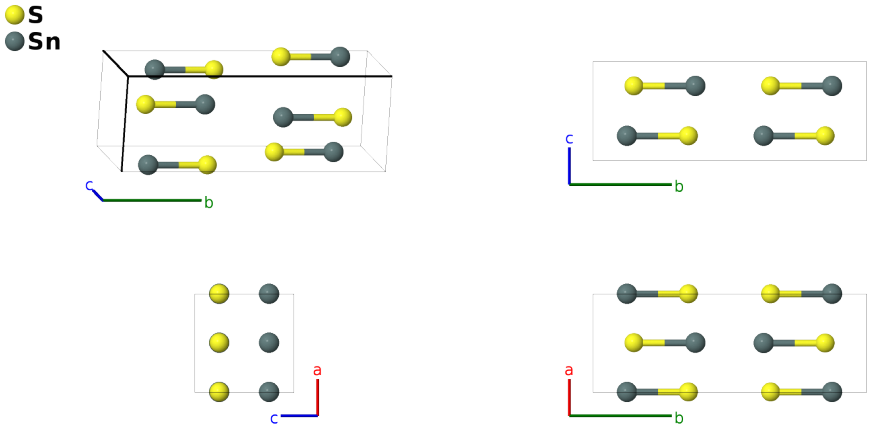
β-SnS Structure: AB_oC8_63_c_c-004

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/8MTK

https://aflow.org/p/AB_oC8_63_c_c-004



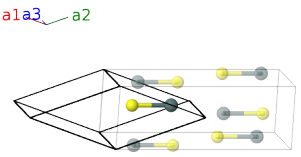
Prototype	SSn
AFLOW prototype label	AB_oC8_63_c_c-004
ICSD	52106
Pearson symbol	oC8
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=AB_oC8_63_c_c-004 --params=`$a, b/a, c/a, y_1, y_2$

Other compounds with this structure
AgCa, CaGe, PtU, TlI

- This is the high-temperature structure of SnS, stable above 875K (Villars, 2018). The ground state system, α-SnS, the mineral herzenbergite, has the $B29$ structure, more commonly listed as the GeS ($B16$) structure.
- We use the data taken by (Chattopadhyay, 1985) at 1000K.
- The ICSD entry for this structure shifts the position of the sulfur atom by $a/2\hat{x}$ from that given in the paper (Chattopadhyay, 1986). The atomic positions are consisted with the published figure of the structure, so we use the original data rather than that in the ICSD.
- β-SnS and CrB ($B33$) have the same AFLOW label, AB_oC8_63_c_c. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Sn I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Sn I

References

[1] T. Chattopadhyay, J. Pannetier, and H. G. von Schnering, *Neutron diffraction study of the structural phase transition in SnS and SnSe*, J. Phys. Chem. Solids **47**, 879–885 (1985), doi:10.1016/0022-3697(86)90059-4.

Found in

[1] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Sulfur-Tin Binary Phase Diagram (1990 Sharma R.C.). Copyright ©2006-2018 ASM International.