

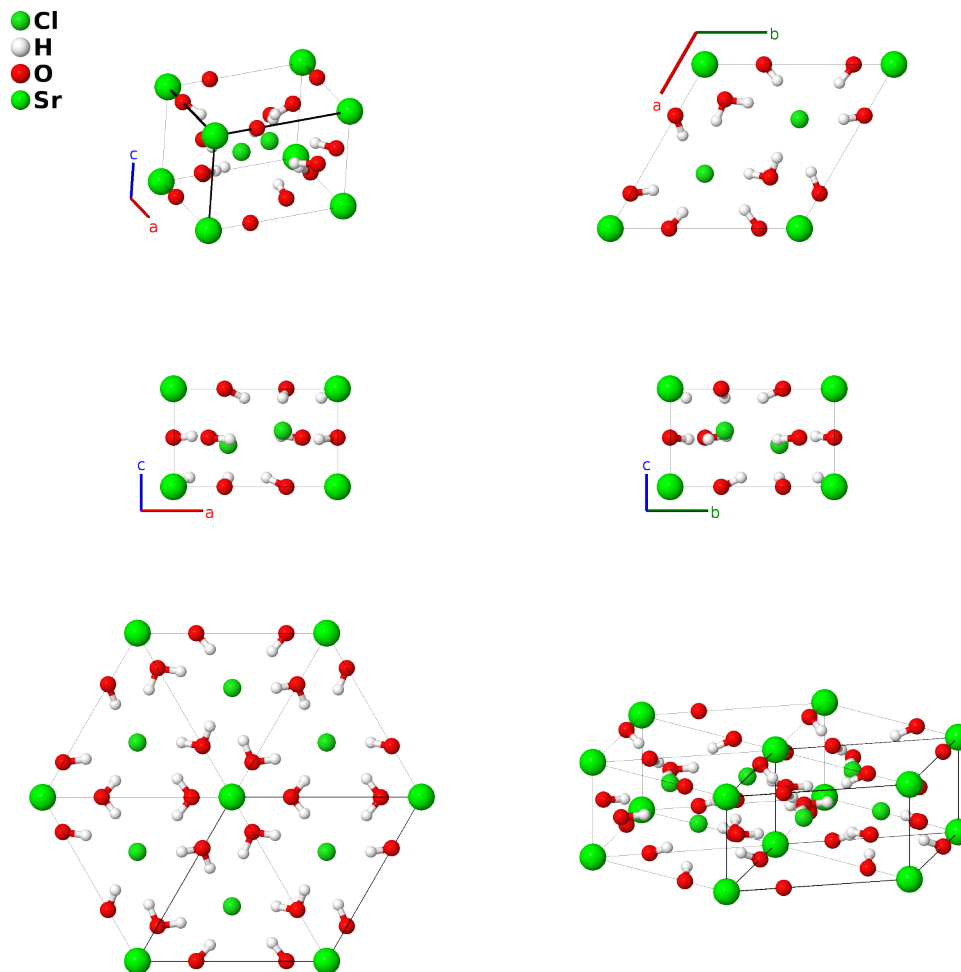
SrCl₂·(H₂O)₆ Structure: A2B12C6D_hP21_150_d_2g_ef_a-001

This structure originally had the label `A2B12C6D_hP21_150_d_2g_ef_a`. Calls to that address will be redirected here.

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<https://aflow.org/p/FX47>

https://aflow.org/p/A2B12C6D_hP21_150_d_2g_ef_a-001



Prototype	Cl ₂ H ₁₂ O ₆ Sr
AFLOW prototype label	A2B12C6D_hP21_150_d_2g_ef_a-001
ICSD	59143
Pearson symbol	hP21
Space group number	150
Space group symbol	<i>P</i> 321
AFLOW prototype command	<code>aflow --proto=A2B12C6D_hP21_150_d_2g_ef_a-001 --params=a, c/a, z₂, x₃, x₄, x₅, y₅, z₅, x₆, y₆, z₆</code>

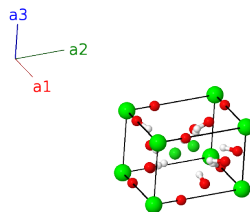
Other compounds with this structure

$\text{CaCl}_2 \cdot (\text{H}_2\text{O})_6$, $\text{CaBr}_2 \cdot (\text{H}_2\text{O})_6$

- This is a redetermination of the $I1_3$ structure. In addition to locating the hydrogen atoms in the water molecule, (Agron, 1986) show that the space group is $P321$ #150, not $P\bar{3}$ #147.

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	0	$=$	0	(1a)	Sr I
\mathbf{B}_2	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2d)	Cl I
\mathbf{B}_3	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2d)	Cl I
\mathbf{B}_4	$x_3 \mathbf{a}_1$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(3e)	O I
\mathbf{B}_5	$x_3 \mathbf{a}_2$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(3e)	O I
\mathbf{B}_6	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}}$	(3e)	O I
\mathbf{B}_7	$x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3f)	O II
\mathbf{B}_8	$x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3f)	O II
\mathbf{B}_9	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3f)	O II
\mathbf{B}_{10}	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6g)	H I
\mathbf{B}_{11}	$-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6g)	H I
\mathbf{B}_{12}	$-(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6g)	H I
\mathbf{B}_{13}	$y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(6g)	H I
\mathbf{B}_{14}	$(x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(6g)	H I
\mathbf{B}_{15}	$-x_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(6g)	H I
\mathbf{B}_{16}	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6g)	H II
\mathbf{B}_{17}	$-y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6g)	H II
\mathbf{B}_{18}	$-(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6g)	H II
\mathbf{B}_{19}	$y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(6g)	H II
\mathbf{B}_{20}	$(x_6 - y_6) \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(6g)	H II
\mathbf{B}_{21}	$-x_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(6g)	H II

References

- [1] 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.

Found in

- [1] P. Villars, *PAULING FILE* (2016). In: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg SpringerMaterials.