Table 32A-2-001. NH_4IO_3. Fractional coordinates in phase III [71Kev]. T = 25 °C. A spherical model was taken for the NH_4-ion.

Atom	x	y	z
I	−0.01124 (8)	0	0.00895 (8)
O (1)	0.174 (2)	−0.004 (3)	0.222 (1)
O (2)	−0.240 (2)	0.033 (1)	0.156 (2)
O (3)	0.037 (2)	0.304 (1)	0.047 (2)
NH_4	0.002 (2)	0.262 (1)	0.503 (3)

Table 32A-2-002. NH_4IO_3. Anisotropic temperature parameters in phase III [71Kev]. T = 25 °C. b_{ij} is defined by Eq. (b) in Introduction. An isotropic model was taken for the NH_4-ion.

	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
I	0.0071 (1)	0.00299 (4)	0.0073 (1)	0.0009 (2)	0.0020 (1)	−0.0005 (2)
O (1)	0.015 (2)	0.013 (2)	0.010 (2)	0.009 (3)	−0.006 (2)	−0.003 (3)
O (2)	0.013 (2)	0.008 (1)	0.011 (2)	0.003 (1)	0.009 (1)	−0.002 (1)
O (3)	0.022 (3)	0.005 (1)	0.015 (2)	−0.002 (1)	−0.003 (2)	−0.001 (1)
NH_4	0.012 (1)	0.006	0.012	0	0	0

Table 32A-2-003. NH_4IO_3. Fractional coordinates and anisotropic temperature parameters [$\cdot 10^{-4}$] in phase II [79Bis]. $T \approx 100$ °C. b_{ij} is defined by Eq. (b) in Introduction.

Atom	x	y	z
I(1)	0	0.0033(2)	0.0232(2)
I(2)	0.5	–0.0060(2)	0.5117(2)
NH_4(1)	0	0.246(4)	0.509(7)
NH_4(2)	0.5	0.253(6)	0.005(8)
O(1)	0.207(2)	0.045(2)	0.191(2)
O(2)	0.710(2)	0.004(2)	0.686(2)
O(3)	0	0.308(4)	–0.045(4)
O(4)	0.5	0.305(3)	0.572(3)

	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
I(1)	70(3)	33(5)	68(3)	0	0	5(6)
I(2)	72(3)	28(5)	64(3)	0	0	0(3)
NH_4(1)	45(53)	37(48)	183(80)	0	0	1(22)
NH_4(2)	213(82)	173(85)	106(69)	0	0	1(34)
O(1)	187(20)	83(15)	156(31)	17(15)	–15(26)	3(15)
O(2)	285(27)	140(23)	153(32)	–112(20)	–162(29)	19(23)
O(3)	462(76)	105(34)	298(78)	0	0	–108(44)
O(4)	421(64)	34(20)	124(39)	0	0	23(31)

Table 32A-2-004. NH_4IO_3. Interatomic distances [Å] in phase III [71Kev]. T = 25 °C.

I – O (1)	1.806 (8)	I – O (1)	2.830 (8)
I – O (2)	1.765 (8)	I – O (2)	2.778 (9)
I – O (3)	1.836 (12)	I – O (3)	2.819 (11)
O (1) – O (2)	2.71 (1)	N – O (2)	2.86 (2)
O (2) – O (3)	2.78 (2)	N – O (3)	2.94 (2)
O (1) – O (3)	2.81 (2)	N – O (3)	3.00 (2)
		N – O (1)	3.00 (2)

Table 32A-2-005. NH_4IO_3. Interatomic angles [°] in phase III [71Kev]. T = 25 °C.

O (1) – I – O (2)	102.3°	O (1) – N – O (2)	96.2°
O (1) – I – O (3)	105.5°	O (3) – N – O (3)′	89.9°
O (2) – I – O (3)	105.6°	O (1) – N – O (3)	109.6°
		O (1) – N – O (3)′	92.8°
		O (2) – N – O (3)	129.4°
		O (2) – N – O (3)′	115.1°

Table 32A-2-006. NH_4IO_3. Interatomic distances [Å] and angles [°] in phase II [79Bis]. $T \approx$ 100 °C.

Distances	[Å]	Distances	[Å]	Angles	[°]
I(1)–O(1)	1.76	N(1)–O(1)	3.57	O(1)–I(1)–O(1)	98.4
I(1)–O(1)	1.76	N(1)–O(1)	3.08	O(1)–I(1)–O(3)	99.6
I(1)–O(2)	2.87	N(1)–O(2)	3.13	O(1)–I(1)–O(3)	99.6
I(1)–O(2)	2.87	N(1)–O(2)	3.23	O(2)–I(2)–O(2)	99.9
I(1)–O(3)	2.81	N(1)–O(3)	3.62	O(2)–I(2)–O(4)	104.0
I(1)–O(3)	1.78	N(1)–O(3)	2.93	O(2)–I(2)–O(4)	104.0
I(2)–O(1)	2.84	N(1)–O(4)	3.28		
I(2)–O(1)	2.84	N(2)–O(1)	2.91		
I(2)–O(2)	1.76	N(2)–O(1)	3.52		
I(2)–O(2)	1.76	N(2)–O(2)	3.33		
I(2)–O(4)	2.86	N(2)–O(2)	3.34		
I(2)–O(4)	1.80	N(2)–O(3)	3.27		
		N(2)–O(4)	2.85		
		N(2)–O(4)	3.70		

Table 32A-2-007. NH_4IO_3. Unit cell parameters at different temperatures [75Vis].

Phase	T [°C]	a [Å]	b [Å]	c [Å]	V [Å^3]
III	20	6.403 (2)	9.168 (4)	6.337 (2)	374.6 (4)
	80	6.413	9.156	6.411	376.5
II	83	6.426	9.104	6.466	378.3
I	120	4.556			

Table 32A-2-008. NH_4IO_3. Refractive indices at T = 25 and 100 °C [77Mit].

λ [μm]		0.6438	0.5791	0.5461	0.4358
T = 25 °C	n_a	1.7570	1.7654	1.7701	1.7994
	n_b	1.7717	1.7808	1.7861	1.8181
	n_c	1.8275	1.8378	1.8437	1.8806
T = 100 °C	n_a		1.7461	1.7513	1.7803
	n_b		1.7875	1.7930	1.8266
	n_c		1.8402	1.8465	1.8844

Table 32A-2-009. NH_4IO_3. Frequency of q = 0 optical modes obtained from Raman scattering [74Sal]. T = RT.

ν [THz]	Polarization
1.60	–
2.40	B (TO)
3.10	A (TO)
3.99	A + B (TO)
4.80	B (TO)
5.25	(LO)
7.19	(LO)
8.99	B
9.79	A
11.10	A + B
21.89	A
22.18	B
22.79	A + B