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addenda and errata

Normal-mode analysis of the structures of perovskites with tilted octahedra. Erratum

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There is an error in the mode assignment for hettotype 9, $[a^-b^+a^-]$, discussed in the paper by Darlington [*Acta Cryst.* (2002). A**58**, 66–71], which has been pointed out by Dr Kevin Knight, Rutherford Appleton Laboratory, Didcot, Oxon, England. In this paper, a mode involving displacements of the anions of hettotype 9 was labelled $[(\frac{1}{2}, 0, \frac{1}{2}), M_1]$ rather than $[(\frac{1}{2}, 0, \frac{1}{2}), M_2]$. Both modes involve *plus-like* distortion of the octahedra. In the corrected Tables 1–4 shown below, this mode, which is only found in hettotype 9, has been labelled K_2 rather than H_2. Therefore, there are not seven but eight normal modes of the cubic phase required to describe the displacements found in the nine hettotypes considered. The weights of K_2 in all the materials examined in the original paper with the structure of hettotype 9 [labelled $W(H_1)$ in the original Table 4] are correct, unaltered by the change in the labelling of the mode. It should be noted that $[(\frac{1}{2}, 0, \frac{1}{2}), M_2]$ is a longitudinal mode – the seven other modes are all transverse. The weights of K_2 are not significantly different from zero in the 15 structures examined.

Table 1
The nine hettotypes.

Number	+/− notation	$[M_i\, R_j]$	Multiplicity	True unit cell	Space group
1	$a^0a^0c^-$	R_3	2 × 2 × 2	$2^{1/2} \times 2^{1/2} \times 2$	$I4/mcm$ (140)
2	$a^-b^0a^-$	$R_1 = R_3$	2 × 2 × 2	$2^{1/2} \times 2 \times 2^{1/2}$	$Imma$ (74)
3	$a^-a^-a^-$	$R_1 = R_2 = R_3$	2 × 2 × 2	$2^{1/2} \times 2^{1/2} \times 2^{1/2}$	$R\bar{3}c$ (167)
4	$a^0a^0c^+$	M_3	2 × 2 × 1	$2^{1/2} \times 2^{1/2} \times 1$	$P4/mbm$ (127)
5	$a^+a^+c^0$	$M_1 = M_2$	2 × 2 × 2	2 × 2 × 2	$I4/mmm$ (139)
6	$a^+a^+a^+$	$M_1 = M_2 = M_3$	2 × 2 × 2	2 × 2 × 2	$Im\bar{3}$ (204)
7	$a^0b^-c^+$	R_2, M_3	2 × 2 × 2	2 × 2 × 2	$Cmcm$ (63)
8	$a^+a^+c^-$	$M_1 = M_2, R_3$	2 × 2 × 2	2 × 2 × 2	$P4_2/nmc$ (137)
9	$a^-b^+a^-$	$R_1 = R_3, M_2$	2 × 2 × 2	$2^{1/2} \times 2 \times 2^{1/2}$	$Pnma$ (62)

Table 2
Atomic displacements in the seven normal modes, the symbol used in the construction of the Landau potential, and character of each mode.

Normal mode	Displacement	Symbol	Character
$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}), \Gamma_{25}$	OI(y) = −OII(z)	R_1	Octahedral minus tilt
$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}), \Gamma_{25}$	OI(x) = −OIII(z)	R_2	Octahedral minus tilt
$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}), \Gamma_{25}$	OII(x) = −OIII(y)	R_3	Octahedral minus tilt
$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}), \Gamma_{15}$	OI(y) = OII(z)	G_{O1}	Octahedral minus distortion
$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}), \Gamma_{15}$	OI(x) = OIII(z)	G_{O2}	Octahedral minus distortion
$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}), \Gamma_{15}$	OII(x) = OIII(y)	G_{O3}	Octahedral minus distortion
$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}), \Gamma_{15}$	$A(x)$	G_{A1}	A cation displacement
$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}), \Gamma_{15}$	$A(y)$	G_{A2}	A cation displacement
$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}), \Gamma_{15}$	$A(z)$	G_{A3}	A cation displacement
$(0, \frac{1}{2}, \frac{1}{2}), M_3$	OI(y) = −OII(z)	M_1	Octahedral plus tilt
$(\frac{1}{2}, 0, \frac{1}{2}), M_3$	OI(x) = −OIII(z)	M_2	Octahedral plus tilt
$(\frac{1}{2}, \frac{1}{2}, 0), M_3$	OII(x) = −OIII(y)	M_3	Octahedral plus tilt
$(0, \frac{1}{2}, \frac{1}{2}), M_1$	OI(y) = OII(z)	H_1	Octahedral plus distortion
$(\frac{1}{2}, 0, \frac{1}{2}), M_1$	OI(x) = OIII(z)	H_2	Octahedral plus distortion
$(\frac{1}{2}, \frac{1}{2}, 0), M_1$	OII(x) = OIII(y)	H_3	Octahedral plus distortion
$(0, \frac{1}{2}, \frac{1}{2}), M_2$	OII(y) = −OI(z)	K_1	Octahedral plus distortion
$(\frac{1}{2}, 0, \frac{1}{2}), M_2$	OI(z) = −OIII(x)	K_2	Octahedral plus distortion
$(\frac{1}{2}, \frac{1}{2}, 0), M_2$	OIII(x) = −OII(y)	K_3	Octahedral plus distortion
$(\frac{1}{2}, 0, 0), M_5'$	OIII(y)	X_{O12}	Octahedral distortion
$(\frac{1}{2}, 0, 0), M_5'$	OIII(z)	X_{O13}	Octahedral distortion
$(0, \frac{1}{2}, 0), M_5'$	OII(z)	X_{O23}	Octahedral distortion
$(0, \frac{1}{2}, 0), M_5'$	OII(x)	X_{O21}	Octahedral distortion
$(0, 0, \frac{1}{2}), M_5'$	OI(x)	X_{O31}	Octahedral distortion
$(0, 0, \frac{1}{2}), M_5'$	OI(y)	X_{O32}	Octahedral distortion
$(\frac{1}{2}, 0, 0), M_5'$	$A(y)$	X_{A12}	Cation displacement
$(\frac{1}{2}, 0, 0), M_5'$	$A(z)$	X_{A13}	Cation displacement
$(0, \frac{1}{2}, 0), M_5'$	$A(z)$	X_{A23}	Cation displacement
$(0, \frac{1}{2}, 0), M_5'$	$A(x)$	X_{A21}	Cation displacement
$(0, 0, \frac{1}{2}), M_5'$	$A(x)$	X_{A31}	Cation displacement
$(0, 0, \frac{1}{2}), M_5'$	$A(y)$	X_{A32}	Cation displacement

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Table 3
The space group, possible condensed modes and non-zero pseudocubic spontaneous macrostrain in the nine hettotypes.

Number	Space group	Allowed modes	Macrostrain
1	*I*4/*mcm* (140)	R_3	$\varepsilon_{11} = \varepsilon_{22}; \varepsilon_{33}$
2	*Imma* (74)	$R_1 = R_3$ $G_{O1} = G_{O3}$ $G_{A1} = G_{A3}$	$\varepsilon_{11} = \varepsilon_{33}; \varepsilon_{22}; \varepsilon_{31}$
3	$R\bar{3}c$ (167)	$R_1 = R_2 = R_3$	$\varepsilon_{11} = \varepsilon_{22} = \varepsilon_{33}; \varepsilon_{23} = \varepsilon_{31} = \varepsilon_{12}$
4	*P*4/*mbm* (127)	M_3	$\varepsilon_{11} = \varepsilon_{22}; \varepsilon_{33}$
5	*I*4/*mmm* (139)	$M_1 = M_2$ $H_1 = H_2 \neq H_3$	$\varepsilon_{11} = \varepsilon_{22}; \varepsilon_{33}$
6	$Im\bar{3}$ (204)	$M_1 = M_2 = M_3$ $H_1 = H_2 = H_3$	$\varepsilon_{11} = \varepsilon_{22} = \varepsilon_{33}$
7	*Cmcm* (63)	R_2 M_3 G_{O2} G_{A2} H_3 X_{O32} X_{A32}	$\varepsilon_{11}; \varepsilon_{22}; \varepsilon_{33}$
8	$P4_2/nmc$ (137)	R_3 $M_1 = M_2$ G_{O3} $H_1 = H_2$ $X_{O13} = X_{O23}$ $X_{A13} = X_{A23}$	$\varepsilon_{11} = \varepsilon_{22}; \varepsilon_{33}$
9	*Pnma* (62)	$R_1 = R_3$ M_2 $G_{O1} = G_{O3}$ $G_{A1} = G_{A3}$ K_2 $X_{O21} = X_{O23}$ $X_{A21} = X_{A23}$	$\varepsilon_{11} = \varepsilon_{33}; \varepsilon_{22}; \varepsilon_{31}$

Table 4
Weights of condensed modes in units of u Å^2.

Hettotype	Material	$W(R_i)$	$W(M_i)$	$W(X_{Aij})$	$W(X_{Oij})$	$W(G_{Ai})$	$W(G_{Oi})$	$W(H_i)$	$W(K_i)$	Ref.†	Entry
1 R_3	$SrTiO_3$, 77 K	0.0726								1	1
	$SrZrO_3$, 1223 K	1.6971								2	2
2 $R_1 = R_3$	$BaCeO_3$, 573 K	6.7294				0.0586	0.1460			3	3
3 $R_1 = R_2 = R_3$	$BaCeO_3$, 773 K	5.2701								3	4
	$LaGeO_3$, 673 K	4.3662								4	5
4 M_3	$NaNbO_3$, 888 K		0.9520							5	6
	$NaTaO_3$, 878 K		0.8965							5	7
5 $M_1 = M_2$	No available data										
6 $M_1 = M_2 = M_3$	$CaCu_3Ti_4O_{12}$		10.2753					0.2031		6	8
	$Tb_{0.67}Cu_3Ti_4O_{12}$		9.9740					0.1964		6	9
	$CaCu_3Mn_4O_{12}$		9.2271					0.1323		7	10
	$Li_{0.36}WO_3$		5.0358					0.0060		8	11
	$Na_{0.73}WO_3$		0.3953					0.0000		8	12
	$Na_{0.54}WO_3$		0.3657					0.0000		8	13
7 R_2, M_3	$NaNbO_3$, 813 K	0.8442	1.2912	0.0082	0.0012	0.0001	0.0002	0.0042		5	14
	$NaTaO_3$, 803 K	0.9408	1.1623	0.0808	0.0048	0.0000	0.0067	0.0013		5	15
	$SrZrO_3$, 973 K	3.1806	0.8497	0.4539	0.0063	0.0154	0.0118	0.0002		2	16
8 $M_1 = M_2$, R_3	$CaFeTi_2O_6$	4.3399	7.3194	0.3690	0.1987		0.0508	0.0015		9	17
9 $R_1 = R_3$, M_2	$BaCeO_3$, 473 K	7.2126	0.5108	0.8058	0.0503	0.0775	0.1518		0.0002	3	18
	$SrZrO_3$	5.8137	1.2545	1.7364	0.0958	0.0471	0.1209		0.0001	2	19
	$LaGeO_3$	5.0130	0.4181	1.1826	0.0162	0.0713	0.1034		0.0002	4	20
	$PrFeO_3$	7.4537	1.7425	8.3611	0.2237	0.3453	0.1390		0.0000	10	21
	$NdFeO_3$	8.3981	1.9033	10.7150	0.2898	0.4901	0.1649		0.0000	10	22
	$SmFeO_3$	9.6041	2.3606	15.1215	0.4215	0.7547	0.1970		0.0005	10	23
	$EuFeO_3$	10.0301	2.5231	17.2613	0.5149	0.9157	0.2237		0.0000	10	24
	$GdFeO_3$	10.2814	2.6910	19.5499	0.5419	1.0893	0.2683		0.0000	10	25
	$TbFeO_3$	11.1054	2.7621	20.4797	0.6507	1.1498	0.2368		0.0000	8	26
	$DyFeO_3$	11.5369	2.9724	22.5061	0.7089	1.3311	0.2471		0.0002	8	27
	$HoFeO_3$	12.0370	3.0026	23.8465	0.7804	1.4574	0.2704		0.0002	10	28
	$ErFeO_3$	12.8142	3.1006	24.9061	0.8218	1.5771	0.3205		0.0000	10	29
	$TmFeO_3$	13.1795	3.0947	25.1013	0.9675	1.6745	0.2982		0.0000	10	30
	$YbFeO_3$	13.6153	3.2967	26.7549	1.0592	1.7761	0.3007		0.0000	10	31
	$LuFeO_3$	14.3837	3.2072	27.5146	1.0463	1.8962	0.2892		0.0000	10	32

† References: (1) Unoki & Sakudo (1967); (2) Kennedy *et al.* (1999); (3) Knight (1995); (4) Howard & Kennedy (1999); (5) Darlington & Knight (1999); (6) Bochu *et al.* (1979); (7) Chenevas *et al.* (1975); (8) Wiseman & Dickens (1976); (9) Leinenweber & Parise (1995); (10) Marezio *et al.* (1970).