

H₂S 70 GPa Structure: A2B_oP12_26_abc_ab-001

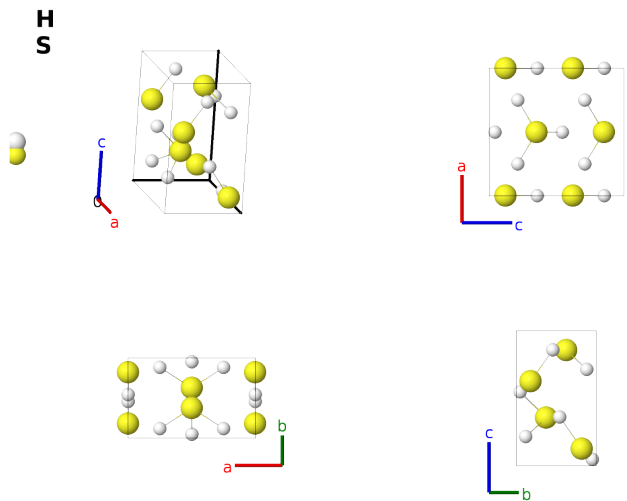
This structure previously used the label(s) **A2B_oP12_26_abc_ab.H2S**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/PC8F>

https://aflow.org/prototype-encyclopedia/A2B_oP12_26_abc_ab-001



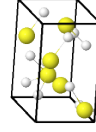
Prototype	H ₂ S
AFLOW prototype label	A2B_oP12_26_abc_ab-001
Pearson symbol	oP12
Space group number	26
Space group symbol	<i>Pmc</i> 2 ₁
AFLOW prototype command	<code>aflow --proto=A2B_oP12_26_abc_ab-001</code> <code>--params=a, b/a, c/a, y₁, z₁, y₂, z₂, y₃, z₃, y₄, z₄, x₅, y₅, z₅</code>

- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of H₂S in the range 40 – 80 GPa. The data presented here was computed at 70 GPa.
- 70 GPa H₂S has the same AFLOW label as β -SeO₂, A2B_oP12_26_abc_ab. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

a3
a2
a1

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2a)	H I
$\mathbf{B}_2$	$= -y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	H I
$\mathbf{B}_3$	$= y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2a)	S I
$\mathbf{B}_4$	$= -y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	S I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2b)	H II
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2b)	H II
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2b)	S II
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2b)	S II
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	H III
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	H III
$\mathbf{B}_{11}$	$= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	H III
$\mathbf{B}_{12}$	$= -x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	H III

References

- [1] Y. Li, J. Hao, H. Liu, Y. Li, and Y. Ma, *The metallization and superconductivity of dense hydrogen sulfide*, J. Chem. Phys. **140**, 174712 (2014), doi:10.1063/1.4874158.

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