Article

Supplementary Materials: Modeling the OEC with Two New Biomimetic Models: Preparations, Structural Characterization, and Water Photolysis Studies of a Ba–Mn Box Type Complex and a Mn_4N_6 Planar-Diamond Cluster

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Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Ba(1)	0.53994(4)	0.33567(2)	0.34099(2)	0.02186(15)
Mn(2)	0.42089(9)	0.21949(6)	0.46053(6)	0.0249(3)
N(1)	0.2701(4)	0.1768(3)	0.4465(3)	0.0220(14)
C(2)	0.2366(6)	0.1785(5)	0.5188(4)	0.0315(19)
C(3)	0.3414(6)	0.1584(5)	0.5832(4)	0.036(2)
N(4)	0.4405(5)	0.1994(3)	0.5695(3)	0.0237(14)
C(11)	0.1880(6)	0.1630(4)	0.3811(4)	0.0244(16)
C(12)	0.2193(6)	0.1589(4)	0.3069(4)	0.0213(16)
C(13)	0.1359(6)	0.1308(4)	0.2414(4)	0.0276(18)
C(14)	0.1560(6)	0.1253(4)	0.1702(4)	0.0285(18)
C(15)	0.2598(7)	0.1483(4)	0.1615(4)	0.0320(19)
C(16)	0.3424(6)	0.1756(4)	0.2245(4)	0.0278(18)
C(17)	0.3256(6)	0.1815(4)	0.2978(4)	0.0211(16)
C(41)	0.5331(6)	0.2065(4)	0.6290(4)	0.0285(18)
C(42)	0.6336(6)	0.2475(4)	0.6177(4)	0.0209(16)
C(43)	0.7212(6)	0.2670(4)	0.6846(4)	0.0285(18)
C(44)	0.8152(6)	0.3062(4)	0.6818(4)	0.0326(19)
C(45)	0.8277(6)	0.3289(4)	0.6117(4)	0.0288(18)
C(46)	0.7459(6)	0.3091(4)	0.5451(4)	0.0276(18)
C(47)	0.6475(6)	0.2681(4)	0.5469(4)	0.0263(18)
O(111)	0.0869(4)	0.1492(3)	0.3815(3)	0.0285(12)
O(171)	0.4102(4)	0.2097(3)	0.3548(3)	0.0258(12)
O(411)	0.5354(4)	0.1845(3)	0.6954(3)	0.0364(14)
O(471)	0.5733(4)	0.2495(3)	0.4779(3)	0.0325(13)
N(5)	0.4801(5)	0.4298(3)	0.5684(3)	0.0220(13)
C(6)	0.5867(6)	0.4560(4)	0.6217(4)	0.0319(19)
C(7)	0.5926(6)	0.4449(4)	0.7058(4)	0.0261(17)
N(8)	0.7013(5)	0.4721(3)	0.7547(3)	0.0273(15)
C(51)	0.3856(7)	0.4709(4)	0.5518(4)	0.0308(19)
C(52)	0.2845(6)	0.4415(4)	0.4917(4)	0.0202(16)
C(53)	0.1818(6)	0.4802(4)	0.4832(4)	0.0335(19)
C(54)	0.0858(7)	0.4583(5)	0.4270(5)	0.044(2)
C(55)	0.0928(7)	0.3985(5)	0.3774(5)	0.044(2)

C(56)	0.1938(7)	0.3597(4)	0.3856(4)	0.0309(19)
C(57)	0.2926(6)	0.3778(4)	0.4437(4)	0.0249(17)
C(81)	0.7256(6)	0.5471(4)	0.7642(4)	0.0213(16)
C(82)	0.8448(6)	0.5694(4)	0.8083(4)	0.0225(16)
C(83)	0.8670(6)	0.6494(4)	0.8145(4)	0.0295(18)
C(84)	0.9727(7)	0.6757(5)	0.8500(5)	0.043(2)
C(85)	1.0630(7)	0.6250(5)	0.8799(5)	0.051(3)
C(86)	1.0424(6)	0.5479(5)	0.8736(5)	0.044(2)
C(87)	0.9339(6)	0.5199(4)	0.8389(4)	0.0327(19)
O(511)	0.3817(4)	0.5345(3)	0.5859(3)	0.0294(12)
O(571)	0.3871(4)	0.3398(3)	0.4500(3)	0.0256(11)
O(811)	0.6523(4)	0.5967(3)	0.7382(3)	0.0260(12)
O(871)	0.9158(4)	0.4426(3)	0.8327(3)	0.0387(14)
O(200)	0.6858(6)	0.1991(4)	0.3598(4)	0.071(2)
C(200)	0.6877(15)	0.1271(11)	0.4143(10)	0.176(8)

Table S2. Bond lengths (Å) and angles (°) for **1**.

Chemical Bond	Bond Lengths (Å)	Chemical Bond	Bond Lengths (Å)
Ba(1)-O(411)	2.636(5)	N(5)-C(6)	1.459(9)
Ba(1)-O(511)	2.648(5)	N(5)-H(5)	0.85(4)
Ba(1)-O(811)	2.658(5)	C(6)-C(7)	1.512(10)
Ba(1)-O(171)	2.754(5)	C(6)-H(6[a])	0.9700
Ba(1)-O(471)	2.816(5)	C(6)-H(6B)	0.9700
Ba(1)-O(571)	3.074(5)	C(7)-N(8)	1.453(9)
Ba(1)-Mn(2)	3.5510(12)	C(7)-H(7A)	0.9700
Mn(2)-O(471)	1.877(5)	C(7)-H(7B)	0.9700
Mn(2)-O(171)	1.883(5)	N(8)-C(81)	1.334(9)
Mn(2)-N(1)	1.938(5)	N(8)-H(8)	0.87(4)
Mn(2)-N(4)	1.944(6)	C(51)-O(511)	1.271(8)
Mn(2)-O(571)	2.125(5)	C(51)-C(52)	1.487(10)
N(1)-C(11)	1.338(8)	C(52)-C(53)	1.394(10)
N(1)-C(2)	1.474(9)	C(52)-C(57)	1.425(9)
C(2)-C(3)	1.509(10)	C(53)-C(54)	1.372(10)
C(2)-H(2A)	0.9700	C(53)-H(53)	0.9300
C(2)-H(2B)	0.9700	C(54)-C(55)	1.388(10)
C(3)-N(4)	1.486(9)	C(54)-H(54)	0.9300
C(3)-H(3A)	0.9700	C(55)-C(56)	1.379(10)
C(3)-H(3B)	0.9700	C(55)-H(55)	0.9300
N(4)-C(41)	1.328(9)	C(56)-C(57)	1.395(10)
C(11)-O(111)	1.264(8)	C(56)-H(56)	0.9300
C(11)-C(12)	1.495(9)	C(57)-O(571)	1.309(8)
C(12)-C(17)	1.412(9)	C(81)-O(811)	1.237(8)
C(12)-C(13)	1.413(9)	C(81)-C(82)	1.503(9)
C(13)-C(14)	1.377(10)	C(82)-C(87)	1.374(10)
C(13)-H(13)	0.9300	C(82)-C(83)	1.412(9)
C(14)-C(15)	1.382(10)	C(83)-C(84)	1.352(10)
C(14)-H(14)	0.9300	C(83)-H(83)	0.9300
C(15)-C(16)	1.374(10)	C(84)-C(85)	1.397(11)
C(15)-H(15)	0.9300	C(84)-H(84)	0.9300
C(16)-C(17)	1.398(9)	C(85)-C(86)	1.360(11)
C(16)-H(16)	0.9300	C(85)-H(85)	0.9300
C(17)-O(171)	1.330(8)	C(86)-C(87)	1.387(10)
C(41)-O(411)	1.249(8)	C(86)-H(86)	0.9300
C(41)-C(42)	1.484(10)	C(87)-O(871)	1.359(9)
C(42)-C(47)	1.383(9)	O(511)-Ba(1)	2.648(5)
C(42)-C(43)	1.411(9)	O(811)-Ba(1)	2.658(5)

C(43)-C(44)	1.350(10)	O(871)-H(87)	0.85(4)
C(43)-H(43)	0.9300	O(200)-C(200)	1.586(18)
C(44)-C(45)	1.375(10)	O(200)-H(200)	0.8200
C(44)-H(44)	0.9300	C(200)-H(20A)	0.9600
C(45)-C(46)	1.373(9)	C(200)-H(20B)	0.9600
C(45)-H(45)	0.9300	C(200)-H(20C)	0.9600
C(46)-C(47)	1.407(10)	O(100)-C(100)	1.486(13)
C(46)-H(46)	0.9300	O(100)-H(100)	0.8200
C(47)-O(471)	1.357(8)	C(100)-H(10A)	0.9600
O(411)-Ba(1)	2.636(5)	C(100)-H(10B)	0.9600
N(5)-C(51)	1.320(9)	C(100)-H(10C)	0.9600

Angle Atom Site	**Angles (°)**	**Angle Atom Site**	**Angles (°)**
O(411)-Ba(1)-O(511)	120.81(16)	C(47)-C(46)-H(46)	119.2
O(411)-Ba(1)-O(811)	75.91(14)	O(471)-C(47)-C(42)	124.1(7)
O(511)-Ba(1)-O(811)	91.95(14)	O(471)-C(47)-C(46)	117.1(6)
O(411)-Ba(1)-O(171)	97.69(15)	C(42)-C(47)-C(46)	118.8(6)
O(511)-Ba(1)-O(171)	140.07(14)	C(17)-O(171)-Mn(2)	129.3(4)
O(811)-Ba(1)-O(171)	87.29(14)	C(17)-O(171)-Ba(1)	124.4(4)
O(411)-Ba(1)-O(471)	139.51(16)	Mn(2)-O(171)-Ba(1)	98.20(18)
O(511)-Ba(1)-O(471)	94.13(15)	C(41)-O(411)-Ba(1)	169.9(5)
O(811)-Ba(1)-O(471)	126.37(14)	C(47)-O(471)-Mn(2)	126.6(5)
O(171)-Ba(1)-O(471)	56.24(14)	C(47)-O(471)-Ba(1)	124.9(4)
O(411)-Ba(1)-O(571)	142.68(14)	Mn(2)-O(471)-Ba(1)	96.27(18)
O(511)-Ba(1)-O(571)	82.08(13)	C(51)-N(5)-C(6)	123.1(6)
O(811)-Ba(1)-O(571)	74.13(13)	C(51)-N(5)-H(5)	111(8)
O(171)-Ba(1)-O(571)	59.34(13)	C(6)-N(5)-H(5)	123(8)
O(471)-Ba(1)-O(571)	54.23(13)	N(5)-C(6)-C(7)	113.7(6)
O(411)-Ba(1)-Mn(2)	129.28(12)	N(5)-C(6)-H(6A)	108.8
O(511)-Ba(1)-Mn(2)	109.45(11)	C(7)-C(6)-H(6A)	108.8
O(811)-Ba(1)-Mn(2)	97.10(10)	N(5)-C(6)-H(6B)	108.8
O(171)-Ba(1)-Mn(2)	31.66(9)	C(7)-C(6)-H(6B)	108.8
O(471)-Ba(1)-Mn(2)	31.70(10)	H(6A)-C(6)-H(6B)	107.7
O(571)-Ba(1)-Mn(2)	36.53(9)	N(8)-C(7)-C(6)	110.1(6)
O(471)-Mn(2)-O(171)	88.6(2)	N(8)-C(7)-H(7A)	109.6
O(471)-Mn(2)-N(1)	173.4(2)	C(6)-C(7)-H(7A)	109.6
O(171)-Mn(2)-N(1)	92.4(2)	N(8)-C(7)-H(7B)	109.6
O(471)-Mn(2)-N(4)	92.7(2)	C(6)-C(7)-H(7B)	109.6
O(171)-Mn(2)-N(4)	164.2(2)	H(7A)-C(7)-H(7B)	108.2
N(1)-Mn(2)-N(4)	84.6(2)	C(81)-N(8)-C(7)	121.8(6)
O(471)-Mn(2)-O(571)	84.4(2)	C(81)-N(8)-H(8)	129(8)
O(171)-Mn(2)-O(571)	92.40(19)	C(7)-N(8)-H(8)	108(8)

N(1)-Mn(2)-O(571)	102.1(2)	O(511)-C(51)-N(5)	120.6(7)
N(4)-Mn(2)-O(571)	103.4(2)	O(511)-C(51)-C(52)	120.9(7)
O(471)-Mn(2)-Ba(1)	52.04(14)	N(5)-C(51)-C(52)	118.5(6)
O(171)-Mn(2)-Ba(1)	50.14(14)	C(53)-C(52)-C(57)	121.4(7)
N(1)-Mn(2)-Ba(1)	132.55(16)	C(53)-C(52)-C(51)	117.1(6)
N(4)-Mn(2)-Ba(1)	139.55(17)	C(57)-C(52)-C(51)	121.5(6)
O(571)-Mn(2)-Ba(1)	59.42(13)	C(54)-C(53)-C(52)	120.5(7)
C(11)-N(1)-C(2)	117.1(6)	C(54)-C(53)-H(53)	119.8
C(11)-N(1)-Mn(2)	129.4(5)	C(52)-C(53)-H(53)	119.8
C(2)-N(1)-Mn(2)	111.7(4)	C(53)-C(54)-C(55)	119.2(8)
N(1)-C(2)-C(3)	106.7(6)	C(53)-C(54)-H(54)	120.4
N(1)-C(2)-H(2A)	110.4	C(55)-C(54)-H(54)	120.4
C(3)-C(2)-H(2A)	110.4	C(56)-C(55)-C(54)	120.8(7)
N(1)-C(2)-H(2B)	110.4	C(56)-C(55)-H(55)	119.6
C(3)-C(2)-H(2B)	110.4	C(54)-C(55)-H(55)	119.6
H(2A)-C(2)-H(2B)	108.6	C(55)-C(56)-C(57)	122.2(7)
N(4)-C(3)-C(2)	108.6(6)	C(55)-C(56)-H(56)	118.9
N(4)-C(3)-H(3A)	110.0	C(57)-C(56)-H(56)	118.9
C(2)-C(3)-H(3A)	110.0	O(571)-C(57)-C(56)	120.7(7)
N(4)-C(3)-H(3B)	110.0	O(571)-C(57)-C(52)	123.3(6)
C(2)-C(3)-H(3B)	110.0	C(56)-C(57)-C(52)	115.9(7)
H(34)-C(3)-H(3B)	108.3	O(811)-C(81)-N(8)	121.2(6)
C(41)-N(4)-C(3)	117.4(6)	O(811)-C(81)-C(82)	121.0(6)
C(41)-N(4)-Mn(2)	129.4(5)	N(8)-C(81)-C(82)	117.8(6)
C(3)-N(4)-Mn(2)	112.3(4)	C(87)-C(82)-C(83)	117.9(7)
O(111)-C(11)-N(1)	121.5(6)	C(87)-C(82)-C(81)	126.5(6)
O(111)-C(11)-C(12)	119.7(6)	C(83)-C(82)-C(81)	115.5(6)
N(1)-C(11)-C(12)	118.7(6)	C(84)-C(83)-C(82)	120.4(7)
C(17)-C(12)-C(13)	118.1(6)	C(84)-C(83)-H(83)	119.8
C(17)-C(12)-C(11)	124.7(6)	C(82)-C(83)-H(83)	119.8
C(13)-C(12)-C(11)	117.2(6)	C(83)-C(84)-C(85)	121.2(8)
C(14)-C(13)-C(12)	121.8(7)	C(83)-C(84)-H(84)	119.4
C(14)-C(13)-H(13)	119.1	C(85)-C(849-H(84)	119.4
C(12)-C(13)-H(13)	119.1	C(86)-C(85)-C(84)	118.7(8)
C(13)-C(14)-C(15)	119.8(7)	C(86)-C(85)-H(85)	120.7
C(13)-C(14)-H(14)	120.1	C(84)-C(85)-H(85)	120.7
C(15)-C(14)-H(14)	120.1	C(85)-C(86)-C(87)	120.8(7)
C(16)-C(15)-C(14)	119.4(7)	C(85)-C(86)-H(86)	119.6
C(16)-C(15)-H(15)	120.3	C(87)-C(86)-H(86)	119.6
C(14)-C(15)-H(15)	120.3	O(871)-C(87)-C(82)	119.3(7)
C(15)-C(16)-C(17)	122.5(7)	O(871)-C(87)-C(86)	119.7(7)

C(15)-C(16)-H(16)	118.8	C(82)-C(87)-C(86)	120.9(7)
C(17)-C(16)-H(16)	118.8	C(51)-O(511)-Ba(1)	157.2(5)
O(171)-C(17)-C(16)	117.9(6)	C(57)-O(571)-Mn(2)	130.3(4)
O(171)-C(17)-C(12)	123.7(6)	C(57)-O(571)-Ba(1)	129.8(4)
C(16)-C(17)-C(12)	118.4(6)	Mn(2)-O(571)-Ba(1)	84.05(15)
O(411)-C(41)-N(4)	122.0(7)	C(81)-O(811)-Ba(1)	161.7(5)
O(411)-C(41)-C(42)	118.8(6)	C(87)-O(871)-H(87)	133(9)
N(4)-C(41)-C(42)	119.0(6)	C(200)-O(200)-H(200)	109.5
C(47)-C(42)-C(43)	117.8(7)	O(200)-C(200)-H(20A)	109.5
C(47)-C(42)-C(41)	125.0(6)	O(200)-C(200)-H(20B)	109.5
C(43)-C(42)-C(41)	117.3(6)	H(20A)-C(200)-H(20B)	109.5
C(44)-C(43)-C(42)	122.7(7)	O(200)-C(200)-H(20C)	109.5
C(44)-C(43)-H(43)	118.7	H(20A)-C(200)-H(20C)	109.5
C(42)-C(43)-H(43)	118.7	H(20B)-C(200)-H(20C)	109.5
C(43)-C(44)-C(45)	119.7(7)	C(100)-O(100)-H(100)	109.5
C(43)-C(44)-H(44)	120.1	O(100)-C(100)-H(10A)	109.5
C(45)-C(44)-H(44)	120.1	O(100)-C(100)-H(10B)	109.5
C(46)-C(45)-C(44)	119.4(7)	H(10A)-C(100)-H(10B)	109.5
C(46)-C(45)-H(45)	120.3	O(100)-C(100)-H(10C)	109.5
C(44)-C(45)-H(45)	120.3	H(10A)-C(100)-H(10C)	109.5
C(45)-C(46)-C(47)	121.7(7)	H(10B)-C(100)-H(10C)	109.5
C(45)-C(46)-H(46)	119.2		

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ba(1)	0.0210(2)	0.0256(2)	0.0166(2)	-0.0017(2)	0.00144(17)	0.0002(2)
Mn(2)	0.0232(6)	0.0328(7)	0.0148(6)	0.0035(5)	-0.0010(5)	-0.0083(5)
N(1)	0.014(3)	0.026(4)	0.020(3)	-0.003(3)	-0.007(3)	-0.003(3)
C(2)	0.013(4)	0.054(6)	0.025(4)	0.002(4)	-0.001(3)	-0.009(4)
C(3)	0.044(5)	0.041(5)	0.023(4)	0.004(4)	0.008(4)	-0.009(4)
N(4)	0.022(3)	0.025(3)	0.022(3)	0.003(3)	0.002(3)	-0.002(3)
C(11)	0.028(4)	0.015(4)	0.028(4)	0.002(3)	0.005(3)	-0.001(4)
C(12)	0.019(4)	0.017(4)	0.024(4)	-0.001(3)	0.000(3)	0.008(3)
C(13)	0.019(4)	0.025(4)	0.035(5)	-0.009(3)	0.001(3)	-0.001(3)
C(14)	0.023(4)	0.037(5)	0.020(4)	-0.011(3)	-0.005(3)	0.007(4)
C(15)	0.039(5)	0.025(5)	0.027(4)	-0.002(3)	0.001(4)	0.002(4)
C(16)	0.027(4)	0.035(5)	0.023(4)	-0.006(3)	0.009(3)	0.003(4)
C(17)	0.020(4)	0.018(4)	0.024(4)	-0.003(3)	0.005(3)	0.006(3)
C(41)	0.031(5)	0.026(4)	0.023(4)	-0.009(3)	-0.002(4)	0.000(4)
C(42)	0.019(4)	0.024(4)	0.017(4)	0.004(3)	0.000(3)	0.005(3)
C(43)	0.019(4)	0.045(5)	0.022(4)	0.009(3)	0.006(3)	0.009(4)
C(44)	0.022(4)	0.038(5)	0.032(5)	-0.002(4)	-0.002(4)	0.000(4)
C(45)	0.023(4)	0.024(4)	0.033(4)	0.005(4)	-0.001(3)	-0.001(4)
C(46)	0.026(4)	0.030(4)	0.023(4)	0.001(3)	0.000(3)	-0.003(3)
C(47)	0.018(4)	0.035(5)	0.019(4)	-0.004(3)	-0.006(3)	0.002(4)
O(111)	0.022(3)	0.030(3)	0.028(3)	-0.006(2)	-0.002(2)	-0.009(2)
O(171)	0.019(3)	0.035(3)	0.021(3)	-0.007(2)	0.002(2)	-0.001(2)
O(411)	0.023(3)	0.068(4)	0.012(3)	0.008(2)	-0.005(2)	-0.008(3)
O(471)	0.021(3)	0.050(3)	0.021(3)	0.005(2)	-0.001(2)	-0.004(2)
N(5)	0.019(3)	0.024(4)	0.020(3)	0.002(3)	0.002(3)	-0.006(3)
C(6)	0.025(4)	0.029(5)	0.040(5)	-0.008(4)	0.006(4)	-0.012(4)
C(7)	0.020(4)	0.022(4)	0.033(4)	0.001(3)	0.001(3)	-0.001(3)
N(8)	0.023(4)	0.026(4)	0.028(4)	0.000(3)	-0.002(3)	0.001(3)
C(51)	0.043(5)	0.027(5)	0.024(4)	-0.002(3)	0.012(4)	-0.002(4)
C(52)	0.023(4)	0.021(4)	0.017(4)	0.000(3)	0.005(3)	0.001(3)
C(53)	0.034(5)	0.029(5)	0.034(5)	0.003(4)	0.006(4)	0.002(4)
C(54)	0.026(5)	0.044(6)	0.051(6)	-0.014(4)	-0.006(4)	0.014(4)
C(55)	0.044(6)	0.035(5)	0.039(5)	-0.009(4)	-0.013(4)	0.009(4)
C(56)	0.039(5)	0.020(4)	0.030(4)	-0.002(3)	0.003(4)	-0.003(4)
C(57)	0.030(5)	0.023(4)	0.020(4)	0.011(3)	0.003(3)	-0.003(4)
C(81)	0.028(4)	0.025(4)	0.011(4)	-0.001(3)	0.006(3)	0.001(4)
C(82)	0.021(4)	0.022(4)	0.020(4)	-0.001(3)	0.000(3)	0.003(3)
C(83)	0.026(4)	0.029(5)	0.032(4)	-0.003(3)	0.007(4)	0.004(4)

C(84)	0.028(5)	0.027(5)	0.068(6)	-0.012(4)	0.005(4)	-0.007(4)
C(85)	0.028(5)	0.031(5)	0.080(7)	-0.004(5)	-0.007(5)	0.007(4)
C(86)	0.022(5)	0.036(5)	0.064(6)	0.002(4)	-0.004(4)	0.014(4)
C(87)	0.027(5)	0.021(4)	0.044(5)	-0.007(4)	0.002(4)	0.001(4)
O(511)	0.031(3)	0.030(3)	0.024(3)	-0.008(2)	0.003(2)	-0.004(2)
O(571)	0.029(3)	0.022(3)	0.022(3)	0.005(2)	0.003(2)	-0.001(2)
O(811)	0.024(3)	0.026(3)	0.025(3)	0.001(2)	0.003(2)	0.008(2)
O(871)	0.025(3)	0.031(3)	0.051(4)	-0.003(3)	-0.005(3)	0.002(3)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **1**.

Atom	x	y	z	U(eq)
H(2A)	0.1766	0.1413	0.5166	0.038
H(2B)	0.2091	0.2293	0.5270	0.038
H(3A)	0.3313	0.1739	0.6325	0.044
H(3A)	0.3543	0.1032	0.5843	0.044
H(13)	0.0656	0.1155	0.2465	0.033
H(14)	0.1000	0.1061	0.1281	0.034
H(15)	0.2736	0.1454	0.1135	0.038
H(16)	0.4120	0.1907	0.2181	0.033
H(43)	0.7139	0.2522	0.7325	0.034
H(44)	0.8714	0.3177	0.7272	0.039
H(45)	0.8910	0.3574	0.6093	0.035
H(46)	0.7558	0.3231	0.4976	0.033
H(6A)	0.5967	0.5103	0.6124	0.038
H(6B)	0.6492	0.4282	0.6108	0.038
H(7A)	0.5313	0.4733	0.7177	0.031
H(7B)	0.5834	0.3908	0.7159	0.031
H(53)	0.1785	0.5211	0.5158	0.040
H(54)	0.0169	0.4832	0.4223	0.053
H(55)	0.0286	0.3845	0.3381	0.053
H(56)	0.1961	0.3202	0.3513	0.037
H(83)	0.8084	0.6841	0.7940	0.035
H(84)	0.9856	0.7286	0.8545	0.051
H(85)	11.356	0.6436	0.9037	0.061
H(86)	11.019	0.5134	0.8928	0.053
H(200)	0.7410	0.2267	0.3788	0.107
H(20A)	0.7290	0.1400	0.4664	0.264
H(20B)	0.7240	0.0844	0.3970	0.264
H(20C)	0.6111	0.1132	0.4124	0.264
H(100)	0.8058	0.3259	0.3385	0.112
H(10A)	0.6935	0.4499	0.2760	0.168
H(10B)	0.7814	0.4038	0.2447	0.168
H(10C)	0.8244	0.4613	0.3139	0.168
H(5)	0.477(10)	0.396(5)	0.534(5)	0.135
H(8)	0.746(8)	0.433(5)	0.769(7)	0.135
H(87)	0.959(9)	0.404(5)	0.848(7)	0.135

Table S5. Torsion angles (°) for **1**.

Torsion Angle Site	Torsion Angles (°)	Torsion Angle Site	Torsion Angles (°)
O(411)-Ba(1)-Mn(2)-O(471)	123.1(2)	O(411)-Ba(1)-O(171)-C(17)	-32.7(5)
O(511)-Ba(1)-Mn(2)-O(471)	-64.7(2)	O(511)-Ba(1)-O(171)-C(17)	132.5(4)
O(811)-Ba(1)-Mn(2)-O(471)	-159.4(2)	O(811)-Ba(1)-O(171)-C(17)	42.7(5)
O(171)-Ba(1)-Mn(2)-O(471)	127.7(3)	O(471)-Ba(1)-O(171)-C(17)	-179.1(5)
O(571)-Ba(1)-Mn(2)-O(471)	-108.5(2)	O(571)-Ba(1)-O(171)-C(17)	115.8(5)
O(411)-Ba(1)-Mn(2)-O(171)	-4.6(2)	Mn(2)-Ba(1)-O(171)-C(17)	150.9(6)
O(511)-Ba(1)-Mn(2)-O(171)	167.6(2)	O(411)-Ba81)-O(171)-Mn(2)	176.40(18)
O(811)-Ba(1)-Mn(2)-O(171)	73.0(2)	O(511)-Ba(1)-O(171)-Mn(2)	-18.4(3)
O(471)-Ba(1)-Mn(2)-O(171)	-127.7(3)	O(811)-Ba(1)-O(171)-Mn(2)	-108.22(19)
O(571)-Ba(1)-Mn(2)-O(171)	123.8(2)	O(471)-Ba(1)-O(171)-Mn(2)	30.01(17)
O(411)-Ba(1)-Mn(2)-N(1)	-50.7(3)	O(571)-Ba(1)-O(171)Mn(2)	-35.08(15)
O(511)-Ba(1)-Mn(2)-N(1)	121.5(3)	N(4)-C(41)-O(411)-Ba(1)	-107(3)
O(811)-Ba(1)-Mn(2)-N(1)	26.8(3)	C(42)-C(41)-O(411-Ba(1)	67(3)
O(171)-Ba(1)-Mn(2)-N(1)	-46.1(3)	C(42)-C(47)-O(471)-Mn(2)	19.3(10)
O(471)-Ba(1)-Mn(2)-N(1)	-173.8(3)	C(46)-C(47)-O(471)-Mn(2)	-162.7(5)
O(571)-Ba(1)-Mn(2)-N(1)	77.7(3)	C(42)-C(47)-O(471)-Ba(1)	152.3(5)
O(411)-Ba(1)-Mn(2)-N(4)	157.7(3)	C(46)-C(47)-O(471)-Ba(1)	-29.6(9)
O(511)-Ba(1)-Mn(2)-N(4)	-30.1(3)	O(171)-Mn(2)-O(471)-C(47)	-179.7(6)
O(811)-Ba(1)-Mn(2)-N(4)	-124.7(3)	N(1)-Mn(2)-O(471)-C(47)	-81(2)
O(171)-Ba(1)-Mn(2)-N(4)	162.3(3)	N(4)-Mn(2)-O(471)-C(47)	-15.4(6)
O(471)-Ba(1)-Mn(2)-N(4)	34.6(3)	O(571)-Mn(2)-O(471)-C(47)	87.8(6)
O(571)-Ba(1)-Mn(2)-N(4)	-73.9(3)	Ba(1)-Mn(2)-O(471)-C(47)	142.9(6)
O(411)-Ba(1)-Mn(2)-O(571)	-128.5(2)	O(171)-Mn(2)-O(471)-Ba(1)	37.42(19)
O(511)-Ba(1)-Mn(2)-O(571)	43.74(18)	N(1)-Mn(2)-O(471)-Ba(1)	136.1(19)
O(811)-Ba(1)-Mn(2)-O(571)	-50.87(17)	N(4)-Mn(2)-O(471)-Ba(1)	-158.3(2)
O(171)-Ba(1)-Mn(2)-O(571)	-123.8(2)	O(571)-Mn(2)-O(471)-Ba(1)	-55.13(17)
O(471)-Ba(1)-Mn(2)-O(571)	108.5(2)	O(411)-Ba(1)-O(471)-C(47)	128.5(5)
O(471)-Mn(2)-N(1)-C(11)	-110.1(19)	O(511)-Ba(1)-O(471)-C(47)	-22.6(5)
O(171)-Mn(2)-N(1)-C(11)	-11.7(6)	O(811)-Ba(1)-O(471)-C(47)	-118.1(5)
N(4)-Mn(2)-N(1)-C(11)	-176.1(6)	O(171)-Ba(1)-O(471)-C(47)	-173.8(6)
O(571)-Mn(2)-N(1)-C(11)	81.3(6)	O(571)-Ba(1)-O(471)-C(47)	-99.7(5)
Ba(1)-Mn(2)-N(1)-C(11)	22.0(7)	Mn(2)-Ba(1)-O(471)-C(47)	-143.8(6)
O(471)-Mn(2)-N(1)-C(2)	86(2)	O(411)-Ba(1)-O(471)-Mn(2)	-87.6(3)
O(171)-Mn(2)-N(1)-C(2)	-175.8(5)	O(511)-Ba(1)-O(471)-Mn(2)	121.2(2)
N(4)-Mn(2)-N(1)-C(2)	19.7(5)	O(811)-Ba(1)-O(471)-Mn(2)	25.8(3)
O(571)-Mn(2)-N(1)-C(2)	-82.9(5)	O(171)-Ba(1)-O(471)-Mn(2)	-29.98(16)
Ba(1)-Mn(2)-N(1)-C(2)	-142.2(4)	O(571)-Ba(1)-O(471)-Mn(2)	44.09(17)
C(11)-N(1)-C(2)-C(3)	154.7(6)	C(51)-N(5)-C(6)-C(7)	80.1(9)
Mn(2)-N(1)-C(2)-C(3)	-39.0(7)	N(5)-C(6)-C(7)-N(8)	179.7(6)
N(1)-C(2)-C(3)-N(4)	42.1(8)	C(6)-C(7)-N(8)-C(81)	73.3(9)
C(2)-C(3)-N(4)-C(41)	162.0(6)	C(6)-N(5)-C(51)-O(511)	-4.4(11)
C(2)-C(3)-N(4)-Mn(2)	-27.6(7)	C(6)-N(5)-C(51)-C(52)	174.8(6)
O(471)-Mn(2)-N(4)-C(41)	-0.2(6)	O(511)-C(51)-C(52)-C(53)	-9.6(10)
O(171)-Mn(2)-N(4)-C(41)	94.3(10)	N(5)-C(51)-C(52)-C(53)	171.1(6)
N(1)-Mn(2)-N(4)-C(41)	173.8(6)	O(511)-C(51)-C(52)-C(57)	169.0(6)
O(571)-Mn(2)-N(4)-C(41)	-85.0(6)	N(5)-C(51)-C(52)-C(57)	-10.3(10)
Ba(1)-Mn(2)-N(4)-C(41)	-26.8(8)	C(57)-C(52)-C(53)-C(54)	-1.0(11)

O(471)-Mn(2)-N(4)-C(3)	-169.0(5)	C(51)-C(52)-C(53)-C(54)	177.5(7)
O(171)-Mn(2)-N(4)-C(3)	-74.6(10)	C(52)-C(53)-C(54)-C(55)	-1.8(12)
N(1)-Mn(2)-N(4)-C(3)	4.9(5)	C(53)-C(54)-C(55)-C(56)	2.1(13)
O(571)-Mn(2)-N(4)-C(3)	106.1(5)	C(54)-C(55)-C(56)-C(57)	0.5(13)
Ba(1)-Mn(2)-N(4)-C(3)	164.3(4)	C(55)-C(56)-C(57)-O(571)	-180.0(7)
C(2)-N(1)-C(11)-O(111)	-2.5(10)	C(55)-C(56)-C(57)-C(52)	-3.2(11)
Mn(2)-N(1)-C(11)-O(111)	-165.9(5)	C(53)-C(52)-C(57)-O(5718	-179.8(6)
C(2)-N(1)-C(11)-C(12)	-178.5(6)	C(51)-C(52)-C(57)-O(571)	1.6(10)
Mn(2)-N(1)-C(11)-C(12)	18.0(9)	C(53)-C(52)-C(57)-C(56)	3.4(10)
O(111)-C(11)-C(12)-C(17)	172.5(6)	C(51)-C(52)-C(57)-C(56)	-175.1(6)
N(1)-C(11)-C(12)-C(17)	-11.3(10)	C(7)-N(8)-C(81)-O(811)	7.4(10)
O(111)-C(11)-C(12)-C(13)	-7.2(10)	C(7)-N(8)-C(81)-C(82)	-173.1(6)
N(1)-C(11)-C(12)-C(13)	168.9(6)	O(8119-C(81)-C(82)-c(87)	-178.8(7)
C(17)-C(12)-C(13)-C(14)	-0.2(10)	N(8)-C(81)-C(82)-C(87)	1.7(11)
C(11)-C(12)-C(13)-C(14)	179.5(6)	O(811)-C(81)-C(82)-C(83)	-2.6(9)
C(12)-C(13)-C(14)-C(15)	-0.5(11)	N(8)-C(81)-C(82)-C(83)	177.9(6)
C(13)-C(14)-C(15)-C(16)	0.8(11)	C(87)-C(82)-C(83)-C(84)	-0.5(11)
C(14)-C(15)-C(16)-C(17)	-0.4(11)	C(81)-C(82)-C(83)-C(84)	-177.0(7)
C(15)-C(16)-C(17)-O(171)	-179.0(6)	C(82)-C(83)-C(84)-C(85)	1.3(12)
C(15)-C(16)-C(17)-C(12)	-0.4(11)	C(83)-C(84)-C(85)-C(86)	-0.7(14)
C(13)-C(12)-C(17)-O(171)	179.2(6)	C(84)-C(85)-C(86)-C(87)	-0.7(14)
C(11)-C(12)-C(17)-O(171)	-0.5(11)	C(83)-C(82)-C(87)-O(871)	-178.8(7)
C(13)-C(12)-C(17)-C(16)	0.7(10)	C(81)-C(82)-C(87)-O(871)	-2.7(12)
C(11)-C(12)-C(17)-C(16)	-179.1(6)	C(83)-C(82)-C(87)-C(86)	-1.0(12)
C(3)-N(4)-C(41)-O(411)	-4.9(10)	C(81)-C(82)-C(87)-C(86)	175.2(7)
Mn(2)-N(4)-C(41)-O(411)	-173.3(5)	C(85)-C(86)-C(87)-O(871)	179.4(8)
C(3)-N(4)-C(41)-C(42)	-179.6(6)	C(85)-C(86)-C(87)-C(82)	1.6(14)
Mn(2)-N(4)-C(41)-C(42)	12.0(10)	N(5)-C(51)-O(511)-Ba(1)	28.2(16)
O(411)-C(41)-C(42)-C(47)	173.2(7)	C(52)-C(51)-O(511)-Ba(1)	-151.0(9)
N(4)-C(41)-C(42)-C(47)	-11.9(11)	C(56)-C(57)-O(571)-Mn(2)	-54.9(8)
O(411)-C(41)-C(42)-C(43)	-6.9(10)	C(52)-C(57)-O(571)-Mn(2)	128.6(6)
N(4)-C(41)-C(42)-C(43)	168.0(6)	C(56)-C(57)-O(571)-Ba(1)	67.1(8)
C(47)-C(42)-C(43)-C(44)	1.7(11)	C(52)-C(57)-O(571)-Ba(1)	-109.5(6)
C(41)-C(42)-C(43)-C(44)	-178.1(7)	O(471)-Mn(2)-O(571)-C(57)	-172.3(6)
C(42)-C(43)-C(44)-C(45)	0.3(12)	O(171)-Mn(2)-O(571)-C(57)	99.4(5)
C(43)-C(44)-C(45)-C(46)	-2.2(11)	N(1)-Mn(2)-O(571)-C(57)	6.4(6)
C(44)-C(45)-C(46)-C(47)	2.1(11)	N(4)-Mn(2)-O(571)-C(57)	-80.8(6)
C(43)-C(42)-C(47)-O(471)	176.2(6)	Ba(1)-Mn(2)-O(571)-C(57)	139.0(6)
C(41)-C(42)-C(47)-O(471)	-3.9(11)	O(471)-Mn(2)-O(571)-Ba(1)	48.71(16)
C(43)-C(42)-C(47)-C(46)	-1.8(10)	O(171)-Mn(2)-O(571)-Ba(1)	-39.65(16)
C(41)-C(42)-C(47)-C(46)	178.1(7)	N(1)-Mn(2)-O(571)-Ba(1)	-132.60(18)
C(45)-C(46)-C(47)-O(471)	-178.2(7)	N(4)-Mn(2)-O(571)-Ba(1)	140.16(18)
C(45)-C(46)-C(47)-C(42)	0.0(11)	O(411)-Ba(1)-O(571)-C(57)	-50.4(6)
C(16)-C(17)-O(171)-Mn(2)	-175.5(5)	O(511)-Ba(1)-O(571)-C(57)	81.7(5)
C(12)-C(17)-O(171)-Mn(2)	5.9(9)	O(811)-Ba(1)-O(571)-C(57)	-12.6(5)
C(16)-C(17)-O(171)-Ba(1)	42.9(8)	O(171)-Ba(1)-O(571)-C(57)	-109.0(6)
C(12)-C(17)-O(171)-Ba(1)	-135.6(5)	O(471)-Ba(1)-O(571)-C(57)	-177.3(6)
O(471)-Mn(2)-O(171)-C(17)	172.6(6)	Mn(2)-Ba(1)-O(571)-C(57)	-139.4(6)
N(1)-Mn(2)-O(171)-C(17)	-0.9(6)	O(411)-Ba(1)-O(571)-Mn(2)	89.1(3)
N(4)-Mn(2)-O(171)-C(17)	77.6(10)	O(511)-Ba(1)-O(571)-Mn(2)	-138.84(16)
O(571)-Mn(2)-O(171)-C(17)	-103.1(5)	O(811)-Ba(1)-O(571)-Mn(2)	126.84(17)

Ba(1)-Mn(2)-O(171)-C(17)	-148.8(6)	O(171)-Ba(1)-O(571)-Mn(2)	30.45(14)
O(471)-Mn(2)-O(171)-Ba(1)	-38.6(2)	O(471)-Ba(1)-O(571)-Mn(2)	-37.89(15)
N(1)-Mn(2)-O(171)-Ba(1)	147.9(2)	N(8)-C(81)-O(811)-Ba(1)	-12.3(18)
N(4)-Mn(2)-O(171)-Ba(1)	-133.6(8)	C(82)-C(81)-O(811)-Ba(1)	168.3(10)
O(571)-Mn(2)-O(171)-Ba(1)	45.70(18)		

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Mn(1)	9393(1)	813(1)	5593(1)	27(1)
Mn(2)	8568(1)	-1848(1)	5181(1)	29(1)
N(1)	7991(8)	1994(8)	5469(5)	50(2)
C(2)	8023(11)	3166(12)	5418(8)	65(4)
C(3)	7065(11)	3901(11)	5369(8)	64(3)
C(4)	6013(11)	3342(11)	5351(8)	64(3)
C(5)	5996(10)	2107(11)	5415(7)	58(3)
C(6)	6989(9)	1484(10)	5465(6)	50(3)
C(7)	7001(9)	151(10)	5554(6)	49(3)
N(8)	8035(6)	-317(7)	5528(5)	40(2)
O(9)	6635(9)	-45(8)	6264(6)	81(3)
C(10)	6259(16)	-1166(13)	6429(10)	96(6)
N(11)	9277(10)	-2621(10)	6203(6)	66(3)
C(12)	8642(15)	-3324(16)	6563(9)	95(5)
C(13)	8930(20)	-3630(20)	7311(13)	138(9)
C(14)	9920(20)	-3180(20)	7683(11)	126(8)
C(15)	10554(15)	-2485(17)	7305(8)	89(5)
C(16)	10249(11)	-2151(12)	6573(7)	58(3)
C(17)	10940(10)	-1446(13)	6119(7)	61(3)
N(18)	10286(6)	-826(7)	5539(4)	34(2)
O(19)	11635(11)	-836(12)	6632(7)	113(4)
C(20)	12633(17)	-270(20)	6372(13)	129(8)
N(21)	9801(9)	1032(10)	6795(6)	63(3)
C(22)	9336(15)	394(15)	7309(8)	88(5)
C(23)	9760(20)	530(20)	8058(10)	131(8)
C(24)	10650(20)	1290(20)	8288(10)	133(9)
C(25)	11090(16)	1880(20)	7754(9)	110(7)
C(26)	10648(11)	1740(13)	7010(7)	65(3)
C(27)	11044(11)	2481(12)	6387(8)	64(3)
N(28)	10665(7)	2049(7)	5688(4)	38(2)
O(29)	10630(9)	3663(9)	6504(6)	89(3)
C(30)	11150(20)	4575(14)	6133(14)	139(9)
Cl(31)	6905(3)	-2871(3)	4803(2)	75(1)

Table S7. Bond lengths (Å) and angles (°) for **2**.

Chemical bond	Bond Lengths (Å)	Chemical bond	Bond Lengths (Å)
Mn(1)-N(28)	2.048(8)	C(12)-H(12)	0.9300
Mn(1)-N(8)	2.051(8)	C(13)-C(14)	1.35(3)
Mn(1)-N(18)#1	2.120(7)	C(13)-H(13)	0.9300
Mn(1)-N(1)	2.123(9)	C(14)-C(15)	1.35(3)
Mn(1)-N(18)	2.141(8)	C(14)-H(14)	0.9300
Mn(1)-N(21)	2.143(10)	C(15)-C(16)	1.356(18)
Mn(1)-Mn(2)	3.203(2)	C(15)-H(15)	0.9300
Mn(1)-Mn(2)#1	3.206(2)	C(16)-C(17)	1.477(18)
Mn(2)-N(28)#1	1.939(8)	C(17)-O(19)	1.328(16)
Mn(2)-N(8)	1.971(8)	C(17)-N(18)	1.385(14)
Mn(2)-N(11)	2.081(11)	C(17)-H(17)	0.9800
Mn(2)-Cl(31)	2.305(4)	N(18)-Mn(1)#1	2.120(7)
Mn(2)-N(18)	2.353(8)	O(19)-C(20)	1.49(2)
Mn(2)-Mn(1)#1	3.206(2)	C(20)-H(20A)	0.9600
N(1)-C(2)	1.324(15)	C(20)-H(20B)	0.9600
N(1)-C(6)	1.328(14)	C(20)-H(20C)	0.9600
C(2)-C(3)	1.403(18)	N(21)-C(26)	1.298(16)
C(2)-H(2)	0.9300	N(21)-C(22)	1.353(17)
C(3)-C(4)	1.403(18)	C(22)-C(23)	1.36(2)
C(3)-H(3)	0.9300	C(22)-H(22)	0.9300
C(4)-C(5)	1.395(17)	C(23)-C(24)	1.38(3)
C(4)-H(4)	0.9300	C(23)-H(23)	0.9300
C(5)-C(6)	1.370(16)	C(24)-C(25)	1.34(3)
C(5)-H(5)	0.9300	C(24)-H(24)	0.9300
C(6)-C(7)	1.508(16)	C(25)-C(26)	1.362(19)
C(7)-N(8)	1.351(13)	C(25)-H(25)	0.9300
C(7)-O(9)	1.424(14)	C(26)-C(27)	1.526(19)
C(7)-H(7)	0.9800	C(27)-N(28)	1.352(14)
O(9)-C(10)	1.386(16)	C(27)-O(29)	1.447(16)
C(10)-H(10A)	0.9600	C(27)-H(27)	0.9800
C(10)-H(10B)	0.9600	N(28)-Mn(2)#1	1.939(8)
C(10)-H(10C)	0.9600	O(29)-C(30)	1.42(2)
N(11)-C(12)	1.330(17)	C(30)-H(30A)	0.9600
N(11)-C(16)	1.351(17)	C(30)-H(30B)	0.9600
C(12)-C(13)	1.37(3)	C(30)-H(30C)	0.9600
Angle Atom Site	**Angles (°)**	**Angle Atom Site**	**Angles (°)**
N(28)-Mn(1)-N(8)	175.2(3)	O(9)-C(10)-H(10A)	109.5
N(28)-Mn(1)-N(18)#1	80.3(3)	O(9)-C(10)-H(10B)	109.5
N(8)-Mn(1)-N(18)#1	102.2(3)	H(10A)-C(10)-H(10B)	109.5
N(28)-Mn(1)-N(1)	98.5(3)	O(9)-C(10)-H(10C)	109.5
N(8)-Mn(1)-N(1)	77.1(3)	H(10A)-C(10)-H(10C)	109.5
N(18)#1-Mn(1)-N(1)	98.9(3)	H(10B)-C(10)-H(10C)	109.5
N(28)-Mn(1)-N(18)	102.7(3)	C(12)-N(11)-C(16)	120.6(13)
N(8)-Mn(1)-N(18)	81.9(3)	C(12)-N(11)-Mn(2)	119.3(11)
N(18)#1-Mn(1)-N(18)	78.2(3)	C(16)-N(11)-Mn(2)	117.8(8)
N(1)-Mn(1)-N(18)	157.7(3)	N(11)-C(12)-C(13)	123(2)

N(28)-Mn(1)-N(21)	77.9(4)	N(11)-C(12)-H(12)	118.5
N(8)-Mn(1)-N(21)	100.4(4)	C(13)-C(12)-H(12)	118.5
N(18)#1-Mn(1)-N(21)	155.7(4)	C(14)-C(13)-C(12)	117(2)
N(1)-Mn(1)-N(21)	94.8(4)	C(14)-C(13)-H(13)	121.6
N(18)-Mn(1)-N(21)	96.2(4)	C(12)-C(13)-H(13)	121.6
N(28)-Mn(1)-Mn(2)	148.4(2)	C(15)-C(14)-C(13)	119.1(19)
N(8)-Mn(1)-Mn(2)	36.4(2)	C(15)-C(14)-H(14)	120.5
N(18)#1-Mn(1)-Mn(2)	83.2(2)	C(13)-C(14)-H(14)	120.5
N(1)-Mn(1)-Mn(2)	110.6(2)	C(14)-C(15)-C(16)	123.9(19)
N(18)-Mn(1)-Mn(2)	47.3(2)	C(14)-C(15)-H(15)	118.0
N(21)-Mn(1)-Mn(2)	110.6(3)	C(16)-C(15)-H(15)	118.0
N(28)-Mn(1)-Mn(2)#1	35.3(2)	N(11)-C(16)-C(15)	116.3(14)
N(8)-Mn(1)-Mn(2)#1	148.2(2)	N(11)-C(16)-C(17)	117.0(11)
N(18)#1-Mn(1)-Mn(2)#1	47.2(2)	C(15)-C(16)-C(17)	126.2(14)
N(1)-Mn(1)-Mn(2)#1	111.6(3)	O(19)-C(17)-N(18)	118.4(12)
N(18)-Mn(1)-Mn(2)#1	82.8(2)	O(19)-C(17)-C(16)	104.0(12)
N(21)-Mn(1)-Mn(2)#1	108.9(3)	N(18)-C(17)-C(16)	112.6(10)
Mn(2)-Mn(1)-Mn(2)#1	117.90(5)	O(19)-C(17)-H(17)	107.1
N(28)#1-Mn(2)-N(8)	124.9(4)	N(18)-C(17)-H(17)	107.1
N(28)#1-Mn(2)-N(11)	118.5(4)	C(16)-C(17)-H(17)	107.1
N(8)-Mn(2)-N(11)	101.3(4)	C(17)-N(18)-Mn(1)#1	123.6(8)
N(28)#1-Mn(2)-Cl(31)	101.6(2)	C(17)-N(18)-Mn(1)	128.8(8)
N(8)-Mn(2)-Cl(31)	102.9(2)	Mn(1)#1-N(18)-Mn(1)	101.8(3)
N(11)-Mn(2)-Cl(31)	105.2(3)	C(17)-N(18)-Mn(2)	108.9(7)
N(28)#1-Mn(2)-N(18)	76.8(3)	Mn(1)#1-N(18)-Mn(2)	91.4(3)
N(8)-Mn(2)-N(18)	78.4(3)	Mn(1)-N(18)-Mn(2)	90.8(3)
N(11)-Mn(2)-N(18)	75.4(4)	C(17)-O(19)-C(20)	116.8(15)
Cl(31)-Mn(2)-N(18)	178.4(2)	O(19)-C(20)-H(20A)	109.5
N(28)#1-Mn(2)-Mn(1)	97.2(2)	O(19)-C(20)-H(20B)	109.5
N(8)-Mn(2)-Mn(1)	38.1(2)	H(20A)-C(20)-H(20B)	109.5
N(11)-Mn(2)-Mn(1)	96.9(3)	O(19)-C(20)-H(20C)	109.5
Cl(31)-Mn(2)-Mn(1)	139.03(11)	H(20A)-C(20)-H(20C)	109.5
N(18)-Mn(2)-Mn(1)	41.95(19)	H(20B)-C(20)-H(20C)	109.5
N(28)#1-Mn(2)-Mn(1)#1	37.6(2)	C(26)-N(21)-C(22)	120.6(13)
N(8)-Mn(2)-Mn(1)#1	97.1(2)	C(26)-N(21)-Mn(1)	114.3(9)
N(11)-Mn(2)-Mn(1)#1	107.4(3)	C(22)-N(21)-Mn(1)	124.6(11)
Cl(31)-Mn(2)-Mn(1)#1	137.20(12)	N(21)-C(22)-C(23)	118.9(19)
N(18)-Mn(2)-Mn(1)#1	41.37(18)	N(21)-C(22)-H(22)	120.5
Mn(1)-Mn(2)-Mn(1)#1	62.10(5)	C(23)-C(22)-H(22)	120.5
C(2)-N(1)-C(6)	117.8(11)	C(22)-C(23)-C(24)	120.5(19)
C(2)-N(1)-Mn(1)	126.9(8)	C(22)-C(23)-H(23)	119.7

C(6)-N(1)-Mn(1)	115.3(8)	C(24)-C(23)-H(23)	119.7
N(1)-C(2)-C(3)	124.0(12)	C(25)-C(24)-C(23)	118.0(17)
N(1)-C(2)-H(2)	118.0	C(25)-C(24)-H(24)	121.0
C(3)-C(2)-H(2)	118.0	C(23)-C(24)-H(24)	121.0
C(2)-C(3)-C(4)	117.2(12)	C(24)-C(25)-C(26)	120.2(18)
C(2)-C(3)-H(3)	121.4	C(24)-C(25)-H(25)	119.9
C(4)-C(3)-H(3)	121.4	C(26)-C(25)-H(25)	119.9
C(5)-C(4)-C(3)	118.0(12)	N(21)-C(26)-C(25)	121.7(15)
C(5)-C(4)-H(4)	121.0	N(21)-C(26)-C(27)	115.8(11)
C(3)-C(4)-H(4)	121.0	C(25)-C(26)-C(27)	122.2(14)
C(6)-C(5)-C(4)	119.4(12)	N(28)-C(27)-O(29)	113.1(11)
C(6)-C(5)-H(5)	120.3	N(28)-C(27)-C(26)	112.5(10)
C(4)-C(5)-H(5)	120.3	O(29)-C(27)-C(26)	104.2(11)
N(1)-C(6)-C(5)	123.4(11)	N(28)-C(27)-H(27)	109.0
N(1)-C(6)-C(7)	115.8(10)	O(29)-C(27)-H(27)	109.0
C(5)-C(6)-C(7)	120.7(11)	C(26)-C(27)-H(27)	109.0
N(8)-C(7)-O(9)	112.4(10)	C(27)-N(28)-Mn(2)#1	130.7(8)
N(8)-C(7)-C(6)	112.2(9)	C(27)-N(28)-Mn(1)	117.2(8)
O(9)-C(7)-C(6)	104.4(9)	Mn(2)#1-N(28)-Mn(1)	107.0(4)
N(8)-C(7)-H(7)	109.2	C(30)-O(29)-C(27)	114.4(12)
O(9)-C(7)-H(7)	109.2	O(29)-C(30)-H(30A)	109.5
C(6)-C(7)-H(7)	109.2	O(29)-C(30)-H(30B)	109.5
C(7)-N(8)-Mn(2)	134.0(7)	H(30A)-C(30)-H(30B)	109.5
C(7)-N(8)-Mn(1)	118.5(7)	O(29)-C(30)-H(30C)	109.5
Mn(2)-N(8)-Mn(1)	105.5(3)	H(30A)-C(30)-H(30C)	109.5
C(10)-O(9)-C(7)	119.1(11)	H(30B)-C(30)-H(30C)	109.5

Symmetry transformations used to generate equivalent atoms: –x+½; y+½; -z+½; -x; -y; -z; x-½; -y-½; z-½.

Table S8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

Atom	U11	U22	U33	U23	U13	U12
Mn(1)	27(1)	29(1)	26(1)	-4(1)	8(1)	-2(1)
Mn(2)	30(1)	26(1)	33(1)	0(1)	9(1)	0(1)
N(1)	49(6)	43(5)	61(6)	-11(4)	15(5)	-6(4)
C(2)	64(8)	64(9)	70(9)	22(7)	18(7)	-3(7)
C(3)	69(9)	43(7)	77(9)	-1(6)	7(7)	5(6)
C(4)	62(8)	52(7)	80(9)	-10(6)	11(7)	14(6)
C(5)	52(7)	57(8)	65(8)	6(6)	9(6)	3(6)
C(6)	46(7)	53(7)	53(7)	2(5)	16(5)	1(5)
C(7)	48(6)	52(7)	50(7)	-8(5)	14(5)	-5(5)
N(8)	27(4)	37(5)	57(5)	-8(4)	13(4)	-3(4)
O(9)	108(8)	69(6)	75(6)	-9(5)	46(6)	-20(6)
C(10)	132(15)	60(9)	111(13)	6(9)	65(12)	-10(9)
N(11)	68(7)	58(7)	75(7)	17(6)	21(6)	11(6)
C(12)	108(13)	106(13)	83(11)	45(10)	49(10)	-4(10)
C(13)	122(18)	180(20)	123(18)	92(17)	43(15)	31(17)
C(14)	139(19)	170(20)	74(12)	49(14)	42(13)	40(17)
C(15)	93(11)	125(14)	49(8)	17(9)	11(8)	34(10)
C(16)	59(8)	61(8)	54(7)	11(6)	13(6)	20(6)
C(17)	48(7)	81(9)	49(7)	9(6)	-10(6)	-7(6)
N(18)	35(4)	42(5)	24(4)	3(3)	-1(3)	3(4)
O(19)	100(9)	134(11)	98(9)	7(8)	-3(7)	-3(8)
C(20)	94(14)	148(19)	145(19)	39(16)	20(13)	6(14)
N(21)	68(7)	71(7)	54(6)	-13(5)	17(5)	-1(6)
C(22)	115(13)	94(11)	61(9)	28(8)	36(9)	22(10)
C(23)	160(20)	190(20)	56(11)	21(13)	35(12)	-9(18)
C(24)	150(20)	210(30)	43(9)	3(13)	6(11)	-28(19)
C(25)	100(13)	164(19)	59(10)	-13(11)	-8(9)	-30(13)
C(26)	62(8)	85(10)	48(7)	-18(7)	10(6)	-11(7)
C(27)	48(7)	67(8)	75(9)	-26(7)	7(6)	-4(6)
N(28)	34(4)	45(5)	32(4)	-6(4)	-3(3)	-11(4)
O(29)	89(7)	72(7)	106(8)	-37(6)	20(6)	0(6)
C(30)	180(20)	51(10)	210(20)	-17(12)	110(20)	-25(12)
Cl(31)	54(2)	64(2)	109(3)	-11(2)	17(2)	-10(2)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **2**.

Atom	x	y	z	U(eq)
H(2)	8723	3525	5414	78
H(3)	7126	4724	5349	76
H(4)	5346	3781	5299	77
H(5)	5315	1710	5424	70
H(7)	6450	-200	5151	59
H(10A)	6048	-1161	6925	144
H(10B)	6855	-1733	6414	144
H(10C)	5615	-1378	6062	144
H(12)	7972	-3623	6294	115
H(13)	8468	-4116	7552	165
H(14)	10149	-3359	8192	151
H(15)	11245	-2217	7562	107
H(17)	11406	-2007	5884	73
H(20A)	13062	159	6785	193
H(20B)	12378	270	5965	193
H(20C)	13100	-871	6199	193
H(22)	8740	-126	7153	105
H(23)	9437	99	8417	157
H(24)	10936	1384	8798	160
H(25)	11699	2391	7892	132
H(27)	11874	2495	6467	77
H(30A)	10825	5328	6233	209
H(30B)	11026	4429	5598	209
H(30C)	11948	4586	6318	209

Table S10. Torsion angles (°) for **2**.

Torsion Angle Site	Torsion Angles (°)	Torsion Angle Site	Torsion Angles (°)
N(28)-Mn(1)-Mn(2)-N(28)#1	-39.5(6)	Mn(1)-Mn(2)-N(11)-C(16)	-31.9(9)
N(8)-Mn(1)-Mn(2)-N(28)#1	140.5(5)	Mn(1)#1-Mn(2)-N(11)-C(16)	30.9(10)
N(18)#1-Mn(1)-Mn(2)-N(28)#1	19.2(3)	C(16)-N(11)-C(12)-C(13)	-1(3)
N(1)-Mn(1)-Mn(2)-N(28)#1	116.2(4)	Mn(2)-N(11)-C(12)-C(13)	-163.1(17)
N(18)-Mn(1)-Mn(2)-N(28)#1	-61.0(4)	N(11)-C(12)-C(13)-C(14)	-1(3)
N(21)-Mn(1)-Mn(2)-N(28)#1	-140.1(4)	C(12)-C(13)-C(14)-C(15)	0(4)
Mn(2)#1-Mn(1)-Mn(2)-N(28)#1	-13.9(2)	C(13)-C(14)-C(15)-C(16)	3(3)
N(28)-Mn(1)-Mn(2)-N(8)	179.9(6)	C(12)-N(11)-C(16)-C(15)	3(2)
N(18)#1-Mn(1)-Mn(2)-N(8)	-121.3(5)	Mn(2)-N(11)-C(16)-C(15)	165.7(10)
N(1)-Mn(1)-Mn(2)-N(8)	-24.3(5)	C(12)-N(11)-C(16)-C(17)	176.0(13)
N(18)-Mn(1)-Mn(2)-N(8)	158.5(5)	Mn(2)-N(11)-C(16)-C(17)	-21.5(15)
N(21)-Mn(1)-Mn(2)-N(8)	79.4(5)	C(14)-C(15)-C(16)-N(11)	-4(2)
Mn(2)#1-Mn(1)-Mn(2)-N(8)	-154.5(4)	C(14)-C(15)-C(16)-C(17)	-176.3(17)
N(28)-Mn(1)-Mn(2)-N(11)	80.5(5)	N(11)-C(16)-C(17)-O(19)	163.1(12)
N(8)-Mn(1)-Mn(2)-N(11)	-99.5(5)	C(15)-C(16)-C(17)-O(19)	-25(2)
N(18)#1-Mn(1)-Mn(2)-N(11)	139.2(4)	N(11)-C(16)-C(17)-N(18)	33.8(17)
N(1)-Mn(1)-Mn(2)-N(11)	-123.8(4)	C(15)-C(16)-C(17)-N(18)	-154.2(14)
N(18)-Mn(1)-Mn(2)-N(11)	59.0(4)	O(19)-C(17)-N(18)-Mn(1)#1	106.3(13)
N(21)-Mn(1)-Mn(2)-N(11)	-20.1(4)	C(16)-C(17)-N(18)-Mn(1)#1	-132.3(10)
Mn(2)#1-Mn(1)-Mn(2)-N(11)	106.1(3)	O(19)-C(17)-N(18)-Mn(1)	-41.7(16)
N(28)-Mn(1)-Mn(2)-Cl(31)	-156.6(5)	C(16)-C(17)-N(18)-Mn(1)	79.8(13)
N(8)-Mn(1)-Mn(2)-Cl(31)	23.4(5)	O(19)-C(17)-N(18)-Mn(2)	-148.7(11)
N(18)#1-Mn(1)-Mn(2)-Cl(31)	-97.9(3)	C(16)-C(17)-N(18)-Mn(2)	-27.3(13)
N(1)-Mn(1)-Mn(2)-Cl(31)	-0.9(3)	N(28)-Mn(1)-N(18)-C(17)	76.1(9)

N(18)-Mn(1)-Mn(2)-Cl(31)	-178.1(3)	N(8)-Mn(1)-N(18)-C(17)	-102.5(9)
N(21)-Mn(1)-Mn(2)-Cl(31)	102.9(4)	N(18)#1-Mn(1)-N(18)-C(17)	153.2(11)
Mn(2)#1-Mn(1)-Mn(2)-Cl(31)	-131.02(18)	N(1)-Mn(1)-N(18)-C(17)	-122.1(11)
N(28)-Mn(1)-Mn(2)-N(18)	21.5(5)	N(21)-Mn(1)-N(18)-C(17)	-2.8(9)
N(8)-Mn(1)-Mn(2)-N(18)	-158.5(5)	Mn(2)-Mn(1)-N(18)-C(17)	-115.2(10)
N(18)#1-Mn(1)-Mn(2)-N(18)	80.2(3)	Mn(2)#1-Mn(1)-N(18)-C(17)	105.5(9)
N(1)-Mn(1)-Mn(2)-N(18)	177.2(4)	N(28)-Mn(1)-N(18)-Mn(1)#1	-77.1(4)
N(21)-Mn(1)-Mn(2)-N(18)	-79.1(4)	N(8)-Mn(1)-N(18)-Mn(1)#1	104.3(4)
Mn(2)#1-Mn(1)-Mn(2)-N(18)	47.1(3)	N(18)#1-Mn(1)-N(18)-Mn(1)#1	0.0
N(28)-Mn(1)-Mn(2)-Mn(1)#1	-25.6(4)	N(1)-Mn(1)-N(18)-Mn(1)#1	84.7(9)
N(8)-Mn(1)-Mn(2)-Mn(1)#1	154.5(4)	N(21)-Mn(1)-N(18)-Mn(1)#1	-156.0(4)
N(18)#1-Mn(1)-Mn(2)-Mn(1)#1	33.2(2)	Mn(2)-Mn(1)-N(18)-Mn(1)#1	91.6(3)
N(1)-Mn(1)-Mn(2)-Mn(1)#1	130.1(3)	Mn(2)#1-Mn(1)-N(18)-Mn(1)#1	-47.7(2)
N(18)-Mn(1)-Mn(2)-Mn(1)#1	-47.1(3)	N(28)-Mn(1)-N(18)-Mn(2)	-168.7(3)
N(21)-Mn(1)-Mn(2)-Mn(1)#1	-126.1(3)	N(8)-Mn(1)-N(18)-Mn(2)	12.7(3)
Mn(2)#1-Mn(1)-Mn(2)-Mn(1)#1	0.0	N(18)#1-Mn(1)-N(18)-Mn(2)	-91.6(3)
N(28)-Mn(1)-N(1)-C(2)	4.3(11)	N(1)-Mn(1)-N(18)-Mn(2)	-6.9(10)
N(8)-Mn(1)-N(1)-C(2)	-177.6(11)	N(21)-Mn(1)-N(18)-Mn(2)	112.4(3)
N(18)#1-Mn(1)-N(1)-C(2)	-77.1(11)	Mn(2)#1-Mn(1)-N(18)-Mn(2)	-139.3(2)
N(18)-Mn(1)-N(1)-C(2)	-157.7(9)	N(28)#1-Mn(2)-N(18)-C(17)	-111.2(8)
N(21)-Mn(1)-N(1)-C(2)	82.7(11)	N(8)-Mn(2)-N(18)-C(17)	118.5(8)
Mn(2)-Mn(1)-N(1)-C(2)	-163.1(10)	N(11)-Mn(2)-N(18)-C(17)	13.4(8)
Mn(2)#1-Mn(1)-N(1)-C(2)	-29.8(11)	Cl(31)-Mn(2)-N(18)-C(17)	-100(8)
N(28)-Mn(1)-N(1)-C(6)	-173.6(8)	Mn(1)-Mn(2)-N(18)-C(17)	131.8(9)
N(8)-Mn(1)-N(1)-C(6)	4.5(8)	Mn(1)#1-Mn(2)-N(18)-C(17)	-126.4(9)
N(18)#1-Mn(1)-N(1)-	105.0(8)	N(28)#1-Mn(2)-N(18)-Mn(1)#1	15.2(3)

C(6)			
N(18)-Mn(1)-N(1)-C(6)	24.4(14)	N(8)-Mn(2)-N(18)-Mn(1)#1	-115.1(4)
N(21)-Mn(1)-N(1)-C(6)	-95.2(8)	N(11)-Mn(2)-N(18)-Mn(1)#1	139.8(4)
Mn(2)-Mn(1)-N(1)-C(6)	19.0(9)	Cl(31)-Mn(2)-N(18)-Mn(1)#1	27(8)
Mn(2)#1-Mn(1)-N(1)-C(6)	152.3(7)	Mn(1)-Mn(2)-N(18)-Mn(1)#1	-101.8(3)
C(6)-N(1)-C(2)-C(3)	0.7(19)	N(28)#1-Mn(2)-N(18)-Mn(1)	117.0(3)
Mn(1)-N(1)-C(2)-C(3)	-177.1(10)	N(8)-Mn(2)-N(18)-Mn(1)	-13.4(3)
N(1)-C(2)-C(3)-C(4)	-2(2)	N(11)-Mn(2)-N(18)-Mn(1)	-118.5(4)
C(2)-C(3)-C(4)-C(5)	2.6(19)	Cl(31)-Mn(2)-N(18)-Mn(1)	128(8)
C(3)-C(4)-C(5)-C(6)	-2(2)	Mn(1)#1-Mn(2)-N(18)-Mn(1)	101.8(3)
C(2)-N(1)-C(6)-C(5)	-0.3(18)	N(18)-C(17)-O(19)-C(20)	-69.2(19)
Mn(1)-N(1)-C(6)-C(5)	177.8(9)	C(16)-C(17)-O(19)-C(20)	165.0(13)
C(2)-N(1)-C(6)-C(7)	-177.8(11)	N(28)-Mn(1)-N(21)-C(26)	-3.7(10)
Mn(1)-N(1)-C(6)-C(7)	0.3(13)	N(8)-Mn(1)-N(21)-C(26)	-179.1(10)
C(4)-C(5)-C(6)-N(1)	1.1(19)	N(18)#1-Mn(1)-N(21)-C(26)	22.9(16)
C(4)-C(5)-C(6)-C(7)	178.5(11)	N(1)-Mn(1)-N(21)-C(26)	-101.3(10)
N(1)-C(6)-C(7)-N(8)	-7.7(15)	N(18)-Mn(1)-N(21)-C(26)	98.0(10)
C(5)-C(6)-C(7)-N(8)	174.7(10)	Mn(2)-Mn(1)-N(21)-C(26)	144.6(9)
N(1)-C(6)-C(7)-O(9)	114.3(11)	Mn(2)#1-Mn(1)-N(21)-C(26)	13.5(10)
C(5)-C(6)-C(7)-O(9)	-63.4(14)	N(28)-Mn(1)-N(21)-C(22)	-175.6(12)
O(9)-C(7)-N(8)-Mn(2)	93.5(12)	N(8)-Mn(1)-N(21)-C(22)	9.0(12)
C(6)-C(7)-N(8)-Mn(2)	-149.2(9)	N(18)#1-Mn(1)-N(21)-C(22)	-149.0(11)
O(9)-C(7)-N(8)-Mn(1)	-105.4(9)	N(1)-Mn(1)-N(21)-C(22)	86.8(11)
C(6)-C(7)-N(8)-Mn(1)	11.9(12)	N(18)-Mn(1)-N(21)-C(22)	-73.9(12)
N(28)#1-Mn(2)-N(8)-C(7)	112.6(10)	Mn(2)-Mn(1)-N(21)-C(22)	-27.4(12)
N(11)-Mn(2)-N(8)-C(7)	-110.3(11)	Mn(2)#1-Mn(1)-N(21)-C(22)	-158.4(11)
Cl(31)-Mn(2)-N(8)-C(7)	-1.7(11)	C(26)-N(21)-C(22)-C(23)	1(2)
N(18)-Mn(2)-N(8)-C(7)	177.3(11)	Mn(1)-N(21)-C(22)-C(23)	172.9(14)
Mn(1)-Mn(2)-N(8)-C(7)	162.8(13)	N(21)-C(22)-C(23)-C(24)	-1(3)
Mn(1)#1-Mn(2)-N(8)-C(7)	140.2(10)	C(22)-C(23)-C(24)-C(25)	0(4)
N(28)#1-Mn(2)-N(8)-Mn(1)	-50.2(5)	C(23)-C(24)-C(25)-C(26)	1(4)
N(11)-Mn(2)-N(8)-Mn(1)	86.8(5)	C(22)-N(21)-C(26)-C(25)	-1(2)

Cl(31)-Mn(2)-N(8)-Mn(1)	-164.5(3)	Mn(1)-N(21)-C(26)-C(25)	-173.2(14)
N(18)-Mn(2)-N(8)-Mn(1)	14.5(3)	C(22)-N(21)-C(26)-C(27)	-175.6(12)
Mn(1)#1-Mn(2)-N(8)-Mn(1)	-22.6(4)	Mn(1)-N(21)-C(26)-C(27)	12.1(15)
N(28)-Mn(1)-N(8)-C(7)	14(5)	C(24)-C(25)-C(26)-N(21)	0(3)
N(18)#1-Mn(1)-N(8)-C(7)	-105.8(8)	C(24)-C(25)-C(26)-C(27)	174.1(19)
N(1)-Mn(1)-N(8)-C(7)	-9.3(8)	N(21)-C(26)-C(27)-N(28)	-17.4(17)
N(18)-Mn(1)-N(8)-C(7)	178.2(8)	C(25)-C(26)-C(27)-N(28)	167.9(15)
N(21)-Mn(1)-N(8)-C(7)	83.3(8)	N(21)-C(26)-C(27)-O(29)	105.5(13)
Mn(2)-Mn(1)-N(8)-C(7)	-166.0(10)	C(25)-C(26)-C(27)-O(29)	-69.3(18)
Mn(2)#1-Mn(1)-N(8)-C(7)	-119.7(7)	O(29)-C(27)-N(28)-Mn(2)#1	105.2(11)
N(28)-Mn(1)-N(8)-Mn(2)	-180(100)	C(26)-C(27)-N(28)-Mn(2)#1	-137.1(9)
N(18)#1-Mn(1)-N(8)-Mn(2)	60.2(4)	O(29)-C(27)-N(28)-Mn(1)	-103.5(11)
N(1)-Mn(1)-N(8)-Mn(2)	156.7(5)	C(26)-C(27)-N(28)-Mn(1)	14.2(13)
N(18)-Mn(1)-N(8)-Mn(2)	-15.8(4)	N(8)-Mn(1)-N(28)-C(27)	63(4)
N(21)-Mn(1)-N(8)-Mn(2)	-110.6(4)	N(18)#1-Mn(1)-N(28)-C(27)	-175.7(9)
Mn(2)#1-Mn(1)-N(8)-Mn(2)	46.3(7)	N(1)-Mn(1)-N(28)-C(27)	86.6(9)
N(8)-C(7)-O(9)-C(10)	-75.4(16)	N(18)-Mn(1)-N(28)-C(27)	-100.2(8)
C(6)-C(7)-O(9)-C(10)	162.8(13)	N(21)-Mn(1)-N(28)-C(27)	-6.5(9)
N(28)#1-Mn(2)-N(11)-C(12)	-127.1(12)	Mn(2)-Mn(1)-N(28)-C(27)	-116.2(8)
N(8)-Mn(2)-N(11)-C(12)	92.3(12)	Mn(2)#1-Mn(1)-N(28)-C(27)	-157.6(11)
Cl(31)-Mn(2)-N(11)-C(12)	-14.5(12)	N(8)-Mn(1)-N(28)-Mn(2)#1	-139(4)
N(18)-Mn(2)-N(11)-C(12)	167.0(13)	N(18)#1-Mn(1)-N(28)-Mn(2)#1	-18.2(4)
Mn(1)-Mn(2)-N(11)-C(12)	130.7(12)	N(1)-Mn(1)-N(28)-Mn(2)#1	-115.8(4)
Mn(1)#1-Mn(2)-N(11)-C(12)	-166.4(11)	N(18)-Mn(1)-N(28)-Mn(2)#1	57.3(4)
N(28)#1-Mn(2)-N(11)-C(16)	70.2(10)	N(21)-Mn(1)-N(28)-Mn(2)#1	151.0(5)
N(8)-Mn(2)-N(11)-C(16)	-70.3(9)	Mn(2)-Mn(1)-N(28)-Mn(2)#1	41.3(7)
Cl(31)-Mn(2)-N(11)-	-177.2(8)	N(28)-C(27)-O(29)-C(30)	-74.2(17)

C(16) N(18)-Mn(2)-N(11)-C(16)	4.4(9)	C(26)-C(27)-O(29)-C(30)	163.3(15)

Symmetry transformations used to generate equivalent atoms: –x+½, y+½, -z+½; -x, -y, -z; x-½, -y-½, z-½.

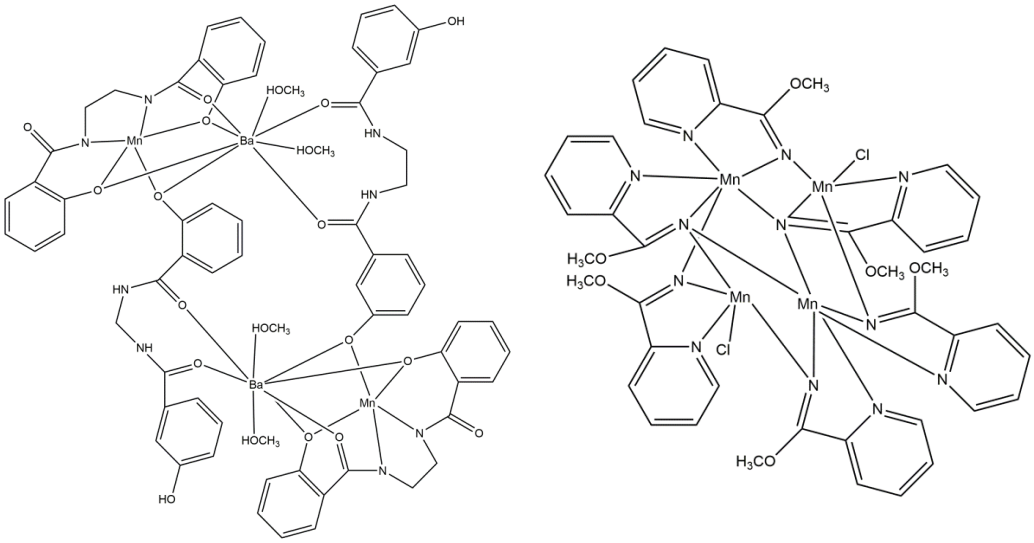
Table S11. Optimized Cartesian Coordinates (Å) obtained with DFT calculations (TPSSh/TZVP) for the $[MnL^1]^-\cdot 2H_2O$ system.

Mn	-0.00065300	0.13910500	0.12746100
N	-1.30634100	1.56349000	0.35114000
C	-0.68374500	2.84330600	0.71776200
H	-1.32511200	3.67424000	0.41736200
H	-0.56296000	2.89495500	1.80740200
C	0.67029300	2.91788900	0.03669200
H	1.31016600	3.66477000	0.51142900
H	0.54998700	3.21019500	-1.01442200
N	1.29743400	1.58862400	0.10873900
C	-2.65737600	1.50486600	0.39438200
C	-3.31808500	0.20486900	0.05970800
C	-4.69249900	0.23578800	-0.21918300
H	-5.18101100	1.20320300	-0.19778300
C	-5.41127600	-0.91436900	-0.51025200
H	-6.47070300	-0.85835800	-0.73290400
C	-4.74823900	-2.14581200	-0.50870300
H	-5.29072900	-3.05917700	-0.73027400
C	-3.39281300	-2.20850200	-0.22570300
H	-2.86940100	-3.15867500	-0.22248400
C	-2.65185000	-1.04299600	0.05892300
C	2.63490500	1.55660400	-0.09781700
C	3.34028500	0.23683900	-0.07278000
C	4.73991300	0.26654400	-0.17768000
H	5.20507100	1.24146300	-0.26670600
C	5.50854300	-0.88745300	-0.16768100
H	6.58806700	-0.82955400	-0.24732500
C	4.86720600	-2.12545800	-0.05866900
H	5.44534600	-3.04382000	-0.05427700
C	3.48707000	-2.18768600	0.04347800
H	2.98126200	-3.14459200	0.11805800
C	2.69706600	-1.01818300	0.04020600
O	-3.36557300	2.49703300	0.67851600
O	-1.35418200	-1.18394300	0.34313200
O	3.30031800	2.59918400	-0.29247900
O	1.37627900	-1.17205600	0.14468000
O	0.06734400	-3.33986500	1.45852600
H	0.78019400	-2.78833300	1.08490000
H	-0.69882500	-2.79394100	1.19858700
O	-0.19888000	-0.00416300	-2.19688300
H	-0.90612500	0.55796800	-2.54400500
H	-0.41538400	-0.89977000	-2.49324900

Table S12. Optimized Cartesian Coordinates (Å) obtained with DFT calculations (TPSSh/TZVP) for the $\{[MnL^1]^-\cdot 2H_2O\}_2$ system.

Mn	1.75966600	-1.72885700	0.08785200
N	3.41541000	-1.57990200	-0.92614700
C	3.41786100	-2.51107700	-2.05990000
H	4.43745100	-2.66627900	-2.41772300
H	2.83266800	-2.08526700	-2.88420200
C	2.78961900	-3.81492900	-1.59529100
H	2.47481900	-4.42364400	-2.44698100
H	3.52050200	-4.40421800	-1.02654500
N	1.63777700	-3.49767900	-0.73645900
C	4.43908900	-0.70942400	-0.81635900
C	4.42875400	0.24399000	0.34081900
C	5.62692400	0.91834900	0.62108700
H	6.48145800	0.68557300	-0.00390600
C	5.73089300	1.84771200	1.64556600
H	6.67367600	2.34509200	1.84304500
C	4.59869200	2.13498300	2.41477800
H	4.65360100	2.86151000	3.21913700
C	3.39843300	1.49219500	2.15664600
H	2.51521000	1.71006600	2.74773200
C	3.28500500	0.53745900	1.12364500
C	0.82044300	-4.53344500	-0.45251200
C	-0.34849200	-4.31165000	0.45899400
C	-1.23521400	-5.38866000	0.61638100
H	-1.00817900	-6.29347800	0.06470600
C	-2.35252000	-5.31906700	1.43474400
H	-3.01836000	-6.16927700	1.52999700
C	-2.60277500	-4.13467100	2.13497300
H	-3.46810200	-4.05411500	2.78504700
C	-1.74472000	-3.05513200	2.00442300
H	-1.92953600	-2.13474600	2.54833500
C	-0.60816200	-3.11410800	1.16864700
O	5.40180000	-0.68383000	-1.61917000
O	2.09239300	-0.02407100	0.92151300
O	1.00211100	-5.67560900	-0.93883600
O	0.16151900	-2.02805500	1.10418700
O	0.49203900	-0.62991300	-1.50905200
Mn	-1.75940200	1.72862800	-0.08772100
N	-3.41481600	1.58214700	0.92723800
C	-3.41564800	2.51397700	2.06046200
H	-4.43490000	2.67059400	2.41862500
H	-2.83068800	2.08789600	2.88478800
C	-2.78602000	3.81684100	1.59497400
H	-2.46985900	4.42536300	2.44628900
H	-3.51654000	4.40695700	1.02661800
N	-1.63520600	3.49790400	0.73539700
C	-4.43905600	0.71207200	0.81910700
C	-4.43049700	-0.24183900	-0.33764700

C	-5.62947500	-0.91524800	-0.61673700
H	-6.48334000	-0.68149400	0.00880800
C	-5.73504200	-1.84488700	-1.64080500
H	-6.67841800	-2.34148500	-1.83741400
C	-4.60365800	-2.13344900	-2.41074500
H	-4.65979800	-2.86024800	-3.21477400
C	-3.40262900	-1.49166000	-2.15371600
H	-2.52002500	-1.71059600	-2.74533900
C	-3.28755800	-0.53663300	-1.12115600
C	-0.81733300	4.53278600	0.44983900
C	0.35047600	4.30943600	-0.46272800
C	1.23725500	5.38603300	-0.62255700
H	1.01109800	6.29159800	-0.07173300
C	2.35352300	5.31515800	-1.44222100
H	3.01943000	6.16510200	-1.53935800
C	2.60269300	4.12979900	-2.14121400
H	3.46716700	4.04825600	-2.79229700
C	1.74459800	3.05059000	-2.00819500
H	1.92860700	2.12941200	-2.55102800
C	0.60913300	3.11090900	-1.17107200
O	-5.40099300	0.68754200	1.62288600
O	-2.09425600	0.02374300	-0.92004100
O	-0.99750000	5.67548600	0.93543900
O	-0.16060900	2.02504400	-1.10402100
O	-0.49271200	0.62900400	1.50985300
H	-0.47357300	-0.73020400	-1.34937700
H	0.56869700	0.34695200	-1.42355600
H	-0.57380400	-0.34726300	1.42517000
H	0.47341200	0.72488400	1.34919100
O	-3.01465300	2.65705800	-2.07623600
H	-2.64638100	2.20549600	-2.84859500
O	3.01376600	-2.65561900	2.07865500
H	2.63716400	-2.20701200	2.84872200
H	3.92177800	-2.32539400	2.02418000
H	-3.92475400	2.33369800	-2.01582100



1 **2**

Scheme S1. Chemdraw structures for **1** (left) and **2** (right).

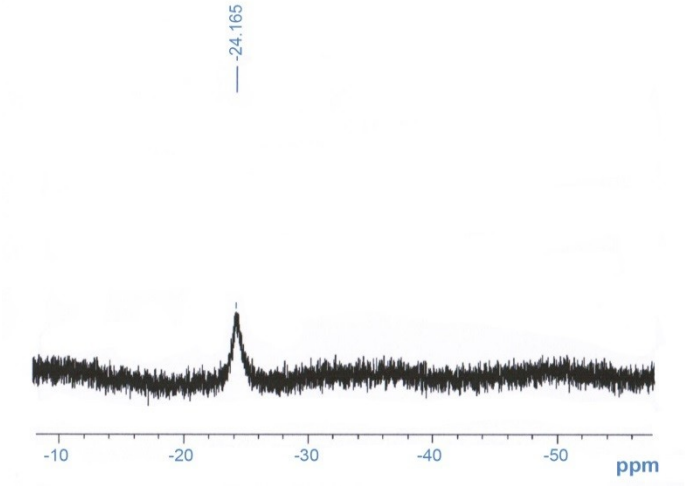


Figure S1. Paramagnetic ^{1}H NMR spectrum for complex **1**.

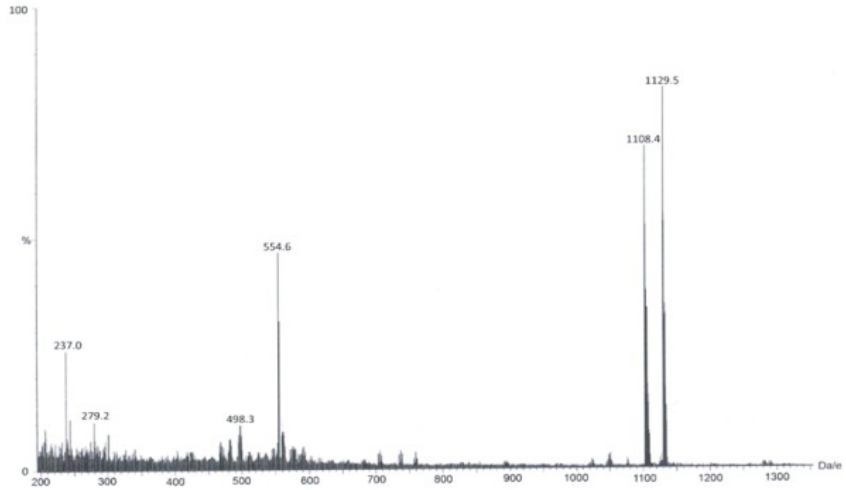


Figure S2. ESI mass spectrum for complex **2**.

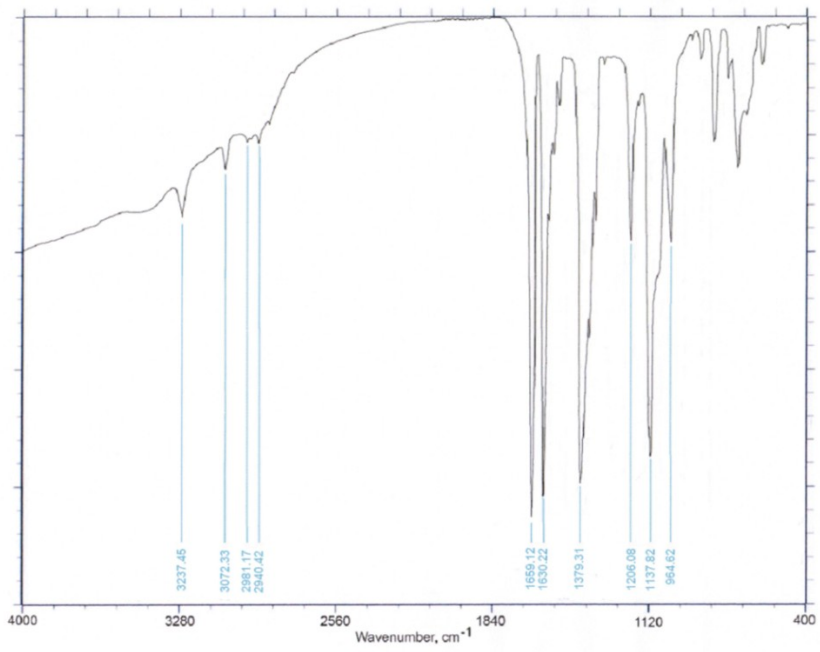


Figure S3. IR spectrum for **2**.