

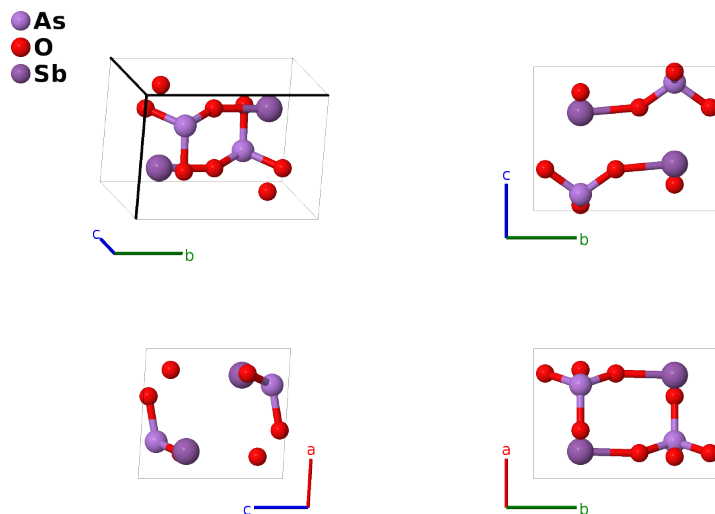
SbAsO₂ Structure:

AB4C_mP12_11_e_2ef_e-001

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<https://afLOW.org/p/C55J>

https://afLOW.org/p/AB4C_mP12_11_e_2ef_e-001



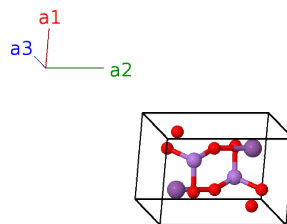
Prototype	AsO ₄ Sb
AFLOW prototype label	AB4C_mP12_11_e_2ef_e-001
ICSD	23316
Pearson symbol	mP12
Space group number	11
Space group symbol	$P2_1/m$
AFLOW prototype command	afLOW --proto=AB4C_mP12_11_e_2ef_e-001 --params=a, b/a, c/a, β , $x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, y_5, z_5$

Other compounds with this structure

SbPO₂

Simple Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	As I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	As I
\mathbf{B}_3	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	O I
\mathbf{B}_4	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	O I
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	O II
\mathbf{B}_6	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	O II
\mathbf{B}_7	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Sb I
\mathbf{B}_8	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Sb I
\mathbf{B}_9	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4f)	O III
\mathbf{B}_{10}	$= -x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4f)	O III
\mathbf{B}_{11}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4f)	O III
\mathbf{B}_{12}	$= x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4f)	O III

References

- [1] P. G. Jones, G. M. Sheldrick, and E. Schwarzmann, *Antimony(III) arsenic(V) oxide*, Acta Crystallogr. Sect. B **36**, 1923–1925 (1980), doi:10.1107/S0567740880007492.

Found in

- [1] A. L. de Jesus Pereira, D. Santamaría-Pérez, R. Vilaplana, D. Errandonea, C. Popescu, E. L. da Silva, J. A. Sans, J. Rodríguez-Carvajal, A. M. noz, P. Rodríguez-Hernández, A. Mujica, S. E. Radescu, A. Beltrán, A. O. de-la Roza, M. Nalin, M. Mollar, and F. J. Manjón, *Experimental and Theoretical Study of SbPO₄ under Compression*, Inorg. Chem. **59**, 287–307 (2020), doi:10.1021/acs.inorgchem.9b02268.