

$D0_{13}$ (AlCl_3) Structure (*Obsolete*): AB3_hP4_164_a_bd-001

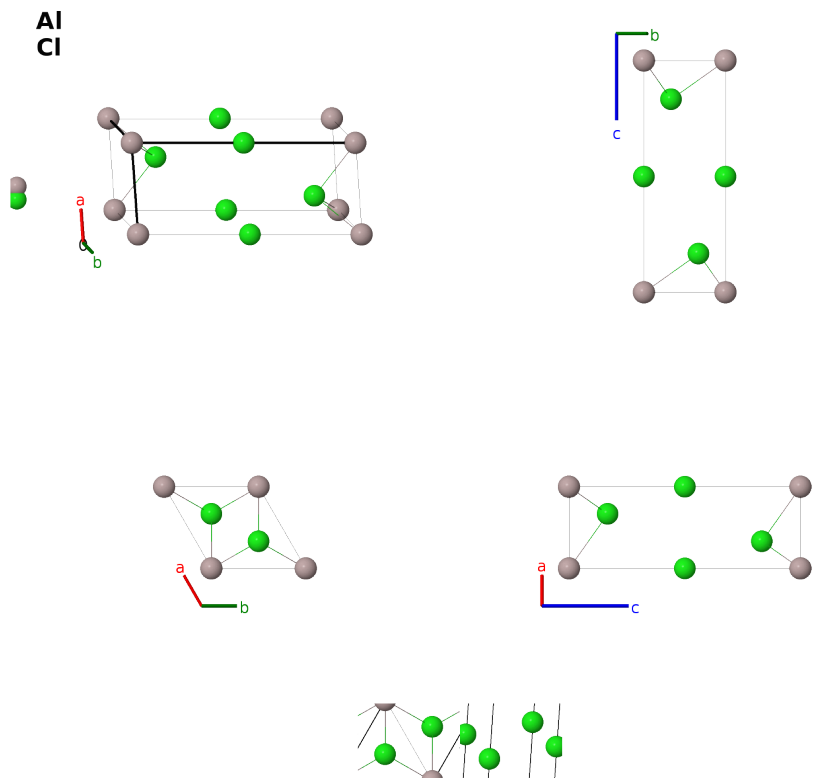
This structure previously used the label(s) **AB3_hP4_164_b_ad**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/K2MJ>

https://aflow.org/prototype-encyclopedia/AB3_hP4_164_a_bd-001

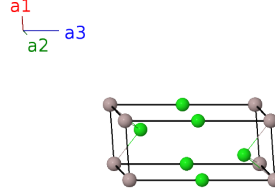


Prototype	AlCl_3
AFLOW prototype label	AB3_hP4_164_a_bd-001
<i>Strukturbericht</i> designation	$D0_{13}$
ICSD	155670
CCDC	1672271
Pearson symbol	hP4
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	<code>aflow --proto=AB3_hP4_164_a_bd-001 --params=a, c/a, z₃</code>

- This structure was suggested by (Laschkarew, 1930) and designated as *Strukturbericht* $D0_{13}$ by (Hermann, 1937). However, in the next edition of *Strukturbericht*, (Gottfried, 1937) changed the AlCl_3 structure to the one found by (Ketelaar, 1935), and designated it as $D0_{15}$. Neither of these structures is currently accepted. The accepted structure is body-centered orthorhombic, space group $C2/m\#12$.

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	Al I
$\mathbf{B}_2$	$=$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}c\hat{\mathbf{z}}$	Cl I
$\mathbf{B}_3$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_3\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	Cl II
$\mathbf{B}_4$	$=$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_3\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$	Cl II

References

- [1] W. E. Laschkarew, *Zur Struktur AlCl_3* , Z. Anorganische und Allgemeine Chemie **193**, 270–276 (1930), doi:10.1002/zaac.19301930123.
- [2] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).
- [3] J. A. A. Ketelaar, *Die Kristallstruktur der Aluminiumhalogenide II*, Z. Krystallogr. **90**, 237–255 (1935), doi:10.1524/zkri.1935.90.1.237.

Found in

- [1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

First cited in

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