

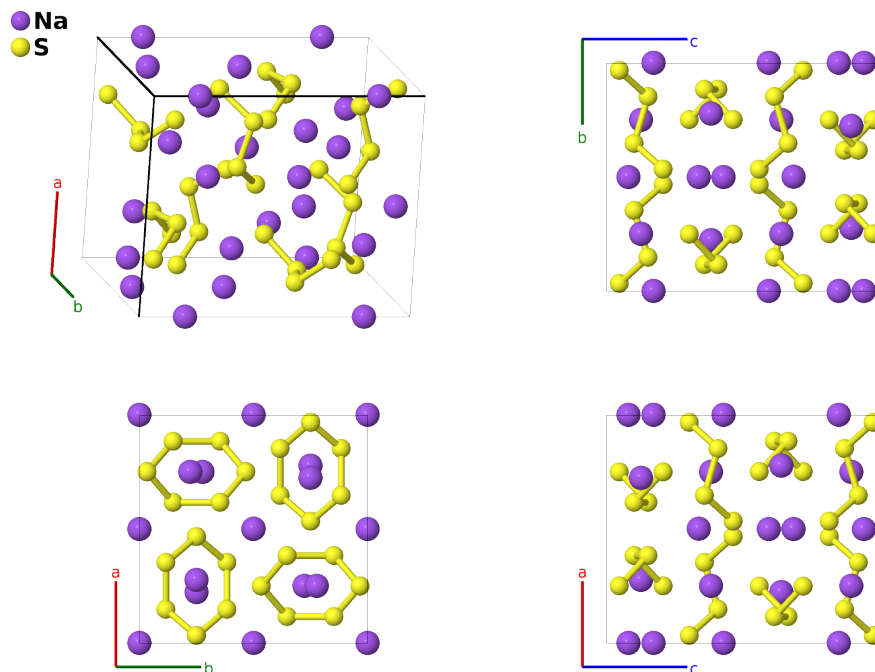
NaS₂ Structure: AB2_tI48_122_cd_2e-001

This structure originally had the label **AB2_tI48_122_cd_2e**. Calls to that address will be redirected here.

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<https://aflow.org/p/Q5KE>

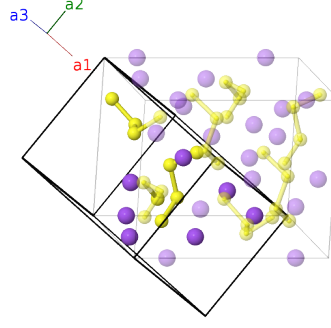
https://aflow.org/p/AB2_tI48_122_cd_2e-001



Prototype	NaS ₂
AFLOW prototype label	AB2_tI48_122_cd_2e-001
ICSD	2586
Pearson symbol	tI48
Space group number	122
Space group symbol	$I\bar{4}2d$
AFLOW prototype command	<pre>aflow --proto=AB2_tI48_122_cd_2e-001 --params=a, c/a, z1, x2, x3, y3, z3, x4, y4, z4</pre>

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2$	$=$	$c z_1 \hat{\mathbf{z}}$	(8c)	Na I
\mathbf{B}_2	$= -z_1 \mathbf{a}_1 - z_1 \mathbf{a}_2$	$=$	$-c z_1 \hat{\mathbf{z}}$	(8c)	Na I
\mathbf{B}_3	$= -(z_1 - \frac{3}{4}) \mathbf{a}_1 - (z_1 - \frac{1}{4}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} - c(z_1 - \frac{1}{4}) \hat{\mathbf{z}}$	(8c)	Na I
\mathbf{B}_4	$= (z_1 + \frac{3}{4}) \mathbf{a}_1 + (z_1 + \frac{1}{4}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + c(z_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(8c)	Na I
\mathbf{B}_5	$= \frac{3}{8} \mathbf{a}_1 + (x_2 + \frac{1}{8}) \mathbf{a}_2 + (x_2 + \frac{1}{4}) \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}}$	(8d)	Na II
\mathbf{B}_6	$= \frac{7}{8} \mathbf{a}_1 - (x_2 - \frac{1}{8}) \mathbf{a}_2 - (x_2 - \frac{3}{4}) \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}}$	(8d)	Na II
\mathbf{B}_7	$= -(x_2 - \frac{7}{8}) \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 - (x_2 - \frac{1}{4}) \mathbf{a}_3$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}}$	(8d)	Na II
\mathbf{B}_8	$= (x_2 + \frac{7}{8}) \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + (x_2 + \frac{3}{4}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}}$	(8d)	Na II
\mathbf{B}_9	$= (y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(16e)	S I
\mathbf{B}_{10}	$= -(y_3 - z_3) \mathbf{a}_1 - (x_3 - z_3) \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(16e)	S I
\mathbf{B}_{11}	$= -(x_3 + z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3$	$=$	$a y_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(16e)	S I
\mathbf{B}_{12}	$= (x_3 - z_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$-a y_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(16e)	S I
\mathbf{B}_{13}	$= (y_3 - z_3 + \frac{3}{4}) \mathbf{a}_1 - (x_3 + z_3 - \frac{1}{4}) \mathbf{a}_2 + (-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(16e)	S I
\mathbf{B}_{14}	$= -(y_3 + z_3 - \frac{3}{4}) \mathbf{a}_1 + (x_3 - z_3 + \frac{1}{4}) \mathbf{a}_2 + (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(16e)	S I
\mathbf{B}_{15}	$= (-x_3 + z_3 + \frac{3}{4}) \mathbf{a}_1 + (-y_3 + z_3 + \frac{1}{4}) \mathbf{a}_2 - (x_3 + y_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a y_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(16e)	S I
\mathbf{B}_{16}	$= (x_3 + z_3 + \frac{3}{4}) \mathbf{a}_1 + (y_3 + z_3 + \frac{1}{4}) \mathbf{a}_2 + (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a y_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(16e)	S I
\mathbf{B}_{17}	$= (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(16e)	S II
\mathbf{B}_{18}	$= -(y_4 - z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - a y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(16e)	S II

$$\begin{aligned}
\mathbf{B}_{19} &= - (x_4 + z_4) \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 - &= & ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (16e) & \text{S II} \\
& \quad (x_4 - y_4) \mathbf{a}_3 \\
\mathbf{B}_{20} &= (x_4 - z_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 + &= & -ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (16e) & \text{S II} \\
& \quad (x_4 - y_4) \mathbf{a}_3 \\
\mathbf{B}_{21} &= \begin{pmatrix} y_4 - z_4 + \frac{3}{4} \\ x_4 + z_4 - \frac{1}{4} \\ -x_4 + y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - &= & -ax_4 \hat{\mathbf{x}} + a \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{4}\right) \hat{\mathbf{z}} & (16e) & \text{S II} \\
& \quad \begin{pmatrix} x_4 + z_4 - \frac{1}{4} \\ -x_4 + y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \\
& \quad \begin{pmatrix} -x_4 + y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{22} &= - \begin{pmatrix} y_4 + z_4 - \frac{3}{4} \\ x_4 - z_4 + \frac{1}{4} \\ x_4 - y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & ax_4 \hat{\mathbf{x}} - a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{4}\right) \hat{\mathbf{z}} & (16e) & \text{S II} \\
& \quad \begin{pmatrix} x_4 - z_4 + \frac{1}{4} \\ x_4 - y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \\
& \quad \begin{pmatrix} x_4 - y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{23} &= \begin{pmatrix} -x_4 + z_4 + \frac{3}{4} \\ -y_4 + z_4 + \frac{1}{4} \\ x_4 + y_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & -ay_4 \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{4}\right) \hat{\mathbf{z}} & (16e) & \text{S II} \\
& \quad \begin{pmatrix} -y_4 + z_4 + \frac{1}{4} \\ x_4 + y_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \\
& \quad \begin{pmatrix} x_4 + y_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{24} &= \begin{pmatrix} x_4 + z_4 + \frac{3}{4} \\ y_4 + z_4 + \frac{1}{4} \\ x_4 + y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & ay_4 \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{4}\right) \hat{\mathbf{z}} & (16e) & \text{S II} \\
& \quad \begin{pmatrix} y_4 + z_4 + \frac{1}{4} \\ x_4 + y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \\
& \quad \begin{pmatrix} x_4 + y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3
\end{aligned}$$

References

- [1] R. Tegman, *The Crystal Structure of Sodium Tetrasulphide, Na₂S₄*, Acta Crystallogr. Sect. B **29**, 1463–1469 (1973), doi:10.1107/S0567740873004735.

Found in

- [1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.