$E6_1$ [$Sr(OH)_2(H_2O)_8$] Structure (*Obsolete*): A8B2C_tP11_123_r_e_b-001

This structure originally had the label `A8B2C_tP11_123_r_f_a`. Calls to that address will be redirected here.

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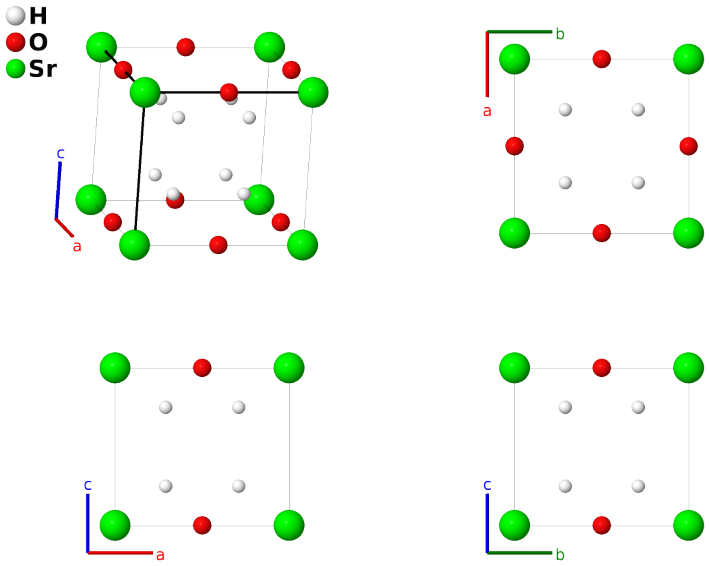
https://aflow.org/p/QEVQ

https://aflow.org/p/A8B2C_tP11_123_r_e_b-001

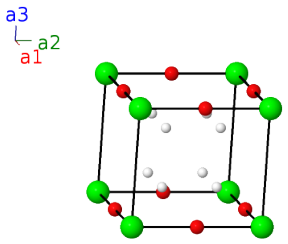


Prototype	$(H_2O)_8(OH)_2Sr$
AFLOW prototype label	A8B2C_tP11_123_r_e_b-001
***Strukturbericht* designation**	$E6_1$
ICSD	none
Pearson symbol	tP11
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=A8B2C_tP11_123_r_e_b-001 --params=`$a, c/a, x_3, z_3$

- 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 It has been superseded by the structure determined by (Ricci, 2005).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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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, $Sr(OH)_2{\cdot}8H_2O$, at 20, 100 and 200 K from neutron diffraction*, Acta Crystallogr. Sect. B **61**, 381–386 (2005), doi:10.1107/S0108768105013480.