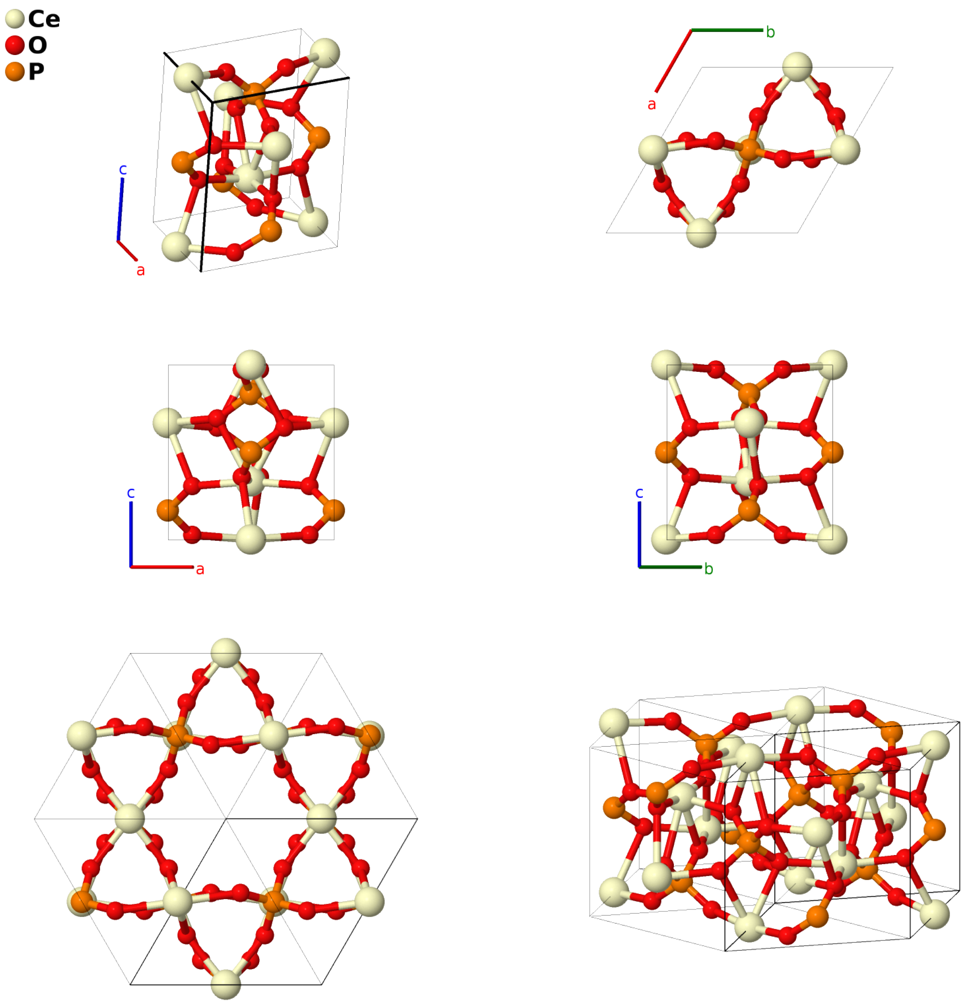
Rhadophane ($CePO_4$) Structure: AB4C_hP18_180_c_k_d-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

---

https://aflow.org/p/QL18

https://aflow.org/p/AB4C_hP18_180_c_k_d-001



Prototype CeO_4P

AFLOW prototype label AB4C_hP18_180_c_k_d-001

Mineral name rhadophane

ICSD 31563

Pearson symbol hP18

Space group number 180

Space group symbol $P6_222$

AFLOW prototype command `aflow --proto=AB4C_hP18_180_c_k_d-001`
`--params=`$a, c/a, x_3, y_3, z_3$

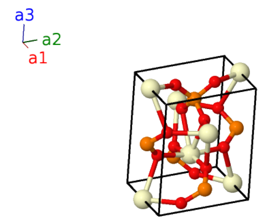
Other compounds with this structure

$LaPO_4$, $NdPO_4$

- This structure can also be found in the enantiomorphic space group $P6_422$ #181.

Hexagonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3c)	Ce I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{2}{3}c\,\hat{\mathbf{z}}$	(3c)	Ce I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(3c)	Ce I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3d)	P I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{6}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	P I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{5}{6}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{5}{6}c\,\hat{\mathbf{z}}$	(3d)	P I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_8}$	=	$-y_3\,\mathbf{a}_1 + (x_3-y_3)\,\mathbf{a}_2 + \left(z_3+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3-2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_3+2)\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_9}$	=	$-(x_3-y_3)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(z_3+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{11}}$	=	$y_3\,\mathbf{a}_1 - (x_3-y_3)\,\mathbf{a}_2 + \left(z_3+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_3+2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_3+2)\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{12}}$	=	$(x_3-y_3)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{13}}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(z_3-\frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_3-2)\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{14}}$	=	$(x_3-y_3)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3-2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{15}}$	=	$-x_3\,\mathbf{a}_1 - (x_3-y_3)\,\mathbf{a}_2 - \left(z_3-\frac{1}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - c\left(z_3-\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{16}}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(z_3-\frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_3-2)\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{17}}$	=	$-(x_3-y_3)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_3+2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{18}}$	=	$x_3\,\mathbf{a}_1 + (x_3-y_3)\,\mathbf{a}_2 - \left(z_3-\frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - c\left(z_3-\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(12k)	O I

References

[1] R. C. L. Mooney, *X-ray diffraction study of cerous phosphate and related crystals. I. Hexagonal modification*, Acta Cryst. **3**, 337–340 (1950), doi:10.1107/S0365110X50000963.

Found in

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