

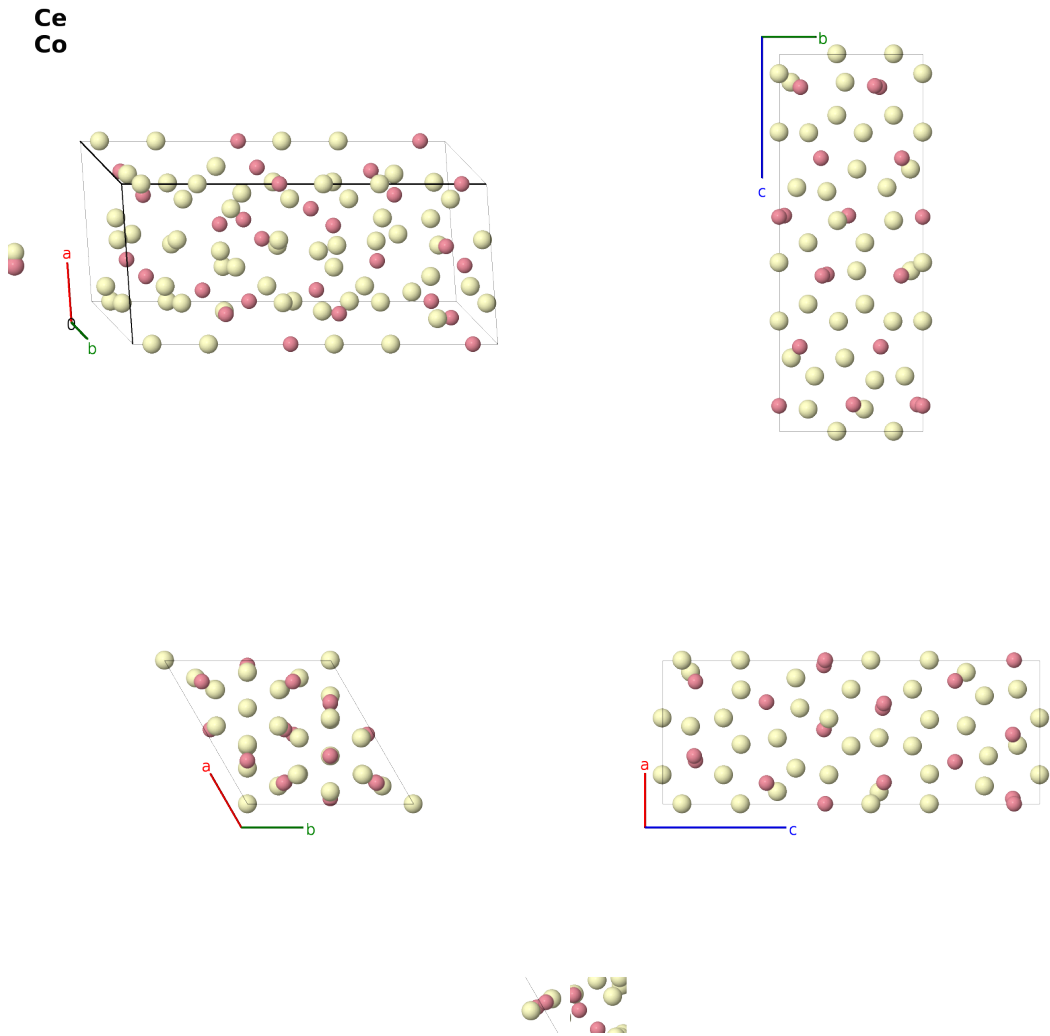
Ce₂₄Co₁₁ Structure: A24B11_hP70_186_2ab7c_ab3c-001

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<https://aflow.org/prototype-encyclopedia/D6S6>

https://aflow.org/prototype-encyclopedia/A24B11_hP70_186_2ab7c_ab3c-001



Prototype	Ce ₂₄ Co ₁₁
AFLOW prototype label	A24B11_hP70_186_2ab7c_ab3c-001
ICSD	102101
CCDC	1660090
Pearson symbol	hP70
Space group number	186

Space group symbol	$P6_3mc$
AFLOW prototype command	aflow --proto=A24B11_hP70_186_2ab7c_ab3c-001 --params= $a, c/a, z_1, z_2, z_3, z_4, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}, x_{12}, z_{12}, x_{13}, z_{13}, x_{14}, z_{14}, x_{15}, z_{15}$

Other compounds with this structure

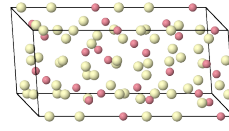
$\text{La}_{24}\text{Ru}_{11}$, $\text{Nd}_{24}\text{Co}_{11}$

- Space group $P6_3mc$ #186 allows an arbitrary placement of the origin of the z -axis. Here we set $z_6 = 0$.

Hexagonal primitive vectors

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

$\mathbf{a}_1$
 $\mathbf{a}_2$
 $\mathbf{a}_3$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Ce I
$\mathbf{B}_2$	$= \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	Ce I
$\mathbf{B}_3$	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(2a)	Ce II
$\mathbf{B}_4$	$= \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	Ce II
$\mathbf{B}_5$	$= z_3 \mathbf{a}_3$	$=$	$c z_3 \hat{\mathbf{z}}$	(2a)	Co I
$\mathbf{B}_6$	$= \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	Co I
$\mathbf{B}_7$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(2b)	Ce III
$\mathbf{B}_8$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2b)	Ce III
$\mathbf{B}_9$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(2b)	Co II
$\mathbf{B}_{10}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2b)	Co II
$\mathbf{B}_{11}$	$= x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-\sqrt{3}a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6c)	Ce IV
$\mathbf{B}_{12}$	$= x_6 \mathbf{a}_1 + 2x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{3}{2}a x_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6c)	Ce IV
$\mathbf{B}_{13}$	$= -2x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-\frac{3}{2}a x_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6c)	Ce IV
$\mathbf{B}_{14}$	$= -x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\sqrt{3}a x_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Ce IV
$\mathbf{B}_{15}$	$= -x_6 \mathbf{a}_1 - 2x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{3}{2}a x_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Ce IV
$\mathbf{B}_{16}$	$= 2x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{3}{2}a x_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Ce IV
$\mathbf{B}_{17}$	$= x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-\sqrt{3}a x_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(6c)	Ce V
$\mathbf{B}_{18}$	$= x_7 \mathbf{a}_1 + 2x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{3}{2}a x_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(6c)	Ce V
$\mathbf{B}_{19}$	$= -2x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-\frac{3}{2}a x_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(6c)	Ce V

$$\begin{aligned}
\mathbf{B}_{61} &= -2x_{14} \mathbf{a}_1 - x_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3 &= -\frac{3}{2}ax_{14} \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} &(6c) &\text{Co IV} \\
\mathbf{B}_{62} &= -x_{14} \mathbf{a}_1 + x_{14} \mathbf{a}_2 + \left(z_{14} + \frac{1}{2}\right) \mathbf{a}_3 &= \sqrt{3}ax_{14} \hat{\mathbf{y}} + c\left(z_{14} + \frac{1}{2}\right) \hat{\mathbf{z}} &(6c) &\text{Co IV} \\
\mathbf{B}_{63} &= -x_{14} \mathbf{a}_1 - 2x_{14} \mathbf{a}_2 + \left(z_{14} + \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{3}{2}ax_{14} \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{14} \hat{\mathbf{y}} + c\left(z_{14} + \frac{1}{2}\right) \hat{\mathbf{z}} &(6c) &\text{Co IV} \\
\mathbf{B}_{64} &= 2x_{14} \mathbf{a}_1 + x_{14} \mathbf{a}_2 + \left(z_{14} + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_{14} \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{14} \hat{\mathbf{y}} + c\left(z_{14} + \frac{1}{2}\right) \hat{\mathbf{z}} &(6c) &\text{Co IV} \\
\mathbf{B}_{65} &= x_{15} \mathbf{a}_1 - x_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 &= -\sqrt{3}ax_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} &(6c) &\text{Co V} \\
\mathbf{B}_{66} &= x_{15} \mathbf{a}_1 + 2x_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 &= \frac{3}{2}ax_{15} \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} &(6c) &\text{Co V} \\
\mathbf{B}_{67} &= -2x_{15} \mathbf{a}_1 - x_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 &= -\frac{3}{2}ax_{15} \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} &(6c) &\text{Co V} \\
\mathbf{B}_{68} &= -x_{15} \mathbf{a}_1 + x_{15} \mathbf{a}_2 + \left(z_{15} + \frac{1}{2}\right) \mathbf{a}_3 &= \sqrt{3}ax_{15} \hat{\mathbf{y}} + c\left(z_{15} + \frac{1}{2}\right) \hat{\mathbf{z}} &(6c) &\text{Co V} \\
\mathbf{B}_{69} &= -x_{15} \mathbf{a}_1 - 2x_{15} \mathbf{a}_2 + \left(z_{15} + \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{3}{2}ax_{15} \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{15} \hat{\mathbf{y}} + c\left(z_{15} + \frac{1}{2}\right) \hat{\mathbf{z}} &(6c) &\text{Co V} \\
\mathbf{B}_{70} &= 2x_{15} \mathbf{a}_1 + x_{15} \mathbf{a}_2 + \left(z_{15} + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_{15} \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{15} \hat{\mathbf{y}} + c\left(z_{15} + \frac{1}{2}\right) \hat{\mathbf{z}} &(6c) &\text{Co V}
\end{aligned}$$

References

- [1] A. C. Larson and D. T. Cromer, *The crystal structure of $Ce_{24}Co_{11}$* , Acta Cryst. **15**, 1224–1227 (1962), doi:10.1107/S0365110X62003254.

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