H-III (300 GPa) Structure: A_mC24_15_2e2f-001

This structure originally had the label `A_mC24_15_2e2f`. Calls to that address will be redirected here.

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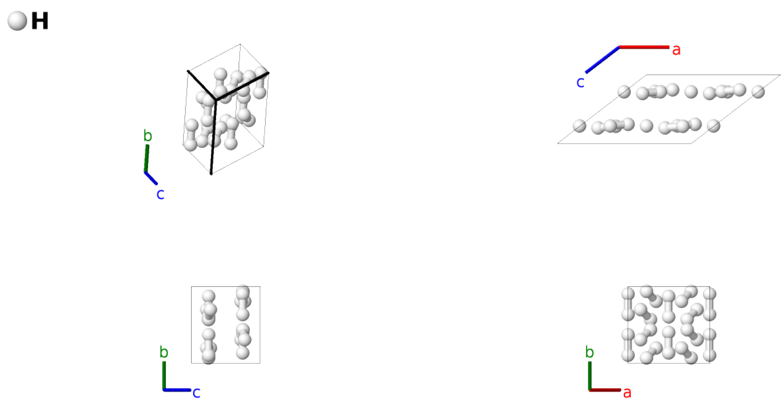
https://aflow.org/p/MULK

https://aflow.org/p/A_mC24_15_2e2f-001

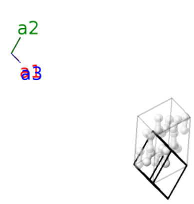


Prototype	H
AFLOW prototype label	A_mC24_15_2e2f-001
ICSD	none
Pearson symbol	mC24
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=A_mC24_15_2e2f-001` `--params=`$a, b/a, c/a, \beta, y_1, y_2, x_3, y_3, z_3, x_4, y_4, z_4$

- This structure was determined by density functional simulations. The authors claim it is in good agreement with experimental data for H-III, and is the lowest energy structure at pressures from approximately 100-250 GPa, including zero-point motion. The data presented here was computed at 300 GPa. If we change our description of the unit cell so that $\mathbf{a}_3 \rightarrow \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$ then all of the primitive vectors for the base-centered orthorhombic structure have approximately equal lengths, and the angles between them are approximately 60°. This structure is very close to exhibiting a face-centered cubic lattice.

Base-centered Monoclinic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} - \tfrac{1}{2}b\,\mathbf{\hat{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} + \tfrac{1}{2}b\,\mathbf{\hat{y}} \\
\mathbf{a_3} &= c\cos\beta\,\mathbf{\hat{x}} + c\sin\beta\,\mathbf{\hat{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\mathbf{\hat{x}} + by_1\,\mathbf{\hat{y}} + \frac{1}{4}c\sin\beta\,\mathbf{\hat{z}}$	(4e)	H I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\mathbf{\hat{x}} - by_1\,\mathbf{\hat{y}} + \frac{3}{4}c\sin\beta\,\mathbf{\hat{z}}$	(4e)	H I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\mathbf{\hat{x}} + by_2\,\mathbf{\hat{y}} + \frac{1}{4}c\sin\beta\,\mathbf{\hat{z}}$	(4e)	H II
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\mathbf{\hat{x}} - by_2\,\mathbf{\hat{y}} + \frac{3}{4}c\sin\beta\,\mathbf{\hat{z}}$	(4e)	H II
$\mathbf{B_5}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\mathbf{\hat{x}} + by_3\,\mathbf{\hat{y}} + cz_3\sin\beta\,\mathbf{\hat{z}}$	(8f)	H III
$\mathbf{B_6}$	=	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_3\,\mathbf{\hat{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	H III
$\mathbf{B_7}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\mathbf{\hat{x}} - by_3\,\mathbf{\hat{y}} - cz_3\sin\beta\,\mathbf{\hat{z}}$	(8f)	H III
$\mathbf{B_8}$	=	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_3\,\mathbf{\hat{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	H III
$\mathbf{B_9}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} + cz_4\sin\beta\,\mathbf{\hat{z}}$	(8f)	H IV
$\mathbf{B_{10}}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	H IV
$\mathbf{B_{11}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} - cz_4\sin\beta\,\mathbf{\hat{z}}$	(8f)	H IV
$\mathbf{B_{12}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	H IV

References

[1] C. J. Pickard and R. J. Needs, *Structure of phase III of solid hydrogen*, Nature Physics **3**, 473–476 (2007), doi:10.1038/nphys625.