

Cl (A18) Structure (*Obsolete*): A_tP16_138_j-001

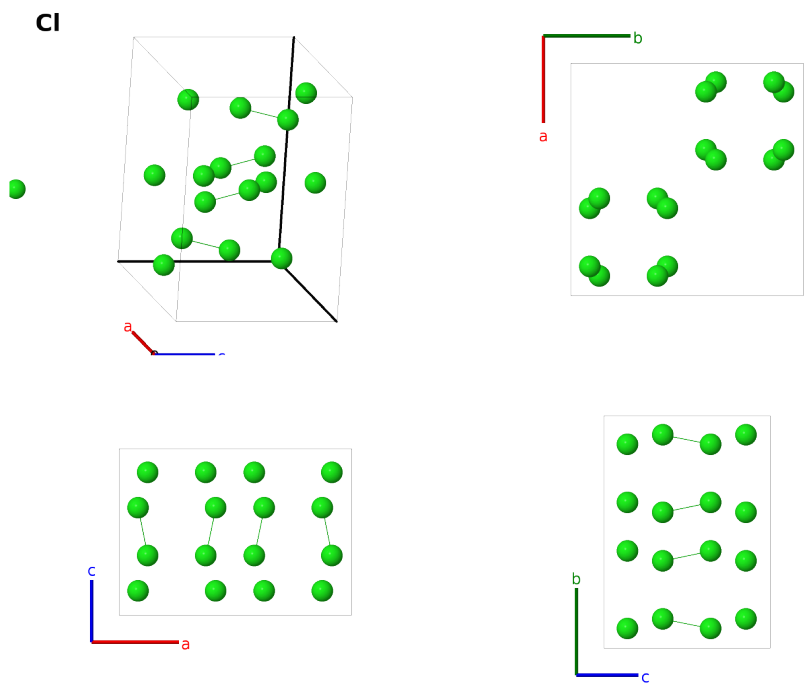
This structure previously used the label(s) **A.tP16_138-j**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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.

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

https://aflow.org/prototype-encyclopedia/A.tP16_138-j-001



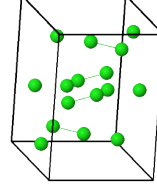
Prototype	Cl
AFLOW prototype label	A_tP16_138_j-001
<i>Strukturbericht</i> designation	A18
ICSD	22406
CCDC	1599150
Pearson symbol	tP16
Space group number	138
Space group symbol	$P4_2/ncm$
AFLOW prototype command	<code>aflow --proto=A_tP16_138_j-001 --params=a, c/a, x₁, y₁, z₁</code>

- As given, this structure has a Cl-Cl bond distance of 1.82Å, far too small for chlorine. The structure was eventually reanalyzed, and found to be similar to molecular iodine (*A14*). See (Donohue, 1982, p. 396) for details. We retain this structure for its historical interest. Note that all atoms are on the general sites of space group $P4_2/nm$ #138.

Simple Tetragonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$

$\mathbf{a}_1$ $\mathbf{a}_2$ $\mathbf{a}_3$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_3$	$= -\left(y_1 - \frac{1}{2}\right) \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(y_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_4$	$= y_1 \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + a\left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_6$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_7$	$= \left(y_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a\left(y_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_8$	$= -y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_9$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_{10}$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_{11}$	$= \left(y_1 + \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(y_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_{12}$	$= -y_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_{13}$	$= x_1 \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} - a\left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_{14}$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_{15}$	$= -\left(y_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-a\left(y_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(16j)	Cl I
$\mathbf{B}_{16}$	$= y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(16j)	Cl I

References

- [1] W. H. Keesom and K. W. Taconis, *On the crystal structure of chlorine*, Physica **3**, 237–242 (1936), doi:10.1016/S0031-8914(36)80226-2.

Found in

[1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017