

Zn₂Mo₃O₈ Structure: A3B8C2_hP26_186_c_ab2c_2b-001

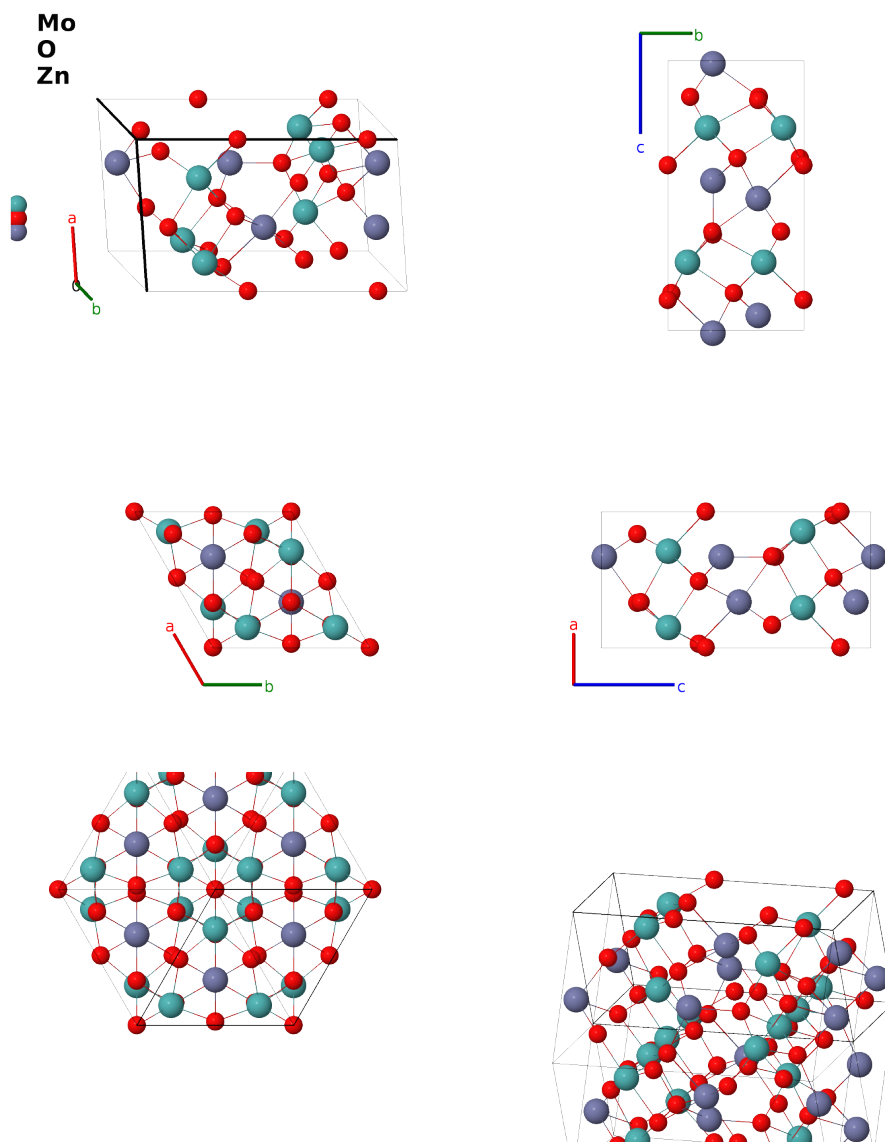
This structure previously used the label(s) **A3B8C2_hP26_186_c_ab2c_2b**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/DG1Q>

https://aflow.org/prototype-encyclopedia/A3B8C2_hP26_186_c_ab2c_2b-001



Prototype

Mo₃O₈Zn₂

AFLOW prototype label

A3B8C2_hP26_186_c_ab2c_2b-001

ICSD

14321

CCDC	1595709
Pearson symbol	hP26
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	aflow --proto=A3B8C2_hP26_186_c_ab2c_2b-001 --params= $a, c/a, z_1, z_2, z_3, z_4, x_5, z_5, x_6, z_6, x_7, z_7$

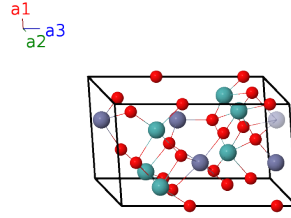
Other compounds with this structure

$\text{Cd}_2\text{Mo}_3\text{O}_8$, $\text{Co}_2\text{Mo}_3\text{O}_8$, $\text{Fe}_2\text{Mo}_3\text{O}_8$ (kamiokite), $\text{Mg}_2\text{Mo}_3\text{O}_8$, $\text{Mn}_2\text{Mo}_3\text{O}_8$, $\text{Ni}_2\text{Mo}_3\text{O}_8$

- Space group $P6_3mc$ #186 does not specify the origin of the z -coordinate. Here we fix it by setting the z -coordinate of the molybdenum atom at $z_5 = 1/4$.

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
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	O 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)	O I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(2b)	Zn I
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2b)	Zn 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)	Zn II
$\mathbf{B}_8$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2b)	Zn II
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\sqrt{3}a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6c)	Mo I
$\mathbf{B}_{10}$	$= x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{3}{2}a x_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6c)	Mo I
$\mathbf{B}_{11}$	$= -2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{3}{2}a x_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6c)	Mo I
$\mathbf{B}_{12}$	$= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\sqrt{3}a x_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Mo I
$\mathbf{B}_{13}$	$= -x_5 \mathbf{a}_1 - 2x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{3}{2}a x_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Mo I
$\mathbf{B}_{14}$	$= 2x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{3}{2}a x_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Mo I
$\mathbf{B}_{15}$	$= x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-\sqrt{3}a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B}_{16}$	$= x_6 \mathbf{a}_1 + 2x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{3}{2}a x_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6c)	O III

$$\begin{aligned}
\mathbf{B}_{17} &= -2x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= -\frac{3}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(6c) &\text{O III} \\
\mathbf{B}_{18} &= -x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= \sqrt{3}ax_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(6c) &\text{O III} \\
\mathbf{B}_{19} &= -x_6 \mathbf{a}_1 - 2x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{3}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(6c) &\text{O III} \\
\mathbf{B}_{20} &= 2x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(6c) &\text{O III} \\
\mathbf{B}_{21} &= x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= -\sqrt{3}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(6c) &\text{O IV} \\
\mathbf{B}_{22} &= x_7 \mathbf{a}_1 + 2x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= \frac{3}{2}ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(6c) &\text{O IV} \\
\mathbf{B}_{23} &= -2x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= -\frac{3}{2}ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(6c) &\text{O IV} \\
\mathbf{B}_{24} &= -x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= \sqrt{3}ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} &(6c) &\text{O IV} \\
\mathbf{B}_{25} &= -x_7 \mathbf{a}_1 - 2x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{3}{2}ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} &(6c) &\text{O IV} \\
\mathbf{B}_{26} &= 2x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} &(6c) &\text{O IV}
\end{aligned}$$

References

- [1] G. B. Ansell and L. Katz, *A Refinement of the Crystal Structure of Zinc Molybdenum(IV) Oxide, $\text{Zn}_2\text{Mo}_3\text{O}_8$* , Acta Cryst. **21**, 482–485 (1966), doi:10.1107/S0365110X66003359.

Found in

- [1] Y. Kanazawa and A. Sasaki, *Structure of Kamiokite*, Acta Crystallogr. Sect. C **42**, 9–11 (1986), doi:10.1107/S0108270186097500.

First cited in

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