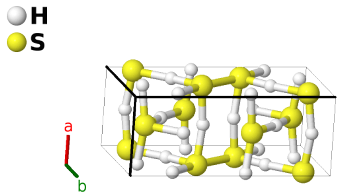
# $H_2S$ (170 GPa) Structure: A2B_oC24_64_2f_f-001

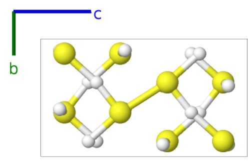
This structure originally had the label `A2B_oC24_64_2f_f`. Calls to that address will be redirected here.

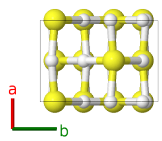
Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

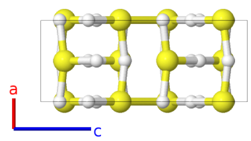
https://aflow.org/p/7FZR

https://aflow.org/p/A2B_oC24_64_2f_f-001



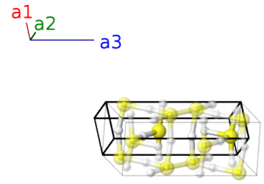




| | |
|---|---|
| **Prototype** | $H_2S$ |
| **AFLOW prototype label** | A2B_oC24_64_2f_f-001 |
| **ICSD** | none |
| **Pearson symbol** | oC24 |
| **Space group number** | 64 |
| **Space group symbol** | $Cmce$ |
| **AFLOW prototype command** | `aflow --proto=A2B_oC24_64_2f_f-001` `--params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3$ |

- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of $H_2S$ for pressures $> 140$ GPa. At 160 GPa it is predicted to be a conventional superconductor with an approximate transition temperature of 80K, however it is unlikely that this is the crystal structure of the 190K superconductor, which is probably the $H_3S$ structure (Bernstein, 2005).
- The data presented here was computed at 170 GPa.

**Base-centered Orthorhombic primitive vectors**

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




**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$ | = | $by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$ | (8f) | H I |
| $\mathbf{B_2}$ | = | $\left(y_1+\frac{1}{2}\right)\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\hat{\mathbf{z}}$ | (8f) | H I |
| $\mathbf{B_3}$ | = | $-\left(y_1-\frac{1}{2}\right)\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\mathbf{a}_2 - \left(z_1-\frac{1}{2}\right)\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{2}\right)\hat{\mathbf{z}}$ | (8f) | H I |
| $\mathbf{B_4}$ | = | $y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$ | = | $-by_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$ | (8f) | H I |
| $\mathbf{B_5}$ | = | $-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (8f) | H II |
| $\mathbf{B_6}$ | = | $\left(y_2+\frac{1}{2}\right)\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\hat{\mathbf{z}}$ | (8f) | H II |
| $\mathbf{B_7}$ | = | $-\left(y_2-\frac{1}{2}\right)\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\mathbf{a}_2 - \left(z_2-\frac{1}{2}\right)\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2-\frac{1}{2}\right)\hat{\mathbf{z}}$ | (8f) | H II |
| $\mathbf{B_8}$ | = | $y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$ | = | $-by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$ | (8f) | H II |
| $\mathbf{B_9}$ | = | $-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (8f) | S I |
| $\mathbf{B_{10}}$ | = | $\left(y_3+\frac{1}{2}\right)\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}}$ | (8f) | S I |
| $\mathbf{B_{11}}$ | = | $-\left(y_3-\frac{1}{2}\right)\mathbf{a}_1 + \left(y_3+\frac{1}{2}\right)\mathbf{a}_2 - \left(z_3-\frac{1}{2}\right)\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3-\frac{1}{2}\right)\hat{\mathbf{z}}$ | (8f) | S I |
| $\mathbf{B_{12}}$ | = | $y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $-by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (8f) | S I |

**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.

[2] 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.