Al_2S_3 Structure: A2B3_hP30_169_2a_3a-001

This structure originally had the label `A2B3_hP30_169_2a_3a`. Calls to that address will be redirected here.

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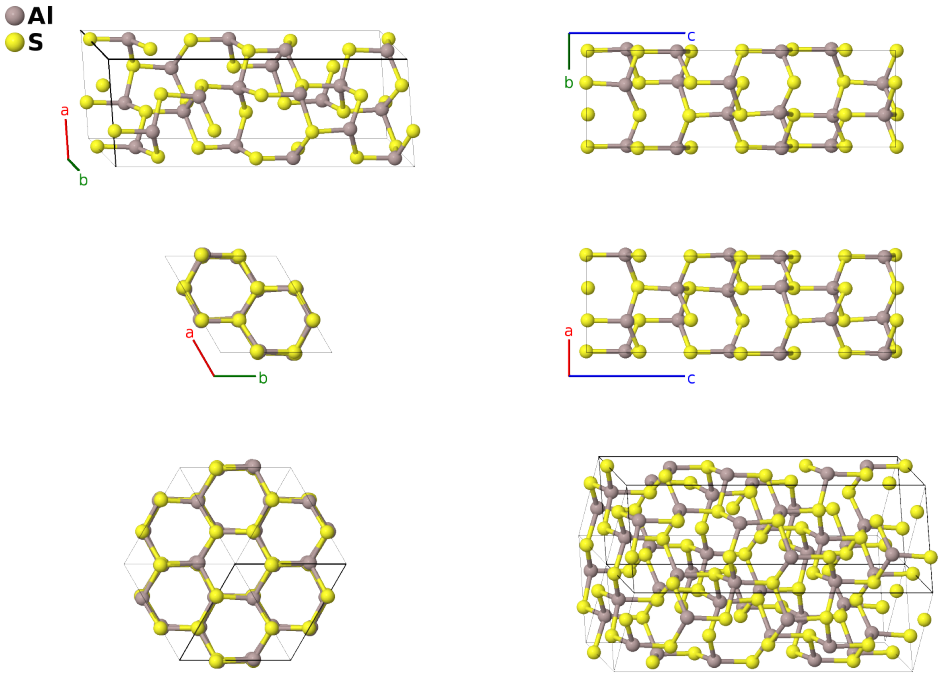
https://aflow.org/p/0WYL

https://aflow.org/p/A2B3_hP30_169_2a_3a-001



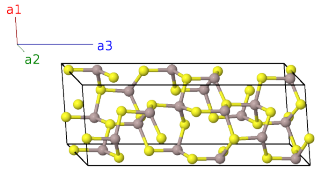
Prototype	Al_2S_3
AFLOW prototype label	A2B3_hP30_169_2a_3a-001
ICSD	300213
Pearson symbol	hP30
Space group number	169
Space group symbol	$P6_1$
AFLOW prototype command	`aflow --proto=A2B3_hP30_169_2a_3a-001 --params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

Other compounds with this structure
In_2S_3

- This structure is the enantiomorph of the Al_2S_3 (A2B3_hP30_170_2a_3a) structure.
- Space group $P6_1$ #169 allows an arbitary choice for the origin of the z-axis. We set this by taking $z_4 = 0$ for the S-I site.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1+y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_1-y_1)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(6a)	Al I
$\mathbf{B_2}$	=	$-y_1\,\mathbf{a}_1 + (x_1-y_1)\,\mathbf{a}_2 + \left(z_1+\frac{1}{3}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1-2y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{3}\right)\hat{\mathbf{z}}$	(6a)	Al I
$\mathbf{B_3}$	=	$-(x_1-y_1)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(z_1+\frac{2}{3}\right)\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_1-y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_1\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_1+2)\,\hat{\mathbf{z}}$	(6a)	Al I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1+y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_1-y_1)\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\hat{\mathbf{z}}$	(6a)	Al I
$\mathbf{B_5}$	=	$y_1\,\mathbf{a}_1 - (x_1-y_1)\,\mathbf{a}_2 + \left(z_1+\frac{5}{6}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_1+2y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{1}{6}c\,(6z_1+5)\,\hat{\mathbf{z}}$	(6a)	Al I
$\mathbf{B_6}$	=	$(x_1-y_1)\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \left(z_1+\frac{1}{6}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_1-y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_1\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{6}\right)\hat{\mathbf{z}}$	(6a)	Al I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2+y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_2-y_2)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6a)	Al II
$\mathbf{B_8}$	=	$-y_2\,\mathbf{a}_1 + (x_2-y_2)\,\mathbf{a}_2 + \left(z_2+\frac{1}{3}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2-2y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{3}\right)\hat{\mathbf{z}}$	(6a)	Al II
$\mathbf{B_9}$	=	$-(x_2-y_2)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(z_2+\frac{2}{3}\right)\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2-y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_2+2)\,\hat{\mathbf{z}}$	(6a)	Al II
$\mathbf{B_{10}}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2+y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_2-y_2)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\hat{\mathbf{z}}$	(6a)	Al II
$\mathbf{B_{11}}$	=	$y_2\,\mathbf{a}_1 - (x_2-y_2)\,\mathbf{a}_2 + \left(z_2+\frac{5}{6}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_2+2y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{6}c\,(6z_2+5)\,\hat{\mathbf{z}}$	(6a)	Al II
$\mathbf{B_{12}}$	=	$(x_2-y_2)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{6}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_2-y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{6}\right)\hat{\mathbf{z}}$	(6a)	Al II
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6a)	S I
$\mathbf{B_{14}}$	=	$-y_3\,\mathbf{a}_1 + (x_3-y_3)\,\mathbf{a}_2 + \left(z_3+\frac{1}{3}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3-2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{3}\right)\hat{\mathbf{z}}$	(6a)	S I
$\mathbf{B_{15}}$	=	$-(x_3-y_3)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(z_3+\frac{2}{3}\right)\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_3+2)\,\hat{\mathbf{z}}$	(6a)	S I
$\mathbf{B_{16}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}}$	(6a)	S I
$\mathbf{B_{17}}$	=	$y_3\,\mathbf{a}_1 - (x_3-y_3)\,\mathbf{a}_2 + \left(z_3+\frac{5}{6}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_3+2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{6}c\,(6z_3+5)\,\hat{\mathbf{z}}$	(6a)	S I
$\mathbf{B_{18}}$	=	$(x_3-y_3)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3+\frac{1}{6}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{6}\right)\hat{\mathbf{z}}$	(6a)	S I
$\mathbf{B_{19}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6a)	S II
$\mathbf{B_{20}}$	=	$-y_4\,\mathbf{a}_1 + (x_4-y_4)\,\mathbf{a}_2 + \left(z_4+\frac{1}{3}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4-2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{3}\right)\hat{\mathbf{z}}$	(6a)	S II
$\mathbf{B_{21}}$	=	$-(x_4-y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(z_4+\frac{2}{3}\right)\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_4+2)\,\hat{\mathbf{z}}$	(6a)	S II

$$\mathbf{B_{22}} = -x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4+\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}} + c\left(z_4+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (6a) \quad \text{S II}$$

$$\mathbf{B_{23}} = y_4\,\mathbf{a}_1 - (x_4-y_4)\,\mathbf{a}_2 + \left(z_4+\tfrac{5}{6}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_4+2y_4)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,(6z_4+5)\,\hat{\mathbf{z}} \quad (6a) \quad \text{S II}$$

$$\mathbf{B_{24}} = (x_4-y_4)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4+\tfrac{1}{6}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4+\tfrac{1}{6}\right)\,\hat{\mathbf{z}} \quad (6a) \quad \text{S II}$$

$$\mathbf{B_{25}} = x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \quad (6a) \quad \text{S III}$$

$$\mathbf{B_{26}} = -y_5\,\mathbf{a}_1 + (x_5-y_5)\,\mathbf{a}_2 + \left(z_5+\tfrac{1}{3}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_5-2y_5)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5+\tfrac{1}{3}\right)\,\hat{\mathbf{z}} \quad (6a) \quad \text{S III}$$

$$\mathbf{B_{27}} = -(x_5-y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(z_5+\tfrac{2}{3}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(3z_5+2)\,\hat{\mathbf{z}} \quad (6a) \quad \text{S III}$$

$$\mathbf{B_{28}} = -x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5+\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}} + c\left(z_5+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (6a) \quad \text{S III}$$

$$\mathbf{B_{29}} = y_5\,\mathbf{a}_1 - (x_5-y_5)\,\mathbf{a}_2 + \left(z_5+\tfrac{5}{6}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_5+2y_5)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,(6z_5+5)\,\hat{\mathbf{z}} \quad (6a) \quad \text{S III}$$

$$\mathbf{B_{30}} = (x_5-y_5)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5+\tfrac{1}{6}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + c\left(z_5+\tfrac{1}{6}\right)\,\hat{\mathbf{z}} \quad (6a) \quad \text{S III}$$

References

[1] B. Eisenmann, *Crystal structure of -dialuminium trisulfide, Al_2S_3*, Z. Kristallogr. **198**, 307–308 (1992), doi:10.1524/zkri.1992.198.14.307.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.