

Andalusite (Al_2SiO_5 , $S0_2$) Structure: A2B5C_oP32_58_eg_3gh_g-001

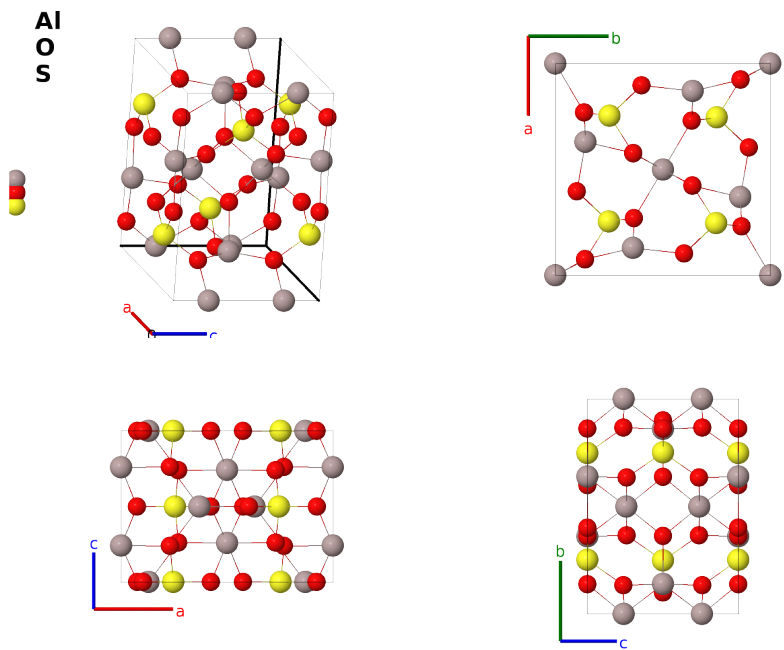
This structure previously used the label(s) **A2B5C_oP32_58_eg_3gh_g**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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.

<https://aflow.org/prototype-encyclopedia/V93J>

https://aflow.org/prototype-encyclopedia/A2B5C_oP32_58_eg_3gh_g-001

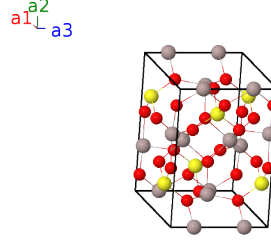


Prototype	$\text{Al}_2\text{O}_5\text{Si}$
AFLOW prototype label	A2B5C_oP32_58_eg_3gh_g-001
<i>Strukturbericht</i> designation	$S0_2$
Mineral name	andalusite
ICSD	100395
CCDC	1659530
Pearson symbol	oP32
Space group number	58
Space group symbol	$Pn\bar{m}$
AFLOW prototype command	<pre>aflow --proto=A2B5C_oP32_58_eg_3gh_g-001 --params=a,b/a,c/a,z1,x2,y2,x3,y3,x4,y4,x5,y5,x6,y6,x7,y7,z7</pre>

- Three crystal polymorphs of Al_2SiO_5 have been characterized, all with Al octahedra and chains of edge-sharing SiO_6 tetrahedra:
 - kyanite ($S0_1$), space group $P\bar{1}$ #2,
 - andalusite ($S0_2$), space group $Pn\bar{1}m$ #58 (this structure), and
 - sillimanite ($S0_3$), space group $Pnma$ #62.
- (Hermann, 1937) listed this as $S0_2$, but also gave it the $H5_3$ designation in the index.

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - c (z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B}_3$	$= -z_1 \mathbf{a}_3$	$=$	$-c z_1 \hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$a x_2 \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}}$	(4g)	Al II
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	$=$	$-a x_2 \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}}$	(4g)	Al II
$\mathbf{B}_7$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	Al II
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	Al II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_{11}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B}_{12}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-a x_4 \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B}_{15}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	O II
$\mathbf{B}_{16}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	O II
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$a x_5 \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}}$	(4g)	O III
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$-a x_5 \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}}$	(4g)	O III
$\mathbf{B}_{19}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	O III

$$\begin{aligned}
\mathbf{B}_{20} &= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4g) & \text{O III} \\
\mathbf{B}_{21} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 = ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} & (4g) & \text{S I} \\
\mathbf{B}_{22} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 = -ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} & (4g) & \text{S I} \\
\mathbf{B}_{23} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4g) & \text{S I} \\
\mathbf{B}_{24} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} & (4g) & \text{S I} \\
\mathbf{B}_{25} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8h) & \text{O IV} \\
\mathbf{B}_{26} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8h) & \text{O IV} \\
\mathbf{B}_{27} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 = -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{O IV} \\
\mathbf{B}_{28} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 = a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{O IV} \\
\mathbf{B}_{29} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (8h) & \text{O IV} \\
\mathbf{B}_{30} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (8h) & \text{O IV} \\
\mathbf{B}_{31} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 = a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{O IV} \\
\mathbf{B}_{32} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 = -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{O IV}
\end{aligned}$$

References

- [1] J. K. Winter and S. Ghose, *Thermal expansion and high-temperature crystal chemistry of the Al_2SiO_4 polymorphs*, Am. Mineral. **64**, 573–586 (1979).
- [2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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.