Cs_7O Structure: A7B_hP24_187_ah2j2kn_j-001

This structure originally had the label `A7B_hP24_187_ai2j2kn_j`. Calls to that address will be redirected here.

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https://aflow.org/p/BZC9

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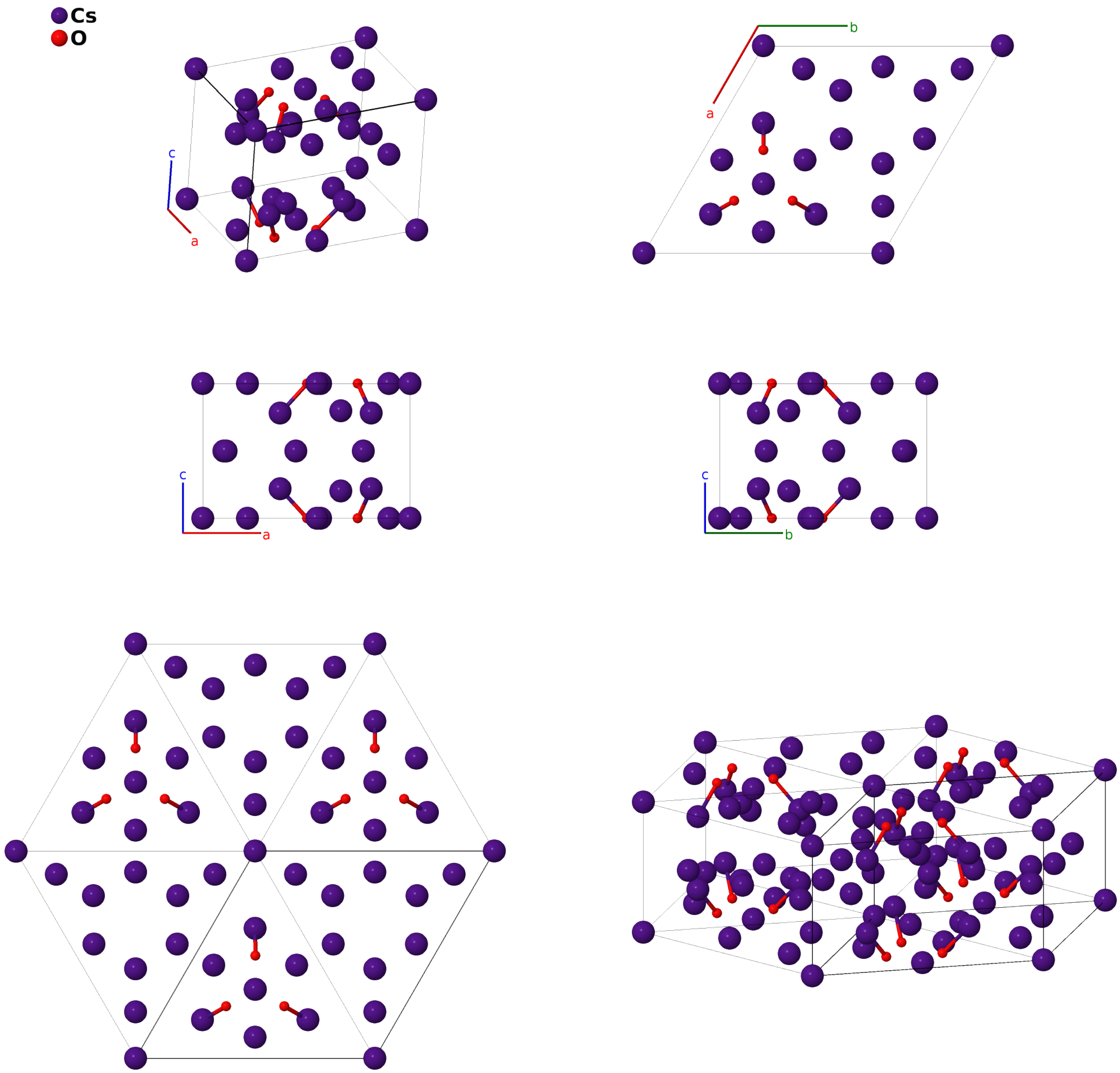


Prototype Cs_7O

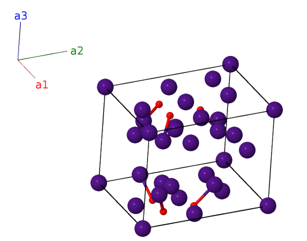
AFLOW prototype label A7B_hP24_187_ah2j2kn_j-001

ICSD	111
Pearson symbol	hP24
Space group number	187
Space group symbol	$P\bar{6}m2$
AFLOW prototype command	`aflow --proto=A7B_hP24_187_ah2j2kn_j-001` `--params=`$a, c/a, z_2, x_3, x_4, x_5, x_6, x_7, x_8, z_8$

- This structure is composed of $Cs_{11}O_3$ molecules, similar to the building blocks of the $Cs_{11}O_3$ structure, interlaced with cesium atoms which have approximately the same spacing as in bcc-Cs.
- Lattice constant data was given at -150°C, while the atomic positions were given at -175°C.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Cs I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2h)	Cs II
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2h)	Cs II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-\sqrt{3}ax_3\,\hat{\mathbf{y}}$	(3j)	Cs III
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3j)	Cs III
$\mathbf{B_6}$	=	$-2x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3j)	Cs III
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-\sqrt{3}ax_4\,\hat{\mathbf{y}}$	(3j)	Cs IV
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$	(3j)	Cs IV
$\mathbf{B_9}$	=	$-2x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$	(3j)	Cs IV
$\mathbf{B_{10}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$-\sqrt{3}ax_5\,\hat{\mathbf{y}}$	(3j)	O I
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_1 + 2x_5\,\mathbf{a}_2$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}$	(3j)	O I
$\mathbf{B_{12}}$	=	$-2x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}$	(3j)	O I
$\mathbf{B_{13}}$	=	$x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	Cs V
$\mathbf{B_{14}}$	=	$x_6\,\mathbf{a}_1 + 2x_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	Cs V
$\mathbf{B_{15}}$	=	$-2x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	Cs V
$\mathbf{B_{16}}$	=	$x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_7\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	Cs VI
$\mathbf{B_{17}}$	=	$x_7\,\mathbf{a}_1 + 2x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_7\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	Cs VI
$\mathbf{B_{18}}$	=	$-2x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_7\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	Cs VI
$\mathbf{B_{19}}$	=	$x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-\sqrt{3}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(6n)	Cs VII

$\mathbf{B_{20}}$	=	$x_8\,\mathbf{a}_1 + 2x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{3}{2}ax_8\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(6n)	Cs VII
$\mathbf{B_{21}}$	=	$-2x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_8\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(6n)	Cs VII
$\mathbf{B_{22}}$	=	$x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\sqrt{3}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(6n)	Cs VII
$\mathbf{B_{23}}$	=	$x_8\,\mathbf{a}_1 + 2x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$\frac{3}{2}ax_8\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(6n)	Cs VII
$\mathbf{B_{24}}$	=	$-2x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_8\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(6n)	Cs VII

References

[1] A. Simon, *Über Alkalimetall-Suboxide. VII. Das metallreichste Cäsiumoxid—Cs_7O*, Z. Anorganische und Allgemeine Chemie **422**, 208–218 (1976), doi:10.1002/zaac.19764220303.

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.