Na_2SO_3 ($G3_2$) Structure: A2B3C_hP12_147_abd_g_d-001

This structure originally had the label `A2B3C_hP12_147_abd_g_d`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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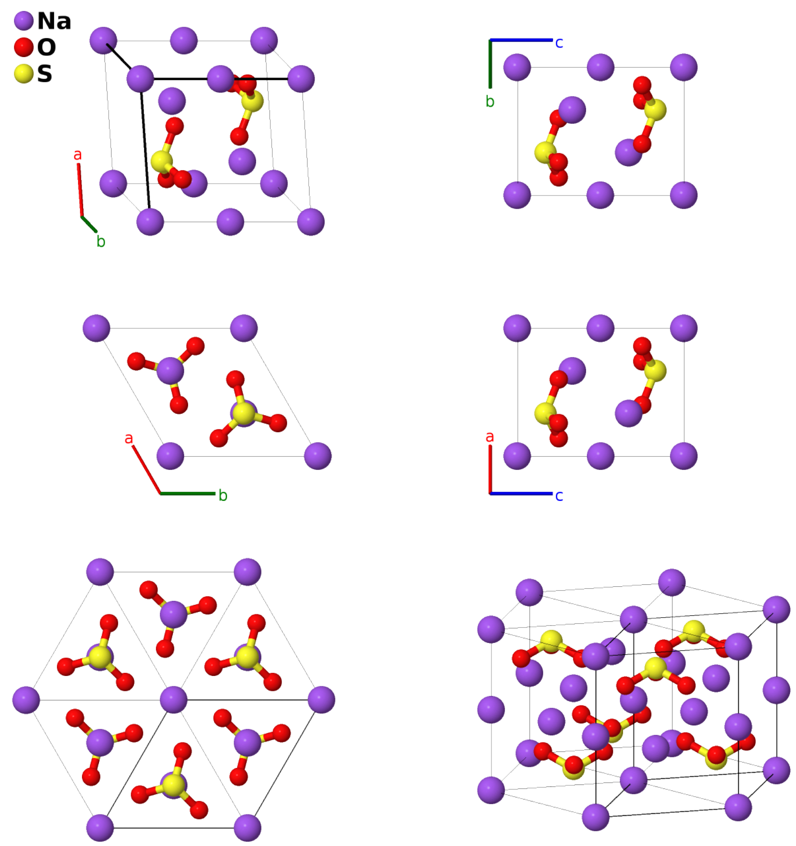
https://aflow.org/p/H9Z3

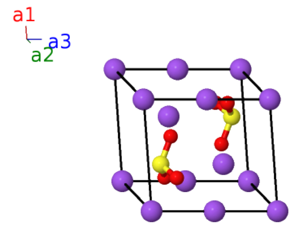
https://aflow.org/p/A2B3C_hP12_147_abd_g_d-001



Prototype	Na_2O_3S
AFLOW prototype label	A2B3C_hP12_147_abd_g_d-001
***Strukturbericht* designation**	$G3_2$
ICSD	31816
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=`$a, c/a, z_3, z_4, x_5, y_5, z_5$

Trigonal (Hexagonal) primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



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
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5 + y_5\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_8}$	=	$-y_5\,\mathbf{a}_1 + \left(x_5 - y_5\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5 - 2y_5\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_9}$	=	$-\left(x_5 - y_5\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_5 - y_5\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_5 + y_5\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{11}}$	=	$y_5\,\mathbf{a}_1 - \left(x_5 - y_5\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_5 + 2y_5\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{12}}$	=	$\left(x_5 - y_5\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_5 - y_5\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6g)	O I

References

[1] W. H. Zachariasen and H. E. Buckley, *The Crystal Lattice of Anhydrous Sodium Sulphite, Na_2SO_3*, Phys. Rev. **37**, 1295–1305 (1931), doi:10.1103/PhysRev.37.1295.