

$E6_1$ $[\text{Sr}(\text{OH})_2(\text{H}_2\text{O})_8]$ Structure (*Obsolete*): A8B2C_tP11_123_r_e_b-001

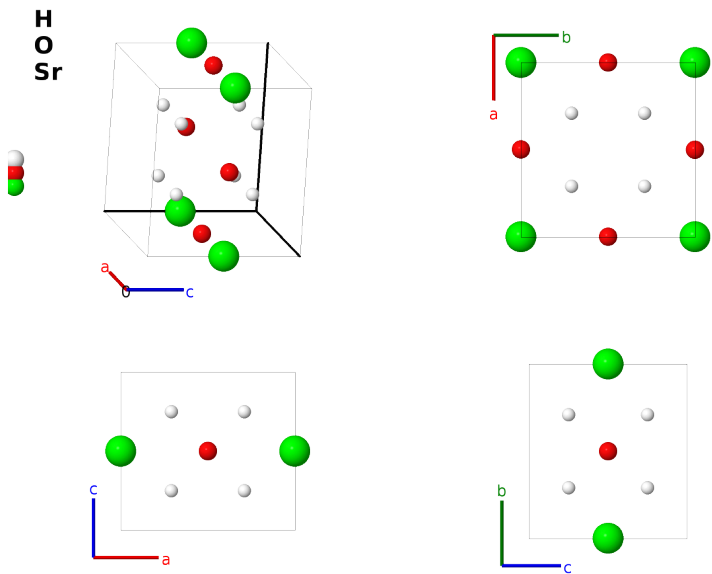
This structure previously used the label(s) **A8B2C.tP11_123.r.f.a.** Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A8B2C_tP11_123_r_e_b-001



Prototype	$(\text{H}_2\text{O})_8(\text{OH})_2\text{Sr}$
AFLOW prototype label	A8B2C.tP11_123_r_e_b-001
<i>Strukturbericht</i> designation	$E6_1$
Pearson symbol	tP11
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	<code>aflow --proto=A8B2C_tP11_123_r_e_b-001 --params=a, c/a, x₃, z₃</code>

- This structure was designated $E6_1$ by (Hermann, 1937). It has been superseded by the structure determined by (Ricci, 2005). We present it for historical interest.

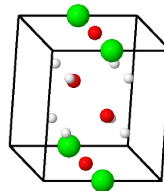
Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$

$\mathbf{a}_1^1 \mathbf{a}_2^2 \mathbf{a}_3^3$



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
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B}_4$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8r)	H I
$\mathbf{B}_5$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8r)	H I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8r)	H I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8r)	H I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8r)	H I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8r)	H I
$\mathbf{B}_{10}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8r)	H I
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8r)	H I

References

- [1] G. Natta, *Constitution of hydroxides and of hydrates. III. Octahydrated strontium hydroxide*, Gazz. chim. Ital. **58**, 870–872 (1928).

Found in

- [1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).
- [2] J. S. Ricci, R. C. Stevens, R. K. McMullan, and W. T. Klooster, *Structure of strontium hydroxide octahydrate, $\text{Sr}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$, at 20, 100 and 200 K from neutron diffraction*, Acta Crystallogr. Sect. B **61**, 381–386 (2005), doi:10.1107/S0108768105013480.

First cited in

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