Table 32A-1-001. KIO_3. Fractional coordinates and equivalent isotropic temperature parameters [$Å^2$] in phase I at T = 523K [87Byr]. Neutron powder diffraction (Rietvelt method). Space group: R3– C_3^4. When the structure was analyzed with space group R3m– C_{3v}^5, fractional coordinates of O atom converged to $x = y = 0.0408(5)$. $B_{eq} = 4\Sigma b_{ij}\boldsymbol{a}_i \cdot \boldsymbol{a}_j/3$, where b_{ij} is defined by Eq. (b) in Introduction.

	x	y	z	B_{eq} [$Å^2$]
K	0.51117(90)	x	x	3.85(6)
I	0.00000	x	x	1.79(4)
O	0.02804(150)	0.05498(153)	–0.39094(47)	5.93(24)

Table 32A-1-002. KIO_3. Fractional coordinates and anisotropic temperature parameters [$Å^2$] in phase III at RT [78Kal]. B_{ij} is defined by Eq. (a) in Introduction.

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{23}	B_{13}
I_1	0	0	0	0.0063(2)	0.0054(2)	0.0057(2)	0.0052(3)	0.0046(3)	0.0056(3)
I_2	–0.0132(1)	0.5067(1)	0.5076(1)	0.0046(2)	0.0049(2)	0.0055(2)	0.0033(3)	0.0038(3)	0.0042(3)
I_3	0.4936(1)	–0.0022(1)	0.5092(1)	0.0062(2)	0.0048(2)	0.0054(2)	0.0038(3)	0.0034(3)	0.0049(3)
I_4	0.4928(1)	0.4913(1)	0.0163(1)	0.0057(2)	0.0050(2)	0.0058(2)	0.0044(3)	0.0048(3)	0.0057(3)
K_1	0.0072(5)	0.0208(5)	0.5116(5)	0.014(1)	0.009(1)	0.016(1)	0.007(1)	0.010(1)	0.016(2)
K_2	0.0047(4)	0.5122(4)	0.0179(4)	0.010(1)	0.011(1)	0.011(1)	0.007(1)	0.005(1)	0.005(2)
K_3	0.5145(4)	0.0023(5)	0.0211(5)	0.011(1)	0.015(1)	0.011(1)	0.013(1)	0.012(2)	0.008(1)
K_4	0.4965(4)	0.5084(4)	0.5292(5)	0.012(1)	0.010(1)	0.010(1)	0.010(1)	0.005(1)	0.009(1)
O_{11}	0.079(1)	–0.152(2)	–0.154(2)	0.008(2)	0.016(2)	0.023(3)	0.002(3)	–0.029(4)	0.005(4)
O_{12}	0.793(1)	–0.199(1)	–0.007(2)	0.017(2)	0.015(2)	0.021(3)	0.012(4)	0.016(4)	0.016(4)
O_{13}	0.845(1)	0.046(2)	0.192(1)	0.013(2)	0.029(3)	0.015(2)	0.027(4)	0.026(4)	0.010(3)
O_{21}	–0.007(1)	0.303(1)	0.317(1)	0.018(2)	0.014(2)	0.021(2)	0.011(4)	–0.013(4)	0.021(4)
O_{22}	0.791(1)	0.343(1)	0.539(2)	0.015(2)	0.015(2)	0.032(3)	0.012(3)	0.033(4)	0.033(4)
O_{23}	0.841(2)	0.586(1)	0.341(2)	0.026(3)	0.013(2)	0.023(3)	0.016(4)	0.016(4)	–0.004(5)
O_{31}	0.533(2)	–0.156(1)	0.309(1)	0.035(3)	0.016(2)	0.019(2)	0.033(5)	0.011(4)	0.034(5)
O_{32}	0.342(1)	–0.203(1)	0.548(2)	0.016(2)	0.012(2)	0.030(3)	0.007(3)	0.028(4)	0.028(4)
O_{33}	0.287(1)	0.024(2)	0.346(1)	0.013(2)	0.029(3)	0.020(2)	0.021(4)	0.034(4)	0.011(4)
O_{41}	0.345(1)	0.339(1)	0.095(1)	0.015(1)	0.016(2)	0.010(2)	–0.020(3)	0.009(3)	0.004(3)
O_{42}	0.286(1)	0.485(1)	–0.188(1)	0.015(2)	0.016(2)	0.021(2)	0.009(4)	0.012(4)	–0.006(4)
O_{43}	0.528(2)	0.297(1)	–0.149(1)	0.036(3)	0.012(2)	0.017(2)	0.030(4)	0.007(3)	0.034(4)

Table 32A-1-003. KIO_3. Fractional coordinates and isotropic temperature parameters [$Å^2$] in phase IV (T = 100 K) and phase V (T = 10 K) [85Luc]. Neutron powder diffraction (Rietvelt method). For each atom, the values for phase IV and phase V are listed in the first and the second lines, respectively. Isotropic temperature parameters were constrained to equal values for each element-type atom. B is defined by Eq. (e) in Introduction.

	x	y	z	B [$Å^2$]
K(1)	–0.0063(51)	0.0266(45)	0.4832(59)	
	–0.0520(49)	0.0389(39)	0.5042(47)	
K(2)	–0.0135(68)	0.4926(61)	0.0022(70)	
	–0.0001(58)	0.4989(54)	–0.0119(55)	0.52(13)
K(3)	0.5117(48)	–0.0027(34)	0.0277(53)	0.34(10)
	0.5012(44)	0.0172(42)	0.0166(47)	
K(4)	0.5014(56)	0.5131(62)	0.5435(66)	
	0.5023(54)	0.5281(54)	0.5212(62)	
I(1)	0.0000	0.0000	0.0000	
	0.0000	0.0000	0.0000	
I(2)	–0.0128(44)	0.5109(35)	0.5060(46)	
	–0.0112(41)	0.5229(35)	0.4890(41)	0.33(6)
I(3)	0.4898(49)	0.0002(50)	0.5208(50)	0.07(8)
	0.4775(47)	0.0200(55)	0.5092(46)	
I(4)	0.5032(45)	0.4879(36)	0.0096(42)	
	0.4891(37)	0.5009(38)	0.0035(38)	
O(11)	0.0697(52)	–0.1727(41)	–0.1360(46)	
	0.0650(44)	–0.1699(41)	–0.1229(41)	
O(12)	0.7789(44)	–0.1952(39)	0.0040(45)	
	0.7668(41)	–0.1819(46)	–0.0169(40)	
O(13)	0.8567(46)	0.0379(47)	–0.2163(50)	
	0.8380(37)	0.0304(42)	–0.2217(36)	
O(21)	0.0308(40)	0.3478(36)	0.3028(45)	
	0.0216(35)	0.3622(37)	0.2938(36)	
O(22)	0.7896(46)	0.3167(38)	0.5014(42)	
	0.7687(41)	0.3270(37)	0.4976(39)	
O(23)	0.8542(41)	0.6065(35)	0.3518(43)	
	0.8298(39)	0.6192(39)	0.3591(40)	0.94(3)
O(31)	0.4987(45)	–0.1746(39)	0.2867(45)	0.45(3)
	0.4910(34)	–0.1666(35)	0.2914(35)	
O(32)	0.3648(48)	–0.1920(45)	0.5799(51)	
	0.3249(48)	–0.1852(43)	0.5628(42)	
O(33)	0.2909(46)	0.0333(38)	0.3685(41)	
	0.2745(44)	0.0601(45)	0.3687(47)	
O(41)	0.3535(55)	0.3207(48)	0.0935(50)	
	0.3549(42)	0.3229(44)	0.0820(39)	
O(42)	0.2839(38)	0.4591(31)	–0.2000(40)	
	0.2747(39)	0.4706(35)	–0.2091(39)	
O(43)	0.5678(44)	0.3078(40)	–0.1335(45)	
	0.5778(43)	0.3420(42)	–0.1366(42)	

Table 32A-1-004. KIO_3. Interatomic distances [Å] and angles [°] in phase I at T = 523 K [87Byr]. The structure was analyzed with space group R3– C_3^4.

IO_3 group		K polyhedra	
I–O	1.775(5)	K...O	3.032(7)
O–I–O	100.8(3)		3.111(8)
			3.280(7)
			3.434(8)

Table 32A-1-005. KIO_3. Interatomic distances [Å] in phase III at RT [78Kal].

IO_3-group							
I_1–O_{11}	1.785(1)	I_2–O_{21}	1.793(1)	I_3–O_{31}	1.795(1)	I_4–O_{41}	1.757(1)
O_{12}	1.780(1)	O_{22}	1.768(1)	O_{32}	1.782(1)	O_{42}	1.810(1)
O_{13}	1.789(1)	O_{23}	1.816(1)	O_{33}	1.792(1)	O_{43}	1.782(1)
...O_{41}	2.702(3)	...O_{11}	2.697(3)	...O_{13}	2.727(3)	...O_{23}	2.659(3)
...O_{33}	2.748(3)	...O_{32}	2.748(3)	...O_{43}	2.737(3)	...O_{31}	2.747(3)
...O_{21}	2.802(3)	...O_{42}	2.787(3)	...O_{23}	2.753(3)	...O_{12}	2.826(3)
O_{11}–O_{12}	2.767(3)	O_{21}–O_{22}	2.682(3)	O_{31}–O_{32}	2.747(3)	O_{41}–O_{42}	2.749(3)
O_{13}	2.722(3)	O_{23}	2.783(3)	O_{33}	2.725(3)	O_{43}	2.698(3)
O_{12}–O_{13}	2.717(3)	O_{22}–O_{23}	2.786(3)	O_{32}–O_{33}	2.732(3)	O_{42}–O_{43}	2.714(3)
K-polyhedra							
K_1–O_{23}	2.788(3)	K_2–O_{13}	3.002(3)	K_3–O_{11}	2.799(3)	K_4–O_{41}	2.791(3)
O_{33}	2.834(4)	O_{43}	3.062(3)	O_{31}	2.840(3)	O_{32}	2.834(3)
O_{13}	2.930(3)	O_{22}	3.070(4)	O_{43}	2.962(3)	O_{22}	2.939(3)
O_{42}	3.002(3)	O_{42}	3.102(3)	O_{32}	3.031(3)	O_{12}	3.003(3)
O_{21}	3.018(3)	O_{23}	3.120(4)	O_{12}	3.059(3)	O_{33}	3.099(4)
O_{31}	3.037(4)	O_{12}	3.179(4)	O_{21}	3.089(3)	O_{42}	3.127(3)
O_{11}	3.242(4)	O_{21}	3.220(4)	O_{41}	3.240(4)	O_{21}	3.209(4)
O_{12}	3.297(4)	O_{11}	3.247(4)	O_{42}	3.294(4)	O_{43}	3.364(4)
O_{43}	3.359(4)	O_{41}	3.294(4)	O_{22}	3.348(4)	O_{23}	3.397(4)
O_{22}	3.406(4)	O_{33}	3.294(4)	O_{13}	3.444(4)	O_{13}	3.463(4)
		O_{31}	3.392(4)	O_{33}	3.491(4)		
		O_{32}	3.409(4)				

Table 32A-1-006. KIO_3. Interatomic distances [Å] and angles [°] in phase IV at T = 100 K (first column) and phase V at T = 10 K (second column) [85Luc].

IO_3 groups											
I(1)–O(11)	1.75(4)	1.66(4)	I(2)–O(21)	1.86(5)	1.76(4)	I(3)–O(31)	1.90(5)	1.87(5)	I(4)–O(41)	1.86(6)	1.82(5)
O(12)	1.88(3)	1.81(3)	O(22)	1.73(5)	1.90(4)	O(32)	1.76(6)	1.89(5)	O(42)	1.78(4)	1.77(4)
O(13)	1.83(4)	1.88(3)	O(23)	1.80(5)	1.81(5)	O(33)	1.74(5)	1.76(5)	O(43)	1.79(5)	1.81(5)
...O(41)	2.67(4)	2.71(3)	...O(11)	2.71(5)	2.85(4)	..O(13)	2.72(5)	2.80(5)	...O(23)	2.66(4)	2.67(4)
...O(33)	2.82(3)	2.68(4)	...O(32)	2.77(5)	2.53(5)	...O(43)	2.63(5)	2.65(5)	...O(31)	2.78(5)	2.77(4)
...O(21)	2.78(3)	2.86(3)	...O(42)	2.86(4)	2.85(4)	...O(22)	2.83(5)	2.72(5)	...O(12)	2.68(5)	2.75(5)
O(11)–O(12)	2.77(6)	2.66(5)	O(21)–O(22)	2.78(5)	2.88(5)	O(31)–O(32)	2.80(6)	2.81(5)	O(41)–O(42)	2.76(5)	2.80(5)
O(13)	2.71(6)	2.75(5)	O(23)	2.75(5)	2.83(5)	O(33)	2.68(5)	2.83(5)	O(43)	2.78(6)	2.78(5)
O(12)–O(13)	2.89(6)	2.66(5)	O(22)–O(23)	2.80(5)	2.75(5)	O(32)–O(33)	2.79(5)	2.79(6)	O(42)–O(43)	2.77(5)	2.77(5)
			O(11)–I(1)–O(12)	99.5(1.6)	100.2(1.6)	O(31)–I(3)–O(32)	99.7(2.3)	96.6(2.2)			
			O(11)–I(1)–O(13)	98.4(1.7)	101.8(1.5)	O(31)–I(3)–O(33)	94.8(2.2)	102.4(2.1)			
			O(12)–I(1)–O(13)	102.5(1.6)	92.6(1.5)	O(32)–I(3)–O(33)	105.8(2.5)	100.2(2.4)			
			O(21)–I(2)–O(22)	101.2(1.9)	104.1(1.7)	O(41)–I(4)–O(42)	98.5(2.1)	102.5(1.9)			
			O(21)–I(2)–O(23)	97.2(2.3)	105.3(2.1)	O(41)–I(4)–O(43)	99.3(2.2)	99.7(2.2)			
			O(22)–I(2)–O(23)	105.2(2.2)	95.8(2.0)	O(42)–I(4)–O(43)	101.7(2.0)	101.4(1.9)			
K polyhedra											
K(1)–O(33)	2.71(6)	3.00(6)	K(2)–O(43)	2.70(6)	2.74(5)	K(3)–O(31)	2.73(6)	2.90(5)	K(4)–O(41)	2.89(6)	2.82(5)
O(23)	2.72(4)	2.73(4)	O(13)	2.95(6)	2.99(5)	O(11)	2.83(5)	2.80(5)	O(32)	2.76(7)	2.92(6)
O(13)	2.84(7)	2.53(5)	O(21)	2.84(7)	2.85(6)	O(12)	2.92(5)	2.95(5)	O(12)	2.95(6)	2.95(5)
O(42)	2.85(5)	2.86(5)	O(22)	3.21(6)	3.13(5)	O(43)	3.00(5)	3.06(5)	O(21)	3.02(5)	3.07(5)
O(21)	3.18(6)	3.37(5)	O(23)	3.15(7)	3.51(6)	O(32)	2.88(5)	2.88(5)	O(22)	3.11(6)	2.95(6)
O(31)	3.15(5)	2.88(5)	O(11)	3.05(7)	2.88(6)	O(22)	3.06(5)	3.08(5)	O(42)	3.03(7)	3.18(6)
O(12)	3.03(5)	3.33(5)	O(12)	3.28(7)	3.47(6)	O(42)	3.41(4)	3.46(4)	O(33)	3.06(5)	3.01(5)
O(22)	3.11(6)	2.96(5)	O(42)	3.20(7)	3.01(6)	O(41)	3.07(6)	2.88(5)	O(23)	3.49(6)	3.15(6)
O(11)	3.69(6)	3.71(5)	O(31)	3.29(6)	3.17(5)	O(21)	3.35(5)	3.34(5)	O(31)	3.56(7)	3.36(6)
O(32)	3.74(6)	3.79(6)	O(41)	3.45(7)	3.39(6)	O(33)	3.56(6)	3.67(6)	O(43)	3:33(7)	
O(41)		3.75(5)	O(33)	3.49(6)	3.63(6)	O(13)	3.73(6)	3.64(5)	O(13)	3.41(6)	3.23(5)
			O(32)	3.70(6)	3.64(6)				O(11)	3.60(6)	3.59(6)

Table 32A-1-007. KIO_3. Static piezoelectric constants [$\cdot 10^{-12}$ C N^{-1}] and piezocoupling coefficients at T = 293 K [95Hau].The specimen was twinned weakly. Piezoelectric behavior was compatible with point group m even though the point group of phase III is 1. See subsection 2b for orthogonal coordinate system.

d_{15}	d_{16}	d_{21}	d_{22}	d_{23}	d_{24}	d_{31}	d_{32}	d_{33}
1(1)	105(7)	105(6)	–108(7)	5(2)	12(3)	–12(3)	0(2)	35(3)

k_t = 0.42 (longitudinal wave propagating along Z_{axis})
k'_{66} = 0.60 (quasi-transversal wave propagating along X_{axis} with displacement near Y_{axis})

Table 32A-1-008. KIO_3. Elastic stiffnesses [$\cdot 10^{10}$ N m^{-2}] and thermoelastic constants $T_{\lambda\mu}$ [$\cdot 10^{-3}$ K^{-1}] [95Hau]. T = 293K. $T_{\lambda\mu}$ = d log $c_{\lambda\mu}$/dT. The specimen was twinned weakly. The elastic behavior was well compatible with point group 3m. See subsection 2b for orthogonal coordinate system.

c_{11}^E	3.983(6)	T_{11}^E	–0.39(2)
c_{13}^E	2.00(15)	$\lvert T_{13}^E \rvert$	< 0.6
c_{14}^E	0.28(2)	T_{14}^E	1.8(10)
c_{33}^D	3.988	T_{33}^D	–0.57(3)
c_{44}^E	1.639(7)	T_{44}^E	–0.79(5)
c_{66}^E	0.578(3)	T_{66}^E	–4.85(10)

Table 32A-1-009. KIO_3. Refractive indices [92Yin1]. T = RT. Principal axes of refractive indices are parallel to orthogonal coordinate system described in subsection 2b.

λ [Å]	4358	4861	5461	5893	6563	7065
n_X	1.8831	1.8599	1.8419	1.8329	1.8227	1.8172
n_Y	1.8867	1.8630	1.8448	1.8358	1.8255	1.8199
n_Z	1.7283	1.7138	1.7024	1.6967	1.6899	1.6863

Table 32A-1-010. KIO_3. Nuclear quadrupole resonance frequencies ν, the quadrupole coupling constant e^2Qq_{zz}/h, and the asymmetric parameters η of ^{127}I [75Bai1]. n: number of lines in the NQR spectrum. Values for $T = 298$ K are from [56Lud].

T	$\nu(\pm\frac{1}{2} \leftrightarrow \pm\frac{3}{2})$	$\nu(\pm\frac{3}{2} \leftrightarrow \pm\frac{5}{2})$	n	e^2Qq_{zz}/h	η
[K]	[MHz]	[MHz]		[MHz]	[%]
4.2	150.567		3		
	149.837				
	149.786				
20	150.548		3		
	149.827				
	149.772				
77	150.046	299.925	4	999.83	2.1
	149.943	299.475		998.45	3.3
	149.256	298.350		994.58	2.1
	149.188	298.200		994.10	1.4
116	149.422		3		
	149.106				
	148.513				
161	148.654	296.930	3	989.98	3.1
	148.190	296.019		986.92	3.1
	147.666	295.050		983.65	2.7
252	146.736		3		
	146.180				
	145.646				
298	145.38	290.71	3	969.0	
	144.91	289.85		966.2	
	144.37	288.82		962.7	
329	144.423		3		
	144.016				
	143.617				
344	142.964		1		
366	142.323		1		