

**No. 39A-17 Rb<sub>2</sub>ZnBr<sub>4</sub>, Rubidium tetrabromozincate***(M* = 555.94)

1a	Ferroelectricity in Rb <sub>2</sub> ZnBr <sub>4</sub> was discovered by Sawada et al. in 1977.					77Saw	
b	phase	V	IV	III	II *)	I	77Saw
	state	(F) <sup>a)</sup>	(F, AF) <sup>a) b)</sup>	F			<sup>a)</sup> 91Yam
	crystal system		monoclinic <sup>c)</sup>	orthorhombic		orthorhombic	<sup>b)</sup> 82Yam
	space group			P2 <sub>1</sub> cn–C <sub>2v</sub> <sup>9</sup>		Pmcn–D <sub>2h</sub> <sup>16</sup>	<sup>c)</sup> 94Kas
	Θ[K]	76.5 <sup>d)</sup>	111.7 <sup>d)</sup>	193.6 <sup>d)</sup>	347 <sup>d)</sup>		<sup>d)</sup> 83Nom
	Another phase was reported to exist below about 50 K, see Fig. 39A-17-004, Fig. 39A-17-007, Fig. 39A-17-008, Fig. 39A-17-020; see also						80Ras
	*) Incommensurate structural modulation was reported along the [001] direction. See 14a.						
	P <sub>s</sub>    [100] in phase III and IV.						77Saw, 91Yam
	Antiferroelectric axis in phase IV:    [010].						82Yam
	P <sub>s</sub> lies in (010) in phase V.						91Yam
	T <sub>melt</sub> = 753 K.						77Saw
	Colorless.						77Saw
	Cleavage plane: (010).						82Yam
	Phase diagram in regard to <i>p</i> : Fig. 39A-17-001;						
	for the low temperature region, some different results were reported: see						87Ale, 92Par, 93Kit1
2a	Crystal growth: solution growth from aqueous solution or melt growth.					77Saw	
3a	Two kinds of settings are currently used for the choice of the unit cell vectors:						
	1: ( <i>a</i> , <i>b</i> , <i>c</i> ), <i>a</i>    <i>P<sub>s</sub></i> in phase III. Space group of phase I: Pmcn.						
	2: ( <i>a'</i> , <i>b'</i> , <i>c'</i> ), <i>b'</i>    <i>P<sub>s</sub></i> in phase III. Space group of phase I: Pcmn.						
	In the following, the choice of setting is additionally written when the case 2 is used.						
	Unit cell parameters:						
	phase I: <i>a</i> = 7.666(3) Å, <i>b</i> = 13.380(2) Å, <i>c</i> = 9.728(1) Å at 368(3) K.						91Nov
	phase II: <i>a</i> = 7.648(2) Å, <i>b</i> = 13.321(1) Å, <i>c</i> = 9.691(1) Å at 293 K for the average structure.						95Nov
	phase III: <i>a</i> = 7.594(4) Å, <i>b</i> = 13.198(5) Å, <i>c</i> = 28.842(9) Å at 140 K.						88Hog
	phase IV, V: <i>a</i> ≈ 2 <i>a</i> <sub>1</sub> , <i>b</i> ≈ 2 <i>b</i> <sub>1</sub> , <i>c</i> ≈ 3 <i>c</i> <sub>1</sub> ; see Fig. 39A-17-002 for β.						94Kas
b	<i>Z</i> = 4 in phase I.					79deP1	
	Positional and temperature parameters: Table 39A-17-001, Table 39A-17-002, Table 39A-17-003, Table 39A-17-004, Table 39A-17-005;						
	see also						95Nov, 96Aze
	Interatomic distances and angles: Table 39A-17-006.						
4	Lattice distortion: Fig. 39A-17-002.						
	Thermal expansion: Fig. 39A-17-003; see also					95She1	
5a	Dielectric constant: Fig. 39A-17-004, Fig. 39A-17-005, Fig. 39A-17-006, Fig. 39A-17-007, Fig. 39A-17-008;						
	see also					78deP1, 81Saw, 81van	

Effect of $p$ : Fig. 39A-17-009; see also Fig. 39A-2-015 in No. 39A-2.					
Memory effect: Fig. 39A-17-010.					
Thermal hysteresis of $\kappa_a$ : see					
b Effect of $E_{\text{bias}}$ on $\kappa$ : Fig. 39A-17-011.					
c Spontaneous polarization and antiferroelectric polarization: Fig. 39A-17-012, Fig. 39A-17-013, Fig. 39A-17-014, Fig. 39A-17-015; see also					
Coercive field: Fig. 39A-17-015.					
Step-like hysteresis loop observed at 0.004 Hz: see					
6a Heat capacity: Fig. 39A-17-016, Fig. 39A-17-017.					
Transition heat, transition entropy: Table 39A-17-007.					
8a Elastic stiffnesses: Table 39A-17-008.					
Sound velocities: Fig. 39A-17-018.					
9a Refractive indices:					
	$T$ [K]	$\lambda$ [nm]	$n_a$	$n_b$	$n_c$
	297(1)	634	1.6518(4)	1.6448(2)	1.6573(2)
	293	589	1.6596(3)	1.6523(3)	1.6642(4)
	297(1)	514.5	1.666	1.659	1.672
Birefringence: Fig. 39A-17-019; see also					
Far-infrared transmission spectra: Fig. 39A-17-020.					
Ultraviolet transmission spectra: see					
b Electrooptic effect and photorefractive effect: Fig. 39A-17-021, Fig. 39A-17-022.					
c Piezoelectric effect: Fig. 39A-17-023.					
d Optical activity: see					
10a Raman scattering: Fig. 39A-17-024, Fig. 39A-17-025; see also					
b Brillouin scattering: Fig. 39A-17-026, Fig. 39A-17-027, Fig. 39A-17-028, Fig. 39A-17-029.					
11 Photoconductivity: Fig. 39A-17-030.					
13a NMR spectra and spin-lattice relaxation time: Fig. 39A-17-031, Fig. 39A-17-032, Fig. 39A-17-033, Fig. 39A-17-034, Fig. 39A-17-035; see also					
<sup>87</sup> Rb quadrupole coupling tensor: Table 39A-17-009; see also					

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NQR: Fig. 39A-17-036; see also	86Ale, 88Bon
NQR under high pressure: Fig. 39A-17-037; see also	87Ale
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14a The diffraction peaks in phase II and III are indexed by four integers $hklm$ defined as $\mathbf{Q} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m(1/3 - \delta)\mathbf{c}^*$ , where $\mathbf{Q}$ is scattering vector and $\delta$ is misfit parameter. Satellite reflections due to structural modulation in phase II: Fig. 39A-17-038, Fig. 39A-17-039, Fig. 39A-17-040, Fig. 39A-17-041; see also	96Aze 79deP2
Effect of $E_{\text{bias}}$ on the satellite reflection intensities in phase II: see	
Intensities of reflections which appear below $\Theta_{\text{V-III}}$ : Fig. 39A-17-042, Fig. 39A-17-043.	
Effect of $p$ on the satellite reflections: Fig. 39A-17-044, Fig. 39A-17-045.	
Anomalous-diffraction studies of modulated structure: see	88Mou
b Neutron diffuse scattering: Fig. 39A-17-046; see also	78deP2
Neutron inelastic scattering: Fig. 39A-17-047, Fig. 39A-17-048, Fig. 39A-17-049; see also	78deP2
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16 Dielectric constants of specimens irradiated with $^2\text{H}^+$ , $^{32}\text{S}^{9+}$ and $\gamma$ -ray: see	88Ben, 95She2
Observation of the incommensurate structure by a transmission electron microscope: see	87Izu
Morphology of single crystals grown in phase II: see	80Jan, 83Dam1, 83Dam2
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