

No. 39A-15 [N(CH₃)₄]₂CuBr₄, Tetramethylammonium tetrabromocuprate
(*M* = 531.45; [D: 555.60])

1a	Ferroelectricity in [N(CH ₃) ₄] ₂ CuBr ₄ was discovered by Wada et al. in 1981.				81Wad	
b	phase	IV	III	II *)	I	81Wad
	state	P	F		P	
	crystal system	monoclinic	orthorhombic		orthorhombic	
	space group	P12 ₁ /c1–C ⁵ _{2h} ^{a)}	Pbc2 ₁ –C ⁵ _{2v} ^{a)}		Pmcn–C ¹⁶ _{2h}	^{a)} 82Has
	Θ[°C]	–37.3 ^{b)}	–33.2 ^{b)}	–2.5 ^{b)}		^{b)} 82Ges2
		[D: –36	–31	–2] ^{c)}		^{c)} 83Ges
	*) Incommensurate structural modulation was found along the <i>b</i> axis. See subsection 14a.					82Has
	Super space group in phase II is P(Pmcn):(s 1 $\bar{1}$).					90Mad
	A high pressure phase was reported at above 2.5 GPa at RT.					95Lor
	<i>P_s</i> [010].					81Wad
	Opaque with dark violet, deliquescent.					81Wad
	ρ _X = 1.91 · 10 ³ kg m ^{–3} .					90Mad
2a	Crystal growth: evaporation method from aqueous solution.					81Wad
b	Crystal form: Fig. 39A-15-001.					
3a	Unit cell parameters:					
	Phase I: <i>a</i> = 9.310(4) Å, <i>b</i> = 15.801(7) Å, <i>c</i> = 12.582(8) Å at 25 °C.					85Has2
	Phase III: <i>a</i> = 9.290(2) Å, <i>b</i> = 31.203(9) Å, <i>c</i> = 12.562(3) Å at –33.5 °C.					85Has2
	For deuterated crystal, <i>a</i> = 9.322(3) Å, <i>b</i> = 15.836(7) Å, <i>c</i> = 12.608(15) Å at 24 °C.					88Has
b	Crystal structure: Fig. 39A-15-002, Fig. 39A-15-003.					
	Positional parameters: Table 39A-15-001, Table 39A-15-002, Table 39A-15-003, Table 39A-15-004, Table 39A-15-005.					
	Temperature dependence of mean-square amplitude: Fig. 39A-15-004.					
4	Thermal expansion: see					91Kah, 84Has
5a	Dielectric constant: Fig. 39A-15-005, Fig. 39A-15-006, Fig. 39A-15-007, Fig. 39A-15-008, Fig. 39A-15-009, Fig. 39A-15-010.					
	Dielectric dispersion: Fig. 39A-15-011.					
	Effect of hydrostatic pressure: Table 39A-15-006, Table 39A-15-007; Fig. 39A-15-012, Fig. 39A-15-013.					
	Phase diagram in regard to <i>p</i> : Fig. 39A-15-014.					
c	Spontaneous polarization: Fig. 39A-15-015, Fig. 39A-15-016.					
6a	Heat capacity: Fig. 39A-15-017.					
	Transition heat, transition entropy: Table 39A-15-008.					
9a	Infrared absorption spectra: see					85Gan
14a	Bragg reflections due to structural modulations: Fig. 39A-15-018; see also					82Has