

AlCl₃ Structure:

AB3_mC16_12_g_ij-001

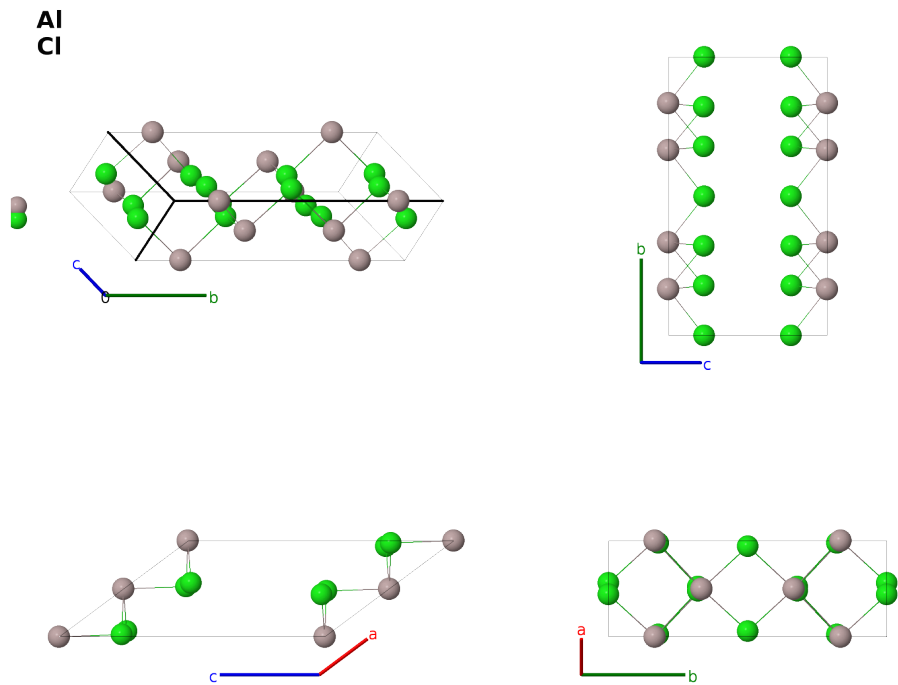
This structure previously used the label(s) **AB3_mC16_12_g_ij**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/2SQ0>

https://aflow.org/prototype-encyclopedia/AB3_mC16_12_g_ij-001



Prototype	AlCl ₃
AFLOW prototype label	AB3_mC16_12_g_ij-001
ICSD	39566
CCDC	1609549
Pearson symbol	mC16
Space group number	12
Space group symbol	C2/m
AFLOW prototype command	<code>aflow --proto=AB3_mC16_12_g_ij-001</code> <code>--params=a, b/a, c/a, β, y_1, x_2, z_2, x_3, y_3, z_3</code>

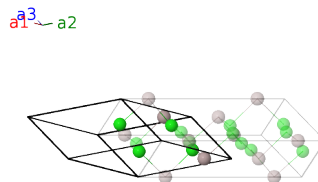
Other compounds with this structure

DyCl₃, ErCl₃, HoCl₃, InCl₃, LuCl₃, α -RuCl₃, TlCl₃, TmCl₃, YbCl₃

- We originally listed this as the $D0_{15}$ structure, but this does not follow the historical record, so we have modified this page and added previous determinations of the structure as follows:
- (Laschkarew, 1930) determined that AlCl₃ was in space group $P\bar{3}m1$ #164. (Hermann, 1937) designated this as the $D0_{13}$ structure.
- (Ketelaar, 1935) determined that the structure was only pseudo-hexagonal, and place it in space group $C2$ #5. (Gottfried, 1937) designated this as the $D0_{15}$ structure. Neither of these works referenced the previous work.
- (Ketelaar, 1947) determined that the space group was actually $C2/m$ #12. Here we present this using the refinement of (Troyanov, 1992).

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
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	$=$	$by_1 \hat{\mathbf{y}}$	(4g)	Al I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2$	$=$	$-by_1 \hat{\mathbf{y}}$	(4g)	Al I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	Cl I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	Cl I
$\mathbf{B}_5$	$= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(8j)	Cl II
$\mathbf{B}_6$	$= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(8j)	Cl II
$\mathbf{B}_7$	$= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(8j)	Cl II
$\mathbf{B}_8$	$= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(8j)	Cl II

References

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- [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).
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- [6] J. A. A. Ketelaar, C. H. MacGillavry, and P. A. Renes, *The crystal structure of aluminium chloride*, Rec. Trav. Chim. Pays-Bas **66**, 501–512 (1947), doi:10.1002/recl.19470660805.

Found in

- [1] P. Villars, *AlCl₃ Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.

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