

Sr[S₂O₆][H₂O]₄ Structure: A10B2C_hP39_171_5c_c_a-001

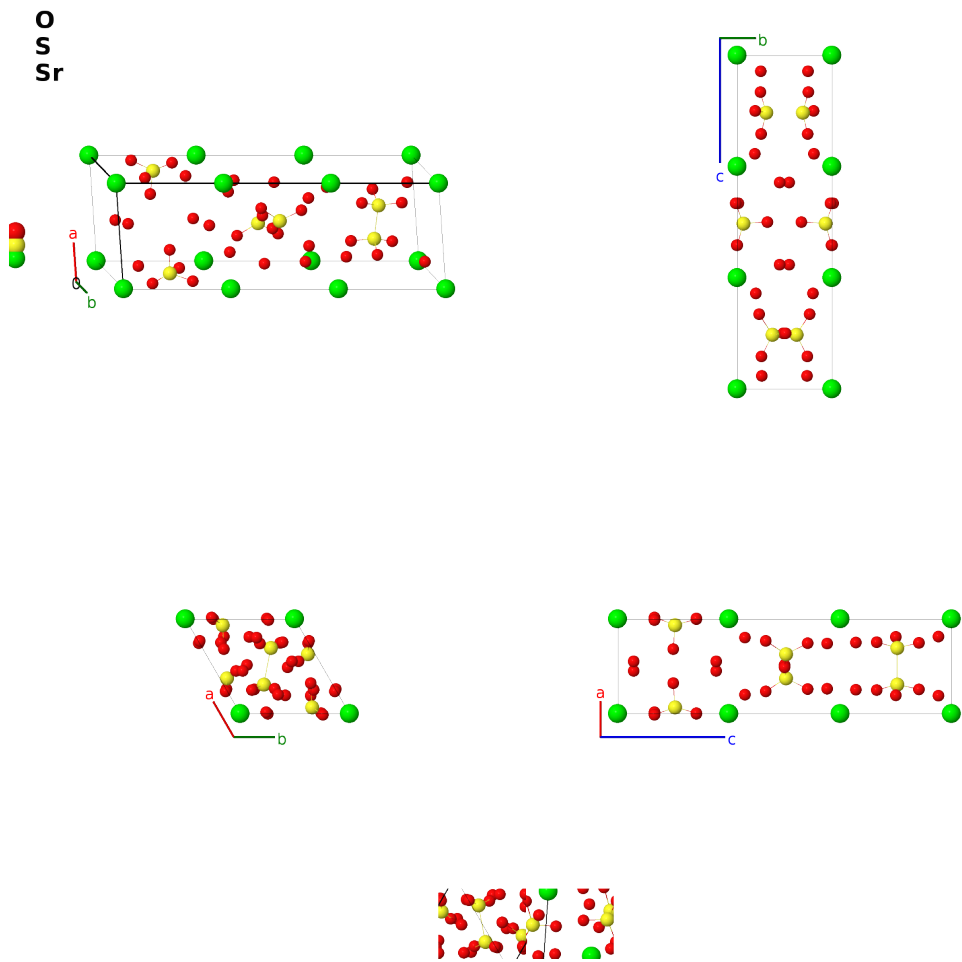
This structure previously used the label(s) **A10B2C_hP39_171_5c_c_a**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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

https://aflow.org/prototype-encyclopedia/A10B2C_hP39_171_5c_c_a-001



Prototype	O ₁₀ S ₂ Sr
AFLOW prototype label	A10B2C_hP39_171_5c_c_a-001
ICSD	2933
CCDC	1592719
Pearson symbol	hP39
Space group number	171

Space group symbol $P6_2$

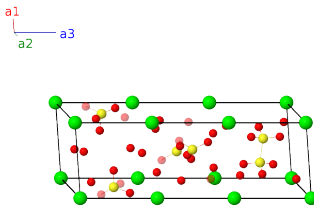
AFLOW prototype command `aflow --proto=A10B2C_hP39_171_5c_c_a-001`
`--params=a, c/a, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7`

Other compounds with this structure

Ca[S₂O₆][H₂O]₄

- This structure is the enantiomorph of the Sr[S₂O₆][H₂O]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 arbitrary choice for the origin of the z -axis. We set this by taking $z_1 = 0$ for the Sr site.

Hexagonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$z_1 \mathbf{a}_3$	=	$cz_1 \hat{\mathbf{z}}$	(3a)	Sr I
$\mathbf{B}_2$	$(z_1 + \frac{2}{3}) \mathbf{a}_3$	=	$\frac{1}{3}c (3z_1 + 2) \hat{\mathbf{z}}$	(3a)	Sr I
$\mathbf{B}_3$	$(z_1 + \frac{1}{3}) \mathbf{a}_3$	=	$c (z_1 + \frac{1}{3}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_5$	$-y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{2}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a (x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{3}c (3z_2 + 2) \hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B}_6$	$-(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{1}{3}) \mathbf{a}_3$	=	$-\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + c (z_2 + \frac{1}{3}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_8$	$y_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{2}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a (-x_2 + 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{3}c (3z_2 + 2) \hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B}_9$	$(x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + (z_2 + \frac{1}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + c (z_2 + \frac{1}{3}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{11}$	$-y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a (x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{3}c (3z_3 + 2) \hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B}_{12}$	$-(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	=	$-\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a (-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{3}c (3z_3 + 2) \hat{\mathbf{z}}$	(6c)	O II

$\mathbf{B}_{15} =$	$(x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{17} =$	$-y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B}_{18} =$	$-(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{20} =$	$y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B}_{21} =$	$(x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{23} =$	$-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{3}c(3z_5 + 2) \hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B}_{24} =$	$-(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{3}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{26} =$	$y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{3}c(3z_5 + 2) \hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B}_{27} =$	$(x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{3}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{29} =$	$-y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + \frac{1}{3}c(3z_6 + 2) \hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B}_{30} =$	$-(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + (z_6 + \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{3}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{32} =$	$y_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + \frac{1}{3}c(3z_6 + 2) \hat{\mathbf{z}}$	(6c)	O V
$\mathbf{B}_{33} =$	$(x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + (z_6 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{3}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{35} =$	$-y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + \frac{1}{3}c(3z_7 + 2) \hat{\mathbf{z}}$	(6c)	S I
$\mathbf{B}_{36} =$	$-(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + (z_7 + \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{3}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{38} =$	$y_7 \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_7 + 2y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + \frac{1}{3}c(3z_7 + 2) \hat{\mathbf{z}}$	(6c)	S I
$\mathbf{B}_{39} =$	$(x_7 - y_7) \mathbf{a}_1 + x_7 \mathbf{a}_2 + (z_7 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	S I

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.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043