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**Ferroelectricity in and Structure of the YMnO<sub>3</sub> Family**

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**Abstract**

The 1963 discovery of ferroelectricity in YMnO<sub>3</sub> was accompanied by an experimental Curie temperature ( $T_c$ ) reported as 913 K; this value was revised to 1270 K in the following decade. Subsequently, YInO<sub>3</sub> was shown to be isostructural with YMnO<sub>3</sub> and later demonstrated to satisfy the structural criteria for ferroelectricity; recent unpublished measurements give  $T_c(\text{YInO}_3) = 835(15)$  K. The experimental  $T_c$  value of 913 K for YMnO<sub>3</sub> is in satisfactory agreement with the calculated 1220(100) K as derived from a very recent structural refinement, the experimental  $T_c$  of 835(15) K for YInO<sub>3</sub> with the calculated 760(120) K. The full YMnO<sub>3</sub> family includes the AMnO<sub>3</sub> subfamily with  $A = \text{Y, Ho, Er, Tm, Yb, Lu, Sc, In}$ ; the AInO<sub>3</sub> subfamily with  $A = \text{Y, Gd, Dy, Ho, Tb}$ ; and the AGaO<sub>3</sub> subfamily with  $A = \text{Y, Ho, Er}$ . The  $T_c$  values of six family members with known structure, in addition to YMnO<sub>3</sub> and YInO<sub>3</sub>, have been structurally derived as 1310(110) K for ErMnO<sub>3</sub>, 1290(165) K for LuMnO<sub>3</sub>, 1270(110) K for YbMnO<sub>3</sub>, 1220(105) K for ScMnO<sub>3</sub>, 540(375) K for InMnO<sub>3</sub> and 1020(100) K for YGaO<sub>3</sub>. The agreement between predicted and experimental  $T_c$  values for ErMnO<sub>3</sub>, LuMnO<sub>3</sub> and YbMnO<sub>3</sub> in addition to that for YMnO<sub>3</sub> and YInO<sub>3</sub> leads to the confident prediction that ScMnO<sub>3</sub>, InMnO<sub>3</sub> and YGaO<sub>3</sub> are new ferroelectrics. The remaining six members of the full YMnO<sub>3</sub> family are also expected to be new ferroelectrics.

**Table S1**

Atomic coordinates of  $\text{ErMnO}_3$  at 293 K,<sup>≡</sup> hypothetical  $x_{\text{I}}$   $y_{\text{I}}$   $z_{\text{I}}$  coordinates above  $T_c$

and atomic ( $\Delta x$ ,  $\Delta y$ ,  $\Delta z$ ) and thermal/static ( $u_{\text{eq}}$ ) displacements in Å

$$a_{\text{II}} = 6.1121(5), c_{\text{II}} = 11.4200(14) \text{ Å} \text{ at 293 K}$$

	Wyckoff position in $P6_3cm$	PHASE II			Wyckoff position in $P6_3/mmc$			PHASE I			
		$x_{\text{II}}$	$y_{\text{II}}$	$z^{\text{A}}$	$x_{\text{I}}$	$y_{\text{I}}$	$z_{\text{I}}$	$\Delta x$	$\Delta y$	$\Delta z^*$	$u_{\text{eq}}$
Er1	2(a)	0	0	0.52244(9)	2(a)	0	0	$\frac{1}{2}$	0	0	0.256 0.092
		0	0	"							
Er2	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.97978(2)	2(a)	0	0	0	0	0	-0.231 0.094
		0	0	"							
Mn	6(c)	0.3396(3)	0	0.24779(17)	2(d)	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	0.076	0.039	-0.025 0.095
		0.6792	0.3396	"							
O2 <sup>A</sup>	6(c)	0.3113(14)	0	0.4123(7)	4(f)	$\frac{2}{3}$	$\frac{1}{3}$	0.4132	-0.269	-0.134	-0.010 0.110
A		0.6226	0.3113	"							
O1 <sup>A</sup>	6(c)	0.6407(12)	0	0.5858(7)	4(f)	$\frac{1}{3}$	$\frac{2}{3}$	0.5868	-0.317	-0.159	-0.011 0.110
A		0.2814	0.6407	"							
O3	2(a)	0	0	0.725(3)	2(b)	0	0	$\frac{3}{4}$	0	0	-0.286 0.100
		0	0	"							
O4	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.2664(13)	2(b)	0	0	$\frac{1}{4}$	0	0	0.187 0.105
		0	0	"							

<sup>≡</sup> van Aken *et al.*, (2001b).

<sup>A</sup>  $z^* = z_{\text{II}} + 0.25027$ ;  $\Delta z = (z^* - z_{\text{I}}) \cdot c$ . See Table 1 for other terms.

<sup>AA</sup> Atoms generally labelled O1 and O2 in this family are labelled O2 and O1 by van Aken *et al.*, (2001b).

**Table S2**

Atomic coordinates of YInO<sub>3</sub> in phase II,<sup>≡</sup> hypothetical  $x_I$   $y_I$   $z_I$  coordinates above  $T_c$  and  $\Delta x$ ,  $\Delta y$ , polar  $\Delta z$  and  $u$  (thermal/static) displacements in Å

$$a_{\text{II}} = 6.260(5), c_{\text{II}} = 12.249(9) \text{ Å}$$

	Wyckoff position in $P6_3cm$	PHASE II			Wyckoff position in $P6_3/mmc$	PHASE I			$u^{\approx\approx}$
		$x_{\text{II}}$	$y_{\text{II}}$	$z^A$		$x_I$	$y_I$	$z_I$	
Y1	2(a)	0 0	0 0	0.5159(8) "	2(a)	0	0	$\frac{1}{2}$	0 0 0.195 0.09
Y2	4(b)	$\frac{2}{3}$ 0	$\frac{1}{3}$ 0	0.9847(5) "	2(a)	0	0	0	-0.187 0.12
In	6(c)	0.334(1) 0.668	0 $0.334$	0.2495 "	2(d)	$\frac{2}{3}$ $\frac{1}{3}$	$\frac{1}{4}$	0.004 0.012 -0.006 0.08	
O1	6(c)	0.309(4) 0.616	0 $0.309$	0.419(2) "	4(f)	$\frac{2}{3}$ $\frac{1}{3}$	0.420	-0.184 -0.087 -0.012 <0	
O2	6(c)	0.632(6) 0.264	0 $0.632$	0.580(3) "	4(f)	$\frac{1}{3}$ $\frac{2}{3}$	0.580	-0.249 -0.126 0.000 0.14	
O3	2(a)	0 0	0 0	0.736(3) "	2(b)	0	0	$\frac{3}{4}$	0 0 -0.171 0.12
O4	4(b)	$\frac{2}{3}$ 0	$\frac{1}{3}$ 0	0.282(2) "	2(b)	0	0	$\frac{1}{4}$	0 0 0.392 0.07

<sup>≡</sup> Pistorius & Kruger (1976).

<sup>A</sup>  $z^* = z_{\text{II}} + 0.2495$ ;  $\Delta z = (z^* - z_I) \cdot c$ . See Table 1 for other terms.

$\approx\approx$   $u^{33}$  for Y and In,  $u_{\text{eq}}$  for O.

**Table S3**

Atomic coordinates of LuMnO<sub>3</sub> in phase II,<sup>≡</sup> hypothetical  $x_I$   $y_I$   $z_I$  coordinates above  $T_c$

and  $\Delta x$ ,  $\Delta y$ , polar  $\Delta z$  and  $u$  (thermal/static) displacements in Å

$$a_{\text{II}} = 6.042(1), c_{\text{II}} = 11.37(1) \text{ Å}$$

	Wyckoff position in $P6_3cm$	PHASE II			Wyckoff position in $P6_3/mmc$	PHASE I			$u^{33}$		
		$x_{\text{II}}$	$y_{\text{II}}$	$z^{\text{A}}$		$x_I$	$y_{\text{II}}$	$z_I$	$\Delta x$		
Lu1	2(a)	0	0	0.5215	2(a)	0	0	$\frac{1}{2}$	0	0	0.244 0.11
		0	0	"							
Lu2	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.9776	2(a)	0	0	0	0	0	-0.254 0.11
		0	0	"							
Mn	6(c)	0.3212	0	0.2510	2(d)	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	-0.085	-0.042	0.011 0.11
		0.6424	0.3212	"							
O1	6(c)	0.3071	0	0.4209	4(f)	$\frac{2}{3}$	$\frac{1}{3}$	0.4151	-0.183	-0.091	0.066 0.08
		0.6142	0.3071	"							
O2	6(c)	0.6328	0	0.5907	4(f)	$\frac{1}{3}$	$\frac{2}{3}$	0.5849	-0.236	-0.118	0.066 0.10
		0.2656	0.6328	"							
O3	2(a)	0	0	0.7346	2(b)	0	0	$\frac{3}{4}$	0	0	-0.175 0.11
		0	0	"							
O4	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.2699	2(b)	0	0	$\frac{1}{4}$	0	0	0.226 0.15
		0	0	"							

<sup>≡</sup> Yakel *et al.* (1963).

<sup>A</sup>  $z^* = z_{\text{II}} + 0.2510$ ;  $\Delta z = (z^* - z_I) \cdot c$ . See Table 1 for other terms.

**Table S4**

Atomic coordinates of YbMnO<sub>3</sub> in phase II,<sup>≡</sup> hypothetical  $x_I$   $y_I$   $z_I$  coordinates above  $T_c$

and  $\Delta x$ ,  $\Delta y$ , polar  $\Delta z$  and  $u$  (thermal/static) displacements in Å

$$a_{\text{II}} = 6.0433(1), c_{\text{II}} = 11.5575(5) \text{ Å}$$

	Wyckoff position in $P6_3cm$	PHASE II			Wyckoff position in $P6_3/mmc$	PHASE I					
		$x_{\text{II}}$	$y_{\text{II}}$	$z^{\text{A}}$		$x_I$	$y_I$	$z_{\text{II}}$	$\Delta x$	$\Delta y$	$\Delta z^*$
Yb1	2(a)	0	0	0.5218(1)	2(a)	0	0	$\frac{1}{2}$	0	-0	0.252 0.11
		0	0	"							
Yb2	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.9806(1)	2(a)	0	0	0	0	-0	-0.224 0.12
		0	0	"							
Mn	6(c)	0.3269(5)	0	0.2476	2(d)	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	-0.045	-0.022	-0.028 0.11
		0.6538	0.3269	"							
O1	6(c)	0.304(2)	0	0.4086(9)	4(f)	$\frac{2}{3}$	$\frac{1}{3}$	0.413	-0.206	-0.101	-0.050 0.14
		0.608	0.304	"							
O2	6(c)	0.644(2)	0	0.5819(8)	4(f)	$\frac{1}{3}$	$\frac{2}{3}$	0.587	-0.157	-0.080	-0.059 0.15
		0.288	0.644	"							
O3	2(a)	0	0	0.726(2)	2(b)	0	0	$\frac{3}{4}$	0	0	-0.277 0.11
		0	0	"							
O4	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.261(1)	2(b)	0	0	$\frac{1}{4}$	0	0	0.127 0.23
		0	0	"							

<sup>≡</sup> Isobe *et al.* (1991).

<sup>A</sup>  $z^* = z_{\text{II}} + 0.2476$ ;  $\Delta z = (z^* - z_I) \cdot c$ . See Table 1 for other terms.

**Table S5(a)**

Atomic coordinates of  $\text{ScMnO}_3$  in phase II,<sup>≡</sup> hypothetical  $x_{\text{I}}$   $y_{\text{I}}$   $z_{\text{I}}$  coordinates above  $T_c$  and  $\Delta x$ ,  $\Delta y$ , polar  $\Delta z$  and  $u$  (thermal/static) displacements in Å

$$a_{\text{II}} = 5.8286(6), c_{\text{II}} = 11.1738(9) \text{ Å}$$

	Wyckoff position in $P6_3cm$			PHASE II			Wyckoff position in $P6_3/mmc$			PHASE I			$u_{\text{eq}}$
		$x_{\text{II}}$	$y_{\text{II}}$	$z^{\text{A}}$		$x_{\text{I}}$	$y_{\text{I}}$	$z_{\text{I}}$	$\Delta x$	$\Delta y$	$\Delta z^*$		
				"					0	0	0.247		
Sc1	2(a)	0	0	0.5221(2)		2(a)	0	0	0	0	0.247	0.06	
		0	0	"									
Sc2	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.9795(2)		2(a)	0	0	0	0	-0.229	0.07	
		0	0	"									
Mn	6(c)	0.3335(1)	0	0.2483(2)		2(d)	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	0.000	0.001	-0.019	0.07
		0.6670	0.3335	"									
O1	6(c)	0.3031(6)	0	0.4166(9)		4(f)	$\frac{2}{3}$	$\frac{1}{3}$	0.4177	-0.203	-0.102	-0.012	0.08
		0.6062	0.3031	"									
O2	6(c)	0.6358(6)	0	0.5811(9)		4(f)	$\frac{1}{3}$	$\frac{2}{3}$	0.5823	-0.208	-0.104	-0.013	0.08
		0.2716	0.6358	"									
O3	2(a)	0	0	0.7158(14)		2(b)	0	0	$\frac{3}{4}$	0	0	-0.380	0.08
		0	0	"									
O4	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.2723(11)		2(b)	0	0	$\frac{1}{4}$	0	0	0.249	0.08
		0	0	"									

<sup>≡</sup> Greedan *et al.*, (1995).

<sup>A</sup>  $z^* = z_{\text{II}} + 0.2483$ ;  $\Delta z = (z^* - z_{\text{I}}) \cdot c$ . See Table 1 for other terms.

**Table S5(b)**

Atomic coordinates of  $\text{ScMnO}_3$  in phase II,<sup>≡</sup> hypothetical  $x_{\text{I}}$   $y_{\text{I}}$   $z_{\text{I}}$  coordinates above  $T_c$

and  $\Delta x$ ,  $\Delta y$ , polar  $\Delta z$  and  $u$  (thermal/static) displacements in Å

$$a_{\text{II}} = 5.8330(1), c_{\text{II}} = 11.1786(10) \text{ Å}$$

	Wyckoff position in $P6_3cm$	PHASE II			Wyckoff position in $P6_3/mmc$	PHASE I					
		$x_{\text{II}}$	$y_{\text{II}}$	$z^{\text{A}}$		$x_{\text{I}}$	$y_{\text{I}}$	$z_{\text{I}}$	$\Delta x$	$\Delta y$	$\Delta z^*$
Sc1	2(a)	0	0	0.522(3)	2(a)	0	0	$\frac{1}{2}$	0	0	0.246 0.11
		0	0	"							
Sc2	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.980(2)	2(a)	0	0	0	0	0	-0.224 0.14
		0	0	"							
Mn	6(c)	0.336(4)	0	0.248	2(d)	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	0.017	0.010	-0.022 0.14
		0.672	0.336	"							
O1	6(c)	0.295(7)	0	0.422(5)	4(f)	$\frac{2}{3}$	$\frac{1}{3}$	0.4175	-0.259	-0.128	0.050 0.16
		0.590	0.295	"							
O2	6(c)	0.638(6)	0	0.587(4)	4(f)	$\frac{1}{3}$	$\frac{2}{3}$	0.5825	-0.192	-0.098	0.050 0.12
		0.276	0.638	"							
O3	2(a)	0	0	0.718(1)	2(b)	0	0	$\frac{3}{4}$	0	0	-0.358 0.14
		0	0	"							
O4	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.279(7)	2(b)	0	0	$\frac{1}{4}$	0	0	0.324 0.17
		0	0	"							

<sup>≡</sup> Xu *et al.*, (1995).

<sup>A</sup>  $z^* = z_{\text{II}} + 0.2457$ ;  $\Delta z = (z^* - z_{\text{I}}) \cdot c$ . See Table 1 for other terms.

**Table S5(c)**

Atomic coordinates of ScMnO<sub>3</sub> in phase II,<sup>≡</sup> hypothetical  $x_I$   $y_I$   $z_I$  coordinates above  $T_c$  and  $\Delta x$ ,  $\Delta y$ , polar  $\Delta z$  and  $u$  (thermal/static) displacements in Å

$$a_{\text{II}} = 5.8364(2), c_{\text{II}} = 11.1812(5) \text{ Å}$$

	Wyckoff position in $P6_3cm$		PHASE II			Wyckoff position in $P6_3/mmc$		PHASE I				$u_{\text{eq}}$
			$x_{\text{II}}$	$y_{\text{II}}$	$z^{\text{A}}$			$x_I$	$y_I$	$z_I$	$\Delta x$	
	$x_{\text{II}}$	$y_{\text{II}}$	$z_I$	$x_I$	$y_I$	$z_I$	$\Delta x$	$\Delta y$	$\Delta z^*$	$u_{\text{eq}}$		
Sc	2(a) 0	0	0.5250(12) "	2(a) 0	0	0 $\frac{1}{2}$	0	0	0.280 0.07	0	0	
Sc	4(b) $\frac{2}{3}$ 0	$\frac{1}{3}$ 0	0.9792(10) "	2(a) 0	0	0 $\frac{1}{2}$	0	0	-0.233 0.07	0	0	
Mn	6(c) 0.3333(2) 0.6666	0 0.3333	0.2457(2) "	2(d) 0	$\frac{2}{3}$ $\frac{1}{3}$	$\frac{1}{4}$	0.000	0.000	-0.048 0.08	0.000	0.000	
O1	6(c) 0.3995(15) 0.7990	0 0.3995	0.4102(13) "	4(f) 0	$\frac{2}{3}$ $\frac{1}{3}$	0.4169 $\frac{1}{3}$	0.446	0.223	-0.066 0.04	-0.066	0.04	
O2	6(c) 0.6381(16) 0.2762	0 0.6381	0.5764(14) "	4(f) 0	$\frac{1}{3}$ $\frac{2}{3}$	0.5823 $\frac{1}{3}$	-0.192	-0.096	-0.066 0.04	-0.066	0.04	
O3	2(a) 0	0 0	0.7245(15) "	2(b) 0	0	$\frac{3}{4}$	0	0	-0.285 0.04	0	0	
O4	4(b) $\frac{2}{3}$ 0	$\frac{1}{3}$ 0	0.2705 <sup>§</sup> "	2(b) 0	0	$\frac{1}{4}$	0	0	0.229 0.04	0	0	

<sup>≡</sup> Bieringer & Greedan (1999).

<sup>A</sup>  $z^* = z_{\text{II}} + 0.2457$ ;  $\Delta z = (z^* - z_I) \cdot c$ . See Table 1 for other terms.

<sup>§</sup> Uncertainty not stated.

**Table S6**

Atomic coordinates of InMnO<sub>3</sub> in phase II,<sup>≈</sup> hypothetical  $x_I$   $y_I$   $z_I$  coordinates above  $T_c$  and  $\Delta x$ ,  $\Delta y$ , polar  $\Delta z$  and  $u$  (thermal/static) displacements in Å

$$a_{\text{II}} = 5.8758(4), c_{\text{II}} = 11.4715(8) \text{ Å}$$

	Wyckoff position in $P6_3cm$	PHASE II			Wyckoff position in $P6_3/mmc$			PHASE I				$u_{\text{eq}}$
		$x_{\text{II}}$	$y_{\text{II}}$	$z^{\text{A}}$	$x_I$	$y_I$	$z_I$	$\Delta x$	$\Delta y$	$\Delta z^*$	$u_{\text{eq}}$	
In1	2(a)	0	0	0.513(5)	2(a)	0	0	$\frac{1}{2}$	0	0	0.145	0.22
		0	0	"								
In2	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.986(4)	2(a)	0	0	0	0	0	-0.164	0.13
		0	0	"								
Mn	6(c)	0.321(5)	0	0.252	2(d)	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	-0.085	-0.041	0.019	0.08
		0.642	0.321	"								
O1	6(c)	0.301(2)	0	0.407(3)	4(f)	$\frac{2}{3}$	$\frac{1}{3}$	0.413	-0.221	-0.109	-0.067	0.14
		0.602	0.301	"								
O2	6(c)	0.654(2)	0	0.577(3)	4(f)	$\frac{1}{3}$	$\frac{2}{3}$	0.587	-0.085	-0.044	-0.074	0.12
		0.308	0.654	"								
O3	2(a)	0	0	0.723(4)	2(b)	0	0	$\frac{3}{4}$	0	0	-0.310	0.03
		0	0	"								
O4	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.261(3)	2(b)	0	0	$\frac{1}{4}$	0	0	0.126	0.18
		0	0	"								

<sup>≈</sup> Greedan *et al.* (1995).

<sup>A</sup>  $z^* = z_{\text{II}} + 0.2525$ ;  $\Delta z = (z^* - z_I) \cdot c$ . See Table 1 for other tables.

**Table S7**

Atomic coordinates of  $\text{YGaO}_3$  in phase II,<sup>≡</sup> hypothetical  $x_{\text{I}}$   $y_{\text{I}}$   $z_{\text{I}}$  coordinates above  $T_c$  and  $\Delta x$ ,  $\Delta y$ , polar  $\Delta z$  and  $u$  (thermal/static) displacements in Å

$$a_{\text{II}} = 6.065(2), c_{\text{II}} = 11.615(4) \text{ Å}$$

	Wyckoff position in $P6_3cm$	PHASE II			Wyckoff position in $P6_3/mmc$	PHASE I			$u^{33}$
		$x_{\text{II}}$	$y_{\text{II}}$	$z^{\text{A}}$		$x_{\text{I}}$	$y_{\text{I}}$	$z_{\text{I}}$	
Y1	2(a)	0	0	0.5195(5)	2(a)	0	0	$\frac{1}{2}$	0 0 0.226 0.08
		0	0	"					
Y2	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.9826(3)	2(a)	0	0	0	-0.202 0.09
		0	0	"					
Ga	6(c)	0.3269(5)	0	0.2479	2(d)	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	-0.045 -0.022 -0.024 0.08
		0.6538	0.3269	"					
O1	6(c)	0.304(2)	0	0.406(2)	4(f)	$\frac{2}{3}$	$\frac{1}{3}$	0.413	-0.206 -0.102 -0.081 0.13
		0.608	0.304	"					
O2	6(c)	0.644(2)	0	0.590(2)	4(f)	$\frac{1}{3}$	$\frac{2}{3}$	0.587	-0.158 -0.081 0.035 0.13
		0.288	0.644	"					
O3	2(a)	0	0	0.732(3)	2(b)	0	0	$\frac{3}{4}$	0 0 -0.209 0.06
		0	0	"					
O4	4(b)	$\frac{2}{3}$	$\frac{1}{3}$	0.264(2)	2(b)	0	0	$\frac{1}{4}$	0 0 0.163 0.09
		0	0	"					

<sup>≡</sup> Geller *et al.*, (1975).

<sup>A</sup>  $z^* = z_{\text{II}} + 0.2479$ ;  $\Delta z = (z^* - z_{\text{I}}) \cdot c$ . See Table 1 for other terms.

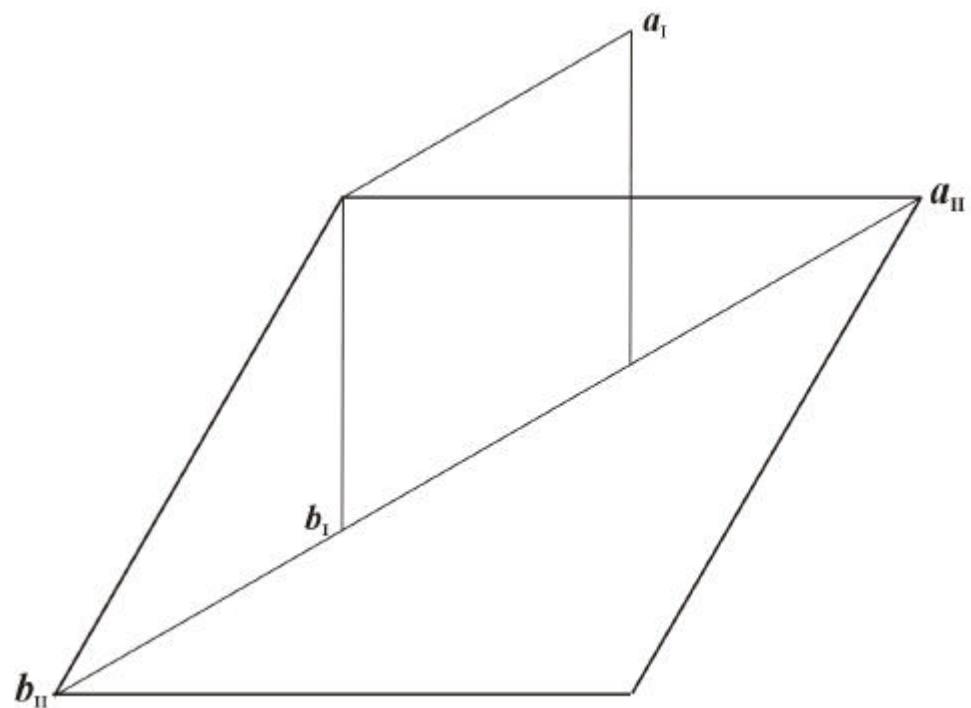
## Figure Captions

**Figure S1** Relationship between the  $\mathbf{a}_1$ ,  $\mathbf{b}_1$  axes in the unit cell of YMnO<sub>3</sub>, phase II |  $P6_3cm$  and the  $\mathbf{a}_2$ ,  $\mathbf{b}_2$  axes in the unit cell of phase I |  $P6_3/mmc$ .

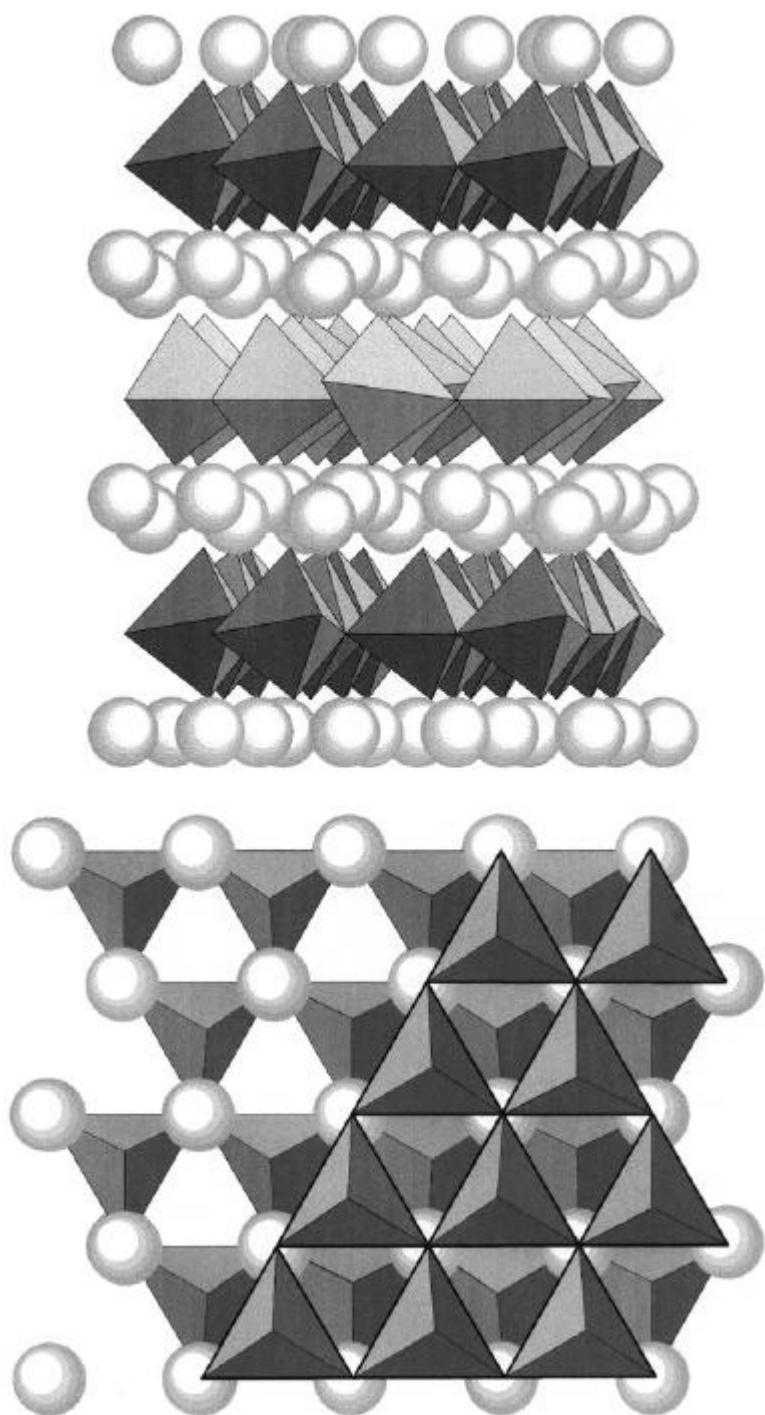
**Figure S2** Reproduction of Fig. 1 from van Aken *et al.*, (2001a) with schematic view of the YMnO<sub>3</sub> structure. The upper panel depicts a view normal to the polar axis, with Y cations represented by spheres and Mn atoms occupying oxygen atom trigonal bipyramids. Corner-sharing by the equatorial oxygens of the MnO<sub>5</sub> groups results in layer formation. The lower panel depicts the structure viewed along the polar axis, with Y cations separating two partially stacked layers.

**Figure S3** Normal probability plot of the ranked atomic-coordinate deviates in ScMnO<sub>3</sub> as determined by Greedan *et al.*, (1995) and Bieringer & Greedan (1999), see Tables S4(a) and (c). The discrepant experimental deviate for  $x(O1)$  has value 59.5. Linear regression on the remaining deviates with a slope of 5.79.

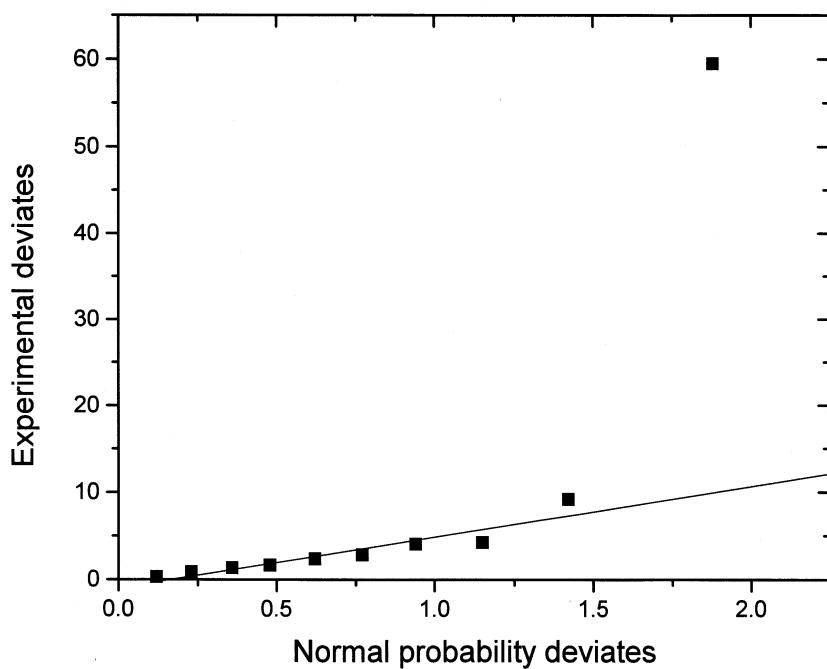
**Figure S4** Normal probability plot of the ranked atomic-coordinate deviates in ScMnO<sub>3</sub> as determined by Greedan *et al.*, (1995) and Xu *et al.*, (1995), see Tables S4(a) and (b). The discrepant experimental deviate for  $x(Mn)$  has value 6.06. Linear regression on the remaining deviates with a slope of 1.10.



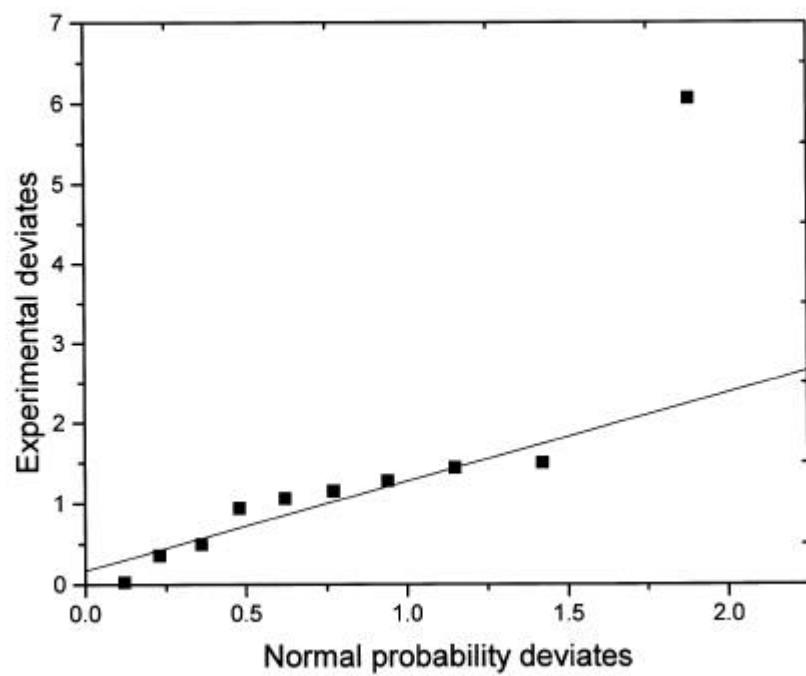
**Figure S1**



**Figure S2**



**Figure S3**



**Figure S4**