

Ta₂NiSe₅ Structure:

AB5C2_mC32_15_e_e2f_f-001

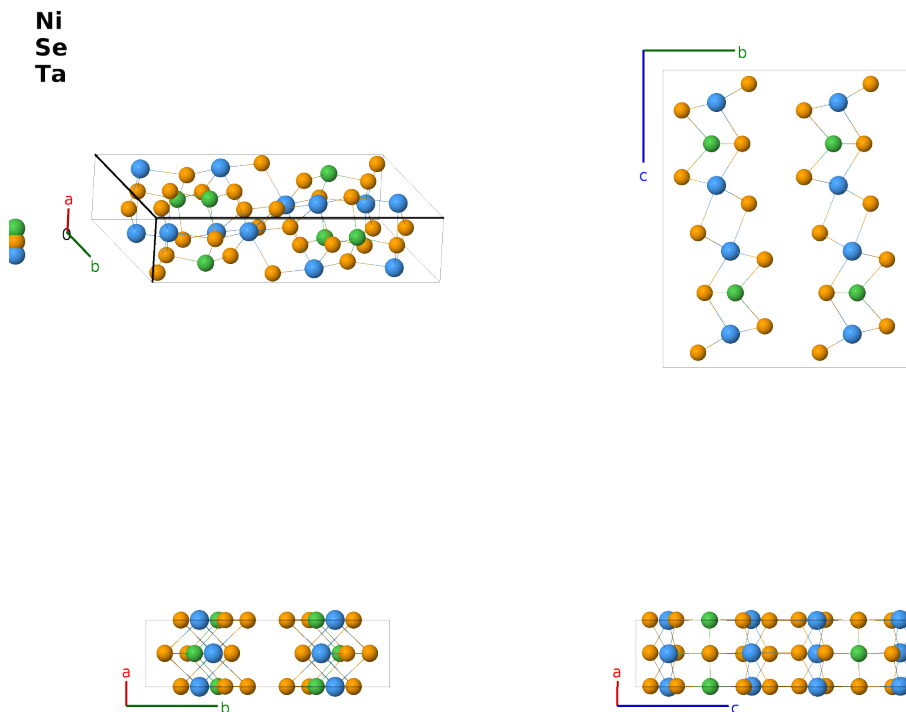
This structure previously used the label(s) **AB5C2_mC32_15_e_e2f_f**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/YFLU>

https://aflow.org/prototype-encyclopedia/AB5C2_mC32_15_e_e2f_f-001



Prototype	NiSe ₅ Ta ₂
AFLOW prototype label	AB5C2_mC32_15_e_e2f_f-001
ICSD	61148
CCDC	1624689
Pearson symbol	mC32
Space group number	15
Space group symbol	C2/c

AFLOW prototype command `aflow --proto=AB5C2_mC32_15_e_e2f_f-001`
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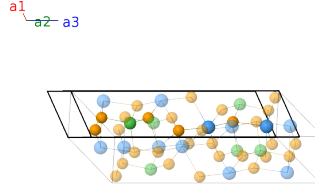
Other compounds with this structure

Ta₂Pd₃Te₅

- Above 328K this transforms into the Ta₂NiS₅ structure.
- When $\beta = 90^\circ$, $x_3 = 1/2$, and $x_4 = x_5 = 0$ this becomes the Ta₂NiS₅ structure.

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Ni I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Ni I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Se I
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Se I
$\mathbf{B}_5$	$= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(8f)	Se II
$\mathbf{B}_6$	$= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Se II
$\mathbf{B}_7$	$= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(8f)	Se II
$\mathbf{B}_8$	$= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Se II
$\mathbf{B}_9$	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(8f)	Se III
$\mathbf{B}_{10}$	$= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Se III
$\mathbf{B}_{11}$	$= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(8f)	Se III
$\mathbf{B}_{12}$	$= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Se III
$\mathbf{B}_{13}$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(8f)	Ta I

$$\mathbf{B}_{14} = \begin{matrix} -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - \\ (z_5 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} - (ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - \\ c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (8f) \quad \text{Ta I}$$

$$\mathbf{B}_{15} = \begin{matrix} -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - \\ z_5 \mathbf{a}_3 \end{matrix} = \begin{matrix} - (ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (8f) \quad \text{Ta I}$$

$$\mathbf{B}_{16} = \begin{matrix} (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \\ (z_5 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} (ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \\ c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (8f) \quad \text{Ta I}$$

References

- [1] S. A. Sunshine and J. A. Ibers, *Structure and physical properties of the new layered ternary chalcogenides tantalum nickel sulfide (Ta_2NiS_5) and tantalum nickel selenide (Ta_2NiSe_5)*, *Inorg. Chem.* **24**, 3611–3614 (1985), doi:10.1021/ic00216a027.

Found in

- [1] F. J. D. Salvo, C. H. Chen, R. M. Fleming, J. V. Waszczak, R. G. Dunn, S. A. Sunshine, and J. A. Ibers, *Physical and structural properties of the new layered compounds Ta_2NiS_5 and Ta_2NiSe_5* , *J. Less-Common Met.* **116**, 51–61 (1986), doi:10.1016/0022-5088(86)90216-X.

First cited in

- 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.