Low Temperature HCl Structure: AB_oC8_36_a_a-001

This structure originally had the label `AB_oC8_36_a_a`. Calls to that address will be redirected here.

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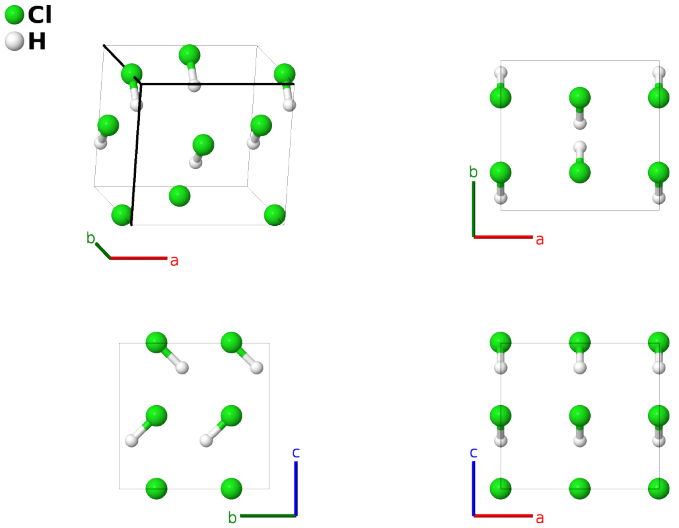
https://aflow.org/p/SAL5

https://aflow.org/p/AB_oC8_36_a_a-001

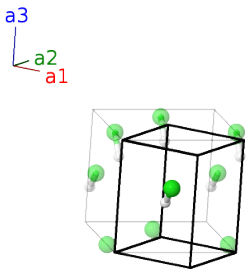


Prototype	ClH
AFLOW prototype label	AB_oC8_36_a_a-001
ICSD	27037
Pearson symbol	oC8
Space group number	36
Space group symbol	$Cmc2_1$
AFLOW prototype command	`aflow --proto=AB_oC8_36_a_a-001 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2$

- We use the 77.4K data for deuterium chloride from (Sándor, 1967). They gave the data in the $Bb2_1m$ setting of space group #36. We used FINDSYM to transform this to the standard $Cmc2_1$ setting.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	H I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	H I

References

[1] E. Sándor and R. F. C. Farrow, *Crystal Structure of Solid Hydrogen Chloride and Deuterium Chloride*, Nature **213**, 217–218 (1967), doi:10.1038/213171a0.