

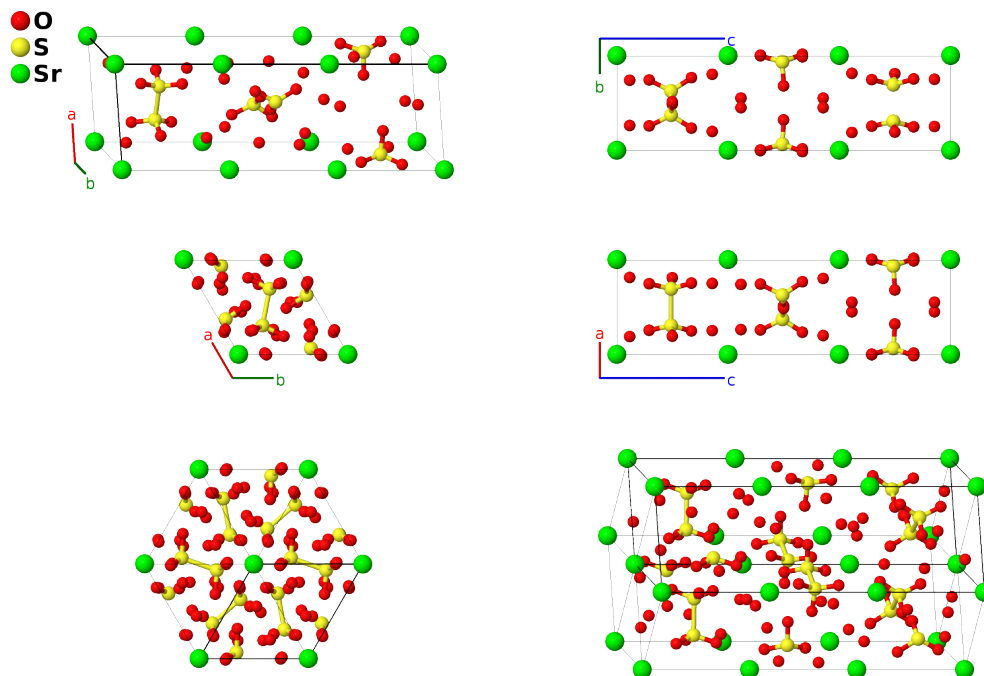
Sr[S₂O₆][H₂O]₄ Structure: A10B2C_hP39_172_5c_c_a-001

This structure originally had the label A10B2C_hP39_172_5c_c.a. Calls to that address will be redirected here.

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<https://aflow.org/p/XXQ8>

https://aflow.org/p/A10B2C_hP39_172_5c_c_a-001

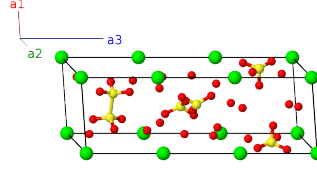


Prototype	O ₁₀ S ₂ Sr
AFLOW prototype label	A10B2C_hP39_172_5c_c_a-001
ICSD	2933
Pearson symbol	hP39
Space group number	172
Space group symbol	<i>P</i> 6 ₄
AFLOW prototype command	<code>aflow --proto=A10B2C_hP39_172_5c_c_a-001 --params=a, c/a, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇</code>

- This structure is the enantiomorph of the Sr[S₂O₆][H₂O]₄ (A10B2C_hP39_171_5c_c.a) structure. Only the non-hydrogen atoms are included in the prototype.
- Space group *P*6₄ #172 allows an arbitrary choice for the origin of the *z*-axis. We set this by taking *z*₁ = 0 for the Sr site.
- The ICSD entry is for space group *P*6₂ #171.

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	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(3a)	Sr I
\mathbf{B}_2	$= (z_1 + \frac{1}{3}) \mathbf{a}_3$	$=$	$c (z_1 + \frac{1}{3}) \hat{\mathbf{z}}$	(3a)	Sr I
\mathbf{B}_3	$= (z_1 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{3}c (3z_1 + 2) \hat{\mathbf{z}}$	(3a)	Sr I
\mathbf{B}_4	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_5	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_2 \hat{\mathbf{y}} + c (z_2 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_6	$= -(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_2 \hat{\mathbf{y}} + \frac{1}{3}c (3z_2 + 2) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_8	$= y_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_2 + 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_2 \hat{\mathbf{y}} + c (z_2 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_9	$= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + (z_2 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_2 \hat{\mathbf{y}} + \frac{1}{3}c (3z_2 + 2) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{10}	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{11}	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{12}	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_3 \hat{\mathbf{y}} + \frac{1}{3}c (3z_3 + 2) \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{13}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{14}	$= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{15}	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_3 \hat{\mathbf{y}} + \frac{1}{3}c (3z_3 + 2) \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{16}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(6c)	O III
\mathbf{B}_{17}	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}} + c (z_4 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O III
\mathbf{B}_{18}	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_4 \hat{\mathbf{y}} + \frac{1}{3}c (3z_4 + 2) \hat{\mathbf{z}}$	(6c)	O III
\mathbf{B}_{19}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(6c)	O III
\mathbf{B}_{20}	$= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}} + c (z_4 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O III
\mathbf{B}_{21}	$= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_4 \hat{\mathbf{y}} + \frac{1}{3}c (3z_4 + 2) \hat{\mathbf{z}}$	(6c)	O III
\mathbf{B}_{22}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6c)	O IV
\mathbf{B}_{23}	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c (z_5 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O IV
\mathbf{B}_{24}	$= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_5 \hat{\mathbf{y}} + \frac{1}{3}c (3z_5 + 2) \hat{\mathbf{z}}$	(6c)	O IV
\mathbf{B}_{25}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6c)	O IV
\mathbf{B}_{26}	$= y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c (z_5 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O IV

$$\begin{aligned}
\mathbf{B}_{27} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{2}{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}} + \frac{1}{3}c(3z_5 + 2) \hat{\mathbf{z}} & (6c) & \text{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) & \text{O V} \\
\mathbf{B}_{29} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \left(z_6 + \frac{1}{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}} + c\left(z_6 + \frac{1}{3}\right) \hat{\mathbf{z}} & (6c) & \text{O V} \\
\mathbf{B}_{30} &= -(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(z_6 + \frac{2}{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}} + \frac{1}{3}c(3z_6 + 2) \hat{\mathbf{z}} & (6c) & \text{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) & \text{O V} \\
\mathbf{B}_{32} &= y_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + \left(z_6 + \frac{1}{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}} + c\left(z_6 + \frac{1}{3}\right) \hat{\mathbf{z}} & (6c) & \text{O V} \\
\mathbf{B}_{33} &= (x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(z_6 + \frac{2}{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}} + \frac{1}{3}c(3z_6 + 2) \hat{\mathbf{z}} & (6c) & \text{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) & \text{S I} \\
\mathbf{B}_{35} &= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \left(z_7 + \frac{1}{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}} + c\left(z_7 + \frac{1}{3}\right) \hat{\mathbf{z}} & (6c) & \text{S I} \\
\mathbf{B}_{36} &= -(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(z_7 + \frac{2}{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}} + \frac{1}{3}c(3z_7 + 2) \hat{\mathbf{z}} & (6c) & \text{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) & \text{S I} \\
\mathbf{B}_{38} &= y_7 \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 + \left(z_7 + \frac{1}{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}} + c\left(z_7 + \frac{1}{3}\right) \hat{\mathbf{z}} & (6c) & \text{S I} \\
\mathbf{B}_{39} &= (x_7 - y_7) \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(z_7 + \frac{2}{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}} + \frac{1}{3}c(3z_7 + 2) \hat{\mathbf{z}} & (6c) & \text{S I}
\end{aligned}$$

References

- [1] R. N. Hargreaves and E. Stanley, *The structure of strontium dithionate tetrahydrate*, Z. Kristallogr. **135**, 399–407 (1972), doi:10.1524/zkri.1972.135.5-6.399.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.