

Al₂S₃ Structure:

A2B3_hP30_170_2a_3a-001

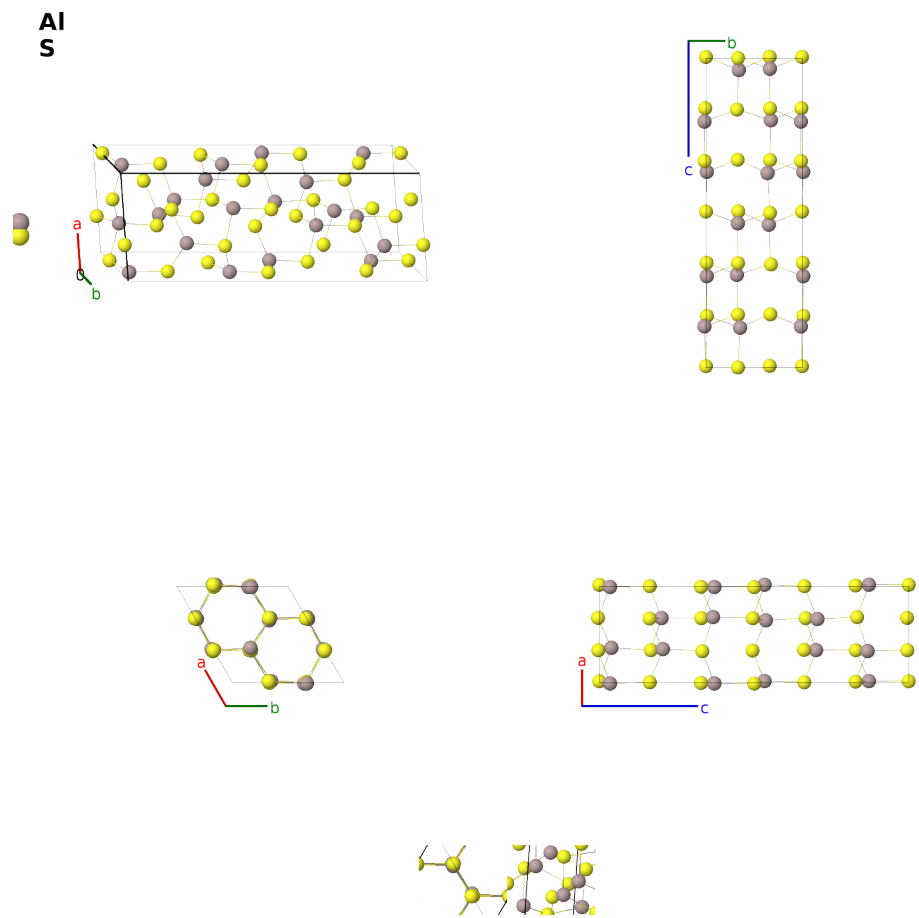
This structure previously used the label(s) **A2B3_hP30_170_2a_3a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/G6GN>

https://aflow.org/prototype-encyclopedia/A2B3_hP30_170_2a_3a-001



Prototype	Al ₂ S ₃
AFLOW prototype label	A2B3_hP30_170_2a_3a-001
ICSD	300213
CCDC	1723843
Pearson symbol	hP30
Space group number	170
Space group symbol	<i>P</i> 6 ₅

AFLOW prototype command `aflow --proto=A2B3_hP30_170_2a_3a-001`
 `--params=a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5`

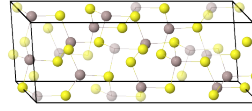
Other compounds with this structure

Ga_xIn_{2-x}Se₃, In₂S₃

- This structure is the enantiomorph of the Al₂S₃ (A2B3_hP30_169_2a_3a) structure. The ICSD information is for that space group.
- Space group $P6_5$ #170 allows an arbitrary choice for the origin of the z -axis. We set this by taking $z_4 = 0$ for the S-I site.

Hexagonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates		Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_1 + y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_1 - y_1) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(6a)		Al I
$\mathbf{B}_2$	$= -y_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + (z_1 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_1 - 2y_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{1}{3}c(3z_1 + 2) \hat{\mathbf{z}}$	(6a)		Al I
$\mathbf{B}_3$	$= -(x_1 - y_1) \mathbf{a}_1 - x_1 \mathbf{a}_2 + (z_1 + \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_1 - y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{3}) \hat{\mathbf{z}}$	(6a)		Al I
$\mathbf{B}_4$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_1 + y_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_1 - y_1) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(6a)		Al I
$\mathbf{B}_5$	$= y_1 \mathbf{a}_1 - (x_1 - y_1) \mathbf{a}_2 + (z_1 + \frac{1}{6}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_1 + 2y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{6}) \hat{\mathbf{z}}$	(6a)		Al I
$\mathbf{B}_6$	$= (x_1 - y_1) \mathbf{a}_1 + x_1 \mathbf{a}_2 + (z_1 + \frac{5}{6}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_1 - y_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_1 \hat{\mathbf{y}} + \frac{1}{6}c(6z_1 + 5) \hat{\mathbf{z}}$	(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
$\mathbf{B}_8$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{3}c(3z_2 + 2) \hat{\mathbf{z}}$	(6a)		Al II
$\mathbf{B}_9$	$= -(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{3}) \hat{\mathbf{z}}$	(6a)		Al II
$\mathbf{B}_{10}$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(6a)		Al II
$\mathbf{B}_{11}$	$= y_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{6}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_2 + 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{6}) \hat{\mathbf{z}}$	(6a)		Al II
$\mathbf{B}_{12}$	$= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + (z_2 + \frac{5}{6}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + \frac{1}{6}c(6z_2 + 5) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{3}c(3z_3 + 2) \hat{\mathbf{z}}$	(6a)		S I

$$\begin{aligned}
\mathbf{B}_{15} &= - (x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{16} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \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(z_3 + \frac{1}{2}) \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{17} &= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{6}) \mathbf{a}_3 = \frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{6}) \hat{\mathbf{z}} & (6a) & \text{S I} \\
\mathbf{B}_{18} &= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{5}{6}) \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}{6}c(6z_3 + 5) \hat{\mathbf{z}} & (6a) & \text{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) & \text{S II} \\
\mathbf{B}_{20} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{21} &= - (x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{22} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \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}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{23} &= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{6}) \mathbf{a}_3 = \frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{6}) \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{24} &= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{5}{6}) \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}{6}c(6z_4 + 5) \hat{\mathbf{z}} & (6a) & \text{S II} \\
\mathbf{B}_{25} &= 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}} & (6a) & \text{S III} \\
\mathbf{B}_{26} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{3}c(3z_5 + 2) \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{27} &= - (x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{3}) \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{28} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \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}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{29} &= y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{6}) \mathbf{a}_3 = \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{6}) \hat{\mathbf{z}} & (6a) & \text{S III} \\
\mathbf{B}_{30} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{6}c(6z_5 + 5) \hat{\mathbf{z}} & (6a) & \text{S III}
\end{aligned}$$

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.

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- D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043