

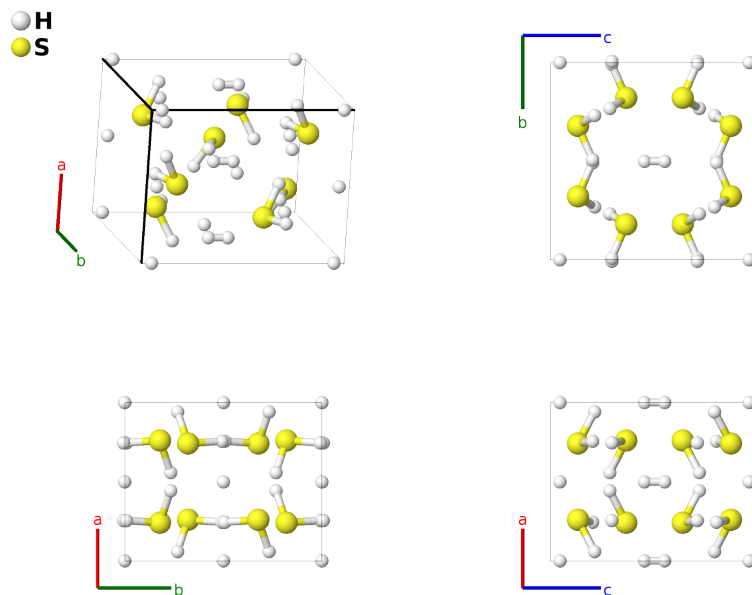
H₃S (5 GPa) Structure: A3B_oI32_23_ef2k_k-001

This structure originally had the label A3B_oI32_23_ij2k_k. Calls to that address will be redirected here.

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<https://aflow.org/p/4LGD>

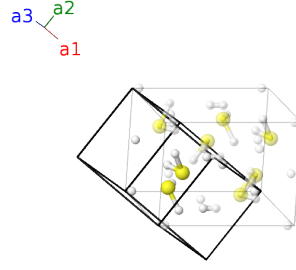
https://aflow.org/p/A3B_oI32_23_ef2k_k-001



Prototype	H ₃ S
AFLOW prototype label	A3B_oI32_23_ef2k_k-001
ICSD	none
Pearson symbol	oI32
Space group number	23
Space group symbol	<i>I</i> 222
AFLOW prototype command	<code>aflow --proto=A3B_oI32_23_ef2k_k-001 --params=a, b/a, c/a, x₁, x₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅</code>

- This structure is found in H₃S in the pressure range 3.5-17 GPa. The data presented here was taken at 5 GPa.

Body-centered Orthorhombic primitive vectors



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

Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}}$	(4e)	H I
\mathbf{B}_2	$= -x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}}$	(4e)	H I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{2}c\hat{\mathbf{z}}$	(4f)	H II
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2}c\hat{\mathbf{z}}$	(4f)	H II
\mathbf{B}_5	$= (y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8k)	H III
\mathbf{B}_6	$= -(y_3 - z_3) \mathbf{a}_1 - (x_3 - z_3) \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8k)	H III
\mathbf{B}_7	$= (y_3 - z_3) \mathbf{a}_1 - (x_3 + z_3) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8k)	H III
\mathbf{B}_8	$= -(y_3 + z_3) \mathbf{a}_1 + (x_3 - z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8k)	H III
\mathbf{B}_9	$= (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8k)	H IV
\mathbf{B}_{10}	$= -(y_4 - z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8k)	H IV
\mathbf{B}_{11}	$= (y_4 - z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8k)	H IV
\mathbf{B}_{12}	$= -(y_4 + z_4) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8k)	H IV
\mathbf{B}_{13}	$= (y_5 + z_5) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + (x_5 + y_5) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8k)	S I
\mathbf{B}_{14}	$= -(y_5 - z_5) \mathbf{a}_1 - (x_5 - z_5) \mathbf{a}_2 - (x_5 + y_5) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8k)	S I
\mathbf{B}_{15}	$= (y_5 - z_5) \mathbf{a}_1 - (x_5 + z_5) \mathbf{a}_2 - (x_5 - y_5) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8k)	S I
\mathbf{B}_{16}	$= -(y_5 + z_5) \mathbf{a}_1 + (x_5 - z_5) \mathbf{a}_2 + (x_5 - y_5) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8k)	S I

References

- [1] T. A. Strobel, P. Ganesh, M. Somayazulu, P. R. C. Kent, and R. J. Hemley, *Novel Cooperative Interactions and Structural Ordering in H_2S-H_2* , Phys. Rev. Lett. **107**, 255503 (2011), doi:10.1103/PhysRevLett.107.255503.