Structural and magnetic properties of iron(II) complexes with 1,4,5,8,9,12-hexaazatriphenylene (HAT)

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Supplementary materials

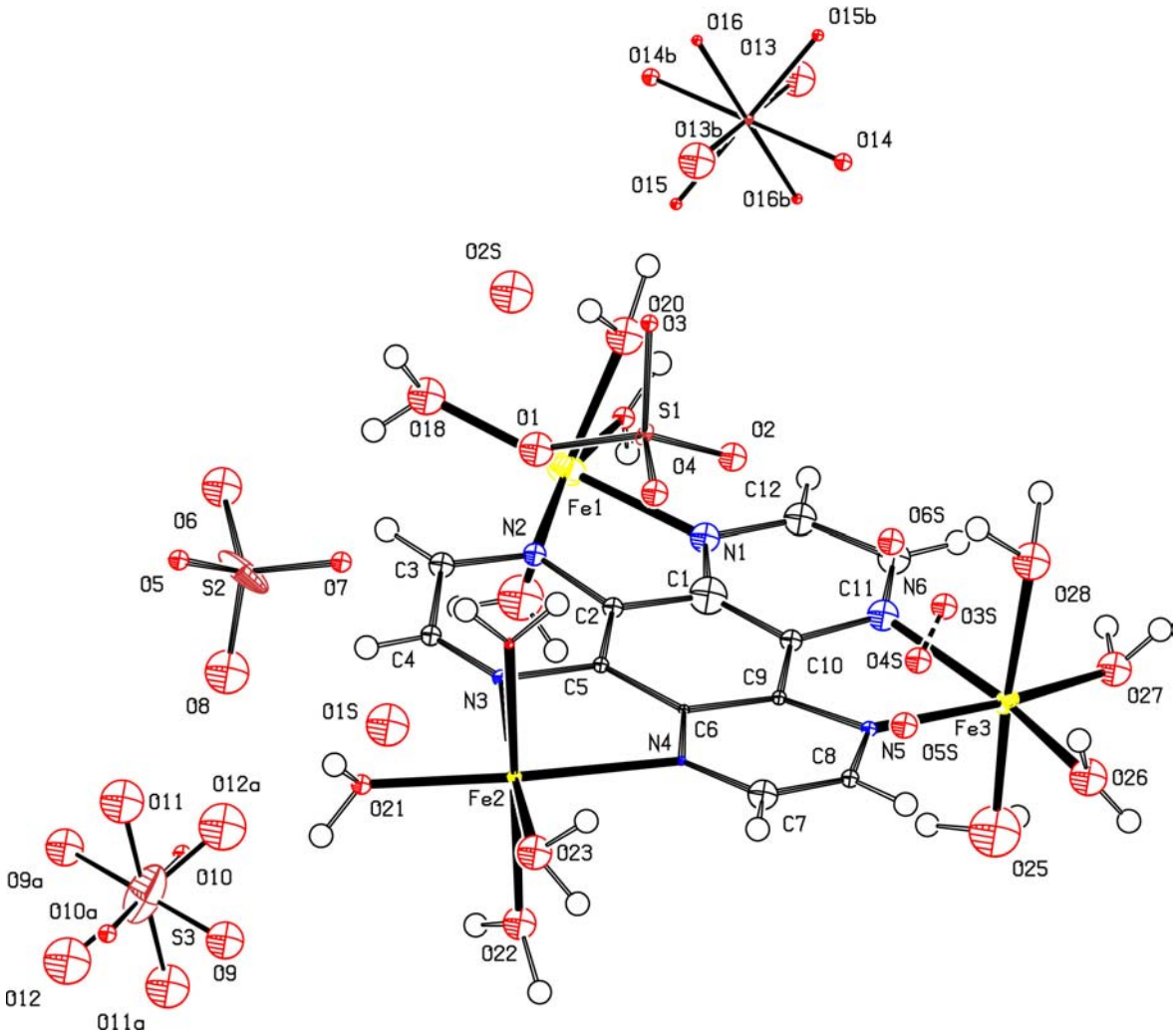

Fig. 1A. ORTEP plot of the asymmetric unit in the crystals structure of **1**.

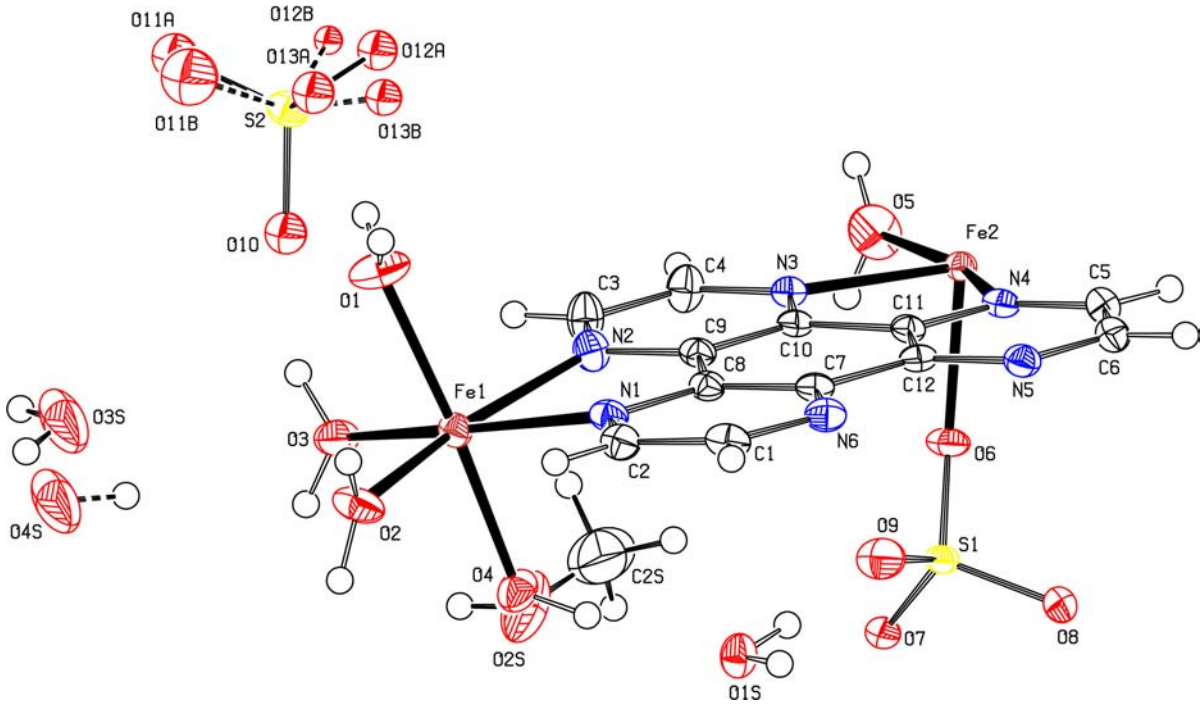

Fig. 2A. ORTEP plot of the asymmetric unit in the crystals structure of **2**.

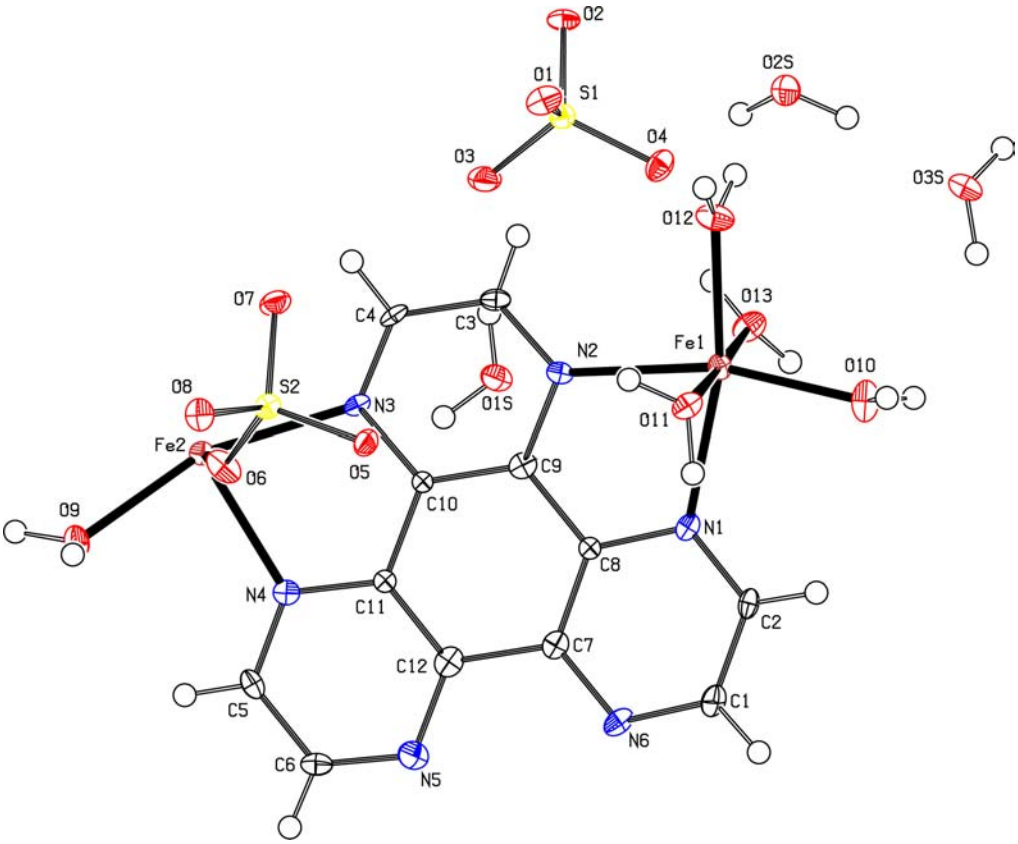

Fig. 3A. ORTEP plot of the asymmetric unit in the crystals structure of **3**.

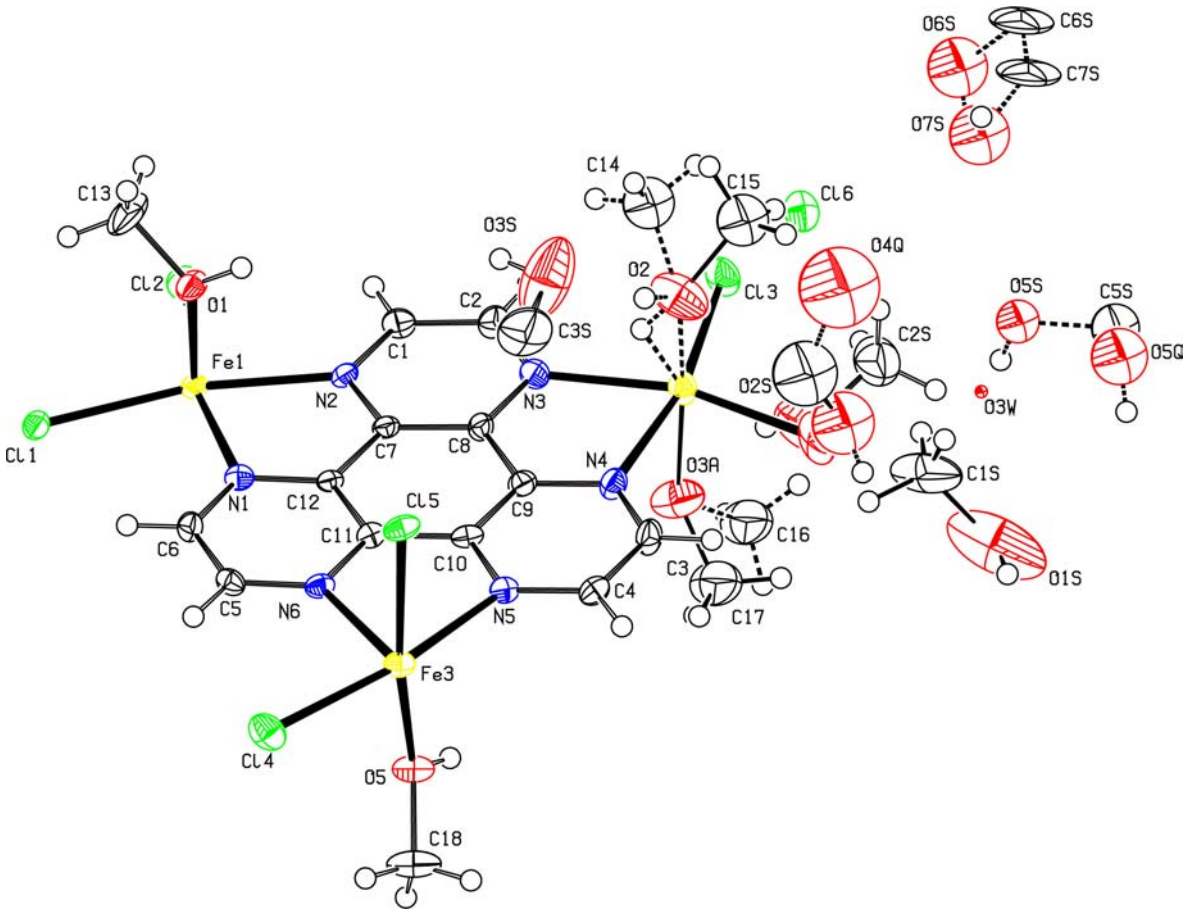

Fig. 4A. ORTEP plot of the asymmetric unit in the crystals structure of **4**.

Table 1A. Positional and thermal parameters for **1**.

Atom	Position	*x*/*a*	*y*/*b*	*z*/*c*	S.o.f.	U_{eq}
Fe(1)	4*e*	0.0867(1)	0.3705(2)	-0.1624(1)	1	0.0220(5)
Fe(2)	4*e*	0.41489(9)	0.3685(1)	0.1575(1)	1	0.0033(4)
Fe(3)	4*e*	0.2529(3)	0.8725(1)	-0.0019(4)	1	0.0102(3)
S(1)	4*e*	0.1535(2)	0.4467(2)	0.1851(2)	1	0.0075(7)
S(2)	4*e*	0.3371(2)	0.0484(4)	0.2993(2)	1	0.033(1)
S(3)	2*d*	0.5	0	0	1	0.051(2)
S(4)	2*a*	0	0	0	1	0.0023(8)
O(1)	4*e*	0.1657(5)	0.3355(7)	0.1445(6)	1	0.021(2)
O(2)	4*e*	0.1443(4)	0.5428(7)	0.1327(5)	1	0.014(2)
O(3)	4*e*	0.0840(4)	0.4324(6)	0.2318(5)	1	0.005
O(4)	4*e*	0.2162(4)	0.4671(6)	0.2551(5)	1	0.012(2)
O(5)	4*e*	0.3605(4)	-0.0216(6)	0.3828(5)	1	0.007(2)
O(6)	4*e*	0.2630(5)	0.0113(8)	0.2511(6)	1	0.028(2)
O(7)	4*e*	0.3297(4)	0.1493(6)	0.3395(5)	1	0.007(2)
O(8)	4*e*	0.3972(5)	0.0483(9)	0.2445(7)	1	0.034(3)
O(9)	4*e*	0.5424(10)	0.0922(15)	0.0600(12)	0.5	0.025(4)
O(10)	4*e*	0.4434(8)	0.0325(12)	-0.0766(9)	0.5	0.006(3)
O(11)	4*e*	0.4550(11)	-0.0399(17)	0.0710(13)	0.5	0.034(5)
O(12)	4*e*	0.5536(12)	-0.0702(18)	-0.0188(14)	0.5	0.040(5)
O(13)	4*e*	0.0535(10)	0.0458(16)	0.0579(12)	0.5	0.023(4)
O(14)	4*e*	-0.0324(8)	0.1084(12)	-0.0426(10)	0.5	0.005(3)
O(15)	4*e*	-0.0636(8)	-0.0601(12)	0.0260(9)	0.5	0.0022(15)
O(16)	4*e*	0.0318(7)	-0.0661(12)	-0.0712(9)	0.5	0.0018(15)
O(17)	4*e*	0.1569(5)	0.3443(6)	-0.2651(6)	1	0.038(3)
O(18)	4*e*	0.0495(4)	0.2110(6)	-0.1619(5)	1	0.025
O(19)	4*e*	0.0119(3)	0.4220(6)	-0.2636(4)	1	0.008(2)
O(20)	4*e*	0.0057(4)	0.4093(7)	-0.0771(5)	1	0.025
O(21)	4*e*	0.4341(3)	0.2088(6)	0.1415(4)	1	0.007(2)
O(22)	4*e*	0.4965(4)	0.3985(6)	0.0687(5)	1	0.019(2)
O(23)	4*e*	0.4985(4)	0.4023(6)	0.2601(5)	1	0.021(2)
O(24)	4*e*	0.3447(4)	0.3400(5)	0.2547(4)	1	0.0016(16)
O(25)	4*e*	0.3271(6)	0.8824(7)	-0.0815(6)	1	0.048(3)
O(26)	4*e*	0.3220(4)	0.9717(6)	0.0769(5)	1	0.025
O(27)	4*e*	0.1914(4)	0.9803(6)	-0.0845(5)	1	0.021(2)
O(28)	4*e*	0.1764(4)	0.8748(7)	0.1029(5)	1	0.025
N(1)	4*e*	0.1294(5)	0.5278(8)	-0.1321(7)	1	0.015(2)
N(2)	4*e*	0.1837(5)	0.3515(8)	-0.0590(6)	1	0.009(2)
N(3)	4*e*	0.3142(5)	0.3375(8)	0.0588(6)	1	0.005(2)
N(4)	4*e*	0.3732(5)	0.5410(7)	0.1255(6)	1	0.0013(16)
N(5)	4*e*	0.3104(5)	0.7328(7)	0.0688(6)	1	0.004(1)
N(6)	4*e*	0.1881(6)	0.7281(9)	-0.0545(7)	1	0.017(3)

Atom	Position	*x*/*a*	*y*/*b*	*z*/*c*	S.o.f.	U_{eq}
C(1)	4*e*	0.1921(2)	0.5409(2)	-0.0629(2)	1	0.026(3)
C(2)	4*e*	0.2215(2)	0.4429(2)	-0.0324(3)	1	0.008(2)
C(5)	4*e*	0.2839(2)	0.4400(2)	0.0306(3)	1	0.004(1)
C(6)	4*e*	0.3168(2)	0.5350(2)	0.0632(3)	1	0.002(1)
C(9)	4*e*	0.2873(2)	0.6330(2)	0.0327(3)	1	0.004(1)
C(10)	4*e*	0.2250(2)	0.6359(2)	-0.0304(3)	1	0.009(2)
C(3)	4*e*	0.2112(2)	0.2556(2)	-0.0299(3)	1	0.011(2)
H(3)	4*e*	0.1867	0.1919	-0.0469	1	0.014
C(4)	4*e*	0.2824(2)	0.2563(2)	0.0304(3)	1	0.007(2)
H(4)	4*e*	0.3040	0.1906	0.0475	1	0.009
C(7)	4*e*	0.3993(6)	0.6324(10)	0.1617(8)	1	0.016(3)
H(7)	4*e*	0.4387	0.6328	0.2069	1	0.019
C(8)	4*e*	0.3680(6)	0.7213(9)	0.1322(7)	1	0.006(2)
H(8)	4*e*	0.3879	0.7841	0.1581	1	0.007
C(11)	4*e*	0.1268(7)	0.7298(11)	-0.1136(8)	1	0.019(3)
H(11)	4*e*	0.1028	0.7937	-0.1307	1	0.023
C(12)	4*e*	0.0990(7)	0.6247(11)	-0.1506(9)	1	0.019(3)
H(12)	4*e*	0.0559	0.6264	-0.1908	1	0.023
H(17A)	4*e*	0.1603	0.2816	-0.3038	1	0.023
H(17B)	4*e*	0.1964	0.3904	-0.2494	1	0.023
H(18A)	4*e*	0.0774	0.1612	-0.1745	1	0.023
H(18B)	4*e*	0.0378	0.1721	-0.1139	1	0.023
H(19A)	4*e*	0.0210	0.4320	-0.3190	1	0.023
H(19B)	4*e*	-0.0293	0.4504	-0.2511	1	0.023
H(20A)	4*e*	-0.0486	0.4212	-0.0752	1	0.023
H(20B)	4*e*	0.0055	0.3680	-0.0281	1	0.023
H(21A)	4*e*	0.4721	0.1750	0.1253	1	0.023
H(21B)	4*e*	0.4354	0.1768	0.1850	1	0.023
H(22A)	4*e*	0.4878	0.3529	0.0163	1	0.023
H(22B)	4*e*	0.5491	0.4315	0.0816	1	0.023
H(23A)	4*e*	0.5292	0.4562	0.2531	1	0.023
H(23B)	4*e*	0.4801	0.4512	0.2981	1	0.023
H(24A)	4*e*	0.3180	0.3835	0.2827	1	0.023
H(24B)	4*e*	0.3395	0.2885	0.3037	1	0.023
H(25A)	4*e*	0.3212	0.8106	-0.1125	1	0.023
H(25B)	4*e*	0.2992	0.9040	-0.1304	1	0.023
H(26A)	4*e*	0.3434	1.0216	0.0553	1	0.023
H(26B)	4*e*	0.3122	0.9554	0.1327	1	0.023
H(27A)	4*e*	0.1507	0.9648	-0.1197	1	0.023
H(27B)	4*e*	0.1625	1.0220	-0.0641	1	0.023
H(28A)	4*e*	0.1216	0.8728	0.0915	1	0.023
H(28B)	4*e*	0.1722	0.8125	0.1478	1	0.023
O(1S)	4*e*	0.4724(2)	0.2738(3)	-0.0666(4)	1	0.032(2)
O(2S)	4*e*	0.0294(2)	0.2824(3)	0.0684(3)	1	0.033(3)
O(3S)	4*e*	0.2714(5)	-0.2093(3)	0.2778(5)	0.33	0.011(2)

Atom	Position	*x*/*a*	*y*/*b*	*z*/*c*	S.o.f.	U_{eq}
O(4S)	4*e*	0.3221(5)	-0.2274(4)	0.3034(5)	0.33	0.011(2)
O(5S)	4*e*	0.3787(5)	-0.2309(4)	0.3261(5)	0.34	0.011(2)
O(6S)	4*e*	0.2132(5)	-0.2762(3)	0.2212(5)	0.34	0.011(2)

Table 1B. Bond distances (Å) in the crystal structure of **1**.

Fe(1)–O(19)	2.031(6)	S(3)–O(11)	1.53(2)
Fe(1)–O(18)	2.101(8)	S(3)–O(9)	1.606(18)
Fe(1)–N(1)	2.137(10)	S(4)–O(13)	1.355(18)
Fe(1)–O(20)	2.147(8)	S(4)–O(15)	1.471(15)
Fe(1)–O(17)	2.177(10)	S(4)–O(16)	1.541(14)
Fe(1)–N(2)	2.224(9)	S(4)–O(14)	1.581(15)
Fe(2)–O(21)	2.041(7)	N(1)–C(12)	1.343(17)
Fe(2)–O(23)	2.083(8)	N(1)–C(1)	1.461(10)
Fe(2)–O(24)	2.114(7)	N(2)–C(3)	1.348(10)
Fe(2)–O(22)	2.170(8)	N(2)–C(2)	1.365(10)
Fe(2)–N(3)	2.249(9)	N(3)–C(4)	1.217(10)
Fe(2)–N(4)	2.312(9)	N(3)–C(5)	1.435(10)
Fe(3)–O(25)	1.936(12)	N(4)–C(6)	1.309(9)
Fe(3)–O(26)	2.042(9)	N(4)–C(7)	1.328(15)
Fe(3)–O(27)	2.072(9)	N(5)–C(8)	1.341(13)
Fe(3)–N(5)	2.237(9)	N(5)–C(9)	1.404(9)
Fe(3)–N(6)	2.242(11)	N(6)–C(11)	1.339(16)
Fe(3)–O(28)	2.258(10)	N(6)–C(10)	1.357(11)
S(1)–O(2)	1.442(9)	C(1)–C(2)	1.3900
S(1)–O(4)	1.481(8)	C(1)–C(10)	1.3900
S(1)–O(3)	1.537(8)	C(2)–C(5)	1.3900
S(1)–O(1)	1.548(9)	C(5)–C(6)	1.3900
S(2)–O(7)	1.416(9)	C(6)–C(9)	1.3900
S(2)–O(8)	1.460(11)	C(9)–C(10)	1.3900
S(2)–O(6)	1.517(10)	C(3)–C(4)	1.4886
S(2)–O(5)	1.566(8)	C(7)–C(8)	1.299(16)
S(3)–O(12)	1.36(2)	C(11)–C(12)	1.491(19)
S(3)–O(10)	1.513(14)		

Table 1C. Bond angles (°) in the crystal structure of **1**.

O(19)–Fe(1)–O(18)	96.9(3)	N(5)–Fe(3)–O(28)	87.3(4)
O(19)–Fe(1)–N(1)	93.6(3)	N(6)–Fe(3)–O(28)	85.9(4)
O(18)–Fe(1)–N(1)	167.3(4)	O(2)–S(1)–O(4)	106.6(5)
O(19)–Fe(1)–O(20)	87.6(3)	O(2)–S(1)–O(3)	108.3(5)
O(18)–Fe(1)–O(20)	88.1(3)	O(4)–S(1)–O(3)	106.0(4)
N(1)–Fe(1)–O(20)	85.2(4)	O(2)–S(1)–O(1)	122.1(5)
O(19)–Fe(1)–O(17)	83.4(3)	O(4)–S(1)–O(1)	108.2(5)
O(18)–Fe(1)–O(17)	94.4(3)	O(3)–S(1)–O(1)	104.6(5)
N(1)–Fe(1)–O(17)	93.9(4)	O(7)–S(2)–O(8)	111.8(6)
O(20)–Fe(1)–O(17)	170.8(3)	O(7)–S(2)–O(6)	111.0(5)
O(19)–Fe(1)–N(2)	165.6(3)	O(8)–S(2)–O(6)	113.2(6)
O(18)–Fe(1)–N(2)	96.9(3)	O(7)–S(2)–O(5)	99.6(5)
N(1)–Fe(1)–N(2)	73.3(4)	O(8)–S(2)–O(5)	109.3(5)
O(20)–Fe(1)–N(2)	97.2(3)	O(6)–S(2)–O(5)	111.0(5)
O(17)–Fe(1)–N(2)	91.3(3)	O(12)–S(3)–O(10)	115.7(10)
O(21)–Fe(2)–O(23)	99.8(3)	O(12)–S(3)–O(11)	113.7(12)
O(21)–Fe(2)–O(24)	92.8(3)	O(10)–S(3)–O(11)	106.0(9)
O(23)–Fe(2)–O(24)	86.6(3)	O(12)–S(3)–O(9)	106.3(11)
O(21)–Fe(2)–O(22)	87.3(3)	O(10)–S(3)–O(9)	118.7(8)
O(23)–Fe(2)–O(22)	87.5(3)	O(11)–S(3)–O(9)	94.6(10)
O(24)–Fe(2)–O(22)	174.0(3)	O(13)–S(4)–O(15)	123.6(10)
O(21)–Fe(2)–N(3)	83.5(3)	O(13)–S(4)–O(16)	113.1(9)
O(23)–Fe(2)–N(3)	172.5(3)	O(15)–S(4)–O(16)	107.4(8)
O(24)–Fe(2)–N(3)	86.6(3)	O(13)–S(4)–O(14)	96.2(10)
O(22)–Fe(2)–N(3)	99.4(3)	O(15)–S(4)–O(14)	106.7(8)
O(21)–Fe(2)–N(4)	159.7(3)	O(16)–S(4)–O(14)	108.4(8)
O(23)–Fe(2)–N(4)	99.1(3)	C(12)–N(1)–C(1)	108.2(9)
O(24)–Fe(2)–N(4)	95.6(3)	C(12)–N(1)–Fe(1)	130.7(8)
O(22)–Fe(2)–N(4)	86.3(3)	C(1)–N(1)–Fe(1)	119.1(6)
N(3)–Fe(2)–N(4)	78.6(3)	C(3)–N(2)–C(2)	119.5(7)
O(25)–Fe(3)–O(26)	85.1(4)	C(3)–N(2)–Fe(1)	123.7(6)
O(25)–Fe(3)–O(27)	86.1(4)	C(2)–N(2)–Fe(1)	116.3(6)
O(26)–Fe(3)–O(27)	102.1(3)	C(4)–N(3)–C(5)	119.2(7)
O(25)–Fe(3)–N(5)	92.3(4)	C(4)–N(3)–Fe(2)	133.5(6)
O(26)–Fe(3)–N(5)	88.4(4)	C(5)–N(3)–Fe(2)	107.2(5)
O(27)–Fe(3)–N(5)	169.1(4)	C(6)–N(4)–C(7)	123.9(9)
O(25)–Fe(3)–N(6)	101.3(4)	C(6)–N(4)–Fe(2)	107.7(5)
O(26)–Fe(3)–N(6)	162.2(4)	C(7)–N(4)–Fe(2)	128.4(7)
O(27)–Fe(3)–N(6)	94.9(4)	C(8)–N(5)–C(9)	110.8(8)
N(5)–Fe(3)–N(6)	74.8(3)	C(8)–N(5)–Fe(3)	134.9(8)
O(25)–Fe(3)–O(28)	172.5(4)	C(9)–N(5)–Fe(3)	113.8(5)
O(26)–Fe(3)–O(28)	87.4(4)	C(11)–N(6)–C(10)	122.3(10)
O(27)–Fe(3)–O(28)	95.7(3)	C(11)–N(6)–Fe(3)	125.5(9)
C(10)–N(6)–Fe(3)	111.5(6)	C(5)–C(6)–C(9)	120.0

C(2)–C(1)–C(10)	120.0	C(6)–C(9)–C(10)	120.0
C(2)–C(1)–N(1)	112.0(4)	C(6)–C(9)–N(5)	124.4(4)
C(10)–C(1)–N(1)	127.9(4)	C(10)–C(9)–N(5)	115.1(4)
N(2)–C(2)–C(1)	118.5(4)	N(6)–C(10)–C(9)	122.7(5)
N(2)–C(2)–C(5)	121.1(4)	N(6)–C(10)–C(1)	116.8(5)
C(1)–C(2)–C(5)	120.0	C(9)–C(10)–C(1)	120.0
C(6)–C(5)–C(2)	120.0	N(2)–C(3)–C(4)	117.0(4)
C(6)–C(5)–N(3)	121.4(4)	N(3)–C(4)–C(3)	124.0(5)
C(2)–C(5)–N(3)	118.6(4)	C(7)–C(8)–N(5)	127.5(11)
N(4)–C(6)–C(5)	124.8(4)	N(6)–C(11)–C(12)	117.1(12)
N(4)–C(6)–C(9)	115.2(4)	N(1)–C(12)–C(11)	126.9(11)

Table 2A. Positional and thermal parameters for **2**.

Atom	Position	*x*/*a*	*y*/*b*	*z*/*c*	S.o.f.	U_{eq}
Fe1	4*e*	0.47167(5)	0.69197(1)	0.00807(3)	1	0.01650(7)
Fe2	4*e*	0.23476(5)	0.55443(1)	0.46072(2)	1	0.01348(7)
S1	4*e*	0.25897(8)	0.45847(2)	0.59147(4)	1	0.0157(1)
S2	4*e*	0.04404(9)	0.69789(2)	-0.30111(5)	1	0.0198(1)
O1	4*e*	0.1928(3)	0.72580(7)	-0.0250(1)	1	0.0305(5)
O2	2*d*	0.5627(3)	0.70717(7)	-0.1442(1)	1	0.0268(4)
O3	2*a*	0.5628(3)	0.75153(6)	0.0873(1)	1	0.0251(4)
O4	4*e*	0.7622(3)	0.66561(6)	0.0552(1)	1	0.0251(4)
O5	4*e*	0.2563(3)	0.60690(6)	0.5728(2)	1	0.0362(5)
O6	4*e*	0.4396(2)	0.44672(6)	0.5271(1)	1	0.0205(4)
O7	4*e*	0.0861(2)	0.43111(5)	0.5464(1)	1	0.0203(4)
O8	4*e*	0.2096(2)	0.50722(5)	0.5778(1)	1	0.0191(4)
O9	4*e*	0.2959(3)	0.44903(6)	0.7046(1)	1	0.0285(4)
O10	4*e*	0.2687(3)	0.70221(6)	-0.2978(1)	1	0.0245(4)
O11A	4*e*	-0.0146(3)	0.64923(7)	-0.3030(2)	0.905(2)	0.0291(5)
O12A	4*e*	-0.0428(3)	0.71855(6)	-0.2036(2)	0.905(2)	0.0219(4)
O13A	4*e*	-0.0403(3)	0.72091(6)	-0.3961(2)	0.905(2)	0.0243(4)
O11B	4*e*	-0.021(4)	0.6672(8)	-0.382(2)	0.095(2)	0.045(6)
O12B	4*e*	-0.044(2)	0.6976(5)	-0.201(1)	0.095(2)	0.011(3)
O13B	4*e*	-0.038(3)	0.7453(6)	-0.361(1)	0.095(2)	0.018(4)
N1	4*e*	0.3700(3)	0.62214(7)	-0.0438(1)	1	0.0170(4)
N2	4*e*	0.3569(3)	0.65999(7)	0.1550(2)	1	0.0202(5)
N3	4*e*	0.2741(3)	0.60616(6)	0.3332(1)	1	0.0153(4)
N4	4*e*	0.2143(3)	0.51512(6)	0.3106(2)	1	0.0161(4)
N5	4*e*	0.2101(3)	0.47517(6)	0.1056(2)	1	0.0180(4)
N6	4*e*	0.2841(3)	0.52889(7)	-0.0727(2)	1	0.0185(4)
C1	4*e*	0.3224(3)	0.55653(8)	-0.1541(2)	1	0.0205(5)
H1	4*e*	0.3196	0.5447	-0.2231	1	0.025
C2	4*e*	0.3667(3)	0.60272(8)	-0.1401(2)	1	0.0192(5)

Atom	Position	*x*/*a*	*y*/*b*	*z*/*c*	S.o.f.	U_{eq}
H2	4*e*	0.3946	0.6203	-0.1997	1	0.023
C3	4*e*	0.3481(4)	0.67760(8)	0.2528(2)	1	0.0253(6)
H3	4*e*	0.3700	0.7085	0.2625	1	0.030
C4	4*e*	0.3063(4)	0.65021(8)	0.3417(2)	1	0.0231(6)
H4	4*e*	0.3012	0.6636	0.4089	1	0.028
C5	4*e*	0.1790(3)	0.47098(8)	0.2964(2)	1	0.0193(5)
H5	4*e*	0.1552	0.4527	0.3555	1	0.023
C6	4*e*	0.1770(3)	0.45146(8)	0.1938(2)	1	0.0192(5)
H6	4*e*	0.1514	0.4205	0.1874	1	0.023
C7	4*e*	0.2858(3)	0.54815(8)	0.0253(2)	1	0.0161(5)
C8	4*e*	0.3256(3)	0.59458(8)	0.0396(2)	1	0.0153(5)
C9	4*e*	0.3205(3)	0.61483(8)	0.1453(2)	1	0.0161(5)
C10	4*e*	0.2798(3)	0.58825(7)	0.2335(2)	1	0.0148(5)
C11	4*e*	0.2464(3)	0.53974(7)	0.2206(2)	1	0.0149(5)
C12	4*e*	0.2460(3)	0.52005(8)	0.1191(2)	1	0.0160(5)
H1A	4*e*	0.124(3)	0.7412(6)	0.0264(11)	1	0.019
H2A	4*e*	0.4630(18)	0.7062(9)	-0.1961(14)	1	0.019
H3A	4*e*	0.6930(16)	0.7615(7)	0.089(2)	1	0.019
H4A	4*e*	0.811(3)	0.6773(5)	0.1199(12)	1	0.019
H5A	4*e*	0.3846(16)	0.6168(8)	0.5821(19)	1	0.019
H1B	4*e*	0.113(3)	0.7185(7)	-0.0830(11)	1	0.019
H2B	4*e*	0.6912(17)	0.7078(9)	-0.1706(17)	1	0.019
H3B	4*e*	0.469(2)	0.7732(6)	0.1077(19)	1	0.019
H4B	4*e*	0.782(4)	0.6353(4)	0.0507(16)	1	0.019
H5B	4*e*	0.161(2)	0.6228(7)	0.6103(17)	1	0.019
O1S	4*e*	0.8253(3)	0.57692(5)	0.0931(1)	1	0.0221(4)
H1SA	4*e*	0.803(4)	0.5530(5)	0.0454(11)	1	0.019
H1SB	4*e*	0.787(4)	0.5677(7)	0.1603(9)	1	0.019
O2S	4*e*	0.1132(4)	0.31025(8)	0.7437(2)	0.818(4)	0.0451(8)
H2S	4*e*	0.0914	0.2829	0.7409	0.818(4)	0.054
C2S	4*e*	0.1804(7)	0.32532(16)	0.6444(5)	0.818(4)	0.073(2)
H2S1	4*e*	0.2356	0.3554	0.6518	0.818(4)	0.110
H2S2	4*e*	0.0671	0.3257	0.5940	0.818(4)	0.110
H2S3	4*e*	0.2845	0.3052	0.6194	0.818(4)	0.110
O3S	4*e*	0.3738(5)	0.3660(1)	0.4040(4)	0.818(4)	0.118(1)
O4S	4*e*	0.2868(18)	0.3487(5)	0.5247(13)	0.18	0.118(1)
H3S	4*e*	0.360(10)	0.3905(6)	0.3601(15)	0.818(4)	0.142
H4S	4*e*	0.293(5)	0.3277(10)	0.470(2)	0.182(4)	0.142
H3T	4*e*	0.342(8)	0.3702(14)	0.4746(12)	0.818(4)	0.142
H4T	4*e*	0.164(3)	0.348(2)	0.560(3)	0.182(4)	0.142

Table 2B. Bond distances (Å) in the crystal structure of **2**.

Fe(1)–O(2)	2.0572(17)	N(1)–C(2)	1.332(3)
Fe(1)–O(3)	2.0935(17)	N(1)–C(8)	1.359(3)
Fe(1)–O(1)	2.1072(18)	N(2)–C(3)	1.331(3)
Fe(1)–O(4)	2.1192(17)	N(2)–C(9)	1.356(3)
Fe(1)–N(2)	2.211(2)	N(3)–C(4)	1.318(3)
Fe(1)–N(1)	2.2517(19)	N(3)–C(10)	1.355(3)
Fe(2)–O(8)	2.0281(16)	N(4)–C(5)	1.332(3)
Fe(2)–O(5)	2.0883(19)	N(4)–C(11)	1.359(3)
Fe(2)–O(6)	2.1273(16)	N(5)–C(6)	1.327(3)
Fe(2)–O(7)	2.1370(16)	N(5)–C(12)	1.353(3)
Fe(2)–N(4)	2.2060(19)	N(6)–C(1)	1.332(3)
Fe(2)–N(3)	2.2243(19)	N(6)–C(7)	1.349(3)
S(1)–O(9)	1.4552(18)	C(1)–C(2)	1.401(3)
S(1)–O(8)	1.4809(16)	C(3)–C(4)	1.405(3)
S(1)–O(6)	1.4843(16)	C(5)–C(6)	1.405(3)
S(1)–O(7)	1.4861(17)	C(7)–C(8)	1.403(3)
S(2)–O(12B)	1.386(15)	C(7)–C(12)	1.464(3)
S(2)–O(11B)	1.41(2)	C(8)–C(9)	1.450(3)
S(2)–O(13A)	1.464(2)	C(9)–C(10)	1.383(3)
S(2)–O(10)	1.4717(18)	C(10)–C(11)	1.454(3)
S(2)–O(11A)	1.484(2)	C(11)–C(12)	1.395(3)
S(2)–O(12A)	1.4873(19)	O(2S)–C(2S)	1.398(6)
S(2)–O(13B)	1.665(17)		

Table 2C. Bond angles (°) in the crystal structure of **2**.

O(2)–Fe(1)–O(3)	99.78(7)	O(5)–Fe(2)–O(6)	85.01(7)
O(2)–Fe(1)–O(1)	89.04(7)	O(8)–Fe(2)–O(7)	94.02(6)
O(3)–Fe(1)–O(1)	86.01(7)	O(5)–Fe(2)–O(7)	86.01(7)
O(2)–Fe(1)–O(4)	93.46(7)	O(6)–Fe(2)–O(7)	169.29(6)
O(3)–Fe(1)–O(4)	86.19(7)	O(8)–Fe(2)–N(4)	104.44(7)
O(1)–Fe(1)–O(4)	172.11(7)	O(5)–Fe(2)–N(4)	163.86(7)
O(2)–Fe(1)–N(2)	166.58(7)	O(6)–Fe(2)–N(4)	95.28(7)
O(3)–Fe(1)–N(2)	93.58(7)	O(7)–Fe(2)–N(4)	91.73(7)
O(1)–Fe(1)–N(2)	93.21(7)	O(8)–Fe(2)–N(3)	178.01(7)
O(4)–Fe(1)–N(2)	86.09(7)	O(5)–Fe(2)–N(3)	88.07(7)
O(2)–Fe(1)–N(1)	91.27(7)	O(6)–Fe(2)–N(3)	85.95(6)
O(3)–Fe(1)–N(1)	168.52(7)	O(7)–Fe(2)–N(3)	87.92(6)
O(1)–Fe(1)–N(1)	97.38(7)	N(4)–Fe(2)–N(3)	75.87(7)
O(4)–Fe(1)–N(1)	90.05(7)	O(9)–S(1)–O(8)	109.15(10)
N(2)–Fe(1)–N(1)	75.33(7)	O(9)–S(1)–O(6)	111.54(10)
O(8)–Fe(2)–O(5)	91.66(7)	O(8)–S(1)–O(6)	109.70(9)
O(8)–Fe(2)–O(6)	92.06(6)	O(9)–S(1)–O(7)	111.76(10)

O(8)–S(1)–O(7)	108.72(9)	C(4)–N(3)–C(10)	116.69(19)
O(6)–S(1)–O(7)	105.89(9)	C(4)–N(3)–Fe(2)	129.62(15)
O(12B)–S(2)–O(11B)	121.1(12)	C(10)–N(3)–Fe(2)	113.50(14)
O(12B)–S(2)–O(13A)	125.3(6)	C(5)–N(4)–C(11)	116.09(19)
O(11B)–S(2)–O(13A)	67.4(10)	C(5)–N(4)–Fe(2)	129.27(15)
O(12B)–S(2)–O(10)	114.2(6)	C(11)–N(4)–Fe(2)	114.62(14)
O(11B)–S(2)–O(10)	110.9(10)	C(6)–N(5)–C(12)	116.3(2)
O(13A)–S(2)–O(10)	109.73(11)	C(1)–N(6)–C(7)	116.0(2)
O(12B)–S(2)–O(11A)	84.0(7)	N(6)–C(1)–C(2)	122.7(2)
O(11B)–S(2)–O(11A)	45.4(10)	N(1)–C(2)–C(1)	121.9(2)
O(13A)–S(2)–O(11A)	110.05(11)	N(2)–C(3)–C(4)	121.1(2)
O(10)–S(2)–O(11A)	109.90(11)	N(3)–C(4)–C(3)	122.3(2)
O(12B)–S(2)–O(12A)	24.5(7)	N(4)–C(5)–C(6)	121.3(2)
O(11B)–S(2)–O(12A)	137.2(10)	N(5)–C(6)–C(5)	123.0(2)
O(13A)–S(2)–O(12A)	109.42(11)	N(6)–C(7)–C(8)	121.6(2)
O(10)–S(2)–O(12A)	109.95(10)	N(6)–C(7)–C(12)	119.5(2)
O(11A)–S(2)–O(12A)	107.77(11)	C(8)–C(7)–C(12)	118.98(19)
O(12B)–S(2)–O(13B)	106.0(9)	N(1)–C(8)–C(7)	121.8(2)
O(11B)–S(2)–O(13B)	97.3(11)	N(1)–C(8)–C(9)	117.6(2)
O(13A)–S(2)–O(13B)	30.3(6)	C(7)–C(8)–C(9)	120.6(2)
O(10)–S(2)–O(13B)	104.3(6)	N(2)–C(9)–C(10)	121.4(2)
O(11A)–S(2)–O(13B)	136.3(6)	N(2)–C(9)–C(8)	118.5(2)
O(12A)–S(2)–O(13B)	84.4(6)	C(10)–C(9)–C(8)	120.1(2)
S(1)–O(6)–Fe(2)	140.39(10)	N(3)–C(10)–C(9)	121.5(2)
S(1)–O(7)–Fe(2)	129.93(10)	N(3)–C(10)–C(11)	118.47(19)
S(1)–O(8)–Fe(2)	136.65(10)	C(9)–C(10)–C(11)	120.0(2)
C(2)–N(1)–C(8)	115.9(2)	N(4)–C(11)–C(12)	122.3(2)
C(2)–N(1)–Fe(1)	130.61(16)	N(4)–C(11)–C(10)	117.31(19)
C(8)–N(1)–Fe(1)	113.05(14)	C(12)–C(11)–C(10)	120.4(2)
C(3)–N(2)–C(9)	116.9(2)	N(5)–C(12)–C(11)	121.1(2)
C(3)–N(2)–Fe(1)	128.34(16)	N(5)–C(12)–C(7)	119.1(2)
C(9)–N(2)–Fe(1)	113.94(15)	C(11)–C(12)–C(7)	119.8(2)

Table 3A. Positional and thermal parameters for **3**.

Atom	Position	*x*/*a*	*y*/*b*	*z*/*c*	S.o.f.	U_{eq}
Fe(1)	4*e*	0.04906(8)	0.32414(2)	0.88263(4)	1	0.0107(2)
Fe(2)	4*e*	0.25412(8)	0.54698(2)	0.58968(4)	1	0.0097(1)
S(1)	4*e*	-0.4914(1)	0.27349(3)	0.59910(6)	1	0.0113(2)
S(2)	4*e*	-0.2544(1)	0.52086(3)	0.61088(6)	1	0.0104(2)
O(1)	4*e*	-0.7138(4)	0.2817(1)	0.5793(2)	1	0.0163(7)
O(2)	4*e*	-0.4110(4)	0.23370(9)	0.5328(2)	1	0.0142(6)
O(3)	4*e*	-0.3770(4)	0.3232(1)	0.5876(2)	1	0.0202(7)
O(4)	4*e*	-0.4636(4)	0.2544(1)	0.6975(2)	1	0.0159(7)

Atom	Position	*x*/*a*	*y*/*b*	*z*/*c*	S.o.f.	U_{eq}
O(5)	4*e*	-0.3060(4)	0.49892(9)	0.7021(2)	1	0.0136(6)
O(6)	4*e*	-0.0683(4)	0.55416(9)	0.6188(2)	1	0.0159(7)
O(7)	4*e*	-0.2149(4)	0.47725(9)	0.5449(2)	1	0.0166(7)
O(8)	4*e*	-0.4234(4)	0.55538(9)	0.5734(2)	1	0.0154(7)
O(9)	4*e*	0.2222(4)	0.62920(9)	0.5666(2)	1	0.0149(6)
O(10)	4*e*	-0.0083(4)	0.2838(1)	1.0047(2)	1	0.0188(7)
O(11)	4*e*	-0.2442(4)	0.3610(1)	0.8920(2)	1	0.0162(7)
O(12)	4*e*	-0.0675(4)	0.27293(9)	0.7797(2)	1	0.0172(7)
O(13)	4*e*	0.3437(4)	0.2881(1)	0.8704(2)	1	0.0167(7)
O(1S)	4*e*	-0.3940(4)	0.39502(9)	0.7312(2)	1	0.0167(7)
O(2S)	4*e*	0.1794(4)	0.31047(9)	1.2366(2)	1	0.0197(7)
O(3S)	4*e*	-0.7981(4)	0.3424(1)	0.4229(2)	1	0.0214(7)
N(1)	4*e*	0.1687(4)	0.3933(1)	0.9680(2)	1	0.0094(7)
N(2)	4*e*	0.1316(4)	0.3845(1)	0.7781(2)	1	0.0095(8)
N(3)	4*e*	0.2221(4)	0.4707(1)	0.6624(2)	1	0.0079(7)
N(4)	4*e*	0.2946(4)	0.5665(1)	0.7409(2)	1	0.0107(8)
N(5)	4*e*	0.3107(5)	0.5799(1)	0.9366(2)	1	0.0154(8)
N(6)	4*e*	0.2510(4)	0.4912(1)	1.0528(2)	1	0.0124(8)
C(1)	4*e*	0.2175(5)	0.4481(1)	1.1027(3)	1	0.014(1)
H(1)	4*e*	0.2209	0.4504	1.1681	1	0.016
C(2)	4*e*	0.1770(5)	0.3997(1)	1.0608(2)	1	0.0113(9)
H(2)	4*e*	0.1556	0.3699	1.0991	1	0.014
C(3)	4*e*	0.1211(5)	0.3815(1)	0.6851(3)	1	0.0120(9)
H(3)	4*e*	0.0799	0.3500	0.6573	1	0.014
C(4)	4*e*	0.1698(5)	0.4244(1)	0.6269(3)	1	0.0108(9)
H(4)	4*e*	0.1653	0.4200	0.5618	1	0.013
C(5)	4*e*	0.3276(5)	0.6133(1)	0.7798(3)	1	0.013(1)
H(5)	4*e*	0.3463	0.6425	0.7414	1	0.015
C(6)	4*e*	0.3346(5)	0.6192(1)	0.8774(3)	1	0.0123(9)
H(6)	4*e*	0.3575	0.6527	0.9020	1	0.015
C(7)	4*e*	0.2463(5)	0.4859(1)	0.9581(3)	1	0.0111(9)
C(8)	4*e*	0.2030(5)	0.4374(1)	0.9160(2)	1	0.0092(8)
C(9)	4*e*	0.1889(5)	0.4318(1)	0.8149(3)	1	0.0099(9)
C(10)	4*e*	0.2282(5)	0.4749(1)	0.7581(2)	1	0.0084(8)
C(11)	4*e*	0.2703(5)	0.5256(1)	0.7996(2)	1	0.0096(8)
C(12)	4*e*	0.2757(5)	0.5318(1)	0.8975(3)	1	0.0118(9)
H(9A)	4*e*	0.286(3)	0.647(1)	0.517(1)	1	0.014
H(10A)	4*e*	0.082(2)	0.2613(9)	1.033(2)	1	0.014
H(11A)	4*e*	-0.284(5)	0.375(1)	0.8356(9)	1	0.014
H(12A)	4*e*	0.019(2)	0.2463(8)	0.763(2)	1	0.014
H(13A)	4*e*	0.403(4)	0.283(1)	0.8129(8)	1	0.014
H(9B)	4*e*	0.088(2)	0.640(1)	0.575(1)	1	0.014
H(10B)	4*e*	-0.144(2)	0.279(1)	1.019(2)	1	0.014
H(11B)	4*e*	-0.245(5)	0.3845(8)	0.941(1)	1	0.014
H(12B)	4*e*	-0.198(2)	0.270(1)	0.755(2)	1	0.014

Atom	Position	*x*/*a*	*y*/*b*	*z*/*c*	S.o.f.	U_{eq}
H(13B)	4*e*	0.428(3)	0.283(1)	0.921(1)	1	0.014
H(1S)	4*e*	-0.380(5)	0.3727(6)	0.682(1)	1	0.014
H(2S)	4*e*	-0.355(5)	0.4288(5)	0.722(2)	1	0.014
H(3S)	4*e*	0.285(3)	0.2877(8)	1.221(2)	1	0.014
H(4S)	4*e*	0.201(4)	0.3241(9)	1.296(1)	1	0.014
H(5S)	4*e*	-0.733(4)	0.3736(5)	0.420(2)	1	0.014
H(6S)	4*e*	-0.762(5)	0.3226(7)	0.475(1)	1	0.014

Table 3B. Bond distances (Å) in the crystal structure of **3**.

Fe(1)–O(10)	2.050(3)	N(1)–C(8)	1.361(4)
Fe(1)–O(12)	2.086(2)	N(2)–C(3)	1.321(5)
Fe(1)–O(11)	2.116(3)	N(2)–C(9)	1.358(4)
Fe(1)–O(13)	2.119(3)	N(3)–C(4)	1.322(4)
Fe(1)–N(2)	2.205(3)	N(3)–C(10)	1.361(4)
Fe(1)–N(1)	2.261(3)	N(4)–C(5)	1.325(4)
Fe(2)–O(7)	2.018(2)	N(4)–C(11)	1.342(4)
Fe(2)–O(8)	2.107(2)	N(5)–C(6)	1.315(5)
Fe(2)–O(9)	2.122(2)	N(5)–C(12)	1.357(5)
Fe(2)–O(6)	2.134(2)	N(6)–C(1)	1.323(5)
Fe(2)–N(3)	2.205(3)	N(6)–C(7)	1.350(5)
Fe(2)–N(4)	2.212(3)	C(1)–C(2)	1.402(5)
S(1)–O(1)	1.472(3)	C(3)–C(4)	1.404(5)
S(1)–O(3)	1.472(3)	C(5)–C(6)	1.392(5)
S(1)–O(2)	1.479(2)	C(7)–C(8)	1.394(5)
S(1)–O(4)	1.485(3)	C(7)–C(12)	1.463(5)
S(2)–O(5)	1.453(2)	C(8)–C(9)	1.442(5)
S(2)–O(6)	1.471(2)	C(9)–C(10)	1.383(5)
S(2)–O(7)	1.474(3)	C(10)–C(11)	1.441(5)
S(2)–O(8)	1.490(3)	C(11)–C(12)	1.398(5)
N(1)–C(2)	1.325(4)		

Table 3C. Bond angles (°) in the crystal structure of **3**.

O(10)–Fe(1)–O(12)	102.23(10)	O(11)–Fe(1)–N(2)	87.77(10)
O(10)–Fe(1)–O(11)	89.62(10)	O(13)–Fe(1)–N(2)	91.05(10)
O(12)–Fe(1)–O(11)	90.43(10)	O(10)–Fe(1)–N(1)	90.01(10)
O(10)–Fe(1)–O(13)	91.62(10)	O(12)–Fe(1)–N(1)	167.06(10)
O(12)–Fe(1)–O(13)	89.25(10)	O(11)–Fe(1)–N(1)	85.43(10)
O(11)–Fe(1)–O(13)	178.76(10)	O(13)–Fe(1)–N(1)	94.62(10)
O(10)–Fe(1)–N(2)	164.64(11)	N(2)–Fe(1)–N(1)	74.69(10)
O(12)–Fe(1)–N(2)	92.93(10)	O(7)–Fe(2)–O(8)	92.06(10)

O(7)–Fe(2)–O(9)	98.26(10)	C(9)–N(2)–Fe(1)	115.1(2)
O(8)–Fe(2)–O(9)	88.69(9)	C(4)–N(3)–C(10)	116.8(3)
O(7)–Fe(2)–O(6)	95.84(10)	C(4)–N(3)–Fe(2)	129.0(2)
O(8)–Fe(2)–O(6)	168.23(10)	C(10)–N(3)–Fe(2)	113.4(2)
O(9)–Fe(2)–O(6)	81.57(9)	C(5)–N(4)–C(11)	117.0(3)
O(7)–Fe(2)–N(3)	99.43(10)	C(5)–N(4)–Fe(2)	128.3(2)
O(8)–Fe(2)–N(3)	103.90(10)	C(11)–N(4)–Fe(2)	114.5(2)
O(9)–Fe(2)–N(3)	157.83(10)	C(6)–N(5)–C(12)	116.2(3)
O(6)–Fe(2)–N(3)	83.42(10)	C(1)–N(6)–C(7)	116.6(3)
O(7)–Fe(2)–N(4)	175.16(10)	N(6)–C(1)–C(2)	122.6(3)
O(8)–Fe(2)–N(4)	88.99(10)	N(1)–C(2)–C(1)	121.6(3)
O(9)–Fe(2)–N(4)	86.49(10)	N(2)–C(3)–C(4)	122.3(3)
O(6)–Fe(2)–N(4)	83.87(10)	N(3)–C(4)–C(3)	121.6(3)
N(3)–Fe(2)–N(4)	75.74(10)	N(4)–C(5)–C(6)	120.9(3)
O(1)–S(1)–O(3)	110.26(15)	N(5)–C(6)–C(5)	123.4(3)
O(1)–S(1)–O(2)	109.04(14)	N(6)–C(7)–C(8)	121.1(3)
O(3)–S(1)–O(2)	109.45(15)	N(6)–C(7)–C(12)	120.2(3)
O(1)–S(1)–O(4)	109.12(15)	C(8)–C(7)–C(12)	118.7(3)
O(3)–S(1)–O(4)	109.38(15)	N(1)–C(8)–C(7)	121.8(3)
O(2)–S(1)–O(4)	109.58(14)	N(1)–C(8)–C(9)	116.7(3)
O(5)–S(2)–O(6)	110.57(15)	C(7)–C(8)–C(9)	121.4(3)
O(5)–S(2)–O(7)	108.78(14)	N(2)–C(9)–C(10)	121.7(3)
O(6)–S(2)–O(7)	109.31(15)	N(2)–C(9)–C(8)	118.8(3)
O(5)–S(2)–O(8)	111.47(14)	C(10)–C(9)–C(8)	119.5(3)
O(6)–S(2)–O(8)	106.27(14)	N(3)–C(10)–C(9)	121.1(3)
O(7)–S(2)–O(8)	110.41(15)	N(3)–C(10)–C(11)	118.5(3)
S(2)–O(6)–Fe(2)	137.08(15)	C(9)–C(10)–C(11)	120.3(3)
S(2)–O(7)–Fe(2)	144.01(16)	N(4)–C(11)–C(12)	121.9(3)
S(2)–O(8)–Fe(2)	128.26(15)	N(4)–C(11)–C(10)	117.5(3)
C(2)–N(1)–C(8)	116.3(3)	C(12)–C(11)–C(10)	120.5(3)
C(2)–N(1)–Fe(1)	128.7(2)	N(5)–C(12)–C(11)	120.6(3)
C(8)–N(1)–Fe(1)	113.9(2)	N(5)–C(12)–C(7)	120.0(3)
C(3)–N(2)–C(9)	116.4(3)	C(11)–C(12)–C(7)	119.5(3)
C(3)–N(2)–Fe(1)	128.5(2)		

Table 4A. Positional and thermal parameters for **4**.

Atom	Position	*x*/*a*	*y*/*b*	*z*/*c*	S.o.f.	U_{eq}
Fe(1)	4*e*	0.91680(9)	0.92497(5)	0.46225(4)	1	0.0152(2)
Fe(2)	4*e*	1.3460(1)	0.56768(5)	0.30709(5)	1	0.0224(2)
Fe(3)	4*e*	1.5173(1)	1.01636(5)	0.09411(5)	1	0.0169(2)
Cl(1)	4*e*	0.8366(2)	1.07683(8)	0.46607(8)	1	0.0183(3)
Cl(2)	4*e*	0.7516(2)	0.8430(1)	0.57621(9)	1	0.0296(4)
Cl(3)	4*e*	1.2098(2)	0.45040(9)	0.3990(1)	1	0.0315(4)

Atom	Position	*x*/*a*	*y*/*b*	*z*/*c*	S.o.f.	U_{eq}
Cl(4)	4*e*	1.5049(2)	1.16979(9)	0.06628(9)	1	0.0285(3)
Cl(5)	4*e*	1.2808(2)	1.01698(9)	0.01625(8)	1	0.0197(3)
Cl(6)	4*e*	0.7827(2)	0.8092(1)	0.28397(9)	1	0.0296(3)
O(1)	4*e*	0.7345(5)	0.9416(3)	0.3818(2)	1	0.0243(9)
H(1A)	4*e*	0.7468	0.9054	0.3565	1	0.037
O(2)	4*e*	1.1775(8)	0.5918(4)	0.2184(3)	0.645(10)	0.052(2)
H(2A)	4*e*	1.1443	0.6397	0.1888	1	0.079
O(2A)	4*e*	1.1775(8)	0.5918(4)	0.2184(3)	0.355(10)	0.052(2)
H(2B)	4*e*	1.2012	0.6214	0.2450	0.355(10)	0.079
O(3)	4*e*	1.5365(6)	0.5636(4)	0.3824(3)	0.823(10)	0.049(2)
O(3A)	4*e*	1.5365(6)	0.5636(4)	0.3824(3)	0.18	0.049(2)
O(4)	4*e*	1.5423(8)	0.5012(3)	0.2312(4)	1	0.052(2)
O(5)	4*e*	1.7152(5)	0.9936(3)	0.1689(2)	1	0.0254(9)
H(5A)	4*e*	1.7343	0.9427	0.1963	1	0.038
N(1)	4*e*	1.0937(6)	0.9723(3)	0.3468(3)	1	0.0157(9)
N(2)	4*e*	1.0311(5)	0.8044(3)	0.4282(3)	1	0.0152(9)
N(3)	4*e*	1.1946(6)	0.6655(3)	0.3662(3)	1	0.021(1)
N(4)	4*e*	1.4316(6)	0.6985(3)	0.2304(3)	1	0.020(1)
N(5)	4*e*	1.4974(6)	0.8716(3)	0.1478(3)	1	0.0159(9)
N(6)	4*e*	1.3289(6)	1.0070(3)	0.2040(3)	1	0.016(1)
C(1)	4*e*	0.9992(7)	0.7219(4)	0.4630(3)	1	0.022(1)
H(1)	4*e*	0.9210	0.7094	0.5098	1	0.026
C(2)	4*e*	1.0793(7)	0.6530(4)	0.4316(3)	1	0.022(1)
H(2)	4*e*	1.0505	0.5966	0.4575	1	0.026
C(3)	4*e*	1.5439(7)	0.7169(4)	0.1645(3)	1	0.023(1)
H(3)	4*e*	1.6034	0.6712	0.1454	1	0.028
C(4)	4*e*	1.5772(7)	0.8047(4)	0.1215(3)	1	0.020(1)
H(4)	4*e*	1.6554	0.8151	0.0746	1	0.024
C(5)	4*e*	1.2444(7)	1.0704(3)	0.2339(3)	1	0.017(1)
H(5)	4*e*	1.2642	1.1281	0.2072	1	0.020
C(6)	4*e*	1.1250(7)	1.0531(4)	0.3051(3)	1	0.019(1)
H(6)	4*e*	1.0669	1.0998	0.3231	1	0.023
C(7)	4*e*	1.1464(6)	0.8182(3)	0.3601(3)	1	0.015(1)
C(8)	4*e*	1.2285(7)	0.7494(3)	0.3289(3)	1	0.017(1)
C(9)	4*e*	1.3509(7)	0.7664(4)	0.2570(3)	1	0.018(1)
C(10)	4*e*	1.3831(7)	0.8530(4)	0.2164(3)	1	0.017(1)
C(11)	4*e*	1.2967(7)	0.9239(3)	0.2461(3)	1	0.015(1)
C(12)	4*e*	1.1787(6)	0.9071(3)	0.3171(3)	1	0.013(1)
C(13)	4*e*	0.5583(8)	0.9718(6)	0.3956(5)	1	0.046(2)
H(13A)	4*e*	0.4983	0.9245	0.4311	1	0.068
H(13B)	4*e*	0.5124	0.9927	0.3451	1	0.068
H(13C)	4*e*	0.5449	1.0186	0.4201	1	0.068
C(14)	4*e*	0.996(3)	0.584(2)	0.235(2)	0.355(10)	0.061(3)
H(14A)	4*e*	0.9424	0.6170	0.1878	0.355(10)	0.091
H(14B)	4*e*	0.9461	0.6073	0.2793	0.355(10)	0.091

Atom	Position	*x*/*a*	*y*/*b*	*z*/*c*	S.o.f.	U_{eq}
H(14C)	4*e*	0.9777	0.5238	0.2484	0.355(10)	0.091
C(15)	4*e*	1.106(2)	0.5227(9)	0.2004(8)	0.645(10)	0.061(3)
H(15A)	4*e*	1.1621	0.5151	0.1496	0.645(10)	0.091
H(15B)	4*e*	0.9856	0.5391	0.1975	0.645(10)	0.091
H(15C)	4*e*	1.1229	0.4688	0.2424	0.645(10)	0.091
C(16)	4*e*	1.644(5)	0.490(3)	0.417(2)	0.177(10)	0.060(3)
H(16A)	4*e*	1.7609	0.5015	0.4007	0.177(10)	0.090
H(16B)	4*e*	1.6263	0.4415	0.3988	0.177(10)	0.090
H(16C)	4*e*	1.6189	0.4749	0.4746	0.177(10)	0.090
C(17)	4*e*	1.711(1)	0.5601(7)	0.3694(7)	0.823(10)	0.060(3)
H(17A)	4*e*	1.7601	0.5061	0.3579	0.823(10)	0.090
H(17B)	4*e*	1.7518	0.5632	0.4169	0.823(10)	0.090
H(17C)	4*e*	1.7446	0.6086	0.3244	0.823(10)	0.090
C(18)	4*e*	1.8711(8)	1.0330(5)	0.1450(4)	1	0.040(2)
H(18A)	4*e*	1.9455	1.0062	0.1077	1	0.060
H(18B)	4*e*	1.9261	1.0247	0.1918	1	0.060
H(18C)	4*e*	1.8466	1.0946	0.1194	1	0.060
H(19A)	4*e*	1.557(17)	0.441(2)	0.260(5)	1	0.163
H(19B)	4*e*	1.535(16)	0.498(6)	0.179(3)	1	0.163
O(1S)	4*e*	1.900(2)	0.315(1)	0.334(1)	0.50	0.129(8)
H(1S)	4*e*	1.9522	0.3369	0.2897	0.50	0.194
O(2S)	4*e*	1.551(1)	0.3638(5)	0.4947(5)	1	0.103(3)
H(2S)	4*e*	1.5186	0.3820	0.5343	1	0.154
O(3S)	4*e*	0.017(1)	0.7415(5)	0.1528(4)	1	0.097(3)
H(3S)	4*e*	-0.0542	0.7612	0.1845	1	0.145
O(4S)	4*e*	1.519(4)	0.558(2)	0.074(2)	0.25	0.088(9)
O(4Q)	4*e*	1.278(5)	0.566(3)	-0.007(3)	0.25	0.15(2)
H(4S)	4*e*	1.6162	0.5662	0.0513	0.25	0.132
O(5S)	4*e*	1.541(2)	0.252(1)	0.297(1)	0.25	0.042(5)
H(5S)	4*e*	1.5940	0.2610	0.3287	0.25	0.063
O(5Q)	4*e*	1.677(3)	0.229(2)	0.186(1)	0.25	0.072(7)
H(5Q)	4*e*	1.7752	0.2425	0.1788	0.25	0.108
O(6S)	4*e*	0.959(4)	0.685(2)	-0.145(2)	0.25	0.081(6)
H(6S)	4*e*	0.8602	0.6742	-0.1366	0.25	0.122
O(7S)	4*e*	0.849(4)	0.600(2)	0.015(2)	0.25	0.081(6)
H(7S)	4*e*	0.8836	0.5832	0.0592	0.25	0.122
O(3W)	4*e*	0.612(3)	0.355(2)	0.203(2)	0.119(12)	0.003(8)
C(1S)	4*e*	1.716(2)	0.356(1)	0.337(2)	0.50	0.088(8)
H(1S1)	4*e*	1.6501	0.3232	0.3852	0.50	0.131
H(1S2)	4*e*	1.6700	0.3550	0.2904	0.50	0.131
H(1S3)	4*e*	1.7106	0.4153	0.3386	0.50	0.131
C(2S)	4*e*	1.508(1)	0.2745(5)	0.5129(6)	1	0.059(2)
H(2S1)	4*e*	1.6077	0.2372	0.4992	1	0.089
H(2S2)	4*e*	1.4199	0.2744	0.4819	1	0.089
H(2S3)	4*e*	1.4679	0.2532	0.5695	1	0.089

Atom	Position	*x*/*a*	*y*/*b*	*z*/*c*	S.o.f.	U_{eq}
C(3S)	4*e*	0.077(1)	0.8114(6)	0.0879(5)	1	0.058(2)
C(4S)	4*e*	1.394(3)	0.608(2)	0.019(2)	0.25	0.096(7)
C(4Q)	4*e*	1.394(3)	0.608(2)	0.019(2)	0.25	0.096(7)
C(5S)	4*e*	1.637(2)	0.182(1)	0.2652(9)	0.25	0.053(4)
C(5Q)	4*e*	1.637(2)	0.182(1)	0.2652(9)	0.25	0.053(4)
C(6S)	4*e*	0.987(5)	0.726(3)	-0.088(3)	0.25	0.11(2)
C(7S)	4*e*	0.902(5)	0.685(2)	-0.028(3)	0.25	0.11(2)

Table 4B. Bond distances (Å) in the crystal structure of **4**.

Fe(1)–N(2)	2.217(4)	O(6S)–C(6S)	1.413(19)
Fe(1)–N(1)	2.256(4)	O(7S)–C(7S)	1.435(19)
Fe(1)–Cl(2)	2.3483(16)	N(1)–C(6)	1.325(7)
Fe(1)–Cl(1)	2.4475(15)	N(1)–C(12)	1.347(7)
Fe(1)–Cl(1)	2.5044(15)	N(2)–C(1)	1.330(7)
Fe(2)–N(3)	2.231(5)	N(2)–C(7)	1.358(7)
Fe(2)–O(4)	2.233(6)	N(3)–C(2)	1.324(7)
Fe(2)–N(4)	2.267(5)	N(3)–C(8)	1.358(7)
Fe(2)–Cl(3)	2.3559(16)	N(4)–C(3)	1.320(7)
Fe(3)–N(6)	2.210(4)	N(4)–C(9)	1.346(7)
Fe(3)–N(5)	2.255(4)	N(5)–C(4)	1.328(7)
Fe(3)–Cl(4)	2.3597(17)	N(5)–C(10)	1.362(7)
Fe(3)–Cl(5)	2.4302(15)	N(6)–C(5)	1.326(7)
Fe(3)–Cl(5)	2.5108(15)	N(6)–C(11)	1.359(7)
O(1)–C(13)	1.418(7)	C(1)–C(2)	1.404(8)
O(2)–C(15)	1.467(14)	C(3)–C(4)	1.429(8)
O(3)–C(17)	1.371(11)	C(5)–C(6)	1.417(8)
O(5)–C(18)	1.429(7)	C(7)–C(8)	1.405(7)
O(4Q)–C(4Q)	1.429(19)	C(7)–C(12)	1.443(7)
O(5Q)–C(5Q)	1.378(17)	C(8)–C(9)	1.438(7)
O(1S)–C(1S)	1.510(16)	C(9)–C(10)	1.402(8)
O(2S)–C(2S)	1.462(10)	C(10)–C(11)	1.428(8)
O(3S)–C(3S)	1.411(10)	C(11)–C(12)	1.407(7)

Table 4C. Bond angles (°) in the crystal structure of **4**.

N(2)–Fe(1)–N(1)	75.13(16)	N(2)–Fe(1)–Cl(1)	92.66(12)
N(2)–Fe(1)–Cl(2)	91.13(12)	N(1)–Fe(1)–Cl(1)	86.09(12)
N(1)–Fe(1)–Cl(2)	166.21(13)	Cl(2)–Fe(1)–Cl(1)	95.86(6)
N(2)–Fe(1)–Cl(1)	164.63(12)	Cl(1)–Fe(1)–Cl(1)	86.72(5)
N(1)–Fe(1)–Cl(1)	89.51(12)	N(3)–Fe(2)–O(4)	163.65(18)
Cl(2)–Fe(1)–Cl(1)	104.21(6)	N(3)–Fe(2)–N(4)	75.16(16)

O(4)–Fe(2)–N(4)	89.15(17)	C(4)–N(5)–Fe(3)	129.5(4)
N(3)–Fe(2)–Cl(3)	92.85(12)	C(10)–N(5)–Fe(3)	113.1(3)
O(4)–Fe(2)–Cl(3)	103.01(13)	C(5)–N(6)–C(11)	116.4(4)
N(4)–Fe(2)–Cl(3)	167.73(13)	C(5)–N(6)–Fe(3)	129.2(4)
N(6)–Fe(3)–N(5)	75.35(16)	C(11)–N(6)–Fe(3)	114.4(3)
N(6)–Fe(3)–Cl(4)	92.09(13)	N(2)–C(1)–C(2)	122.3(5)
N(5)–Fe(3)–Cl(4)	167.12(12)	N(3)–C(2)–C(1)	122.2(5)
N(6)–Fe(3)–Cl(5)	163.98(13)	N(4)–C(3)–C(4)	122.3(5)
N(5)–Fe(3)–Cl(5)	88.69(12)	N(5)–C(4)–C(3)	120.5(5)
Cl(4)–Fe(3)–Cl(5)	103.92(6)	N(6)–C(5)–C(6)	122.1(5)
N(6)–Fe(3)–Cl(5)	89.41(12)	N(1)–C(6)–C(5)	121.9(5)
N(5)–Fe(3)–Cl(5)	85.86(12)	N(2)–C(7)–C(8)	122.1(5)
Cl(4)–Fe(3)–Cl(5)	97.03(6)	N(2)–C(7)–C(12)	118.4(5)
Cl(5)–Fe(3)–Cl(5)	87.94(5)	C(8)–C(7)–C(12)	119.5(5)
Fe(1)–Cl(1)–Fe(1)	93.28(5)	N(3)–C(8)–C(7)	120.7(5)
Fe(3)–Cl(5)–Fe(3)	92.06(5)	N(3)–C(8)–C(9)	118.8(5)
C(6)–N(1)–C(12)	116.6(5)	C(7)–C(8)–C(9)	120.5(5)
C(6)–N(1)–Fe(1)	129.7(4)	N(4)–C(9)–C(10)	121.7(5)
C(12)–N(1)–Fe(1)	113.6(3)	N(4)–C(9)–C(8)	118.9(5)
C(1)–N(2)–C(7)	115.9(5)	C(10)–C(9)–C(8)	119.4(5)
C(1)–N(2)–Fe(1)	129.5(4)	N(5)–C(10)–C(9)	121.0(5)
C(7)–N(2)–Fe(1)	114.5(3)	N(5)–C(10)–C(11)	118.3(5)
C(2)–N(3)–C(8)	116.8(5)	C(9)–C(10)–C(11)	120.7(5)
C(2)–N(3)–Fe(2)	129.2(4)	N(6)–C(11)–C(12)	121.2(5)
C(8)–N(3)–Fe(2)	114.0(4)	N(6)–C(11)–C(10)	118.8(5)
C(3)–N(4)–C(9)	117.0(5)	C(12)–C(11)–C(10)	120.0(5)
C(3)–N(4)–Fe(2)	129.8(4)	N(1)–C(12)–C(11)	121.8(5)
C(9)–N(4)–Fe(2)	113.1(3)	N(1)–C(12)–C(7)	118.3(4)
C(4)–N(5)–C(10)	117.5(5)	C(11)–C(12)–C(7)	119.9(5)