

CsB₉O₁₄ Structure:

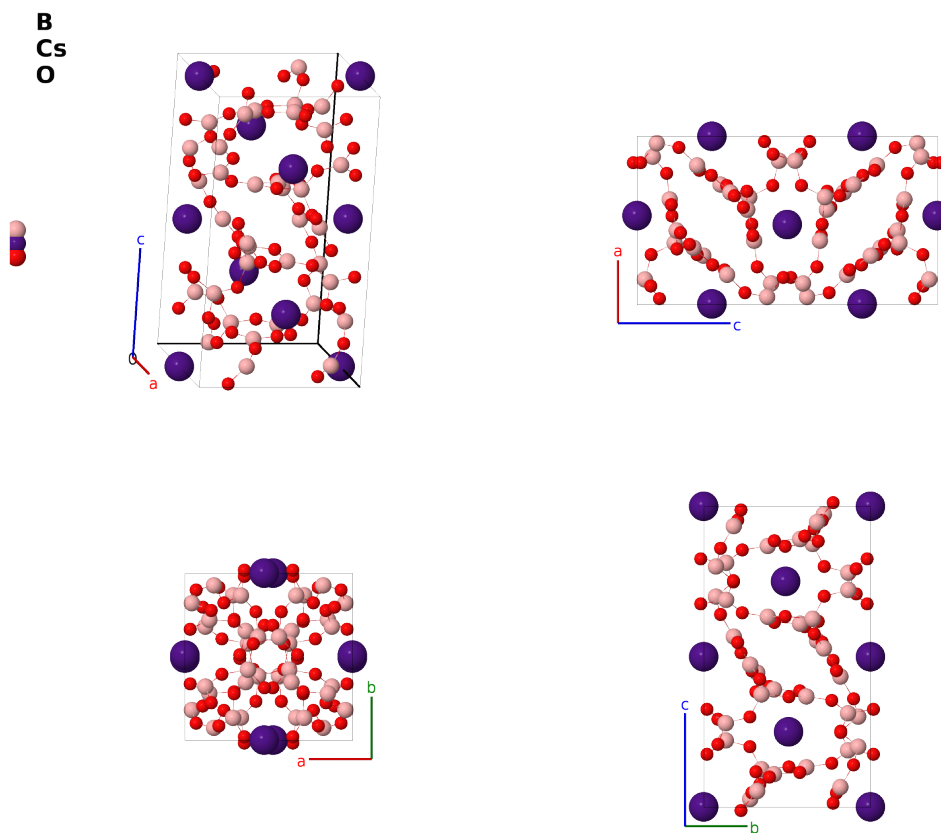
A9BC14_oP96_17_9e_ac_14e-001

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- 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/GTF0>

https://aflow.org/prototype-encyclopedia/A9BC14_oP96_17_9e_ac_14e-001



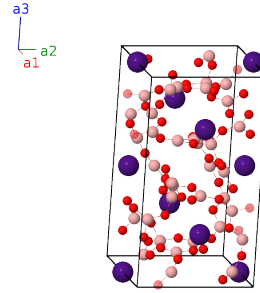
Prototype	B ₉ CsO ₁₄
AFLOW prototype label	A9BC14_oP96_17_9e_ac_14e-001
ICSD	99793
CCDC	1659006
Pearson symbol	oP96
Space group number	17
Space group symbol	$P222_1$

AFLOW prototype command `aflow --proto=A9BC14_oP96_17_9e_ac_14e-001`
 `--params=a, b/a, c/a, x1, y2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18, y18, z18, x19, y19, z19, x20, y20, z20, x21, y21, z21, x22, y22, z22, x23, y23, z23, x24, y24, z24, x25, y25, z25`

- (Wright, 2003) call this Cs₂0.9B₂O₃. The ICSD labels the structure as Cs₂O(B₂O₃)₉.
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Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1$	$=$	$ax_1 \hat{\mathbf{x}}$	(2a)	Cs I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2a)	Cs I
$\mathbf{B}_3$	$= y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Cs II
$\mathbf{B}_4$	$= -y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Cs II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B}_7$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B}_8$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4e)	B II
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	B II
$\mathbf{B}_{11}$	$= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	B II
$\mathbf{B}_{12}$	$= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4e)	B II
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4e)	B III
$\mathbf{B}_{14}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	B III
$\mathbf{B}_{15}$	$= -x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	B III
$\mathbf{B}_{16}$	$= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4e)	B III
$\mathbf{B}_{17}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4e)	B IV
$\mathbf{B}_{18}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	B IV
$\mathbf{B}_{19}$	$= -x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	B IV
$\mathbf{B}_{20}$	$= x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4e)	B IV
$\mathbf{B}_{21}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4e)	B V

$\mathbf{B}_{63} =$	$-x_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 - (z_{17} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{17} \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} - c(z_{17} - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O VI
$\mathbf{B}_{64} =$	$x_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 - z_{17} \mathbf{a}_3$	$=$	$ax_{17} \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} - cz_{17} \hat{\mathbf{z}}$	(4e)	O VI
$\mathbf{B}_{65} =$	$x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$ax_{18} \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B}_{66} =$	$-x_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 + (z_{18} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{18} \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B}_{67} =$	$-x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 - (z_{18} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{18} \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} - c(z_{18} - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B}_{68} =$	$x_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 - z_{18} \mathbf{a}_3$	$=$	$ax_{18} \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} - cz_{18} \hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B}_{69} =$	$x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3$	$=$	$ax_{19} \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}}$	(4e)	O VIII
$\mathbf{B}_{70} =$	$-x_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 + (z_{19} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{19} \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} + c(z_{19} + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O VIII
$\mathbf{B}_{71} =$	$-x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 - (z_{19} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{19} \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} - c(z_{19} - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O VIII
$\mathbf{B}_{72} =$	$x_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 - z_{19} \mathbf{a}_3$	$=$	$ax_{19} \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}}$	(4e)	O VIII
$\mathbf{B}_{73} =$	$x_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3$	$=$	$ax_{20} \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}}$	(4e)	O IX
$\mathbf{B}_{74} =$	$-x_{20} \mathbf{a}_1 - y_{20} \mathbf{a}_2 + (z_{20} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{20} \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} + c(z_{20} + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O IX
$\mathbf{B}_{75} =$	$-x_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 - (z_{20} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{20} \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} - c(z_{20} - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O IX
$\mathbf{B}_{76} =$	$x_{20} \mathbf{a}_1 - y_{20} \mathbf{a}_2 - z_{20} \mathbf{a}_3$	$=$	$ax_{20} \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} - cz_{20} \hat{\mathbf{z}}$	(4e)	O IX
$\mathbf{B}_{77} =$	$x_{21} \mathbf{a}_1 + y_{21} \mathbf{a}_2 + z_{21} \mathbf{a}_3$	$=$	$ax_{21} \hat{\mathbf{x}} + by_{21} \hat{\mathbf{y}} + cz_{21} \hat{\mathbf{z}}$	(4e)	O X
$\mathbf{B}_{78} =$	$-x_{21} \mathbf{a}_1 - y_{21} \mathbf{a}_2 + (z_{21} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{21} \hat{\mathbf{x}} - by_{21} \hat{\mathbf{y}} + c(z_{21} + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O X
$\mathbf{B}_{79} =$	$-x_{21} \mathbf{a}_1 + y_{21} \mathbf{a}_2 - (z_{21} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{21} \hat{\mathbf{x}} + by_{21} \hat{\mathbf{y}} - c(z_{21} - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O X
$\mathbf{B}_{80} =$	$x_{21} \mathbf{a}_1 - y_{21} \mathbf{a}_2 - z_{21} \mathbf{a}_3$	$=$	$ax_{21} \hat{\mathbf{x}} - by_{21} \hat{\mathbf{y}} - cz_{21} \hat{\mathbf{z}}$	(4e)	O X
$\mathbf{B}_{81} =$	$x_{22} \mathbf{a}_1 + y_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3$	$=$	$ax_{22} \hat{\mathbf{x}} + by_{22} \hat{\mathbf{y}} + cz_{22} \hat{\mathbf{z}}$	(4e)	O XI
$\mathbf{B}_{82} =$	$-x_{22} \mathbf{a}_1 - y_{22} \mathbf{a}_2 + (z_{22} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{22} \hat{\mathbf{x}} - by_{22} \hat{\mathbf{y}} + c(z_{22} + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O XI
$\mathbf{B}_{83} =$	$-x_{22} \mathbf{a}_1 + y_{22} \mathbf{a}_2 - (z_{22} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{22} \hat{\mathbf{x}} + by_{22} \hat{\mathbf{y}} - c(z_{22} - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O XI
$\mathbf{B}_{84} =$	$x_{22} \mathbf{a}_1 - y_{22} \mathbf{a}_2 - z_{22} \mathbf{a}_3$	$=$	$ax_{22} \hat{\mathbf{x}} - by_{22} \hat{\mathbf{y}} - cz_{22} \hat{\mathbf{z}}$	(4e)	O XI
$\mathbf{B}_{85} =$	$x_{23} \mathbf{a}_1 + y_{23} \mathbf{a}_2 + z_{23} \mathbf{a}_3$	$=$	$ax_{23} \hat{\mathbf{x}} + by_{23} \hat{\mathbf{y}} + cz_{23} \hat{\mathbf{z}}$	(4e)	O XII
$\mathbf{B}_{86} =$	$-x_{23} \mathbf{a}_1 - y_{23} \mathbf{a}_2 + (z_{23} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{23} \hat{\mathbf{x}} - by_{23} \hat{\mathbf{y}} + c(z_{23} + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O XII
$\mathbf{B}_{87} =$	$-x_{23} \mathbf{a}_1 + y_{23} \mathbf{a}_2 - (z_{23} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{23} \hat{\mathbf{x}} + by_{23} \hat{\mathbf{y}} - c(z_{23} - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O XII
$\mathbf{B}_{88} =$	$x_{23} \mathbf{a}_1 - y_{23} \mathbf{a}_2 - z_{23} \mathbf{a}_3$	$=$	$ax_{23} \hat{\mathbf{x}} - by_{23} \hat{\mathbf{y}} - cz_{23} \hat{\mathbf{z}}$	(4e)	O XII
$\mathbf{B}_{89} =$	$x_{24} \mathbf{a}_1 + y_{24} \mathbf{a}_2 + z_{24} \mathbf{a}_3$	$=$	$ax_{24} \hat{\mathbf{x}} + by_{24} \hat{\mathbf{y}} + cz_{24} \hat{\mathbf{z}}$	(4e)	O XIII
$\mathbf{B}_{90} =$	$-x_{24} \mathbf{a}_1 - y_{24} \mathbf{a}_2 + (z_{24} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{24} \hat{\mathbf{x}} - by_{24} \hat{\mathbf{y}} + c(z_{24} + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O XIII
$\mathbf{B}_{91} =$	$-x_{24} \mathbf{a}_1 + y_{24} \mathbf{a}_2 - (z_{24} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{24} \hat{\mathbf{x}} + by_{24} \hat{\mathbf{y}} - c(z_{24} - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O XIII
$\mathbf{B}_{92} =$	$x_{24} \mathbf{a}_1 - y_{24} \mathbf{a}_2 - z_{24} \mathbf{a}_3$	$=$	$ax_{24} \hat{\mathbf{x}} - by_{24} \hat{\mathbf{y}} - cz_{24} \hat{\mathbf{z}}$	(4e)	O XIII
$\mathbf{B}_{93} =$	$x_{25} \mathbf{a}_1 + y_{25} \mathbf{a}_2 + z_{25} \mathbf{a}_3$	$=$	$ax_{25} \hat{\mathbf{x}} + by_{25} \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}}$	(4e)	O XIV
$\mathbf{B}_{94} =$	$-x_{25} \mathbf{a}_1 - y_{25} \mathbf{a}_2 + (z_{25} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{25} \hat{\mathbf{x}} - by_{25} \hat{\mathbf{y}} + c(z_{25} + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O XIV
$\mathbf{B}_{95} =$	$-x_{25} \mathbf{a}_1 + y_{25} \mathbf{a}_2 - (z_{25} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{25} \hat{\mathbf{x}} + by_{25} \hat{\mathbf{y}} - c(z_{25} - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O XIV
$\mathbf{B}_{96} =$	$x_{25} \mathbf{a}_1 - y_{25} \mathbf{a}_2 - z_{25} \mathbf{a}_3$	$=$	$ax_{25} \hat{\mathbf{x}} - by_{25} \hat{\mathbf{y}} - cz_{25} \hat{\mathbf{z}}$	(4e)	O XIV

References

- [1] A. C. Wright, R. N. Sinclair, C. E. Stone, K. S. Knight, I. G. Polyakova, N. M. Vedishcheva, and B. A. Shakhmatkin, *Structure of crystalline caesium enneaborate*, Phys. Chem. Glasses **44**, 197–202 (2003).

Found in

- [1] F. Hoffmann, *The Fascination of Crystals and Symmetry* (2015). 230 – The Space Group List Project.

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