

Low Temperature HCl Structure: AB_oC8_36_a_a-001

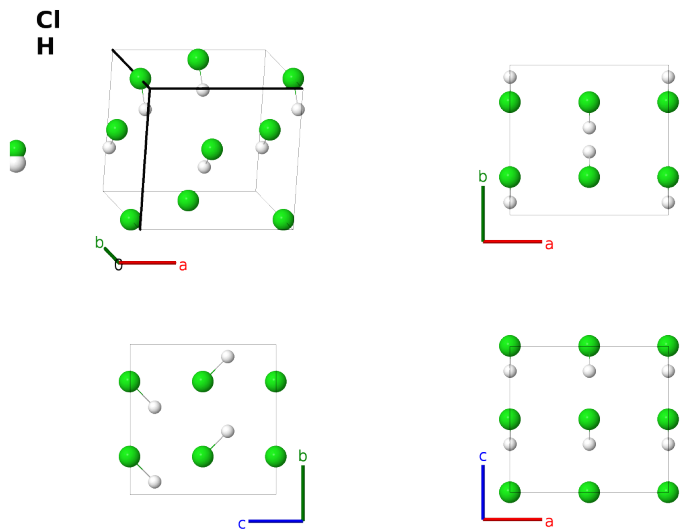
This structure previously used the label(s) **AB_oC8_36_a.a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/SAL5>

https://aflow.org/prototype-encyclopedia/AB_oC8_36_a_a-001

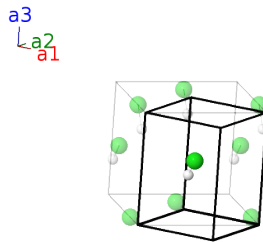


Prototype	ClH
AFLOW prototype label	AB_oC8_36_a_a-001
ICSD	27037
CCDC	1602388
Pearson symbol	oC8
Space group number	36
Space group symbol	$Cmc2_1$
AFLOW prototype command	<code>aflow --proto=AB_oC8_36_a_a-001 --params=a, b/a, c/a, y₁, z₁, y₂, z₂</code>

- 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

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(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.

First cited in

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