S-III Structure: A_tI16_142_f-001

This structure originally had the label `A_tI16_142_f`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

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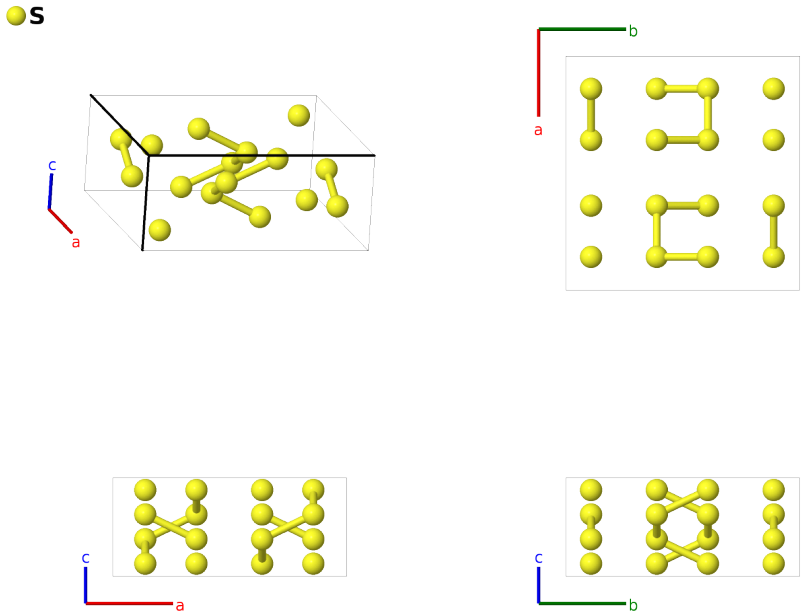
https://aflow.org/p/GC8R

https://aflow.org/p/A_tI16_142_f-001

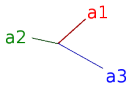


Prototype	S
AFLOW prototype label	A_tI16_142_f-001
ICSD	none
Pearson symbol	tI16
Space group number	142
Space group symbol	$I4_1/acd$
AFLOW prototype command	`aflow --proto=A_tI16_142_f-001 --params=`$a, c/a, x_1$

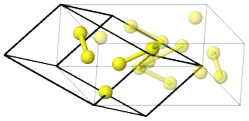
Other compounds with this structure
Se (Se-VII, prepared at 450K and 20 GPa)

- The S-III phase is found when sulfur is pressurized above 36 GPa at 300K. At 300K it is stable up to 83 GPa. This data was taken at 12 GPa and 300K.

Body-centered Tetragonal primitive vectors



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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\left(x_1+\frac{3}{8}\right)\mathbf{a}_1+\left(x_1+\frac{1}{8}\right)\mathbf{a}_2+\left(2x_1+\frac{1}{4}\right)\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}}+a\left(x_1+\frac{1}{4}\right)\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_2}$	=	$-\left(x_1-\frac{3}{8}\right)\mathbf{a}_1-\left(x_1-\frac{1}{8}\right)\mathbf{a}_2-\left(2x_1-\frac{1}{4}\right)\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}}-a\left(x_1-\frac{1}{4}\right)\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_3}$	=	$\left(x_1+\frac{1}{8}\right)\mathbf{a}_1-\left(x_1-\frac{3}{8}\right)\mathbf{a}_2+\frac{3}{4}\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_1+\frac{1}{4}\right)\hat{\mathbf{y}}-\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_4}$	=	$-\left(x_1-\frac{1}{8}\right)\mathbf{a}_1+\left(x_1+\frac{3}{8}\right)\mathbf{a}_2+\frac{3}{4}\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_1-\frac{1}{4}\right)\hat{\mathbf{y}}-\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_5}$	=	$-\left(x_1-\frac{5}{8}\right)\mathbf{a}_1-\left(x_1-\frac{7}{8}\right)\mathbf{a}_2-\left(2x_1-\frac{3}{4}\right)\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_1-\frac{1}{4}\right)\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_6}$	=	$\left(x_1+\frac{5}{8}\right)\mathbf{a}_1+\left(x_1+\frac{7}{8}\right)\mathbf{a}_2+\left(2x_1+\frac{3}{4}\right)\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_1+\frac{1}{4}\right)\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_7}$	=	$-\left(x_1-\frac{7}{8}\right)\mathbf{a}_1+\left(x_1+\frac{5}{8}\right)\mathbf{a}_2+\frac{1}{4}\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}}-a\left(x_1-\frac{1}{4}\right)\hat{\mathbf{y}}+\frac{5}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_8}$	=	$\left(x_1+\frac{7}{8}\right)\mathbf{a}_1-\left(x_1-\frac{5}{8}\right)\mathbf{a}_2+\frac{1}{4}\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}}+a\left(x_1+\frac{1}{4}\right)\hat{\mathbf{y}}+\frac{5}{8}c\,\hat{\mathbf{z}}$	(16f)	S I

References

[1] O. Degtyareva, E. Gregoryanz, M. Somayazulu, P. Dera, H. Mao, and R. J. Hemley, *Novel chain structures in group VI elements*, Nat. Mater. **4**, 152–155 (2005), doi:10.1038/nmat1294.