Supporting Information

$BaMn_9^{II}(VO_4)_6(OH)_2$: a homospin ferrimagnet with a broken spinel-lattice of B-site

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Figure S1. Energy-dispersive X-ray spectroscopy of $BaMn_9(VO_4)_6(OH)_2$.

Figure S2. Simulated and experimental XRD powder patterns for $BaMn_9(VO_4)_6(OH)_2$.

Table S1. Atomic coordinates and equivalent isotropic displacement parameters for $BaMn_9(VO_4)_6(OH)_2$.

Table S2. Bond lengths [A] and angles [deg] for $BaMn_9(VO_4)_6(OH)_2$.

Table S3. Anisotropic displacement parameters for $BaMn_9(VO_4)_6(OH)_2$.

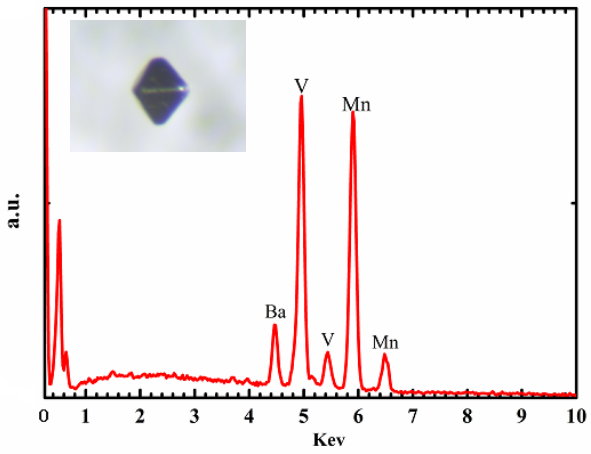

Figure S1. Energy-dispersive X-ray spectroscopy of $BaMn_9(VO_4)_6(OH)_2$.

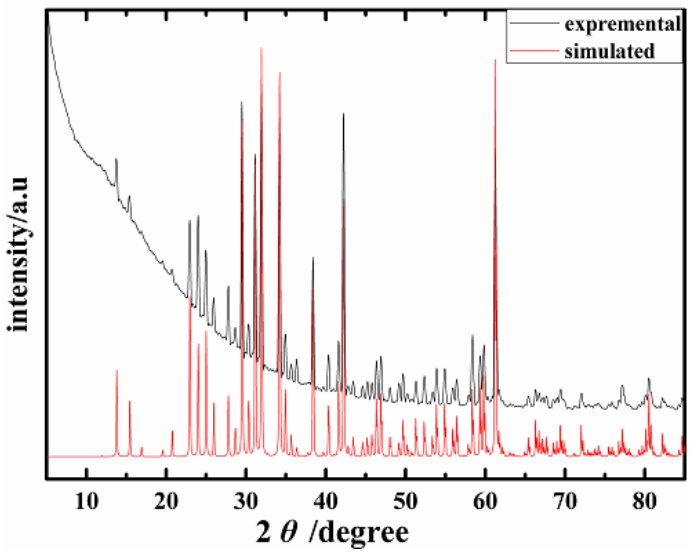

Figure S2. Simulated and experimental XRD powder patterns for $BaMn_9(VO_4)_6(OH)_2$.

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for $BaMn_9(VO_4)_6(OH)_2$. U(eq) is defined as one third of the trace of the orthogonalized

Uij tensor.

atom	x	y	z	U(eq)
Ba	0	-5000	-5000	13(1)
Mn(1)	3247(1)	-3247(1)	-8247(1)	9(1)
Mn(2)	5000	0	-10000	8(1)
Mn(3)	4948(1)	-1598(1)	-8065(1)	11(1)
V	4076(1)	-2541(1)	-5729(1)	7(1)
O(1)	4799(2)	-1705(2)	-6423(2)	12(1)
O(2)	4913(2)	-3305(2)	-8212(2)	11(1)
O(3)	6554(2)	-1554(2)	-8446(2)	11(1)
O(4)	4931(2)	-1690(2)	-9969(2)	9(1)
O(5)	3277(2)	-1567(2)	-8330(2)	10(1)

Table 2. Bond lengths [A] and angles [deg] for $BaMn_9(VO_4)_6(OH)_2$.

Mn(1)-O(2)#1	2.142(2)	Mn(1)-O(5)	2.160(2)
Mn(2)-O(4)	2.172(2)	Mn(3)-O(3)	2.1199(18)
Mn(3)-O(1)	2.121(2)	Mn(3)-O(4)#6	2.166(2)
Mn(3)-O(5)	2.172(2)	Mn(3)-O(2)	2.201(2)
Mn(3)-O(4)	2.447(2)	V-O(1)	1.675(3)
V-O(5)#1	1.722(3)	V-O(2)#8	1.735(3)
V-O(4)#9	1.770(2)	O(2)#1-Mn(1)-O(2)	89.19(10)
O(2)#1-Mn(1)-O(5)#2	85.93(9)	O(2)-Mn(1)-O(5)#2	175.12(9)
O(2)#2-Mn(1)-O(5)#2	91.03(9)	O(5)#2-Mn(1)-O(5)#1	93.85(9)
O(4)#3-Mn(2)-O(4)#4	88.67(8)	O(4)#3-Mn(2)-O(4)	91.33(8)
O(4)#3-Mn(2)-O(4)#7	180.00(12)	O(3)-Mn(3)-O(1)	108.60(11)
O(3)-Mn(3)-O(4)#6	83.81(11)	O(1)-Mn(3)-O(4)#6	102.29(9)
O(3)-Mn(3)-O(5)	157.47(11)	O(1)-Mn(3)-O(5)	93.90(9)
O(4)#6-Mn(3)-O(5)	90.45(9)	O(3)-Mn(3)-O(2)	91.49(9)
O(1)-Mn(3)-O(2)	91.10(9)	O(4)#6-Mn(3)-O(2)	166.59(9)
O(5)-Mn(3)-O(2)	89.14(9)	O(3)-Mn(3)-O(4)	77.25(9)
O(1)-Mn(3)-O(4)	171.37(10)	O(4)#6-Mn(3)-O(4)	84.43(12)
O(5)-Mn(3)-O(4)	80.52(8)	O(2)-Mn(3)-O(4)	82.28(9)
O(1)-V-O(5)#1	109.11(12)	O(1)-V-O(2)#8	106.23(12)
O(5)#1-V-O(2)#8	111.44(11)	O(1)-V-O(4)#9	107.92(11)
O(5)#1-V-O(4)#9	112.51(11)	O(2)#8-V-O(4)#9	109.38(12)

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

Table 3. Anisotropic displacement parameters (A^2 x 10^3) for $BaMn_9(VO_4)_6(OH)_2$. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a*

b* U12].

atom	U11	U22	U33	U23	U13	U12
Ba	13(1)	13(1)	13(1)	-3(1)	3(1)	-3(1)
Mn(1)	9(1)	9(1)	9(1)	0(1)	0(1)	0(1)
Mn(2)	8(1)	8(1)	8(1)	0(1)	0(1)	0(1)
Mn(3)	10(1)	9(1)	13(1)	2(1)	1(1)	-1(1)
V	7(1)	7(1)	6(1)	-1(1)	0(1)	0(1)
O(1)	13(1)	13(1)	11(1)	1(1)	1(1)	-1(1)
O(2)	10(1)	10(1)	13(1)	3(1)	0(1)	0(1)
O(3)	11(1)	11(1)	11(1)	-1(1)	1(1)	-1(1)
O(4)	8(1)	9(1)	11(1)	2(1)	-1(1)	-1(1)
O(5)	10(1)	8(1)	12(1)	1(1)	0(1)	1(1)