α-S ($A16$) Structure: A_oF128_70_4h-001
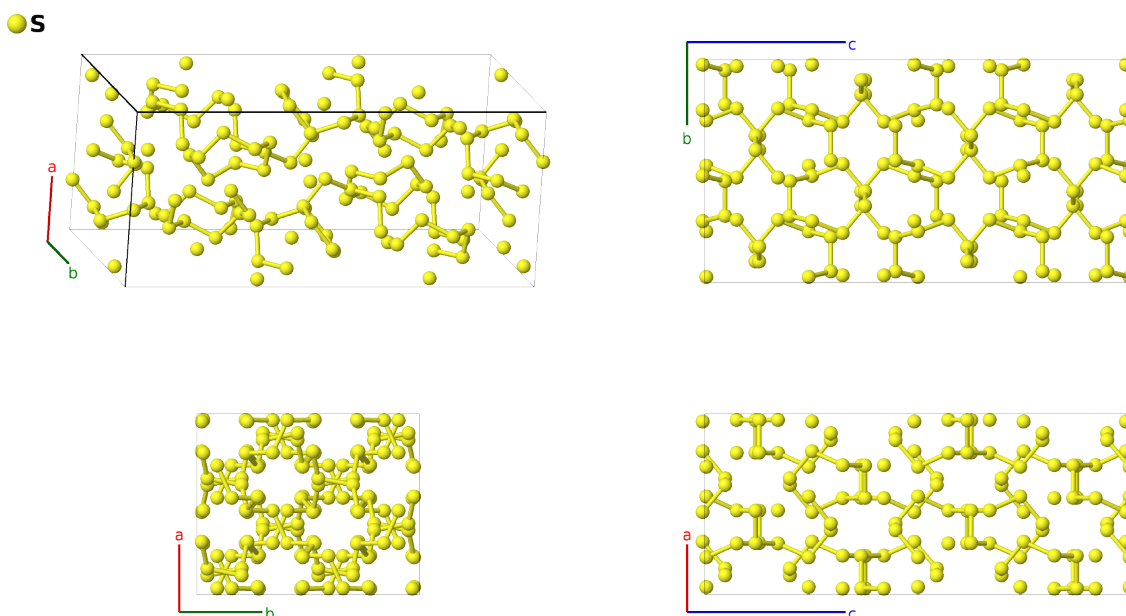
This structure originally had the label `A_oF128_70_4h`. Calls to that address will be redirected here.

https://aflow.org/p/MYP4

https://aflow.org/p/A_oF128_70_4h-001

Prototype	S
AFLOW prototype label	A_oF128_70_4h-001
***Strukturbericht* designation**	$A16$
ICSD	63082
Pearson symbol	oF128
Space group number	70
Space group symbol	$Fddd$
AFLOW prototype command	aflow --proto=A_oF128_70_4h-001
	--params=$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

Face-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
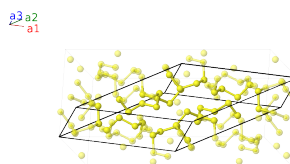
Basis vectors

		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
$\mathbf{B_2}$	$=$	$(x_1 - y_1 + z_1)\,\mathbf{a}_1 +$ $(-x_1 + y_1 + z_1)\,\mathbf{a}_2 -$ $\left(x_1 + y_1 + z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{4}\right)\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(32h)	S I
$\mathbf{B_3}$	$=$	$(x_1 + y_1 - z_1)\,\mathbf{a}_1 -$ $\left(x_1 + y_1 + z_1 - \frac{1}{2}\right)\,\mathbf{a}_2 +$ $(-x_1 + y_1 + z_1)\,\mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{4}\right)\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	S I
$\mathbf{B_4}$	$=$	$-\left(x_1 + y_1 + z_1 - \frac{1}{2}\right)\,\mathbf{a}_1 +$ $(x_1 + y_1 - z_1)\,\mathbf{a}_2 +$ $(x_1 - y_1 + z_1)\,\mathbf{a}_3$	$=$	$ax_1\,\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{4}\right)\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(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
$\mathbf{B_6}$	$=$	$-(x_1 - y_1 + z_1)\,\mathbf{a}_1 +$ $(x_1 - y_1 - z_1)\,\mathbf{a}_2 +$ $\left(x_1 + y_1 + z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{4}\right)\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{4}\right)\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(32h)	S I
$\mathbf{B_7}$	$=$	$-(x_1 + y_1 - z_1)\,\mathbf{a}_1 +$ $\left(x_1 + y_1 + z_1 + \frac{1}{2}\right)\,\mathbf{a}_2 +$ $(x_1 - y_1 - z_1)\,\mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{4}\right)\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	S I
$\mathbf{B_8}$	$=$	$\left(x_1 + y_1 + z_1 + \frac{1}{2}\right)\,\mathbf{a}_1 -$ $(x_1 + y_1 - z_1)\,\mathbf{a}_2 -$ $(x_1 - y_1 + z_1)\,\mathbf{a}_3$	$=$	$-ax_1\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(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
$\mathbf{B_{10}}$	$=$	$(x_2 - y_2 + z_2)\,\mathbf{a}_1 +$ $(-x_2 + y_2 + z_2)\,\mathbf{a}_2 -$ $\left(x_2 + y_2 + z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{4}\right)\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{11}}$	$=$	$(x_2 + y_2 - z_2)\,\mathbf{a}_1 -$ $\left(x_2 + y_2 + z_2 - \frac{1}{2}\right)\,\mathbf{a}_2 +$ $(-x_2 + y_2 + z_2)\,\mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{4}\right)\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{12}}$	$=$	$-\left(x_2 + y_2 + z_2 - \frac{1}{2}\right)\,\mathbf{a}_1 +$ $(x_2 + y_2 - z_2)\,\mathbf{a}_2 +$ $(x_2 - y_2 + z_2)\,\mathbf{a}_3$	$=$	$ax_2\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{4}\right)\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{13}}$	$=$	$(x_2 - y_2 - z_2)\,\mathbf{a}_1 -$ $(x_2 - y_2 + z_2)\,\mathbf{a}_2 -$ $(x_2 + y_2 - z_2)\,\mathbf{a}_3$	$=$	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{14}}$	$=$	$-(x_2 - y_2 + z_2)\,\mathbf{a}_1 +$ $(x_2 - y_2 - z_2)\,\mathbf{a}_2 +$ $\left(x_2 + y_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{4}\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{4}\right)\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{15}}$	$=$	$-(x_2 + y_2 - z_2)\,\mathbf{a}_1 +$ $\left(x_2 + y_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_2 +$ $(x_2 - y_2 - z_2)\,\mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{4}\right)\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	S II

$$\mathbf{B}_{16} = \begin{array}{l}\left(x_2 + y_2 + z_2 + \tfrac{1}{2}\right)\mathbf{a}_1 - \\ \left(x_2 + y_2 - z_2\right)\mathbf{a}_2 - \\ \left(x_2 - y_2 + z_2\right)\mathbf{a}_3\end{array} = -ax_2\,\hat{\mathbf{x}} + b\left(y_2 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ II}$$

$$\mathbf{B}_{17} = \begin{array}{l}\left(-x_3 + y_3 + z_3\right)\mathbf{a}_1 + \\ \left(x_3 - y_3 + z_3\right)\mathbf{a}_2 + \\ \left(x_3 + y_3 - z_3\right)\mathbf{a}_3\end{array} = ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ III}$$

$$\mathbf{B}_{18} = \begin{array}{l}\left(x_3 - y_3 + z_3\right)\mathbf{a}_1 + \\ \left(-x_3 + y_3 + z_3\right)\mathbf{a}_2 - \\ \left(x_3 + y_3 + z_3 - \tfrac{1}{2}\right)\mathbf{a}_3\end{array} = -a\left(x_3 - \tfrac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ III}$$

$$\mathbf{B}_{19} = \begin{array}{l}\left(x_3 + y_3 - z_3\right)\mathbf{a}_1 - \\ \left(x_3 + y_3 + z_3 - \tfrac{1}{2}\right)\mathbf{a}_2 + \\ \left(-x_3 + y_3 + z_3\right)\mathbf{a}_3\end{array} = -a\left(x_3 - \tfrac{1}{4}\right)\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ III}$$

$$\mathbf{B}_{20} = \begin{array}{l}-\left(x_3 + y_3 + z_3 - \tfrac{1}{2}\right)\mathbf{a}_1 + \\ \left(x_3 + y_3 - z_3\right)\mathbf{a}_2 + \\ \left(x_3 - y_3 + z_3\right)\mathbf{a}_3\end{array} = ax_3\,\hat{\mathbf{x}} - b\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ III}$$

$$\mathbf{B}_{21} = \begin{array}{l}\left(x_3 - y_3 - z_3\right)\mathbf{a}_1 - \\ \left(x_3 - y_3 + z_3\right)\mathbf{a}_2 - \\ \left(x_3 + y_3 - z_3\right)\mathbf{a}_3\end{array} = -ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ III}$$

$$\mathbf{B}_{22} = \begin{array}{l}-\left(x_3 - y_3 + z_3\right)\mathbf{a}_1 + \\ \left(x_3 - y_3 - z_3\right)\mathbf{a}_2 + \\ \left(x_3 + y_3 + z_3 + \tfrac{1}{2}\right)\mathbf{a}_3\end{array} = a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + b\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ III}$$

$$\mathbf{B}_{23} = \begin{array}{l}-\left(x_3 + y_3 - z_3\right)\mathbf{a}_1 + \\ \left(x_3 + y_3 + z_3 + \tfrac{1}{2}\right)\mathbf{a}_2 + \\ \left(x_3 - y_3 - z_3\right)\mathbf{a}_3\end{array} = a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ III}$$

$$\mathbf{B}_{24} = \begin{array}{l}\left(x_3 + y_3 + z_3 + \tfrac{1}{2}\right)\mathbf{a}_1 - \\ \left(x_3 + y_3 - z_3\right)\mathbf{a}_2 - \\ \left(x_3 - y_3 + z_3\right)\mathbf{a}_3\end{array} = -ax_3\,\hat{\mathbf{x}} + b\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ III}$$

$$\mathbf{B}_{25} = \begin{array}{l}\left(-x_4 + y_4 + z_4\right)\mathbf{a}_1 + \\ \left(x_4 - y_4 + z_4\right)\mathbf{a}_2 + \\ \left(x_4 + y_4 - z_4\right)\mathbf{a}_3\end{array} = ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ IV}$$

$$\mathbf{B}_{26} = \begin{array}{l}\left(x_4 - y_4 + z_4\right)\mathbf{a}_1 + \\ \left(-x_4 + y_4 + z_4\right)\mathbf{a}_2 - \\ \left(x_4 + y_4 + z_4 - \tfrac{1}{2}\right)\mathbf{a}_3\end{array} = -a\left(x_4 - \tfrac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_4 - \tfrac{1}{4}\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ IV}$$

$$\mathbf{B}_{27} = \begin{array}{l}\left(x_4 + y_4 - z_4\right)\mathbf{a}_1 - \\ \left(x_4 + y_4 + z_4 - \tfrac{1}{2}\right)\mathbf{a}_2 + \\ \left(-x_4 + y_4 + z_4\right)\mathbf{a}_3\end{array} = -a\left(x_4 - \tfrac{1}{4}\right)\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ IV}$$

$$\mathbf{B}_{28} = \begin{array}{l}-\left(x_4 + y_4 + z_4 - \tfrac{1}{2}\right)\mathbf{a}_1 + \\ \left(x_4 + y_4 - z_4\right)\mathbf{a}_2 + \\ \left(x_4 - y_4 + z_4\right)\mathbf{a}_3\end{array} = ax_4\,\hat{\mathbf{x}} - b\left(y_4 - \tfrac{1}{4}\right)\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ IV}$$

$$\mathbf{B}_{29} = \begin{array}{l}\left(x_4 - y_4 - z_4\right)\mathbf{a}_1 - \\ \left(x_4 - y_4 + z_4\right)\mathbf{a}_2 - \\ \left(x_4 + y_4 - z_4\right)\mathbf{a}_3\end{array} = -ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ IV}$$

$$\mathbf{B}_{30} = \begin{array}{l}-\left(x_4 - y_4 + z_4\right)\mathbf{a}_1 + \\ \left(x_4 - y_4 - z_4\right)\mathbf{a}_2 + \\ \left(x_4 + y_4 + z_4 + \tfrac{1}{2}\right)\mathbf{a}_3\end{array} = a\left(x_4 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + b\left(y_4 + \tfrac{1}{4}\right)\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ IV}$$

$$\mathbf{B}_{31} = \begin{array}{l}-\left(x_4 + y_4 - z_4\right)\mathbf{a}_1 + \\ \left(x_4 + y_4 + z_4 + \tfrac{1}{2}\right)\mathbf{a}_2 + \\ \left(x_4 - y_4 - z_4\right)\mathbf{a}_3\end{array} = a\left(x_4 + \tfrac{1}{4}\right)\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ IV}$$

$$\mathbf{B}_{32} = \begin{array}{l}\left(x_4 + y_4 + z_4 + \tfrac{1}{2}\right)\mathbf{a}_1 - \\ \left(x_4 + y_4 - z_4\right)\mathbf{a}_2 - \\ \left(x_4 - y_4 + z_4\right)\mathbf{a}_3\end{array} = -ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \qquad (32\mathrm{h}) \qquad \mathrm{S\ IV}$$

References

[1] S. J. Rettig and J. Trotter, *Refinement of the structure of orthorhombic sulfur, α-S_8*, Acta Crystallogr. Sect. C **43**, 2260–2262 (1987), doi:10.1107/S0108270187088152.