H_3S (130 GPa) Structure: A3B_hR4_160_b_a-001

This structure originally had the label `A3B_hR4_160_b_a`. Calls to that address will be redirected here.

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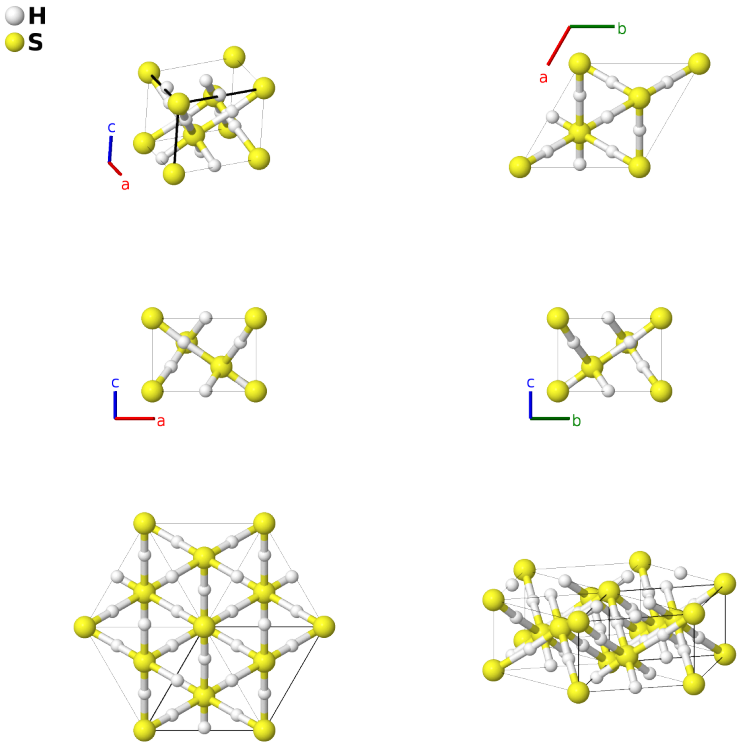
https://aflow.org/p/P2LA

https://aflow.org/p/A3B_hR4_160_b_a-001



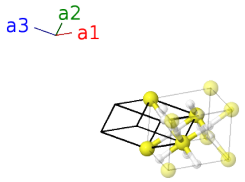
Prototype	H_3S
AFLOW prototype label	A3B_hR4_160_b_a-001
ICSD	291501
Pearson symbol	hR4
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=A3B_hR4_160_b_a-001 --params=`$a, c/a, x_1, x_2, z_2$

- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of H_3S for pressures between 90 and 150 GPa. When $c/a \to \sqrt{8}$, $x_2 \to 1/2$ and $z_2 \to 0$ this structure continuously evolves into the cubic 200 GPa H_3S structure.

- The data presented here was computed at 130 GPa.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(1a)	S I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(3b)	H I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(3b)	H I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(3b)	H I

References

[1] D. Duan, Y. Liu, F. T. 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**, 6968 (2014), doi:10.1038/srep06968.