$Sr[S_2O_6][H_2O]_4$ Structure: A10B2C_hP39_171_5c_c_a-001

This structure originally had the label `A10B2C_hP39_171_5c_c_a`. Calls to that address will be redirected here.

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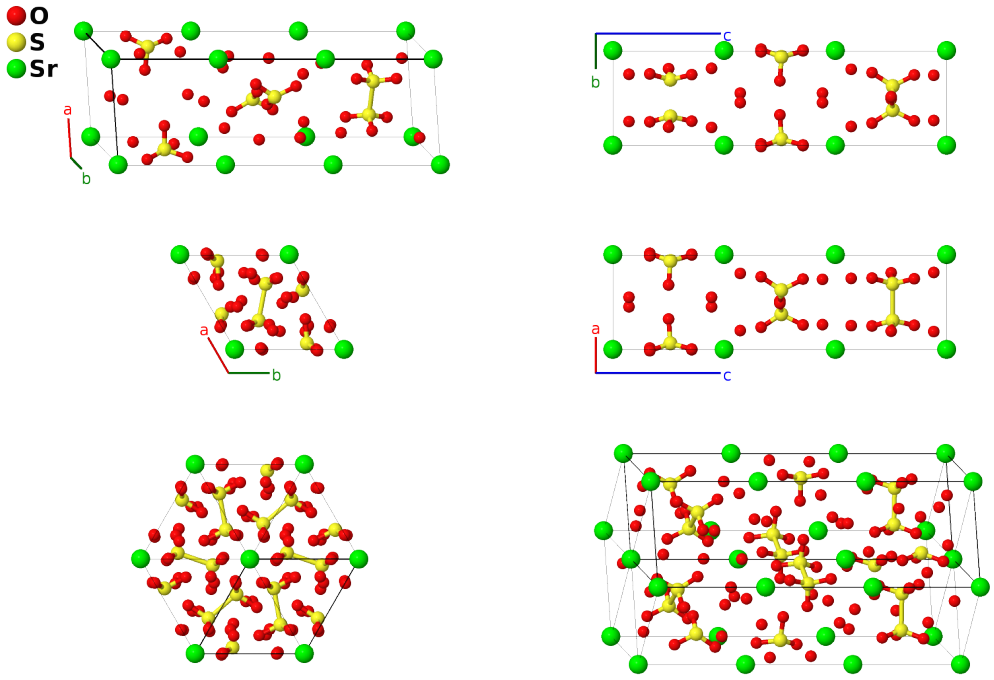
https://aflow.org/p/WCPM

https://aflow.org/p/A10B2C_hP39_171_5c_c_a-001

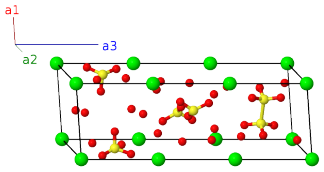


Prototype	$O_{10}S_2Sr$
AFLOW prototype label	A10B2C_hP39_171_5c_c_a-001
ICSD	2933
Pearson symbol	hP39
Space group number	171
Space group symbol	$P6_2$
AFLOW prototype command	`aflow --proto=A10B2C_hP39_171_5c_c_a-001 --params=`$a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- This structure is the enantiomorph of the $Sr[S_2O_6][H_2O]_4$ (A10B2C_hP39_172_5c_c_a) structure. Only the non-hydrogen atoms are included in the prototype.
- Space group $P6_2$ #171 allows an arbitary choice for the origin of the z-axis. We set this by taking $z_1 = 0$ for the Sr site.

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(3a)	Sr I
$\mathbf{B_2}$	=	$\left(z_1+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{3}c\,(3z_1+2)\,\hat{\mathbf{z}}$	(3a)	Sr I
$\mathbf{B_3}$	=	$\left(z_1+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(3a)	Sr I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1+y_2\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2+y_2)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_2-y_2)\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_1+(x_2-y_2)\,\mathbf{a}_2+\left(z_2+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2-2y_2)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}+\frac{1}{3}c\,(3z_2+2)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_6}$	=	$-(x_2-y_2)\,\mathbf{a}_1-x_2\,\mathbf{a}_2+\left(z_2+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2-y_2)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1-y_2\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2+y_2)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_2-y_2)\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_8}$	=	$y_2\,\mathbf{a}_1-(x_2-y_2)\,\mathbf{a}_2+\left(z_2+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_2+2y_2)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}+\frac{1}{3}c\,(3z_2+2)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_9}$	=	$(x_2-y_2)\,\mathbf{a}_1+x_2\,\mathbf{a}_2+\left(z_2+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_2-y_2)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1+y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{11}}$	=	$-y_3\,\mathbf{a}_1+(x_3-y_3)\,\mathbf{a}_2+\left(z_3+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3-2y_3)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+\frac{1}{3}c\,(3z_3+2)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{12}}$	=	$-(x_3-y_3)\,\mathbf{a}_1-x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{13}}$	=	$-x_3\,\mathbf{a}_1-y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{14}}$	=	$y_3\,\mathbf{a}_1-(x_3-y_3)\,\mathbf{a}_2+\left(z_3+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_3+2y_3)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+\frac{1}{3}c\,(3z_3+2)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{15}}$	=	$(x_3-y_3)\,\mathbf{a}_1+x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{17}}$	=	$-y_4\,\mathbf{a}_1+(x_4-y_4)\,\mathbf{a}_2+\left(z_4+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4-2y_4)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+\frac{1}{3}c\,(3z_4+2)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{18}}$	=	$-(x_4-y_4)\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{19}}$	=	$-x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{20}}$	=	$y_4\,\mathbf{a}_1-(x_4-y_4)\,\mathbf{a}_2+\left(z_4+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_4+2y_4)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+\frac{1}{3}c\,(3z_4+2)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{21}}$	=	$(x_4-y_4)\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{22}}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{23}}$	=	$-y_5\,\mathbf{a}_1+(x_5-y_5)\,\mathbf{a}_2+\left(z_5+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5-2y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+\frac{1}{3}c\,(3z_5+2)\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{24}}$	=	$-(x_5-y_5)\,\mathbf{a}_1-x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	O IV

$\mathbf{B_{25}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5+y_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5-y_5)\;\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{26}}$	=	$y_5\,\mathbf{a}_1 - (x_5-y_5)\;\mathbf{a}_2 + \left(z_5+\frac{2}{3}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5+2y_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_5+2)\;\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{27}}$	=	$(x_5-y_5)\;\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5+\frac{1}{3}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5-y_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{3}\right)\;\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{28}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6+y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6-y_6)\;\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B_{29}}$	=	$-y_6\,\mathbf{a}_1 + (x_6-y_6)\;\mathbf{a}_2 + \left(z_6+\frac{2}{3}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6-2y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_6+2)\;\hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B_{30}}$	=	$-(x_6-y_6)\;\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \left(z_6+\frac{1}{3}\right)\;\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6-y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{3}\right)\;\hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B_{31}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6+y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6-y_6)\;\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B_{32}}$	=	$y_6\,\mathbf{a}_1 - (x_6-y_6)\;\mathbf{a}_2 + \left(z_6+\frac{2}{3}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_6+2y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_6+2)\;\hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B_{33}}$	=	$(x_6-y_6)\;\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \left(z_6+\frac{1}{3}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_6-y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{3}\right)\;\hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B_{34}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6c)	S I
$\mathbf{B_{35}}$	=	$-y_7\,\mathbf{a}_1 + (x_7-y_7)\;\mathbf{a}_2 + \left(z_7+\frac{2}{3}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7-2y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_7+2)\;\hat{\mathbf{z}}$	(6c)	S I
$\mathbf{B_{36}}$	=	$-(x_7-y_7)\;\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \left(z_7+\frac{1}{3}\right)\;\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + c\left(z_7+\frac{1}{3}\right)\;\hat{\mathbf{z}}$	(6c)	S I
$\mathbf{B_{37}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6c)	S I
$\mathbf{B_{38}}$	=	$y_7\,\mathbf{a}_1 - (x_7-y_7)\;\mathbf{a}_2 + \left(z_7+\frac{2}{3}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_7+2y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_7+2)\;\hat{\mathbf{z}}$	(6c)	S I
$\mathbf{B_{39}}$	=	$(x_7-y_7)\;\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \left(z_7+\frac{1}{3}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + c\left(z_7+\frac{1}{3}\right)\;\hat{\mathbf{z}}$	(6c)	S I

References

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