

TaInS <sub>2</sub>	<i>hP4</i>	(187) <i>P-6m2</i> – gda
--------------------	------------	--------------------------

# **InTaS<sub>2</sub> 1s** [1]

Structural features: Directly superposed close-packed S layers; Ta in trigonal prismatic, In in linear voids (stacking sequence AbAα). TaS<sub>6</sub> trigonal prisms share edges to form infinite slabs; In in linear coordination between the slabs.

Eppinga R., Wiegers G.A. (1980) [1]

InS<sub>2</sub>Ta

$a = 0.331$ ,  $c = 0.873$  nm,  $c/a = 2.637$ ,  $V = 0.0828$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	<i>2g</i>	<i>3m.</i>	0	0	0.31		tetrahedron Ta <sub>3</sub> In
Ta2	<i>1d</i>	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		anticuboctahedron S <sub>6</sub> Ta <sub>6</sub>
In3	<i>1a</i>	<i>-6m2</i>	0	0	0		hexagonal bipyramid S <sub>2</sub> In <sub>6</sub>

Experimental: powder, diffractometer, X-rays

References: [1] Eppinga R., Wiegers G.A. (1980), Physica B+C (Amsterdam) 99, 121-127.