H_3Cl (400 GPa) Structure: AB3_mP16_10_mn_3m3n-001

This structure previously used the label(s) `AB3_mP16_10_mn_3m3n`. Calls to these addresses will be redirected here.

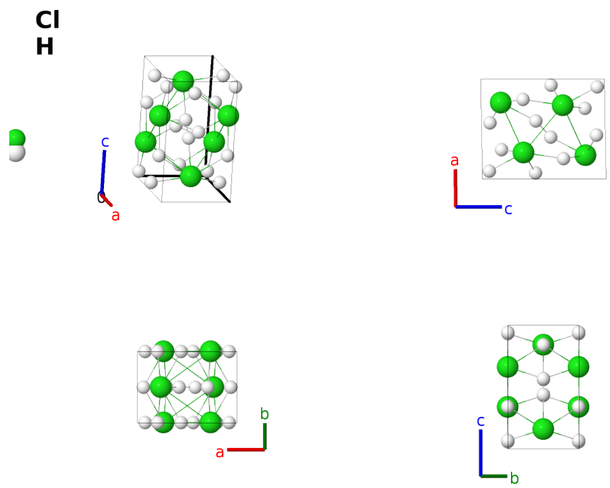
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/1EYW

https://aflow.org/prototype-encyclopedia/AB3_mP16_10_mn_3m3n-001

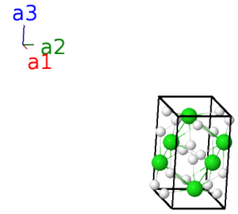


Prototype	ClH_3
AFLOW prototype label	AB3_mP16_10_mn_3m3n-001
Pearson symbol	mP16
Space group number	10
Space group symbol	$P2/m$
AFLOW prototype command	`aflow --proto=AB3_mP16_10_mn_3m3n-001` `--params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8$

- This structure was found via first-principles calculations. The data presented here was computed at a pressure of 400 GPa.
- (Zeng, 2017) do not provide a value for β, so it is assumed to be near 90°. Using exactly 90° results in space group $Pnnm$ #58, so we set $\beta = 91°$, yielding the proposed space group $P2/m$ #10.

Simple Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(2m)	Cl I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(2m)	Cl I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(2m)	H I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(2m)	H I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2m)	H II
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(2m)	H II
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(2m)	H III
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(2m)	H III
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(2n)	Cl II
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(2n)	Cl II
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(2n)	H IV
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(2n)	H IV
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(2n)	H V
$\mathbf{B_{14}}$	=	$-x_7\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(2n)	H V
$\mathbf{B_{15}}$	=	$x_8\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(2n)	H VI
$\mathbf{B_{16}}$	=	$-x_8\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(2n)	H VI

References

[1] Q. Zeng, S. Yu, D. Li, A. R. Oganov, and G. Frapper, *Emergence of novel hydrogen chlorides under high pressure*, Phys. Chem. Chem. Phys. **19**, 8236–8242 (2017), doi:10.1039/C6CP08708F.

First cited in

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