

InNbS₂ Structure:

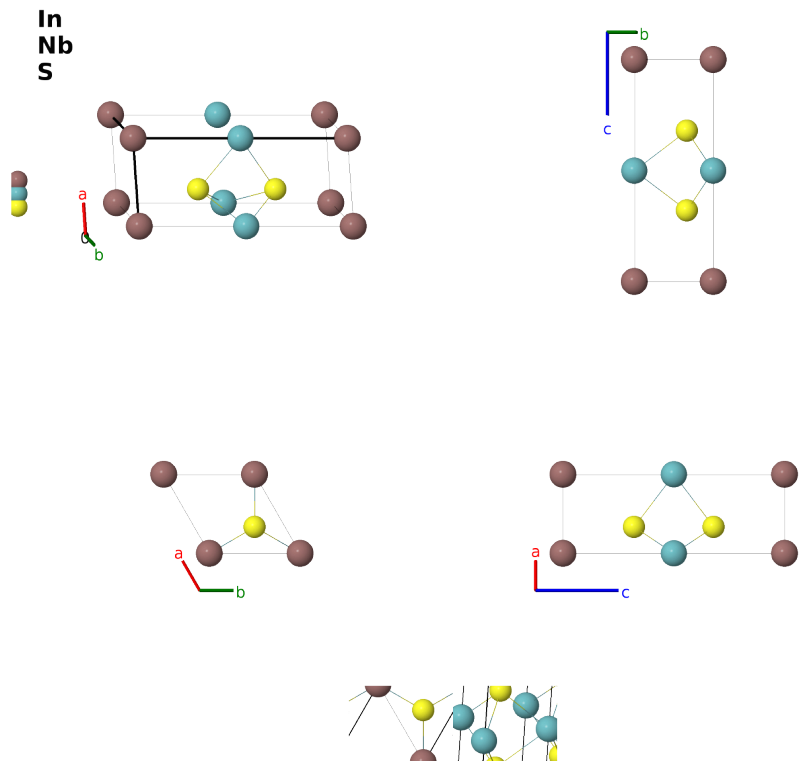
ABC2_hP4_187_a_b_h-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/GUVX>

https://aflow.org/prototype-encyclopedia/ABC2_hP4_187_a_b_h-001



Prototype	InNbS ₂
AFLOW prototype label	ABC2_hP4_187_a_b_h-001
ICSD	74702
CCDC	1635391
Pearson symbol	hP4
Space group number	187
Space group symbol	$P\bar{6}m2$
AFLOW prototype command	<code>aflow --proto=ABC2_hP4_187_a_b_h-001</code> <code>--params=a, c/a, z₃</code>

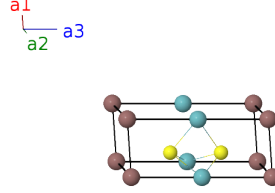
Other compounds with this structure

InTaS₂, InTaSe₂, TiNbS₂, TiNbSe₂, TiTaS₂, TiTaSe₂

- 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 InNbS_2 , which is why we and the ICSD choose it as the prototype of the structure, even though (Eppinga, 1980) give it as Tl_xTaS_2 .
- The value $z_3 = 0.32$ for the sulfur (2c) site is inferred from the value given for Ta_xInSe_2 by (Eppinga, 1980).

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(1a) In I
$\mathbf{B}_2$	$=$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}c\hat{\mathbf{z}}$	(1b) Nb I
$\mathbf{B}_3$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_3\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(2h) S I
$\mathbf{B}_4$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - z_3\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$	(2h) S I

References

- [1] R. Eppinga and G. A. Wieggers, *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.).

First cited in

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