Supporting Information

$KNa_3Mn_7(PO_4)_6$: 2D Spin Frustrated Magnetic Material with a Diamond-like Chain Structure

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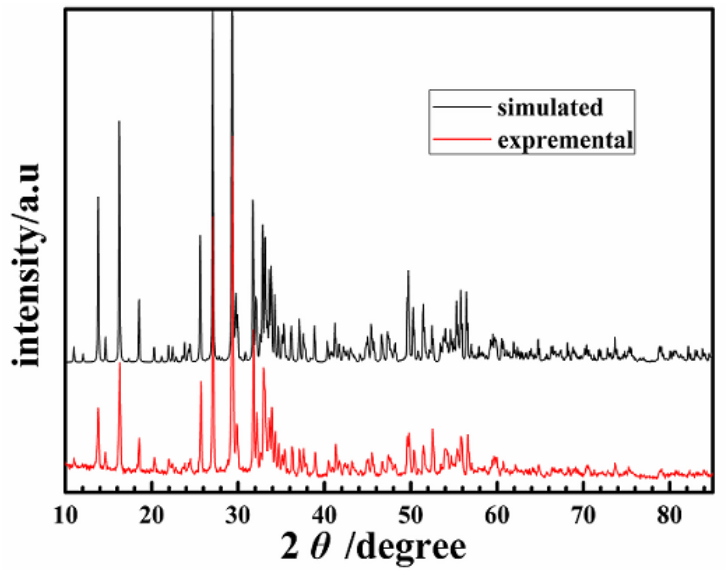

Figure S1. Simulated (black line) and experimental (red line) powder X-ray (Cu Kα) diffraction patterns of $KNa_3Mn_7(PO_4)_6$.

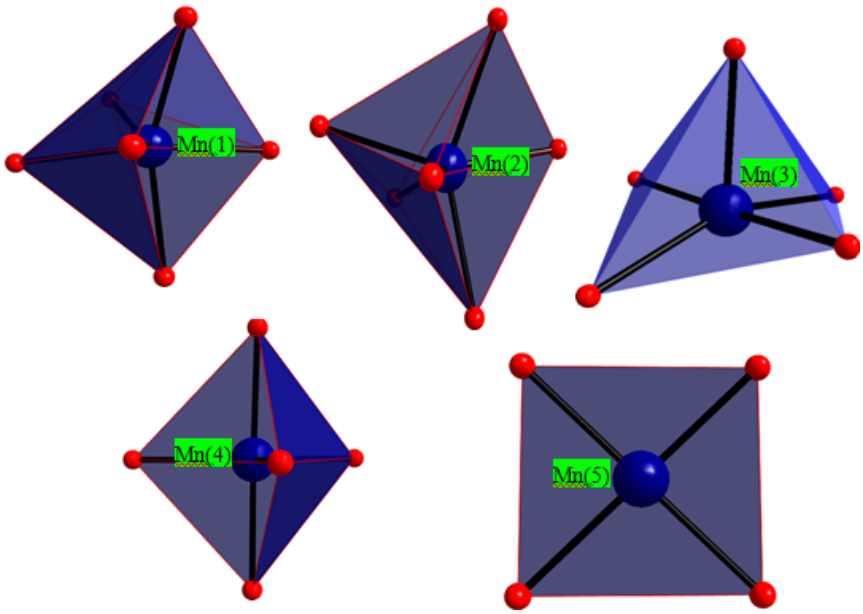

Figure S2. Different polyhedra built by Mn atoms.

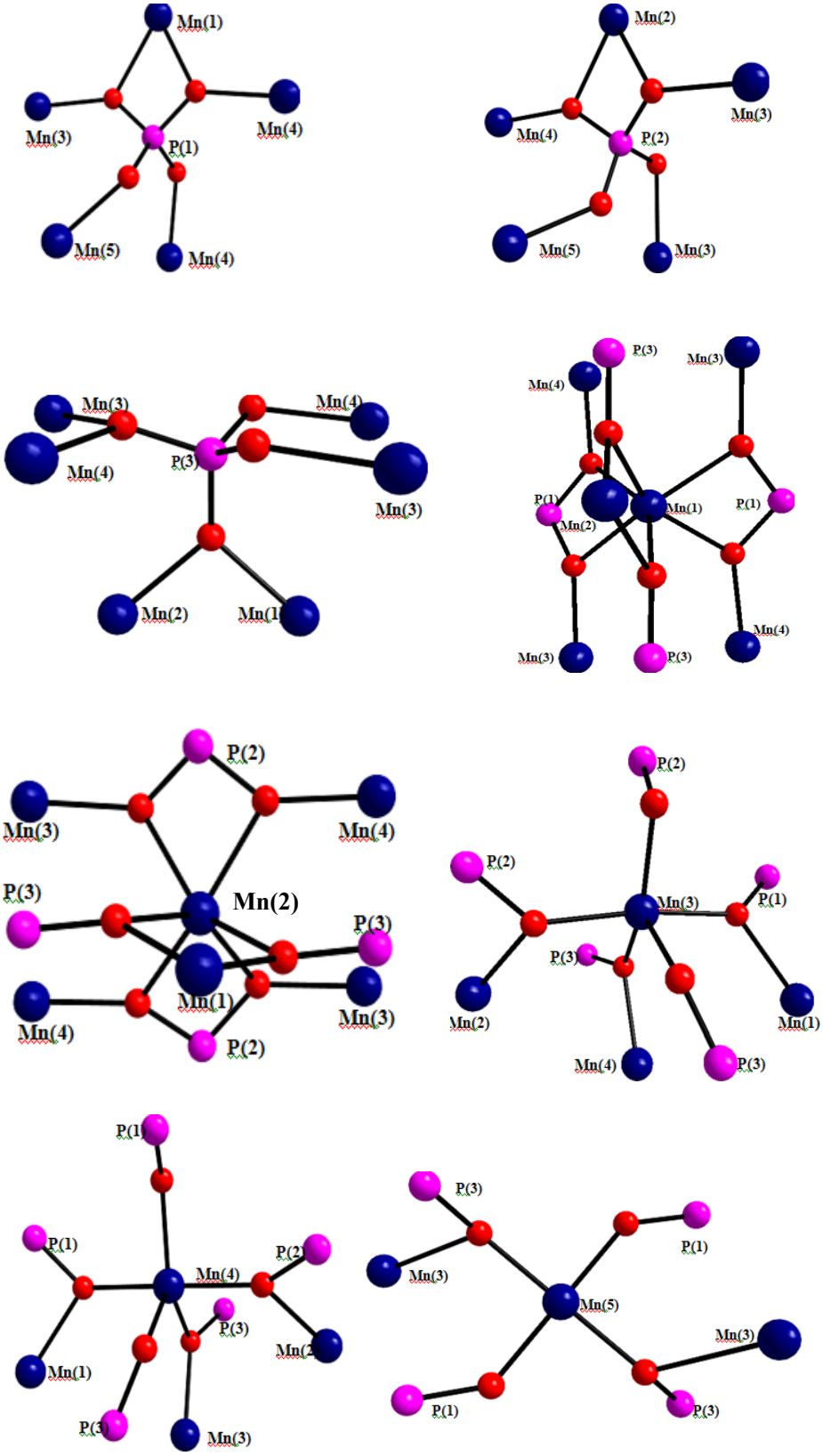

Figure S3. Oxygen-coordination environment of Mn and P atoms.

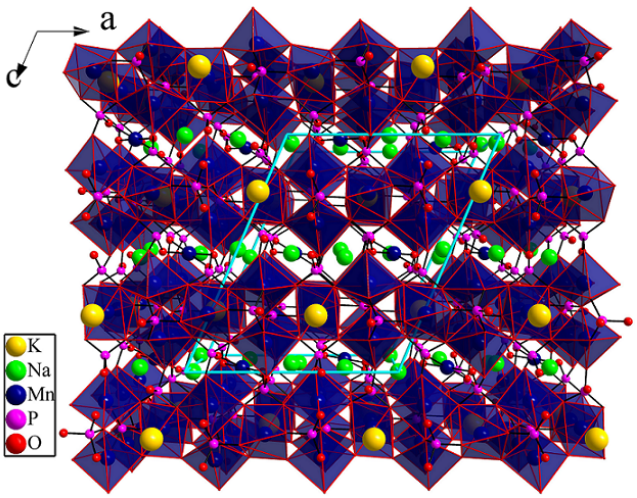

Figure S4. Perspective view of $KNa_3Mn_7(PO_4)_6$. The transparent blue polyhedra respect the pseudo-two-dimensional slabs.

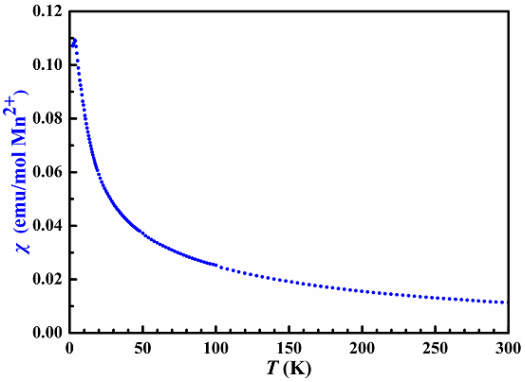

Figure S5. Dc magnetic susceptibility measured at 0.1 T for $KNa_3Mn_7(PO_4)_6$.

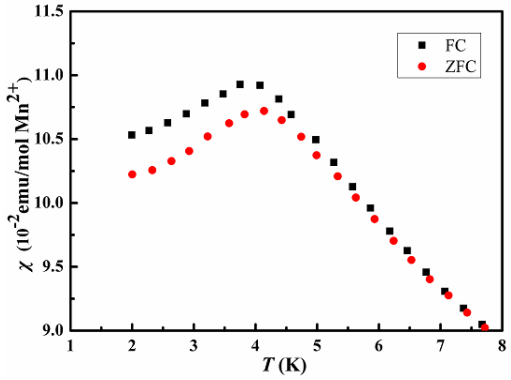

Figure S6. The low-temperature susceptibility for $KNa_3Mn_7(PO_4)_6$ measured at 500 Oe with field-cooling (FC) and zero-field-cooling (ZFC) regimes.

Table S1. Crystal data and structure refinement of $KNa_3Mn_7(PO_4)_6$.

	$KNa_3Mn_7(PO_4)_6$
space group	*C 2/c*
a/ Å	13.165(8)
b/ Å	10.907(6)
c/ Å	15.960(1)
β/°	113.243(9)
V/ $Å^3$	2106(2)
Z	4
$D_{calcd}/g.cm^{-3}$	3.351
μ(Mo-Ka)/mm^{-1}	6.139
GOF on F^2	0.932
R1, wR2[I>2σ (I)][a]	0.0517, 0.0961
R1, wR2(all data)	0.0945, 0.1181

[a] $R1 = \sum||Fo| - |Fc||/\sum|Fo|$, $wR2 = \{\sum w[(Fo)^2 - (Fc)^2]^2/\sum w[(Fo)^2]^2\}^{1/2}$

Table S2. Atomic coordinates and equivalent isotropic displacement parameters of $KNa_3Mn_7(PO_4)_6$.

	x	y	z	U(eq)
K	-5000	2622(3)	-2500	80(1)
Na(1)	-2500	2500	-5000	46(2)
Na(2)	-187(3)	2395(3)	-173(3)	39(1)
Mn(1)	0	1212(1)	-2500	12(1)
Mn(2)	0	4176(1)	-2500	16(1)
Mn(3)	-3176(1)	394(1)	-3746(1)	13(1)
Mn(4)	1892(1)	-6(1)	-3599(1)	13(1)
Mn(5)	-2500	-2500	-5000	61(1)
P(1)	-878(1)	-3(2)	-4206(1)	11(1)
P(2)	-4065(1)	-8(2)	-5714(1)	12(1)
P(3)	-2113(2)	2707(2)	-2298(1)	13(1)
O(1)	-1546(3)	597(4)	-3703(3)	15(1)
O(2)	339(3)	128(4)	-3509(3)	15(1)
O(3)	-924(3)	2678(4)	-2260(3)	16(1)
O(4)	-3459(4)	212(4)	-6354(3)	19(1)
O(5)	-2112(4)	2008(4)	-1465(4)	21(1)
O(6)	-1081(4)	717(4)	-5065(3)	20(1)
O(7)	-2457(3)	4063(4)	-2274(3)	13(1)
O(8)	-3960(4)	1114(4)	-5121(3)	20(1)
O(9)	-3604(4)	-1091(4)	-5068(3)	19(1)
O(10)	-1131(4)	-1359(4)	-4406(4)	21(1)
O(11)	-2949(4)	2163(5)	-3183(4)	29(2)
O(12)	-4732(3)	238(4)	-3605(3)	20(1)

Table S3. Selected bond lengths and angles of $KNa_3Mn_7(PO_4)_6$.

K-O(10)#1	3.022(6)	K-O(12)#4	3.239(6)	K-O(2)#1	3.291(6)
K-O(11)#3	3.325(5)	Na(1)-O(8)#5	2.393(5)	Na(1)-O(6)#3	2.726(5)
Na(1)-O(1)#5	2.850(5)	Na(2)-O(8)#6	2.269(5)	Na(2)-O(10)#7	2.350(6)
Na(2)-O(6)#8	2.404(6)	Na(2)-O(9)#1	2.427(6)	Na(2)-O(3)#3	3.094(7)
Mn(1)-O(3)	2.133(5)	Mn(1)-O(3)#8	2.133(5)	Mn(1)-O(2)#8	2.181(5)
Mn(1)-O(2)	2.181(5)	Mn(1)-O(1)	2.280(4)	Mn(1)-O(1)#3	2.280(4)
Mn(2)-O(3)#3	2.159(5)	Mn(2)-O(3)	2.159(5)	Mn(2)-O(4)#6	2.232(4)
Mn(2)-O(4)#5	2.232(4)	Mn(2)-O(12)#1	2.252(5)	Mn(2)-O(12)#9	2.252(5)
Mn(3)-O(7)#10	2.094(5)	Mn(3)-O(11)#3	2.099(5)	Mn(3)-O(1)	2.130(5)
Mn(3)-O(12)#3	2.154(5)	Mn(3)-O(8)	2.170(5)	Mn(4)-O(4)#11	2.105(5)
Mn(4)-O(2)	2.111(5)	Mn(4)-O(6)#11	2.119(5)	Mn(4)-O(7)#12	2.192(5)
Mn(4)-O(5)#8	2.213(5)	Mn(5)-O(10)#13	2.085(4)	Mn(5)-O(10)	2.085(4)
Mn(5)-O(9)#13	2.088(5)	Mn(5)-O(9)	2.088(5)	P(1)-O(6)	1.510(5)
P(1)-O(10)	1.522(5)	P(1)-O(1)	1.550(5)	P(1)-O(2)	1.554(4)
P(2)-O(8)#3	1.520(5)	P(2)-O(9)	1.528(5)	P(2)-O(4)	1.543(5)
P(2)-O(12)#15	1.547(5)	P(3)-O(11)	1.527(5)	P(3)-O(5)	1.532(6)
P(3)-O(3)	1.543(5)	P(3)-O(7)	1.551(5)	O(3)-Mn(1)-O(3)	82.9(3)
O(3)#3-Mn(1)-O(2)	88.66(19)	O(3)-Mn(1)-O(2)	146.74(8)	O(3)-Mn(1)-O(2)	88.66(9)
O(2)#8-Mn(1)-O(2)	114.3(3)	O(3)#3-Mn(1)-O(1)	89.38(17)	O(3)-Mn(1)-O(1)	116.91(8)
O(2)#8-Mn(1)-O(1)	95.01(17)	O(2)-Mn(1)-O(1)	66.00(16)	O(2)-Mn(1)-O(1)	95.01(7)
O(2)-Mn(1)-O(1)#3	66.00(16)	O(3)#8-Mn(1)-O(1)#8	89.38(17)	O(2)-Mn(1)-O(1)	95.01(7)
O(1)-Mn(1)-O(1)#8	145.7(2)	O(3)-Mn(2)-O(3)#8	81.7(2)	O(3)-Mn(2)-O(4)	118.34(9)
O(3)-Mn(2)-O(4)#5	88.75(17)	O(4)#6-Mn(2)-O(4)#5	145.2(3)	O(3)-Mn(2)-O(12)	88.65(9)
O(3)#8-Mn(2)-O(12)	143.30(8)	O(4)#6-Mn(2)-O(12)#1	64.97(17)	O(4)-Mn(2)-O(12)	96.61(8)
O(3)#8-Mn(2)-O(12)	88.65(19)	O(4)#6-Mn(2)-O(12)#9	96.61(18)	O(12)-Mn(2)-O(2)	118.1(3)
O(7)-Mn(3)-O(11)#3	111.0(2)	O(11)-Mn(3)-O(1)#3	85.37(18)	O(7)-Mn(3)-O(1)	87.72(8)
O(7)-Mn(3)-O(12)#3	88.09(18)	O(11)-Mn(3)-O(12)#3	90.50(19)	O(1)-Mn(3)-O(12)	172.6(9)
O(7)-Mn(3)-O(12)	88.09(18)	O(7)#10-Mn(3)-O(8)#3	157.2(19)	O(11)-Mn(3)-O(8)	91.7(2)
O(12)-Mn(3)-O(8)#3	92.37(18)	O(1)-Mn(3)-O(8)	93.84(19)	O(7)-Mn(3)-O(9)	95.36(8)
O(11)#3-Mn(3)-O(9)	152.7(2)	O(1)-Mn(3)-O(9)	89.08(17)	O(12)-Mn(3)-O(9)	97.4(18)
O(8)-Mn(3)-O(9)	61.98(17)	O(4)#11-Mn(4)-O(2)	177.28(9)	O(4)-Mn(4)-O(6)	92.1(19)
O(2)-Mn(4)-O(6)#11	88.66(19)	O(2)-Mn(4)-O(7)#12	89.26(18)	O(6)-Mn(4)-O(7)	130.6(2)
O(4)-Mn(4)-O(5)#8	89.75(18)	O(2)-Mn(4)-O(5)#8	92.32(18)	O(6)-Mn(4)-O(5)	114.50(19)
O(10)-Mn(5)-O(10)	180.0(2)	O(10)-Mn(5)-O(9)#13	92.48(19)	O(10)-Mn(5)-O(9)	87.5(19)
O(9)#13-Mn(5)-O(9)	180.00(1)	O(10)-Mn(5)-O(5)#10	98.83(18)	O(9)-Mn(5)-O(5)	100.28(18)
O(9)-Mn(5)-O(5)#10	79.72(18)	O(10)#13-Mn(5)-O(5)	98.83(18)	O(10)-Mn(5)-O(5)	81.7(18)
O(9)#13-Mn(5)-O(5)	79.72(18)	O(6)-P(1)-O(10)	111.6(3)	O(6)#3-P(1)-O(1)	108.5(3)
O(6)-P(1)-O(1)#3	108.5(3)	O(10)-P(1)-O(1)#3	113.3(3)	O(6)-P(1)-O(2)	111.4(3)
O(1)-P(1)-O(2)	103.1(3)	O(8)-P(2)-O(9)	106.7(3)	O(8)-P(2)-O(4)	110.1(3)
O(9)-P(2)-O(4)	113.3(3)	O(8)-P(2)-O(12)#15	112.6(3)	O(9)-P(2)-O(12)	111.9(3)
O(4)-P(2)-O(12)#15	102.4(3)	O(11)-P(3)-O(5)	111.3(3)	O(11)-P(3)-O(3)#3	112.2(3)
O(5)-P(3)-O(3)#3	107.6(3)	O(11)-P(3)-O(7)	106.4(3)	O(5)-P(3)-O(7)	110.7(3)

O(3)-P(3)-O(7)	108.6(3)

Symmetry transformations used to generate equivalent atoms: #1 -x-1/2,y+1/2,-z-1/2; #2 x-1/2,y+1/2,z; #3 x,y,z; #4 -x-1,y,-z-1/2; #5 -x-1/2,-y+1/2,-z-1; #6 x+1/2,-y+1/2,z+1/2; #7 x,-y,z+1/2; #8 -x,y,-z-1/2; #9 x+1/2,y+1/2,z #10 -x-1/2,y-1/2,-z-1/2; #11 -x,-y,-z-1; #12 x+1/2,y-1/2,z; #13 -x-1/2,-y-1/2,-z-1; #14 x,-y,z-1/2; #15 -x-1,-y,-z-1; #16 x-1/2,y-1/2,z.