

CeCo₄B₄ Structure: A4BC4_tP18_137_g_a_g-001

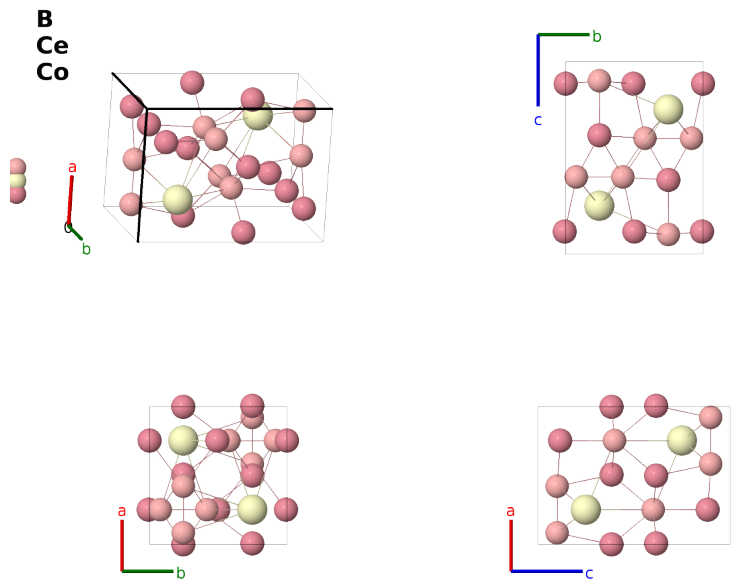
This structure previously used the label(s) **A4BC4_tP18_137_g_b_g**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A4BC4_tP18_137_g_a_g-001

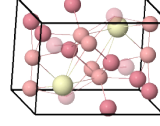


Prototype	B ₄ CeCo ₄
AFLOW prototype label	A4BC4_tP18_137_g_a_g-001
ICSD	654433
CCDC	1765753
Pearson symbol	tP18
Space group number	137
Space group symbol	$P4_2/nmc$
AFLOW prototype command	<pre>aflow --proto=A4BC4_tP18_137_g_a_g-001 --params=a, c/a, y₂, z₂, y₃, z₃</pre>

Simple Tetragonal primitive vectors

a₁
a₂
a₃

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2a)	Ce I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2a)	Ce I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + a y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8g)	B I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - a (y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8g)	B I
$\mathbf{B}_5$	$= -(y_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	B I
$\mathbf{B}_6$	$= y_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a y_2 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	B I
$\mathbf{B}_7$	$= \frac{3}{4} \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + a (y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8g)	B I
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - a y_2 \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8g)	B I
$\mathbf{B}_9$	$= (y_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c (z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	B I
$\mathbf{B}_{10}$	$= -y_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a y_2 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c (z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	B I
$\mathbf{B}_{11}$	$= \frac{1}{4} \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8g)	Co I
$\mathbf{B}_{12}$	$= \frac{1}{4} \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - a (y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8g)	Co I
$\mathbf{B}_{13}$	$= -(y_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Co I
$\mathbf{B}_{14}$	$= y_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a y_3 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Co I
$\mathbf{B}_{15}$	$= \frac{3}{4} \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + a (y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8g)	Co I
$\mathbf{B}_{16}$	$= \frac{3}{4} \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8g)	Co I
$\mathbf{B}_{17}$	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Co I
$\mathbf{B}_{18}$	$= -y_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a y_3 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Co I

References

- [1] Y. B. Kuzma and N. S. Bilonizhko, *Crystal structure of the compounds CeCo₄B₄ and its analogs*, Sov. Phys. Crystallogr. **16**, 897–898 (1972).

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

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