

**No. M18 Sb<sub>5</sub>O<sub>7</sub>I, Antimony (III) oxide iodide***(M* = 847.70)

1a	Sb <sub>5</sub> O <sub>7</sub> I crystallizes in several polytypes (see 1b below). Ferroelectric activity in Sb <sub>5</sub> O <sub>7</sub> I of 2MA type was first reported by Nitsche et al. in 1977.	77Nit															
b	Eight polytypes of Sb <sub>5</sub> O <sub>7</sub> I are known: Table M18-001. Most abundant polytype is 2MC-Sb <sub>5</sub> O <sub>7</sub> I (or α-Sb <sub>5</sub> O <sub>7</sub> I), which undergoes a phase transition at Θ = 208 °C. But it shows only an elastic anomaly <sup>a)</sup> . Ferroelectric polytype is 2MA-Sb <sub>5</sub> O <sub>7</sub> I (or β-Sb <sub>5</sub> O <sub>7</sub> I). Data shown below concern primarily with 2MA-Sb <sub>5</sub> O <sub>7</sub> I.	<sup>a)</sup> 73Kra															
<table><tr><td>phase</td><td>II</td><td>I</td></tr><tr><td>state</td><td>F</td><td>P</td></tr><tr><td>crystal system</td><td>monoclinic</td><td>hexagonal</td></tr><tr><td>space group</td><td>Pc – C<sub>s</sub><sup>2</sup></td><td>P6̄ – C<sub>3h</sub><sup>1</sup></td></tr><tr><td>Θ [°C]</td><td colspan="2">165</td></tr></table>		phase	II	I	state	F	P	crystal system	monoclinic	hexagonal	space group	Pc – C <sub>s</sub> <sup>2</sup>	P6̄ – C <sub>3h</sub> <sup>1</sup>	Θ [°C]	165		77Nit
phase	II	I															
state	F	P															
crystal system	monoclinic	hexagonal															
space group	Pc – C <sub>s</sub> <sup>2</sup>	P6̄ – C <sub>3h</sub> <sup>1</sup>															
Θ [°C]	165																
ρ = 5.55 · 10 <sup>3</sup> kg m <sup>-3</sup> . Transparent, colorless.		75Kra															
2a	Crystal growth: vacuum sublimation growth technique, see	74Kra, 77Nit															
b	Crystal form: flat pseudo-hexagonal prism.	75Kra															
3a	Unit cell parameters: a = 6.759(3) Å, b = 12.718(6) Å, c = 13.405(6) Å, β = 120.1(1)°; see also Table M18-001.	77Nit															
b	Crystal structure: Z = 4 in phase II, Z = 2 in phase I. Table M18-002, Table M18-003; Fig. M18-001, Fig. M18-002. Fractional coordinates and thermal parameters of 2MC-Sb <sub>5</sub> O <sub>7</sub> I: see	77Nit 75Kra															
5b	Ferroelectric hysteresis loop: see	77Nit															
c	P <sub>s</sub> = 5 · 10 <sup>-3</sup> C m <sup>-2</sup> at RT. P <sub>s</sub> is not reversible but reorientable by ± 120° by coercive fields of 200...500 kV m <sup>-1</sup> .	77Nit															
8a	Elastic stiffness measured by ultrasonic techniques: Fig. M18-003.																
b	Spontaneous strain: 2 · 10 <sup>-2</sup> . Coercive stress at 20 °C: 1.8 · 10 <sup>6</sup> N m <sup>-2</sup> ; see also Table M18-001.	77Nit															
9a	Refractive indices of 2MC-Sb <sub>5</sub> O <sub>7</sub> I: n <sub>1</sub> = 2.25, n <sub>2</sub> = 2.30(6) for the two main vibration directions in the a-c plane. Double refraction in the a-c plane: Δn = 3.8 · 10 <sup>-2</sup> for 2MC-Sb <sub>5</sub> O <sub>7</sub> I and 3.5 · 10 <sup>-2</sup> for 2MA-Sb <sub>5</sub> O <sub>7</sub> I at RT for λ = 632.8 nm. Birefringence of 2MA-Sb <sub>5</sub> O <sub>7</sub> I: Fig. M18-004. Temporal change in the birefringence by light illumination (photorefractive effect): see	77Nit 81Fri															
e	Nonlinear susceptibilities for SHG of Nd-glass laser (λ = 1.06 μm) is about an order of magnitude below that of quartz.	77Nit															
10a	Raman scattering: Table M18-004; Fig. M18-005, Fig. M18-006. Raman scattering of 2MC-Sb <sub>5</sub> O <sub>7</sub> I: Fig. M18-007; see also	75Pre															