$D0_{15}$ ($AlCl_3$) Structure (*Obsolete*): AB3_mC16_5_c_3c-001

This structure originally had the label `AB3_mC16_5_c_3c`. Calls to that address will be redirected here.

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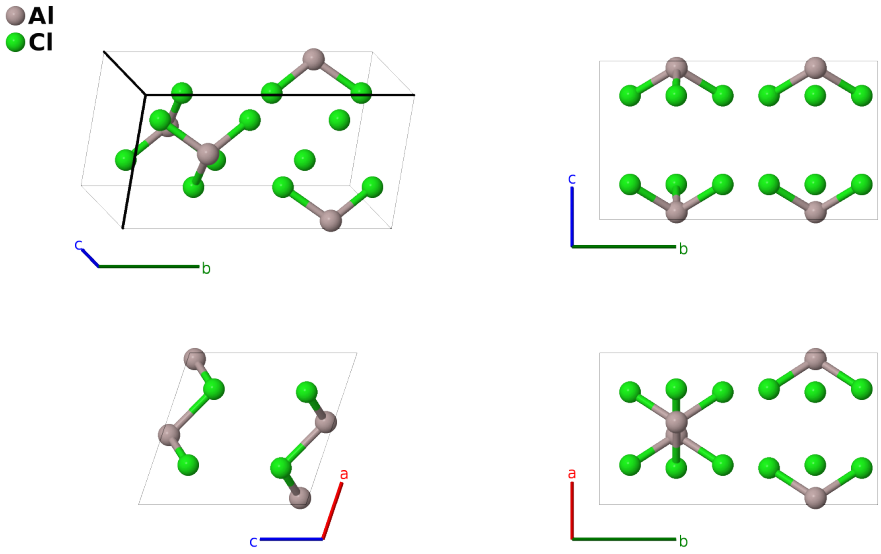
https://aflow.org/p/RSL8

https://aflow.org/p/AB3_mC16_5_c_3c-001

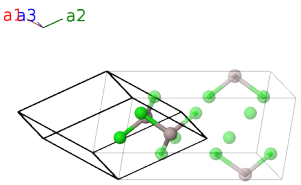


Prototype	$AlCl_3$
AFLOW prototype label	AB3_mC16_5_c_3c-001
***Strukturbericht* designation**	$D0_{15}$
ICSD	none
Pearson symbol	mC16
Space group number	5
Space group symbol	$C2$
AFLOW prototype command	`aflow --proto=AB3_mC16_5_c_3c-001 --params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

- This structure was suggested by (Ketelaar, 1935) and given the *Strukturbericht* designation $D0_{15}$ by (Gottfried, 1395) 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.

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Found in

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