

High-pressure (200GPa) H₃S Structure: A3B_cI8_229_b_a-001

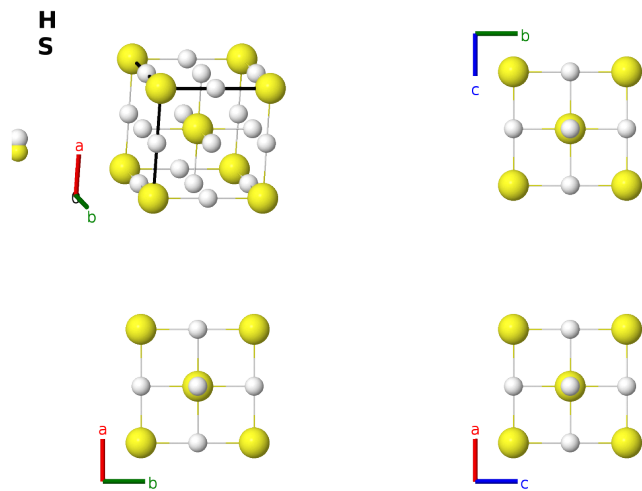
This structure previously used the label(s) **A3B_cI8_229_b_a**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/VV0Z>

https://aflow.org/prototype-encyclopedia/A3B_cI8_229_b_a-001



Prototype	H ₃ S
AFLOW prototype label	A3B_cI8_229_b_a-001
ICSD	291502
CCDC	1723599
Pearson symbol	cI8
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A3B_cI8_229_b_a-001 --params=a</code>

Other compounds with this structure

La₂O₃, Nd₂O₃

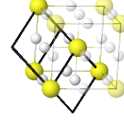
- (Duan, 2014) predicted that this structure of H₃S would be a conventional superconductor at temperatures above 191 K and a pressure of 200 GPa. (Drozdov, 2015) found a superconductor in the hydrogen-sulfur system at 203 K and pressure near 200 GPa. (Bernstein, 2015) showed that this structure is the ground state of the H–S system near 200 GPa. Both La₂O₃ and Nd₂O₃ 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

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

a1



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) S I
$\mathbf{B}_2$	$=$	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{x}$	(6b) H I
$\mathbf{B}_3$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{y}$	(6b) H I
$\mathbf{B}_4$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{2}a\hat{z}$	(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 $(\text{H}_2\text{S})_2\text{H}_2$ with high- T_c superconductivity*, Sci. Rep. **4**, 6968 (2014), doi:10.1038/srep06968.
- [2] A. P. Drozdov, M. I. Erements, 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.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017