Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Synthesis, Characterization, and Mechanism Analysis of *S*=2 Quasi-One-Dimensional Ferromagnetic Semiconductor $Pb_2Mn(VO_4)_2(OH)$

Suyun Zhang,[a] Hongping Xiang,*[a] Wenbin Guo,[a] Yingying Tang[a,b], Meiyan Cui[a,b] and Zhangzhen He*[a]

[a]State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, P. R. China.

[b]University of Chinese Academy of Sciences, Beijing, 100049, P. R. China.

E-mail: xianghp@fjirsm.ac.cn, hcz1988@hotmail.com or hezz@fjirsm.ac.cn.

Tel/Fax: +86-591-63173255.

Table S1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for $Pb_2Mn(VO_4)_2(OH)$.

atom	x	y	z	U(eq)
Pb(1)	2702(1)	2500	7529(1)	19(1)
Pb(2)	6695(1)	2500	15934(1)	26(1)
Mn(1)	0	0	0	8(1)
V(1)	407(2)	2500	3359(2)	9(1)
V(2)	4495(2)	2500	11759(2)	9(1)
O(1)	-1701(9)	2500	-752(9)	10(2)
O(2)	-116(7)	130(9)	2160(7)	16(1)
O(3)	-780(11)	2500	4597(10)	21(2)
O(4)	2676(10)	2500	4540(10)	21(2)
O(5)	5590(10)	2500	10426(11)	26(2)
O(6)	2113(9)	2500	10588(9)	12(2)
O(7)	5116(7)	235(9)	12989(7)	14(1)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table S2.Selected bond length (Å) and bond angles (°) in$Pb_2Mn(VO_4)_2(OH)$.

Pb(1)-O(7)#1	2.531(5)	Pb(1)-O(7)#2	2.531(5)
Pb(1)-O(4)	2.617(8)	Pb(1)-O(2)#3	2.652(6)
Pb(1)-O(2)#4	2.652(6)	Pb(1)-O(5)	2.701(8)
Pb(2)-O(7)#5	2.573(6)	Pb(2)-O(7)#6	2.573(5)
Pb(2)-O(3)#7	2.604(8)	Pb(2)-O(1)#8	2.718(8)
Pb(2)-O(7)	2.800(2)	Pb(2)-O(7)#9	2.800(2)
Mn-O(2)#9	1.932(6)	Mn-O(2)	1.932(6)
Mn-O(1)	1.973(4)	Mn-O(1)#10	1.973(4)
Mn-O(6)#3	2.160(5)	Mn-O(6)#11	2.160(5)
Mn-Mn#12	3.084(3)	Mn-Mn#13	3.084(3)
V(1)-O(3)	1.651(8)	V(1)-O(4)	1.673(7)
V(1)-O(2)	1.761(6)	V(1)-O(2)#9	1.761(6)
V(2)-O(5)	1.670(8)	V(2)-O(7)#9	1.724(6)
V(2)-O(7)	1.724(6)	V(2)-O(6)	1.742(7)
Mn#12-O(1)-Mn	102.8(3)	Mn#14-O(6)-Mn#4	91.1(3)

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

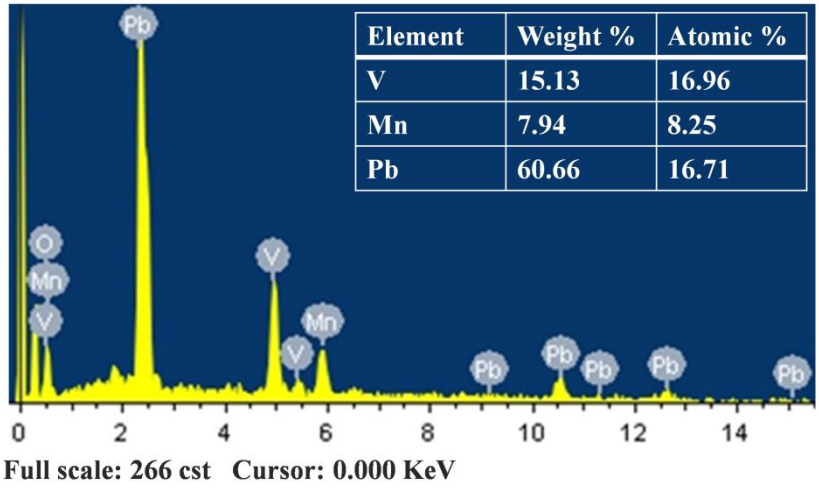

Figure S1. The EDS analysis of $Pb_2Mn(VO_4)_2(OH)$ confirms the Pb/Mn/V/O elemental composition.

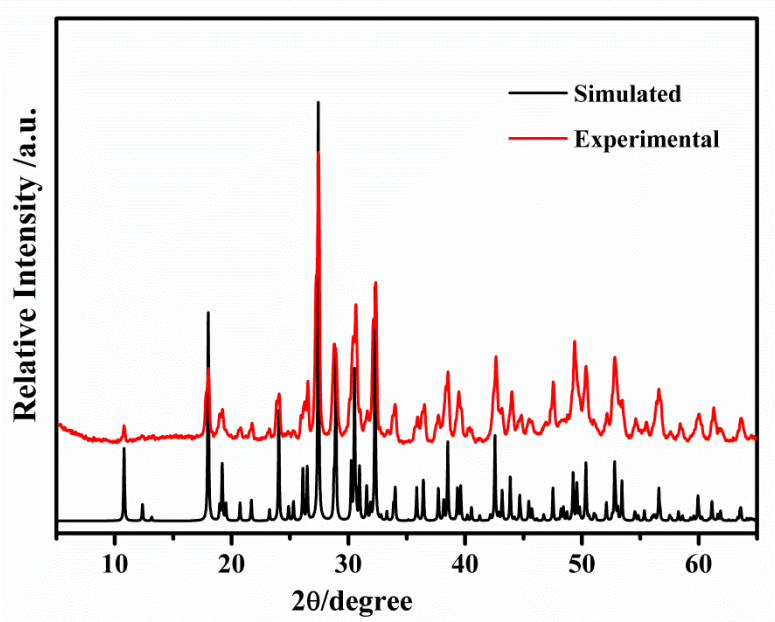

Figure S2. Experimental and calculated powder X-ray diffraction patterns of $Pb_2Mn(VO_4)_2(OH)$.

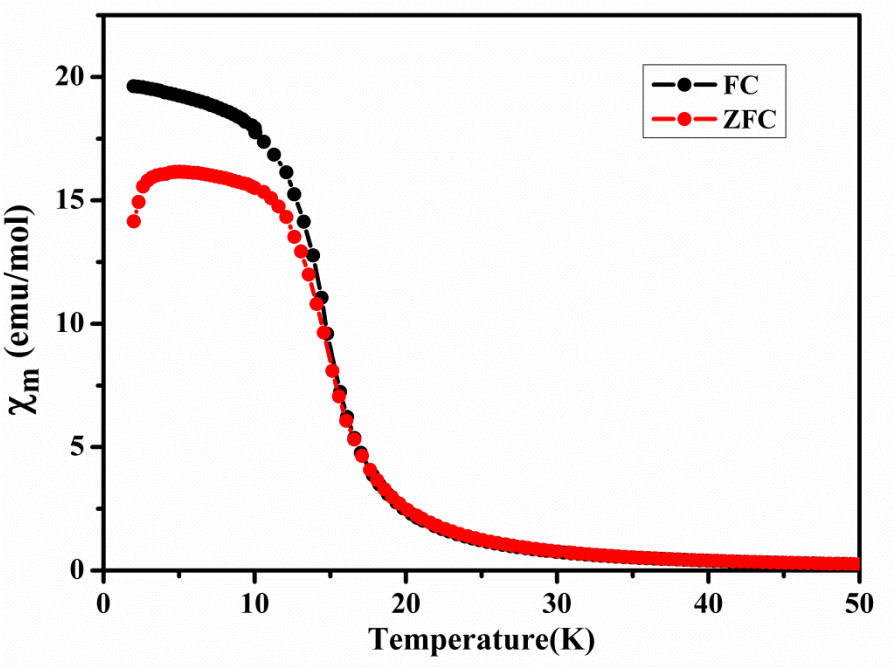

Figure S3. Field cooled (*FC*) and zero-field cooled (*ZFC*) plots of χ_m *vs. T* at *H* = 500 Oe.

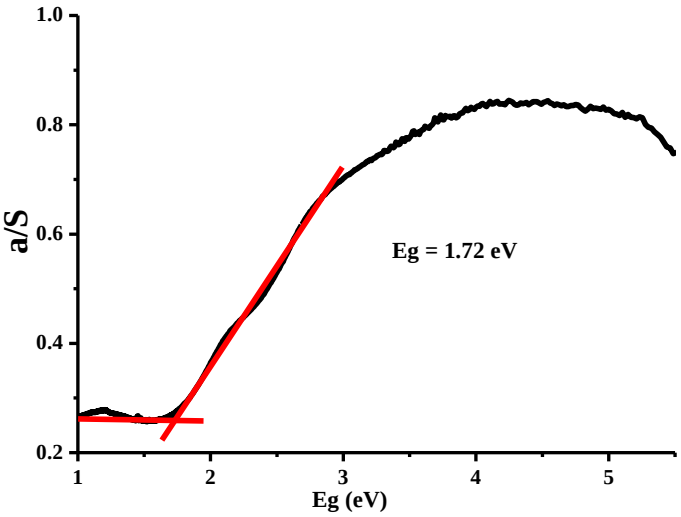

Figure S4. Diffuse reflectance spectrum of $Pb_2Mn(VO_4)_2(OH)$.

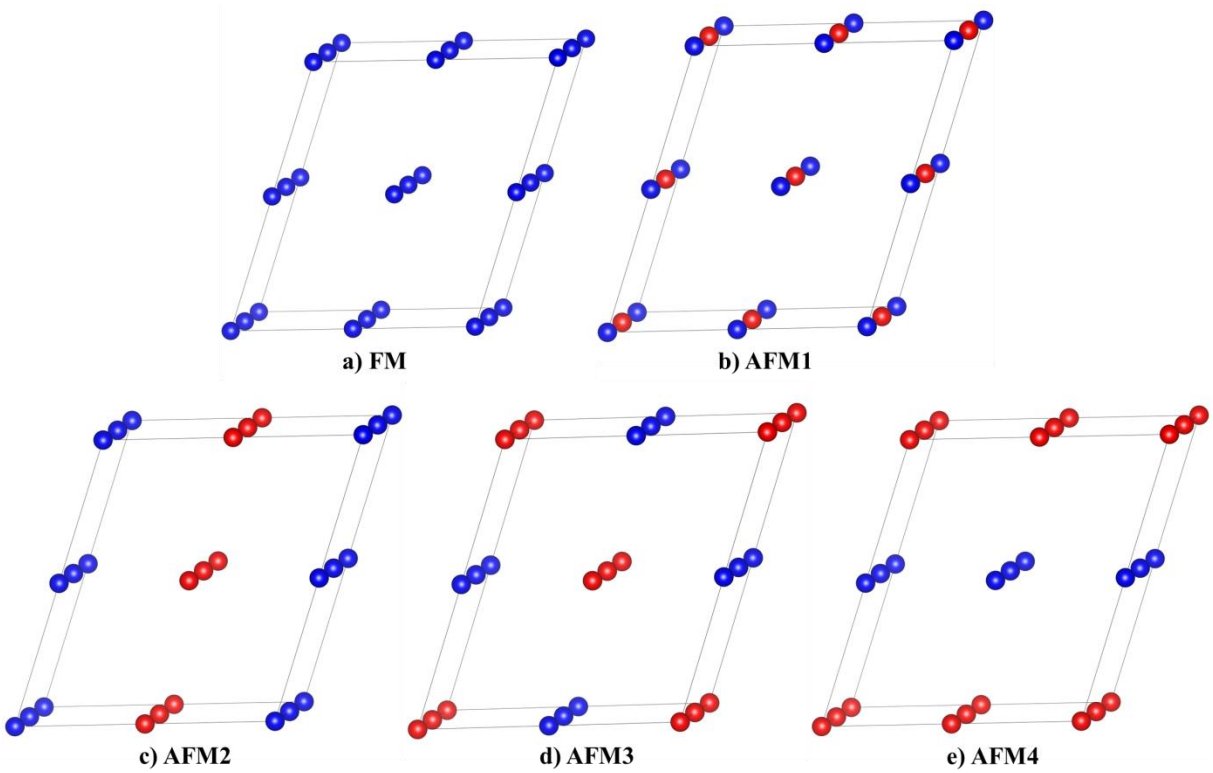

Figure S5. Five magnetic structures are designed as (a) FM, (b) AFM1, (c) AFM2, (d) AFM3, and (e) AFM4, to figure out the magnetic ground state of $Pb_2Mn(VO_4)_2(OH)$. Blue and red spheres indicate different orientations of the spin moments residing on the Mn^{3+} ions, which are the only atoms shown.