H_2S (90 GPa) Structure: A2B_aP6_2_aei_i-001

This structure originally had the label `A2B_aP6_2_aei_i`. Calls to that address will be redirected here.

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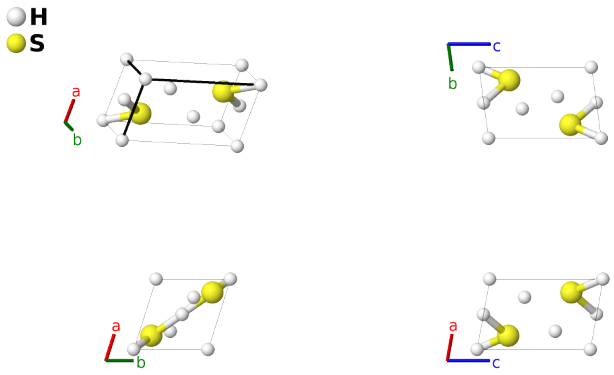
https://aflow.org/p/Q769

https://aflow.org/p/A2B_aP6_2_aei_i-001

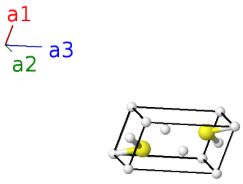


Prototype	H_2S
AFLOW prototype label	A2B_aP6_2_aei_i-001
ICSD	none
Pearson symbol	aP6
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	`aflow --proto=A2B_aP6_2_aei_i-001 --params=`$a, b/a, c/a, \alpha, \beta, \gamma, x_3, y_3, z_3, x_4, y_4, z_4$

- This structure was found by first-principles electronic structure calculations and is predicted to be the stable structure of H_2S in the range 80-140 GPa. The data presented here was computed at 90 GPa.
- (Li, 2014) place the hydrogen atoms on (1g), (1f) and (2i) sites, with sulfur atoms on (2i) sites. We have changed the origin so that the hydrogen atoms are now on (1a), (1e) and (2i) sites.

Triclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\cos\gamma\,\hat{\mathbf{x}} + b\sin\gamma\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c_x\,\hat{\mathbf{x}} + c_y\,\hat{\mathbf{y}} + c_z\,\hat{\mathbf{z}}$$
$$c_x = c\cos\beta$$
$$c_y = c(\cos\alpha - \cos\beta\cos\gamma)/\sin\gamma$$
$$c_z = \sqrt{c^2 - c_x^2 - c_y^2}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	H I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}\,(a + b\cos\gamma)\,\hat{\mathbf{x}} + \frac{1}{2} b \sin\gamma\,\hat{\mathbf{y}}$	(1e)	H II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} + (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} + c_z z_3\,\hat{\mathbf{z}}$	(2i)	H III
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} - (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} - c_z z_3\,\hat{\mathbf{z}}$	(2i)	H III
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + by_4\cos\gamma + c_x z_4)\,\hat{\mathbf{x}} + (by_4\sin\gamma + c_y z_4)\,\hat{\mathbf{y}} + c_z z_4\,\hat{\mathbf{z}}$	(2i)	S I
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + by_4\cos\gamma + c_x z_4)\,\hat{\mathbf{x}} - (by_4\sin\gamma + c_y z_4)\,\hat{\mathbf{y}} - c_z z_4\,\hat{\mathbf{z}}$	(2i)	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.