

Four coordination clusters using fluorenyl and carbazyl phosphonates as ligands

Yun-Sheng Ma,^{*,a,b} Wang-Shui Cai,^a Bin Chen,^a Jian-Yu Chang,^a Xiao-Yan Tang,^a and Rong-Xin Yuan^{*,a}

BVS calculations for compound 1, 2, 3 and 4.

Compound 1

Co1

		Co ²⁺			Co ³⁺
1.692	2.041	0.38936	1.7	2.041	0.39787
1.692	2.065	0.36491	1.7	2.065	0.37288
1.692	2.169	0.27549	1.7	2.169	0.28152
1.692	2.193	0.25819	1.7	2.193	0.26383
1.84	2.175	0.40438	1.84	2.175	0.40438
1.84	2.196	0.38207	1.84	2.196	0.38207
		2.0744			2.1026

Co2

		Co2+			Co3+
1.692	1.928	0.52843	1.7	1.928	0.53998
1.692	1.958	0.48728	1.7	1.958	0.49793
1.692	1.989	0.44812	1.7	1.989	0.45791
1.692	2.449	0.12926	1.7	2.449	0.13208
1.84	2.086	0.51434	1.84	2.086	0.51434
		2.1074			2.1423

Compound 2

Mn1

		Mn2+			Mn3+			Mn4+
1.765	2.343	0.20968	1.732	2.343	0.19179	1.75	2.343	0.20135
1.765	1.956	0.59677	1.732	1.956	0.54585	1.75	1.956	0.57306
1.765	2.154	0.34947	1.732	2.154	0.31965	1.75	2.154	0.33558
1.765	1.935	0.63162	1.732	1.935	0.57773	1.75	1.935	0.60653
1.765	1.909	0.67761	1.732	1.909	0.61979	1.75	1.909	0.65068
1.765	1.911	0.67395	1.732	1.911	0.61645	1.75	1.911	0.64718
		3.1391			2.8713			3.0144

Mn2

		Mn2+			Mn3+			Mn4+
1.765	2.189	0.31792	1.732	2.189	0.2908	1.75	2.189	0.30529
1.765	1.993	0.53998	1.732	1.993	0.49391	1.75	1.993	0.51853
1.765	1.975	0.5669	1.732	1.975	0.51853	1.75	1.975	0.54438
1.765	2.127	0.37592	1.732	2.127	0.34384	1.75	2.127	0.36098
1.765	1.91	0.67578	1.732	1.91	0.61811	1.75	1.91	0.64893
1.765	1.881	0.73087	1.732	1.881	0.66851	1.75	1.881	0.70184
		3.2074			2.9337			3.08

Mn3

		Mn2+			Mn3+			Mn4+
1.765	1.889	0.71524	1.732	1.889	0.65421	1.75	1.889	0.68683
1.765	2.065	0.4445	1.732	2.065	0.40657	1.75	2.065	0.42684
1.765	2.196	0.31196	1.732	2.196	0.28535	1.75	2.196	0.29957
1.765	1.827	0.84572	1.732	1.827	0.77356	1.75	1.827	0.81212
1.849	2.077	0.53998	1.837	2.077	0.52275	1.822	2.077	0.50198
1.849	2.096	0.51295	1.837	2.096	0.49659	1.822	2.096	0.47686
		3.37			3.139			3.204

Mn4

		Mn2+			Mn3+			Mn4+
1.765	1.921	0.65598	1.732	1.921	0.60001	1.75	1.921	0.62992
1.765	2.177	0.3284	1.732	2.177	0.30038	1.75	2.177	0.31536
1.765	2.049	0.46414	1.732	2.049	0.42454	1.75	2.049	0.4457
1.765	1.865	0.76317	1.732	1.865	0.69805	1.75	1.865	0.73285
1.765	1.979	0.56081	1.732	1.979	0.51295	1.75	1.979	0.53853
1.765	2.183	0.32312	1.732	2.183	0.29555	1.75	2.183	0.31028
		3.0956			2.8315			2.9726

Mn5

		Mn2+			Mn3+			Mn4+
1.765	2.055	0.45667	1.732	2.055	0.41771	1.75	2.055	0.43853
1.765	1.933	0.63505	1.732	1.933	0.58086	1.75	1.933	0.60982
1.765	2.008	0.51853	1.732	2.008	0.47429	1.75	2.008	0.49793
1.765	1.815	0.8736	1.732	1.815	0.79906	1.75	1.815	0.83889
1.849	2.07	0.5503	1.837	2.07	0.53274	1.822	2.07	0.51157
1.849	2.247	0.34107	1.837	2.247	0.33018	1.822	2.247	0.31706
		3.375			3.1348			3.2134

Compound 3

Mn1

		Mn2+			Mn3+			Mn4+
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1.765	1.852	0.790464	1.732	1.852	0.723016	1.75	1.852	0.759059
1.765	1.918	0.661323	1.732	1.918	0.604894	1.75	1.918	0.635048
1.765	1.946	0.613123	1.732	1.946	0.560807	1.75	1.946	0.588764
1.765	1.986	0.550297	1.732	1.986	0.503341	1.75	1.986	0.528434
1.765	2.22	0.292372	1.732	2.22	0.267424	1.75	2.22	0.280756
1.765	2.249	0.270331	1.732	2.249	0.247264	1.75	2.249	0.259591
		3.177909			2.906746			3.051652

Mn2

		Mn2+			Mn3+			Mn4+
1.765	1.883	0.726934	1.732	1.883	0.664907	1.75	1.883	0.698054
1.765	1.908	0.67944	1.732	1.908	0.621465	1.75	1.908	0.652446
1.765	1.933	0.635048	1.732	1.933	0.580861	1.75	1.933	0.609818
1.765	1.966	0.580861	1.732	1.966	0.531298	1.75	1.966	0.557784
1.765	2.141	0.361962	1.732	2.141	0.331077	1.75	2.141	0.347581
1.765	2.311	0.228624	1.732	2.311	0.209116	1.75	2.311	0.219541
		3.21287			2.938724			3.085224

Mn3

		Mn2+			Mn3+			Mn4+
1.765	1.81	0.885483	1.732	1.81	0.809927	1.75	1.81	0.850303
1.765	1.928	0.643688	1.732	1.928	0.588764	1.75	1.928	0.618115
1.849	2.063	0.560807	1.837	2.063	0.54291	1.822	2.063	0.521341
1.849	2.109	0.495245	1.837	2.109	0.479441	1.822	2.109	0.460393
1.765	2.123	0.380006	1.732	2.123	0.347581	1.75	2.123	0.364909
1.765	2.216	0.29555	1.732	2.216	0.270331	1.75	2.216	0.283807
		3.26078			3.038955			3.098868

Mn4

		Mn2+			Mn3+			Mn4+
1.765	1.886	0.721064	1.732	1.886	0.659538	1.75	1.886	0.692417
1.765	1.894	0.705641	1.732	1.894	0.64543	1.75	1.894	0.677606
1.765	1.939	0.624833	1.732	1.939	0.571518	1.75	1.939	0.600009
1.765	1.947	0.611468	1.732	1.947	0.559293	1.75	1.947	0.587175
1.765	2.234	0.281516	1.732	2.234	0.257495	1.75	2.234	0.270331
1.765	2.298	0.2368	1.732	2.298	0.216594	1.75	2.298	0.227392
		3.181322			2.909868			3.054929

Mn5

		Mn2+			Mn3+			Mn4+
1.765	1.849	0.796899	1.732	1.849	0.728902	1.75	1.849	0.765239
1.765	1.933	0.635048	1.732	1.933	0.580861	1.75	1.933	0.609818
1.849	2.059	0.566903	1.837	2.059	0.548812	1.822	2.059	0.527007

1.849	2.072	0.54733	1.837	2.072	0.529864	1.822	2.072	0.508813
1.765	2.132	0.370874	1.732	2.132	0.339229	1.75	2.132	0.35614
1.765	2.208	0.302009	1.732	2.208	0.27624	1.75	2.208	0.290011
		3.219064			3.003907			3.057027

Compound 4

Mn1

		Mn2+			Mn3+			Mn4+
1.765	2.155	0.348522	1.732	2.155	0.318783	1.75	2.155	0.334675
1.765	2.155	0.348522	1.732	2.155	0.318783	1.75	2.155	0.334675
1.765	2.2	0.30861	1.732	2.2	0.282277	1.75	2.2	0.296349
1.849	2.245	0.342916	1.837	2.245	0.331973	1.822	2.245	0.318783
1.765	2.262	0.260998	1.732	2.262	0.238728	1.75	2.262	0.250628
1.765	2.262	0.260998	1.732	2.262	0.238728	1.75	2.262	0.250628
		1.870566			1.729272			1.78574

Mn2

		Mn2+			Mn3+			Mn4+
1.765	2.104	0.40003	1.732	2.104	0.365896	1.75	2.104	0.384137
1.765	2.104	0.40003	1.732	2.104	0.365896	1.75	2.104	0.384137
1.765	2.311	0.228624	1.732	2.311	0.209116	1.75	2.311	0.219541
1.849	2.211	0.37592	1.837	2.211	0.363924	1.822	2.211	0.349465
1.765	2.311	0.228624	1.732	2.311	0.209116	1.75	2.311	0.219541
1.765	2.464	0.151194	1.732	2.464	0.138293	1.75	2.464	0.145187
		1.784423			1.652242			1.702008

Mn3

		Mn2+			Mn3+			Mn4+
1.765	1.927	0.64543	1.732	1.927	0.590357	1.75	1.927	0.619788
1.765	1.935	0.631625	1.732	1.935	0.57773	1.75	1.935	0.606531
1.765	1.95	0.606531	1.732	1.95	0.554777	1.75	1.95	0.582433
1.765	2.25	0.269601	1.732	2.25	0.246597	1.75	2.25	0.25889
1.765	2.298	0.2368	1.732	2.298	0.216594	1.75	2.298	0.227392
1.765	1.863	0.76731	1.732	1.863	0.701837	1.75	1.863	0.736825
		3.157297			2.887893			3.031858

Mn4

		Mn2+			Mn3+			Mn4+
1.765	1.91	0.675777	1.732	1.91	0.618115	1.75	1.91	0.648929
1.765	1.91	0.675777	1.732	1.91	0.618115	1.75	1.91	0.648929
1.765	1.937	0.62822	1.732	1.937	0.574616	1.75	1.937	0.603261
1.849	2.279	0.312809	1.837	2.279	0.302827	1.822	2.279	0.290795
1.765	1.937	0.62822	1.732	1.937	0.574616	1.75	1.937	0.603261

1.765	2.288	0.243287	1.732	2.288	0.222528	1.75	2.288	0.233621
		3.16409			2.910815			3.028796

Mn5

		Mn2+			Mn3+			Mn4+
1.765	2.149	0.35422	1.732	2.149	0.323995	1.75	2.149	0.340147
1.765	2.201	0.307777	1.732	2.201	0.281516	1.75	2.201	0.29555
1.765	2.265	0.25889	1.732	2.265	0.2368	1.75	2.265	0.248605
1.849	2.268	0.322248	1.837	2.268	0.311965	1.822	2.268	0.299571
1.765	2.265	0.25889	1.732	2.265	0.2368	1.75	2.265	0.248605
1.765	2.149	0.35422	1.732	2.149	0.323995	1.75	2.149	0.340147
		1.856246			1.71507			1.772622

Mn6

		Mn2+			Mn3+			Mn4+
1.765	1.867	0.759059	1.732	1.867	0.69429	1.75	1.867	0.728902
1.765	1.928	0.643688	1.732	1.928	0.588764	1.75	1.928	0.618115
1.765	1.943	0.618115	1.732	1.943	0.565373	1.75	1.943	0.593557
1.765	1.943	0.618115	1.732	1.943	0.565373	1.75	1.943	0.593557
1.765	2.264	0.259591	1.732	2.264	0.237441	1.75	2.264	0.249277
1.765	2.378	0.190757	1.732	2.378	0.17448	1.75	2.378	0.183178
		3.089325			2.82572			2.966586

Mn7

		Mn2+			Mn3+			Mn4+
1.765	2.09	0.415456	1.732	2.09	0.380006	1.75	2.09	0.39895
1.765	2.216	0.29555	1.732	2.216	0.270331	1.75	2.216	0.283807
1.765	2.216	0.29555	1.732	2.216	0.270331	1.75	2.216	0.283807
1.849	2.201	0.386219	1.837	2.201	0.373894	1.822	2.201	0.359039
1.765	2.395	0.18219	1.732	2.395	0.166645	1.75	2.395	0.174952
1.765	2.09	0.415456	1.732	2.09	0.380006	1.75	2.09	0.39895
		1.99042			1.841213			1.899506

Mn8

		Mn2+			Mn3+			Mn4+
1.765	1.924	0.650685	1.732	1.924	0.595164	1.75	1.924	0.624833
1.765	1.924	0.650685	1.732	1.924	0.595164	1.75	1.924	0.624833
1.765	1.939	0.624833	1.732	1.939	0.571518	1.75	1.939	0.600009
1.849	2.233	0.35422	1.837	2.233	0.342916	1.822	2.233	0.329292
1.765	1.939	0.624833	1.732	1.939	0.571518	1.75	1.939	0.600009
1.765	2.347	0.207428	1.732	2.347	0.189728	1.75	2.347	0.199187
		3.112684			2.866007			2.978163

O					Sum
O17	0.30861	0.590357	0.590357		1.489325
O18	0.151194	0.701837	0.701837	0.222528	1.777396
O19	0.69429	0.69429	0.18219	0.189728	1.7605
O20	0.307777	0.565373	0.565373		1.438523

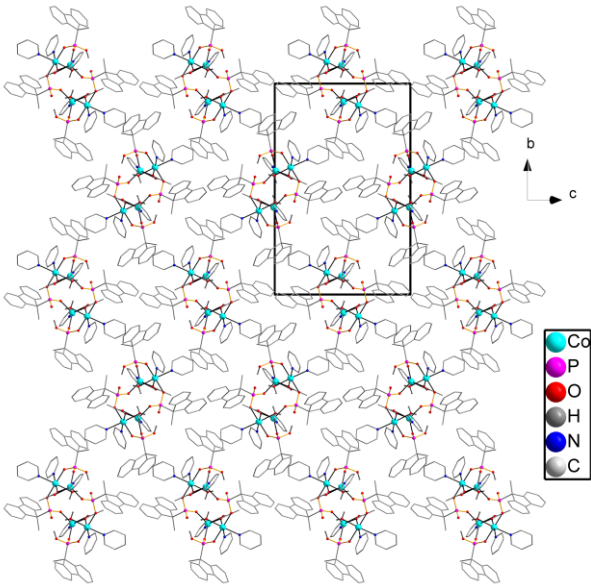


Fig. S1 Packing diagram of **1** viewed along a-axis.

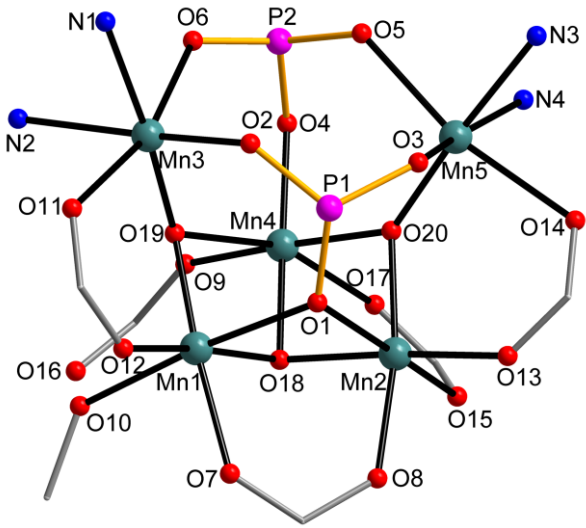


Fig. S2 Inorganic core of compound **3**.

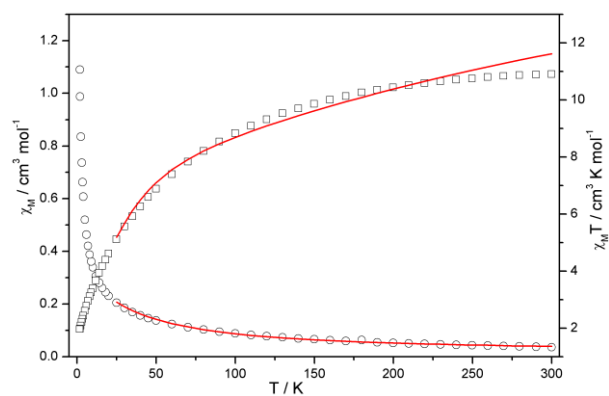


Fig. S3 Temperature dependence of χ_M ($\circ$) and $\chi_M T$ ($\square$) values for **3**. The solid lines correspond to the best-fit curves using the parameters described in the text.

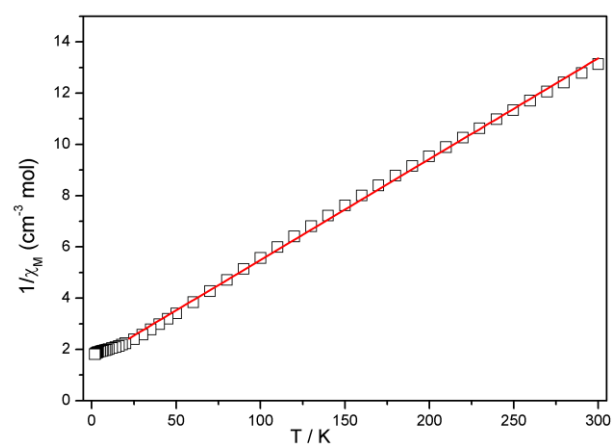


Fig. S4 $1/\chi_M$ versus T for **4**.

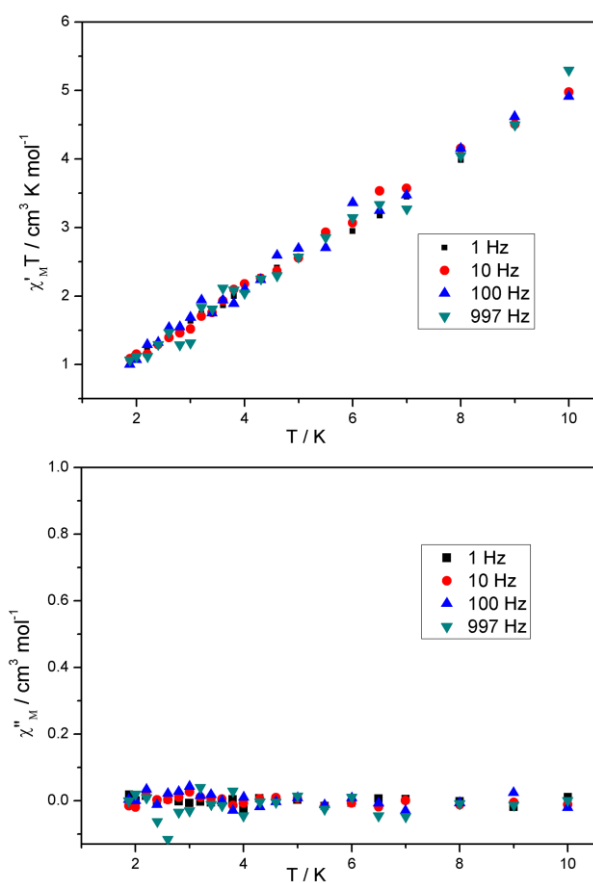


Fig. S5 Plots of ac susceptibility versus temperature for **4**.

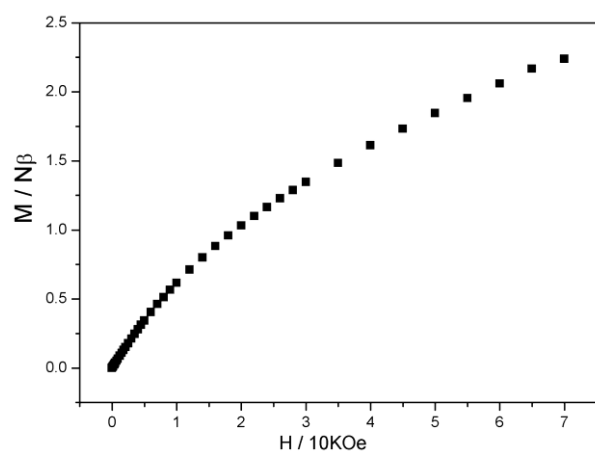


Fig. S6 Field dependent magnetization for **2** at 2 K.

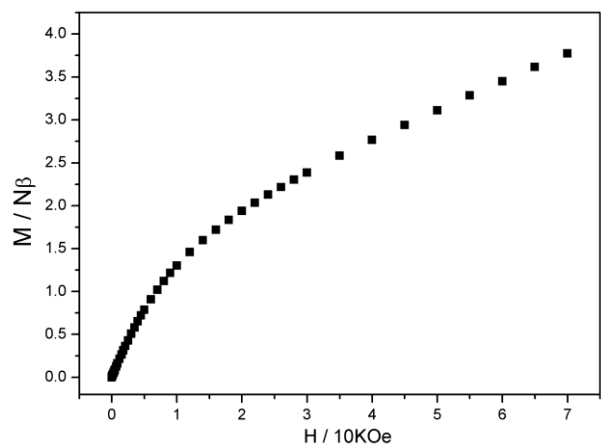


Fig. S7 Field dependent magnetization for **3** at 2 K.

Table S1 Selected bond lengths and angles for **1**

Co1-O2	2.041(2)	Co2-O6A	1.928(3)
Co1-O4	2.065(2)	Co2-O1	1.958(2)
Co1-O7A	2.169(3)	Co2-O8	1.989(3)
Co1-N1	2.175(3)	Co2-N3	2.086(3)
Co1-O9	2.193(3)	Co2-O7	2.449(1)
Co1-N2	2.196(3)	P2-O5	1.548(3)
O2-Co1-O4	179.29(10)	O7A-Co1-N1	92.05(13)
O2-Co1-O7A	93.02(11)	O7A-Co1-N2	175.61(12)
O2-Co1-O9	87.23(10)	O1-Co2-O8	108.91(12)
O2-Co1-N1	90.22(11)	O1-Co2-N3	104.20(12)
O2-Co1-N2	91.25(12)	O1-Co2-O6A	114.49(12)
O4-Co1-O9	92.14(11)	O8-Co2-N3	96.46(15)
O4-Co1-N1	90.40(12)	O8-Co2-O6A	128.18(13)
O4-Co1-N2	89.14(14)	O6A-Co2-N3	98.97(15)
O4-Co1-O7A	86.61(13)	O7-Co2-O8	57.62(1)
O9-Co1-N1	177.41(11)	O7-Co2-O6A	92.04(2)
O9-Co1-N2	93.66(13)	O7-Co2-O1	93.76(2)
O7A-Co1-O9	87.59(12)	O7-Co2-N3	152.60(3)
N1-Co1-N2	86.88(14)		

Table S2 Selected bond lengths and angles for **2**

Mn1-O1	2.343(3)	Mn3-O19	1.827(2)
Mn1-O7	1.956(3)	Mn3-N1	2.077(3)
Mn1-O10	2.154(3)	Mn3-N2	2.096(3)
Mn1-O12	1.935(3)	Mn4-O4	1.921(2)
Mn1-O18	1.909(2)	Mn4-O9	2.177(3)
Mn1-O19	1.911(2)	Mn4-O17	2.049(3)
Mn2-O1	2.189(3)	Mn4-O18	1.865(2)

Mn2-O8	1.993(3)	Mn4-O19	1.979(2)
Mn2-O13	1.975(3)	Mn4-O20	2.183(3)
Mn2-O15	2.127(3)	Mn5-O3	2.055(3)
Mn2-O18	1.910(2)	Mn5-O5	1.933(3)
Mn2-O20	1.881(3)	Mn5-O14	2.008(3)
Mn3-O2	1.889(3)	Mn5-O20	1.815(2)
Mn3-O6	2.065(3)	Mn5-N3	2.070(3)
Mn3-O11	2.196(3)	Mn5-N4	2.247(3)
O1-Mn1-O7	87.62(10)	O1-Mn2-O8	84.28(10)
O1-Mn1-O10	166.90(10)	O1-Mn2-O13	91.22(10)
O1-Mn1-O12	97.91(10)	O1-Mn2-O15	170.68(11)
O1-Mn1-O18	81.08(10)	O1-Mn2-O18	85.23(10)
O1-Mn1-O19	83.62(10)	O1-Mn2-O20	91.56(11)
O7-Mn1-O10	96.90(11)	O8-Mn2-O13	86.20(11)
O7-Mn1-O12	84.08(11)	O8-Mn2-O15	86.56(11)
O7-Mn1-O18	91.08(11)	O8-Mn2-O18	90.67(10)
O7-Mn1-O19	170.69(11)	O8-Mn2-O20	172.56(12)
O10-Mn1-O12	94.79(11)	O13-Mn2-O15	86.45(11)
O10-Mn1-O18	86.53(10)	O13-Mn2-O18	175.49(11)
O10-Mn1-O19	91.00(10)	O13-Mn2-O20	100.09(11)
O12-Mn1-O18	175.10(11)	O15-Mn1-O18	96.61(11)
O12-Mn1-O19	100.21(11)	O15-Mn1-O20	97.73(11)
O18-Mn1-O19	84.48(10)	O18-Mn1-O20	82.82(10)
O2-Mn3-O6	98.83(11)	O4-Mn4-O9	96.75(10)
O2-Mn3-O11	90.20(11)	O4-Mn4-O17	92.82(11)
O2-Mn3-O19	96.07(11)	O4-Mn4-O18	172.33(11)
O2-Mn3-N1	89.87(12)	O4-Mn4-O19	91.65(10)
O2-Mn3-N2	166.77(12)	O4-Mn4-O20	99.17(10)
O6-Mn3-O11	165.58(11)	O9-Mn4-O17	84.67(10)
O6-Mn3-O19	96.05(11)	O9-Mn4-O18	89.06(10)
O6-Mn3-N1	88.09(12)	O9-Mn4-O19	85.94(10)
O6-Mn3-N2	86.84(11)	O9-Mn4-O20	161.01(10)
O11-Mn3-O19	94.13(10)	O17-Mn4-O18	92.70(11)
O11-Mn3-N1	80.67(12)	O17-Mn4-O19	170.02(10)
O11-Mn3-N2	82.08(11)	O17-Mn4-O20	84.26(10)
O19-Mn3-N1	172.14(12)	O18-Mn4-O19	83.74(10)
O19-Mn3-N2	95.20(11)	O18-Mn4-O20	76.10(10)
N1-Mn3-N2	78.32(13)	O19-Mn4-O20	103.83(10)
O3-Mn5-O5	99.12(11)	O5-Mn5-N4	84.08(12)
O3-Mn5-O14	89.06(11)	O14-Mn5-O20	96.23(12)
O3-Mn5-O20	94.94(11)	O14-Mn5-N3	83.45(12)
O3-Mn5-N3	91.50(12)	O14-Mn5-N4	85.61(12)
O3-Mn5-N4	166.92(11)	O20-Mn5-N3	173.55(12)

O5-Mn5-O14	166.43(12)	O20-Mn5-N4	97.51(11)
O5-Mn5-O20	93.85(11)	N3-Mn5-N4	76.05(12)
O5-Mn5-N3	85.52(12)	Mn2-O18-Mn4	105.48(11)
Mn1-O1-Mn2	84.33(9)	Mn2-O20-Mn4	95.06(10)
Mn1-O18-Mn2	105.73(11)	Mn2-O20-Mn5	123.89(13)
Mn1-O18-Mn4	97.21(11)	Mn3-O19-Mn4	136.56(14)
Mn1-O19-Mn3	125.67(13)	Mn4-O20-Mn5	129.95(14)
Mn1-O19-Mn4	93.40(10)		

Table S3 Selected bond lengths and angles for **3**

Mn1-O1	2.249(2)	Mn3-O19	1.810(2)
Mn1-O7	1.986(3)	Mn3-N1	2.063(3)
Mn1-O10	2.220(2)	Mn3-N2	2.109(3)
Mn1-O12	1.946(3)	Mn4-O4	1.894(3)
Mn1-O18	1.918(3)	Mn4-O9	1.947(3)
Mn1-O19	1.852(3)	Mn4-O17	2.234(3)
Mn2-O1	2.311(3)	Mn4-O18	1.886(2)
Mn2-O8	1.966(3)	Mn4-O19	2.298(3)
Mn2-O13	1.933(3)	Mn4-O20	1.939(3)
Mn2-O15	2.141(3)	Mn5-O3	1.934(3)
Mn2-O18	1.884(2)	Mn5-O5	2.132(3)
Mn2-O20	1.908(3)	Mn5-O14	2.208(3)
Mn3-O2	1.928(3)	Mn5-O20	1.849(2)
Mn3-O6	2.123(3)	Mn5-N3	2.059(3)
Mn3-O11	2.216(3)	Mn5-N4	2.072(3)
O1-Mn1-O7	87.00(10)	O1-Mn2-O8	89.07(10)
O1-Mn1-O10	175.07(10)	O1-Mn2-O13	91.69(10)
O1-Mn1-O12	90.58(10)	O1-Mn2-O15	174.58(10)
O1-Mn1-O18	84.77(10)	O1-Mn2-O18	83.82(10)
O1-Mn1-O19	92.37(11)	O1-Mn2-O20	84.69(10)
O7-Mn1-O10	88.07(11)	O8-Mn2-O13	86.45(11)
O7-Mn1-O12	85.65(11)	O8-Mn2-O15	93.22(11)
O7-Mn1-O18	87.37(11)	O8-Mn2-O18	88.10(11)
O7-Mn1-O19	173.07(11)	O8-Mn2-O20	170.38(11)
O10-Mn1-O12	88.97(11)	O13-Mn2-O15	93.36(11)
O11-Mn1-O18	95.07(11)	O13-Mn2-O18	173.00(11)
O10-Mn1-O19	92.53(11)	O13-Mn2-O20	101.01(11)
O12-Mn1-O18	171.80(11)	O15-Mn2-O18	91.34(11)
O12-Mn1-O19	101.26(11)	O15-Mn2-O20	92.39(11)
O18-Mn1-O19	85.71(11)	O18-Mn2-O20	83.97(11)
O2-Mn3-O6	102.41(11)	O4-Mn4-O9	98.79(11)
O2-Mn3-O11	86.13(11)	O4-Mn4-O17	170.58(11)
O2-Mn3-O19	96.87(11)	O4-Mn4-O18	99.08(10)

O2-Mn3-N1	89.44(12)	O4-Mn4-O19	91.10(11)
O2-Mn3-N2	164.92(12)	O4-Mn4-O20	83.99(12)
O6-Mn3-O11	165.05(10)	O9-Mn4-O17	86.80(11)
O6-Mn3-O19	94.65(11)	O9-Mn4-O18	98.62(11)
O6-Mn3-N1	83.85(11)	O9-Mn4-O19	88.25(10)
O6-Mn3-N2	86.67(11)	O9-Mn4-O20	171.20(12)
O11-Mn3-O19	96.50(10)	O17-Mn4-O18	88.05(10)
O11-Mn3-N1	83.99(12)	O17-Mn4-O19	161.29(9)
O11-Mn3-N2	82.59(12)	O17-Mn4-O20	84.62(10)
O19-Mn3-N1	173.69(12)	O18-Mn4-O19	74.87(10)
O19-Mn3-N2	94.32(12)	O18-Mn4-O20	83.06(11)
N1-Mn3-N2	79.49(12)	O19-Mn4-O20	100.51(10)
O3-Mn5-O5	100.07(11)	O5-Mn5-N4	85.89(11)
O3-Mn5-O14	85.96(10)	O14-Mn5-O20	94.46(11)
O3-Mn5-O20	95.37(12)	O14-Mn5-N3	82.25(11)
O3-Mn5-N3	88.24(12)	O14-Mn5-N4	85.95(11)
O3-Mn5-N4	166.43(12)	O20-Mn5-N3	174.95(12)
O5-Mn5-O14	167.25(10)	O20-Mn5-N4	96.10(12)
O5-Mn5-O20	96.13(10)	N3-Mn5-N4	79.88(12)
O5-Mn5-N3	86.69(11)	Mn2-O18-Mn4	97.02(11)
Mn1-O1-Mn2	83.15(9)	Mn2-O20-Mn4	94.44(11)
Mn1-O18-Mn2	105.52(13)	Mn2-O20-Mn5	125.40(14)
Mn1-O18-Mn4	105.79(11)	Mn3-O19-Mn4	127.78(12)
Mn1-O19-Mn4	93.34(10)	Mn4-O20-Mn5	137.53(14)
Mn1-O19-Mn3	125.52(15)		

Table S4 Selected bond lengths and angles for **4**

Mn1-O1	2.262(3)	Mn5-O1	2.265(3)
Mn1-O13	2.155(3)	Mn5-O15	2.149(3)
Mn1-O17	2.200(3)	Mn5-O20	2.201(3)
Mn1-N7	2.245(4)	Mn5-N6	2.268(4)
Mn2-O4	2.104(2)	Mn6-O2	1.928(2)
Mn2-O14	2.311(3)	Mn6-O7	2.264(3)
Mn2-O18	2.464(4)	Mn6-O10	1.943(3)
Mn2-N10	2.211(5)	Mn6-O16	2.378(3)
Mn3-O3	1.951(2)	Mn6-O19	1.867(2)
Mn3-O5	1.935(3)	Mn6-O20	1.943(2)
Mn3-O7	2.298(3)	Mn7-O11	2.090(2)
Mn3-O14	2.251(3)	Mn7-O16	2.216(3)
Mn3-O17	1.927(2)	Mn7-O19	2.395(4)
Mn3-O18	1.863(2)	Mn7-N5	2.201(5)
Mn4-O6	1.937(3)	Mn8-O9	1.924(3)
Mn4-O8	1.910(3)	Mn8-O12	1.939(3)

Mn4-O18	2.288(3)	Mn8-O19	2.347(4)
Mn4-N9	2.279(4)	Mn8-N8	2.233(4)
O1-Mn1-O13	89.88(9)	O4-Mn2-O14	86.78(9)
O1-Mn1-O17	78.43(9)	O4-Mn2-O18	84.00(9)
O1-Mn1-N7	99.79(12)	O4-Mn2-N10	89.79(11)
O1-Mn1-O1A	87.95(10)	O4-Mn2-O4A	99.74(10)
O1-Mn1-O13A	176.67(10)	O4-Mn2-O14A	158.19(11)
O13-Mn1-O17	103.62(9)	O14-Mn2-O18	75.96(9)
O13-Mn1-N7	78.08(11)	O14-Mn2-N10	111.16(12)
O13-Mn1-O13A	92.17(11)	O14-Mn2-O14A	80.17(9)
O17-Mn1-N7	177.48(17)	O18-Mn2-N10	170.34(15)
O3-Mn3-O5	97.74(10)	O6-Mn4-O8	88.58(11)
O3-Mn3-O7	87.99(10)	O6-Mn4-O18	85.88(10)
O3-Mn3-O14	83.26(10)	O6-Mn4-N9	91.77(12)
O3-Mn3-O17	91.76(11)	O6-Mn4-O6A	90.35(11)
O3-Mn3-O18	171.39(12)	O6-Mn4-O8A	178.36(12)
O5-Mn3-O7	98.52(10)	O8-Mn4-O18	95.28(10)
O5-Mn3-O14	85.94(11)	O8-Mn4-N9	87.02(12)
O5-Mn3-O17	168.69(12)	O8-Mn4-O8A	92.46(12)
O5-Mn3-O18	88.01(11)	O18-Mn4-N9	176.67(16)
O7-Mn3-O14	170.66(10)	O1-Mn5-O15	88.37(10)
O7-Mn3-O17	87.89(12)	O1-Mn5-O20	77.94(10)
O7-Mn3-O18	97.54(12)	O1-Mn5-N6	94.11(11)
O14-Mn3-O17	89.12(12)	O1-Mn5-O1A	87.78(10)
O14-Mn3-O18	90.79(13)	O1-Mn5-O15A	175.31(10)
O17-Mn3-O18	81.89(11)	O15-Mn5-O20	103.85(10)
O2-Mn6-O7	88.57(10)	O15-Mn5-N6	83.50(10)
O2-Mn6-O10	97.44(11)	O15-Mn5-O15A	95.35(11)
O2-Mn6-O16	85.54(10)	O20-Mn5-N6	168.85(16)
O2-Mn6-O19	168.79(13)	O9-Mn8-O12	87.12(11)
O2-Mn6-O20	90.93(11)	O9-Mn8-O19	95.23(10)
O7-Mn6-O10	97.56(10)	O9-Mn8-N8	87.16(12)
O7-Mn6-O16	173.69(10)	O9-Mn8-O9A	91.13(12)
O7-Mn6-O19	99.28(130)	O9-Mn8-O12A	178.22(12)
O7-Mn6-O20	87.64(13)	O12-Mn8-O19	85.26(10)
O10-Mn6-O16	85.47(10)	O12-Mn8-N8	92.42(12)
O10-Mn6-O19	89.49(12)	O12-Mn8-O12A	94.63(12)
O10-Mn6-O20	170.23(12)	O19-Mn8-N8	176.57(17)
O16-Mn6-O19	86.25(13)	O9A-Mn8-O19	95.23(10)
O16-Mn6-O20	90.18(13)	O12A-Mn8-O19	85.26(10)
O19-Mn6-O20	81.48(12)	O9A-Mn8-N8	87.16(12)
O11-Mn7-O16	85.10(9)	Mn1-O1-Mn5	91.51(8)
O11-Mn7-O19	84.45(9)	Mn3-O7-Mn6	119.62(16)

O11-Mn7-N5	96.99(10)	Mn2-O14-Mn3	93.00(10)
O11-Mn7-O11A	102.96(10)	Mn6-O16-Mn7	92.30(10)
O11-Mn7-O16A	160.52(11)	Mn1-O17-Mn3	117.91(12)
O16-Mn7-O19	78.66(10)	Mn3-O17-Mn3A	95.82(15)
O16-Mn7-N5	99.62(11)	Mn2-O18-Mn3	98.83(12)
O16A-Mn7-O16	82.16(11)	Mn2-O18-Mn4	120.05(15)
O19-Mn7-N5	177.68(14)	Mn3-O18-Mn4	117.50(11)
Mn6A-O19-Mn7	101.40(13)	Mn3-O18-Mn3A	100.31(16)
Mn6A-O19-Mn8	115.49(13)	Mn6-O19-Mn7	101.40(13)
Mn5-O20-Mn6	117.20(13)	Mn6-O19-Mn8	115.49(13)
Mn6-O20-Mn6A	95.71(15)	Mn6-O19-Mn6A	101.01(18)
Mn7-O19-Mn8	119.32(16)		