No. 39A-16 K_2ZnBr_4, Potassium tetrabromozincate

(M = 463.20)

1a Ferroelectricity in K_2ZnBr_4 was first reported by Shimizu et al. in 1990. 90Shi

b Stable transition sequence:

phase	(IV) *)	III	II	I	90Shi
state		F			
crystal system		monoclinic	monoclinic	orhorhombic	
space group		$P2_1-C_2^{2\,a)}$	$P2_1/m-C_{2h}^{2\,a)}$	$Pmcn-D_{2h}^{16\,a)}$	[a]) 94Mas [b]) 90Shi
Θ [K]		93 [b])	155 [b])	491 [c])	[c]) 94Mas

*) Phase was suggested by dielectric anomalies. However, it was not confirmed by other measurements. 90Shi

Metastable transition sequence **):

phase	IVβ	IIIβ	IIβ ***)	I	94Mas
state	(F)	(F)		P	
crystal system	monoclinic	orthorhombic	orthorhombic	orhorhombic	
space group	$Cc-C_s^4$	$P2_1cn-C_{2v}^9$		$Pmcn-C_{2h}^{16}$	
Θ [K]	143	292	561		

**) On cooling from above about 470 K, the crystal undergoes different series of transitions through metastable phases. The metastable phases are denoted by β. 90Shi, 94Mas

***) Incommensurately modulated structure along the c axis.

2a Crystal growth: Bridgman method from melt at about 380 °C, or evaporation method from aqueous solution at 100 °C. 90Shi

3a Unit cell parameters:

phase	T [K]	a [Å]	b [Å]	c [Å]	β [°]	
I	564	7.712(4)	13.344(11)	9.513(6)		94Mas
II	296	9.181(2)	7.499(1)	7.218(1)	108.99(1)	92Kas
III	123	9.018(9)	7.436(7)	7.229(6)	108.77(7)	92Kas

b Z = 4 in phase I, Z = 2 in phases II and III, Z = 12 in phase IIIβ, Z = 48 in phase IVβ. 94Mas
Crystal structure of phase I: Table 39A-16-001.
Crystal structure of phase II: Table 39A-16-002, Table 39A-16-003; Fig. 39A-16-001.
Crystal structure of phase III: Table 39A-16-004, Table 39A-16-005; Fig. 39A-16-002.
See also 93Fab, 94Joc

5a Dielectric constant: Fig. 39A-16-003, Fig. 39A-16-004.
Curie-Weiss law: $\kappa_b = \kappa_\infty + C/(T - \Theta_p)$ with κ_∞ = 8.1, $C = 3.1 \cdot 10^3$ K, Θ_p = 155.2 K. 94Joc
Dielectric dispersion: Fig. 39A-16-005, Fig. 39A-16-006.

c Spontaneous polarization: Fig. 39A-16-007.

6a	Heat capacity: Fig. 39A-16-008, Fig. 39A-16-009. Transition heat and transition entropy of II–I transition: ΔQ_m = 499.7 J mol^{-1}, ΔS_m = 3.91 J K^{-1} mol^{-1}.	95Tak
14a	Bragg reflections due to structural modulation in phase IIβ: Fig. 39A-16-010.	