Thenardite [Na_2SO_4 (V), $H1_7$] Structure: A2B4C_oF56_70_e_h_a-001

This structure previously used the label(s) `A2B4C_oF56_70_g_h_a`. Calls to these addresses will be redirected here.

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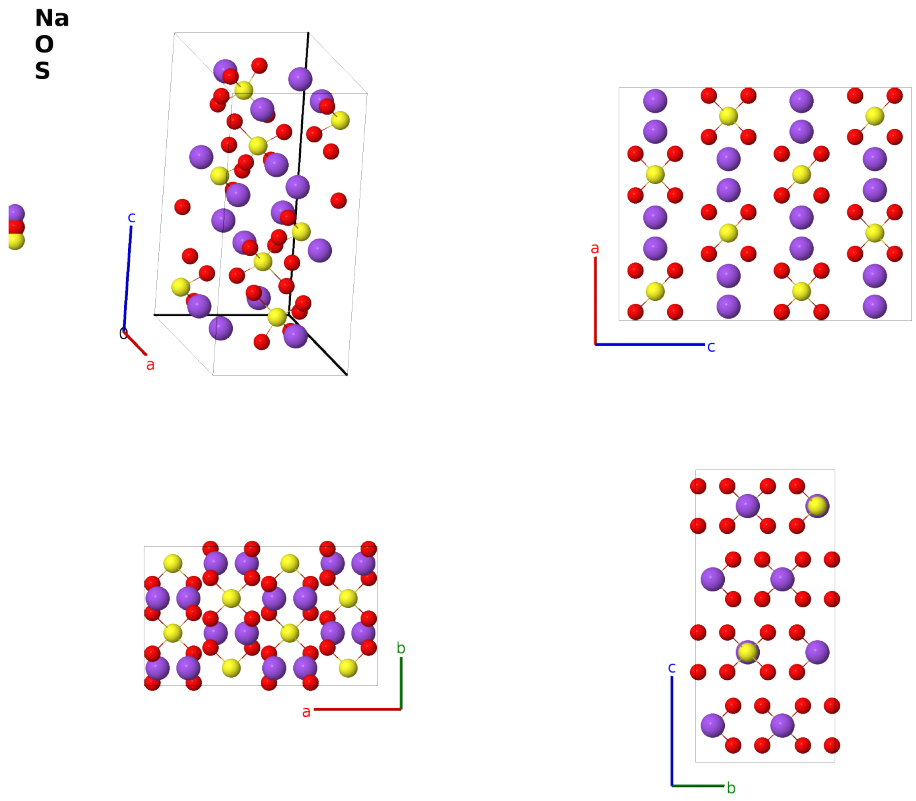
https://aflow.org/prototype-encyclopedia/8CBQ

https://aflow.org/prototype-encyclopedia/A2B4C_oF56_70_e_h_a-001



Prototype	Na_2O_4S
AFLOW prototype label	A2B4C_oF56_70_e_h_a-001
***Strukturbericht* designation**	$H1_7$
Mineral name	thenardite
ICSD	2895
CCDC	1592687
Pearson symbol	oF56
Space group number	70

Space group symbol $Fddd$

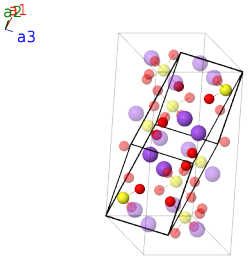
AFLOW prototype command `aflow --proto=A2B4C_oF56_70_e_h_a-001 --params=`$a, b/a, c/a, x_2, x_3, y_3, z_3$

Other compounds with this structure
Ag_2SO_4, Ag_2SeO_4, Cd_2SiO_4, Cr_2SO_4, Cr_2SiO_4, Hg_2GeO_4, Na_2MoO_4, Na_2SeO_4

- Na_2SO_4 has eight known anhydrous phases. For now we have
  - Na_2SO_4 III and
  - Thenardite (Na_2SO_4 V, $H1_7$) (this structure).
- The thenardite phase is "reported to be stable between 32°C and about 180°C" (Nord, 1973), however the data reported here was taken on synthetic thenardite at 25°C.
- The AFLOW label protocol moves the sodium atoms from the reported (16g) site to the (16e) site. This involves shifting the axes so that $\hat{z} \to \hat{x} \to \hat{y} \to \hat{z}$.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8a)	S I
$\mathbf{B_2}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}b\,\hat{\mathbf{y}} + \frac{7}{8}c\,\hat{\mathbf{z}}$	(8a)	S I
$\mathbf{B_3}$	=	$-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_5}$	=	$\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Na I
$\mathbf{B_7}$	=	$(-x_3 + y_3 + z_3)\,\mathbf{a}_1 + (x_3 - y_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3 - z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(32h)	O I
$\mathbf{B_8}$	=	$(x_3 - y_3 + z_3)\,\mathbf{a}_1 + (-x_3 + y_3 + z_3)\,\mathbf{a}_2 - \left(x_3 + y_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(32h)	O I
$\mathbf{B_9}$	=	$(x_3 + y_3 - z_3)\,\mathbf{a}_1 - \left(x_3 + y_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + (-x_3 + y_3 + z_3)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32h)	O I

$\mathbf{B_{10}}$	$=$	$-\left(x_3+y_3+z_3-\frac{1}{2}\right)\mathbf{a}_1+$ $(x_3+y_3-z_3)\,\mathbf{a}_2+$ $(x_3-y_3+z_3)\,\mathbf{a}_3$	$=$	$ax_3\,\hat{\mathbf{x}}-b\left(y_3-\frac{1}{4}\right)\hat{\mathbf{y}}-c\left(z_3-\frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	O I
$\mathbf{B_{11}}$	$=$	$(x_3-y_3-z_3)\,\mathbf{a}_1-$ $(x_3-y_3+z_3)\,\mathbf{a}_2-$ $(x_3+y_3-z_3)\,\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(32h)	O I
$\mathbf{B_{12}}$	$=$	$-(x_3-y_3+z_3)\,\mathbf{a}_1+$ $(x_3-y_3-z_3)\,\mathbf{a}_2+$ $\left(x_3+y_3+z_3+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_3+\frac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_3+\frac{1}{4}\right)\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(32h)	O I
$\mathbf{B_{13}}$	$=$	$-(x_3+y_3-z_3)\,\mathbf{a}_1+$ $\left(x_3+y_3+z_3+\frac{1}{2}\right)\mathbf{a}_2+$ $(x_3-y_3-z_3)\,\mathbf{a}_3$	$=$	$a\left(x_3+\frac{1}{4}\right)\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	O I
$\mathbf{B_{14}}$	$=$	$\left(x_3+y_3+z_3+\frac{1}{2}\right)\mathbf{a}_1-$ $(x_3+y_3-z_3)\,\mathbf{a}_2-$ $(x_3-y_3+z_3)\,\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}}+b\left(y_3+\frac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_3+\frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	O I

References

[1] A. C. Nord, *Refinement of the Crystal Structure of Thenardite Na_2SO_4 (V)*, Acta Chem. Scand. **27**, 814–822 (1973).

First cited in

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