

Sillimanite (Al_2SiO_5 , $S0_3$) Structure: A2B5C_oP32_62_ac_3cd_c-001

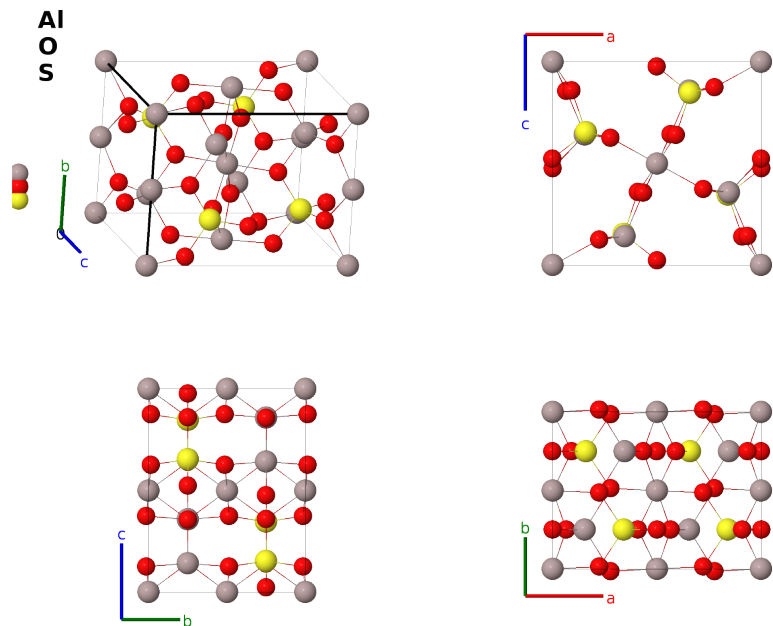
This structure previously used the label(s) **A2B5C_oP32_62.bc.3cd.c**. Calls to these addresses will be redirected here.

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- 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/XCRT>

https://aflow.org/prototype-encyclopedia/A2B5C_oP32_62_ac_3cd_c-001

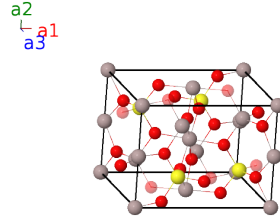


Prototype	$\text{Al}_2\text{O}_5\text{Si}$
AFLOW prototype label	A2B5C_oP32_62_ac_3cd_c-001
<i>Strukturbericht</i> designation	$S0_3$
Mineral name	sillimanite
ICSD	85200
CCDC	1645142
Pearson symbol	oP32
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	<pre>aflow --proto=A2B5C_oP32_62_ac_3cd_c-001 --params=a,b/a,c/a,x2,z2,x3,z3,x4,z4,x5,z5,x6,z6,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 $Pn\bar{m}$ #58, and
 - sillimanite ($S0_3$), space group $Pnma$ #62 (this structure).
- We use the ambient pressure data of (Yang, 1997).
- (Yang, 1997) give the Wyckoff positions in the $Pbnm$ setting of space group #62. We use FINDSYM to transform this to the standard $Pnma$ setting. This involves a rotation of the principle axes and a shift of the set of aluminum atoms from the (4a) to the (4b) Wyckoff position.
- (Hermann, 1937) defined this as $S0_3$, but also listed it as $H5_2$ 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
$\mathbf{B}_1$	$=$	0	$=$	0	Al I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	Al I
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} b \hat{\mathbf{y}}$	Al I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	Al I
$\mathbf{B}_5$	$=$	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	Al II
$\mathbf{B}_6$	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	Al II
$\mathbf{B}_7$	$=$	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	Al II
$\mathbf{B}_8$	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	Al II
$\mathbf{B}_9$	$=$	$x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	O I
$\mathbf{B}_{10}$	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	O I
$\mathbf{B}_{11}$	$=$	$-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	O I
$\mathbf{B}_{12}$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	O I
$\mathbf{B}_{13}$	$=$	$x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	O II
$\mathbf{B}_{14}$	$=$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	O II
$\mathbf{B}_{15}$	$=$	$-x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	O II
$\mathbf{B}_{16}$	$=$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	O II

$$\begin{aligned}
\mathbf{B}_{17} &= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3 &= ax_5 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} &(4c) & \text{O III} \\
\mathbf{B}_{18} &= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{O III} \\
\mathbf{B}_{19} &= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -ax_5 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} &(4c) & \text{O III} \\
\mathbf{B}_{20} &= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{O III} \\
\mathbf{B}_{21} &= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3 &= ax_6 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(4c) & \text{S I} \\
\mathbf{B}_{22} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{S I} \\
\mathbf{B}_{23} &= -x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(4c) & \text{S I} \\
\mathbf{B}_{24} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \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}} &(8d) & \text{O IV} \\
\mathbf{B}_{26} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{O IV} \\
\mathbf{B}_{27} &= -x_7 \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} + b \left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(8d) & \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}} &(8d) & \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}} &(8d) & \text{O IV} \\
\mathbf{B}_{30} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 + y_7 \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{O IV} \\
\mathbf{B}_{31} &= x_7 \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= ax_7 \hat{\mathbf{x}} - b \left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(8d) & \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}} &(8d) & \text{O IV}
\end{aligned}$$

References

- [1] H. Yang, R. M. Hazen, L. W. Finger, C. T. Prewitt, and R. T. Downs, *Compressibility and crystal structure of sillimanite, Al_2SiO_5 , at high pressure*, Phys. Chem. of Minerals **25**, 39–47 (1997), doi:10.1007/s002690050084.
- [2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

First cited in

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.