

D_{015} (AlCl_3) Structure (*Obsolete*): AB3_mC16_5_c_3c-001

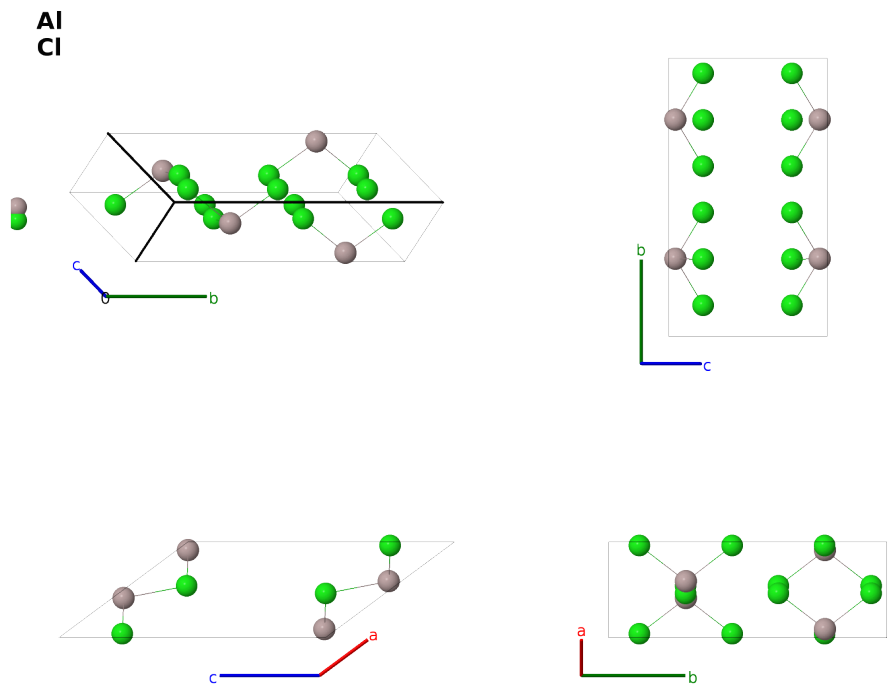
This structure previously used the label(s) **AB3_mC16_5_c_3c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/RSL8>

https://aflow.org/prototype-encyclopedia/AB3_mC16_5_c_3c-001

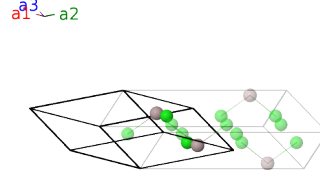


Prototype	AlCl_3
AFLOW prototype label	AB3_mC16_5_c_3c-001
<i>Strukturbericht</i> designation	D_{015}
Pearson symbol	mC16
Space group number	5
Space group symbol	C_2
AFLOW prototype command	<pre>aflow --proto=AB3_mC16_5_c_3c-001 --params=a,b/a,c/a,β,x_1,y_1,z_1,x_2,y_2,z_2,x_3,y_3,z_3,x_4,y_4,z_4</pre>

- This structure was suggested by (Ketelaar, 1935) and given the *Strukturbericht* designation $D0_{15}$ by (Gottfried, 1935) with no reference to the $D0_{13}$ structure of (Laschkarew, 1930) found in (Hermann, 1937).
- Ketelaar gave a description of the unit cell a hexagonal setting, but the atomic positions resolve into the body-centered monoclinic cell shown here. This structure, however, has a lower symmetry than the currently accepted structure, which we previously designated $D0_{15}$. The current accepted structure is body-centered orthorhombic, space group $C2/m$ #12.

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$(x_1 - y_1) \mathbf{a}_1 + (x_1 + y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B}_2$	$-(x_1 + y_1) \mathbf{a}_1 - (x_1 - y_1) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B}_3$	$(x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B}_4$	$-(x_2 + y_2) \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B}_5$	$(x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4c)	Cl II
$\mathbf{B}_6$	$-(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4c)	Cl II
$\mathbf{B}_7$	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4c)	Cl III
$\mathbf{B}_8$	$-(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4c)	Cl III

References

- [1] J. A. A. Ketelaar, *Die Kristallstruktur der Aluminiumhalogenide II*, Z. Krystallogr. **90**, 237–255 (1935), doi:10.1524/zkri.1935.90.1.237.
- [2] W. E. Laschkarew, *Zur Struktur $AlCl_3$* , Z. Anorganische und Allgemeine Chemie **193**, 270–276 (1930), doi:10.1002/zaac.19301930123.
- [3] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

Found in

- [1] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

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- 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.