

S-III Structure: A_tI16_142_f-001

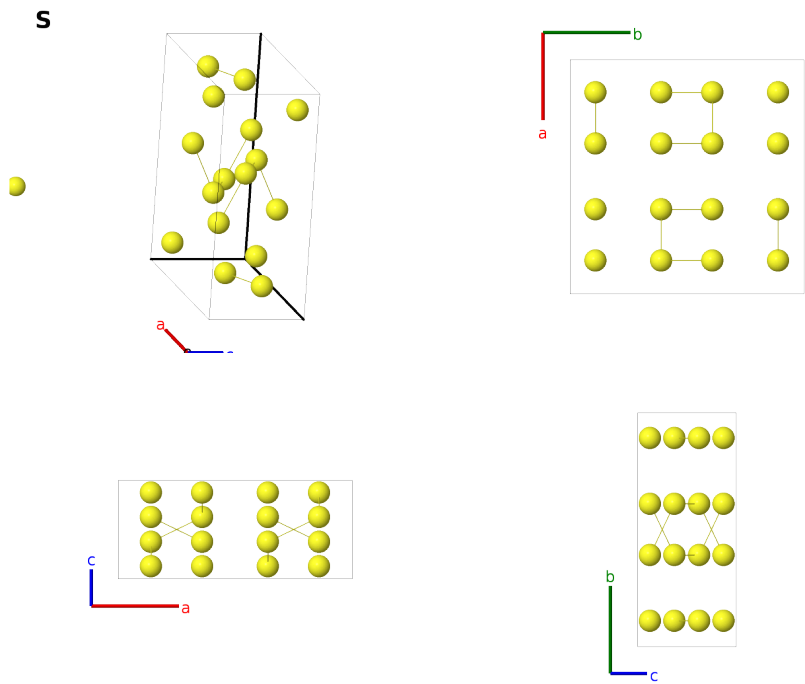
This structure previously used the label(s) **A_tI16_142_f**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/GC8R>

https://aflow.org/prototype-encyclopedia/A_tI16_142_f-001



Prototype	S
AFLOW prototype label	A_tI16_142_f-001
Pearson symbol	tI16
Space group number	142
Space group symbol	$I4_1/acd$
AFLOW prototype command	<code>aflow --proto=A_tI16_142_f-001 --params=a, c/a, x₁</code>

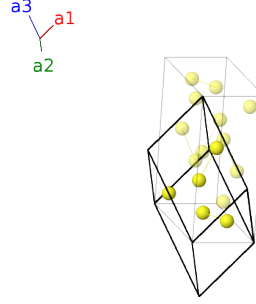
Other compounds with this structure

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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \begin{pmatrix} x_1 + \frac{3}{8} \\ 2x_1 + \frac{1}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_1 + \frac{1}{8} \\ 2x_1 + \frac{1}{4} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{4}\right) \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B}_2$	$= -\begin{pmatrix} x_1 - \frac{3}{8} \\ 2x_1 - \frac{1}{4} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_1 - \frac{1}{8} \\ 2x_1 - \frac{1}{4} \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{4}\right) \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B}_3$	$= \begin{pmatrix} x_1 + \frac{1}{8} \\ 2x_1 + \frac{3}{4} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_1 - \frac{3}{8} \\ 2x_1 + \frac{3}{4} \end{pmatrix} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{4}\right) \hat{\mathbf{y}} - \frac{1}{8}c \hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B}_4$	$= -\begin{pmatrix} x_1 - \frac{1}{8} \\ 2x_1 + \frac{3}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_1 + \frac{3}{8} \\ 2x_1 + \frac{3}{4} \end{pmatrix} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{4}\right) \hat{\mathbf{y}} - \frac{1}{8}c \hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B}_5$	$= -\begin{pmatrix} x_1 - \frac{5}{8} \\ 2x_1 - \frac{3}{4} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_1 - \frac{7}{8} \\ 2x_1 - \frac{3}{4} \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{4}\right) \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B}_6$	$= \begin{pmatrix} x_1 + \frac{5}{8} \\ 2x_1 + \frac{3}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_1 + \frac{7}{8} \\ 2x_1 + \frac{3}{4} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{4}\right) \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B}_7$	$= -\begin{pmatrix} x_1 - \frac{7}{8} \\ 2x_1 + \frac{1}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_1 + \frac{5}{8} \\ 2x_1 + \frac{1}{4} \end{pmatrix} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{4}\right) \hat{\mathbf{y}} + \frac{5}{8}c \hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B}_8$	$= \begin{pmatrix} x_1 + \frac{7}{8} \\ 2x_1 + \frac{1}{4} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_1 - \frac{5}{8} \\ 2x_1 + \frac{1}{4} \end{pmatrix} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{4}\right) \hat{\mathbf{y}} + \frac{5}{8}c \hat{\mathbf{z}}$	(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.

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