

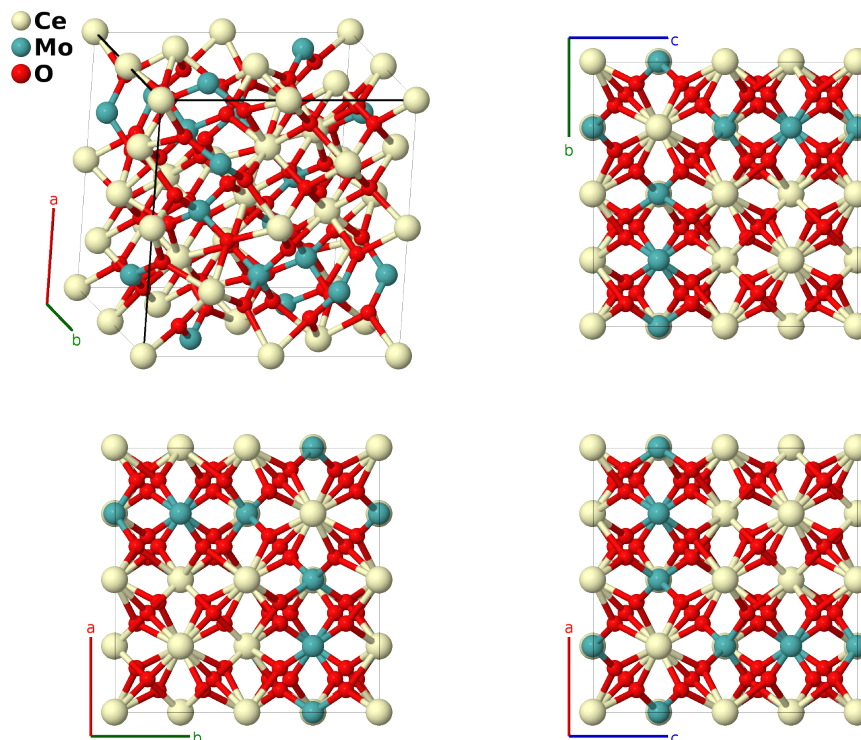
Ce₅Mo₃O₁₆ Structure: A5B3C16_cP96_222_ce_d_fi-001

This structure originally had the label A5B3C16_cP96_222_ce_d_fi. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

<https://aflow.org/p/3NUA>

https://aflow.org/p/A5B3C16_cP96_222_ce_d_fi-001



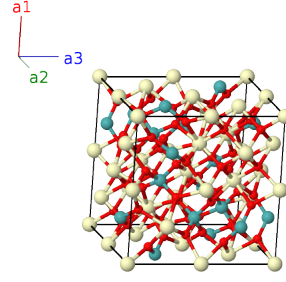
Prototype	Ce ₅ Mo ₃ O ₁₆
AFLOW prototype label	A5B3C16_cP96_222_ce_d_fi-001
ICSD	none
Pearson symbol	cP96
Space group number	222
Space group symbol	$Pn\bar{3}n$
AFLOW prototype command	<code>aflow --proto=A5B3C16_cP96_222_ce_d_fi-001 --params=a, x3, x4, x5, y5, z5</code>

Other compounds with this structure

CdTm₄MoO₃O₁₆, CdY₄Mo₃O₁₆, La₅Mo₃O₁₆, Nd₅Mo₃O₁₆

Simple Cubic primitive vectors

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



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}_{29}	$\frac{3}{4} \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(12e)	Ce II
\mathbf{B}_{30}	$\frac{3}{4} \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + a (x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(12e)	Ce 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.