NaS_2 Structure: AB2_tI48_122_cd_2e-001

This structure previously used the label(s) `AB2_tI48_122_cd_2e`. Calls to these addresses will be redirected here.

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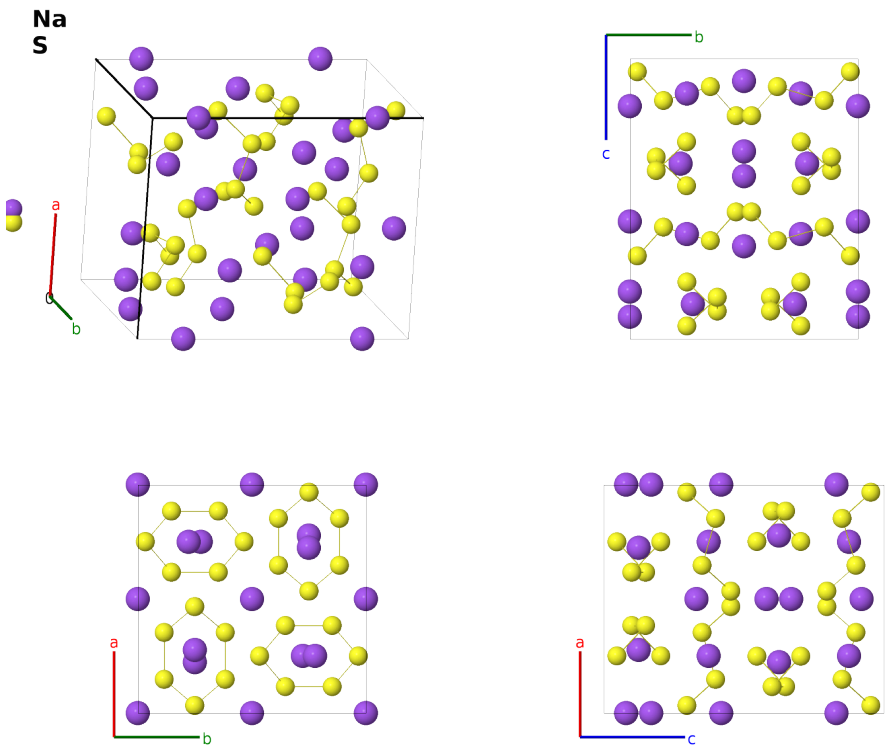
https://aflow.org/prototype-encyclopedia/Q5KE

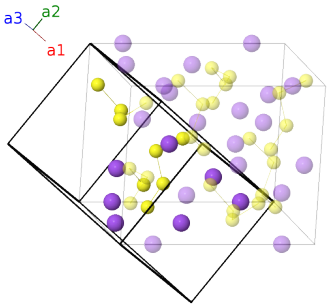
https://aflow.org/prototype-encyclopedia/AB2_tI48_122_cd_2e-001



Prototype	NaS_2
AFLOW prototype label	AB2_tI48_122_cd_2e-001
ICSD	2586
CCDC	1592461
Pearson symbol	tI48
Space group number	122
Space group symbol	$I\bar{4}2d$
AFLOW prototype command	`aflow --proto=AB2_tI48_122_cd_2e-001 --params=`$a, c/a, z_1, x_2, x_3, y_3, z_3, x_4, y_4, z_4$

Body-centered Tetragonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(8c)	Na I
$\mathbf{B_2}$	=	$-z_1\,\mathbf{a}_1 - z_1\,\mathbf{a}_2$	=	$-cz_1\,\hat{\mathbf{z}}$	(8c)	Na I
$\mathbf{B_3}$	=	$-\left(z_1 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(z_1 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Na I
$\mathbf{B_4}$	=	$\left(z_1 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(z_1 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Na I
$\mathbf{B_5}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \left(x_2 + \frac{1}{8}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8d)	Na II
$\mathbf{B_6}$	=	$\frac{7}{8}\,\mathbf{a}_1 - \left(x_2 - \frac{1}{8}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8d)	Na II
$\mathbf{B_7}$	=	$-\left(x_2 - \frac{7}{8}\right)\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(8d)	Na II
$\mathbf{B_8}$	=	$\left(x_2 + \frac{7}{8}\right)\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(8d)	Na II
$\mathbf{B_9}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16e)	S I
$\mathbf{B_{10}}$	=	$-(y_3 - z_3)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - (x_3 + y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16e)	S I
$\mathbf{B_{11}}$	=	$-(x_3 + z_3)\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 - (x_3 - y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16e)	S I
$\mathbf{B_{12}}$	=	$(x_3 - z_3)\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16e)	S I
$\mathbf{B_{13}}$	=	$\left(y_3 - z_3 + \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_3 + z_3 - \frac{1}{4}\right)\,\mathbf{a}_2 + \left(-x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	S I
$\mathbf{B_{14}}$	=	$-\left(y_3 + z_3 - \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_3 - z_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_3 - y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	S I
$\mathbf{B_{15}}$	=	$\left(-x_3 + z_3 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(-y_3 + z_3 + \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_3 + y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	S I
$\mathbf{B_{16}}$	=	$\left(x_3 + z_3 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(y_3 + z_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	S I
$\mathbf{B_{17}}$	=	$(y_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16e)	S II

$\mathbf{B_{18}}$	$= -(y_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16e)	S II
$\mathbf{B_{19}}$	$= -(x_4 + z_4)\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 - (x_4 - y_4)\,\mathbf{a}_3$	$=$	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16e)	S II
$\mathbf{B_{20}}$	$= (x_4 - z_4)\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 + (x_4 - y_4)\,\mathbf{a}_3$	$=$	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16e)	S II
$\mathbf{B_{21}}$	$= \left(y_4 - z_4 + \frac{3}{4}\right)\mathbf{a}_1 - \left(x_4 + z_4 - \frac{1}{4}\right)\mathbf{a}_2 + \left(-x_4 + y_4 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(16e)	S II
$\mathbf{B_{22}}$	$= -\left(y_4 + z_4 - \frac{3}{4}\right)\mathbf{a}_1 + \left(x_4 - z_4 + \frac{1}{4}\right)\mathbf{a}_2 + \left(x_4 - y_4 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(16e)	S II
$\mathbf{B_{23}}$	$= \left(-x_4 + z_4 + \frac{3}{4}\right)\mathbf{a}_1 + \left(-y_4 + z_4 + \frac{1}{4}\right)\mathbf{a}_2 - \left(x_4 + y_4 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-ay_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(16e)	S II
$\mathbf{B_{24}}$	$= \left(x_4 + z_4 + \frac{3}{4}\right)\mathbf{a}_1 + \left(y_4 + z_4 + \frac{1}{4}\right)\mathbf{a}_2 + \left(x_4 + y_4 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$ay_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(16e)	S II

References

[1] R. Tegman, *The Crystal Structure of Sodium Tetrasulphide, Na_2S_4*, 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.

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