Supplementary Material for (19 pages):

Synthesis and structure of $[Fe(TPA)Cl_2](ClO_4)$ and $[\{Fe(TPA)Cl\}_2O](ClO_4)_2$ where TPA = tris-(2-pyridylmethyl)amine

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Table S1a. Fractional atomic coordinates for **1**.

Atom	x	y	z
Fe(1)	0.32926(4)	0.02948(3)	0.26981(2)
Cl(1)	0.34563(8)	-0.05465(5)	0.15604(4)
Cl(2)	0.22045(7)	0.14832(5)	0.20773(4)
Cl(3)	0.66509(8)	0.13263(4)	0.60366(4)
O(1)	0.6512(3)	0.04054(13)	0.5924(1)
O(2)	0.7589(3)	0.1487(2)	0.67642(13)
O(3)	0.7354(3)	0.1708(1)	0.53058(12)
O(4)	0.5134(3)	0.1695(2)	0.6148(2)
N(1)	0.1153(3)	-0.0089(2)	0.3270(1)
N(2)	0.4194(3)	-0.0740(2)	0.3511(1)
N(3)	0.5513(2)	0.0880(2)	0.2750(1)
N(4)	0.3343(3)	0.0951(1)	0.39206(13)
C(11)	0.0296(3)	-0.0775(2)	0.3036(2)
C(12)	-0.0995(3)	-0.1041(2)	0.3480(2)
C(13)	-0.1422(3)	-0.0575(2)	0.4186(2)
C(14)	-0.0548(3)	0.0128(2)	0.4432(2)
C(15)	0.0734(3)	0.0368(2)	0.3955(2)
C(16)	0.1713(3)	0.1141(2)	0.4151(2)
C(21)	0.4472(3)	-0.1564(2)	0.3283(2)
C(22)	0.4681(4)	-0.2220(2)	0.3858(2)
C(23)	0.4560(4)	-0.2026(2)	0.4697(2)

C(24)	0.4294(4)	-0.1176(2)	0.4944(2)
C(25)	0.4147(3)	-0.0550(2)	0.4336(2)
C(26)	0.4095(3)	0.0391(2)	0.4560(2)
C(31)	0.6705(3)	0.0650(2)	0.2249(2)
C(32)	0.8102(3)	0.1095(2)	0.2267(2)
C(33)	0.8277(3)	0.1782(2)	0.2812(2)
C(34)	0.7059(3)	0.2000(2)	0.3344(2)
C(35)	0.5697(3)	0.1535(2)	0.3292(2)
C(36)	0.4284(3)	0.1750(2)	0.3810(2)
H(11)	0.0588	-0.1087	0.2549
H(12)	-0.1576	-0.1532	0.3307
H(13)	-0.2311	-0.0740	0.4498
H(14)	-0.0817	0.0445	0.4920
H(15)	0.1651	0.1266	0.4731
H(16)	0.1354	0.1625	0.3840
H(21)	0.4527	-0.1700	0.2705
H(22)	0.4902	-0.2793	0.3680
H(23)	0.4659	-0.2470	0.5104
H(24)	0.4214	-0.1030	0.5519
H(25)	0.3536	0.0450	0.5069
H(26)	0.5128	0.0588	0.4638
H(31)	0.6585	0.0175	0.1878
H(32)	0.8928	0.0931	0.1908

H(33)	0.9217	0.2101	0.2825
H(34)	0.7164	0.2459	0.3735
H(35)	0.4598	0.1962	0.4341
H(36)	0.3683	0.2178	0.3533

Table S1b. Thermal parameters for the non-hydrogen atoms of **1**.

Atom	U11	U22	U33	U12	U13	U23
Fe(1)	.013	.017	.011	-.001	.000	-.002
C1(1)	.026	.028	.013	-.006	.001	-.008
C1(2)	.018	.026	.019	-.001	-.003	.004
C1(3)	.020	.013	.013	-.002	-.001	-.001
O(1)	.033	.014	.031	-.002	-.016	.000
O(2)	.054	.031	.018	-.018	-.012	.002
O(3)	.031	.030	.017	-.001	.004	.003
O(4)	.032	.031	.045	.010	.015	.001
N(1)	.016	.021	.013	-.001	-.002	.000
N(2)	.016	.019	.018	.001	.002	-.002
N(3)	.014	.019	.016	.000	.001	-.002
N(4)	.013	.017	.015	.003	-.001	-.002
C(11)	.018	.024	.018	-.002	-.002	-.001
C(12)	.019	.030	.023	-.007	-.003	.001
C(13)	.017	.034	.027	-.001	.004	.003
C(14)	.019	.034	.019	.004	.005	-.003

C(15)	.016	.022	.018	.005	-.001	.000
C(16)	.017	.021	.019	.004	.000	-.005
C(21)	.022	.021	.027	.002	-.001	-.009
C(22)	.035	.019	.042	.002	-.001	-.002
C(23)	.042	.023	.038	-.001	-.004	.008
C(24)	.028	.025	.022	-.001	-.001	.005
C(25)	.013	.022	.016	.001	.001	.001
C(26)	.023	.023	.011	.002	-.003	-.003
C(31)	.016	.020	.018	.000	.001	-.005
C(32)	.014	.023	.023	-.001	.002	-.001
C(33)	.016	.018	.025	-.003	-.004	.002
C(34)	.020	.016	.018	.000	-.004	.000
C(35)	.016	.015	.015	.001	-.004	-.002
C(36)	.017	.015	.019	.002	-.002	-.004

Table S2a. Fractional atomic coordinates for **2**.

Atom	x	y	z
Fe1	0.04807(3)	0.00372(2)	0.37350(3)
Cl1	-0.00860(6)	-0.12985(3)	0.30383(5)
Cl2	0.47846(6)	0.32189(3)	0.38818(5)
O11	0.0000	0.0000	0.5000
O21	0.4250(2)	0.28572(11)	0.4708(1)
O22	0.4165(2)	0.28519(13)	0.2798(2)

O23	0.6145(2)	0.30272(12)	0.4192(2)
O24	0.4610(2)	0.41146(10)	0.3867(1)
N1	-0.1189(2)	0.07415(11)	0.2846(1)
N2	0.1335(2)	0.02630(11)	0.2311(2)
N3	0.2455(2)	-0.00980(10)	0.4732(2)
N4	0.1149(2)	0.13627(10)	0.3996(2)
C11	-0.2262(2)	0.04344(13)	0.2104(2)
C12	-0.3339(2)	0.0917(2)	0.1634(2)
C13	-0.3327(2)	0.1748(2)	0.1945(2)
C14	-0.2238(2)	0.2079(1)	0.2711(2)
C15	-0.1184(2)	0.15553(13)	0.3155(2)
C16	-0.0001(2)	0.18402(12)	0.4065(2)
C21	0.1506(2)	-0.0319(1)	0.1579(2)
C22	0.2174(3)	-0.0164(1)	0.0810(2)
C23	0.2672(3)	0.0625(2)	0.0758(2)
C24	0.2502(2)	0.1239(1)	0.1501(2)
C25	0.1819(2)	0.10285(12)	0.2263(2)
C26	0.1587(2)	0.16921(13)	0.3041(2)
C31	0.3103(2)	-0.08336(13)	0.4995(2)
C32	0.4277(3)	-0.0888(2)	0.5805(2)
C33	0.4838(3)	-0.0165(2)	0.6373(2)
C34	0.4190(2)	0.0585(2)	0.6094(2)
C35	0.2993(2)	0.06006(13)	0.5291(2)

C36	0.2183(2)	0.13839(13)	0.5077(2)
H11	-0.2276	-0.0139	0.1896
H12	-0.4077	0.0681	0.1106
H13	-0.4061	0.2091	0.1634
H14	-0.2211	0.2652	0.2928
H15	-0.0128	0.1749	0.4781
H16	0.0135	0.2421	0.3972
H21	0.1149	-0.0861	0.1594
H22	0.2289	-0.0596	0.0321
H23	0.3123	0.0748	0.0227
H24	0.2840	0.1787	0.1491
H25	0.0945	0.2064	0.2612
H26	0.2370	0.1991	0.3347
H31	0.2733	-0.1327	0.4605
H32	0.4702	-0.1413	0.5978
H33	0.5647	-0.0189	0.6939
H34	0.4563	0.1089	0.6451
H35	0.1800	0.1449	0.5669
H36	0.2728	0.1849	0.5071

Table S2b. Thermal parameters for the non-hydrogen atoms of **2**.

Atom	U11	U22	U33	U12	U13	U23
Fe1	0.0166(2)	0.0082(1)	0.0163(2)	-0.00119(11)	0.00879(12)	-0.00097(11)

Cl1	0.0331(3)	0.0115(2)	0.0251(3)	-0.0067(2)	0.0174(3)	-0.0058(2)
Cl2	0.0304(3)	0.0157(2)	0.0251(3)	-0.0075(2)	0.0152(3)	-0.0056(2)
O11	0.0180(11)	0.0154(10)	0.0164(10)	-0.0020(8)	0.0086(9)	-0.0002(8)
O21	0.0271(10)	0.0278(9)	0.0276(9)	-0.0069(7)	0.0120(8)	0.0026(7)
O22	0.059(1)	0.0345(10)	0.0287(10)	-0.0021(10)	0.0153(10)	-0.0091(8)
O23	0.0307(12)	0.0327(11)	0.068(2)	-0.0037(8)	0.0288(11)	-0.0131(10)
O24	0.0426(12)	0.0167(8)	0.0315(10)	-0.0005(7)	0.0102(9)	0.0014(7)
N1	0.0203(10)	0.0127(8)	0.0165(9)	0.0006(7)	0.0084(8)	0.0019(7)
N2	0.0215(10)	0.0129(8)	0.0186(10)	-0.0004(7)	0.0096(8)	-0.0010(7)
N3	0.0175(9)	0.0126(8)	0.0209(9)	0.0013(7)	0.0110(8)	0.0018(7)
N4	0.0190(10)	0.0104(8)	0.0183(9)	0.0003(7)	0.0099(8)	0.0020(7)
C11	0.0245(12)	0.0154(10)	0.0169(10)	-0.0026(9)	0.0082(9)	0.0002(8)
C12	0.0204(13)	0.0274(12)	0.0214(12)	-0.0033(9)	0.0048(10)	0.0018(9)
C13	0.0209(13)	0.0249(12)	0.0257(12)	0.0048(9)	0.0059(10)	0.0069(9)
C14	0.0241(12)	0.0162(10)	0.0247(12)	0.0032(9)	0.0096(10)	0.0024(9)
C15	0.0191(11)	0.0128(9)	0.0196(11)	-0.0011(8)	0.0097(9)	0.0009(8)
C16	0.0217(12)	0.0106(9)	0.0199(11)	-0.0001(8)	0.0093(9)	-0.0018(8)
C21	0.032(1)	0.0150(10)	0.0244(12)	-0.0017(9)	0.0164(11)	-0.0029(9)
C22	0.038(2)	0.0218(11)	0.0261(13)	0.0001(10)	0.0201(12)	-0.0025(9)
C23	0.029(1)	0.0301(13)	0.0223(12)	-0.0023(10)	0.0147(11)	0.0011(10)
C24	0.0228(12)	0.0195(10)	0.0221(11)	-0.0034(9)	0.0109(10)	0.0033(9)
C25	0.0163(11)	0.0121(9)	0.0174(10)	0.0016(7)	0.0061(9)	0.0029(8)
C26	0.0256(12)	0.0133(9)	0.0235(11)	-0.0025(8)	0.0145(10)	0.0018(8)

C31	0.0194(12)	0.0145(10)	0.0281(12)	0.0023(8)	0.0118(10)	0.0033(9)
C32	0.026(1)	0.0217(11)	0.0310(13)	0.0072(9)	0.0144(11)	0.0106(10)
C33	0.0235(13)	0.0275(12)	0.0220(12)	0.0041(9)	0.0071(10)	0.0084(9)
C34	0.0240(13)	0.0235(11)	0.0200(11)	-0.0010(9)	0.0098(10)	0.0014(9)
C35	0.0206(12)	0.0141(9)	0.0157(10)	-0.0004(8)	0.0093(9)	0.0018(8)
C36	0.0182(11)	0.0137(10)	0.0217(11)	-0.0018(8)	0.0075(9)	-0.0035(8)

Table S3a. Fractional atomic coordinates for **3**.

Atom	x	y	z
Fe1	0.04156(3)	0.10058(3)	0.49387(4)
Cl1	0.14655(6)	0.37983(7)	0.87412(7)
Cl2	0.09064(6)	0.05987(7)	0.40205(7)
N2	-0.07424(18)	0.1505(2)	0.3836(2)
N3	0.14518(17)	0.0849(2)	0.6430(2)
N4	0.01190(17)	0.1716(2)	0.5875(2)
N5	0.07160(19)	0.2428(2)	0.4842(2)
O1	0.0000	0.0000	0.5000
O2	0.22606(18)	0.4124(2)	0.9374(2)
O3	0.1090(2)	0.3860(2)	0.9266(2)
O4	0.1030(2)	0.4301(2)	0.7829(2)
O5	0.14667(18)	0.28952(19)	0.8493(2)
C1	-0.1077(2)	0.1531(3)	0.2845(3)
H1	-0.0785	0.1362	0.2589

C2	-0.1830(3)	0.1875(3)	0.2179(3)
H2	-0.2049	0.1824	0.1471
C3	-0.2238(3)	0.2204(3)	0.2565(3)
H3	-0.2811	0.2517	0.2042
C4	-0.1885(2)	0.2177(3)	0.3595(3)
H4	-0.2211	0.2441	0.3784
C5	-0.1145(2)	0.1818(3)	0.4210(3)
C6	-0.0750(2)	0.1683(3)	0.5328(3)
H6A	-0.0929	0.2146	0.5597
H6B	-0.0988	0.1087	0.5323
C7	0.2149(2)	0.0530(3)	0.6659(3)
H7	0.2236	0.0469	0.6182
C8	0.2755(3)	0.0338(3)	0.7635(3)
H8	0.3244	0.0064	0.7747
C9	0.2650(3)	0.0487(3)	0.8396(3)
H9	0.3042	0.0424	0.9083
C10	0.1942(2)	0.0804(3)	0.8169(3)
H10	0.1808	0.0845	0.8669
C11	0.1342(2)	0.0971(3)	0.7173(3)
C12	0.0521(2)	0.1239(3)	0.6845(3)
H12A	0.0500	0.1633	0.7389
H12B	0.0221	0.0775	0.6796
C13	0.0868(3)	0.2734(3)	0.4183(3)

H13	0.1033	0.2244	0.3891
C14	0.0789(3)	0.3605(3)	0.3921(4)
H14	0.0814	0.3658	0.3320
C15	0.0535(4)	0.4186(4)	0.4335(5)
H15	0.0430	0.4837	0.4016
C16	0.0386(4)	0.3874(3)	0.5025(4)
H16	0.0214	0.4265	0.5332
C17	0.0493(2)	0.2991(3)	0.5266(3)
C18	0.0414(2)	0.2640(3)	0.6077(3)
H18A	0.0987	0.2665	0.6781
H18B	0.0012	0.2968	0.6103

Table S3b. Thermal parameters for the non-hydrogen atoms of **3**.

Atom	U11	U22	U33	U12	U13	U23
Fe1	0.0322(3)	0.0220(3)	0.0292(3)	-0.0016(2)	0.0208(2)	0.0005(2)
Cl1	0.0481(6)	0.0331(6)	0.0397(5)	-0.0062(4)	0.0292(5)	-0.0104(5)
Cl2	0.0457(5)	0.0319(6)	0.0389(5)	0.0010(4)	0.0315(4)	0.0033(4)
N2	0.0378(17)	0.0240(18)	0.0333(17)	0.0044(13)	0.0217(15)	0.0042(14)
N3	0.0317(16)	0.0234(17)	0.0309(16)	-0.0026(12)	0.0190(13)	-0.0011(14)
N4	0.0343(16)	0.0227(17)	0.0349(16)	-0.0054(13)	0.0235(14)	-0.0012(14)
N5	0.0441(19)	0.0263(19)	0.0439(18)	-0.0017(15)	0.0300(16)	-0.0033(15)
O1	0.0375(19)	0.0196(19)	0.0375(19)	-0.0050(15)	0.0265(17)	-0.0030(16)
O2	0.0528(18)	0.060(2)	0.0530(18)	-0.0185(15)	0.0323(15)	-0.0276(17)

O3	0.074(2)	0.043(2)	0.071(2)	-0.0204(16)	0.0570(19)	-0.0188(16)
O4	0.074(2)	0.064(3)	0.062(2)	0.0201(18)	0.0349(18)	-0.008(2)
O5	0.065(2)	0.0327(18)	0.0591(18)	-0.0191(14)	0.0403(16)	-0.0118(15)
C1	0.041(2)	0.036(3)	0.041(2)	0.0009(18)	0.0258(19)	0.0017(19)
C2	0.045(2)	0.049(3)	0.038(2)	0.005(2)	0.021(2)	-0.001(2)
C3	0.040(2)	0.042(3)	0.054(3)	0.008(2)	0.023(2)	0.008(2)
C4	0.037(2)	0.031(2)	0.058(3)	0.0026(19)	0.031(2)	0.0046(18)
C5	0.0323(19)	0.025(2)	0.040(2)	-0.0024(16)	0.0234(18)	-0.0013(17)
C6	0.040(2)	0.025(2)	0.043(2)	-0.0046(17)	0.0305(19)	-0.0013(18)
C7	0.044(2)	0.033(2)	0.039(2)	-0.0116(18)	0.0246(19)	-0.004(2)
C8	0.045(2)	0.044(3)	0.042(2)	-0.005(2)	0.017(2)	0.009(2)
C9	0.047(3)	0.047(3)	0.033(2)	-0.006(2)	0.0121(19)	0.005(2)
C10	0.044(2)	0.041(3)	0.032(2)	-0.0028(18)	0.0223(18)	-0.006(2)
C11	0.041(2)	0.023(2)	0.0343(19)	-0.0051(16)	0.0243(17)	-0.0058(17)
C12	0.040(2)	0.032(2)	0.032(2)	-0.0052(16)	0.0235(17)	-0.0069(18)
C13	0.057(3)	0.036(3)	0.058(3)	0.001(2)	0.040(2)	-0.004(2)
C14	0.096(4)	0.036(3)	0.082(4)	-0.002(2)	0.068(3)	-0.016(3)
C15	0.144(6)	0.030(3)	0.112(5)	0.005(3)	0.097(5)	-0.007(3)
C16	0.113(5)	0.025(3)	0.102(4)	-0.006(3)	0.085(4)	-0.004(3)
C17	0.049(2)	0.027(2)	0.052(2)	-0.0085(19)	0.033(2)	-0.009(2)
C18	0.045(2)	0.024(2)	0.051(2)	-0.0083(18)	0.035(2)	-0.0001(18)

Table S4a. Fractional atomic coordinates for **4**.

Atom	x	y	z
Fe(1)	0.60744(4)	0.16527(4)	0.78645(4)
Fe(2)	0.36985(4)	0.15955(3)	0.70780(4)
Cl(1)	0.63572(7)	0.13903(7)	0.93183(7)
Cl(2)	0.33946(8)	0.13349(7)	0.56226(7)
Cl(3)	0.79677(8)	0.11507(7)	0.50259(8)
Cl(4)	0.67539(8)	0.40318(7)	0.49892(8)
O(1)	0.4883(2)	0.1678(2)	0.7459(2)
O(2)	0.7914(4)	0.0918(2)	0.5823(3)
O(3)	0.8427(5)	0.0584(3)	0.4740(4)
O(4)	0.7066(4)	0.1295(4)	0.4403(4)
O(5)	0.8420(3)	0.1890(3)	0.5166(4)
O(6)	0.6452(3)	0.3241(2)	0.4745(3)
O(7)	0.7425(4)	0.4251(3)	0.4718(5)
O(8)	0.7013(7)	0.4096(4)	0.5902(4)
O(9)	0.6039(3)	0.4575(3)	0.4666(5)
O(10)	0.3903(9)	0.1797(8)	0.1068(10)
N(11)	0.7524(3)	0.1596(2)	0.8146(3)
N(12)	0.6111(2)	0.0553(2)	0.7247(3)
N(13)	0.6163(3)	0.2925(2)	0.7932(3)
N(14)	0.6168(2)	0.2032(2)	0.6612(2)
N(21)	0.2242(3)	0.1497(2)	0.6840(3)
N(22)	0.3757(2)	0.0482(2)	0.7692(3)

N(23)	0.3537(2)	0.2857(2)	0.7026(2)
N(24)	0.3627(2)	0.1936(2)	0.8359(3)
C(111)	0.8133(3)	0.1250(3)	0.8859(3)
C(112)	0.9015(3)	0.1198(3)	0.8981(4)
C(113)	0.9304(4)	0.1538(3)	0.8372(4)
C(114)	0.8684(4)	0.1872(3)	0.7633(4)
C(115)	0.7793(3)	0.1883(3)	0.7535(3)
C(116)	0.7092(3)	0.2257(3)	0.6735(3)
C(121)	0.6249(4)	-0.0153(3)	0.7655(4)
C(122)	0.6302(4)	-0.0838(3)	0.7233(4)
C(123)	0.6255(4)	-0.0803(3)	0.6363(4)
C(124)	0.6136(4)	-0.0078(3)	0.5957(4)
C(125)	0.6041(3)	0.0591(3)	0.6405(3)
C(126)	0.5808(3)	0.1383(3)	0.5970(3)
C(131)	0.6428(4)	0.3369(3)	0.8655(3)
C(132)	0.6396(4)	0.4183(3)	0.8635(4)
C(133)	0.6067(5)	0.4557(3)	0.7818(4)
C(134)	0.5790(4)	0.4097(3)	0.7062(3)
C(135)	0.5848(3)	0.3286(3)	0.7139(3)
C(136)	0.5588(3)	0.2745(2)	0.6353(3)
C(211)	0.1615(3)	0.1187(3)	0.6120(3)
C(212)	0.0722(4)	0.1134(3)	0.6028(4)
C(213)	0.0478(3)	0.1412(3)	0.6674(4)

C(214)	0.1122(3)	0.1714(3)	0.7430(4)
C(215)	0.2006(3)	0.1755(3)	0.7495(3)
C(216)	0.2705(3)	0.2108(3)	0.8295(3)
C(221)	0.3693(3)	-0.0214(3)	0.7281(3)
C(222)	0.3780(4)	-0.0918(3)	0.7723(4)
C(223)	0.3918(4)	-0.0903(3)	0.8617(4)
C(224)	0.3949(4)	-0.0187(3)	0.9027(4)
C(225)	0.3891(3)	0.0493(3)	0.8553(3)
C(226)	0.4046(3)	0.1291(3)	0.9002(3)
C(231)	0.3230(3)	0.3298(3)	0.6294(3)
C(232)	0.3219(4)	0.4108(3)	0.6328(4)
C(233)	0.3535(4)	0.4474(3)	0.7136(4)
C(234)	0.3849(4)	0.4024(3)	0.7894(3)
C(235)	0.3846(3)	0.3212(3)	0.7812(3)
C(236)	0.4173(3)	0.2675(3)	0.8603(3)
H(111)	0.7943	0.1035	0.9292
H(112)	0.9424	0.0932	0.9478
H(113)	0.9919	0.1541	0.8463
H(114)	0.8861	0.2093	0.7193
H(115)	0.7145	0.2813	0.6795
H(116)	0.7199	0.2099	0.6229
H(121)	0.6311	-0.0177	0.8252
H(122)	0.6369	-0.1330	0.7526

H(123)	0.6305	-0.1268	0.6063
H(124)	0.6118	-0.0035	0.5375
H(125)	0.5178	0.1430	0.5708
H(126)	0.6052	0.1423	0.5529
H(131)	0.6648	0.3114	0.9210
H(132)	0.6594	0.4481	0.9163
H(133)	0.6033	0.5115	0.7779
H(134)	0.5562	0.4337	0.6498
H(135)	0.4980	0.2597	0.6180
H(136)	0.5674	0.3005	0.5879
H(211)	0.1781	0.0999	0.5660
H(212)	0.0291	0.0905	0.5517
H(213)	-0.0129	0.1400	0.6610
H(214)	0.0964	0.1892	0.7900
H(215)	0.2633	0.1902	0.8801
H(216)	0.2625	0.2663	0.8275
H(221)	0.3586	-0.0220	0.6672
H(222)	0.3748	-0.1405	0.7427
H(223)	0.3988	-0.1380	0.8938
H(224)	0.4010	-0.0165	0.9624
H(225)	0.3794	0.1290	0.9438
H(226)	0.4670	0.1384	0.9272
H(231)	0.3014	0.3044	0.5738

H(232)	0.2998	0.4409	0.5803
H(233)	0.3537	0.5032	0.7172
H(234)	0.4061	0.4266	0.8456
H(235)	0.4096	0.2922	0.9087
H(236)	0.4785	0.2556	0.8752

Table S4b. Thermal parameters for the non-hydrogen atoms of **4**.

Atom	U11	U22	U33	U12	U13	U23
Fe(1)	0.0189(3)	0.0178(3)	0.0119(3)	-0.0015(2)	0.0066(2)	0.0009(2)
Fe(2)	0.0188(3)	0.0172(3)	0.0107(3)	0.0004(2)	0.0057(2)	0.0010(2)
Cl(1)	0.0271(6)	0.0354(6)	0.0145(5)	0.0000(5)	0.0074(4)	0.0073(5)
Cl(2)	0.0318(6)	0.0328(6)	0.0145(6)	-0.0000(5)	0.0073(5)	-0.0038(5)
Cl(3)	0.0336(6)	0.0354(6)	0.0188(6)	-0.0034(5)	0.0101(5)	0.0054(5)
Cl(4)	0.0383(7)	0.0334(6)	0.0206(6)	-0.0122(5)	0.0122(5)	0.0022(5)
O(1)	0.0186(13)	0.020(2)	0.014(2)	0.0011(12)	0.0073(12)	0.0008(12)
O(2)	0.128(5)	0.039(2)	0.076(4)	0.025(3)	0.079(4)	0.021(2)
O(3)	0.149(6)	0.062(3)	0.095(5)	0.015(3)	0.102(4)	-0.004(3)
O(4)	0.090(5)	0.103(5)	0.083(5)	-0.006(4)	-0.039(4)	-0.025(4)
O(5)	0.063(3)	0.041(2)	0.099(4)	-0.008(2)	0.040(3)	0.020(3)
O(6)	0.054(3)	0.036(2)	0.052(3)	-0.006(2)	0.023(2)	-0.005(2)
O(7)	0.096(4)	0.049(3)	0.253(9)	0.032(3)	0.140(6)	0.056(4)
O(8)	0.242(10)	0.101(5)	0.042(4)	-0.097(6)	0.016(5)	-0.003(3)
O(9)	0.047(3)	0.042(3)	0.221(8)	0.004(2)	0.061(4)	-0.005(4)

O(10)	0.21(1)	0.26(1)	0.33(2)	0.008(11)	0.151(13)	0.018(12)
N(11)	0.021(2)	0.032(2)	0.016(2)	-0.001(2)	0.006(2)	0.000(2)
N(12)	0.022(2)	0.024(2)	0.021(2)	0.003(2)	0.011(2)	0.002(2)
N(13)	0.027(2)	0.019(2)	0.019(2)	-0.004(2)	0.011(2)	-0.001(2)
N(14)	0.023(2)	0.023(2)	0.014(2)	-0.001(2)	0.008(2)	-0.001(2)
N(21)	0.025(2)	0.026(2)	0.020(2)	0.003(2)	0.006(2)	0.003(2)
N(22)	0.022(2)	0.021(2)	0.021(2)	-0.001(2)	0.009(2)	0.005(2)
N(23)	0.025(2)	0.020(2)	0.013(2)	0.001(2)	0.007(1)	0.000(2)
N(24)	0.020(2)	0.025(2)	0.019(2)	-0.003(2)	0.010(2)	-0.002(2)
C(111)	0.025(2)	0.046(3)	0.014(2)	0.000(2)	0.005(2)	-0.000(2)
C(112)	0.023(2)	0.048(3)	0.034(3)	0.001(2)	0.006(2)	0.002(3)
C(113)	0.025(3)	0.049(3)	0.050(4)	-0.004(2)	0.011(3)	0.003(3)
C(114)	0.033(3)	0.040(3)	0.042(3)	-0.006(2)	0.021(3)	0.001(3)
C(115)	0.026(2)	0.025(2)	0.024(3)	-0.006(2)	0.011(2)	-0.002(2)
C(116)	0.028(2)	0.034(3)	0.021(3)	-0.002(2)	0.016(2)	0.001(2)
C(121)	0.044(3)	0.025(2)	0.027(3)	0.006(2)	0.018(2)	0.004(2)
C(122)	0.066(4)	0.022(3)	0.041(4)	0.009(3)	0.027(3)	0.003(2)
C(123)	0.056(4)	0.027(3)	0.041(4)	0.009(3)	0.025(3)	-0.006(2)
C(124)	0.039(3)	0.031(3)	0.031(3)	0.002(2)	0.020(2)	-0.008(2)
C(125)	0.022(2)	0.022(2)	0.026(3)	0.003(2)	0.011(2)	-0.004(2)
C(126)	0.032(2)	0.031(2)	0.020(3)	0.001(2)	0.016(2)	0.000(2)
C(131)	0.041(3)	0.024(2)	0.018(2)	-0.011(2)	0.011(2)	-0.002(2)
C(132)	0.060(4)	0.026(2)	0.021(3)	-0.012(3)	0.014(3)	-0.005(2)

C(133)	0.080(5)	0.020(2)	0.038(4)	-0.008(3)	0.024(3)	-0.001(2)
C(134)	0.055(3)	0.024(2)	0.022(3)	-0.002(2)	0.012(2)	0.001(2)
C(135)	0.036(3)	0.024(2)	0.016(2)	-0.003(2)	0.012(2)	0.003(2)
C(136)	0.032(2)	0.021(2)	0.018(2)	0.001(2)	0.014(2)	0.008(2)
C(211)	0.026(2)	0.032(3)	0.023(3)	-0.003(2)	0.004(2)	-0.000(2)
C(212)	0.030(3)	0.042(3)	0.029(3)	-0.003(2)	0.003(2)	0.001(2)
C(213)	0.021(2)	0.041(3)	0.049(4)	0.001(2)	0.007(2)	-0.003(3)
C(214)	0.023(2)	0.036(3)	0.043(3)	0.003(2)	0.017(2)	0.002(2)
C(215)	0.025(2)	0.020(2)	0.026(3)	0.001(2)	0.011(2)	0.004(2)
C(216)	0.029(3)	0.042(3)	0.025(3)	-0.005(2)	0.017(2)	-0.008(2)
C(221)	0.038(3)	0.025(2)	0.024(3)	-0.009(2)	0.012(2)	-0.001(2)
C(222)	0.051(3)	0.022(2)	0.041(4)	-0.002(2)	0.013(3)	0.007(2)
C(223)	0.045(3)	0.036(3)	0.038(3)	-0.012(3)	0.012(3)	0.015(3)
C(224)	0.038(3)	0.042(3)	0.026(3)	-0.014(2)	0.012(2)	0.007(2)
C(225)	0.022(2)	0.030(2)	0.015(2)	-0.003(2)	0.005(2)	0.008(2)
C(226)	0.036(3)	0.030(2)	0.013(2)	-0.006(2)	0.010(2)	0.001(2)
C(231)	0.040(3)	0.022(2)	0.022(3)	0.004(2)	0.010(2)	-0.000(2)
C(232)	0.048(3)	0.020(2)	0.031(3)	0.006(2)	0.007(2)	0.007(2)
C(233)	0.055(4)	0.017(2)	0.042(4)	0.003(2)	0.009(3)	-0.002(2)
C(234)	0.042(3)	0.023(2)	0.026(3)	0.001(2)	0.008(2)	-0.006(2)
C(235)	0.023(2)	0.022(2)	0.022(3)	0.002(2)	0.009(2)	-0.001(2)
C(236)	0.026(2)	0.025(2)	0.017(2)	-0.001(2)	0.010(2)	-0.003(2)