

α -S (A16) Structure: A_oF128_70_4h-001

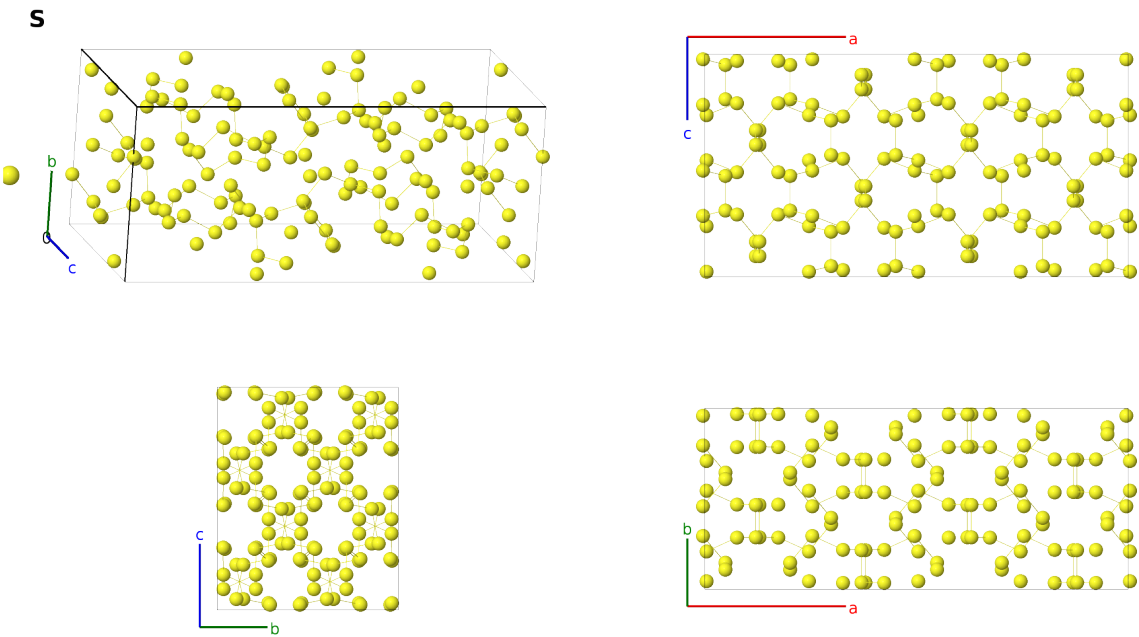
This structure previously used the label(s) **A_oF128_70_4h**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/MYP4>

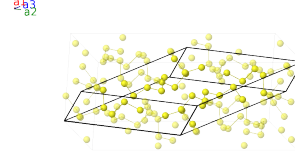
https://aflow.org/prototype-encyclopedia/A_oF128_70_4h-001



Prototype	S
AFLOW prototype label	A_oF128_70_4h-001
<i>Strukturbericht</i> designation	A16
ICSD	63082
CCDC	1161500
Pearson symbol	oF128
Space group number	70
Space group symbol	<i>Fddd</i>
AFLOW prototype command	<code>aflow --proto=A_oF128_70_4h-001</code> <code>--params=<i>a</i>,<i>b</i>/<i>a</i>,<i>c</i>/<i>a</i>,<i>x</i>₁,<i>y</i>₁,<i>z</i>₁,<i>x</i>₂,<i>y</i>₂,<i>z</i>₂,<i>x</i>₃,<i>y</i>₃,<i>z</i>₃,<i>x</i>₄,<i>y</i>₄,<i>z</i>₄</code>

Face-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$(-x_1 + y_1 + z_1)\mathbf{a}_1 +$ $(x_1 - y_1 + z_1)\mathbf{a}_2 +$ $(x_1 + y_1 - z_1)\mathbf{a}_3$	$=$	$ax_1\hat{\mathbf{x}} + by_1\hat{\mathbf{y}} + cz_1\hat{\mathbf{z}}$	(32h) S I
$\mathbf{B}_2$	$=$	$(x_1 - y_1 + z_1)\mathbf{a}_1 +$ $(-x_1 + y_1 + z_1)\mathbf{a}_2 -$ $(x_1 + y_1 + z_1 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{4})\hat{\mathbf{x}} - b(y_1 - \frac{1}{4})\hat{\mathbf{y}} + cz_1\hat{\mathbf{z}}$	(32h) S I
$\mathbf{B}_3$	$=$	$(x_1 + y_1 - z_1)\mathbf{a}_1 -$ $(x_1 + y_1 + z_1 - \frac{1}{2})\mathbf{a}_2 +$ $(-x_1 + y_1 + z_1)\mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{4})\hat{\mathbf{x}} + by_1\hat{\mathbf{y}} - c(z_1 - \frac{1}{4})\hat{\mathbf{z}}$	(32h) S I
$\mathbf{B}_4$	$=$	$-(x_1 + y_1 + z_1 - \frac{1}{2})\mathbf{a}_1 +$ $(x_1 + y_1 - z_1)\mathbf{a}_2 +$ $(x_1 - y_1 + z_1)\mathbf{a}_3$	$=$	$ax_1\hat{\mathbf{x}} - b(y_1 - \frac{1}{4})\hat{\mathbf{y}} - c(z_1 - \frac{1}{4})\hat{\mathbf{z}}$	(32h) S I
$\mathbf{B}_5$	$=$	$(x_1 - y_1 - z_1)\mathbf{a}_1 -$ $(x_1 - y_1 + z_1)\mathbf{a}_2 -$ $(x_1 + y_1 - z_1)\mathbf{a}_3$	$=$	$-ax_1\hat{\mathbf{x}} - by_1\hat{\mathbf{y}} - cz_1\hat{\mathbf{z}}$	(32h) S I
$\mathbf{B}_6$	$=$	$-(x_1 - y_1 + z_1)\mathbf{a}_1 +$ $(x_1 - y_1 - z_1)\mathbf{a}_2 +$ $(x_1 + y_1 + z_1 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{4})\hat{\mathbf{x}} + b(y_1 + \frac{1}{4})\hat{\mathbf{y}} - cz_1\hat{\mathbf{z}}$	(32h) S I
$\mathbf{B}_7$	$=$	$-(x_1 + y_1 - z_1)\mathbf{a}_1 +$ $(x_1 + y_1 + z_1 + \frac{1}{2})\mathbf{a}_2 +$ $(x_1 - y_1 - z_1)\mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{4})\hat{\mathbf{x}} - by_1\hat{\mathbf{y}} + c(z_1 + \frac{1}{4})\hat{\mathbf{z}}$	(32h) S I
$\mathbf{B}_8$	$=$	$(x_1 + y_1 + z_1 + \frac{1}{2})\mathbf{a}_1 -$ $(x_1 + y_1 - z_1)\mathbf{a}_2 -$ $(x_1 - y_1 + z_1)\mathbf{a}_3$	$=$	$-ax_1\hat{\mathbf{x}} + b(y_1 + \frac{1}{4})\hat{\mathbf{y}} + c(z_1 + \frac{1}{4})\hat{\mathbf{z}}$	(32h) S I
$\mathbf{B}_9$	$=$	$(-x_2 + y_2 + z_2)\mathbf{a}_1 +$ $(x_2 - y_2 + z_2)\mathbf{a}_2 +$ $(x_2 + y_2 - z_2)\mathbf{a}_3$	$=$	$ax_2\hat{\mathbf{x}} + by_2\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(32h) S II
$\mathbf{B}_{10}$	$=$	$(x_2 - y_2 + z_2)\mathbf{a}_1 +$ $(-x_2 + y_2 + z_2)\mathbf{a}_2 -$ $(x_2 + y_2 + z_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{4})\hat{\mathbf{x}} - b(y_2 - \frac{1}{4})\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(32h) S II
$\mathbf{B}_{11}$	$=$	$(x_2 + y_2 - z_2)\mathbf{a}_1 -$ $(x_2 + y_2 + z_2 - \frac{1}{2})\mathbf{a}_2 +$ $(-x_2 + y_2 + z_2)\mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{4})\hat{\mathbf{x}} + by_2\hat{\mathbf{y}} - c(z_2 - \frac{1}{4})\hat{\mathbf{z}}$	(32h) S II
$\mathbf{B}_{12}$	$=$	$-(x_2 + y_2 + z_2 - \frac{1}{2})\mathbf{a}_1 +$ $(x_2 + y_2 - z_2)\mathbf{a}_2 +$ $(x_2 - y_2 + z_2)\mathbf{a}_3$	$=$	$ax_2\hat{\mathbf{x}} - b(y_2 - \frac{1}{4})\hat{\mathbf{y}} - c(z_2 - \frac{1}{4})\hat{\mathbf{z}}$	(32h) S II

$$\begin{aligned}
\mathbf{B}_{13} &= \begin{pmatrix} (x_2 - y_2 - z_2) \mathbf{a}_1 - \\ (x_2 - y_2 + z_2) \mathbf{a}_2 - \\ (x_2 + y_2 - z_2) \mathbf{a}_3 \end{pmatrix} = -ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}} & (32h) & \text{S II} \\
\mathbf{B}_{14} &= \begin{pmatrix} -(x_2 - y_2 + z_2) \mathbf{a}_1 + \\ (x_2 - y_2 - z_2) \mathbf{a}_2 + \\ (x_2 + y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_2 + \frac{1}{4}\right) \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{4}\right) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}} & (32h) & \text{S II} \\
\mathbf{B}_{15} &= \begin{pmatrix} -(x_2 + y_2 - z_2) \mathbf{a}_1 + \\ (x_2 + y_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_2 - y_2 - z_2) \mathbf{a}_3 \end{pmatrix} = a \left(x_2 + \frac{1}{4}\right) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{4}\right) \hat{\mathbf{z}} & (32h) & \text{S II} \\
\mathbf{B}_{16} &= \begin{pmatrix} (x_2 + y_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_2 + y_2 - z_2) \mathbf{a}_2 - \\ (x_2 - y_2 + z_2) \mathbf{a}_3 \end{pmatrix} = -ax_2 \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{4}\right) \hat{\mathbf{z}} & (32h) & \text{S II} \\
\mathbf{B}_{17} &= \begin{pmatrix} (-x_3 + y_3 + z_3) \mathbf{a}_1 + \\ (x_3 - y_3 + z_3) \mathbf{a}_2 + \\ (x_3 + y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}} & (32h) & \text{S III} \\
\mathbf{B}_{18} &= \begin{pmatrix} (x_3 - y_3 + z_3) \mathbf{a}_1 + \\ (-x_3 + y_3 + z_3) \mathbf{a}_2 - \\ (x_3 + y_3 + z_3 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_3 - \frac{1}{4}\right) \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{4}\right) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}} & (32h) & \text{S III} \\
\mathbf{B}_{19} &= \begin{pmatrix} (x_3 + y_3 - z_3) \mathbf{a}_1 - \\ (x_3 + y_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 + \\ (-x_3 + y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -a \left(x_3 - \frac{1}{4}\right) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{4}\right) \hat{\mathbf{z}} & (32h) & \text{S III} \\
\mathbf{B}_{20} &= \begin{pmatrix} -(x_3 + y_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 + y_3 - z_3) \mathbf{a}_2 + \\ (x_3 - y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = ax_3 \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{4}\right) \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{4}\right) \hat{\mathbf{z}} & (32h) & \text{S III} \\
\mathbf{B}_{21} &= \begin{pmatrix} (x_3 - y_3 - z_3) \mathbf{a}_1 - \\ (x_3 - y_3 + z_3) \mathbf{a}_2 - \\ (x_3 + y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = -ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} & (32h) & \text{S III} \\
\mathbf{B}_{22} &= \begin{pmatrix} -(x_3 - y_3 + z_3) \mathbf{a}_1 + \\ (x_3 - y_3 - z_3) \mathbf{a}_2 + \\ (x_3 + y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{x}} + b \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} & (32h) & \text{S III} \\
\mathbf{B}_{23} &= \begin{pmatrix} -(x_3 + y_3 - z_3) \mathbf{a}_1 + \\ (x_3 + y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_3 - y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (32h) & \text{S III} \\
\mathbf{B}_{24} &= \begin{pmatrix} (x_3 + y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_3 + y_3 - z_3) \mathbf{a}_2 - \\ (x_3 - y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -ax_3 \hat{\mathbf{x}} + b \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (32h) & \text{S III} \\
\mathbf{B}_{25} &= \begin{pmatrix} (-x_4 + y_4 + z_4) \mathbf{a}_1 + \\ (x_4 - y_4 + z_4) \mathbf{a}_2 + \\ (x_4 + y_4 - z_4) \mathbf{a}_3 \end{pmatrix} = ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (32h) & \text{S IV} \\
\mathbf{B}_{26} &= \begin{pmatrix} (x_4 - y_4 + z_4) \mathbf{a}_1 + \\ (-x_4 + y_4 + z_4) \mathbf{a}_2 - \\ (x_4 + y_4 + z_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_4 - \frac{1}{4}\right) \hat{\mathbf{x}} - b \left(y_4 - \frac{1}{4}\right) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (32h) & \text{S IV} \\
\mathbf{B}_{27} &= \begin{pmatrix} (x_4 + y_4 - z_4) \mathbf{a}_1 - \\ (x_4 + y_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 + \\ (-x_4 + y_4 + z_4) \mathbf{a}_3 \end{pmatrix} = -a \left(x_4 - \frac{1}{4}\right) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{4}\right) \hat{\mathbf{z}} & (32h) & \text{S IV} \\
\mathbf{B}_{28} &= \begin{pmatrix} -(x_4 + y_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 + y_4 - z_4) \mathbf{a}_2 + \\ (x_4 - y_4 + z_4) \mathbf{a}_3 \end{pmatrix} = ax_4 \hat{\mathbf{x}} - b \left(y_4 - \frac{1}{4}\right) \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{4}\right) \hat{\mathbf{z}} & (32h) & \text{S IV} \\
\mathbf{B}_{29} &= \begin{pmatrix} (x_4 - y_4 - z_4) \mathbf{a}_1 - \\ (x_4 - y_4 + z_4) \mathbf{a}_2 - \\ (x_4 + y_4 - z_4) \mathbf{a}_3 \end{pmatrix} = -ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (32h) & \text{S IV}
\end{aligned}$$

$$\mathbf{B}_{30} = \begin{matrix} -(x_4 - y_4 + z_4) \mathbf{a}_1 + \\ (x_4 - y_4 - z_4) \mathbf{a}_2 + \\ (x_4 + y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a \left(x_4 + \frac{1}{4}\right) \hat{\mathbf{x}} + b \left(y_4 + \frac{1}{4}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} \quad (32h) \quad \text{S IV}$$

$$\mathbf{B}_{31} = \begin{matrix} -(x_4 + y_4 - z_4) \mathbf{a}_1 + \\ (x_4 + y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_4 - y_4 - z_4) \mathbf{a}_3 \end{matrix} = a \left(x_4 + \frac{1}{4}\right) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{4}\right) \hat{\mathbf{z}} \quad (32h) \quad \text{S IV}$$

$$\mathbf{B}_{32} = \begin{matrix} (x_4 + y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_4 + y_4 - z_4) \mathbf{a}_2 - \\ (x_4 - y_4 + z_4) \mathbf{a}_3 \end{matrix} = -ax_4 \hat{\mathbf{x}} + b \left(y_4 + \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{4}\right) \hat{\mathbf{z}} \quad (32h) \quad \text{S IV}$$

References

- [1] S. J. Rettig and J. Trotter, *Refinement of the structure of orthorhombic sulfur, α -S₈*, Acta Crystallogr. Sect. C **43**, 2260–2262 (1987), doi:10.1107/S0108270187088152.

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