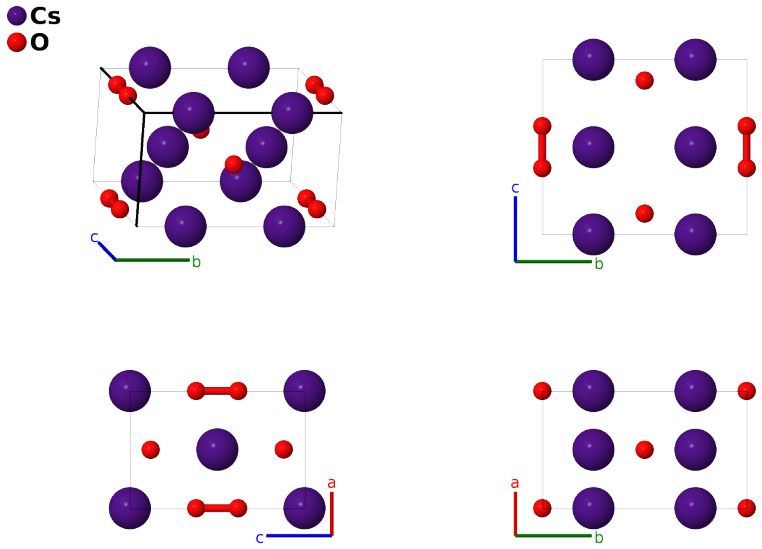
CsO Structure: AB_oI8_71_e_g-001

This structure originally had the label `AB_oI8_71_g_i`. Calls to that address will be redirected here.

Cite this page as: 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/p/2UZJ

https://aflow.org/p/AB_oI8_71_e_g-001

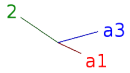


Prototype	CsO
AFLOW prototype label	AB_oI8_71_e_g-001
ICSD	25529
Pearson symbol	oI8
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	`aflow --proto=AB_oI8_71_e_g-001 --params=`$a, b/a, c/a, x_1, y_2$

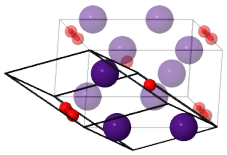
Other compounds with this structure
RbO, NaC

- (Massaliski, 1990) credits the discovery of this structure to (Rengade, 1909), but we have been unable to obtain a copy of this reference. (Downs, 2003) quotes (Wyckoff, 1963) giving an $Immm - oI8$ structure for CsO. Since this is the same space group and Pearson symbol as found in Massaliski we use Wyckoff's data.
- In the absence of the original article, we provide the ICSD link to the work of (Föppl, 1957).

Body-centered Orthorhombic primitive vectors



$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}}$	(4e)	Cs I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}}$	(4e)	Cs I
$\mathbf{B_3}$	=	$y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_4}$	=	$-y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}}$	(4g)	O I

References

[1] M. E. Rengade, , Compt. Rend. **148**, 1199–1202 (1909).

[2] H. Föppl, *Die Kristallstrukturen der Alkaliperoxyde*, Z. Anorganische und Allgemeine Chemie **291**, 12–50 (1957), doi:10.1002/zaac.19572910104.

Found in

[1] T. B. Massalski, H. Okamoto, P. R. Subramanian, and L. Kacprzak, eds., *Binary Alloy Phase Diagrams*, vol. 2 (ASM International, Materials Park, Ohio, USA, 1990), 2^{nd} edn. Cd-Ce to Hf-Rb.

[2] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

[3] R. W. G. Wyckoff, *Crystal Structures*, vol. 1 (Interscience Publishers, New York, 1963), second edn.