

A new metal-organic framework of Mn^{II}–chelidamic acid consolidated by octamer water cluster

Hossein Eshtiagh-Hosseini and Masoud Mirzaei

Table 1S Crystal data and structure refinement for **1**.

Empirical formula	C ₁₄ H ₂₂ Mn ₂ N ₂ O ₁₈	
Formula weight	616.22	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	<i>a</i> = 9.4351(5) Å	$\alpha = 87.8480(10)^\circ$.
	<i>b</i> = 10.8065(6) Å	$\beta = 74.0430(10)^\circ$.
	<i>c</i> = 11.1035(6) Å	$\gamma = 80.0070(10)^\circ$.
Volume	1071.92(10) Å ³	
<i>Z</i>	2	
Density (calculated)	1.909 Mg/m ³	
Absorption coefficient	1.276 mm ⁻¹	
<i>F</i> (000)	628	
Crystal size	0.18 × 0.15 × 0.12 mm ³	
Theta range for data collection	1.91 to 28.00°.	
Index ranges	-12 ≤ <i>h</i> ≤ 12, -14 ≤ <i>k</i> ≤ 14, -14 ≤ <i>l</i> ≤ 14	
Reflections collected	11959	
Independent reflections	5180 [<i>R</i> (int) = 0.0293]	
Completeness to theta = 28.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.830 and 0.743	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	5180 / 0 / 333	
Goodness-of-fit on <i>F</i> ²	1.031	
Final <i>R</i> indices [for 4220 rfln with <i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0422, <i>wR</i> 2 = 0.1044	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0554, <i>wR</i> 2 = 0.1128	
Largest diff. peak and hole	0.755 and -0.669 e.Å ⁻³	

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

	x	y	z	U(eq)
Mn(1)	3634(1)	9256(1)	1318(1)	12(1)
Mn(2)	4763(1)	5864(1)	1565(1)	15(1)
O(1)	1890(2)	8700(2)	3032(2)	16(1)
O(2)	1099(2)	8674(2)	5113(2)	14(1)
O(3)	5278(2)	10788(2)	757(2)	13(1)
O(4)	6451(2)	12085(2)	1502(2)	14(1)
O(5)	3779(2)	12040(2)	6202(2)	15(1)
O(6)	3961(2)	4296(2)	514(2)	14(1)
O(7)	2290(2)	3009(2)	717(2)	20(1)
O(8)	4395(2)	6533(2)	3638(2)	16(1)
O(9)	3493(2)	6138(2)	5664(2)	18(1)
O(10)	198(2)	2966(2)	5514(2)	14(1)
O(11)	5732(2)	7827(2)	1404(2)	13(1)
O(12)	3116(2)	7289(2)	891(2)	14(1)
O(1W)	1709(3)	10327(2)	871(2)	29(1)
O(2W)	6687(3)	4694(3)	1982(2)	40(1)
N(1)	3737(2)	10245(2)	3008(2)	11(1)
N(2)	3132(3)	4814(2)	2931(2)	12(1)
C(1)	2846(3)	10015(2)	4141(2)	11(1)
C(2)	2834(3)	10605(3)	5223(2)	12(1)
C(3)	3802(3)	11462(3)	5150(2)	11(1)
C(4)	4740(3)	11705(3)	3978(2)	11(1)
C(5)	4650(3)	11074(2)	2946(2)	10(1)
C(6)	1865(3)	9057(3)	4092(3)	12(1)
C(7)	5553(3)	11336(3)	1637(2)	12(1)
C(8)	2453(3)	3971(3)	2551(3)	12(1)
C(9)	1446(3)	3318(3)	3356(3)	13(1)
C(10)	1141(3)	3535(3)	4644(3)	12(1)
C(11)	1870(3)	4389(3)	5045(3)	13(1)
C(12)	2827(3)	5011(3)	4171(3)	12(1)
C(13)	2929(3)	3731(3)	1145(3)	13(1)

C(14)	3628(3)	5967(3)	4542(3)	13(1)
O(3W)	291(2)	6923(2)	1907(2)	26(1)
O(4W)	8423(3)	9091(2)	1468(2)	31(1)
O(5W)	8985(3)	1288(4)	2435(3)	20(1)
O(6W)	9576(4)	4678(4)	1220(4)	46(1)
O(5WA)	9065(14)	1841(11)	2342(12)	31(3)
O(6WA)	9640(30)	4130(20)	180(20)	118(7)

Table 3S Bond lengths [Å] and angles [°] for **1**.

Mn(1)-O(1W)	2.146(2)	O(6)-Mn(2)#2	2.288(2)
Mn(1)-N(1)	2.227(2)	O(7)-C(13)	1.244(3)
Mn(1)-O(3)#1	2.2489(19)	O(8)-C(14)	1.270(3)
Mn(1)-O(1)	2.286(2)	O(9)-C(14)	1.235(3)
Mn(1)-O(11)	2.312(2)	O(10)-C(10)	1.333(3)
Mn(1)-O(12)	2.355(2)	O(10)-H(10)	0.8501
Mn(1)-O(3)	2.4122(19)	O(11)-H(11A)	0.8500
Mn(1)-H(1W1)	2.1881	O(11)-H(11B)	0.8502
Mn(2)-O(2W)	2.174(3)	O(12)-H(12A)	0.8500
Mn(2)-O(12)	2.252(2)	O(12)-H(12B)	0.8500
Mn(2)-N(2)	2.270(2)	O(1W)-H(1W1)	0.8500
Mn(2)-O(6)#2	2.288(2)	O(1W)-H(1W2)	0.8500
Mn(2)-O(8)	2.354(2)	O(2W)-H(2W1)	0.8500
Mn(2)-O(6)	2.4266(19)	O(2W)-H(2W2)	0.8500
Mn(2)-O(11)	2.433(2)	N(1)-C(5)	1.334(3)
O(1)-C(6)	1.244(3)	N(1)-C(1)	1.348(3)
O(2)-C(6)	1.264(3)	N(2)-C(8)	1.341(3)
O(3)-C(7)	1.268(3)	N(2)-C(12)	1.344(3)
O(3)-Mn(1)#1	2.2489(19)	C(1)-C(2)	1.378(4)
O(4)-C(7)	1.247(3)	C(1)-C(6)	1.516(4)
O(5)-C(3)	1.338(3)	C(2)-C(3)	1.395(4)
O(5)-H(5)	0.8500	C(2)-H(2A)	0.9500
O(6)-C(13)	1.269(3)	C(3)-C(4)	1.403(4)

C(4)-C(5)	1.384(4)	O(3W)-H(3W2)	0.8501
C(4)-H(4A)	0.9500	O(4W)-H(4W1)	0.8500
C(5)-C(7)	1.513(4)	O(4W)-H(4W2)	0.8500
C(8)-C(9)	1.385(4)	O(5W)-H(5W1)	0.8501
C(8)-C(13)	1.520(4)	O(5W)-H(5W2)	0.8500
C(9)-C(10)	1.399(4)	O(6W)-H(6W1)	0.8500
C(9)-H(9A)	0.9500	O(6W)-H(6W2)	0.8500
C(10)-C(11)	1.394(4)	O(5WA)-H(5W3)	0.8501
C(11)-C(12)	1.374(4)	O(5WA)-H(5W4)	0.8501
C(11)-H(11C)	0.9500	O(6WA)-H(6W4)	0.8500
C(12)-C(14)	1.512(4)	O(6WA)-H(6W3)	0.8500
O(3W)-H(3W1)	0.9964		
O(1W)-Mn(1)-N(1)	103.03(9)	O(3)#1-Mn(1)-H(1W1)	90.2
O(1W)-Mn(1)-O(3)#1	85.76(8)	O(1)-Mn(1)-H(1W1)	89.7
N(1)-Mn(1)-O(3)#1	137.82(8)	O(11)-Mn(1)-H(1W1)	165.8
O(1W)-Mn(1)-O(1)	83.27(8)	O(12)-Mn(1)-H(1W1)	117.6
N(1)-Mn(1)-O(1)	70.61(8)	O(3)-Mn(1)-H(1W1)	79.4
O(3)#1-Mn(1)-O(1)	151.40(7)	O(2W)-Mn(2)-O(12)	168.47(9)
O(1W)-Mn(1)-O(11)	166.76(8)	O(2W)-Mn(2)-N(2)	92.39(10)
N(1)-Mn(1)-O(11)	90.20(8)	O(12)-Mn(2)-N(2)	99.10(8)
O(3)#1-Mn(1)-O(11)	84.47(7)	O(2W)-Mn(2)-O(6)#2	88.58(8)
O(1)-Mn(1)-O(11)	101.28(7)	O(12)-Mn(2)-O(6)#2	83.65(7)
O(1W)-Mn(1)-O(12)	95.04(9)	N(2)-Mn(2)-O(6)#2	136.73(8)
N(1)-Mn(1)-O(12)	135.97(8)	O(2W)-Mn(2)-O(8)	80.62(8)
O(3)#1-Mn(1)-O(12)	82.65(7)	O(12)-Mn(2)-O(8)	102.63(7)
O(1)-Mn(1)-O(12)	72.14(7)	N(2)-Mn(2)-O(8)	69.10(7)
O(11)-Mn(1)-O(12)	74.88(7)	O(6)#2-Mn(2)-O(8)	152.79(7)
O(1W)-Mn(1)-O(3)	98.44(8)	O(2W)-Mn(2)-O(6)	98.64(9)
N(1)-Mn(1)-O(3)	68.79(7)	O(12)-Mn(2)-O(6)	86.53(7)
O(3)#1-Mn(1)-O(3)	69.13(8)	N(2)-Mn(2)-O(6)	68.13(7)
O(1)-Mn(1)-O(3)	138.66(7)	O(6)#2-Mn(2)-O(6)	68.97(8)
O(11)-Mn(1)-O(3)	86.39(7)	O(8)-Mn(2)-O(6)	137.16(7)
O(12)-Mn(1)-O(3)	147.52(7)	O(2W)-Mn(2)-O(11)	96.14(10)
O(1W)-Mn(1)-H(1W1)	22.6	O(12)-Mn(2)-O(11)	74.44(7)
N(1)-Mn(1)-H(1W1)	84.9	N(2)-Mn(2)-O(11)	140.27(7)

O(6)#2-Mn(2)-O(11)	82.35(7)	C(12)-N(2)-Mn(2)	120.33(18)
O(8)-Mn(2)-O(11)	74.15(6)	N(1)-C(1)-C(2)	122.8(2)
O(6)-Mn(2)-O(11)	147.20(7)	N(1)-C(1)-C(6)	113.1(2)
C(6)-O(1)-Mn(1)	119.40(17)	C(2)-C(1)-C(6)	124.1(2)
C(7)-O(3)-Mn(1)#1	130.44(18)	C(1)-C(2)-C(3)	118.7(3)
C(7)-O(3)-Mn(1)	117.82(17)	C(1)-C(2)-H(2A)	120.6
Mn(1)#1-O(3)-Mn(1)	110.87(8)	C(3)-C(2)-H(2A)	120.6
C(3)-O(5)-H(5)	114.3	O(5)-C(3)-C(2)	118.5(2)
C(13)-O(6)-Mn(2)#2	130.48(17)	O(5)-C(3)-C(4)	122.5(2)
C(13)-O(6)-Mn(2)	118.47(17)	C(2)-C(3)-C(4)	119.0(2)
Mn(2)#2-O(6)-Mn(2)	111.03(8)	C(5)-C(4)-C(3)	117.7(2)
C(14)-O(8)-Mn(2)	119.83(17)	C(5)-C(4)-H(4A)	121.2
C(10)-O(10)-H(10)	114.1	C(3)-C(4)-H(4A)	121.2
Mn(1)-O(11)-Mn(2)	100.82(7)	N(1)-C(5)-C(4)	123.8(3)
Mn(1)-O(11)-H(11A)	119.8	N(1)-C(5)-C(7)	115.0(2)
Mn(2)-O(11)-H(11A)	94.8	C(4)-C(5)-C(7)	121.2(2)
Mn(1)-O(11)-H(11B)	111.2	O(1)-C(6)-O(2)	125.0(2)
Mn(2)-O(11)-H(11B)	122.3	O(1)-C(6)-C(1)	116.6(2)
H(11A)-O(11)-H(11B)	107.9	O(2)-C(6)-C(1)	118.4(2)
Mn(2)-O(12)-Mn(1)	105.08(8)	O(4)-C(7)-O(3)	125.6(3)
Mn(2)-O(12)-H(12A)	125.2	O(4)-C(7)-C(5)	118.8(2)
Mn(1)-O(12)-H(12A)	95.5	O(3)-C(7)-C(5)	115.6(2)
Mn(2)-O(12)-H(12B)	105.3	N(2)-C(8)-C(9)	123.9(3)
Mn(1)-O(12)-H(12B)	121.9	N(2)-C(8)-C(13)	114.5(2)
H(12A)-O(12)-H(12B)	105.4	C(9)-C(8)-C(13)	121.6(2)
Mn(1)-O(1W)-H(1W1)	81.5	C(8)-C(9)-C(10)	118.0(2)
Mn(1)-O(1W)-H(1W2)	124.1	C(8)-C(9)-H(9A)	121.0
H(1W1)-O(1W)-H(1W2)	108.4	C(10)-C(9)-H(9A)	121.0
Mn(2)-O(2W)-H(2W1)	116.6	O(10)-C(10)-C(11)	117.8(2)
Mn(2)-O(2W)-H(2W2)	132.1	O(10)-C(10)-C(9)	123.8(2)
H(2W1)-O(2W)-H(2W2)	99.9	C(11)-C(10)-C(9)	118.3(2)
C(5)-N(1)-C(1)	118.0(2)	C(12)-C(11)-C(10)	119.3(3)
C(5)-N(1)-Mn(1)	122.37(18)	C(12)-C(11)-H(11C)	120.3
C(1)-N(1)-Mn(1)	119.63(17)	C(10)-C(11)-H(11C)	120.3
C(8)-N(2)-C(12)	117.4(2)	N(2)-C(12)-C(11)	123.1(2)
C(8)-N(2)-Mn(2)	122.31(18)	N(2)-C(12)-C(14)	114.9(2)

C(11)-C(12)-C(14)	122.0(2)	H(3W1)-O(3W)-H(3W2)	107.9
O(7)-C(13)-O(6)	126.0(3)	H(4W1)-O(4W)-H(4W2)	100.6
O(7)-C(13)-C(8)	118.1(2)	H(5W1)-O(5W)-H(5W2)	108.3
O(6)-C(13)-C(8)	116.0(2)	H(6W1)-O(6W)-H(6W2)	97.2
O(9)-C(14)-O(8)	125.7(3)	H(5W3)-O(5WA)-H(5W4)	84.0
O(9)-C(14)-C(12)	119.0(2)	H(6W4)-O(6WA)-H(6W3)	80.7
O(8)-C(14)-C(12)	115.2(2)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z #2 -x+1,-y+1,-z

Table 4S Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Mn(1)	14(1)	14(1)	9(1)	-2(1)	-2(1)	-5(1)
Mn(2)	21(1)	16(1)	10(1)	1(1)	-4(1)	-8(1)
O(1)	21(1)	21(1)	10(1)	-2(1)	-3(1)	-13(1)
O(2)	16(1)	19(1)	10(1)	-1(1)	-3(1)	-9(1)
O(3)	17(1)	14(1)	10(1)	-2(1)	-4(1)	-7(1)
O(4)	17(1)	18(1)	11(1)	-2(1)	-5(1)	-10(1)
O(5)	19(1)	19(1)	9(1)	-2(1)	-4(1)	-10(1)
O(6)	18(1)	15(1)	13(1)	1(1)	-4(1)	-9(1)
O(7)	22(1)	27(1)	13(1)	-7(1)	1(1)	-16(1)
O(8)	21(1)	16(1)	13(1)	0(1)	-5(1)	-10(1)
O(9)	29(1)	19(1)	12(1)	1(1)	-8(1)	-13(1)
O(10)	16(1)	16(1)	12(1)	-1(1)	-1(1)	-9(1)
O(11)	13(1)	19(1)	7(1)	-4(1)	-4(1)	-3(1)
O(12)	14(1)	19(1)	11(1)	0(1)	-2(1)	-7(1)
O(1W)	27(1)	40(2)	19(1)	10(1)	-7(1)	-3(1)
O(2W)	42(2)	55(2)	14(1)	1(1)	-7(1)	16(1)
N(1)	10(1)	12(1)	11(1)	-2(1)	-3(1)	-3(1)
N(2)	14(1)	13(1)	11(1)	-2(1)	-4(1)	-5(1)
C(1)	10(1)	12(1)	11(1)	-1(1)	-2(1)	-2(1)

C(2)	12(1)	14(1)	10(1)	-1(1)	-3(1)	-3(1)
C(3)	13(1)	11(1)	11(1)	-2(1)	-6(1)	0(1)
C(4)	12(1)	12(1)	12(1)	-1(1)	-5(1)	-3(1)
C(5)	9(1)	10(1)	12(1)	0(1)	-5(1)	-1(1)
C(6)	12(1)	12(1)	14(1)	-1(1)	-4(1)	-4(1)
C(7)	13(1)	13(1)	10(1)	-2(1)	-4(1)	-2(1)
C(8)	13(1)	13(1)	12(1)	-2(1)	-5(1)	-4(1)
C(9)	13(1)	12(1)	15(1)	-2(1)	-4(1)	-4(1)
C(10)	10(1)	12(1)	14(1)	1(1)	-2(1)	-2(1)
C(11)	15(1)	12(1)	12(1)	-1(1)	-4(1)	-4(1)
C(12)	15(1)	11(1)	14(1)	-1(1)	-7(1)	-4(1)
C(13)	15(1)	11(1)	13(1)	0(1)	-4(1)	-4(1)
C(14)	15(1)	12(1)	15(1)	-1(1)	-6(1)	-4(1)
O(3W)	22(1)	39(1)	19(1)	-2(1)	-4(1)	-13(1)
O(4W)	39(2)	37(1)	20(1)	5(1)	-11(1)	-7(1)
O(5W)	16(2)	36(2)	9(1)	-3(1)	-6(1)	0(2)
O(6W)	30(2)	44(2)	69(3)	-16(2)	-20(2)	-4(2)

Table 5S Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**.

	x	y	z	U(eq)
H(5)	4393	12550	6099	22
H(10)	-134	2391	5228	21
H(11A)	6423	7615	736	19
H(11B)	6130	8050	1942	19
H(12A)	3148	7439	127	21
H(12B)	2268	7075	1215	21
H(1W1)	2047	10929	1106	44
H(1W2)	1641	10469	129	44
H(2W1)	6519	4292	2666	60
H(2W2)	7565	4825	1927	60
H(2A)	2180	10430	6004	14
H(4A)	5414	12282	3895	13
H(9A)	976	2741	3043	15
H(11C)	1707	4540	5914	16
H(3W1)	198	6992	2819	39
H(3W2)	81	6215	1775	39
H(4W1)	8941	9605	1620	47
H(4W2)	9002	8398	1489	47
H(5W1)	8137	1526	2297	31
H(5W2)	8885	1386	3211	31
H(6W1)	10402	4175	1095	69
H(6W2)	9782	5066	530	69
H(5W3)	8284	1573	2302	47
H(5W4)	8921	1470	3043	47
H(6W4)	9403	3405	313	177
H(6W3)	10326	3788	508	177

Table 6S Torsion angles [°] for **1**.

O(1W)-Mn(1)-O(1)-C(6)	-113.3(2)	O(6)-Mn(2)-O(8)-C(14)	3.0(3)
N(1)-Mn(1)-O(1)-C(6)	-6.9(2)	O(11)-Mn(2)-O(8)-C(14)	171.2(2)
O(3)#1-Mn(1)-O(1)-C(6)	178.50(19)	O(1W)-Mn(1)-O(11)-Mn(2)	-57.2(4)
O(11)-Mn(1)-O(1)-C(6)	79.3(2)	N(1)-Mn(1)-O(11)-Mn(2)	122.14(8)
O(12)-Mn(1)-O(1)-C(6)	149.2(2)	O(3)#1-Mn(1)-O(11)-Mn(2)	-99.78(7)
O(3)-Mn(1)-O(1)-C(6)	-18.2(3)	O(1)-Mn(1)-O(11)-Mn(2)	51.88(8)
O(1W)-Mn(1)-O(3)-C(7)	107.4(2)	O(12)-Mn(1)-O(11)-Mn(2)	-15.92(6)
N(1)-Mn(1)-O(3)-C(7)	6.59(19)	O(3)-Mn(1)-O(11)-Mn(2)	-169.13(7)
O(3)#1-Mn(1)-O(3)-C(7)	-170.5(2)	O(2W)-Mn(2)-O(11)-Mn(1)	-170.06(8)
O(1)-Mn(1)-O(3)-C(7)	18.0(2)	O(12)-Mn(2)-O(11)-Mn(1)	16.70(7)
O(11)-Mn(1)-O(3)-C(7)	-85.03(19)	N(2)-Mn(2)-O(11)-Mn(1)	-68.81(13)
O(12)-Mn(1)-O(3)-C(7)	-139.15(19)	O(6)#2-Mn(2)-O(11)-Mn(1)	102.20(8)
O(1W)-Mn(1)-O(3)-Mn(1)#1	-82.15(10)	O(8)-Mn(2)-O(11)-Mn(1)	-91.65(8)
N(1)-Mn(1)-O(3)-Mn(1)#1	177.07(11)	O(6)-Mn(2)-O(11)-Mn(1)	73.46(14)
O(3)#1-Mn(1)-O(3)-Mn(1)#1	0.0	O(2W)-Mn(2)-O(12)-Mn(1)	-52.6(5)
O(1)-Mn(1)-O(3)-Mn(1)#1	-171.55(9)	N(2)-Mn(2)-O(12)-Mn(1)	123.12(8)
O(11)-Mn(1)-O(3)-Mn(1)#1	85.45(9)	O(6)#2-Mn(2)-O(12)-Mn(1)	-100.48(8)
O(12)-Mn(1)-O(3)-Mn(1)#1	31.33(17)	O(8)-Mn(2)-O(12)-Mn(1)	52.65(9)
O(2W)-Mn(2)-O(6)-C(13)	96.5(2)	O(6)-Mn(2)-O(12)-Mn(1)	-169.69(8)
O(12)-Mn(2)-O(6)-C(13)	-93.9(2)	O(11)-Mn(2)-O(12)-Mn(1)	-16.68(7)
N(2)-Mn(2)-O(6)-C(13)	7.35(19)	O(1W)-Mn(1)-O(12)-Mn(2)	-171.17(8)
O(6)#2-Mn(2)-O(6)-C(13)	-178.4(2)	N(1)-Mn(1)-O(12)-Mn(2)	-56.54(13)
O(8)-Mn(2)-O(6)-C(13)	11.0(2)	O(3)#1-Mn(1)-O(12)-Mn(2)	103.77(8)
O(11)-Mn(2)-O(6)-C(13)	-147.72(18)	O(1)-Mn(1)-O(12)-Mn(2)	-89.91(9)
O(2W)-Mn(2)-O(6)-Mn(2)#2	-85.11(10)	O(11)-Mn(1)-O(12)-Mn(2)	17.54(7)
O(12)-Mn(2)-O(6)-Mn(2)#2	84.52(9)	O(3)-Mn(1)-O(12)-Mn(2)	74.43(14)
N(2)-Mn(2)-O(6)-Mn(2)#2	-174.22(11)	O(1W)-Mn(1)-N(1)-C(5)	-98.7(2)
O(6)#2-Mn(2)-O(6)-Mn(2)#2	0.0	O(3)#1-Mn(1)-N(1)-C(5)	-0.6(3)
O(8)-Mn(2)-O(6)-Mn(2)#2	-170.61(9)	O(1)-Mn(1)-N(1)-C(5)	-176.7(2)
O(11)-Mn(2)-O(6)-Mn(2)#2	30.70(17)	O(11)-Mn(1)-N(1)-C(5)	81.4(2)
O(2W)-Mn(2)-O(8)-C(14)	-89.6(2)	O(12)-Mn(1)-N(1)-C(5)	149.60(18)
O(12)-Mn(2)-O(8)-C(14)	101.7(2)	O(3)-Mn(1)-N(1)-C(5)	-4.62(19)
N(2)-Mn(2)-O(8)-C(14)	6.6(2)	O(1W)-Mn(1)-N(1)-C(1)	80.7(2)
O(6)#2-Mn(2)-O(8)-C(14)	-157.5(2)	O(3)#1-Mn(1)-N(1)-C(1)	178.92(17)

O(1)-Mn(1)-N(1)-C(1)	2.79(19)	N(1)-C(1)-C(6)-O(2)	172.8(2)
O(11)-Mn(1)-N(1)-C(1)	-99.1(2)	C(2)-C(1)-C(6)-O(2)	-7.5(4)
O(12)-Mn(1)-N(1)-C(1)	-30.9(2)	Mn(1)#1-O(3)-C(7)-O(4)	6.8(4)
O(3)-Mn(1)-N(1)-C(1)	174.8(2)	Mn(1)-O(3)-C(7)-O(4)	175.0(2)
O(2W)-Mn(2)-N(2)-C(8)	-103.5(2)	Mn(1)#1-O(3)-C(7)-C(5)	-175.77(16)
O(12)-Mn(2)-N(2)-C(8)	77.3(2)	Mn(1)-O(3)-C(7)-C(5)	-7.5(3)
O(6)#2-Mn(2)-N(2)-C(8)	-13.1(3)	N(1)-C(5)-C(7)-O(4)	-178.8(2)
O(8)-Mn(2)-N(2)-C(8)	177.5(2)	C(4)-C(5)-C(7)-O(4)	3.9(4)
O(6)-Mn(2)-N(2)-C(8)	-5.2(2)	N(1)-C(5)-C(7)-O(3)	3.5(4)
O(11)-Mn(2)-N(2)-C(8)	153.89(18)	C(4)-C(5)-C(7)-O(3)	-173.8(2)
O(2W)-Mn(2)-N(2)-C(12)	75.6(2)	C(12)-N(2)-C(8)-C(9)	1.3(4)
O(12)-Mn(2)-N(2)-C(12)	-103.5(2)	Mn(2)-N(2)-C(8)-C(9)	-179.6(2)
O(6)#2-Mn(2)-N(2)-C(12)	166.08(18)	C(12)-N(2)-C(8)-C(13)	-176.1(2)
O(8)-Mn(2)-N(2)-C(12)	-3.4(2)	Mn(2)-N(2)-C(8)-C(13)	3.1(3)
O(6)-Mn(2)-N(2)-C(12)	174.0(2)	N(2)-C(8)-C(9)-C(10)	-1.3(4)
O(11)-Mn(2)-N(2)-C(12)	-27.0(3)	C(13)-C(8)-C(9)-C(10)	175.9(2)
C(5)-N(1)-C(1)-C(2)	0.4(4)	C(8)-C(9)-C(10)-O(10)	-179.8(3)
Mn(1)-N(1)-C(1)-C(2)	-179.1(2)	C(8)-C(9)-C(10)-C(11)	-0.2(4)
C(5)-N(1)-C(1)-C(6)	-179.9(2)	O(10)-C(10)-C(11)-C(12)	-178.7(2)
Mn(1)-N(1)-C(1)-C(6)	0.6(3)	C(9)-C(10)-C(11)-C(12)	1.7(4)
N(1)-C(1)-C(2)-C(3)	-1.0(4)	C(8)-N(2)-C(12)-C(11)	0.3(4)
C(6)-C(1)-C(2)-C(3)	179.4(2)	Mn(2)-N(2)-C(12)-C(11)	-178.9(2)
C(1)-C(2)-C(3)-O(5)	179.5(2)	C(8)-N(2)-C(12)-C(14)	179.8(2)
C(1)-C(2)-C(3)-C(4)	0.7(4)	Mn(2)-N(2)-C(12)-C(14)	0.6(3)
O(5)-C(3)-C(4)-C(5)	-178.7(2)	C(10)-C(11)-C(12)-N(2)	-1.8(4)
C(2)-C(3)-C(4)-C(5)	0.2(4)	C(10)-C(11)-C(12)-C(14)	178.7(3)
C(1)-N(1)-C(5)-C(4)	0.5(4)	Mn(2)#2-O(6)-C(13)-O(7)	-6.2(4)
Mn(1)-N(1)-C(5)-C(4)	179.9(2)	Mn(2)-O(6)-C(13)-O(7)	171.8(2)
C(1)-N(1)-C(5)-C(7)	-176.8(2)	Mn(2)#2-O(6)-C(13)-C(8)	173.55(17)
Mn(1)-N(1)-C(5)-C(7)	2.7(3)	Mn(2)-O(6)-C(13)-C(8)	-8.4(3)
C(3)-C(4)-C(5)-N(1)	-0.8(4)	N(2)-C(8)-C(13)-O(7)	-176.4(3)
C(3)-C(4)-C(5)-C(7)	176.3(2)	C(9)-C(8)-C(13)-O(7)	6.2(4)
Mn(1)-O(1)-C(6)-O(2)	-169.9(2)	N(2)-C(8)-C(13)-O(6)	3.8(4)
Mn(1)-O(1)-C(6)-C(1)	9.6(3)	C(9)-C(8)-C(13)-O(6)	-173.6(3)
N(1)-C(1)-C(6)-O(1)	-6.7(4)	Mn(2)-O(8)-C(14)-O(9)	171.6(2)
C(2)-C(1)-C(6)-O(1)	173.0(3)	Mn(2)-O(8)-C(14)-C(12)	-8.5(3)

N(2)-C(12)-C(14)-O(9)	-174.9(3)	N(2)-C(12)-C(14)-O(8)	5.2(4)
C(11)-C(12)-C(14)-O(9)	4.7(4)	C(11)-C(12)-C(14)-O(8)	-175.2(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z #2 -x+1,-y+1,-z

Table 7S Hydrogen bonds for **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5)...O(8)#3	0.85	1.72	2.548(3)	162
O(10)-H(10)...O(2)#4	0.85	1.70	2.537(3)	169
O(11)-H(11A)...O(7)#2	0.85	1.80	2.646(3)	171
O(11)-H(11B)...O(5)#3	0.85	2.08	2.833(3)	147
O(12)-H(12A)...O(4)#1	0.85	1.82	2.655(3)	168
O(12)-H(12B)...O(3W)#5	0.85	1.85	2.685(3)	169
O(1W)-H(1W1)...O(7)#6	0.85	2.31	3.032(3)	143
O(1W)-H(1W2)...O(4W)#1	0.85	1.83	2.681(3)	175
O(2W)-H(2W1)...O(9)#7	0.85	1.89	2.702(3)	159
O(2W)-H(2W2)...O(6W)#5	0.85	1.82	2.620(5)	155
O(3W)-H(3W1)...O(10)#4	0.99	1.79	2.776(3)	172
O(3W)-H(3W2)...O(6W)#8	0.85	1.97	2.813(4)	171
O(3W)-H(3W2)...O(6WA)#2	0.85	2.15	2.60(2)	113
O(4W)-H(4W1)...O(5W)#6	0.85	2.07	2.831(4)	148
O(4W)-H(4W2)...O(3W)#9	0.85	1.95	2.790(4)	167
O(5W)-H(5W1)...O(4)#10	0.85	2.02	2.848(4)	165
O(5W)-H(5W2)...O(2)#7	0.85	1.86	2.704(4)	170
O(6W)-H(6W1)...O(7)#9	0.85	1.95	2.795(4)	177
O(6W)-H(6W2)...O(6W)#11	0.85	1.89	2.706(9)	159
O(5WA)-H(5W3)...O(4)#10	0.85	2.14	2.836(13)	139
O(5WA)-H(5W4)...O(2)#7	0.85	2.04	2.827(13)	153
O(6WA)-H(6W3)...O(7)#9	0.85	1.97	2.79(2)	162

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z #2 -x+1,-y+1,-z #3 -x+1,-y+2,-z+1

#4 -x,-y+1,-z+1 #5 x,y,z #6 x,y+1,z #7 -x+1,-y+1,-z+1

#8 x-1,y,z #9 x+1,y,z #10 x,y-1,z #11 -x+2,-y+1,-z

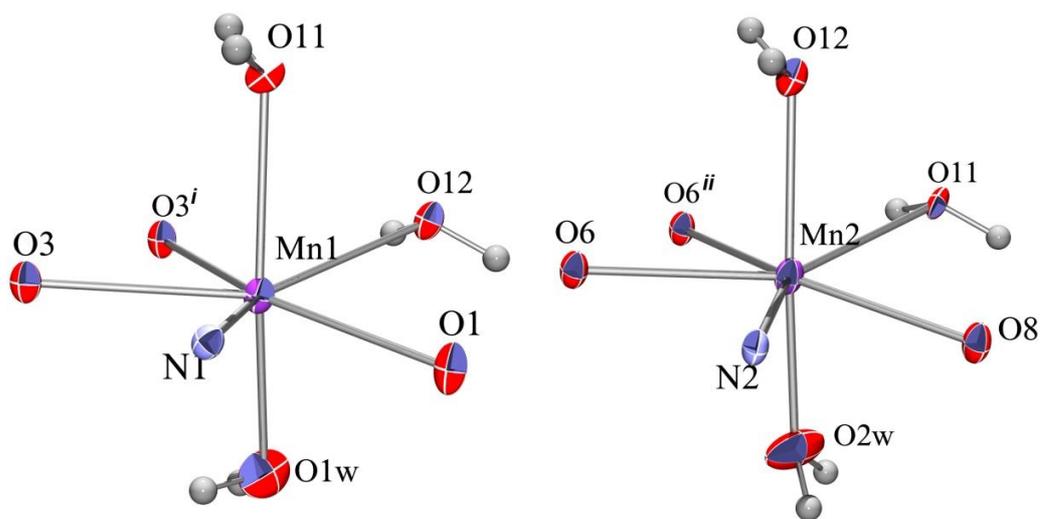


Figure 1S ORTEP-3 drawing of coordination polyhedra of Mn atoms. Displacement ellipsoids are drawn for the probability of 50 % and hydrogen atoms are shown as spheres of arbitrary radii. Symmetry operators: *i*) $1 - x, 2 - y, -z$; *ii*) $1 - x, 1 - y, -z$.

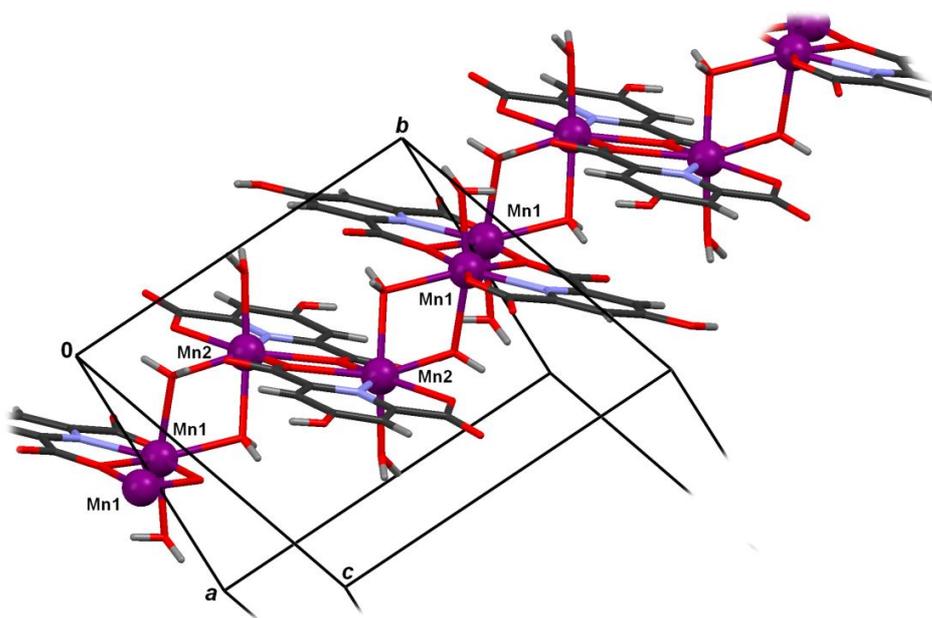


Figure 2S A staircase-like coordination polymer of **1** extending in the direction $[010]$. In each centrosymmetric "stair" Mn atoms are labelled. Manganese atoms are shown as spheres of arbitrary radii.