

H₂S (15 GPa) Structure: A2B_mP12_13_2g_ef-001

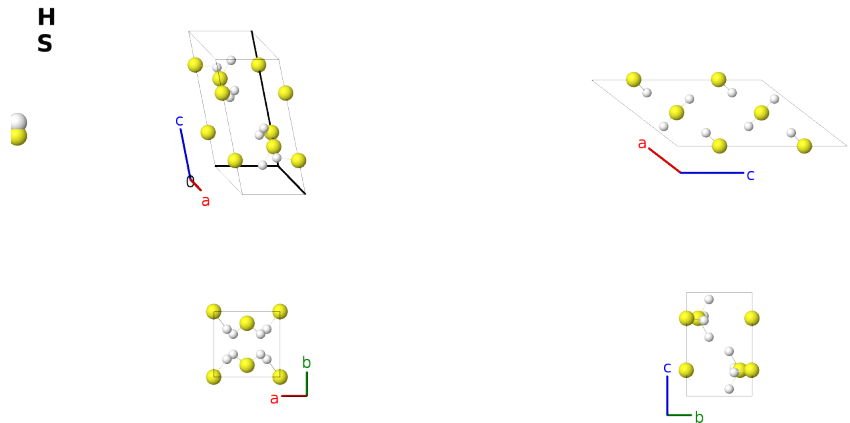
This structure previously used the label(s) **A2B_mP12_13_2g_ef**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/VYK4>

https://aflow.org/prototype-encyclopedia/A2B_mP12_13_2g_ef-001

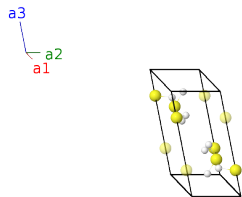


Prototype	H ₂ S
AFLOW prototype label	A2B_mP12_13_2g_ef-001
Pearson symbol	mP12
Space group number	13
Space group symbol	$P2/c$
AFLOW prototype command	<code>aflow --proto=A2B_mP12_13_2g_ef-001</code> <code>--params=a, b/a, c/a, β, y_1, y_2, x_3, y_3, z_3, x_4, y_4, z_4</code>

- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of H₂S in the range 10 – 30 GPa, which does not agree with the experimental phase diagram (Shimizu, 1995). The data presented here was computed at 15 GPa.

Simple Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(2e)	S I
$\mathbf{B}_2$	$= -y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(2e)	S I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\left(\frac{a}{2} + \frac{c \cos \beta}{4}\right) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(2f)	S II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\left(\frac{a}{2} + \frac{3c \cos \beta}{4}\right) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(2f)	S II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4g)	H I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	H I
$\mathbf{B}_7$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4g)	H I
$\mathbf{B}_8$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	H I
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4g)	H II
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	H II
$\mathbf{B}_{11}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4g)	H II
$\mathbf{B}_{12}$	$= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	H II

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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