Sc_2S_3 Structure: A3B2_oF80_70_fh_2e-001

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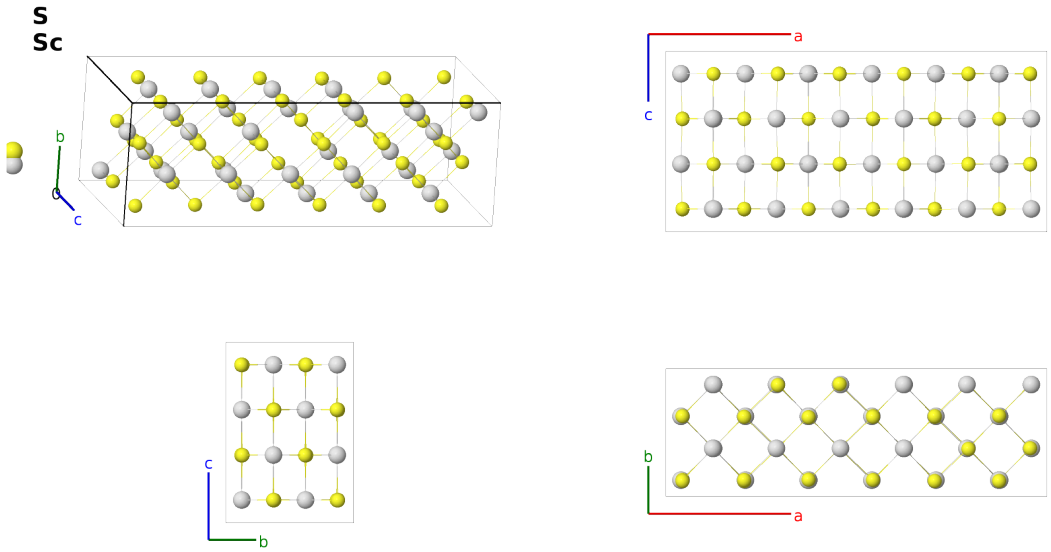
https://aflow.org/prototype-encyclopedia/HQ18

https://aflow.org/prototype-encyclopedia/A3B2_oF80_70_fh_2e-001



Prototype	S_3Sc_2
AFLOW prototype label	A3B2_oF80_70_fh_2e-001
ICSD	22236
CCDC	1599011
Pearson symbol	oF80
Space group number	70
Space group symbol	$Fddd$
AFLOW prototype command	`aflow --proto=A3B2_oF80_70_fh_2e-001 --params=`$a, b/a, c/a, x_1, x_2, y_3, x_4, y_4, z_4$

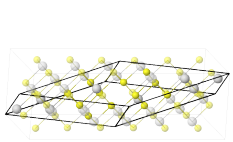
Other compounds with this structure

Dy_2Se_3, Dy_2Te_3, Eu_2Se_3, Eu_2Te_3, Lu_2Se_3, Sc_2Se_3, Y_2Se_3, Y_2Te_3, Yb_2Se_3

- This structure has been rotated from the orientation given by (Dismukes, 1964).

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
$\mathbf{B_1}$	=	$-\left(x_1-\frac{1}{4}\right)\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_1 - \left(x_1-\frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_1-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc I
$\mathbf{B_3}$	=	$\left(x_1+\frac{3}{4}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 + \left(x_1+\frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_1+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_1+\frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc I
$\mathbf{B_5}$	=	$-\left(x_2-\frac{1}{4}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc II
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_1 - \left(x_2-\frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc II
$\mathbf{B_7}$	=	$\left(x_2+\frac{3}{4}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc II
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2+\frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_2+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2+\frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc II
$\mathbf{B_9}$	=	$y_3\,\mathbf{a}_1 - \left(y_3-\frac{1}{4}\right)\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_{10}}$	=	$-\left(y_3-\frac{1}{4}\right)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(y_3-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_{11}}$	=	$-y_3\,\mathbf{a}_1 + \left(y_3+\frac{3}{4}\right)\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_{12}}$	=	$\left(y_3+\frac{3}{4}\right)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(y_3+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + b\left(y_3+\frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_{13}}$	=	$(-x_4+y_4+z_4)\,\mathbf{a}_1 + (x_4-y_4+z_4)\,\mathbf{a}_2 + (x_4+y_4-z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{14}}$	=	$(x_4-y_4+z_4)\,\mathbf{a}_1 + (-x_4+y_4+z_4)\,\mathbf{a}_2 - \left(x_4+y_4+z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{x}} - b\left(y_4-\frac{1}{4}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{15}}$	=	$(x_4+y_4-z_4)\,\mathbf{a}_1 - \left(x_4+y_4+z_4-\frac{1}{2}\right)\,\mathbf{a}_2 + (-x_4+y_4+z_4)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{16}}$	=	$-\left(x_4+y_4+z_4-\frac{1}{2}\right)\,\mathbf{a}_1 + (x_4+y_4-z_4)\,\mathbf{a}_2 + (x_4-y_4+z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - b\left(y_4-\frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{17}}$	=	$(x_4-y_4-z_4)\,\mathbf{a}_1 - (x_4-y_4+z_4)\,\mathbf{a}_2 - (x_4+y_4-z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{18}}$	=	$-(x_4-y_4+z_4)\,\mathbf{a}_1 + (x_4-y_4-z_4)\,\mathbf{a}_2 + \left(x_4+y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{x}} + b\left(y_4+\frac{1}{4}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(32h)	S II

$\mathbf{B_{19}}$	$= -(x_4 + y_4 - z_4)\,\mathbf{a}_1 + \left(x_4 + y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_4 - y_4 - z_4)\,\mathbf{a}_3$	$= a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{20}}$	$= \left(x_4 + y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_4 + y_4 - z_4)\,\mathbf{a}_2 - (x_4 - y_4 + z_4)\,\mathbf{a}_3$	$= -ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32h)	S II

References

[1] J. P. Dismukes and J. G. White, *The Preparation, Properties, and Crystal Structures of Some Scandium Sulfides in the Range Sc_2S_3-ScS*, Inorg. Chem. **3**, 1220–1228 (1964), doi:10.1021/ic50019a004.

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