

Supporting Information

Synthesis and characterization of a series of manganese phosphonate complexes with various valences and nuclearity

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Table S1. Selected bond angles [°] for **1**

O1-Mn1-O6	82.33(9)	O16-Mn4-O34	80.01(8)	O41-Mn7-O21	177.12(9)
O1-Mn1-O10	173.33(9)	O20-Mn4-O34	83.77(8)	O5-Mn8-O4	81.20(9)
O6-Mn1-O10	93.88(9)	O30-Mn4-O34	171.24(8)	O5-Mn8-O22	94.75(9)
O1-Mn1-O14	93.76(9)	O3-Mn5-O33	97.20(10)	O4-Mn8-O22	175.42(9)
O6-Mn1-O14	152.77(9)	O3-Mn5-O21	89.11(9)	O5-Mn8-O8A	172.01(9)
O10-Mn1-O14	87.10(9)	O33-Mn5-O21	173.09(9)	O4-Mn8-O8A	97.39(9)
O1-Mn1-O29	94.63(9)	O3-Mn5-O39	169.03(10)	O22-Mn8-O8A	86.33(10)
O6-Mn1-O29	106.90(10)	O33-Mn5-O39	87.51(10)	O5-Mn8-O36	87.65(10)
O10-Mn1-O29	91.72(9)	O21-Mn5-O39	85.79(10)	O4-Mn8-O36	94.82(9)
O14-Mn1-O29	100.26(9)	O3-Mn5-O31	95.89(9)	O22-Mn8-O36	87.11(10)
O6-Mn2-O1	82.30(9)	O33-Mn5-O31	88.11(11)	O8A-Mn8-O36	100.32(10)
O6-Mn2-O11	173.90(10)	O21-Mn5-O31	94.04(10)	O5-Mn8-O34	87.92(8)
O1-Mn2-O11	94.09(9)	O39-Mn5-O31	94.16(10)	O4-Mn8-O34	89.70(8)
O6-Mn2-O19A	93.42(9)	O3-Mn5-O25	86.70(8)	O22-Mn8-O34	88.01(9)
O1-Mn2-O19A	152.48(10)	O33-Mn5-O25	93.20(10)	O8A-Mn8-O34	84.20(9)
O11-Mn2-O19A	87.51(9)	O21-Mn5-O25	84.34(9)	O36-Mn8-O34	173.12(8)
O6-Mn2-O26	93.95(10)	O39-Mn5-O25	83.13(9)	O5-Mn9-O4	80.93(9)
O1-Mn2-O26	106.15(10)	O31-Mn5-O25	176.93(9)	O5-Mn9-O18	165.07(10)
O11-Mn2-O26	91.78(10)	O3-Mn6-O2	81.31(9)	O4-Mn9-O18	95.70(9)
O19A-Mn2-O26	101.25(10)	O3-Mn6-O13	172.71(9)	O5-Mn9-O23	93.24(9)
O15-Mn3-O12	171.49(9)	O2-Mn6-O13	97.01(9)	O4-Mn9-O23	172.25(10)
O15-Mn3-O2	89.51(9)	O3-Mn6-O24	94.56(9)	O18-Mn9-O23	88.64(9)
O12-Mn3-O2	92.32(9)	O2-Mn6-O24	174.10(10)	O5-Mn9-O40	91.76(10)
O15-Mn3-O28	87.16(11)	O13-Mn6-O24	86.55(10)	O4-Mn9-O40	95.48(9)
O12-Mn3-O28	90.18(11)	O3-Mn6-O32	88.61(9)	O18-Mn9-O40	103.06(10)
O2-Mn3-O28	173.49(10)	O2-Mn6-O32	95.61(9)	O23-Mn9-O40	89.77(10)
O15-Mn3-O1	97.22(9)	O13-Mn6-O32	98.63(10)	O5-Mn9-O35	85.59(8)
O12-Mn3-O1	91.02(9)	O24-Mn6-O32	88.48(10)	O4-Mn9-O35	90.71(8)
O2-Mn3-O1	91.82(8)	O3-Mn6-O35	87.53(8)	O18-Mn9-O35	79.89(9)
O28-Mn3-O1	94.15(9)	O2-Mn6-O35	88.95(8)	O23-Mn9-O35	83.72(9)
O15-Mn3-O42	85.86(10)	O13-Mn6-O35	85.34(9)	O40-Mn9-O35	172.82(8)
O12-Mn3-O42	85.94(10)	O24-Mn6-O35	86.65(9)	O17-Mn10-O9A	171.77(10)
O2-Mn3-O42	87.18(9)	O32-Mn6-O35	173.52(9)	O17-Mn10-O4	89.53(9)
O28-Mn3-O42	87.00(9)	O5-Mn7-O37	96.76(10)	O9A-Mn10-O4	92.62(9)
O1-Mn3-O42	176.76(10)	O5-Mn7-O38	169.93(10)	O17-Mn10-O27A	87.66(10)
O2-Mn4-O3	80.94(9)	O37-Mn7-O38	87.55(10)	O9A-Mn10-O27A	89.47(10)
O2-Mn4-O16	95.93(9)	O5-Mn7-O25	89.22(9)	O4-Mn10-O27A	174.23(10)
O3-Mn4-O16	165.26(9)	O37-Mn7-O25	173.31(10)	O17-Mn10-O6A	97.30(9)
O2-Mn4-O20	173.03(10)	O38-Mn7-O25	86.07(10)	O9A-Mn10-O6A	90.55(9)
O3-Mn4-O20	93.63(10)	O5-Mn7-O41	94.81(9)	O4-Mn10-O6A	92.35(8)
O16-Mn4-O20	88.23(9)	O37-Mn7-O41	86.14(11)	O27A-Mn10-O6A	93.01(9)
O2-Mn4-O30	96.64(9)	O38-Mn7-O41	94.56(10)	O17-Mn10-O7	86.93(10)
O3-Mn4-O30	92.24(9)	O25-Mn7-O41	96.36(10)	O9A-Mn10-O7	85.25(10)
O16-Mn4-O30	102.44(9)	O5-Mn7-O21	88.00(8)	O4-Mn10-O7	87.09(9)
O20-Mn4-O30	87.89(10)	O37-Mn7-O21	92.94(10)	O27A-Mn10-O7	87.72(9)
O2-Mn4-O34	91.42(8)	O38-Mn7-O21	82.67(9)	O6A-Mn10-O7	175.73(10)
O3-Mn4-O34	85.65(8)	O25-Mn7-O21	84.25(9)		

^a Symmetry transformations used to generate equivalent atoms: A: $-x, y, -z + 3/2$.

Table S2. Hydrogen Bond Distances (Å) and Bond Angles (°) for compounds **2** and **3**

Complex	D-H...A	d(D-H)	d(H...A)	<DHA	d(D...A)	Symmetry code
2	O9-H9B...O4&	0.853	2.017	159.97	2.834	$-y, x-y, z$
	O10-H10A...O7#	0.820	2.017	144.44	2.727	$-x+y-1, -x, z$
3	O2-H2A...O3&	0.820	1.774	172.64	2.590	$-x+1/2, -y+1, -z+1$
	O7-H7A...O5	0.820	1.777	163.45	2.573	
	O6-H6A...O3	0.820	1.906	160.30	2.693	

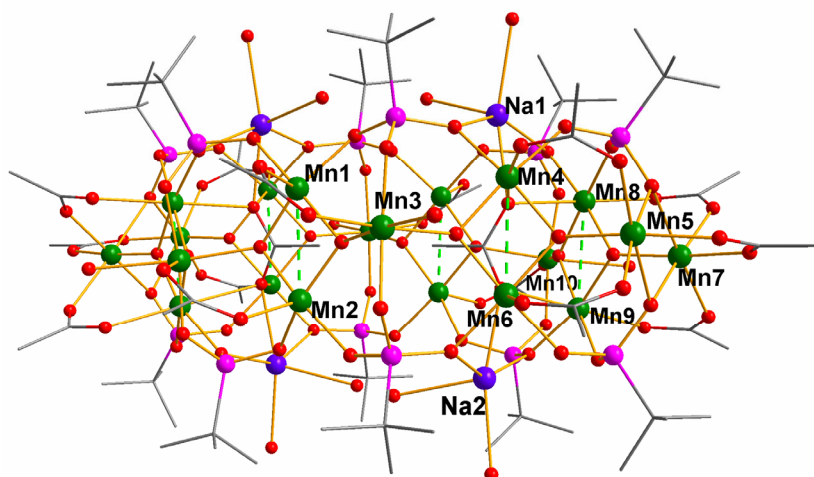


Fig. S1. The structure of compound **1** along c axis. Color code: green, Mn; orange, Na; purple, P; red, O; gray, C. Hydrogen atoms have been omitted for clarity.

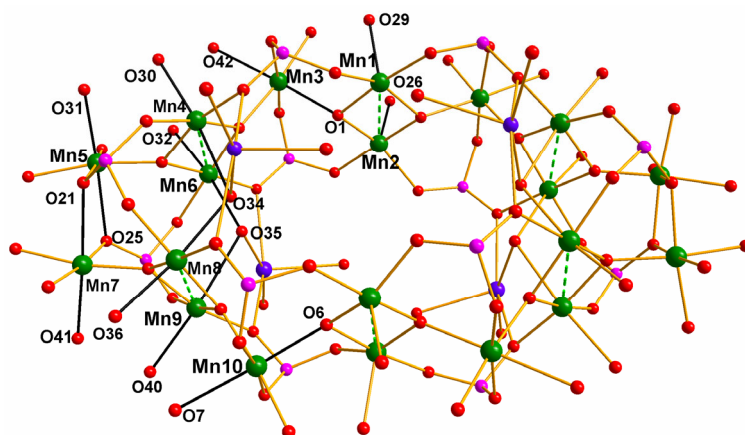


Fig. S2. The structure of compound **1**. The Jahn-Teller elongated axes of the nine Mn(III) ions are highlighted in black. Color code: green, Mn; pink, Na; purple, P; red, O. Hydrogen atoms and carbon atoms have been omitted for clarity.

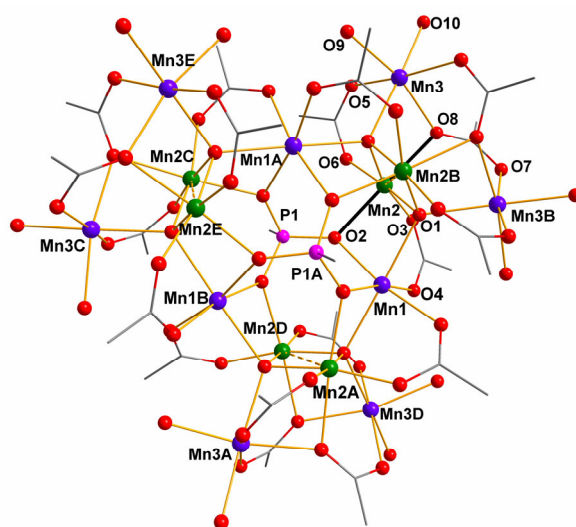


Fig. S3. The structure of compound **2**. The Jahn-Teller elongated axes of the Mn(III) ions are highlighted in black. Color code: Mn^{III}: green; Mn^{II}: pink; purple, P; red, O. Hydrogen atoms and carbon atoms have been omitted for clarity.

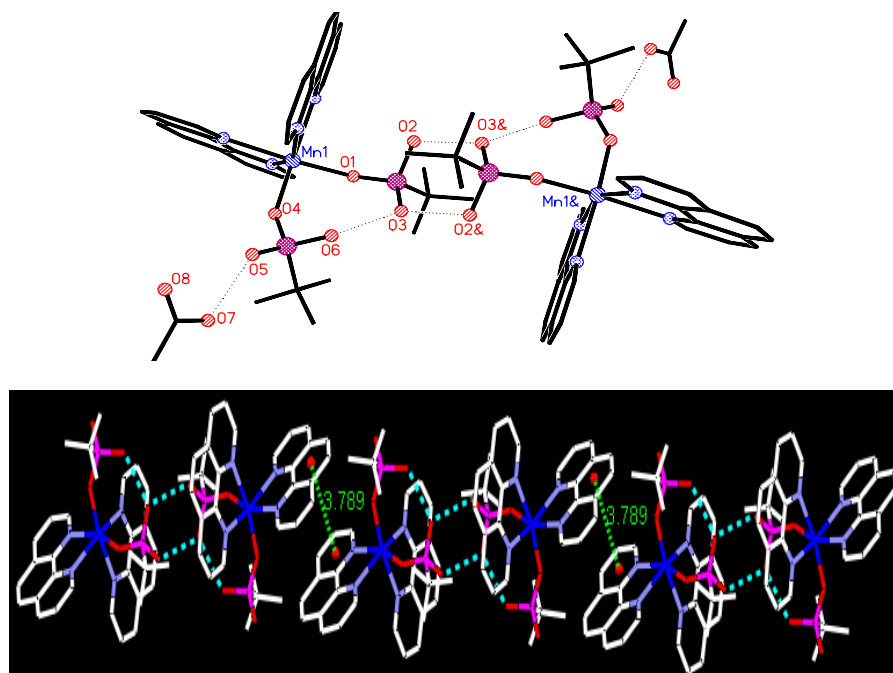


Fig. S4 The view of the hydrogen-bonded dinuclear complex for **3** (top) and the one-dimensional packing diagram for compound **3** (bottom). Dotted lines show hydrogen bonding interactions

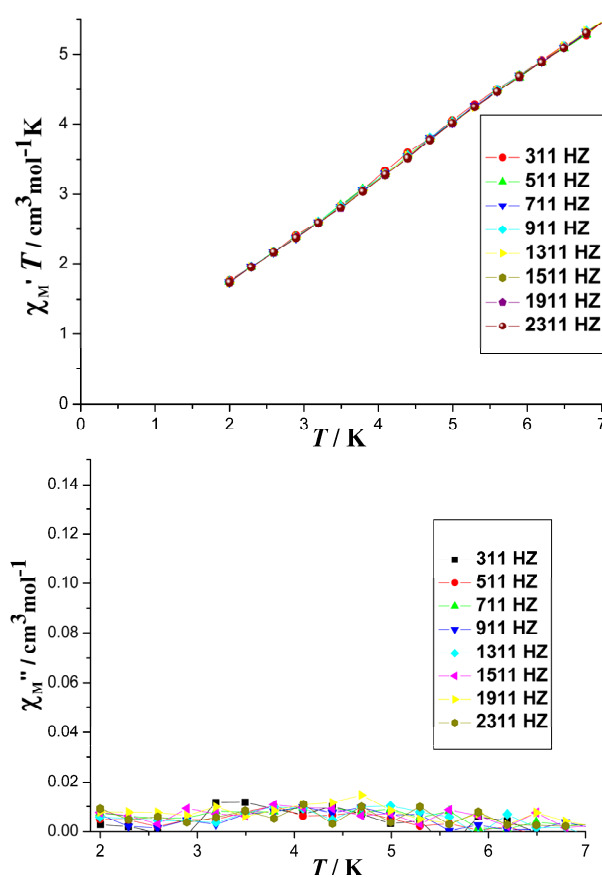


Fig. S5. In-phase ($\chi'_M T$) (top) and out-phase (χ''_M) (bottom) AC susceptibility versus T for complex **2** measured in a 3.0 G AC field oscillating at the indicated frequencies.