

CsO Structure:

AB_oI8_71_e_g-001

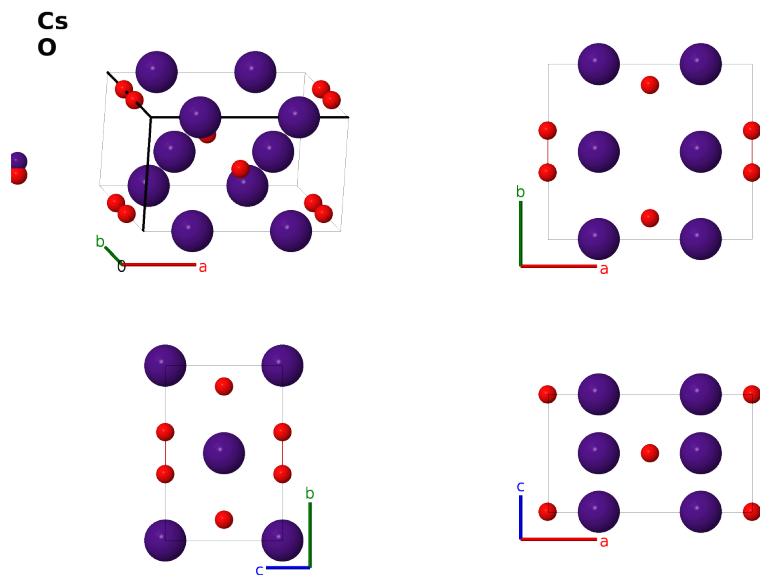
This structure previously used the label(s) **AB_oI8_71_g_i**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/2UZJ>

https://aflow.org/prototype-encyclopedia/AB_oI8_71_e_g-001



Prototype	CsO
AFLOW prototype label	AB_oI8_71_e_g-001
ICSD	25529
CCDC	1601183
Pearson symbol	oI8
Space group number	71
Space group symbol	<i>Immm</i>
AFLOW prototype command	<code>aflow --proto=AB_oI8_71_e_g-001</code> <code>--params=a,b/a,c/a,x₁,y₂</code>

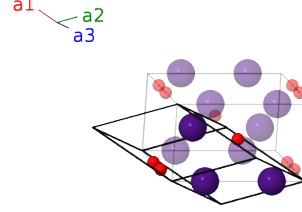
Other compounds with this structure

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

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



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), 2nd 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.

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