

H₂S (170 GPa) Structure:

A2B_oC24_64_2f_f-001

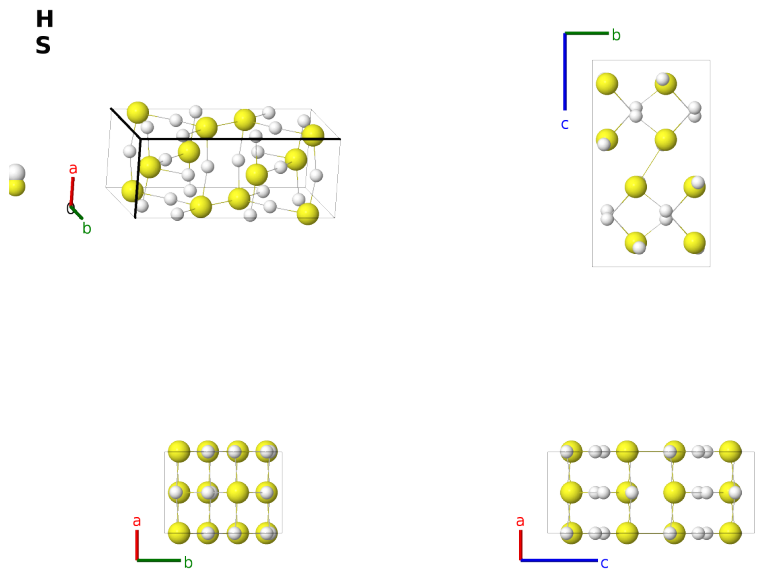
This structure previously used the label(s) **A2B_oC24_64_2f_f**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/7FZR>

https://aflow.org/prototype-encyclopedia/A2B_oC24_64_2f_f-001



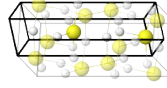
Prototype	H ₂ S
AFLOW prototype label	A2B_oC24_64_2f_f-001
Pearson symbol	oC24
Space group number	64
Space group symbol	<i>Cmce</i>
AFLOW prototype command	<code>aflow --proto=A2B_oC24_64_2f_f-001</code> <code>--params=a, b/a, c/a, y₁, z₁, y₂, z₂, y₃, z₃</code>

- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of H₂S for pressures > 140 GPa. At 160 GPa it is predicted to be a conventional superconductor with an approximate transition temperature of 80K, however it is unlikely that this is the crystal structure of the 190K superconductor, which is probably the H₃S structure (Bernstein, 2005).
- The data presented here was computed at 170 GPa.

Base-centered Orthorhombic primitive vectors

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

$\mathbf{a}_1$
 $\mathbf{a}_2$
 $\mathbf{a}_3$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8f)	H I
$\mathbf{B}_2$	$= \left(y_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	H I
$\mathbf{B}_3$	$= -\left(y_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	H I
$\mathbf{B}_4$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(8f)	H I
$\mathbf{B}_5$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8f)	H II
$\mathbf{B}_6$	$= \left(y_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	H II
$\mathbf{B}_7$	$= -\left(y_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	H II
$\mathbf{B}_8$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8f)	H II
$\mathbf{B}_9$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8f)	S I
$\mathbf{B}_{10}$	$= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	S I
$\mathbf{B}_{11}$	$= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	S I
$\mathbf{B}_{12}$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8f)	S I

References

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- [2] N. Bernstein, C. S. Hellberg, M. D. Johannes, I. I. Mazin, and M. J. Mehl, *What superconducts in sulfur hydrides under pressure and why*, Phys. Rev. B **91**, 060511(R) (2015), doi:10.1103/PhysRevB.91.060511.

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