

$\text{In}_2\text{Si}[\text{PO}_4]_3\text{O}_{0.5}$ *hP50* $(176) P6_3/m - i^2h^3fe$  **$\text{In}_4\text{Si}_2\text{P}_6\text{O}_{25}$**  [1]

Structural features:  $\text{InO}_6$  octahedra share vertices with  $\text{PO}_4$  and  $\text{SiO}_4$  tetrahedra (statistical occupation of two face-linked tetrahedra for the latter) to form a 3D-framework.

Hanawa M. et al. (2000) [1]

 $\text{In}_2\text{O}_{12.50}\text{P}_3\text{Si}$  $a = 0.85149$ ,  $c = 0.77481$  nm,  $c/a = 0.910$ ,  $V = 0.4865$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.0	0.022	0.0	0.083	
O2	12 <i>i</i>	1	0.4381	0.1427	0.0864		single atom P
O3	6 <i>h</i>	<i>m</i> ..	0.0366	0.1923	$\frac{1}{4}$		
O4	6 <i>h</i>	<i>m</i> ..	0.1348	0.5163	$\frac{1}{4}$		single atom P
P5	6 <i>h</i>	<i>m</i> ..	0.36448	0.03735	$\frac{1}{4}$		tetrahedron O <sub>4</sub>
In6	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0436		octahedron O <sub>6</sub>
Si7	4 <i>e</i>	3..	0	0	0.2033	0.5	

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0  $\frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays,  $R = 0.044$ ,  $T = 296$  K

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Hanawa M., Kobayashi T., Imoto H. (2000), *Z. Anorg. Allg. Chem.* 626, 216-222.