

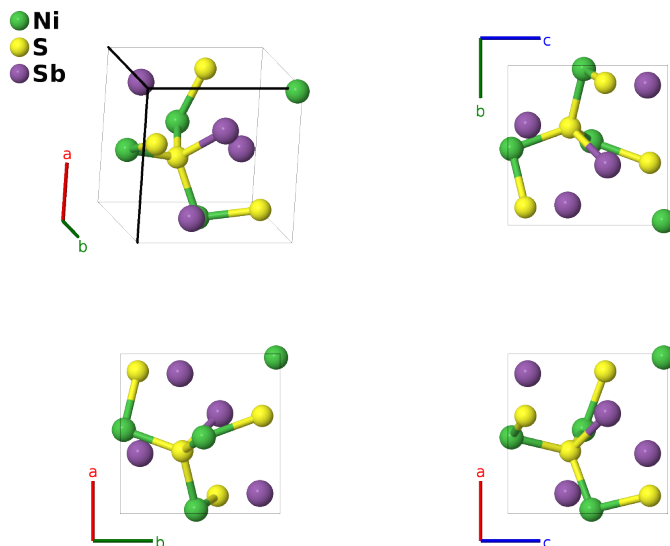
Ullmanite (NiSSb, $F0_1$) Structure: ABC_cP12_198_a_a_a-001

This structure originally had the label ABC_cP12_198_a_a_a. Calls to that address will be redirected here.

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<https://aflow.org/p/VHP8>

https://aflow.org/p/ABC_cP12_198_a_a_a-001



Prototype	NiSSb
AFLOW prototype label	ABC_cP12_198_a_a_a-001
<i>Strukturbericht</i> designation	$F0_1$
Mineral name	ullmanite
ICSD	44606
Pearson symbol	cP12
Space group number	198
Space group symbol	$P2_13$
AFLOW prototype command	<code>aflow --proto=ABC_cP12_198_a_a_a-001 --params=a, x_1, x_2, x_3</code>

Other compounds with this structure

AsBaPt, AsCoS (cobaltite), AsPdS, AsPdSe, BiIrS, BiIrSe, BiNiSe, BiPdSe, BiPtSe, BiRhS, BiRhSe, CaPtSi, CrPtSb, EuPtSi, IrLaSi, IrPSe, IrSSb, IrSSe, IrSbSe, PRhSe, PdSSb, PdSbSe, RhSSb, RhSbSe, (Co, Ni)SbS

- (Ewald, 1928) originally designated CoAsS as *Strukturbericht* $F1$. This was later changed to $F0_1$. We follow (Parthé, 1993) in using NiSbS as the prototype for this structure.

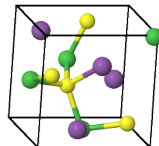
- The Sb (4a) Wyckoff parameter (x_3) has been corrected from 0.875 to 0.625, which matches the bonding distances given by (Y. Takéuchi, 1957) (corrected on 2021/05/10).

Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(4a)	Ni I
\mathbf{B}_2	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Ni I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Ni I
\mathbf{B}_4	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - x_1 \mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(4a)	Ni I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(4a)	S I
\mathbf{B}_6	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	S I
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	S I
\mathbf{B}_8	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(4a)	S I
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(4a)	Sb I
\mathbf{B}_{10}	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Sb I
\mathbf{B}_{11}	$= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Sb I
\mathbf{B}_{12}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(4a)	Sb I

References

- [1] Y. Takéuchi, *The Absolute Structure of Ullmanite, NiSbS*, Mineralogical Journal **2**, 90–102 (1957), doi:10.2465/minerj1953.2.90.
- [2] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).
- [3] Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types, Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., doi:10.1007/978-3-662-02909-1_3.