

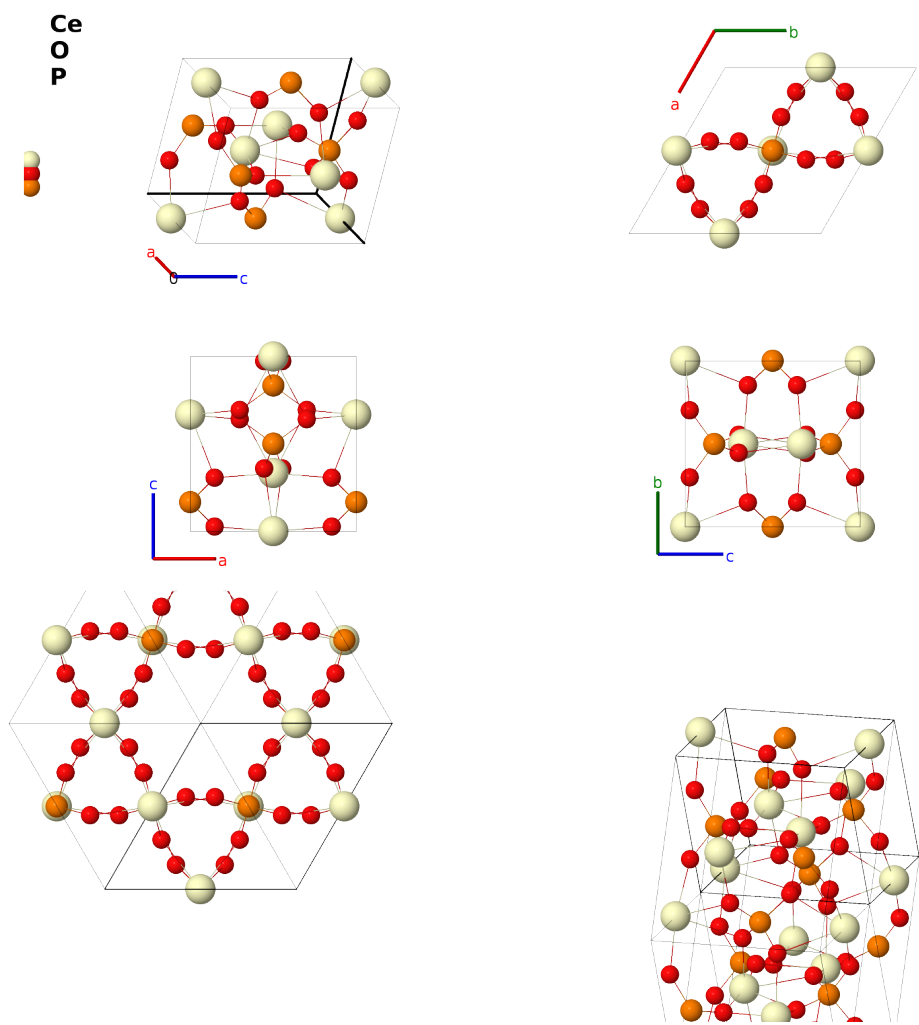
Rhadophane (CePO₄) Structure: AB4C_hP18_180_c_k_d-001

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<https://aflow.org/prototype-encyclopedia/QL18>

https://aflow.org/prototype-encyclopedia/AB4C_hP18_180_c_k_d-001



Prototype	CeO ₄ P
AFLOW prototype label	AB4C_hP18_180_c_k_d-001
Mineral name	rhadophane
ICSD	31563
CCDC	1605580
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= $a, c/a, x_3, y_3, z_3$

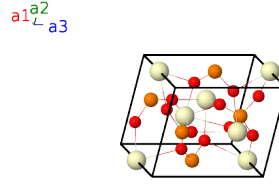
Other compounds with this structure

LaPO₄, NdPO₄

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

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \hat{\mathbf{z}}
\end{aligned}$$



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
$\mathbf{B}_8$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{3}c (3z_3 + 2) \hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B}_9$	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{11}$	$= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{3}c (3z_3 + 2) \hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B}_{12}$	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B}_{13}$	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - (z_3 - \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} - \frac{1}{3}c (3z_3 - 2) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{15}$	$= -x_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - c (z_3 - \frac{1}{3}) \hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B}_{16}$	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} - \frac{1}{3}c (3z_3 - 2) \hat{\mathbf{z}}$	(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

$$\mathbf{B}_{18} = x_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 - \left(z_3 - \frac{1}{3}\right) \mathbf{a}_3 = \frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{3}\right) \hat{\mathbf{z}} \quad (12k) \quad \text{O I}$$

References

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Found in

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

First cited in

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