32 KIO_3 family

32A Pure compounds

No. 32A-1 KIO_3, Potassium iodate

(M = 214.00)

1a Ferroelectricity in KIO_3 was discovered by Herlach in 1961. 61Her

b

phase	V	VI	III	II	I
state		F	F	F	
crystal system	triclinic [a])	triclinic [a])	triclinic [b])	monoclinic [c]) [d])	trigonal [c]) [e])
space group	P1–C_1^{1} [a])	P1–C_1^{1} [a])	P1–C_1^{1} [b])	Cm–C_s^{3} [c]) [d])	(R3m–C_{3v}^{5} [c]) [e]) or R3–C_3^{4} [f]))
Θ [°C]	–190 *)	–18, –10 **)	70	212	

61Her

[a]) 85Luc
[b]) 65Fil
[c]) 72Cra
[d]) 73Ham
[e]) 75Cra
[f]) 87Byr

Spontaneous polarization below $\Theta_{II–I}$ consists of two components; $P_s = P_{sp} + P_{sf}$. Pyroelectric component P_{sp} is parallel to the rotation axis 3 of phase I and cannot be reversed by electric field. Ferroelectric component P_{sf} is perpendicular to P_{sp} and parallel to one of the three (pseudo) mirror planes of phase I. P_{sf} can be reoriented among three possible directions, at an angle of 120° to each other, by electric field. 73Shu

T_{melt} = 560 °C. 70Hel

$\rho_X = 3.96 \cdot 10^3$ kg m^{-3} at 300 K. 84Luc

Transparent, colorless.

*) Different value –163 °C was reported. 71Sal

**) –10 °C on heating, –18 °C on cooling. 61Her

2a Crystal growth: hydrothermal method [a]) [b]), temperature-gradient method [c]) [d]), combined method of convection and evaporation [e]).

[a]) 61Her
[b]) 70Hel
[c]) 62Kas
[d]) 70Mat
[e]) 74Ham

Solubility in H_2O: Fig. 32A-1-001.

b Orthogonal coordinate system: $\boldsymbol{Z} \parallel P_{sp}$, $\boldsymbol{Y} \parallel P_{sf}$. The X axis is perpendicular to the mirror or pseudomirror plane in ferroelectric phases. Referring to the pseudocubic cell described in subsection 3a, $\boldsymbol{X} \parallel \langle \bar{1}01 \rangle$, $\boldsymbol{Y} \parallel \langle 1\bar{2}1 \rangle$, $\boldsymbol{Z} \parallel [111]$. 95Hau

3a Unit cell parameters:

phase I: a = 6.404(1) Å, α = 58.33(1)° at 215 °C. 73Ham

a' = 4.4973(1) Å, α' = 89.218(2)° at 523 K. 87Byr

phase II: a = 12.797(2) Å, b = 12.644(2) Å, c = 7.705(1) Å, β = 144.63(1)° at 161 °C. 73Ham

phase III: a = 7.7436(4) Å, b = 7.7183(4) Å, c = 7.7328(5) Å, α = 108.986(4)°, β = 109.449(4)°, γ = 109.209(5)° at 300 K. 84Luc

a = 7.710(10) Å, b = 7.701(7) Å, c = 7.698(6) Å, α = 109.06(6)°, β = 109.27(10)°, γ = 109.20(10)° at RT. 78Kal

phase IV: a = 7.6982(4) Å, b = 7.6597(2) Å, c = 7.6912(5) Å, α = 108.999(5)°, β = 109.745(2)°, γ = 109.085(5)° at 100 K. 85Luc

	phase V: a = 7.6818(5) Å, b = 7.6504(3) Å, c = 7.6896(5) Å, α = 109.062(5)°, β = 109.786(2)°, γ = 109.012(5)° at 10 K. Crystallographic axes $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$ are related with the basic vectors $\boldsymbol{a'}$, $\boldsymbol{b'}$, $\boldsymbol{c'}$ of the pseudocubic cell [87Byr] as follows: In phase I: $\boldsymbol{a} = \boldsymbol{a'} + \boldsymbol{c'}$, $\boldsymbol{b} = \boldsymbol{a'} + \boldsymbol{b'}$, $\boldsymbol{c} = \boldsymbol{b'} + \boldsymbol{c'}$. In phase II: $\boldsymbol{a} = 2\boldsymbol{a'} - 2\boldsymbol{b'}$, $\boldsymbol{b} = 2\boldsymbol{a'} + 2\boldsymbol{b'}$, $\boldsymbol{c} = -\boldsymbol{a'} + \boldsymbol{b'} + \boldsymbol{c'}$. In phase III, IV, V: $\boldsymbol{a} = \boldsymbol{a'} - \boldsymbol{b'} + \boldsymbol{c'}$, $\boldsymbol{b} = \boldsymbol{a'} + \boldsymbol{b'} - \boldsymbol{c'}$, $\boldsymbol{c} = -\boldsymbol{a'} + \boldsymbol{b'} + \boldsymbol{c'}$.	85Luc
b	Z = 2 [a]) or 1 [b]) in phase I; Z = 8 [a]) in phase II; Z = 4 [a]) in phase III. Positional and temperature parameters: Table 32A-1-001, Table 32-A-1-002, Table 32-A-1-003; for phase III see also Interatomic distances and angles: Table 32A-1-004, Table 32A-1-005, Table 32A-1-006. Crystal structures: Fig. 32A-1-002, Fig. 32A-1-003.	[a]) 73Ham [b]) 87Byr 84Luc
4	Lattice distortions: see	61Her, 73Ham, 95Hau
5a	Dielectric constant: Fig. 32A-1-004, Fig. 32A-1-005, Fig. 32A-1-006; see also	 71Sal
b	Effect of E_{bias} on κ: Fig. 32A-1-007.	
c	Spontaneous polarization P_{sf}: Fig. 32A-1-008, Fig. 32A-1-009.	
d	Pyroelectricity: $dP_{sp}/dT = 5.8(5) \cdot 10^{-5}$ C m^{-2} K^{-1} at RT, along [111] direction of the pseudocubic cell.	72Cra
6a	Transition enthalpy and entropy measured by differential scanning calorimetry: ΔH_{III-II} = 46 J mol^{-1}, ΔS_{III-II} = 0.13 J K^{-1} mol^{-1}; ΔH_{II-I} = 46 J mol^{-1}, ΔS_{II-I} = 0.09 J K^{-1} mol^{-1}.	85Loi
7a	Piezoelectric constants and piezoelectric coupling coefficients: Table 32A-1-007; see also	 71Sal, 72Sal
8a	Elastic stiffness: Table 32A-1-008; Fig. 32A-1-010.	
9a	Refractive indices: Table 32A-1-009; see also Optical axial angle: Fig. 32A-1-011, Fig. 32A-1-012. Birefringence: Fig. 32A-1-012. Optical absorption: see Optical reflectance: see Infrared spectra: see	87Yin 67Ver, 89Xia 89Sza 72Bai, 73Bal, 75Bai2
b	Electrooptic effect: Fig. 32A-1-013; see also	72Sal
e	Susceptibility for second harmonic generation: $d_{23} = 1.2 \left\| d_{31}^{LiIO_3} \right\|$, $d_{21} = 1.8 \left\| d_{31}^{LiIO_3} \right\|$ See subsection 2b for orthogonal coordinate system. SHG: see	92Yin1 65Fil, 69Ber, 93Xiu
10a	Raman scattering: see	73Bal, 74Sal

11	Electrical conductivity: Fig. 32A-1-014.	
13a	NQR: Table 32A-1-010; Fig. 32A-1-015, Fig. 32A-1-016, Fig. 32A-1-017; see also	61Her, 75Bai2, 81Bai
c	Mössbauer effect: Fig. 32A-1-018, Fig. 32A-1-019.	
16	Detwinning or poling procedure: see	72Cra, 73Shu, 91Xiu, 92Yin2