SiS_2 ($C42$) Structure: A2B_oI12_72_j_a-001

This structure originally had the label `A2B_oI12_72_j_a`. Calls to that address will be redirected here.

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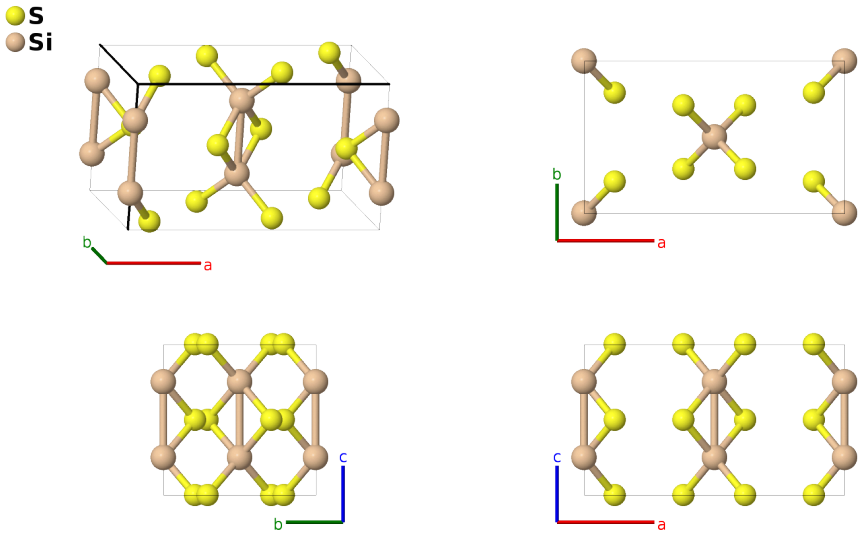
https://aflow.org/p/PYBC

https://aflow.org/p/A2B_oI12_72_j_a-001



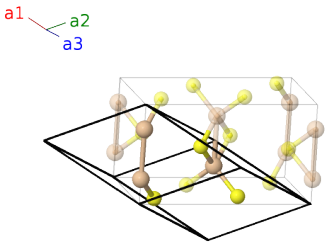
Prototype	S_2Si
AFLOW prototype label	A2B_oI12_72_j_a-001
***Strukturbericht* designation**	$C42$
ICSD	27205
Pearson symbol	oI12
Space group number	72
Space group symbol	$Ibam$
AFLOW prototype command	`aflow --proto=A2B_oI12_72_j_a-001 --params=`$a, b/a, c/a, x_2, y_2$

Other compounds with this structure

$SeSi_2$

Body-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_3}$	=	$y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + (x_2+y_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}}$	(8j)	S I
$\mathbf{B_4}$	=	$-y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - (x_2+y_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}}$	(8j)	S I
$\mathbf{B_5}$	=	$\left(y_2+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2-\frac{1}{2}\right)\,\mathbf{a}_2 - (x_2-y_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	S I
$\mathbf{B_6}$	=	$-\left(y_2-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2+\frac{1}{2}\right)\,\mathbf{a}_2 + (x_2-y_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	S I

References

[1] J. Peters and B. Krebs, *Silicon disulphide and silicon diselenide: a reinvestigation*, Acta Crystallogr. Sect. B **38**, 1270–1272 (1982), doi:10.1107/S0567740882005469.