H_3Cl (20 GPa) Structure: AB3_mC16_9_a_3a-001

This structure originally had the label `AB3_mC16_9_a_3a`. Calls to that address will be redirected here.

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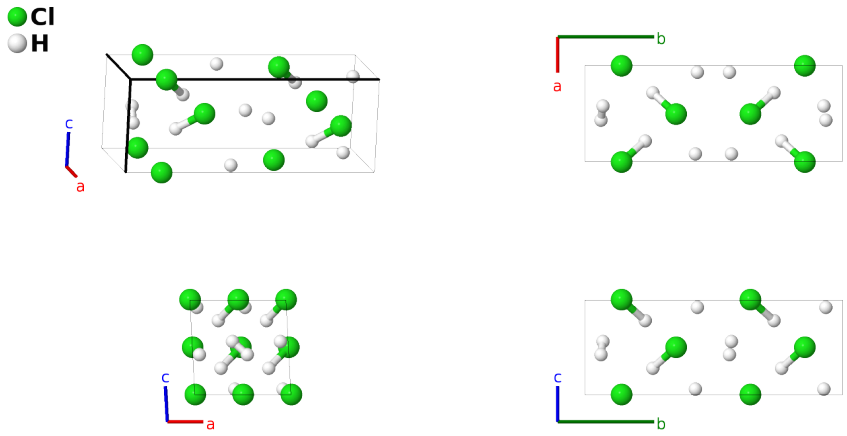
https://aflow.org/p/QYSB

https://aflow.org/p/AB3_mC16_9_a_3a-001

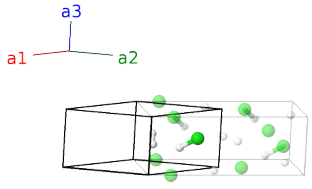


Prototype	ClH_3
AFLOW prototype label	AB3_mC16_9_a_3a-001
ICSD	671645
Pearson symbol	mC16
Space group number	9
Space group symbol	Cc
AFLOW prototype command	`aflow --proto=AB3_mC16_9_a_3a-001 --params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

- This structure was found via first-principles calculations. The data presented here was computed at a pressure of 20 GPa.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$(x_1 - y_1)\ \mathbf{a}_1 + (x_1 + y_1)\ \mathbf{a}_2 + z_1\ \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos\beta)\ \hat{\mathbf{x}} + by_1\ \hat{\mathbf{y}} + cz_1 \sin\beta\ \hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B_2}$	=	$(x_1 + y_1)\ \mathbf{a}_1 + (x_1 - y_1)\ \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\ \mathbf{a}_3$	=	$\left(ax_1 + c\left(z_1 + \frac{1}{2}\right)\cos\beta\right)\ \hat{\mathbf{x}} - by_1\ \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\sin\beta\ \hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B_3}$	=	$(x_2 - y_2)\ \mathbf{a}_1 + (x_2 + y_2)\ \mathbf{a}_2 + z_2\ \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos\beta)\ \hat{\mathbf{x}} + by_2\ \hat{\mathbf{y}} + cz_2 \sin\beta\ \hat{\mathbf{z}}$	(4a)	H I
$\mathbf{B_4}$	=	$(x_2 + y_2)\ \mathbf{a}_1 + (x_2 - y_2)\ \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\ \mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\ \hat{\mathbf{x}} - by_2\ \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\ \hat{\mathbf{z}}$	(4a)	H I
$\mathbf{B_5}$	=	$(x_3 - y_3)\ \mathbf{a}_1 + (x_3 + y_3)\ \mathbf{a}_2 + z_3\ \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos\beta)\ \hat{\mathbf{x}} + by_3\ \hat{\mathbf{y}} + cz_3 \sin\beta\ \hat{\mathbf{z}}$	(4a)	H II
$\mathbf{B_6}$	=	$(x_3 + y_3)\ \mathbf{a}_1 + (x_3 - y_3)\ \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\ \mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\ \hat{\mathbf{x}} - by_3\ \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\ \hat{\mathbf{z}}$	(4a)	H II
$\mathbf{B_7}$	=	$(x_4 - y_4)\ \mathbf{a}_1 + (x_4 + y_4)\ \mathbf{a}_2 + z_4\ \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos\beta)\ \hat{\mathbf{x}} + by_4\ \hat{\mathbf{y}} + cz_4 \sin\beta\ \hat{\mathbf{z}}$	(4a)	H III
$\mathbf{B_8}$	=	$(x_4 + y_4)\ \mathbf{a}_1 + (x_4 - y_4)\ \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\ \mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\ \hat{\mathbf{x}} - by_4\ \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\ \hat{\mathbf{z}}$	(4a)	H III

References

[1] D. Duan, X. Huang, F. Tian, Y. Liu, D. Li, H. Yu, B. Liu, W. Tian, and T. Cui, *Predicted Formation of H_3^+ in Solid Halogen Polyhydrides at High Pressures*, J. Phys. Chem. A **119**, 11059–11065 (2015), doi:10.1021/acs.jpca.5b08183.