

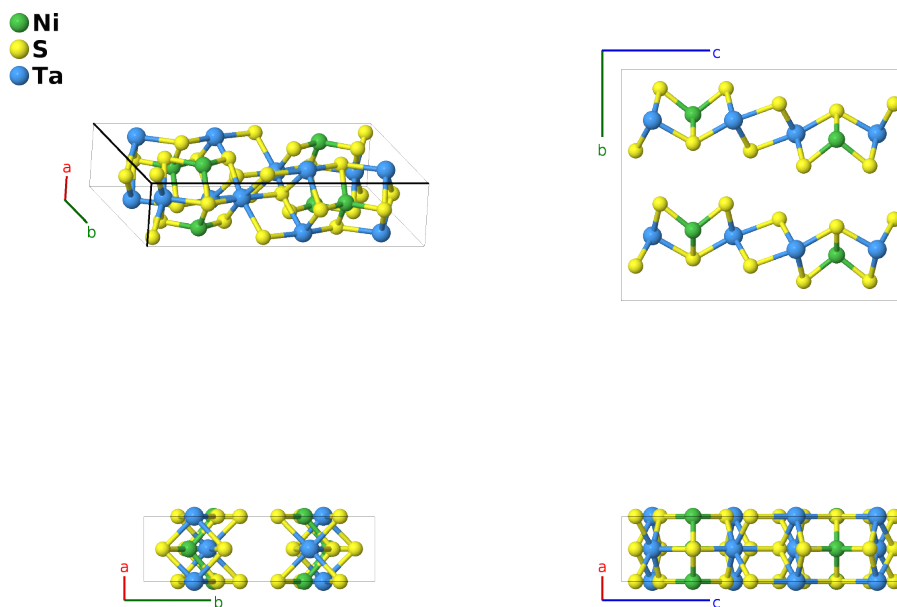
Ta₂NiS₅ Structure: AB5C2_oC32_63_c_c2f_f-004

This structure originally had the label AB5C2_oC32_63_c_c2f_f. Calls to that address will be redirected here.

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

https://aflow.org/p/AB5C2_oC32_63_c_c2f_f-004

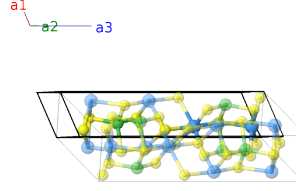


Prototype	NiS ₅ Ta ₂
AFLOW prototype label	AB5C2_oC32_63_c_c2f_f-004
ICSD	61147
Pearson symbol	oC32
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=AB5C2_oC32_63_c_c2f_f-004 --params=a, b/a, c/a, y1, y2, y3, z3, y4, z4, y5, z5</code>

Other compounds with this structure

Ta₂NiSe₅ (above 328K)

Base-centered Orthorhombic primitive vectors



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

Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Ni 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)	Ni 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)	S 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)	S I
\mathbf{B}_5	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8f)	S II
\mathbf{B}_6	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	S II
\mathbf{B}_7	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	S II
\mathbf{B}_8	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8f)	S II
\mathbf{B}_9	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f)	S III
\mathbf{B}_{10}	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	S III
\mathbf{B}_{11}	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	S III
\mathbf{B}_{12}	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8f)	S III
\mathbf{B}_{13}	$= -y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8f)	Ta I
\mathbf{B}_{14}	$= y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Ta I
\mathbf{B}_{15}	$= -y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Ta I
\mathbf{B}_{16}	$= y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8f)	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)* Ta_2NiS_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.