$InTaS_2$ Structure: AB2C_hP4_187_a_g_d-002

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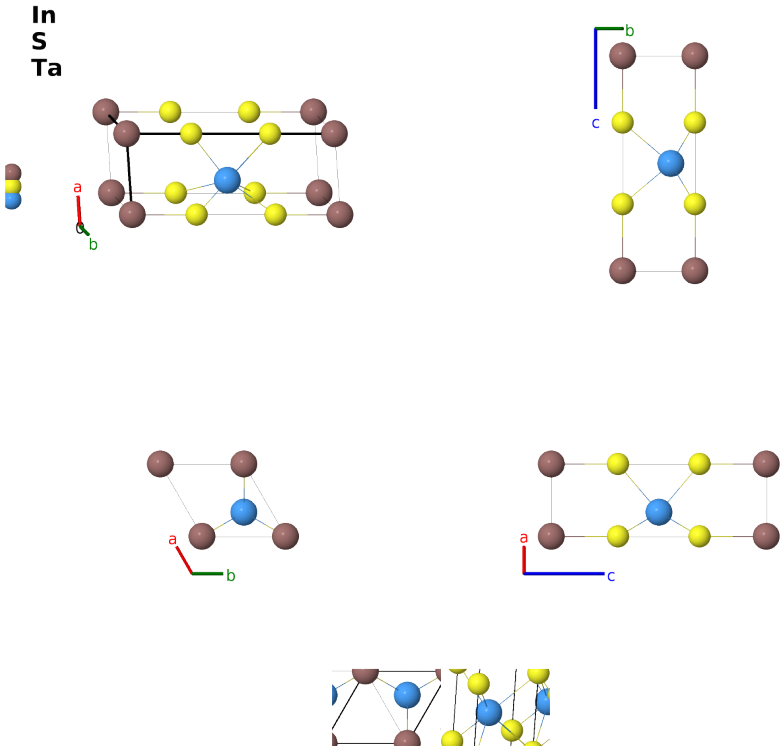
https://aflow.org/prototype-encyclopedia/4SXA

https://aflow.org/prototype-encyclopedia/AB2C_hP4_187_a_g_d-002



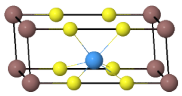
Prototype	InS_2Ta
AFLOW prototype label	AB2C_hP4_187_a_g_d-002
ICSD	74703
CCDC	1635392
Pearson symbol	hP4
Space group number	187
Space group symbol	$P\bar{6}m2$
AFLOW prototype command	`aflow --proto=AB2C_hP4_187_a_g_d-002 --params=`$a, c/a, z_3$

Other compounds with this structure
$BiNbSe_2$, $InNbSe_2$, $PbTaS_2$, $SnNbSe_2$

- Many, if not all, of the compounds listed here have sub-stoichiometric occupation on the (1a) site. The site is reported as fully occupied in $InTaS_2$.
- The value $z_3 = 0.32$ for the sulfur (2c) site is inferred from the value given for Pb_xTaS_2 by (Eppinga, 1980).
- $LiAgC_2$ and $InTaS_2$ have the same AFLOW label, AB2C_hP4_187_a_g_d. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	In I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1d)	Ta I
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2g)	S I
$\mathbf{B_4}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(2g)	S I

References

[1] R. Eppinga and G. A. Wiegers, *A generalized scheme for niobium and tantalum dichalcogenides intercalated with post-transition elements*, Physica B+C **99**, 121–127 (1980), doi:10.1016/0378-4363(80)90219-3.

Found in

[1] R. Sankar, G. N. Rao, I. P. Muthuselvam, G. Bian, H. Zheng, G. P.-J. Chen, T.-R. Chang, S. Xu, G. S. Murgan, C.-H. Lin, W.-L. Lee, H.-T. Jeng, M. Hasan, and F.-C. Chou, *Single crystal growth and physical property characterization of $PbTaSe_2$ as a noncentrosymmetric type-II superconductor*, doi:10.48550/arXiv.1511.05295. ArXiv:1511.05295 [cond-mat.supr-con] (We have not been able to find an archival reference for this paper. Users who know of such a reference are encouraged to contact us.).

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