

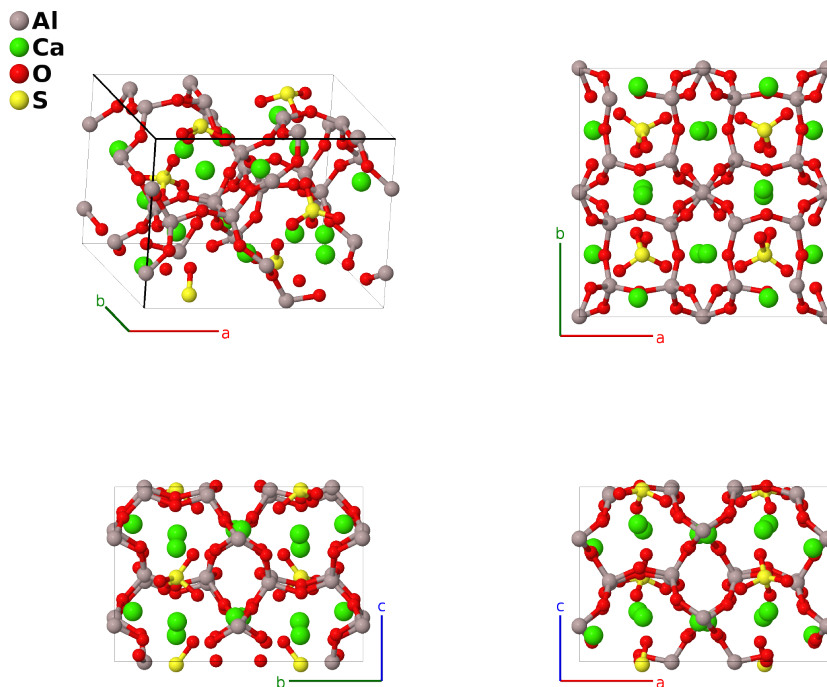
# Ca<sub>4</sub>Al<sub>6</sub>O<sub>16</sub>S Structure: A6B4C16D\_oP108\_27\_abcd4e\_4e\_16e\_e-001

This structure originally had the label A6B4C16D\_oP108\_27\_abcd4e\_4e\_16e\_e. Calls to that address will be redirected here.

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<https://aflow.org/p/TBPX>

[https://aflow.org/p/A6B4C16D\\_oP108\\_27\\_abcd4e\\_4e\\_16e\\_e-001](https://aflow.org/p/A6B4C16D_oP108_27_abcd4e_4e_16e_e-001)



Prototype	Al <sub>6</sub> Ca <sub>4</sub> O <sub>16</sub> S
AFLOW prototype label	A6B4C16D_oP108_27_abcd4e_4e_16e_e-001
ICSD	80361
Pearson symbol	oP108
Space group number	27
Space group symbol	<i>Pcc2</i>
AFLOW prototype command	<pre>aflow --proto=A6B4C16D_oP108_27_abcd4e_4e_16e_e-001       --params=a, b/a, c/a, z1, z2, z3, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10,       y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17,       z17, x18, y18, z18, x19, y19, z19, x20, y20, z20, x21, y21, z21, x22, y22, z22, x23, y23, z23, x24, y24, z24,       x25, y25, z25, x26, y26, z26, x27, y27, z27, x28, y28, z28, x29, y29, z29</pre>

## Other compounds with this structure

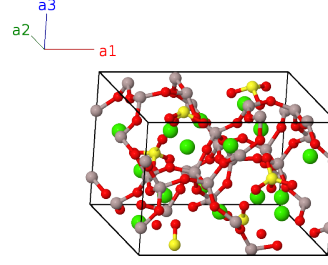
Sr<sub>4</sub>Al<sub>6</sub>O<sub>16</sub>S

## Simple Orthorhombic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1 =$	$z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B}_2 =$	$(z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B}_3 =$	$\frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2b)	Al II
$\mathbf{B}_4 =$	$\frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Al II
$\mathbf{B}_5 =$	$\frac{1}{2} \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + cz_3 \hat{\mathbf{z}}$	(2c)	Al III
$\mathbf{B}_6 =$	$\frac{1}{2} \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2c)	Al III
$\mathbf{B}_7 =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2d)	Al IV
$\mathbf{B}_8 =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2d)	Al IV
$\mathbf{B}_9 =$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4e)	Al V
$\mathbf{B}_{10} =$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4e)	Al V
$\mathbf{B}_{11} =$	$x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Al V
$\mathbf{B}_{12} =$	$-x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Al V
$\mathbf{B}_{13} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4e)	Al VI
$\mathbf{B}_{14} =$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4e)	Al VI
$\mathbf{B}_{15} =$	$x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Al VI
$\mathbf{B}_{16} =$	$-x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Al VI
$\mathbf{B}_{17} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4e)	Al VII
$\mathbf{B}_{18} =$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4e)	Al VII
$\mathbf{B}_{19} =$	$x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Al VII
$\mathbf{B}_{20} =$	$-x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Al VII
$\mathbf{B}_{21} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4e)	Al VIII
$\mathbf{B}_{22} =$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4e)	Al VIII
$\mathbf{B}_{23} =$	$x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Al VIII
$\mathbf{B}_{24} =$	$-x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Al VIII
$\mathbf{B}_{25} =$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B}_{26} =$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B}_{27} =$	$x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B}_{28} =$	$-x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Ca I





## References

- [1] N. J. Calos, C. H. L. Kennard, A. K. Whittaker, and R. L. Davis, *Structure of calcium aluminate sulfate  $Ca_4Al_6O_{16}S$* , J. Solid State Chem. **119**, 1–7 (1995), doi:10.1016/0022-4596(95)80002-7.

## Found in

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