$AlCl_3$ Structure: AB3_mC16_12_g_ij-001

This structure originally had the label `AB3_mC16_12_g_ij`. Calls to that address will be redirected here.

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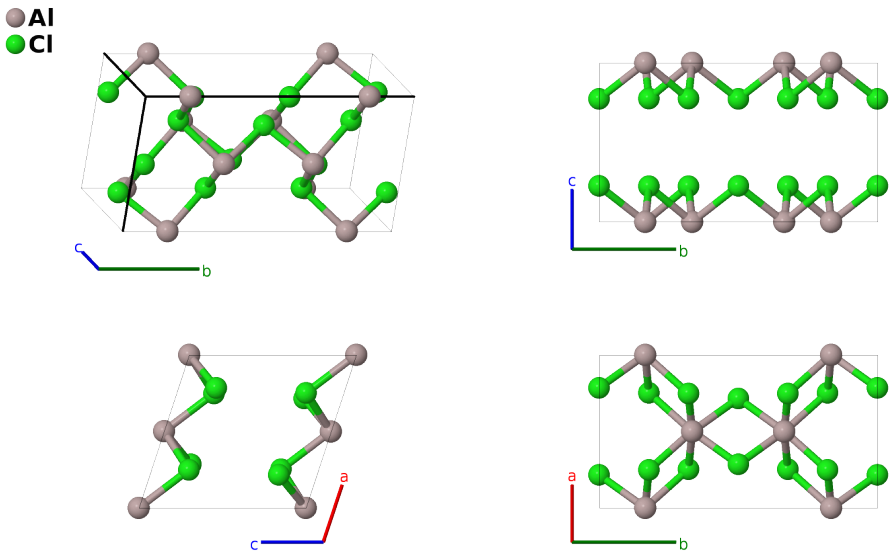
https://aflow.org/p/2SQ0

https://aflow.org/p/AB3_mC16_12_g_ij-001



Prototype	$AlCl_3$
AFLOW prototype label	AB3_mC16_12_g_ij-001
ICSD	39566
Pearson symbol	mC16
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=AB3_mC16_12_g_ij-001 --params=`$a, b/a, c/a, \beta, y_1, x_2, z_2, x_3, y_3, z_3$

Other compounds with this structure

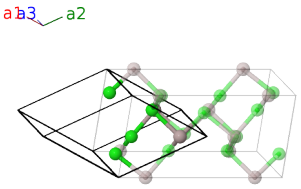
$DyCl_3$, $ErCl_3$, $HoCl_3$, $InCl_3$, $LuCl_3$, α-$RuCl_3$, $TlCl_3$, $TmCl_3$, YbCl3

- 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 $AlCl_3$ 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

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}\end{aligned}$$



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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[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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[1] P. Villars, *$AlCl_3$ Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.