$I1_3$ [$SrCl_2 \cdot (H_2O)_6$] (*Obsolete*) Structure: A2B6C_hP9_162_c_k_b-001

This structure previously used the label(s) `A2B6C_hP9_162_d_k_a`. 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.

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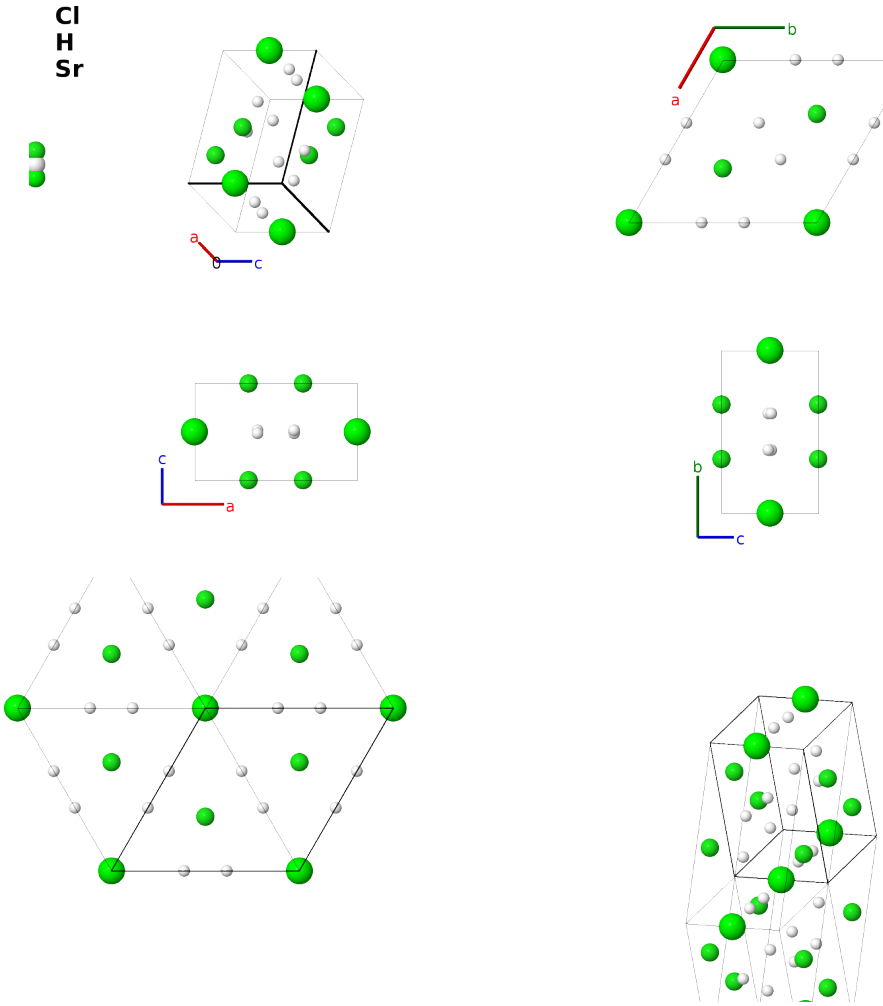
https://aflow.org/prototype-encyclopedia/WZ1P

https://aflow.org/prototype-encyclopedia/A2B6C_hP9_162_c_k_b-001



Prototype	$Cl_2(H_2O)_6Sr$
AFLOW prototype label	A2B6C_hP9_162_c_k_b-001
***Strukturbericht* designation**	$I1_3$
Pearson symbol	hP9
Space group number	162

Space group symbol $P\bar{3}1m$

AFLOW prototype command `aflow --proto=A2B6C_hP9_162_c_k_b-001 --params=`$a, c/a, x_3, z_3$

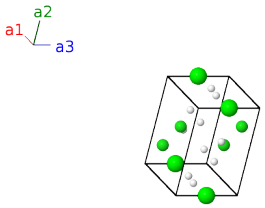
Other compounds with this structure

$CaCl_2{\cdot}(H_2O)_6$, $CaBr_2{\cdot}(H_2O)_6$, $SrBr_2{\cdot}(H_2O)_6$, $CaI_2{\cdot}(H_2O)_6$, $SrI_2{\cdot}(H_2O)_6$, $BaI_2{\cdot}(H_2O)_6$

- (Hermann, 1937) gives this the *Strukturbericht* designation $I1_3$, but gives the prototype as $K_2Pt(SCN)_6$. As we discussed on the $K_2Pt(SCN)_6$ ($H6_3$) page, the difference between these two structures is significant, so we will use the original $H6_3$ designation for $K_2Pt(SCN)_6$, and $I1_3$ for $SrCl_2{\cdot}(H_2O)_6$.
- In any case, (Aagon, 1986) and others have shown that the correct space group of this structure is $P321$ #150. We discuss the corrected structure on the $SrCl_2{\cdot}(H_2O)_6$ page.
- Using the notation of (Gottfried, 1937) this could also be designated the $J1_3$ structure. That designation was never used in any *Strukturbericht* volume, so we will use $I1_3$ here.
- The positions of the hydrogen atoms in the water molecules were not determined, so we only provide the positions of the oxygen atoms (labeled as H2O).

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Sr I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Cl I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Cl I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6k)	H I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6k)	H I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(6k)	H I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6k)	H I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6k)	H I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - cz_3\,\hat{\mathbf{z}}$	(6k)	H I

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First cited in

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