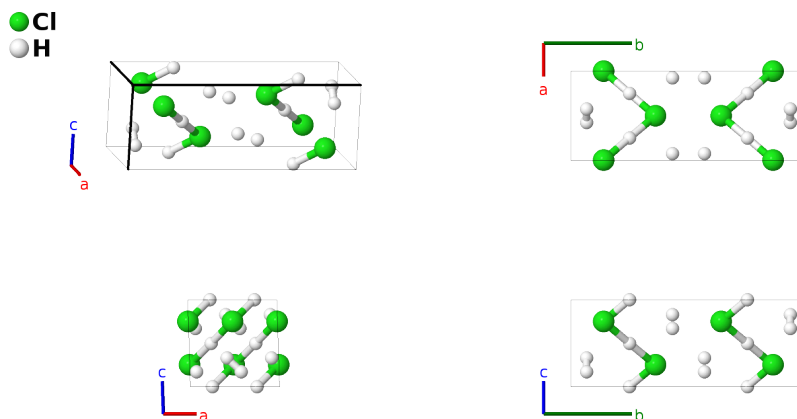# H_3Cl (50 GPa) Structure: AB3_mC16_15_e_af-001

This structure originally had the label `AB3_mC16_15_e_cf`. Calls to that address will be redirected here.

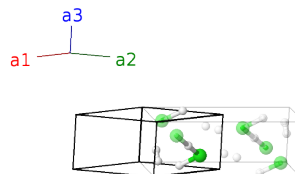https://aflow.org/p/T96Y

https://aflow.org/p/AB3_mC16_15_e_af-001

Prototype	ClH_3
AFLOW prototype label	AB3_mC16_15_e_af-001
ICSD	671644
Pearson symbol	mC16
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	aflow --proto=AB3_mC16_15_e_af-001 --params=$a, b/a, c/a, \beta, y_2, x_3, y_3, z_3$

- This structure was found via first-principles calculations. The data presented here was computed at a pressure of 50 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
$\mathbf{B_1}$	=	0	=	0	(4a)	H I
$\mathbf{B_2}$	=	$\frac{1}{2}\mathbf{a_3}$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4a)	H I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + \frac{1}{4}\mathbf{a_3}$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} + \frac{3}{4}\mathbf{a_3}$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_5}$	=	$(x_3 - y_3)\,\mathbf{a_1} + (x_3 + y_3)\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	H II
$\mathbf{B_6}$	=	$-(x_3 + y_3)\,\mathbf{a_1} - (x_3 - y_3)\,\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	H II
$\mathbf{B_7}$	=	$-(x_3 - y_3)\,\mathbf{a_1} - (x_3 + y_3)\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	H II
$\mathbf{B_8}$	=	$(x_3 + y_3)\,\mathbf{a_1} + (x_3 - y_3)\,\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	H II

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.