

Ce₅Mo₃O₁₆ Structure: A5B3C16_cP96_222_ce_d-fi-001

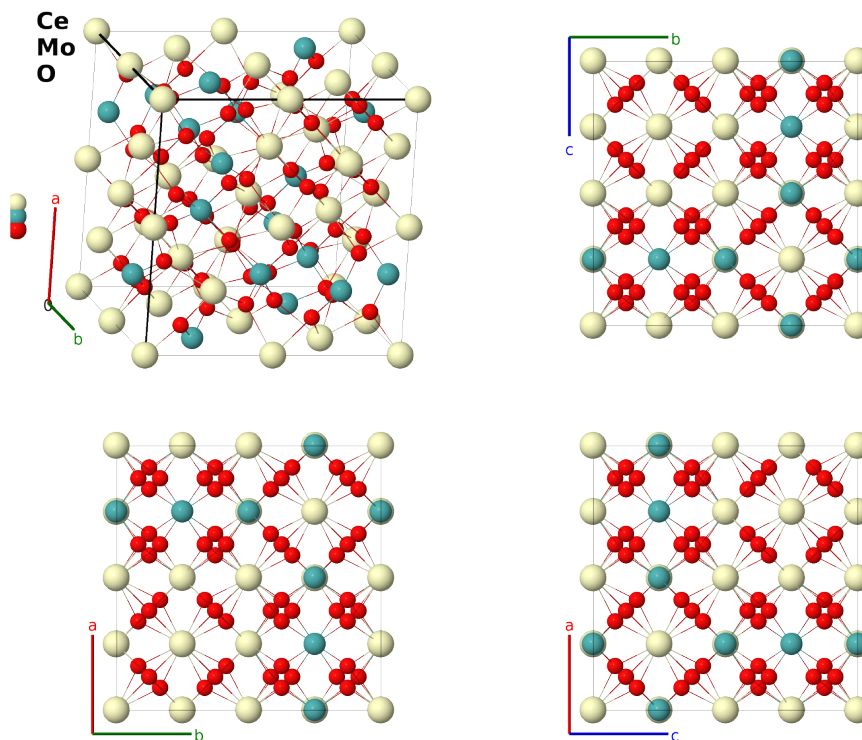
This structure previously used the label(s) **A5B3C16_cP96_222_ce_d-fi**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/3NUA>

https://aflow.org/prototype-encyclopedia/A5B3C16_cP96_222_ce_d-fi-001



Prototype	Ce ₅ Mo ₃ O ₁₆
AFLOW prototype label	A5B3C16_cP96_222_ce_d-fi-001
Pearson symbol	cP96
Space group number	222
Space group symbol	$Pn\bar{3}n$
AFLOW prototype command	<code>aflow --proto=A5B3C16_cP96_222_ce_d-fi-001 --params=a, x₃, x₄, x₅, y₅, z₅</code>

Other compounds with this structure

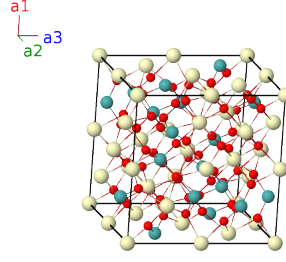
CdTm₄MoO₃O₁₆, CdY₄Mo₃O₁₆, La₅Mo₃O₁₆, Nd₅Mo₃O₁₆, Nd₄SmMo₃O₁₆, Pr₅Mo₃O₁₆

Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(8c) Ce I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(8c) Ce I
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(8c) Ce I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(8c) Ce I
$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{z}}$	(8c) Ce I
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(8c) Ce I
$\mathbf{B}_7$	$=$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(8c) Ce I
$\mathbf{B}_8$	$=$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(8c) Ce I
$\mathbf{B}_9$	$=$	$\frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12d) Mo I
$\mathbf{B}_{10}$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12d) Mo I
$\mathbf{B}_{11}$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{z}}$	(12d) Mo I
$\mathbf{B}_{12}$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(12d) Mo I
$\mathbf{B}_{13}$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(12d) Mo I
$\mathbf{B}_{14}$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12d) Mo I
$\mathbf{B}_{15}$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12d) Mo I
$\mathbf{B}_{16}$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12d) Mo I
$\mathbf{B}_{17}$	$=$	$\frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(12d) Mo I
$\mathbf{B}_{18}$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(12d) Mo I
$\mathbf{B}_{19}$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12d) Mo I
$\mathbf{B}_{20}$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(12d) Mo I
$\mathbf{B}_{21}$	$=$	$x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12e) Ce II
$\mathbf{B}_{22}$	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12e) Ce II
$\mathbf{B}_{23}$	$=$	$\frac{1}{4} \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12e) Ce II
$\mathbf{B}_{24}$	$=$	$\frac{1}{4} \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12e) Ce II
$\mathbf{B}_{25}$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + a x_3 \hat{\mathbf{z}}$	(12e) Ce II
$\mathbf{B}_{26}$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(12e) Ce II
$\mathbf{B}_{27}$	$=$	$-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(12e) Ce II
$\mathbf{B}_{28}$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(12e) Ce II

$$\mathbf{B}_{96} = \begin{pmatrix} z_5 + \frac{1}{2} \\ y_5 + \frac{1}{2} \\ x_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_5 + \frac{1}{2} \\ x_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \\ y_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 = a \begin{pmatrix} z_5 + \frac{1}{2} \\ y_5 + \frac{1}{2} \\ x_5 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} y_5 + \frac{1}{2} \\ x_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + a \begin{pmatrix} x_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \\ y_5 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} \quad (48i) \quad \text{O II}$$

References

- [1] P.-H. Hubert, *Contribution à l'étude des molybdites des terres rares: II. Molybdites cubiques $Pn\bar{3}n$* , Bull. Soc. Chim. Fr. pp. 475–477 (1975).

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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