

S-II Structure: A_hP9_154_ac-001

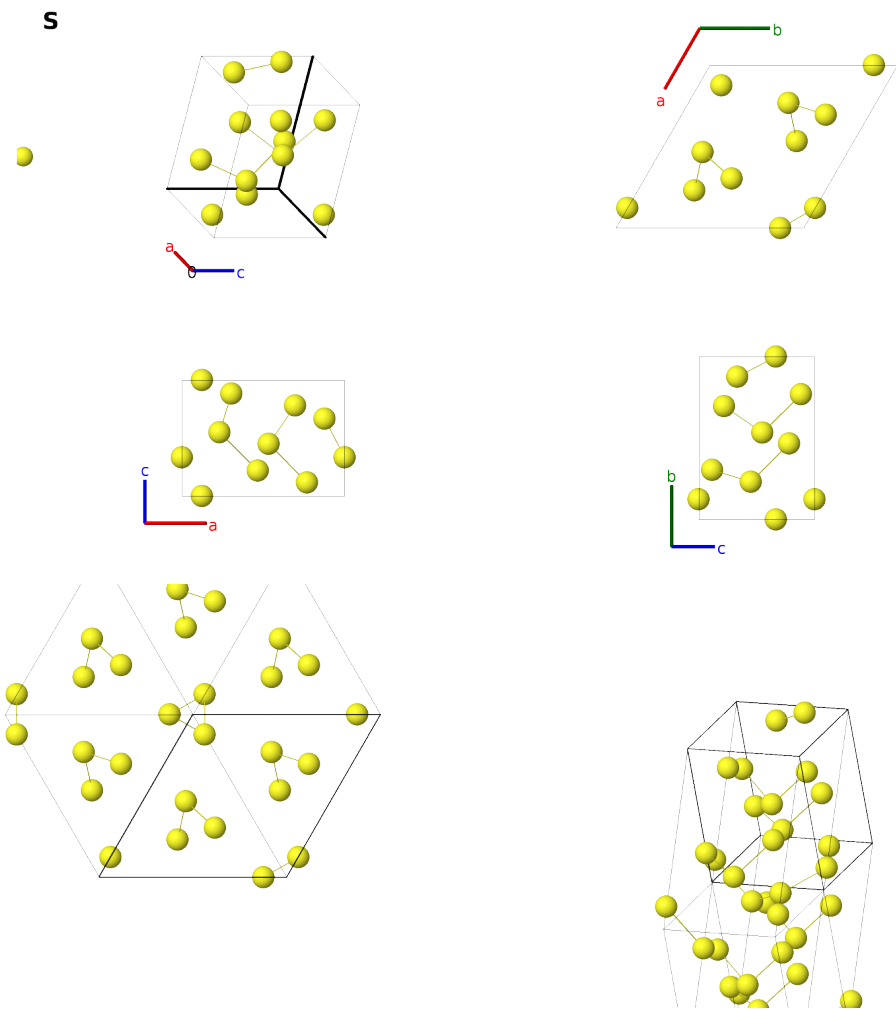
This structure previously used the label(s) **A_hP9_154_bc**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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

https://aflow.org/prototype-encyclopedia/A_hP9_154_ac-001

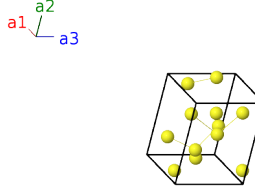


Prototype	S
AFLOW prototype label	A_hP9_154_ac-001
Pearson symbol	hP9
Space group number	154
Space group symbol	$P3_221$

AFLOW prototype command `aflow --proto=A_hP9_154_ac-001`
 `--params=a, c/a, x1, x2, y2, z2`

- The S-II phase is found when sulfur is heated and pressurized above 3 GPa. This data was taken at 5.8 GPa and 800K.

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_3$	=	$\frac{1}{2}ax_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	S I
$\mathbf{B}_2$	$x_1 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	=	$\frac{1}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3a)	S I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	=	$-ax_1 \hat{\mathbf{x}}$	(3a)	S I
$\mathbf{B}_4$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(6c)	S II
$\mathbf{B}_5$	$-y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{2}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{3}c(3z_2 + 2) \hat{\mathbf{z}}$	(6c)	S II
$\mathbf{B}_6$	$-(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{1}{3}) \mathbf{a}_3$	=	$-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	S II
$\mathbf{B}_7$	$y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(6c)	S II
$\mathbf{B}_8$	$(x_2 - y_2) \mathbf{a}_1 - y_2 \mathbf{a}_2 - (z_2 - \frac{1}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	S II
$\mathbf{B}_9$	$-x_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 - (z_2 - \frac{2}{3}) \mathbf{a}_3$	=	$-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} - \frac{1}{3}c(3z_2 - 2) \hat{\mathbf{z}}$	(6c)	S II

References

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

First cited in

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