Table M18-001. Sb_5O_7I. Polytypes of Sb_5O_7I and their properties [77Nit].

	Modified Ramsdell symbol	2MC	2MA	4MC	4MA	$6MC_1$	$6MA_1$	$6MA_2$	$8MC_1$
	Former symbol	α	β	γ	η	ζ	δ	ε	κ
Low-temp. phase	Relative abundance [%]	85	11	2	0.7	0.7	0.2	0.3	0.1
	Space group	$P2_1/c$	Pc	$P2_1/c$	Pc				
	Lattice parameters: a [Å]	6.772	6.759	6.766	6.765	6.77	6.77	6.77	6.77
	b [Å]	12.726	12.718	25.458	25.462	38.46	38.6	38.50	51.00
	c [Å]	13.392	13.405	13.405	13.402	13.40	13.40	13.40	13.40
	β [deg]	120.1	120.1	120.1	120.1	120.1	120.1	120.1	120.1
	Formula units per cell (Z)	4	4	8	8	12	12	12	16
	Optical extinction angle [deg]	13	0	0	8	6	4	0	0
	Piezoelectric, ferroelectric	–	+	–	+	–	+	+	–
	Coercive stress at 20°C *) [10^{+6} N/m^2]	1.5	1.8	0.5	0.7	0.2	0.9	0.8	
	Spontaneous strain [10^{-2}] **)	8	2	6	7	7	7	7	7
	Coercive field [10^2 kV m^{-1}]	–	2	–	4–6	–	8–10	8–10	–
	Spontaneous polarization [10^{-3} Cm^{-2}]	–	5	–		–			–
	Θ [°C]	208	165	184	182	189	195	175	190
	Modified Ramsdell symbol	2HC	2HA	4TC	4HA	6TC	6HA	6HA	
High-temp. phase	Space group	P6/m	P $\bar{6}$	P $\bar{3}$ m	P $\bar{6}$	P $\bar{3}$	P $\bar{6}$	P $\bar{6}$	
	Lattice parameters: a [Å]	6.77	6.78	6.78	6.78	6.79	6.77	6.77	6.73
	c [Å]	12.80	12.86	25.68	25.72	38.61	38.51	38.53	51.10
	Formula units per cell (Z)	2	2	4	4	6	6	6	8

*) Stress required for convertation of three orientation states into each other (mechanical switching).
**) Derived with the procedure of Aizu [70Aiz].

Table M18-002. Sb_5O_7I (polytype 2MA). Fractional coordinates [$\cdot 10^{-4}$] [78Kra]. Non-primed and primed numbers in the brackets of the first column indicate that corresponding atoms are located in the lower and upper half of a unit cell along *b* axis, as explicitely shown in Fig. M18-002(a). Note that Fig. M18-002(a) represents a polytype 2MC, in which only the positions of Sb(1′), Sb(2′) and Sb(3′) differ from those for polytype 2MA.

	x	*y*	*z*
Sb (1)	−701 (7)	2345 (1)	4079 (3)
Sb (1′)	39 (7)	7548 (1)	4301 (3)
Sb (2)	3206 (7)	2460 (2)	2652 (3)
Sb (2′)	2914 (7)	7541 (2)	2352 (4)
Sb (3)	−3561 (7)	2451 (1)	700 (3)
Sb (3′)	−3859 (6)	7652 (1)	917 (3)
Sb (4)	2931 (7)	551 (1)	802 (3)
Sb (5)	3028 (7)	4520 (1)	807 (3)
Sb (4′)	−3664 (7)	5551 (1)	−800 (3)
Sb (5′)	−3581 (7)	9519 (1)	−805 (3)
I (1)	0	0	2500
I (2)	−654 (5)	4997 (2)	2504 (3)
O (1)	6396 (41)	2484 (13)	4163 (22)
O (1′)	3073 (37)	7513 (11)	824 (20)
O (2)	509 (49)	1678 (17)	432 (26)
O (3)	−15 (42)	3858 (14)	125 (30)
O (2′)	−636 (37)	6243 (12)	−42 (19)
O (3′)	−1146 (50)	8429 (17)	−36 (24)
O (4)	4378 (43)	1247 (14)	46 (22)
O (5)	3742 (44)	3367 (15)	36 (22)
O (4′)	4873 (51)	6666 (17)	−354 (26)
O (5′)	4820 (48)	8871 (15)	−140 (24)
O (6)	4744 (54)	1396 (18)	2204 (26)
O (7)	4258 (47)	3665 (15)	2252 (22)
O (6′)	4894 (56)	6316 (17)	2802 (26)
O (7′)	5495 (59)	8567 (20)	2771 (28)

Table M18-003. Sb_5O_7I (polytype 2MA). Interatomic distances [Å] [78Kra]. For the meaning of primes in brackets, such as Sb(2′), see the caption of Table M18-002. Square brackets denote the fourth nearest neighbor.

Sb (1)–O (1)	2.03 (3)	Sb (1′)–O (1′)	2.05 (2)
O (2)	2.00 (3)	O (2′)	1.94 (2)
O (3)	1.97 (2)	O (3′)	1.92 (3)
[O (5)	2.76 (3)]	[O (7′)	3.00 (3)]
I (1)	3.821 (3)	I (1)	3.935 (3)
I (2)	3.988 (4)	I (2)	3.928 (4)
Sb (2)–O (1)	2.09 (2)	Sb (2′)–O (1′)	2.10 (3)
O (6)	1.98 (4)	O (6′)	1.94 (3)
O (7)	1.88 (3)	O (7′)	2.02 (3)
[O (2)	2.78 (3)]	[O (4′)	2.86 (3)
I (1)	3.754 (3)	I (1)	3.754 (4)
I (2)	4.092 (5)	I (2)	4.101 (5)
Sb (3)–O (1)	2.05 (3)	Sb (3′)–O (1′)	2.02 (3)
O (4)	1.96 (2)	O (4′)	1.94 (3)
O (5)	1.96 (2)	O (5′)	1.99 (2)
[O (6)	3.08 (4)]	[O (3′)	2.88 (4)]
I (1)	3.940 (2)	I (1)	3.832 (2)
I (2)	3.930 (4)	I (2)	4.002 (3)
Sb (4)–O (2)	2.04 (3)	Sb (4′)–O (2′)	1.98 (2)
O (4)	1.94 (3)	O (4′)	1.98 (3)
O (6)	1.97 (3)	O (7′)	2.04 (3)
[O (5′)	3.07 (3)]	[O (3)	3.03 (2)]
I (1)	3.756 (6)	I (1)	3.777 (4)
	4.199 (4)		4.178 (5)
I (2)	3.896 (5)	I (2)	3.902 (6)
Sb (5)–O (3)	1.97 (3)	Sb (5′)–O (3′)	2.00 (2)
O (5)	1.99 (3)	O (5′)	1.90 (4)
O (7)	2.00 (3)	O (6′)	1.94 (3)
[O (2′)	3.07 (2)]	[O (4)	3.10 (3)]
I (1)	3.889 (4)	I (1)	3.890 (4)
I (2)	4.118 (5)	I (2)	3.731 (8)
	4.170 (7)		4.188 (5)

Table M18-004. Sb_5O_7I (polytype 2MA and 2MC). Frequencies of Raman scattering lines at RT [cm^{-1}] [79Pre]. Frequencies of strong lines which give similar structures in the Raman spectra for both polytypes are underlined.

ν [cm^{-1}]			
2MA A'	2MC A_g	2MA A''	2MC B_g
34.5	31	33	31
37	39.5	38.5	
41.5	41		40
		46	45.5
48			48.5
		53	
		58	57
		63	70
78	79	75	80
86		88	
	104		
111	110		111
146	145	147	145
149			
		152	
156	156		
161.5			
		165	
		182	182.5
		190	190
213	210	210	212
		232	
262			259
273.5	272		
330.5	330		
394	387		
408	415		
459	456		
	478		
	534		
			568
	600		
	750		