

**No. 41A-2 KLiSO<sub>4</sub>, Potassium lithium sulfate**

(M = 142.10)

1a	Dielectric anomaly associated with a phase transition was observed in KLiSO <sub>4</sub> and the possibility of ferroelectricity was discussed by Ando in 1962.						62And	
b	phase	VI	V	IV	III	II	I	
	crystal system	mono-clinic	hexagonal	hexagonal	hex-agonal	ortho-rhombic	hexagonal	
	space group	P2 <sub>1</sub> –C <sub>2</sub> <sup>a)</sup>	P6 <sub>3</sub> mc–C <sub>6v</sub> <sup>4 b)</sup> P31c–C <sub>3v</sub> <sup>4 c)</sup>	P6 <sub>3</sub> –C <sub>6</sub> <sup>6 c)</sup>		Pcmn–D <sub>2h</sub> <sup>16 d)</sup> Pc2 <sub>1</sub> n–C <sub>2v</sub> <sup>9 d)</sup>	P6 <sub>3</sub> mc–C <sub>6v</sub> <sup>4 d)</sup> P6 <sub>3</sub> /mmc–D <sub>6h</sub> <sup>4 d)</sup>	a) 89Gli b) 80Ban c) 25Bra d) 88Pie
	Θ [K]	190	245 <sup>d)</sup> 201 <sup>b)</sup> 242 <sup>b)</sup>	333	711 <sup>f)</sup> 708 <sup>g)</sup> 712 <sup>d)</sup>	948 <sup>f)</sup> 942 <sup>g)</sup> 935 <sup>d)</sup>		e) 88Zha f) 85Cac g) 86Sor
	Pyroelectric axis    [001].						25Bra	
	Transparent.						25Bra	
	T <sub>melt</sub> = 998 K.						85Cac	
	ρ <sub>X</sub> = 2.397 · 10 <sup>3</sup> kg m <sup>–3</sup> .						88Zha	
2a	Crystal growth: slow evaporation of aqueous solution of 2 KHSO <sub>4</sub> and Li <sub>2</sub> CO <sub>3</sub> . Amorphous state at $p \geq 1.2 \cdot 10^{10}$ Pa.						62And	
3a	Unit cell parameters:							
	Phase I: $a = 5.295$ Å, $c = 8.706$ Å at 950 K.						88Pie	
	Phase II: See						88Pie	
	Phase III: $a = 5.160(3)$ Å, $c = 8.633(4)$ Å at 398 K.						85Sch	
	$a = 5.160(3)$ Å, $c = 8.634(4)$ Å at 568 K.						85Sch	
	Phase IV: $a = 5.147(3)$ Å, $c = 8.633(4)$ Å at 293 K.						85Sch	
	Phase V: $a = 5.129$ Å, $c = 8.639$ Å at 200 K.						88Zha	
	Phase VI: $a = 5.134(3)$ Å, $b = 5.102(2)$ Å, $c = 8.646(5)$ Å, $\gamma = 119.13(4)^\circ$ at 160 K.						89Gli	
b	Crystal structure of phase III and phase IV: Table 41A-2-001, Table 41A-2-002. Crystal structure of phase IV: Table 41A-2-003; Fig. 41A-2-001, Fig. 41A-2-002. $Z = 2$ in phase V. Crystal structure of phase V (200K): Fig. 41A-2-003, Fig. 41A-2-004. Fractional coordinates and temperature factors: Table 41A-2-004. Interatomic distances: Table 41A-2-005. r.m.s. displacement: Table 41A-2-006; Fig. 41A-2-005.						88Zha	
4	Tensile spontaneous strain and linear thermal expansion coefficient were measured at different heating rates. Temperature dependence of unit cell parameters $a$ and $c$ : Fig. 41A-2-006.						86Kan	
5a	Temperature dependence of dielectric constants: Fig. 41A-2-007, Fig. 41A-2-008, Fig. 41A-2-009. Phase diagram with respect to $p$ : Fig. 41A-2-010. $d\Theta/dp$ : see						85Fuj2	
c	Spontaneous polarization: see						84Fuj	
d	Temperature dependence of pyroelectric coefficient: Fig. 41A-2-011.							
6a	Heat capacity: Fig. 41A-2-012, Fig. 41A-2-013.							
b	Thermal conductivity: Fig. 41A-2-014.							

7a	Temperature dependence of piezoelectric constants: see	82Mro
8a	Temperature dependence of inverse of elastic compliance: Fig. 41A-2-015. Elastic stiffness constant determined by ultrasonic measurement: Fig. 41A-2-016, Fig. 41A-2-017, Fig. 41A-2-018. Elastic stiffness constant determined by Brillouin scattering: Table 41A-2-007, Table 41A-2-008; Fig. 41A-2-019, Fig. 41A-2-020. See also	83Dro, 86Pim
9a	Reflective index: $n_o = 1.4738$ for $\lambda = 546.1$ nm. Birefringence: $\Delta n = 0.0006$ for $\lambda = 546.1$ nm. Temperature dependence of birefringence of (100) plate: Fig. 41A-2-021. See also Optical absorption due to Cu <sup>2+</sup> <sup>a)</sup> , Mn <sup>2+</sup> <sup>b)</sup> , VO <sup>2+</sup> <sup>c)</sup> , Cr <sup>3+</sup> <sup>d)</sup> ions.	30Wes 64Smi  85Iva <sup>a)</sup> 84Lak <sup>b)</sup> 83Lak1 <sup>c)</sup> 83Lak2 <sup>d)</sup> 82Aly
c	Elasto-optic constants at RT: Table 41A-2-009. See also	90Cza
d	Infrared absorption for A and E <sub>1</sub> modes: Fig. 41A-2-022. Electro-optic constant: $ r_{13} - r_{33}  = 1.60(16) \cdot 10^{-12}$ mV <sup>-1</sup> for $\lambda = 546$ nm. Temperature dependence of electro-optic coefficient at 632.8 nm: Fig. 41A-2-023. Optical rotatory power: $\rho = 41(2) \cdot 10^2$ m <sup>-1</sup> for $\lambda = 546$ nm. Optical rotatory power: Table 41A-2-010. Optical activity: see Nonlinear optical susceptibilities: $d_{31}/d_{36}^{\text{KDP}} = 0.8$ , $d_{33}/d_{36}^{\text{KDP}} = 1.5$ at RT for $\lambda = 694.3$ nm.	64Smi 64Smi 79Per 68Son
10a	Raman scattering spectra: Table 41A-2-011, Table 41A-2-012; Fig. 41A-2-024 Fig. 41A-2-025..	
b	Brillouin scattering: temperature dependence of $\rho v^2$ for the longitudinal acoustic wave propagating along [100] direction: Fig. 41A-2-026, along [001] direction: Fig. 41A-2-027. For a longitudinal acoustic wave propagating along [001]: see	89Mro, 87Pim, 86Pim, 83Dro
13a	NMR: temperature dependence of the frequency separation of <sup>7</sup> Li line: Fig. 41A-2-028. NMR of <sup>39</sup> K line: Fig. 41A-2-029, Fig. 41A-2-030, Fig. 41A-2-031, Fig. 41A-2-032, Fig. 41A-2-033. Spin-lattice relaxation time of <sup>39</sup> K: Fig. 41A-2-034.	
b	ESR of SO <sub>4</sub> <sup>-</sup> : Table 41A-2-013. ESR of Cu <sup>2+</sup> : Table 41A-2-014. ESR of Ti <sup>2+</sup> : Fig. 41A-2-035, Fig. 41A-2-036, Fig. 41A-2-037, Fig. 41A-2-038, Fig. 41A-2-039, Fig. 41A-2-041. ESR of CrO <sub>4</sub> <sup>3-</sup> : Fig. 41A-2-040. See also	86YuJ1

For doped $\text{SeO}_4^-$ , see	85Mae
ESR of $\text{Cu}^{2+}$ <sup>a)</sup> , $\text{Tl}^{2+}$ <sup>b)</sup> , $\text{Cr}^{3+}$ <sup>c)</sup> , $\text{NH}_3^+$ <sup>d)</sup> :	<sup>a)</sup> 84Lak <sup>b)</sup> 86Efi <sup>c)</sup> 86Con <sup>d)</sup> 86Mur
See also	86YuJ2
14a Neutron diffraction: Fig. 41A-2-042, Fig. 41A-2-043, Fig. 41A-2-044, Fig. 41A-2-045.	
b Dispersion relation of acoustic mode in phase IV: Fig. 41A-2-046, Fig. 41A-2-047, Fig. 41A-2-048.	
Diffuse scattering at RT: see	94Wel
15a Domain structure in the temperature range 33...300 K: see	85Cac
Wedge-shaped and striped domains were observed by polarized light.	86Sor
Domains were observed by neutron diffraction study in the temperature range 15...189 K.	92Sav