

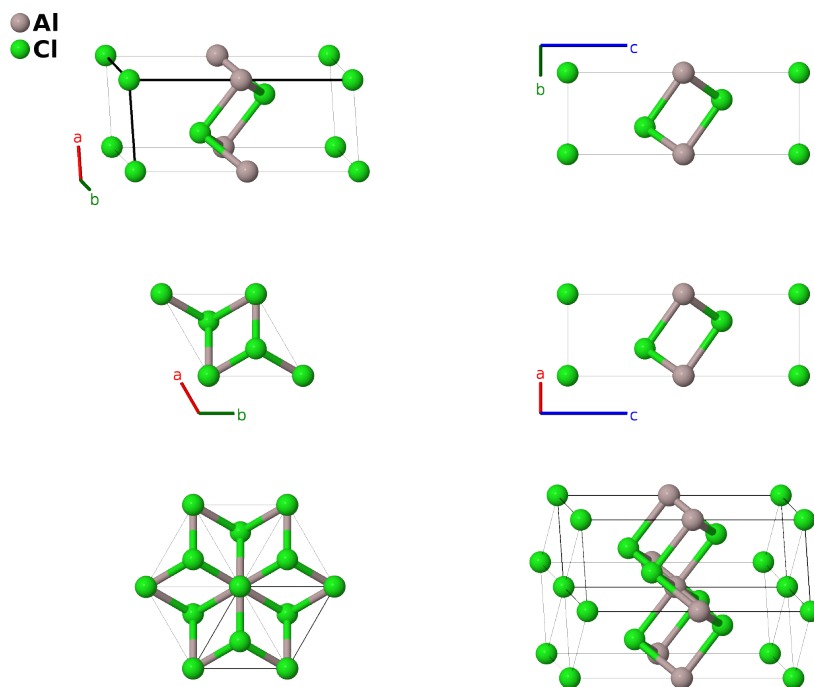
# $D_{013}$ ( $\text{AlCl}_3$ ) Structure (*Obsolete*): AB3\_hP4\_164\_a\_bd-001

This structure originally had the label AB3\_hP4\_164\_b\_ad. Calls to that address will be redirected here.

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<https://aflow.org/p/K2MJ>

[https://aflow.org/p/AB3\\_hP4\\_164\\_a\\_bd-001](https://aflow.org/p/AB3_hP4_164_a_bd-001)



Prototype	$\text{AlCl}_3$
AFLOW prototype label	AB3_hP4_164_a_bd-001
<i>Strukturbericht</i> designation	$D_{013}$
ICSD	155670
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*  $D_{013}$  by (Hermann, 1937). However, in the next edition of *Strukturbericht*, (Gottfried, 1937) changed the  $\text{AlCl}_3$  structure to the one found by (Ketellar, 1935), and designated it as  $D_{015}$ . Neither of these structures is currently accepted. The accepted structure is body-centered orthorhombic, space group  $C2/m\#12$ .

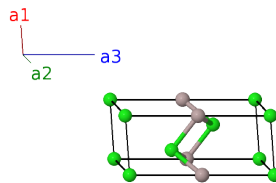
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## Trigonal (Hexagonal) primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



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## Basis vectors

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