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Redetermination of the crystal structure of barium tetrafluorozincate, $BaZnF_4$, at 295 K and 113 K

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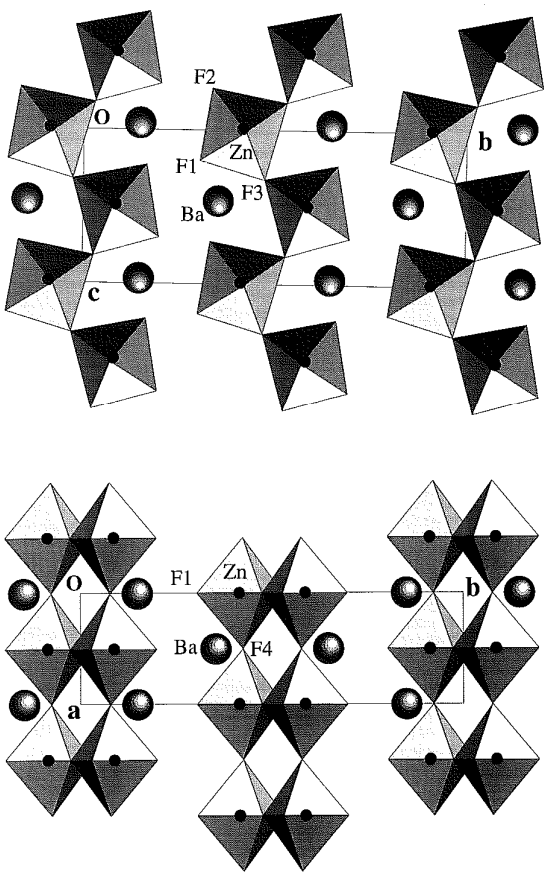

Source of material: Crystals of the title compound were synthesized from the melts of high purity binary components BaF_2 and ZnF_2 (ratio 1:1) in a graphite crucible under argon atmosphere. The melt has been held at 1073 K for three hours and then slowly cooled down to the solidification temperature.

The present investigation yields the same results as in ref. 1. and $BaZnF_4$ keeps the same structure till 113 K. The isostructural BaMnF4 presents an incommensurate phase below 247 K (see ref. 2). The Raman investigation of $BaZnF_4$ performed in the 10 K - 300 K temperature range shows the occurence of a slow dynamics which could correspond to precursor states of an instability (see ref. 3). A neutron scattering investigation of the low frequency dynamics, at various temperatures has been recently performed.

1. Barium tetrafluorozincate, $BaZnF_4$ at 295 K

BaF_4Zn, orthorhombic, $Cmc2_1$ (No. 36), a =4.1974(6) Å, b =14.546(3) Å, c =5.8391(8) Å, V =356.5 Å^3, Z =4, $R(F)$ =0.027, $R_w(F^2)$ =0.071.

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless sphere, diameter 0.25 mm
Wavelength:	Mo K_α radiation (0.71070 Å)
μ:	176.33 cm^{-1}
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	ω/2θ
$T_{measurement}$:	295 K
$2\theta_{max}$:	100°
$N(hkl)_{unique}$:	1072
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	37
Program:	SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ba	4a	1/2	0.35235(3)	0.4626(1)	0.00653(9)	0.0186(1)	0.0146(1)	0	0	0.0067(1)
Zn	4a	0	0.41317(5)	0[a]	0.0092(2)	0.0086(2)	0.0084(2)	0	0	0.0007(2)
F(1)	4a	0	0.3017(3)	0.2003(9)	0.018(2)	0.010(1)	0.014(2)	0	0	0.001(1)
F(2)	4a	0	0.3326(4)	−0.2705(9)	0.012(2)	0.021(2)	0.015(2)	0	0	−0.007(2)
F(3)	4a	0	0.4715(3)	0.3241(9)	0.022(2)	0.011(1)	0.016(2)	0	0	−0.005(1)
F(4)	4a	1/2	0.4227(5)	0.012(1)	0.008(1)	0.040(3)	0.024(2)	0	0	0.009(2)

a: arbitrabily fixed for definition of the origin

2. Barium tetrafluorozincate, $BaZnF_4$ at 113 K

BaF_4Zn, orthorhombic, $Cmc2_1$ (No. 36), a =4.184(1) Å, b =14.496(4) Å, c =5.825(2) Å, V =353.3 Å^3, Z =4, $R(F)$ =0.024, $R_w(F^2)$ =0.059.

Table 3. Parameters used for the X-ray data collection

Crystal:	colorless sphere, diameter 0.25 mm
Wavelength:	Mo $K\alpha$ radiation (0.71070 Å)
μ:	177.91 cm^{-1}
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	ω/2θ
$T_{measurement}$:	113 K
$2\theta_{max}$:	100°
N(hkl)$_{unique}$:	1060
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
N($param$)$_{refined}$:	37
Program:	SHELXL-93

Table 4. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ba	4a	1/2	0.35232(2)	0.4614(1)	0.00257(7)	0.00830(8)	0.00660(8)	0	0	0.00306(8)
Zn	4a	0	0.41301(4)	0	0.0035(2)	0.0040(2)	0.0039(2)	0	0	0.0002(1)
F(1)	4a	0	0.3020(3)	0.1997(7)	0.010(1)	0.005(1)	0.007(1)	0	0	0.0004(8)
F(2)	4a	0	0.3331(3)	−0.2708(7)	0.007(1)	0.009(1)	0.006(1)	0	0	−0.0002(9)
F(3)	4a	0	0.4709(2)	0.3256(7)	0.010(1)	0.005(1)	0.009(1)	0	0	−0.0024(9)
F(4)	4a	1/2	0.4225(3)	0.0126(8)	0.005(1)	0.016(1)	0.013(1)	0	0	0.004(1)

a: arbitrabily fixed for definition of the origin

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