In_3Se_4 Structure: A3B4_hR7_166_ac_2c-001

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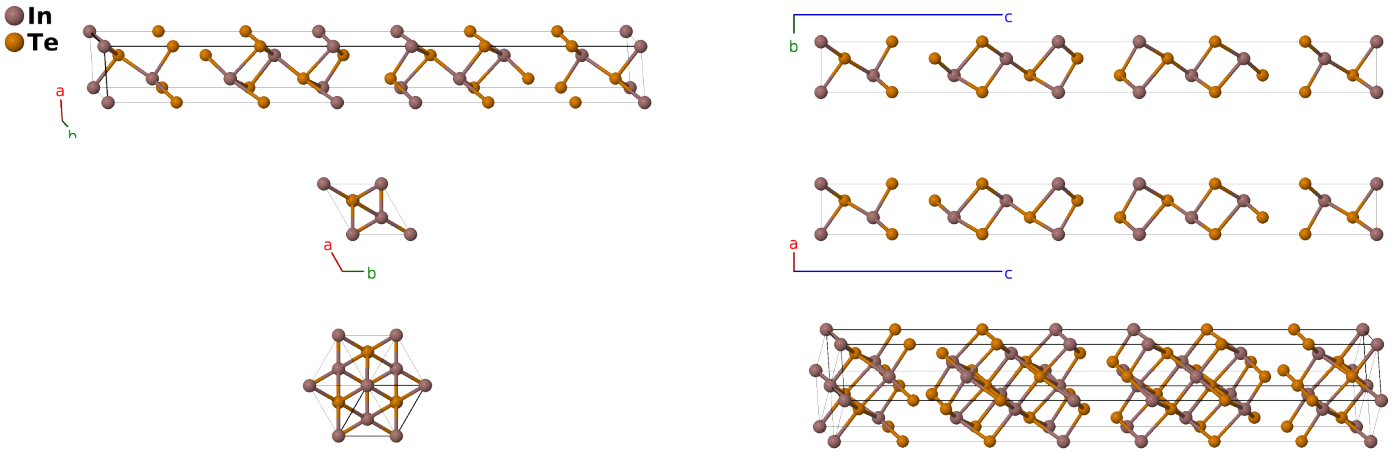
https://aflow.org/p/DJRQ

https://aflow.org/p/A3B4_hR7_166_ac_2c-001



Prototype	In_3Te_4
AFLOW prototype label	A3B4_hR7_166_ac_2c-001
ICSD	44655
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A3B4_hR7_166_ac_2c-001 --params=`$a, c/a, x_2, x_3, x_4$

Other compounds with this structure
Bi_3Te_4, Fe_3S_4 (smythite), In_3Se_4

- (Geller, 1965) created this structure under pressures of about 35 kBar, but works such as (Villars, 2018) list it as the room temperature structure for In_3Te_4.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	In I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	In II
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	In II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Te I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Te I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	Te II
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	Te II

References

[1] S. Geller, A. jayaraman, and J. G. W. Hull, *Crystal chemistry and superconductivity of pressure-induced phases in the In-Te system*, J. Phys. Chem. Solids **26**, 353–361 (1965), doi:10.1016/0022-3697(65)90164-2.

[2] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Indium-Tellurium Binary Phase Diagram (1998 Budanova N.Y.). Copyright ©2006-2018 ASM International.

Found in

[1] G. Han, Z.-G. Chen, C. Sun, L. Yang, L. Cheng, Z. Li, W. Lu, Z. M. Gibbs, G. J. Snyder, K. Jack, J. Drennan, and J. Zou, *A new crystal: layer-structured rhombohedral In_3Se_4*, CrystEngComm **16**, 393–398 (2014), doi:10.1039/c3ce41815d.