High-pressure (200GPa) H_3S Structure: A3B_cI8_229_b_a-001

This structure originally had the label `A3B_cI8_229_b_a`. Calls to that address will be redirected here.

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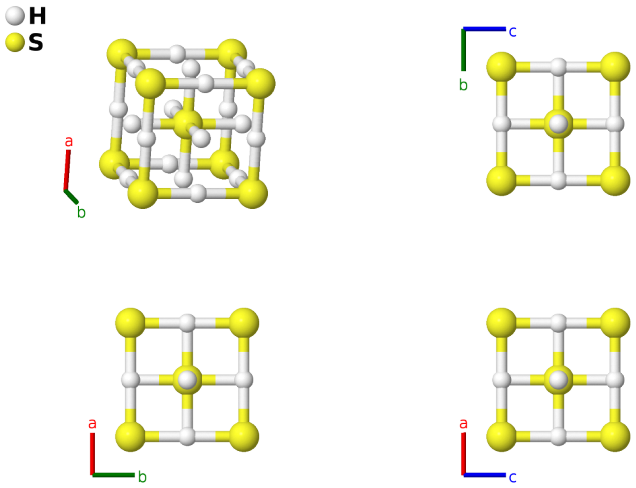
https://aflow.org/p/VV0Z

https://aflow.org/p/A3B_cI8_229_b_a-001



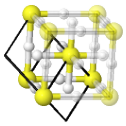
Prototype	H_3S
AFLOW prototype label	A3B_cI8_229_b_a-001
ICSD	291502
Pearson symbol	cI8
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	`aflow --proto=A3B_cI8_229_b_a-001 --params=`a

Other compounds with this structure
La_2O_3, Nd_2O_3

- (Duan, 2014) predicted that this structure of H_3S would be a conventional superconductor at temperatures above 191 K and a pressure of 200 GPa. (Drozdov, 2015) found a superconductor in the hydrogen-sulfur system at 203 K and pressure near 200 GPa. (Bernstein, 2015) showed that this structure is the ground state of the H–S system near 200 GPa. Both La_2O_3 and Nd_2O_3 can form in this structure under ambient conditions, but in both cases the oxygen atoms occupy only 50% of the (6b) Wyckoff positions.
- We have used the fact that all vectors of the form $(\pm a/2\hat{x} \pm a/2\hat{y} \pm a/2\hat{z})$ are primitive vectors of the body-centered cubic lattice to simplify the positions of some atoms in both lattice and Cartesian coordinates.
- The oxides with this structure have a large number of defects, with the oxygen (6b) sites only partially filled.

Body-centered Cubic primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	S I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(6b)	H I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(6b)	H I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{z}}$	(6b)	H I

References

[1] D. Duan, Y. Liu, F. Tian, 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*, Sci. Rep. **4**, 6968 (2014), doi:10.1038/srep06968.

[2] A. P. Drozdov, M. I. Eremets, I. A. Troyan, V. Ksenofontov, and S. I. Shylin, *Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system*, Nature **525**, 73–76 (2015), doi:10.1038/nature14964.

[3] 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.