

Arcanite (β -K₂SO₄, *H*1₆) Structure: A2B4C_oP28_62_2c_2cd_c-001

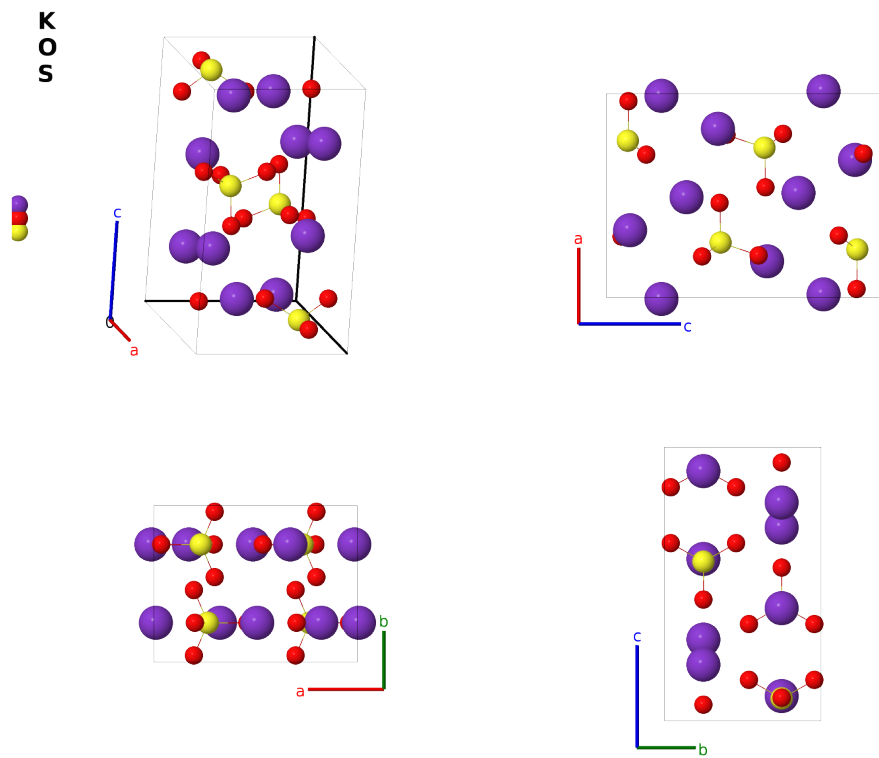
This structure previously used the label(s) **A2B4C_oP28_62_2c_2cd_c**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A2B4C_oP28_62_2c_2cd_c-001



Prototype	K ₂ O ₄ S
AFLOW prototype label	A2B4C_oP28_62_2c_2cd_c-001
Strukturbericht designation	<i>H</i> 1 ₆
Mineral name	arcanite
ICSD	2827
CCDC	1592628
Pearson symbol	oP28
Space group number	62
Space group symbol	<i>Pnma</i>

AFLOW prototype command `aflow --proto=A2B4C_oP28_62_2c_2cd_c-001`
 `--params=a, b/a, c/a, x1, z1, x2, z2, x3, z3, x4, z4, x5, z5, x6, y6, z6`

Other compounds with this structure

Ba₂CoO₄, Ba₂CrO₄, Ba₂GeO₄, Ba₂GeS₄, Ba₂PdD₄, Ba₂SiO₄, Ba₂SiS₄, Ba₂TiS₄, Ca₂CO₄, Ca₂SiO₄, Cs₂CrO₄, Cs₂FeO₄, Cs₂MgD₄, Cs₂MnO₄, Cs₂MoO₄, Cs₂MoS₄, Cs₂MoSe₄, Cs₂RuO₄, Cs₂SO₄, Cs₂SeO₄, Cs₂TeO₄, Cs₂WO₄, Cs₂WS₄, Cs₂ZnD₄, Eu₂PdD₄, Eu₂SiO₄, K₂CrO₄, K₂FeO₄, K₂MnO₄, K₂MoS₄, K₂RuO₄, K₂SeO₄, K₂WS₄, K₂WSe₄, K₂ZnD₄, Rb₂CrO₄, Rb₂MgD₄, Rb₂MgH₄, Rb₂MnO₄, Rb₂MoO₄, Rb₂MoS₄, Rb₂RuO₄, Rb₂SO₄, Rb₂SeO₄, Rb₂WS₄, Rb₂ZnD₄, Sr₂CO₄, Sr₂PdD₄, Sr₂SiO₄, Tl₂CrO₄, Tl₂SO₄, Tl₂SeO₄, (NH₄)₂BeF₄, (NH₄)₂MoS₄, (NH₄)₂SO₄, (NH₄)₂WS₄, (NH₄)₂WSe₄, (NH₄)₂ZnCl₄

- (McGinnety, 1972) gives the atomic positions using the *Pnam* setting of space group #62. We have switched the y- and z-axes to put the crystal in the standard *Pnma* setting.
 - This structure is somewhat similar to Cs₂CuCl₄, but the ICSD recognizes them as different structure types and AFLOW finds a misfit value of 0.2, sufficiently large to justify making this a new prototype.
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Simple Orthorhombic primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B₁	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	K I
B₂	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	K I
B₃	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	K I
B₄	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	K I
B₅	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	K II
B₆	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	K II
B₇	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	K II
B₈	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	K II
B₉	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	O I
B₁₀	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	O I
B₁₁	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	O I
B₁₂	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	O I
B₁₃	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	O II

$$\begin{aligned}
\mathbf{B}_{14} &= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\quad \text{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}} &(4c) &\quad \text{O II} \\
\mathbf{B}_{16} &= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\quad \text{O II} \\
\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) &\quad \text{S I} \\
\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) &\quad \text{S I} \\
\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) &\quad \text{S I} \\
\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) &\quad \text{S I} \\
\mathbf{B}_{21} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(8d) &\quad \text{O III} \\
\mathbf{B}_{22} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) &\quad \text{O III} \\
\mathbf{B}_{23} &= -x_6 \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(8d) &\quad \text{O III} \\
\mathbf{B}_{24} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \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}} - c\left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) &\quad \text{O III} \\
\mathbf{B}_{25} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(8d) &\quad \text{O III} \\
\mathbf{B}_{26} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 + y_6 \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) &\quad \text{O III} \\
\mathbf{B}_{27} &= x_6 \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 + z_6 \mathbf{a}_3 &= ax_6 \hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(8d) &\quad \text{O III} \\
\mathbf{B}_{28} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \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}} + c\left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) &\quad \text{O III}
\end{aligned}$$

References

- [1] J. A. McGinnety, *Redetermination of the structures of potassium sulphate and potassium chromate: the effect of electrostatic crystal forces upon observed bond lengths*, Acta Crystallogr. Sect. B **28**, 2845–2852 (1972), doi:10.1107/S0567740872007022.

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. 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.