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Supplementary Information

Cation, magnetic, and charge ordering in $MnFe_3O_5$

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Table 1. Lattice parameters, atomic coordinates, and isotropic thermal displacements from neutron refinements in *Cmcm* space group of $MnFe_3O_5$ at 5 K. Estimated standard deviations for independent variables are shown in parentheses. (R_{wp} = 12.9 % and R_p = 12.6 %)

a /Å		*b* /Å		*c* /Å	Volume /Å^3	
2.9017(3)		9.8928(7)		12.6083(11)	361.94(5)	
Atom	Site	*x*	*y*	*z*	Occupancy[a]	B_{iso} /Å^2
Fe1	8*f*	½	0.2345(4)	0.1131(3)	1	2.42(12)
Fe2/Mn2	4*a*	0	0	0	0.995(4)/0.005(4)	2.42(12)
Mn/Fe	4*c*	0	0.4812(16)	¼	0.937(4)/0.063(4)	2.42(12)
O1	4*c*	½	0.3188(9)	¼	1	3.00(15)
O2	8*f*	0	0.3469(6)	0.0473(7)	1	3.00(15)
O3	8*f*	0	0.0992(6)	0.1410(7)	1	3.00(15)

[a] Variable occupancies were refined against 400 K neutron data and were fixed in lower temperature refinements.

Table 2. Metal-oxygen bond lengths and metal-metal distances , with mean values < > shown for $MnFe_3O_5$ at 5 K.

Bond	Distance (Å)	Bond	Distance (Å)
Mn-O1 (x 2)	2.165(14)	Fe2-O2 (x 4)	2.180(5)
Mn-O3 (x 4)	2.314(11)	Fe2-O3 (x 2)	2.031(9)
<Mn-O>	2.264(5)	<Fe2-O>	2.130(3)
Fe1-O1	1.917(6)	Fe1-Fe1,	2.9015(3)
Fe1-O2	2.177(10)	Fe2-Fe2,Mn-Mn	
Fe1-O2 (x 2)	2.007(6)	Fe1-Fe2(x 2)	2.989(4)
Fe1-O3 (x 2)	2.005(6)	Fe1-Fe2(x 4)	3.085(4)
<Fe1-O>	2.020(3)		

Table 3. Irreducible representations (IrReps) and basis vectors (BV) for Fe1, Fe2 and Mn spin order in $MnFe_3O_5$ at 5 K, with propagation vector (0 0 0). The magnetically independent atoms are Fe1 at (½, 0.2345, 0.1131), Fe2 at (0, 0, 0) and Mn1 at (0, 0.4812, ¼). The symmetry related positions are generated by the operators 1: (x, y, z), 2: (-x+½, -y+½, z+½), 3: (-x+1, y, -z+½), 4: (x-½, -y+½, -z+1), 5: (-x, -y, z+½) and 6: (-x, -y+1, z+½). The structure was solved using $\Gamma_2\psi_3$, $\Gamma_6\psi_8$ and $\Gamma_6\psi_9$ for Fe1 and Fe2, and $\Gamma_3\psi_4$, $\Gamma_6\psi_8$ and $\Gamma_7\psi_{11}$ for Mn1.

IrReps	Γ_1		Γ_2	Γ_3	Γ_4		Γ_5	Γ_6		Γ_7		Γ_8
BV	ψ_1	ψ_2	ψ_3	ψ_4	ψ_5	ψ_6	ψ_7	ψ_8	ψ_9	ψ_{10}	ψ_{11}	ψ_{12}
Atoms	m_y	m_z	m_x	m_x	m_y	m_z	m_x	m_y	m_z	m_y	m_z	m_x
Fe1_1	+	+	+	+	+	+	+	+	+	+	+	+
Fe1_2	-	+	-	-	-	+	+	+	-	+	-	+
Fe1_3	+	-	-	+	-	+	-	+	-	-	+	+
Fe1_4	-	-	+	-	+	+	-	+	+	-	-	+
Fe2_1			+		+	+		+	+			+
Fe2_5			-		-	+		+	-			+
Mn1_1	+			+		+		+			+	+
Mn1_6	-			-		+		+			-	+

Table 4. The magnetic components and total moment on each magnetic ion in $MnFe_3O_5$ between 5 and 300 K.

Sites		5 K	75 K	150 K	300 K
Fe1	Total	3.9(3)	4.2(2)	3.7(1)	2.4(1)
(μ_B)	x	1.6(1)	0	0	0
	y	1.5(2)	1.4(1)	0	0
	z	3.2(1)	3.9(1)	3.7(1)	2.4(1)
Fe2	Total	3.1(4)	4.1(1)	4.0(1)	2.7(1)
(μ_B)	x	1.7(1)	0	0	0
	y	1.0(2)	0	0	0
	z	2.4(1)	4.1(1)	4.0(1)	2.7(1)
Mn	Total	3.1(6)	1.88(2)	0	0
(μ_B)	x	0	0	0	0
	y	2.6(3)	1.88(2)	0	0
	z	1.7(4)	0	0	0

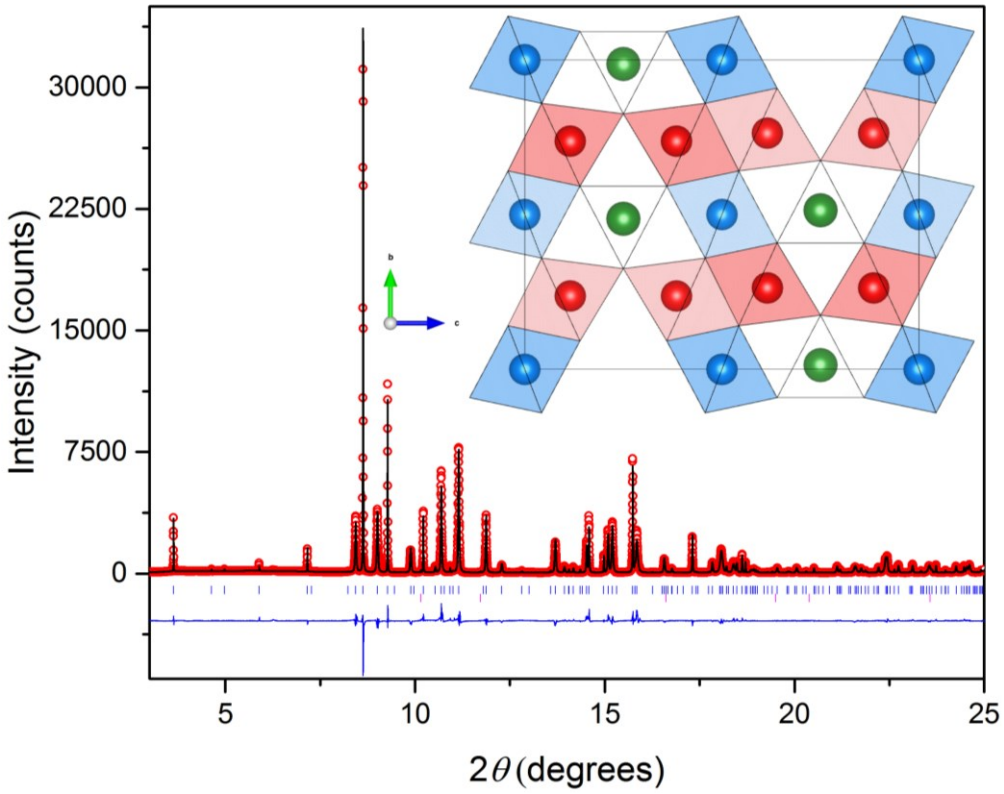

Figure 1. Rietveld fit to synchrotron powder diffraction profiles for $MnFe_3O_5$ at 13 K, with upper tick marks indicating the $MnFe_3O_5$ phase and lower for residual platinum from the sample container during high pressure-temperature synthesis. (R_{wp} = 15.6 % and R_p = 13.2 %) Insert shows the *Cmcm* structure of $MnFe_3O_5$ at 13 K with Fe1 octahedra shown in red, Fe2 in blue and Mn triangular prisms in green. Oxygens are located at the corners of polyhedra.