

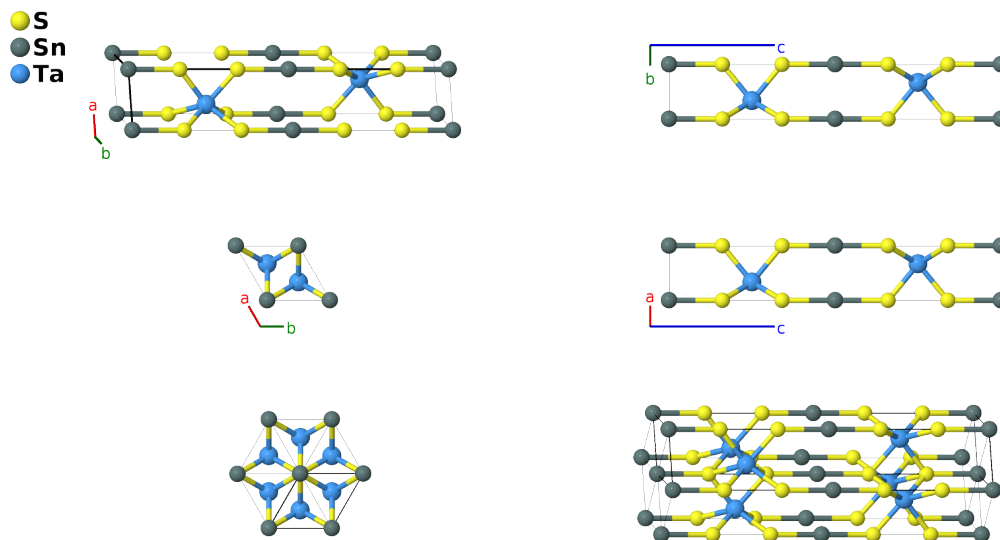
# SnTaS<sub>2</sub> Structure:

## A2BC\_hP8\_194\_e\_a\_c-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/DG69>

[https://aflow.org/p/A2BC\\_hP8\\_194\\_e\\_a\\_c-001](https://aflow.org/p/A2BC_hP8_194_e_a_c-001)



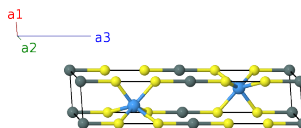
Prototype	S <sub>2</sub> SnTa
AFLOW prototype label	A2BC_hP8_194_e_a_c-001
ICSD	100387
Pearson symbol	hP8
Space group number	194
Space group symbol	<i>P</i> 6 <sub>3</sub> / <i>mmc</i>
AFLOW prototype command	<code>aflow --proto=A2BC_hP8_194_e_a_c-001 --params=a, c/a, z<sub>3</sub></code>

### Other compounds with this structure

SnNbS<sub>2</sub>

### Hexagonal primitive vectors

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



### 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
$\mathbf{B}_5$	=	$z_3 \mathbf{a}_3$	=	$c z_3 \hat{\mathbf{z}}$	(4e) S I
$\mathbf{B}_6$	=	$(z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e) S I
$\mathbf{B}_7$	=	$-z_3 \mathbf{a}_3$	=	$-c z_3 \hat{\mathbf{z}}$	(4e) S I
$\mathbf{B}_8$	=	$-(z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$-c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e) S I

## References

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