

Na₂SO₃ (*G*3₂) Structure: A2B3C_hP12_147_abd_g_d-001

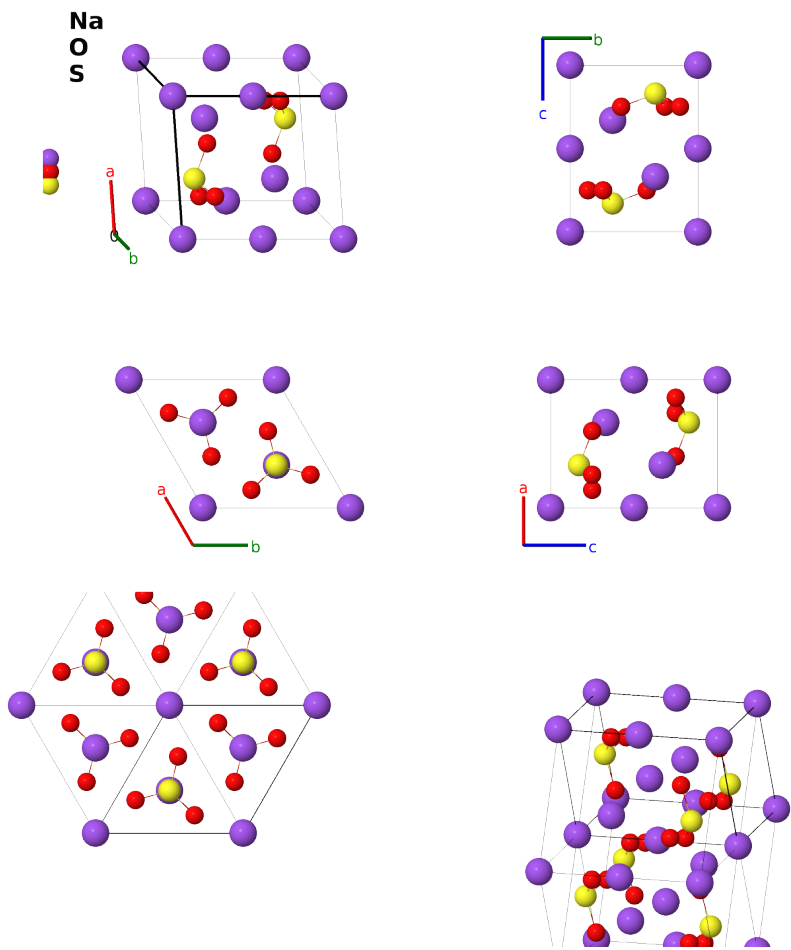
This structure previously used the label(s) **A2B3C_hP12_147_abd_g_d**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/H9Z3>

https://aflow.org/prototype-encyclopedia/A2B3C_hP12_147_abd_g_d-001

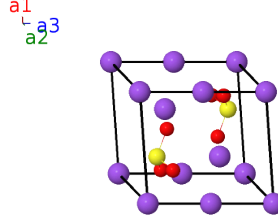


Prototype	Na ₂ O ₃ S
AFLOW prototype label	A2B3C_hP12_147_abd_g_d-001
<i>Strukturbericht</i> designation	<i>G</i> 3 ₂
ICSD	31816
CCDC	1605775
Pearson symbol	hP12

Space group number 147
Space group symbol $P\bar{3}$
AFLOW prototype command `aflow --proto=A2B3C_hP12_147_abd_g_d-001`
`--params=a, c/a, z3, z4, x5, y5, z5`

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(1a)	Na I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(1b)	Na II
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2d)	Na III
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(2d)	Na III
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2d)	S I
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(2d)	S I
$\mathbf{B}_7$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_8$	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_9$	$= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_{11}$	$= y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_{12}$	$= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(6g)	O I

References

- [1] W. H. Zachariasen and H. E. Buckley, *The Crystal Lattice of Anhydrous Sodium Sulphite, Na₂SO₃*, Phys. Rev. **37**, 1295–1305 (1931), doi:10.1103/PhysRev.37.1295.

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