S-II Structure:
A_hP9_154_ac-001

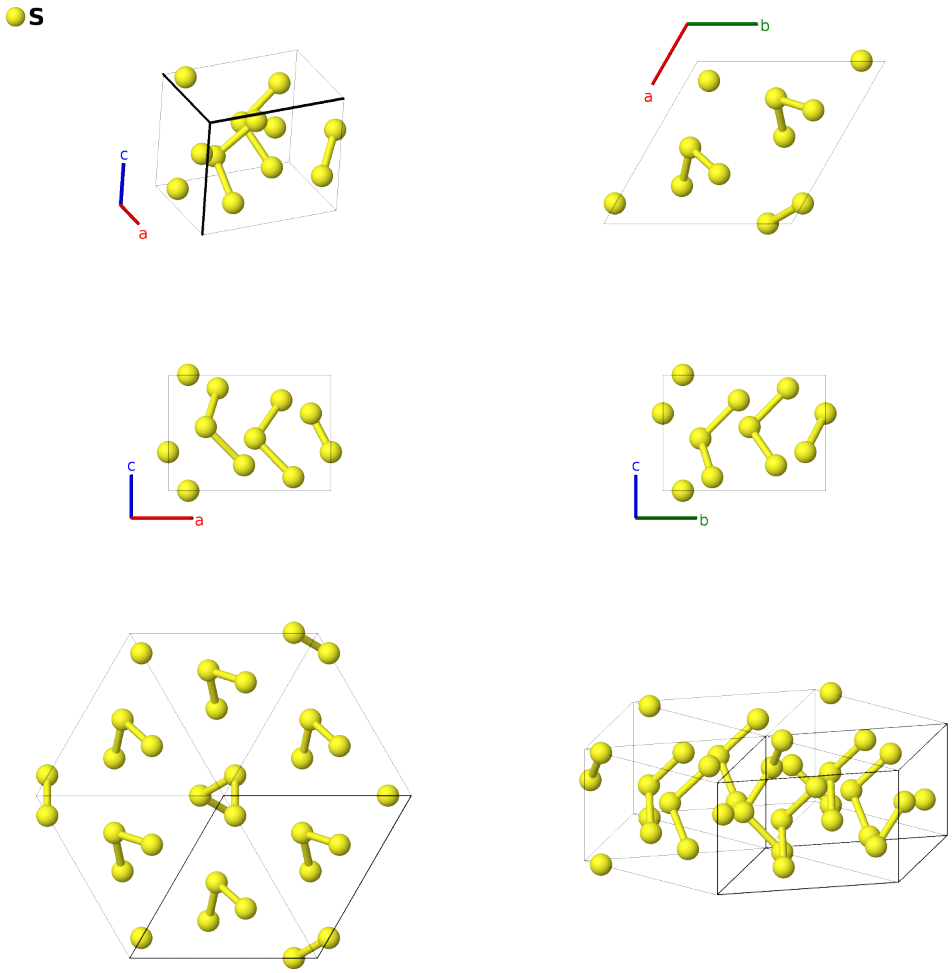
This structure originally had the label `A_hP9_154_bc`. Calls to that address will be redirected here.

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

---

https://aflow.org/p/GAZQ

https://aflow.org/p/A_hP9_154_ac-001

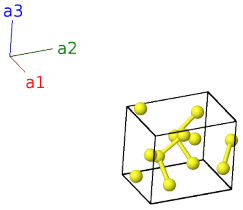


Prototype	S
AFLOW prototype label	A_hP9_154_ac-001
ICSD	none
Pearson symbol	hP9
Space group number	154
Space group symbol	$P3_221$
AFLOW prototype command	`aflow --proto=A_hP9_154_ac-001 --params=`$a, c/a, x_1, x_2, y_2, z_2$

- 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - 2y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_2 + 2)\,\hat{\mathbf{z}}$	(6c)	S II
$\mathbf{B_6}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_8}$	=	$(x_2 - y_2)\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - 2y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	S II
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 - \left(z_2 - \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_2 - 2)\,\hat{\mathbf{z}}$	(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.