H_3S (60 GPa) Structure: A3B_oC64_66_gi2lm_2l-001

This structure originally had the label `A3B_oC64_66_gi2lm_2l`. Calls to that address will be redirected here.

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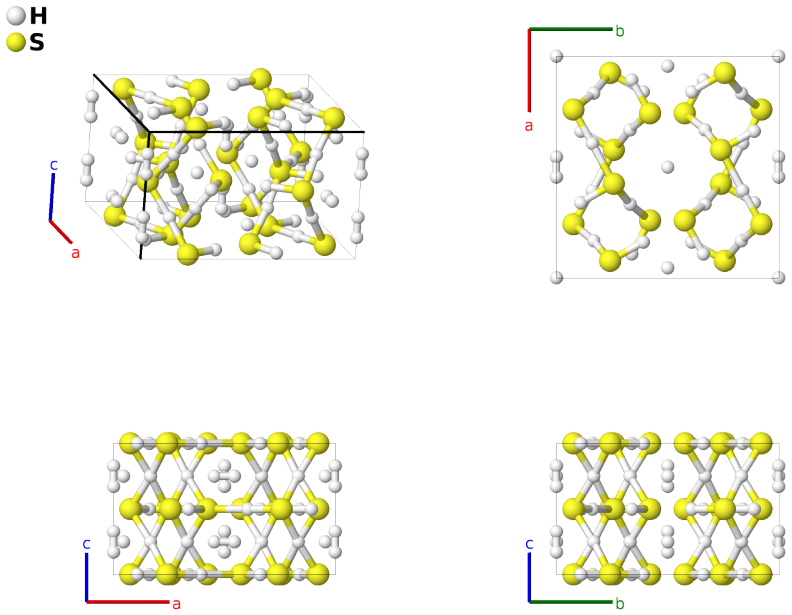
https://aflow.org/p/DQEU

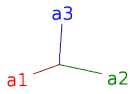
https://aflow.org/p/A3B_oC64_66_gi2lm_2l-001



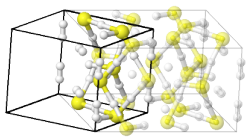
Prototype	H_3S
AFLOW prototype label	A3B_oC64_66_gi2lm_2l-001
ICSD	291500
Pearson symbol	oC64
Space group number	66
Space group symbol	$Cccm$
AFLOW prototype command	`aflow --proto=A3B_oC64_66_gi2lm_2l-001 --params=`$a, b/a, c/a, x_1, z_2, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, z_7$

- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of H_3S for pressures between 40 and 90 GPa. The data presented here was computed at 60 GPa.
- (Hicks, 2019) had a transcription error in the position of the S-I atom. We have corrected that here.

Base-centered Orthorhombic primitive vectors



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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	H I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	H I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	H I
$\mathbf{B_4}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	H I
$\mathbf{B_5}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(8i)	H II
$\mathbf{B_6}$	=	$-\left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8i)	H II
$\mathbf{B_7}$	=	$-z_2\,\mathbf{a}_3$	=	$-cz_2\,\hat{\mathbf{z}}$	(8i)	H II
$\mathbf{B_8}$	=	$\left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8i)	H II
$\mathbf{B_9}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}}$	(8l)	H III
$\mathbf{B_{10}}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}}$	(8l)	H III
$\mathbf{B_{11}}$	=	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8l)	H III
$\mathbf{B_{12}}$	=	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8l)	H III
$\mathbf{B_{13}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}}$	(8l)	H IV
$\mathbf{B_{14}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}}$	(8l)	H IV
$\mathbf{B_{15}}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8l)	H IV
$\mathbf{B_{16}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8l)	H IV
$\mathbf{B_{17}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}}$	(8l)	S I
$\mathbf{B_{18}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}}$	(8l)	S I
$\mathbf{B_{19}}$	=	$-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8l)	S I
$\mathbf{B_{20}}$	=	$(x_5 + y_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8l)	S I
$\mathbf{B_{21}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 + (x_6 + y_6)\,\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}}$	(8l)	S II
$\mathbf{B_{22}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - (x_6 + y_6)\,\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}}$	(8l)	S II
$\mathbf{B_{23}}$	=	$-(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8l)	S II
$\mathbf{B_{24}}$	=	$(x_6 + y_6)\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8l)	S II
$\mathbf{B_{25}}$	=	$(x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16m)	H V

$\mathbf{B_{26}}$	=	$-\left(x_7 - y_7\right)\,\mathbf{a}_1 - \left(x_7 + y_7\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16m)	H V
$\mathbf{B_{27}}$	=	$-\left(x_7 + y_7\right)\,\mathbf{a}_1 - \left(x_7 - y_7\right)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16m)	H V
$\mathbf{B_{28}}$	=	$\left(x_7 + y_7\right)\,\mathbf{a}_1 + \left(x_7 - y_7\right)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16m)	H V
$\mathbf{B_{29}}$	=	$-\left(x_7 - y_7\right)\,\mathbf{a}_1 - \left(x_7 + y_7\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(16m)	H V
$\mathbf{B_{30}}$	=	$\left(x_7 - y_7\right)\,\mathbf{a}_1 + \left(x_7 + y_7\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(16m)	H V
$\mathbf{B_{31}}$	=	$\left(x_7 + y_7\right)\,\mathbf{a}_1 + \left(x_7 - y_7\right)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16m)	H V
$\mathbf{B_{32}}$	=	$-\left(x_7 + y_7\right)\,\mathbf{a}_1 - \left(x_7 - y_7\right)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16m)	H V

References

[1] D. Duan, Y. Liu, F. Tian, D. Li, X. Huang, Z. Zhao, H. Yu, B. Liu, W. Tian, and T. Cui, *Pressure-induced metallization of dense $(H_2S)_2H_2$ with high-T_c superconductivity* **4**, 698 (2014), doi:10.1038/srep06968.

[2] 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–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.