

H₃S (60 GPa) Structure: A3B_oC64_66_gi2lm_2l-001

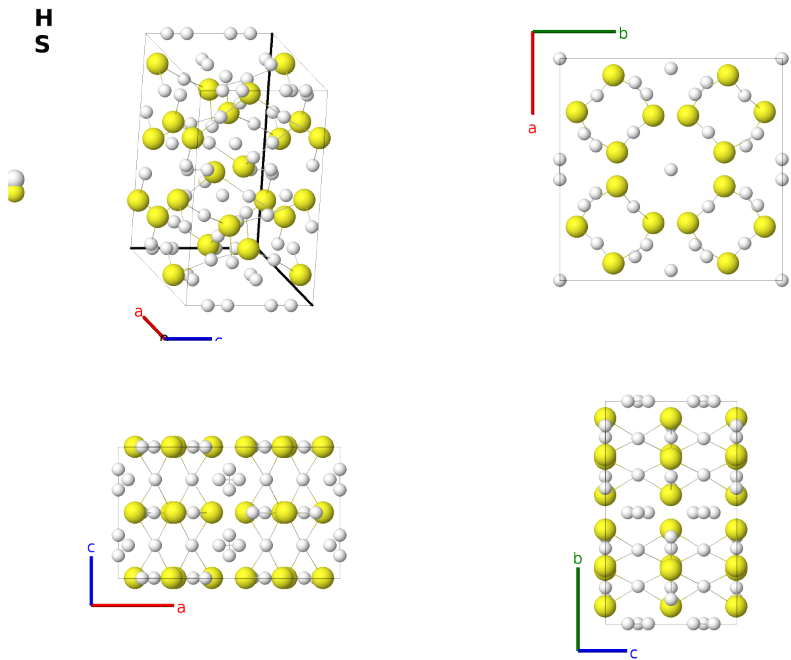
This structure previously used the label(s) A3B_oC64_66_gi2lm_2l. Calls to these addresses will be redirected here.

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- 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/DQEU>

https://aflow.org/prototype-encyclopedia/A3B_oC64_66_gi2lm_2l-001



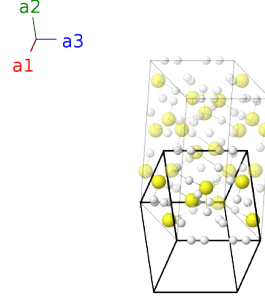
Prototype	H ₃ S
AFLOW prototype label	A3B_oC64_66_gi2lm_2l-001
ICSD	291500
CCDC	1723597
Pearson symbol	oC64
Space group number	66
Space group symbol	<i>Cccm</i>
AFLOW prototype command	<code>aflow --proto=A3B_oC64_66_gi2lm_2l-001 --params=a, b/a, c/a, x₁, z₂, x₃, y₃, x₄, y₄, x₅, y₅, x₆, y₆, x₇, y₇, z₇</code>

- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of H₃S 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

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



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

$$\begin{aligned}
\mathbf{B}_{25} &= \begin{matrix} (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + \\ z_7 \mathbf{a}_3 \end{matrix} = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16m) & \text{H V} \\
\mathbf{B}_{26} &= \begin{matrix} -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 + \\ z_7 \mathbf{a}_3 \end{matrix} = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16m) & \text{H V} \\
\mathbf{B}_{27} &= \begin{matrix} -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - \\ (z_7 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}} & (16m) & \text{H V} \\
\mathbf{B}_{28} &= \begin{matrix} (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - \\ (z_7 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}} & (16m) & \text{H V} \\
\mathbf{B}_{29} &= \begin{matrix} -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - \\ z_7 \mathbf{a}_3 \end{matrix} = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16m) & \text{H V} \\
\mathbf{B}_{30} &= \begin{matrix} (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 - \\ z_7 \mathbf{a}_3 \end{matrix} = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16m) & \text{H V} \\
\mathbf{B}_{31} &= \begin{matrix} (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \\ (z_7 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (16m) & \text{H V} \\
\mathbf{B}_{32} &= \begin{matrix} -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 + \\ (z_7 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (16m) & \text{H V}
\end{aligned}$$

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.

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