(2)	0.051(5)	0.038(5)	0.036(5)	0.000(4)	-0.007(4)	0.003(4)
C(3)	0.072(7)	0.066(6)	0.064(6)	-0.004(6)	0.007(5)	-0.023(5)
C(4)	0.097(9)	0.071(7)	0.078(8)	0.005(7)	0.013(6)	-0.035(6)
C(5)	0.14(1)	0.043(6)	0.045(6)	0.021(7)	-0.009(7)	-0.016(5)
C(6)	0.096(8)	0.041(6)	0.049(6)	-0.017(5)	-0.029(6)	0.002(5)
C(7)	0.055(6)	0.056(5)	0.039(5)	-0.003(5)	-0.007(4)	0.007(4)
C(10)	0.049(5)	0.054(6)	0.043(5)	0.000(5)	0.000(4)	0.002(4)
C(11)	0.043(6)	0.063(6)	0.054(6)	0.010(5)	-0.007(4)	0.005(5)
C(12)	0.052(6)	0.047(5)	0.046(5)	0.001(5)	0.006(4)	0.017(4)
C(13)	0.11(1)	0.060(7)	0.076(8)	-0.019(7)	0.038(8)	0.015(6)
C(14)	0.078(8)	0.066(7)	0.11(1)	-0.036(7)	0.006(8)	0.026(7)
C(15)	0.13(1)	0.044(6)	0.055(7)	-0.023(7)	0.008(7)	-0.005(5)
C(16)	0.105(9)	0.029(5)	0.108(9)	0.006(6)	0.000(8)	0.021(6)
C(17)	0.15(1)	0.064(8)	0.058(8)	-0.023(8)	-0.012(8)	0.026(6)
C(18)	0.12(1)	0.068(7)	0.071(8)	0.058(8)	-0.052(7)	-0.004(6)
C(19)	0.054(8)	0.23(2)	0.057(8)	0.04(1)	-0.018(6)	0.02(1)
C(20)	0.064(9)	0.14(1)	0.14(1)	-0.065(10)	-0.073(9)	0.08(1)
C(22)	0.095(9)	0.106(9)	0.033(5)	0.015(8)	-0.009(5)	0.005(6)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table S-III-1. Complete Bond Lengths (Å) for 6

atom	atom	distance	atom	atom	distance
Fe(1)	Fe(2)	2.527(2)	Fe(1)	C(1)	2.03(1)
Fe(1)	C(10)	1.91(1)	Fe(1)	C(11)	1.75(1)
Fe(1)	C(13)	2.11(1)	Fe(1)	C(14)	2.13(1)
Fe(1)	C(15)	2.12(1)	Fe(1)	C(16)	2.13(1)
Fe(1)	C(17)	2.06(2)	Fe(2)	C(1)	2.00(1)
Fe(2)	C(10)	1.91(1)	Fe(2)	C(12)	1.75(2)
Fe(2)	C(18)	2.09(2)	Fe(2)	C(19)	2.11(1)
Fe(2)	C(20)	2.14(1)	Fe(2)	C(21)	2.14(1)
Fe(2)	C(22)	2.12(2)	Cl	C(25)	1.76(1)
S	C(1)	1.83(1)	S	C(23)	1.81(1)
O(2)	C(10)	1.18(1)	O(3)	C(11)	1.13(1)
O(4)	C(12)	1.15(1)	C(1)	C(2)	1.54(1)
C(2)	C(3)	1.38(2)	C(2)	C(7)	1.37(2)
C(3)	C(4)	1.36(2)	C(4)	C(5)	1.32(2)
C(5)	C(6)	1.34(2)	C(6)	C(7)	1.45(2)
C(13)	C(14)	1.39(2)	C(13)	C(17)	1.34(2)
C(14)	C(15)	1.39(2)	C(15)	C(16)	1.41(2)
C(16)	C(17)	1.37(2)	C(18)	C(19)	1.38(2)
C(18)	C(22)	1.42(2)	C(19)	C(20)	1.40(2)
C(20)	C(21)	1.39(2)	C(21)	C(22)	1.40(2)
C(23)	C(24)	1.52(2)			

Table S-III-2. Complete Bond Lengths (Å) for 7

atom	atom	distance	atom	atom	distance
Fe((1)	Fe((2)	2.523(2)	Fe((1)	C((10)	1.89(1)
Fe((1)	C((11)	1.73(1)	Fe((1)	C((13)	2.103(9)
Fe((1)	C((14)	2.131(9)	Fe((1)	C((15)	2.146(10)
Fe((1)	C((16)	2.111(9)	Fe((1)	C((17)	2.129(9)
Fe((1)	C((1))	2.026(8)	Fe((2)	C((10)	1.902(9)
Fe((2)	C((12)	1.72(1)	Fe((2)	C((18)	2.15(1)
Fe((2)	C((19)	2.132(9)	Fe((2)	C((20)	2.123(9)
Fe((2)	C((21)	2.101(9)	Fe((2)	C((22)	2.117(10)
Fe((2)	C((1))	2.032(8)	S	C((23)	1.785(9)
S	C((1))	1.829(8)	O((2))	C((10)	1.19(1)
O((3))	C((11)	1.16(1)	O((4))	C((12)	1.17(1)
C((13)	C((14)	1.39(1)	C((13)	C((17)	1.39(1)
C((14)	C((15)	1.42(1)	C((15)	C((16)	1.37(1)
C((16)	C((17)	1.40(1)	C((18)	C((19)	1.40(1)
C((18)	C((22)	1.40(1)	C((19)	C((20)	1.40(1)
C((20)	C((21)	1.42(1)	C((21)	C((22)	1.41(1)
C((23)	C((24)	1.38(1)	C((23)	C((28)	1.41(1)
C((24)	C((25)	1.38(1)	C((25)	C((26)	1.39(1)
C((26)	C((27)	1.34(1)	C((27)	C((28)	1.40(1)
C((1))	C((2))	1.50(1)	C((2))	C((3))	1.38(1)
C((2))	C((7))	1.40(1)	C((3))	C((4))	1.37(1)
C((4))	C((5))	1.37(2)	C((5))	C((6))	1.37(1)
C((6))	C((7))	1.39(1)			

Table S-III-3. Complete Bond Lengths (Å) for 15

atom	atom	distance	atom	atom	distance
Fe(1)	Fe(2)	2.530(3)	Fe(1)	C(1)	2.00(2)
Fe(1)	C(10)	1.89(1)	Fe(1)	C(11)	1.74(2)
Fe(1)	C(13)	2.16(2)	Fe(1)	C(14)	2.12(2)
Fe(1)	C(15)	2.10(2)	Fe(1)	C(16)	2.16(2)
Fe(1)	C(17)	2.11(2)	Fe(2)	C(1)	2.02(1)
Fe(2)	C(10)	1.90(2)	Fe(2)	C(12)	1.73(2)
Fe(2)	C(18)	2.15(1)	Fe(2)	C(19)	2.10(1)
Fe(2)	C(20)	2.11(2)	Fe(2)	C(21)	2.15(2)
Fe(2)	C(22)	2.13(2)	S	C(1)	1.82(1)
S	C(23)	1.82(1)	O(2)	C(10)	1.18(1)
O(3)	C(11)	1.16(2)	O(4)	C(12)	1.18(2)
C(1)	C(2)	1.52(2)	C(2)	C(3)	1.39(2)
C(2)	C(7)	1.40(2)	C(3)	C(4)	1.38(2)
C(4)	C(5)	1.37(2)	C(5)	C(6)	1.36(2)
C(5)	C(8)	1.54(2)	C(6)	C(7)	1.38(2)
C(13)	C(14)	1.32(3)	C(13)	C(17)	1.43(3)
C(14)	C(15)	1.40(3)	C(15)	C(16)	1.43(3)
C(16)	C(17)	1.38(2)	C(18)	C(19)	1.40(2)
C(18)	C(22)	1.41(2)	C(19)	C(20)	1.40(2)
C(20)	C(21)	1.40(2)	C(21)	C(22)	1.43(2)
C(23)	C(24)	1.52(2)	C(24)	C(25)	1.50(2)
C(25)	C(26)	1.51(2)			

Table S-III-4. Complete Bond Lengths (Å) for 17

atom	atom	distance	atom	atom	distance
Fe(1)	Fe(2)	2.523(2)	Fe(1)	C(1)	1.997(7)
Fe(1)	C(10)	1.923(8)	Fe(1)	C(11)	1.707(9)
Fe(1)	C(13)	2.120(10)	Fe(1)	C(14)	2.134(9)
Fe(1)	C(15)	2.142(9)	Fe(1)	C(16)	2.097(8)
Fe(1)	C(17)	2.076(9)	Fe(2)	C(1)	1.991(7)
Fe(2)	C(10)	1.913(8)	Fe(2)	C(12)	1.742(9)
Fe(2)	C(18)	2.063(9)	Fe(2)	C(19)	2.08(1)
Fe(2)	C(20)	2.14(1)	Fe(2)	C(21)	2.111(10)
Fe(2)	C(22)	2.084(9)	O(2)	C(10)	1.175(8)
O(3)	C(11)	1.165(9)	O(4)	C(12)	1.143(9)
C(1)	C(2)	1.463(9)	C(2)	C(3)	1.38(1)
C(2)	C(7)	1.41(1)	C(3)	C(4)	1.36(1)
C(4)	C(5)	1.36(1)	C(5)	C(6)	1.36(1)
C(6)	C(7)	1.40(1)	C(13)	C(14)	1.37(1)
C(13)	C(17)	1.37(1)	C(14)	C(15)	1.39(1)
C(15)	C(16)	1.41(1)	C(16)	C(17)	1.40(1)
C(18)	C(19)	1.33(2)	C(18)	C(22)	1.38(1)
C(19)	C(20)	1.40(2)	C(20)	C(21)	1.41(2)
C(21)	C(22)	1.34(1)			

Table S-IV-1. Complete Bond Angles (deg) for 6

atom	atom	atom	angle	atom	atom	atom	angle
Fe(2)	Fe(1)	C(1)	50.6(4)	Fe(2)	Fe(1)	C(10)	48.5(4)
Fe(2)	Fe(1)	C(11)	100.1(5)	Fe(2)	Fe(1)	C(13)	134.6(6)
Fe(2)	Fe(1)	C(14)	106.8(4)	Fe(2)	Fe(1)	C(15)	108.6(4)
Fe(2)	Fe(1)	C(16)	139.1(6)	Fe(2)	Fe(1)	C(17)	170.2(5)
C(1)	Fe(1)	C(10)	97.8(5)	C(1)	Fe(1)	C(11)	93.0(5)
C(1)	Fe(1)	C(13)	98.6(6)	C(1)	Fe(1)	C(14)	99.5(5)
C(1)	Fe(1)	C(15)	131.3(5)	C(1)	Fe(1)	C(16)	161.7(6)
C(1)	Fe(1)	C(17)	128.8(7)	C(10)	Fe(1)	C(11)	88.1(6)
C(10)	Fe(1)	C(13)	149.9(5)	C(10)	Fe(1)	C(14)	113.9(5)
C(10)	Fe(1)	C(15)	86.4(5)	C(10)	Fe(1)	C(16)	96.5(7)
C(10)	Fe(1)	C(17)	133.4(7)	C(11)	Fe(1)	C(13)	116.0(7)
C(11)	Fe(1)	C(14)	152.6(6)	C(11)	Fe(1)	C(15)	135.6(6)
C(11)	Fe(1)	C(16)	98.8(7)	C(11)	Fe(1)	C(17)	89.7(7)
C(13)	Fe(1)	C(14)	38.2(6)	C(13)	Fe(1)	C(15)	63.9(6)
C(13)	Fe(1)	C(16)	63.6(7)	C(13)	Fe(1)	C(17)	37.5(6)
C(14)	Fe(1)	C(15)	38.2(5)	C(14)	Fe(1)	C(16)	64.1(6)
C(14)	Fe(1)	C(17)	63.4(6)	C(15)	Fe(1)	C(16)	38.6(6)
C(15)	Fe(1)	C(17)	63.9(6)	C(16)	Fe(1)	C(17)	38.1(7)
Fe(1)	Fe(2)	C(1)	51.7(3)	Fe(1)	Fe(2)	C(10)	48.6(5)
Fe(1)	Fe(2)	C(12)	100.2(5)	Fe(1)	Fe(2)	C(18)	167.8(5)
Fe(1)	Fe(2)	C(19)	129.8(5)	Fe(1)	Fe(2)	C(20)	104.2(4)
Fe(1)	Fe(2)	C(21)	110.4(5)	Fe(1)	Fe(2)	C(22)	141.5(6)
C(1)	Fe(2)	C(10)	99.0(6)	C(1)	Fe(2)	C(12)	95.1(5)
C(1)	Fe(2)	C(18)	123.8(7)	C(1)	Fe(2)	C(19)	94.4(5)

Table S-IV-1. (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Fe(2)	C(20)	99.1(5)	C(1)	Fe(2)	C(21)	133.3(6)
C(1)	Fe(2)	C(22)	160.1(6)	C(10)	Fe(2)	C(12)	86.2(6)
C(10)	Fe(2)	C(18)	137.2(8)	C(10)	Fe(2)	C(19)	148.5(5)
C(10)	Fe(2)	C(20)	110.9(5)	C(10)	Fe(2)	C(21)	87.0(6)
C(10)	Fe(2)	C(22)	98.4(7)	C(12)	Fe(2)	C(18)	91.3(6)
C(12)	Fe(2)	C(19)	121.1(6)	C(12)	Fe(2)	C(20)	155.6(6)
C(12)	Fe(2)	C(21)	131.6(7)	C(12)	Fe(2)	C(22)	95.7(7)
C(18)	Fe(2)	C(19)	38.5(6)	C(18)	Fe(2)	C(20)	64.3(6)
C(18)	Fe(2)	C(21)	63.4(6)	C(18)	Fe(2)	C(22)	39.4(7)
C(19)	Fe(2)	C(20)	38.3(5)	C(19)	Fe(2)	C(21)	63.4(6)
C(19)	Fe(2)	C(22)	65.7(6)	C(20)	Fe(2)	C(21)	37.9(5)
C(20)	Fe(2)	C(22)	65.4(6)	C(21)	Fe(2)	C(22)	38.4(6)
C(1)	S	C(23)	107.4(5)	Fe(1)	C(1)	Fe(2)	77.7(4)
Fe(1)	C(1)	S	111.9(6)	Fe(1)	C(1)	C(2)	118.9(8)
Fe(2)	C(1)	S	119.1(6)	Fe(2)	C(1)	C(2)	122.9(8)
S	C(1)	C(2)	104.7(7)	C(1)	C(2)	C(3)	120(1)
C(1)	C(2)	C(7)	120(1)	C(3)	C(2)	C(7)	119(1)
C(2)	C(3)	C(4)	121(1)	C(3)	C(4)	C(5)	120(1)
C(4)	C(5)	C(6)	122(1)	C(5)	C(6)	C(7)	118(1)
C(2)	C(7)	C(6)	118(1)	Fe(1)	C(10)	Fe(2)	82.9(5)
Fe(1)	C(10)	O(2)	138(1)	Fe(2)	C(10)	O(2)	138(1)
Fe(1)	C(11)	O(3)	173(1)	Fe(2)	C(12)	O(4)	172(1)
Fe(1)	C(13)	C(14)	72.0(8)	Fe(1)	C(13)	C(17)	69(1)
C(14)	C(13)	C(17)	107(1)	Fe(1)	C(14)	C(13)	69.8(9)

Table S-IV-1. (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Fe(1)	C(14)	C(15)	70.3(8)	C(13)	C(14)	C(15)	107(1)
Fe(1)	C(15)	C(14)	71.5(8)	Fe(1)	C(15)	C(16)	71.1(9)
C(14)	C(15)	C(16)	107(1)	Fe(1)	C(16)	C(15)	70.2(8)
Fe(1)	C(16)	C(17)	68.2(9)	C(15)	C(16)	C(17)	105(1)
Fe(1)	C(17)	C(13)	73.1(9)	Fe(1)	C(17)	C(16)	73(1)
C(13)	C(17)	C(16)	111(1)	Fe(2)	C(18)	C(19)	71.9(9)
Fe(2)	C(18)	C(22)	71.6(9)	C(19)	C(18)	C(22)	110(1)
Fe(2)	C(19)	C(18)	69.6(9)	Fe(2)	C(19)	C(20)	71.8(8)
C(18)	C(19)	C(20)	107(1)	Fe(2)	C(20)	C(19)	69.8(8)
Fe(2)	C(20)	C(21)	71.1(8)	C(19)	C(20)	C(21)	106(1)
Fe(2)	C(21)	C(20)	71.0(8)	Fe(2)	C(21)	C(22)	69.9(9)
C(20)	C(21)	C(22)	111(1)	Fe(2)	C(22)	C(18)	69.0(9)
Fe(2)	C(22)	C(21)	71.7(9)	C(18)	C(22)	C(21)	104(1)
S	C(23)	C(24)	109.4(8)	Cl	C(25)	Cl	110(1)

Table S-IV-2. Complete Bond Angles (deg) for 7

atom	atom	atom	angle	atom	atom	atom	angle
Fe((2)	Fe((1)	C((10)	48.5(3)	Fe((2)	Fe((1)	C((11)	100.7(3)
Fe((2)	Fe((1)	C((13)	168.8(3)	Fe((2)	Fe((1)	C((14)	134.2(3)
Fe((2)	Fe((1)	C((15)	104.9(3)	Fe((2)	Fe((1)	C((16)	106.1(3)
Fe((2)	Fe((1)	C((17)	135.9(3)	Fe((2)	Fe((1)	C((1))	51.7(2)
C((10)	Fe((1)	C((11)	85.7(4)	C((10)	Fe((1)	C((13)	131.6(4)
C((10)	Fe((1)	C((14)	151.0(4)	C((10)	Fe((1)	C((15)	114.8(4)
C((10)	Fe((1)	C((16)	87.2(4)	C((10)	Fe((1)	C((17)	95.0(4)
C((10)	Fe((1)	C((1))	98.2(4)	C((11)	Fe((1)	C((13)	90.4(4)
C((11)	Fe((1)	C((14)	116.7(4)	C((11)	Fe((1)	C((15)	154.0(4)
C((11)	Fe((1)	C((16)	136.7(5)	C((11)	Fe((1)	C((17)	99.8(4)
C((11)	Fe((1)	C((1))	93.6(4)	C((13)	Fe((1)	C((14)	38.5(4)
C((13)	Fe((1)	C((15)	64.3(4)	C((13)	Fe((1)	C((16)	63.7(4)
C((13)	Fe((1)	C((17)	38.3(4)	C((13)	Fe((1)	C((1))	130.2(4)
C((14)	Fe((1)	C((15)	38.9(4)	C((14)	Fe((1)	C((16)	64.0(4)
C((14)	Fe((1)	C((17)	64.7(4)	C((14)	Fe((1)	C((1))	98.3(3)
C((15)	Fe((1)	C((16)	37.6(4)	C((15)	Fe((1)	C((17)	64.4(4)
C((15)	Fe((1)	C((1))	98.6(4)	C((16)	Fe((1)	C((17)	38.6(4)
C((16)	Fe((1)	C((1))	129.7(4)	C((17)	Fe((1)	C((1))	161.9(4)
Fe((1)	Fe((2)	C((10)	48.2(3)	Fe((1)	Fe((2)	C((12)	100.5(3)
Fe((1)	Fe((2)	C((18)	106.2(3)	Fe((1)	Fe((2)	C((19)	107.6(3)
Fe((1)	Fe((2)	C((20)	136.8(3)	Fe((1)	Fe((2)	C((21)	170.8(3)
Fe((1)	Fe((2)	C((22)	134.4(3)	Fe((1)	Fe((2)	C((1))	51.5(2)
C((10)	Fe((2)	C((12)	88.2(4)	C((10)	Fe((2)	C((18)	114.3(4)
C((10)	Fe((2)	C((19)	86.7(4)	C((10)	Fe((2)	C((20)	94.9(4)

Table S-IV-2. (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C((10)	Fe((2)	C((21)	132.5(5)	C((10)	Fe((2)	C((22)	150.5(4)
C((10)	Fe((2)	C((1))	97.7(4)	C((12)	Fe((2)	C((18)	152.6(4)
C((12)	Fe((2)	C((19)	136.7(4)	C((12)	Fe((2)	C((20)	99.6(4)
C((12)	Fe((2)	C((21)	88.7(4)	C((12)	Fe((2)	C((22)	115.6(4)
C((12)	Fe((2)	C((1))	90.7(4)	C((18)	Fe((2)	C((19)	38.0(4)
C((18)	Fe((2)	C((20)	64.8(4)	C((18)	Fe((2)	C((21)	64.8(4)
C((18)	Fe((2)	C((22)	38.4(4)	C((18)	Fe((2)	C((1))	100.8(4)
C((19)	Fe((2)	C((20)	38.4(4)	C((19)	Fe((2)	C((21)	64.5(4)
C((19)	Fe((2)	C((22)	64.2(4)	C((19)	Fe((2)	C((1))	132.5(4)
C((20)	Fe((2)	C((21)	39.3(4)	C((20)	Fe((2)	C((22)	65.4(4)
C((20)	Fe((2)	C((1))	163.9(4)	C((21)	Fe((2)	C((22)	39.1(4)
C((21)	Fe((2)	C((1))	129.7(4)	C((22)	Fe((2)	C((1))	99.0(4)
C((23)	S	C((1))	110.2(4)	Fe((1)	C((10)	Fe((2)	83.3(4)
Fe((1)	C((10)	O((2))	138.2(8)	Fe((2)	C((10)	O((2))	138.5(8)
Fe((1)	C((11)	O((3))	174.1(8)	Fe((2)	C((12)	O((4))	175.3(9)
Fe((1)	C((13)	C((14)	71.9(5)	Fe((1)	C((13)	C((17)	71.9(6)
C((14)	C((13)	C((17)	109.9(9)	Fe((1)	C((14)	C((13)	69.7(6)
Fe((1)	C((14)	C((15)	71.1(6)	C((13)	C((14)	C((15)	106.6(9)
Fe((1)	C((15)	C((14)	70.0(5)	Fe((1)	C((15)	C((16)	69.8(6)
C((14)	C((15)	C((16)	107.0(9)	Fe((1)	C((16)	C((15)	72.6(6)
Fe((1)	C((16)	C((17)	71.4(6)	C((15)	C((16)	C((17)	110.5(9)
Fe((1)	C((17)	C((13)	69.8(5)	Fe((1)	C((17)	C((16)	70.0(5)
C((13)	C((17)	C((16)	105.8(9)	Fe((2)	C((18)	C((19)	70.3(6)
Fe((2)	C((18)	C((22)	69.6(6)	C((19)	C((18)	C((22)	107.5(10)

Table S-IV-2. (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Fe((2)	C((19)	C((18)	71.6(5)	Fe((2)	C((19)	C((20)	70.5(5)
C((18)	C((19)	C((20)	109.9(9)	Fe((2)	C((20)	C((19)	71.1(5)
Fe((2)	C((20)	C((21)	69.5(5)	C((19)	C((20)	C((21)	106.5(9)
Fe((2)	C((21)	C((20)	71.2(5)	Fe((2)	C((21)	C((22)	71.1(5)
C((20)	C((21)	C((22)	108.1(9)	Fe((2)	C((22)	C((18)	72.0(6)
Fe((2)	C((22)	C((21)	69.8(6)	C((18)	C((22)	C((21)	108.0(9)
S	C((23)	C((24)	118.9(7)	S	C((23)	C((28)	122.8(7)
C((24)	C((23)	C((28)	118.0(8)	C((23)	C((24)	C((25)	122.5(9)
C((24)	C((25)	C((26)	118.3(9)	C((25)	C((26)	C((27)	120.5(10)
C((26)	C((27)	C((28)	121.9(10)	C((23)	C((28)	C((27)	118.6(8)
Fe((1)	C((1))	Fe((2)	76.9(3)	Fe((1)	C((1))	S	118.6(4)
Fe((1)	C((1))	C((2))	121.9(5)	Fe((2)	C((1))	S	110.7(4)
Fe((2)	C((1))	C((2))	120.5(5)	S	C((1))	C((2))	106.1(6)
C((1))	C((2))	C((3))	122.2(7)	C((1))	C((2))	C((7))	120.2(7)
C((3))	C((2))	C((7))	117.3(7)	C((2))	C((3))	C((4))	121.4(9)
C((3))	C((4))	C((5))	120.5(10)	C((4))	C((5))	C((6))	120.1(9)
C((5))	C((6))	C((7))	119.4(9)	C((2))	C((7))	C((6))	121.3(9)

Table S-IV-3. Complete Bond Angles (deg) for 15

atom	atom	atom	angle	atom	atom	atom	angle
Fe(2)	Fe(1)	C(1)	51.5(4)	Fe(2)	Fe(1)	C(10)	48.3(5)
Fe(2)	Fe(1)	C(11)	102.2(5)	Fe(2)	Fe(1)	C(13)	110.6(7)
Fe(2)	Fe(1)	C(14)	141.3(8)	Fe(2)	Fe(1)	C(15)	167.1(6)
Fe(2)	Fe(1)	C(16)	128.2(6)	Fe(2)	Fe(1)	C(17)	102.4(6)
C(1)	Fe(1)	C(10)	97.8(6)	C(1)	Fe(1)	C(11)	95.4(7)
C(1)	Fe(1)	C(13)	136.5(9)	C(1)	Fe(1)	C(14)	159.8(7)
C(1)	Fe(1)	C(15)	124.4(8)	C(1)	Fe(1)	C(16)	96.0(6)
C(1)	Fe(1)	C(17)	100.4(7)	C(10)	Fe(1)	C(11)	85.8(6)
C(10)	Fe(1)	C(13)	87.2(7)	C(10)	Fe(1)	C(14)	99.9(9)
C(10)	Fe(1)	C(15)	137.8(8)	C(10)	Fe(1)	C(16)	147.1(7)
C(10)	Fe(1)	C(17)	110.3(8)	C(11)	Fe(1)	C(13)	128(1)
C(11)	Fe(1)	C(14)	95.3(9)	C(11)	Fe(1)	C(15)	90.2(7)
C(11)	Fe(1)	C(16)	122.3(8)	C(11)	Fe(1)	C(17)	155.4(8)
C(13)	Fe(1)	C(14)	36.0(8)	C(13)	Fe(1)	C(15)	62.9(8)
C(13)	Fe(1)	C(16)	62.7(7)	C(13)	Fe(1)	C(17)	39.3(8)
C(14)	Fe(1)	C(15)	38.6(7)	C(14)	Fe(1)	C(16)	63.8(8)
C(14)	Fe(1)	C(17)	64.4(8)	C(15)	Fe(1)	C(16)	39.3(7)
C(15)	Fe(1)	C(17)	65.3(8)	C(16)	Fe(1)	C(17)	37.6(6)
Fe(1)	Fe(2)	C(1)	50.6(4)	Fe(1)	Fe(2)	C(10)	48.0(4)
Fe(1)	Fe(2)	C(12)	101.3(5)	Fe(1)	Fe(2)	C(18)	105.5(5)
Fe(1)	Fe(2)	C(19)	135.7(6)	Fe(1)	Fe(2)	C(20)	168.8(4)
Fe(1)	Fe(2)	C(21)	134.2(4)	Fe(1)	Fe(2)	C(22)	105.4(5)
C(1)	Fe(2)	C(10)	96.7(6)	C(1)	Fe(2)	C(12)	93.3(6)
C(1)	Fe(2)	C(18)	130.1(6)	C(1)	Fe(2)	C(19)	162.4(6)

Table S-IV-3. (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Fe(2)	C(20)	130.9(7)	C(1)	Fe(2)	C(21)	98.7(6)
C(1)	Fe(2)	C(22)	99.3(5)	C(10)	Fe(2)	C(12)	86.9(7)
C(10)	Fe(2)	C(18)	86.4(7)	C(10)	Fe(2)	C(19)	95.4(7)
C(10)	Fe(2)	C(20)	132.3(7)	C(10)	Fe(2)	C(21)	152.1(7)
C(10)	Fe(2)	C(22)	115.2(7)	C(12)	Fe(2)	C(18)	136.6(6)
C(12)	Fe(2)	C(19)	100.1(6)	C(12)	Fe(2)	C(20)	89.8(7)
C(12)	Fe(2)	C(21)	115.2(7)	C(12)	Fe(2)	C(22)	152.7(7)
C(18)	Fe(2)	C(19)	38.3(6)	C(18)	Fe(2)	C(20)	64.5(7)
C(18)	Fe(2)	C(21)	65.9(6)	C(18)	Fe(2)	C(22)	38.5(6)
C(19)	Fe(2)	C(20)	38.7(6)	C(19)	Fe(2)	C(21)	65.3(6)
C(19)	Fe(2)	C(22)	63.8(5)	C(20)	Fe(2)	C(21)	38.4(5)
C(20)	Fe(2)	C(22)	63.7(6)	C(21)	Fe(2)	C(22)	39.1(6)
C(1)	S	C(23)	107.6(6)	Fe(1)	C(1)	Fe(2)	77.9(5)
Fe(1)	C(1)	S	118.8(7)	Fe(1)	C(1)	C(2)	121.3(10)
Fe(2)	C(1)	S	110.5(7)	Fe(2)	C(1)	C(2)	120.7(9)
S	C(1)	C(2)	105.8(9)	C(1)	C(2)	C(3)	121(1)
C(1)	C(2)	C(7)	122(1)	C(3)	C(2)	C(7)	115(1)
C(2)	C(3)	C(4)	120(1)	C(3)	C(4)	C(5)	122(1)
C(4)	C(5)	C(6)	117(1)	C(4)	C(5)	C(8)	119(1)
C(6)	C(5)	C(8)	123(1)	C(5)	C(6)	C(7)	121(1)
C(2)	C(7)	C(6)	122(1)	Fe(1)	C(10)	Fe(2)	83.6(5)
Fe(1)	C(10)	O(2)	138(1)	Fe(2)	C(10)	O(2)	137(1)
Fe(1)	C(11)	O(3)	173(1)	Fe(2)	C(12)	O(4)	175(1)
Fe(1)	C(13)	C(14)	70(1)	Fe(1)	C(13)	C(17)	68(1)

Table S-IV-3. (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(14)	C(13)	C(17)	109(2)	Fe(1)	C(14)	C(13)	73(1)
Fe(1)	C(14)	C(15)	70(1)	C(13)	C(14)	C(15)	109(2)
Fe(1)	C(15)	C(14)	71(1)	Fe(1)	C(15)	C(16)	72(1)
C(14)	C(15)	C(16)	106(1)	Fe(1)	C(16)	C(15)	68(1)
Fe(1)	C(16)	C(17)	69(1)	C(15)	C(16)	C(17)	108(1)
Fe(1)	C(17)	C(13)	72(1)	Fe(1)	C(17)	C(16)	73(1)
C(13)	C(17)	C(16)	105(1)	Fe(2)	C(18)	C(19)	69.0(9)
Fe(2)	C(18)	C(22)	69.9(9)	C(19)	C(18)	C(22)	105(1)
Fe(2)	C(19)	C(18)	72.7(9)	Fe(2)	C(19)	C(20)	70.8(9)
C(18)	C(19)	C(20)	109(1)	Fe(2)	C(20)	C(19)	70(1)
Fe(2)	C(20)	C(21)	72.5(9)	C(19)	C(20)	C(21)	110(1)
Fe(2)	C(21)	C(20)	69.1(10)	Fe(2)	C(21)	C(22)	69.6(9)
C(20)	C(21)	C(22)	104(1)	Fe(2)	C(22)	C(18)	71.6(9)
Fe(2)	C(22)	C(21)	71.3(9)	C(18)	C(22)	C(21)	110(1)
S	C(23)	C(24)	108.4(10)	C(23)	C(24)	C(25)	112(1)
C(24)	C(25)	C(26)	112(1)				

Table S-IV-4. Complete Bond Angles (deg) for 17

atom	atom	atom	angle	atom	atom	atom	angle
Fe(2)	Fe(1)	C(1)	50.7(2)	Fe(2)	Fe(1)	C(10)	48.7(2)
Fe(2)	Fe(1)	C(11)	102.3(3)	Fe(2)	Fe(1)	C(13)	127.2(4)
Fe(2)	Fe(1)	C(14)	103.8(3)	Fe(2)	Fe(1)	C(15)	110.8(3)
Fe(2)	Fe(1)	C(16)	144.6(4)	Fe(2)	Fe(1)	C(17)	165.2(4)
C(1)	Fe(1)	C(10)	98.5(3)	C(1)	Fe(1)	C(11)	95.7(3)
C(1)	Fe(1)	C(13)	91.6(4)	C(1)	Fe(1)	C(14)	97.0(4)
C(1)	Fe(1)	C(15)	131.1(5)	C(1)	Fe(1)	C(16)	155.8(4)
C(1)	Fe(1)	C(17)	120.2(5)	C(10)	Fe(1)	C(11)	90.5(4)
C(10)	Fe(1)	C(13)	147.6(5)	C(10)	Fe(1)	C(14)	110.5(5)
C(10)	Fe(1)	C(15)	87.1(4)	C(10)	Fe(1)	C(16)	102.1(4)
C(10)	Fe(1)	C(17)	141.0(5)	C(11)	Fe(1)	C(13)	119.1(5)
C(11)	Fe(1)	C(14)	153.4(4)	C(11)	Fe(1)	C(15)	132.9(5)
C(11)	Fe(1)	C(16)	96.7(4)	C(11)	Fe(1)	C(17)	89.7(4)
C(13)	Fe(1)	C(14)	37.4(4)	C(13)	Fe(1)	C(15)	63.6(4)
C(13)	Fe(1)	C(16)	64.2(4)	C(13)	Fe(1)	C(17)	38.0(4)
C(14)	Fe(1)	C(15)	37.9(4)	C(14)	Fe(1)	C(16)	63.9(4)
C(14)	Fe(1)	C(17)	63.7(4)	C(15)	Fe(1)	C(16)	38.7(4)
C(15)	Fe(1)	C(17)	65.0(4)	C(16)	Fe(1)	C(17)	39.3(4)
Fe(1)	Fe(2)	C(1)	50.8(2)	Fe(1)	Fe(2)	C(10)	49.0(2)
Fe(1)	Fe(2)	C(12)	103.3(3)	Fe(1)	Fe(2)	C(18)	160.0(5)
Fe(1)	Fe(2)	C(19)	123.1(5)	Fe(1)	Fe(2)	C(20)	102.5(3)
Fe(1)	Fe(2)	C(21)	116.0(4)	Fe(1)	Fe(2)	C(22)	150.6(4)
C(1)	Fe(2)	C(10)	99.0(3)	C(1)	Fe(2)	C(12)	97.5(3)
C(1)	Fe(2)	C(18)	114.2(5)	C(1)	Fe(2)	C(19)	89.0(4)

Table S-IV-4. (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Fe(2)	C(20)	99.3(6)	C(1)	Fe(2)	C(21)	136.8(6)
C(1)	Fe(2)	C(22)	151.6(4)	C(10)	Fe(2)	C(12)	90.0(3)
C(10)	Fe(2)	C(18)	146.3(4)	C(10)	Fe(2)	C(19)	145.0(6)
C(10)	Fe(2)	C(20)	106.4(6)	C(10)	Fe(2)	C(21)	88.4(4)
C(10)	Fe(2)	C(22)	107.4(4)	C(12)	Fe(2)	C(18)	91.2(5)
C(12)	Fe(2)	C(19)	122.9(7)	C(12)	Fe(2)	C(20)	154.2(4)
C(12)	Fe(2)	C(21)	125.1(6)	C(12)	Fe(2)	C(22)	92.6(4)
C(18)	Fe(2)	C(19)	37.3(5)	C(18)	Fe(2)	C(20)	64.0(5)
C(18)	Fe(2)	C(21)	63.7(4)	C(18)	Fe(2)	C(22)	38.8(4)
C(19)	Fe(2)	C(20)	38.6(5)	C(19)	Fe(2)	C(21)	63.8(5)
C(19)	Fe(2)	C(22)	63.4(4)	C(20)	Fe(2)	C(21)	38.7(5)
C(20)	Fe(2)	C(22)	63.8(5)	C(21)	Fe(2)	C(22)	37.1(4)
Fe(1)	C(1)	Fe(2)	78.5(3)	Fe(1)	C(1)	C(2)	126.9(5)
Fe(2)	C(1)	C(2)	128.1(5)	C(1)	C(2)	C(3)	119.1(7)
C(1)	C(2)	C(7)	125.5(7)	C(3)	C(2)	C(7)	115.4(7)
C(2)	C(3)	C(4)	123.5(9)	C(3)	C(4)	C(5)	120.4(9)
C(4)	C(5)	C(6)	119.3(9)	C(5)	C(6)	C(7)	120.7(9)
C(2)	C(7)	C(6)	120.6(8)	Fe(1)	C(10)	Fe(2)	82.3(3)
Fe(1)	C(10)	O(2)	137.5(7)	Fe(2)	C(10)	O(2)	140.3(7)
Fe(1)	C(11)	O(3)	173.7(8)	Fe(2)	C(12)	O(4)	174.4(7)
Fe(1)	C(13)	C(14)	71.8(6)	Fe(1)	C(13)	C(17)	69.2(6)
C(14)	C(13)	C(17)	108(1)	Fe(1)	C(14)	C(13)	70.7(6)
Fe(1)	C(14)	C(15)	71.3(6)	C(13)	C(14)	C(15)	109(1)
Fe(1)	C(15)	C(14)	70.7(6)	Fe(1)	C(15)	C(16)	68.9(5)

Table S-IV-4. (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(14)	C(15)	C(16)	106.4(9)	Fe(1)	C(16)	C(15)	72.4(6)
Fe(1)	C(16)	C(17)	69.5(5)	C(15)	C(16)	C(17)	107.6(10)
Fe(1)	C(17)	C(13)	72.7(6)	Fe(1)	C(17)	C(16)	71.1(6)
C(13)	C(17)	C(16)	107(1)	Fe(2)	C(18)	C(19)	72.2(6)
Fe(2)	C(18)	C(22)	71.4(5)	C(19)	C(18)	C(22)	108(1)
Fe(2)	C(19)	C(18)	70.5(7)	Fe(2)	C(19)	C(20)	72.8(7)
C(18)	C(19)	C(20)	109(1)	Fe(2)	C(20)	C(19)	68.7(7)
Fe(2)	C(20)	C(21)	69.6(6)	C(19)	C(20)	C(21)	104(1)
Fe(2)	C(21)	C(20)	71.7(7)	Fe(2)	C(21)	C(22)	70.4(6)
C(20)	C(21)	C(22)	108(1)	Fe(2)	C(22)	C(18)	69.8(5)
Fe(2)	C(22)	C(21)	72.5(6)	C(18)	C(22)	C(21)	108(1)

Table S-V-1. Least Squares Planes for 6

Plane number 1

Atoms defining plane	Distance
Fe(1)	0.0000
Fe(2)	0.0000
C(1)	0.0000
Additional Atoms	**Distance**
C(10)	0.395

Plane number 2

Atoms defining plane	Distance
Fe(1)	0.0000
Fe(2)	0.0000
C(10)	0.0000
Additional Atoms	**Distance**
C(1)	-0.432

Plane number 3

Atoms defining plane	Distance
C(2)	0.00(1)
C(3)	0.00(1)
C(4)	0.00(1)
C(5)	-0.01(2)
C(6)	0.00(1)
C(7)	0.00(1)

Plane number 4

Atoms defining plane	Distance
C(13)	0.00(1)
C(14)	0.00(1)
C(15)	0.01(1)
C(16)	-0.02(2)
C(17)	0.02(2)
Additional Atoms	**Distance**
Fe(1)	1.754

Table S-V-1. (continued)

Plane number 5

Atoms defining plane	Distance
C(18)	0.00(2)
C(19)	0.00(1)
C(20)	0.01(1)
C(21)	-0.01(1)
C(22)	0.02(2)

Additional Atoms	Distance
Fe(2)	1.756

Summary

plane	mean deviation	χ^2
1	0.0000	0.0
2	0.0000	0.0
3	0.0030	0.3
4	0.0118	3.1
5	0.0097	2.6

Dihedral angles between planes (°)

plane	1	2	3	4
2	164.00			
3	43.23	120.97		
4	50.18	131.86	75.53	
5	49.21	132.29	62.87	95.84

Table S-V-2. Least Squares Planes for 7

Plane number 1

Atoms defining plane	Distance
Fe((1)	0.0000
Fe((2)	0.0000
C((10)	0.0000
Additional Atoms	**Distance**
O((2))	0.020

Plane number 2

Atoms defining plane	Distance
Fe((1)	0.0000
Fe((2)	0.0000
C((1))	0.0000
Additional Atoms	**Distance**
S	1.539

Plane number 3

Atoms defining plane	Distance
C((13)	0.003(9)
C((14)	0.001(8)
C((15)	-0.005(9)
C((16)	0.008(10)
C((17)	-0.007(10)
Additional Atoms	**Distance**
Fe((1)	1.761

Plane number 4

Atoms defining plane	Distance
C((18)	0.002(9)
C((19)	-0.002(9)
C((20)	0.001(10)
C((21)	0.001(9)
C((22)	-0.002(9)
Additional Atoms	**Distance**
Fe((2)	-1.755

Table S-V-2. (continued)

Plane number 5

Atoms defining plane	Distance
C((2))	-0.003(8)
C((3))	0.001(9)
C((4))	0.00(1)
C((5))	0.01(1)
C((6))	-0.01(1)
C((7))	0.007(9)

Plane number 6

Atoms defining plane	Distance
C((23)	0.005(8)
C((24)	0.007(9)
C((25)	-0.018(10)
C((26)	0.014(10)
C((27)	0.001(9)
C((28)	-0.008(8)

Summary

plane	mean deviation	χ^2
1	0.0000	0.0
2	0.0000	0.0
3	0.0050	1.7
4	0.0017	0.2
5	0.0060	2.6
6	0.0089	6.6

Dihedral angles between planes (°)

plane	1	2	3	4	5
2	160.55				
3	45.55	131.65			
4	132.31	50.71	86.76		
5	62.82	136.40	65.20	102.25	
6	62.89	129.26	97.79	141.55	48.25

Table S-V-3. Least Squares Planes for 15

Plane number 1

Atoms defining plane	Distance
C(13)	-0.04(2)
C(14)	0.00(2)
C(15)	0.03(2)
C(16)	-0.03(2)
C(17)	0.04(2)

Additional Atoms	Distance
Fe(1)	1.769

Plane number 2

Atoms defining plane	Distance
C(18)	0.01(2)
C(19)	-0.01(2)
C(20)	0.01(2)
C(21)	0.00(1)
C(22)	0.00(1)

Additional Atoms	Distance
Fe(2)	-1.760

Plane number 3

Atoms defining plane	Distance
Fe(1)	0.0000
Fe(2)	0.0000
C(10)	0.0000

Plane number 4

Atoms defining plane	Distance
Fe(1)	0.0000
Fe(2)	0.0000
C(1)	0.0000

Table S-V-3. (continued)

Plane number 5

Atoms defining plane	Distance
C(2)	-0.01(1)
C(3)	0.02(1)
C(4)	0.00(1)
C(5)	0.00(1)
C(6)	0.00(1)
C(7)	0.01(1)

Summary

plane	mean deviation	χ^2
1	0.0286	12.6
2	0.0046	0.5
3	0.0000	0.0
4	0.0000	0.0
5	0.0079	2.6

Dihedral angles between planes (°)

plane	1	2	3	4
2	88.81			
3	134.53	45.77		
4	47.89	131.34	160.25	
5	113.31	77.32	65.65	133.92

Table S-V-4. Least Squares Planes for 17

Plane number 1

Atoms defining plane	Distance
Fe(1)	0.0000
Fe(2)	0.0000
C(10)	0.0000

Additional Atoms	Distance
O(2)	-0.008
C(1)	-0.345

Plane number 2

Atoms defining plane	Distance
Fe(1)	0.0000
Fe(2)	0.0000
C(1)	0.0000

Additional Atoms	Distance
O(2)	0.593
C(10)	0.323

Plane number 3

Atoms defining plane	Distance
C(2)	0.001(7)
C(3)	0.011(9)
C(4)	-0.01(1)
C(5)	-0.001(9)
C(6)	0.010(8)
C(7)	-0.007(7)

Plane number 4

Atoms defining plane	Distance
C(13)	0.009(9)
C(14)	-0.006(9)
C(15)	0.002(9)
C(16)	0.003(9)
C(17)	-0.009(10)

Additional Atoms	Distance
Fe(1)	-1.753

Table S-V-4. (continued)

Plane number 5

Atoms defining plane	Distance
C(18)	-0.003(9)
C(19)	0.00(1)
C(20)	0.00(1)
C(21)	-0.005(10)
C(22)	0.004(9)

Additional Atoms	Distance
Fe(2)	-1.743

Summary

plane	mean deviation	χ^2
1	0.0000	0.0
2	0.0000	0.0
3	0.0073	5.1
4	0.0059	2.2
5	0.0030	0.5

Dihedral angles between planes (°)

plane	1	2	3	4
2	167.09			
3	85.64	95.36		
4	47.72	131.77	132.72	
5	47.96	132.12	37.70	95.21