Table 32A-3-001. α-$KIO_3 \cdot HIO_3$. Fractional coordinates in phase I at RT [78Tre1]. X-ray data are given in the first column and neutron data in the second. Used crystallographic axes are (*a*′, *b*′, *c*′), the second setting of cell defined in subsection 3b.

Atom	*x*		*y*		*z*	
I(1)	0.12580(2)	0.1261(3)	0.07331(2)	0.0731(3)	0.19741(2)	0.1968(3)
I(2)	0.49283(2)	0.4934(2)	0.29601(2)	0.2956(3)	0.43529(2)	0.4349(5)
K	0.79808(7)	0.7977(4)	0.15951(9)	0.1596(5)	0.24710(12)	0.2478(7)
O(11)	0.0595(3)	0.0589(3)	0.1858(4)	0.1854(4)	0.0482(3)	0.0474(4)
O(12)	0.2278(3)	0.2277(3)	0.2337(4)	0.2335(4)	0.3470(4)	0.3479(4)
O(13)	–0.0303(2)	–0.0301(2)	–0.0132(3)	–0.0125(3)	0.3381(3)	0.3371(3)
O(21)	0.6742(2)	0.6735(2)	0.3491(3)	0.3487(3)	0.4566(3)	0.4574(3)
O(22)	0.4606(2)	0.4604(3)	0.3868(3)	0.3875(3)	0.6416(3)	0.6406(3)
O(23)	0.4275(2)	0.4270(3)	0.0822(2)	0.0827(3)	0.5292(3)	0.5293(4)
H(1)		0		0.5		0
H(2)		0.5		0.5		0

Table 32A-3-002. α-$KIO_3 \cdot HIO_3$. Interatomic distances [Å] and angles in phase I at RT [78Tre1]. X-ray data are given in the first column and neutron data in the second. Symmetry operated atoms are denoted by *.

$I_{(1)}$ group			$I_{(2)}$ group		
$I_{(1)}$–$O_{(11)}$	1.784(3)	1.789(5)	$I_{(2)}$–$O_{(21)}$	1.804(2)	1.792(3)
–$O_{(12)}$	1.787(3)	1.792(4)	–$O_{(22)}$	1.814(2)	1.818(4)
–$O_{(13)}$	1.858(2)	1.856(3)	–$O_{(23)}$	1.845(2)	1.843(4)
...$O_{(21)}$	2.660(3)	2.655(4)	...$O_{(23)}$*	2.653(2)	2.649(4)
...$O_{(11)}$*	2.979(3)	2.969(4)	...$O_{(13)}$*	2.729(3)	2.734(4)
...$O_{(12)}$*	3.500(3)	3.497(4)	...$O_{(23)}$*	2.846(3)	2.850(4)
$O_{(13)}$...H...$O_{(12)}$*	2.483(3)	2.497(4)	$O_{(23)}$...H...$O_{(23)}$*	2.490(3)	2.500(4)
$O_{(11)}$–I–$O_{(12)}$	102°21′ (10)	102°36′ (12)	$O_{(21)}$–I–$O_{(22)}$	99°53′ (6)	99°50′ (12)
$O_{(11)}$–I–$O_{(13)}$	95°33′ (9)	95°00′ (12)	$O_{(21)}$–I–$O_{(23)}$	100°24′ (9)	100°46′ (12)
$O_{(12)}$–I–$O_{(13)}$	98°20′ (6)	97°54′ (10)	$O_{(22)}$–I–$O_{(23)}$	92°50′ (9)	92°54′ (12)

Table 32A-3-003. β-$KIO_3 \cdot HIO_3$. Fractional coordinates and equivalent isotropic temperature parameters at RT [85Sor]. $B_{eq} = 8\ \pi^2(\sigma_1\sigma_2\sigma_3)^{2/3}$, where the σ_i's are the semiaxes of the corresponding thermal vibration ellipsoids.

Atom	*x*	*y*	*z*	B_{eq} [Å^2]
I(1)	0.3276(2)	0.1921(3)	0.0008(1)	0.42
I(2)	0.2271(3)	0.6916(3)	0.0046(1)	0.59
I(3)	0.3161(3)	0.0528	0.3308(2)	0.85
I(4)	0.2533(3)	0.4644(4)	0.1893(1)	0.90
K(1)	0.0154(6)	0.4797(7)	0.3530(2)	1.60
K(2)	0.0348(6)	0.0055(7)	0.1570(2)	1.78
O(11)	0.1498(3)	0.2764(4)	0.9610(2)	1.18
O(12)	0.4407(3)	0.3935(3)	0.9866(1)	0.94
O(13)	0.2871(3)	0.2185(4)	0.0900(1)	1.33
O(21)	0.1252(3)	0.8957(3)	0.0246(1)	1.04
O(22)	0.4160(3)	0.7886(4)	0.0352(2)	1.16
O(23)	0.2540(4)	0.7203(4)	0.9144(1)	1.46
O(31)	0.2723(4)	0.9197(4)	0.2554(1)	1.68
O(32)	0.1252(3)	0.1243(4)	0.3556(1)	1.48
O(33)	0.3909(3)	0.2410(3)	0.2858(2)	1.54
O(41)	0.1909(4)	0.6455(4)	0.1361(1)	1.85
O(42)	0.2555(3)	0.5916(3)	0.2715(1)	1.31
O(43)	0.0738(3)	0.3524(4)	0.2045(1)	1.64
H(22)	0.0086(5)	0.2442(6)	0.0037(3)	2.32
H(42)	0.7595(6)	0.2682(6)	0.2628(3)	2.45

Table 32A-3-004. β-$KIO_3 \cdot HIO_3$. Interatomic distances [Å] at RT [85Sor].

IO_3 group							
I(1)–O(11)	1.830(1)	I(2)–O(21)	1.808(1)	I(3)–O(31)	1.821(1)	I(4)–O(41)	1.794(1)
–O(12)	1.819(1)	–O(22)	1.880(1)	–O(32)	1.795(1)	–O(42)	1.870(1)
–O(13)	1.791(1)	–O(23)	1.792(1)	–O(33)	1.784(1)	–O(43)	1.784(1)
–O(21)	2.687(1)	–O(12)	2.572(1)	–O(23)	3.044(1)	–O(13)	2.695(1)
–O(21)	2.864(1)	–O(41)	2.615(1)	–O(32)	3.014(1)	–O(33)	2.789(1)
–O(32)	2.915(1)	–O(12)	2.918(1)	–O(11)	3.064(1)	–O(43)	3.098(1)
O(11)–O(12)	2.701(2)	O(21)–O(22)	2.638(1)	O(31)–O(32)	2.793(2)	O(41)–O(42)	2.735(1)
–O(13)	2.821(1)	–O(23)	2.758(1)	–O(33)	2.686(2)	–O(43)	2.765(1)
O(12)–O(13)	2.751(1)	O(22)–O(23)	2.792(1)	O(32)–O(33)	2.803(1)	O(42)–O(43)	2.718(1)
K polyhedron				Hydrogen contacts			
K(1)–O(33)	2.696(1)	K(2)–O(43)	2.783(1)	O(22)–H(22)...O(11)		O(42)–H(42)...O(31)	
–O(12)	2.719(2)	–O(21)	2.820(1)	O(22)–O(11)	2.530(1)	O(42)–O(31)	2.487(1)
–O(42)	2.743(1)	–O(31)	2.885(1)	O(22)–H(22)	1.045(2)	O(42)–H(42)	1.067(2)
–O(42)	2.799(1)	–O(13)	2.980(1)	O(11)...H(22)	1.481(2)	O(31)...H(42)	1.422(2)
–O(32)	2.831(1)	–O(22)	2.997(1)				
–O(23)	2.941(1)	–O(31)	3.015(1)				
–O(23)	3.013(1)	–O(13)	3.032(1)				
–O(43)	3.099(1)	–O(41)	3.066(1)				
–O(11)	3.136(1)	–O(33)	3.361(1)				

Table 32A-3-005. γ-$KIO_3 \cdot HIO_3$. Fractional coordinates and anisotropic temperature parameters [$\cdot 10^{-5}$ Å^2] at RT [72Kem]. Fractional coordinates of H atoms are obtained by neutron powder diffraction. U_{ij} is defined by Eq. (d) in Introduction.

Atom	*x*	*y*	*z*
I(1)	0.16889(3)	0.10453(3)	0.65738(1)
I(2)	0.23147(3)	0.38738(3)	0.49976(1)
I(3)	0.66774(3)	0.36784(3)	0.65626(1)
I(4)	0.65247(3)	0.86048(3)	0.63591(1)
K(1)	0.24947(13)	0.87591(13)	0.50359(5)
K(2)	0.14460(14)	0.61345(12)	0.67125(5)
O(11)	0.0535(5)	0.2717(4)	0.6927(2)
O(12)	0.0155(5)	0.9355(4)	0.6699(2)
O(13)	0.0975(5)	0.1415(5)	0.5763(2)
O(21)	–0.0037(5)	0.3582(5)	0.4567(2)
O(22)	0.3206(5)	0.5460(4)	0.4534(2)
O(23)	0.3525(5)	0.2076(4)	0.4744(2)
O(31)	0.4144(4)	0.3927(4)	0.6357(2)
O(32)	0.6466(5)	0.2739(5)	0.7345(2)
O(33)	0.7436(5)	0.5655(4)	0.6852(2)
O(41)	0.4024(5)	0.8100(5)	0.6270(2)
O(42)	0.6652(5)	0.9005(4)	0.7239(2)
O(43)	0.6237(5)	0.0681(4)	0.6097(2)
H(1)	0.552(4)	0.320(4)	0.754(1)
H(2)	0.773(4)	0.842(4)	0.747(1)

Atom	U_{11}	U_{22}	U_{33}	$2U_{12}$	$2U_{23}$	$2U_{13}$
I(1)	1194(8)	1535(9)	1627(10)	–113(15)	–214(16)	227(14)
I(2)	1541(9)	1397(9)	1070(8)	90(15)	52(15)	378(14)
I(3)	1307(8)	1111(8)	1592(9)	–9(14)	–67(15)	287(14)
I(4)	1247(8)	1153(8)	1523(9)	14(14)	324(15)	630(13)
K(1)	1886(38)	2223(41)	1729(37)	–192(62)	435(65)	439(60)
K(2)	1891(38)	1708(37)	2728(46)	–331(61)	52(68)	133(67)
O(11)	2135(148)	1992(145)	2562(167)	180(229)	–1273(249)	817(248)
O(12)	1467(131)	2130(151)	3589(205)	–649(222)	1037(279)	556(257)
O(13)	2284(150)	3400(191)	1514(134)	–577(273)	–74(268)	–156(225)
O(21)	1657(132)	3380(189)	1947(147)	–208(256)	–142(274)	–692(218)
O(22)	2873(167)	2062(147)	1987(152)	–1001(251)	866(240)	1582(257)
O(23)	2381(150)	1794(137)	1934(144)	1003(225)	–258(224)	907(207)
O(31)	1089(111)	2555(153)	2347(151)	392(213)	–5(250)	–370(207)
O(32)	2598(167)	3129(183)	1893(152)	2065(277)	1450(268)	1200(255)
O(33)	2810(168)	1545(135)	2787(180)	–655(239)	–1203(249)	–649(274)
O(41)	1212(124)	3601(192)	2379(165)	–721(246)	337(289)	564(225)
O(42)	2066(137)	2295(146)	1409(123)	–16(228)	85(220)	616(210)
O(43)	3208(172)	1428(126)	1980(148)	860(236)	843(220)	959(257)

Table 32A-3-006. (a) γ-$KIO_3 \cdot HIO_3$. Interatomic distances [Å] and angles [°] at RT [72Kem].

Bond	Length [Å]	Average length [Å]
I(3)–O(31)	1.786 (1.792)	
I(3)–O(33)	1.795 (1.803)	1.792 (1.799)
I(4)–O(41)	1.789 (1.795)	
I(4)–O(43)	1.800 (1.806)	
I(2)–O(21)	1.800 (1.807)	
I(2)–O(22)	1.814 (1.820)	
I(2)–O(23)	1.827 (1.834)	1.810 (1.817)
I(1)–O(11)	1.819 (1.826)	
I(1)–O(12)	1.801 (1.806)	
I(1)–O(13)	1.799 (1.806)	
I(3)–O(32)	1.898 (1.904)	
I(4)–O(42)	1.939 (1.943)	1.919 (1.924)

(b) I...O and K...O distances smaller than 3.5 Å.

Bond	Distance [Å]	Symmetry*	Bond	Distance [Å]	Symmetry*
I(1)–O(31)	3.003	1*	I(3)–O(22)	2.509	2
O(41)	3.045	1*a*	O(43)	2.663	1
O(33)	3.423	3	O(11)	2.828	1*b*
I(2)–O(13)	2.861	1	I(4)–O(23)	2.468	2
O(21)	2.871	2*a*	O(12)	2.628	1*b*
O(31)	3.068	1	O(33)	2.690	1
O(22)	3.218	2			
K(1)–O(13)	2.797	2*a*	K(2)–O(11)	2.929	1
O(13)	2.980	1*c*	O(12)	2.793	1
O(21)	2.799	2*a*	O(21)	2.842	2*a*
O(22)	2.989	1	O(31)	2.808	1
O(23)	2.854	2	O(32)	2.700	3*a*
O(23)	2.910	1*c*	O(33)	2.902	1*d*
O(41)	2.812	1	O(41)	2.702	1
O(43)	2.783	2	O(42)	3.039	3

* (1), x, y, z; (1*a*), $x, y-1, z$; (1*b*), $x+1, y, z$; (1*c*), $x, y+1, z$; (1*d*), $x-1, y, z$; (2), $1-x, 1-y, 1-z$; (2*a*), $-x, 1-y, 1-z$; (3), $1-x, y-\frac{1}{2}, \frac{3}{2}-z$; (3*a*), $1-x, y+\frac{1}{2}, \frac{3}{2}-z$.

Table 32A-3-006 (continued)

(d) O...O distances smaller than 3 Å;
selected angles (for hydrogen bonds see (e)).

Bond	Distance [Å]	Bonds	Angle [°]
O(22)–O(31)	2.918	I(3)–O(32)–O(42)	108.4
O(23)–O(43)	2.933	I(4)–O(42)–O(32)	110.0
O(12)–O(42)	2.886	I(4)–O(42)–O(11)	121.9
O(33)–O(42)	2.950	I(1)–O(11)–O(42)	104.6
O(11)–O(42)	2.710*	O(32)–O(42)–O(11)	100.0
O(42)–O(32)	2.694*		

* Hydrogen bonds.

(e) The geometry of the hydrogen bonds.

Bond	Distance [Å]	Bonds	Angle [°]
O(32)–H(1)	0.92(4)	I(3)–O(32)–H(1)	114(3)
O(42)...H(1)	1.79(4)	I(4)–O(42)...H(1)	106(4)
O(32)...O(42)	2.694(6)	O(32)–H(1)...O(42)	167(4)
O(42)–H(2)	0.98(3)	I(4)–O(42)–H(2)	111(3)
O(11)...H(2)	1.76(3)	I(1)–O(11)...H(2)	105(2)
O(42)...O(11)	2.710(6)	O(42)–H(2)...O(11)	163(3)
		H(2)–O(42)...H(1)	108(3)

Table 32A-3-006 (continued)

(c) Angles [°] around iodine atoms.

	I(2)		I(1)		I(3)		I(4)	
I–O Contacts involved	Bonding O	Angle [°]	Bonding O	Angle [°]	Bonding O	Angle [°]	Bonding O	Angle [°]
Both I–O < 2.00 Å	O(21), O(22)	99.6	O(11), O(12)	101.8	O(31), O(32)	94.2	O(41), O(42)	93.2
	O(22), O(23)	101.5	O(12), O(13)	100.9	O(32), O(33)	96.1	O(42), O(43)	98.2
	O(23), O(21)	99.6	O(13), O(11)	102.2	O(33), O(31)	102.8	O(43), O(41)	96.8
2.40 Å < both I–O < 3.5 Å	O(21), O(22)	109.7	O(31), O(41)	104.6	O(22), O(43)	85.0	O(12), O(33)	86.0
	O(21), O(13)	94.4	O(41), O(33)	96.8	O(22), O(11)	101.0	O(23), O(12)	102.2
	O(13), O(22)	108.7	O(31), O(33)	101.8	O(11), O(43)	84.6	O(33), O(23)	99.0
	O(21), O(31)	81.2						
	O(22), O(31)	55.3						
	O(13), O(31)	64.7						
One I–O < 2.00 Å	O(21), O(22)	167.2	O(11), O(41)	167.5	O(31), O(11)	170.1	O(41), O(12)	169.9
2.40 Å < one I–O < 3.5 Å	O(22), O(13)	178.2	O(12), O(31)	178.3	O(32), O(22)	171.9	O(42), O(23)	176.2
	O(23), O(21)	172.7	O(13), O(33)	172.7	O(33), O(43)	169.2	O(43), O(33)	171.5
	O(21), O(13)	81.9	O(11), O(31)	76.8	O(31), O(22)	83.8	O(41), O(23)	87.8
	O(21), O(21)	75.9	O(11), O(33)	70.9	O(31), O(43)	87.2	O(41), O(33)	90.6
	O(22), O(22)	70.0	O(12), O(33)	78.6	O(32), O(11)	79.9	O(42), O(33)	77.3
	O(23), O(22)	76.0	O(12), O(41)	76.9	O(32), O(43)	87.1	O(42), O(12)	76.7
	O(23), O(13)	79.2	O(13), O(31)	78.4	O(33), O(22)	91.9	O(43), O(12)	86.0
	O(31), O(21)	137.6	O(13), O(41)	90.2	O(33), O(11)	85.8	O(43), O(23)	85.3
	O(31), O(22)	113.6						
	O(31), O(23)	98.9						
	O(22), O(21)	85.1						

Table 32A-3-007. δ-$KIO_3 \cdot HIO_3$. Fractional coordinates and anisotropic temperature parameters at RT [78Ily]. B_{ij} is defined by Eq. (a) in Introduction.

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{23}	
I(1)	0.25626(5)	0.05019(1)	0.0	0.00418(6)	0.000103(2)	0.00191(3)	0.00026(1)	0.00021(2)	0.00114(8)
I(2)	0.25369(5)	0.04991(1)	0.47610(5)	0.00398(6)	0.000225(2)	0.00236(4)	0.00052(2)	–0.00076(2)	–0.00055(11)
I(3)	–0.02561(5)	0.09228(1)	0.73146(6)	0.00366(4)	0.000110(2)	0.00150(2)	–0.00016(1)	–0.00007(1)	–0.00005(7)
K(1)	–0.0046(3)	0.09943(4)	0.2357(2)	0.00695(22)	0.000202(7)	0.00257(10)	–0.00010(6)	0.00002(8)	–0.0002(40)
K(2)	0.0	0.0	0.2287(3)	0.01041(39)	0.000149(10)	0.00319(17)	–0.00022(10)	0.0	0.0
O(11)	0.2243(8)	0.0851(1)	–0.1084(6)	0.0078(9)	0.00016(3)	0.0017(3)	0.0002(3)	0.0009(2)	–0.0013(9)
O(12)	0.0642(9)	0.0503(2)	0.0687(6)	0.0042(7)	0.00025(4)	0.0042(5)	–0.0003(3)	0.0000(2)	0.0022(10)
O(13)	0.1991(10)	0.0171(2)	–0.1275(7)	0.0100(10)	0.00021(3)	0.0030(4)	0.0003(3)	–0.0008(2)	–0.0033(11)
O(21)	0.2124(8)	0.0154(2)	0.5822(7)	0.0091(11)	0.00035(4)	0.0025(4)	0.0005(3)	0.0007(2)	0.0018(11)
O(22)	0.0613(8)	0.0486(2)	0.3994(6)	0.0048(7)	0.00027(3)	0.0022(4)	0.0000(3)	0.0000(2)	–0.0007(9)
O(23)	0.2171(10)	0.0844(2)	0.5774(7)	0.0082(10)	0.00027(4)	0.0033(5)	0.0000(3)	–0.0005(2)	–0.0004(11)
O(31)	–0.0240(7)	0.0467(1)	0.7408(7)	0.0082(7)	0.00006(2)	0.0039(4)	0.0002(2)	0.0000(2)	–0.0032(12)
O(32)	–0.1609(8)	0.0964(2)	0.6050(5)	0.0062(8)	0.00016(3)	0.0022(4)	0.0001(2)	–0.0004(2)	–0.0039(9)
O(33)	–0.1829(9)	0.0992(2)	0.8384(6)	0.0057(8)	0.00024(3)	0.0031(4)	–0.0001(3)	0.0000(2)	0.0030(10)

Table 32A-3-008. δ-$KIO_3 \cdot HIO_3$. Interatomic distances [Å] at RT [78Ily]. Symmetry operated atoms are denoted by *.

IO_3(1) group	IO_3(2) group	IO_3(3) group
I(1)–O(11) = 1.812(6)	I(2)–O(22) = 1.805(7)	I(3)–O(31) = 1.796(5)
–O(12) = 1.795(7)	–O(23) = 1.809(8)	–O(33) = 1.795(7)
–O(13) = 1.951(7)	–O(21) = 1.853(8)	–O(32) = 1.839(6)
...O(32) = 2.347(7)	...O(33) = 2.569(8)	...O(23) = 2.677(8)
...O(22) = 2.702(7)	...O(12) = 2.732(8)	...O(11) = 2.757(7)
...O(21) = 2.804(7)	...O(13) = 2.919(8)	...O(32) = 2.953(6)
		...O(11) = 3.047(8)
O(11)–O(13) = 2.700(10)	O(22)–O(21) = 2.775(11)	O(31)–O(33) = 2.697(10)
–O(12) = 2.785(10)	–O(23) = 2.791(10)	–O(32) = 2.731(11)
O(12)–O(13) = 2.825(10)	O(21)–O(23) = 2.716(11)	O(32)–O(33) = 2.708(10)
K(1) polyhedron	**K(2) polyhedron**	**O–O polyhedron**
K(1)–O(33) = 2.702(7)	K(2)–O(12) = 2.767(8)	O(13)–O(31) = 2.657(10)
–O(12) = 2.809(7)	–O*(12) = 2.767(8)	O(11)–O(32) = 2.682(10)
–O(22) = 2.792(7)	–O(22) = 2.785(7)	O(13)–O(21) = 2.838(10)
–O(23) = 2.818(8)	–O*(22) = 2.785(7)	O(21)–O*(21) = 3.540(11)
–O*(33) = 2.888(8)	–O(21) = 2.958/8)	
–O(11) = 2.893(8)	–O*(21) = 2.958(8)	
–O*(23) = 2.979(8)	–O(13) = 3.021(8)	
–O(32) = 3.177(8)	–O*(13) = 3.021(8)	

Table 32A-3-009. δ-$KIO_3 \cdot HIO_3$. Interatomic angles at RT [78Ily].

O(11)–I(1)–O(12)	100°58′(18′)	O(21)–I(2)–O(22)	98°28′(19′)
O(12)–I(1)–O(13)	98°26′(19′)	O(22)–I(2)–O(23)	101°17′(19′)
O(13)–I(1)–O(11)	92°11′(18′)	O(23)–I(2)–O(21)	95°13′(21′)
O(11)–O(12)–O(13)	57°14′(15′)	O(21)–O(22)–O(23)	58°28′(18′)
O(12)–O(13)–O(11)	60°27′(15′)	O(22)–O(23)–O(21)	60°20′(16′)
O(13)–O(11)–O(12)	62°17′(15′)	O(23)–O(21)–O(22)	61°12′(16′)
O(31)–I(3)–O(32)	85°23′(17′)	O(31)–O(32)–O(33)	59°36′(19′)
O(32)–I(3)–O(33)	98°42′(19′)	O(32)–O(33)–O(31)	60°32′(17′)
O(33)–I(3)–O(31)	85°42′(17′)	O(33)–O(31)–O(32)	59°52′(18′)

Table 32A-3-010. α-$KIO_3 \cdot HIO_3$. NQR data for ^{127}I [83Pet]. ν_1, ν_2: NQR frequency of (1/2 ↔ 3/2) and (3/2 ↔ 5/2) transition, respectively. η: asymmetry parameter. e^2Qq_{zz}/h: nuclear quadrupole coupling constant.

T [K]	$\nu_1\left(\frac{1}{2} \leftrightarrow \frac{3}{2}\right)$ [MHz]	$\nu_1\left(\frac{3}{2} \leftrightarrow \frac{5}{2}\right)$ [MHz]	η	e^2Qq_{zz}/h [MHz]
77	156.15	298.08	0.1933	1000.98
	156.15	311.73	0.0375	1039.40
	192.47	321.04	0.4058	1102.37
	200.12	307.68	0.5033	1072.02
300	163.60	309.35	0.2129	1040.44
	170.92	295.57	0.3558	1008.94

Table 32A-3-011. β-$KIO_3 \cdot HIO_3$. NQR data for ^{127}I [83Pet]. ν_1, ν_2: NQR frequency of (1/2 ↔ 3/2) and (3/2 ↔ 5/2) transition, respectively. η: asymmetry parameter. e^2Qq_{zz}/h: nuclear quadrupole coupling constant.

T [K]	$\nu_1\left(\frac{1}{2} \leftrightarrow \frac{3}{2}\right)$ [MHz]	$\nu_1\left(\frac{3}{2} \leftrightarrow \frac{5}{2}\right)$ [MHz]	η	e^2Qq_{zz}/h [MHz]
77	149.32	294.72	0.1015	984.45
	157.54	311.64	0.0924	1040.60
	196.15	311.37	0.4652	1078.73
	196.15	322.22	0.4231	1109.65
300	146.97	289.08	0.1142	966.14
	154.77	305.87	0.0964	1021.48
	193.06	304.45	0.4732	1055.99
	193.40	315.40	0.4322	1087.54

Table 32A-3-012. γ-$KIO_3 \cdot HIO_3$, γ-$KIO_3 \cdot DIO_3$. NQR data for ^{127}I at T = 77 K [83Pet]. ν_1, ν_2: NQR frequency of (1/2 ↔ 3/2) and (3/2 ↔ 5/2) transition, respectively. η: asymmetry parameter. e^2Qq_{zz}/h: nuclear quadrupole coupling constant.

Sample	$\nu_1\left(\frac{1}{2} \leftrightarrow \frac{3}{2}\right)$ [MHz]	$\nu_1\left(\frac{3}{2} \leftrightarrow \frac{5}{2}\right)$ [MHz]	η	e^2Qq_{zz}/h [MHz]
γ-$KIO_3 \cdot HIO_3$	148.62	296.35	0.0482	988.29
	155.60	306.68	0.1069	1024.63
	221.68	326.57	0.5529	1146.65
	222.47	327.21	0.5548	1149.22
γ-$KIO_3 \cdot DIO_3$	148.47	296.15	0.0454	987.58
	155.68	306.75	0.1079	1024.91
	222.71	326.85	0.5573	1148.41
	223.10	327.56	0.5568	1150.82

Table 32A-3-013. δ-$KIO_3 \cdot HIO_3$. ^{127}I NQR frequencies at T = 77K [83Pet]. ν_1, ν_2: NQR frequency of (1/2 ↔ 3/2) and (3/2 ↔ 5/2) transition, respectively.

$\nu_1\left(\frac{1}{2} \leftrightarrow \frac{3}{2}\right)$ [MHz]	$\nu_1\left(\frac{3}{2} \leftrightarrow \frac{5}{2}\right)$ [MHz]	$\nu_1\left(\frac{1}{2} \leftrightarrow \frac{3}{2}\right)$ [MHz]	$\nu_1\left(\frac{3}{2} \leftrightarrow \frac{5}{2}\right)$ [MHz]
153.50	304.44	222.00	331.70
157.90	309.99	235.84	
158.20	310.84	236.82	333.6
164.75	321.34	241.05	
165.77	322.92		