

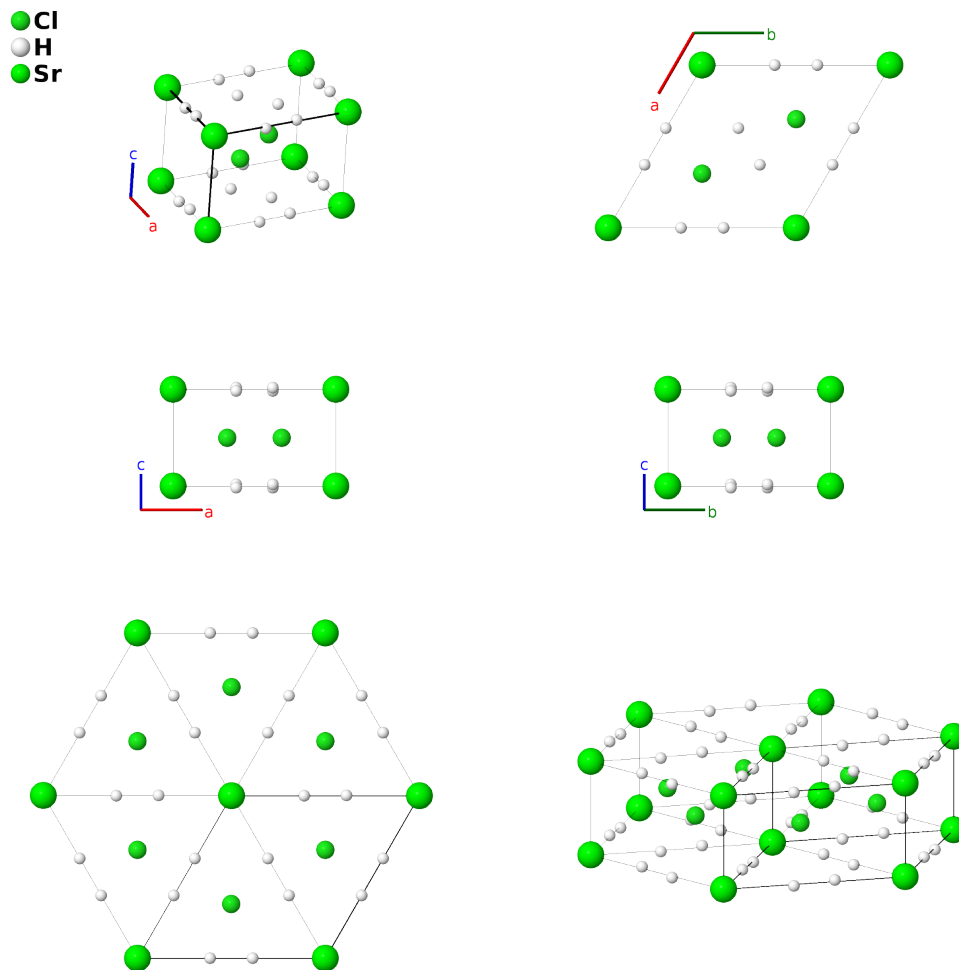
# $I1_3$ $[\text{SrCl}_2 \cdot (\text{H}_2\text{O})_6]$ (*Obsolete*) Structure: A2B6C\_hP9\_162\_c\_k\_b-001

This structure originally had the label A2B6C\_hP9\_162\_d\_k\_a. Calls to that address will be redirected here.

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<https://afLOW.org/p/WZ1P>

[https://afLOW.org/p/A2B6C\\_hP9\\_162\\_c\\_k\\_b-001](https://afLOW.org/p/A2B6C_hP9_162_c_k_b-001)



Prototype	$\text{Cl}_2(\text{H}_2\text{O})_6\text{Sr}$
AFLOW prototype label	A2B6C_hP9_162_c_k_b-001
<i>Strukturbericht</i> designation	$I1_3$
ICSD	none
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, x3, z3`

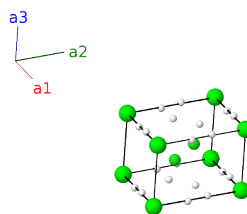
### Other compounds with this structure

$\text{CaCl}_2 \cdot (\text{H}_2\text{O})_6$ ,  $\text{CaBr}_2 \cdot (\text{H}_2\text{O})_6$ ,  $\text{SrBr}_2 \cdot (\text{H}_2\text{O})_6$ ,  $\text{CaI}_2 \cdot (\text{H}_2\text{O})_6$ ,  $\text{SrI}_2 \cdot (\text{H}_2\text{O})_6$ ,  $\text{BaI}_2 \cdot (\text{H}_2\text{O})_6$

- (Hermann, 1937) gives this the *Strukturbericht* designation  $I1_3$ , but gives the prototype as  $\text{K}_2\text{Pt}(\text{SCN})_6$ . As we discussed on the  $\text{K}_2\text{Pt}(\text{SCN})_6$  ( $H6_3$ ) page, the difference between these two structures is significant, so we will use the original  $H6_3$  designation for  $\text{K}_2\text{Pt}(\text{SCN})_6$ , and  $I1_3$  for  $\text{SrCl}_2 \cdot (\text{H}_2\text{O})_6$ .
- 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  $\text{SrCl}_2 \cdot (\text{H}_2\text{O})_6$  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

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



### 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

### References

- [1] Z. Herrmann, *Über die Struktur des Strontiumchlorid-Hexahydrats*, *Z. Anorganische und Allgemeine Chemie* **187**, 231–236 (1930), doi:10.1002/zaac.19301870121.
- [2] P. A. Agron and W. R. Busing, *Calcium and strontium dichloride hexahydrates by neutron diffraction*, *Acta Crystallogr. Sect. C* **42**, 141–143 (1986), doi:10.1107/S0108270186097007.
- [3] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

## Found in

- [1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).