$SnTaS_2$ Structure: A2BC_hP8_194_e_a_c-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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.

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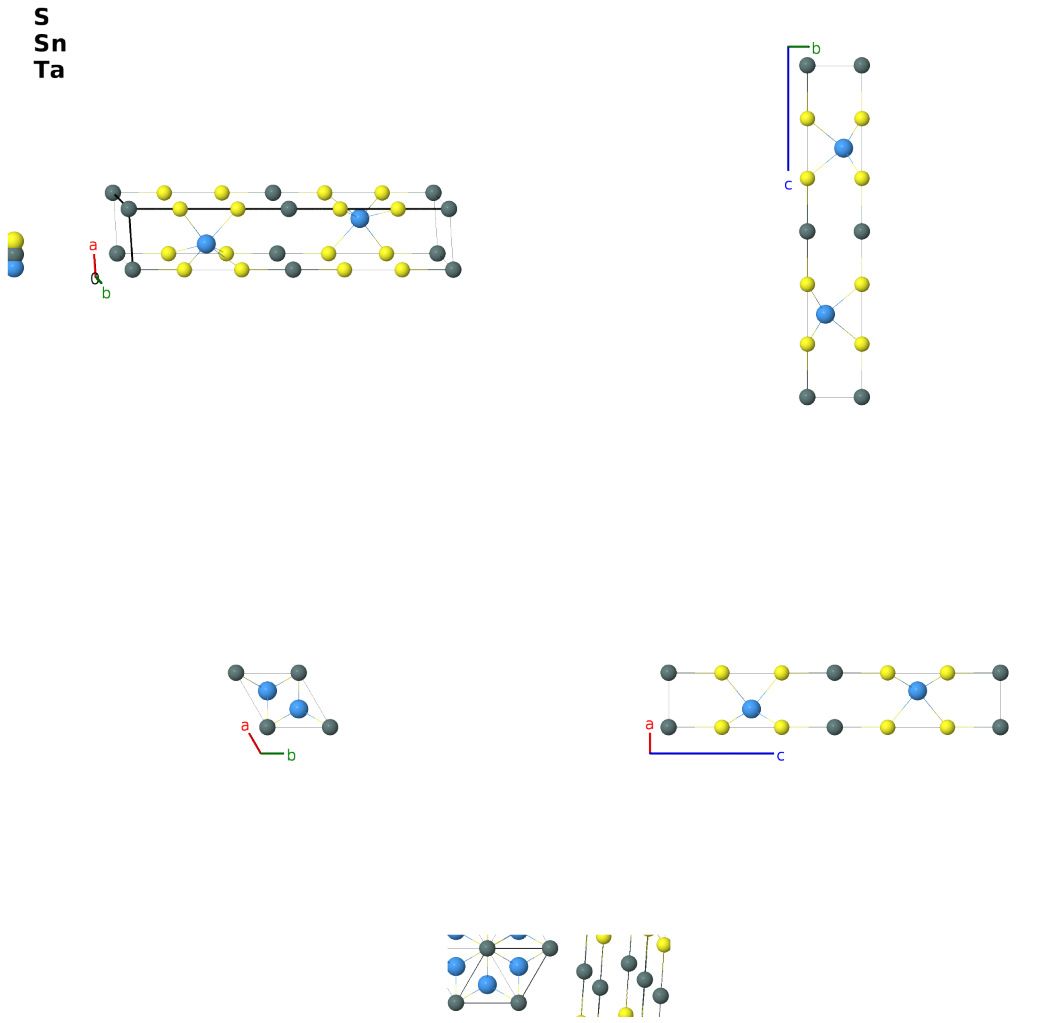
https://aflow.org/prototype-encyclopedia/DG69

https://aflow.org/prototype-encyclopedia/A2BC_hP8_194_e_a_c-001



Prototype	S_2SnTa
AFLOW prototype label	A2BC_hP8_194_e_a_c-001
ICSD	100387
CCDC	1659523
Pearson symbol	hP8
Space group number	194

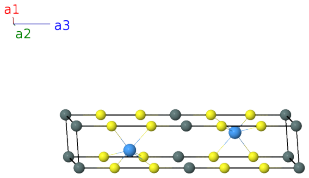
Space group symbol $P6_3/mmc$

AFLOW prototype command `aflow --proto=A2BC_hP8_194_e_a_c-001 --params=`$a, c/a, z_3$

Other compounds with this structure
Bi_xNbS_2, $PbNbS_2$, $SnNbS_2$

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	(2a)	Sn I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Sn I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Ta I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Ta I
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B_6}$	=	$\left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B_7}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B_8}$	=	$-\left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	S I

References

[1] R. Eppinga and G. A. Wiegers, *The crystal structure of the intercalates $SnTaS_2$ and $SnNbS_2$*, Mater. Res. Bull. **12**, 1057–1062 (1977), doi:10.1016/0025-5408(77)90033-2.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.