

No. 39A-13 K₂CoBr₄, Potassium tetrabromocobaltate*(M* = 456.74)

1a	Ferroelectricity in K ₂ CoBr ₄ was first reported by Suzuki et al. in 1990.				90Suz	
b	Stable phases:					
	phase	III	II	I	90Suz	
	state					
	crystal system		monoclinic	orthorhombic	^{a)} 91Mas	
	space group		P2 ₁ /m–C _{2h} ^{2 a)}	Pmcn–D _{2h} ^{16 a)}	^{b)} 90Suz	
	Θ [K]	143 ^{b)}		491 ^{c)} *)	^{c)} 75Sei	
	*) Different values for Θ _{I-I} have been reported: see				87War, 90Suz	
	Metastable phases: **)					
	phase	(IVβ) ***)	IIIβ	IIβ ****)	I	90Suz
	state	F	F		P	
	crystal system		orthorhombic	orthorhombic	orthorhombic	^{a)} 91Mas
	space group		P2 ₁ cn–C _{2v} ^{9 a)}		Pmcn–D _{2h} ^{16 a)}	^{b)} 90Suz
	Θ [K]	143 ^{b)}		303 ^{b)}	555 ^{c)}	^{c)} 91Mas
	Time-dependent transition from metastable to stable phase: see				90Suz	
	**) The high temperature orthorhombic phase can be brought into low temperatures as a metastable phase by quenching from about 200 °C to about – 50 °C within 1 min. On heating the metastable phase undergoes different phase transitions from those in stable state. The metastable phases are denoted by β.				90Suz	
	***) The phase IVβ was suggested by a small anomaly in dielectric constant.				90Suz	
	However, existence of phase IVβ has not been confirmed by other measurements.					
	****) Incommensurately modulated structure along the <i>c</i> axis.					
2a	Crystal growth: Bridgman method from melt.				90Suz	
3a	Unit cell parameters:					
	Phase I: <i>a</i> = 7.68(1) Å, <i>b</i> = 13.32(2) Å, <i>c</i> = 9.51(1) Å at <i>T</i> = 555 K.				91Mas	
	Phase II: <i>a</i> = 9.141(4) Å, <i>b</i> = 7.457(3) Å, <i>c</i> = 7.222(2) Å, β = 108.93(3)° at <i>T</i> = RT.				91Mas	
b	<i>Z</i> = 4 in phase I, <i>Z</i> = 2 in phase II. <i>Z</i> = 12 in phase IIIβ.				91Mas	
5a	Dielectric constant: Fig. 39A-13-001.					
c	Spontaneous polarization: <i>P</i> _s = 1.1 · 10 ^{–5} C m ^{–2} at 201 K.				90Suz	
14a	Bragg reflections due to structural modulation: Fig. 39A-13-002.					