Table 26A-2-001. $BaMnF_4$. Crystal structure [69Kev]. Fractional coordinates at 298 K.

Atom	*x*	*y*	*z*
Ba	0.4537	0.34383(5)	1/2
Mn	0.0000(4)	0.4160(1)	0
F(1)	0.196(2)	0.2982(6)	0
F(2)	–0.275(3)	0.3363(7)	0
F(3)	0.337(3)	0.4651(7)	0
F(4)	0.016(3)	0.4217(10)	1/2

Table 26A-2-002. $BaMnF_4$. Crystal structure [69Kev]. Temperature parameters at 298 K. Temperature factor b_{ij} is defined by Eq. (b) in Introduction.

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Ba	0.0127(3)	0.00240(3)	0.0103(3)	0.00262(9)	0	0
Mn	0.0099(9)	0.00092(4)	0.0099(5)	0.00007(13)	0	0
F(1)	0.016(3)	0.0007(2)	0.035(5)	–0.0009(7)	0	0
F(2)	0.013(4)	0.0024(4)	0.024(4)	–0.0012(9)	0	0
F(3)	0.022(5)	0.0018(4)	0.050(6)	–0.0061(11)	0	0
F(4)	0.025(6)	0.0057(7)	0.009(3)	0.0038(15)	0	0

Table 26A-2-003. $BaMnF_4$. Crystal structure [69Kev]. Root-mean-square amplitude of thermal vibration of atoms along the principal axes at 298 K.

Atom	*1* [Å]	*2* [Å]	*3* [Å]
Ba	0.096(1)	0.115(2)	0.194(2)
Mn	0.095(1)	0.103(2)	0.134(6)
F(1)	0.090(14)	0.171(18)	0.177(13)
F(2)	0.142(18)	0.147(13)	0.179(16)
F(3)	0.033(42)	0.212(13)	0.245(20)
F(4)	0.089(15)	0.187(21)	0.275(18)

Table 26A-2-004. $BaMnF_4$. Crystal structure [69Kev]. Interatomic distances at 298 K. Symmetry related atoms are denoted by subscripts explained in Table 28-2-006. All atoms lie on mirror planes.

Distance	[Å]	Distance	[Å]
Mn–F(2)	2.037(15)	$Mn–Mn_{i}$	3.922(2)
$Mn–F(3)_{iv}$	2.042(9)	$Mn–Mn_{vi}$	4.222(3)
Mn–F(4)	2.115(1)		
Mn–F(1)	2.129(11)	F(1)–F(3)	2.658(12)
Mn–F(3)	2.151(15)	F(1)–F(2)	2.874(21)
		$F(4)–F(3)_{iv}$	2.919(11)
$Ba–F(1)_{ii}$	2.588(9)	F(3)–F(4)	2.929(17)
$Ba–F(2)_{v}$	2.666(10)	F(1)–F(4)	3.015(13)
Ba–F(1)	2.704(7)	F(2)–F(4)	3.024(17)
Ba–F(4)	2.871(16)	$F(2)–F(3)_{iv}$	3.073(18)
Ba–F(3)	2.880(10)	$F(3)–F(3)_{iv}$	3.173(7)
$Ba–F(2)_{ii}$	3.044(12)		
$Ba–F(4)_{i}$	3.559(15)	$F(1)–F(2)_{ii}$	2.935(10)
$Ba–F(4)_{v}$	3.565(18)	$F(3)–F(2)_{v}$	3.028(23)
		$F(1)–F(2)_{v}$	3.220(21)
$Ba–Ba_{ii}$	4.630(10)		

Table 26A-2-005. $BaMnF_4$. Crystal structure [69Kev]. Interatomic angles at 298 K. Symmetry related atoms are denoted by subscripts, see Table 28A-2-006 for the symmetry nomenclature.

Angles	[°]	Angles	[°]
F(1)–Mn–F(3)	76.8(5)	$F(3)_{iv}–Mn–F(2)$	97.7(7)
F(4)–Mn–F(3)	86.7(5)	$F(3)–Mn–F(3)_{iv}$	98.3(3)
F(2)–Mn–F(1)	87.2(5)	$F(4)–Mn–F(4)_{viii}$	173.0(9)
$F(4)–Mn–F(3)_{iv}$	89.2(4)	$Mn–F(3)–Mn_{i}$	138.6(9)
F(4)–Mn–F(1)	90.5(4)	$Mn–F(4)–Mn_{vi}$	173.0(9)
F(4)–Mn–F(2)	93.5(5)		

Table 26A-2-006. $BaMnF_4$. Symmetry relation nomenclature for crystal structure data [69Kev].

Subscript	Operation	Subscript	Operation
i	$\frac{1}{2}+x, 1-y, z$	vi	$x, y, 1+z$
ii	$\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$	vii	$\frac{1}{2}+x, \frac{1}{2}-y, z-\frac{1}{2}$
iii	$x-\frac{1}{2}, \frac{1}{2}-y, z-\frac{1}{2}$	viii	$x, y, z-1$
iv	$x-\frac{1}{2}, 1-y, z$	ix	$x, \frac{1}{2}+y, \frac{1}{2}+z$
v	$1+x, y, z$	x	$\overline{x}, y, z$

Table 26A-2-007. $BaMnF_4$. Elastic stiffness constants $c_{\lambda\mu}^{\boldsymbol{E}}$ and piezoelectric stress constants $e_{i\lambda}$ [81Loc]. Determined by Brillouin scattering. λ = 488 nm, 514.5 nm. T = 295 K.

Coefficient	Value
Elastic constants	[$\cdot 10^{10}$ N m^{-2}]
c_{11}^E	11.25
c_{22}^E	5.69
c_{33}^E	$7.50^{+0.07}_{-0.28}$
c_{44}^E	1.71
c_{55}^E	3.47
c_{66}^E	1.97
c_{12}^E	3.11(1)
c_{13}^E	6.34(54)
c_{23}^E	3.89(59)
Piezoelectric constants	[C m^{-2}]
e_{15}	0.03
e_{24}	0.69
e_{31}	1.74(9)
e_{32}	2.62(21)
e_{33}	–0.26(60)

Table 26A-2-008. $BaMnF_4$. Frequencies of the lattice vibration modes obtained by Raman spectra in unit of cm^{-1} [81Loc]. The scattering geometries are shown in the top row.

c(*b*,*b*)*a*		*c*(*b*,*c*)*a*		*c*(*a*,*c*)*a*		*c*(*a*,*b*)a	
257 K	86 K	257 K	86 K	257 K	86 K	257 K	86 K
	22.5(5)		22(2) ‡)			30(3)	25(1)
	35.5(5)		34(2) ‡)				37.0(15)
						53(2)	60(1)
							67(1)
71(1)	75.0(15)	71(1)	73(1)				79.0(5)
93(1)						83(1)	87(1)
	100(1)						103(1)
	116(1)		115(2) ‡)	110.0(15)	111(3) †)		116.0(15)
130(1)	127(1)					136(1)	136(1)
			148(1)				149(1)
	156(1) †)		156(1) ‡)				
161(1)	163(1)	160(3) †)	164(1)			160.0(15)	
	174(1)		173(1)			176.0(15)	169.0(25)
196.0(15)			186(1)		183(3)		181.0(15)
	201(1)						200(1)
229(4) †)	224(1)			221(5)	224(1)	221.0(25) ‡)	223.0(25) ‡)
	236(2)	233(5) ‡)	244(4) †) ‡)	238(3)	241.0(15) †)	238(1) ‡)	239(2) ‡)
	249(3) †)						
287(2)	289(1)	287(3) ‡)	289.0(15) ‡)				287.0(25)
	325(1)					327(1)	332.0(15)
	347(2)						
399(2)	407(2) †)	397(5) ‡)	406(1) †)			378(3)	389(3)
						455(3)	455(3)

†) indicates a probable multiple peak
‡) indicates a possible "leak through" peak