

Low Temperature Mo₈O₂₃ Structure: A8B23_mP124_7_16a_46a-001

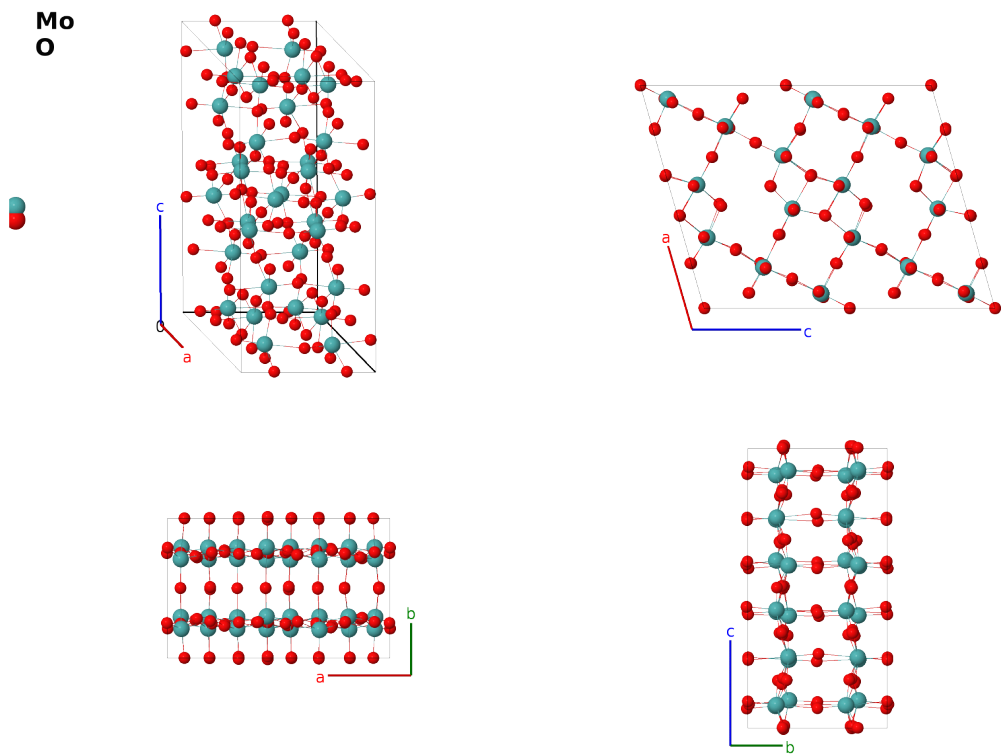
This structure previously used the label(s) **A8B23_mP124_7_16a_46a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/5T76>

https://aflow.org/prototype-encyclopedia/A8B23_mP124_7_16a_46a-001



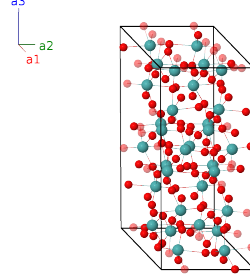
Prototype	Mo ₈ O ₂₃
AFLOW prototype label	A8B23_mP124_7_16a_46a-001
ICSD	202203
CCDC	1706790
Pearson symbol	mP124
Space group number	7
Space group symbol	<i>Pc</i>
AFLOW prototype command	<code>aflow --proto=A8B23_mP124_7_16a_46a-001</code> <code>--params=a, b/a, c/a, β, $x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15},$</code>

$y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}, x_{22}, y_{22},$
 $z_{22}, x_{23}, y_{23}, z_{23}, x_{24}, y_{24}, z_{24}, x_{25}, y_{25}, z_{25}, x_{26}, y_{26}, z_{26}, x_{27}, y_{27}, z_{27}, x_{28}, y_{28}, z_{28}, x_{29}, y_{29}, z_{29},$
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 $z_{44}, x_{45}, y_{45}, z_{45}, x_{46}, y_{46}, z_{46}, x_{47}, y_{47}, z_{47}, x_{48}, y_{48}, z_{48}, x_{49}, y_{49}, z_{49}, x_{50}, y_{50}, z_{50}, x_{51}, y_{51}, z_{51},$
 $x_{52}, y_{52}, z_{52}, x_{53}, y_{53}, z_{53}, x_{54}, y_{54}, z_{54}, x_{55}, y_{55}, z_{55}, x_{56}, y_{56}, z_{56}, x_{57}, y_{57}, z_{57}, x_{58}, y_{58}, z_{58}, x_{59},$
 $y_{59}, z_{59}, x_{60}, y_{60}, z_{60}, x_{61}, y_{61}, z_{61}, x_{62}, y_{62}, z_{62}$

- This data was taken at 100K. Above 285K the structure exhibits an incommensurate charge density wave, which is approximated by the high temperature Mo_8O_{23} structure.

Simple Monoclinic primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
 \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	Mo I
$\mathbf{B}_2$	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Mo I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	Mo II
$\mathbf{B}_4$	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Mo II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	Mo III
$\mathbf{B}_6$	$x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Mo III
$\mathbf{B}_7$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	Mo IV
$\mathbf{B}_8$	$x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Mo IV
$\mathbf{B}_9$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	Mo V
$\mathbf{B}_{10}$	$x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Mo V
$\mathbf{B}_{11}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	Mo VI
$\mathbf{B}_{12}$	$x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Mo VI
$\mathbf{B}_{13}$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	Mo VII
$\mathbf{B}_{14}$	$x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Mo VII
$\mathbf{B}_{15}$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	Mo VIII

$\mathbf{B}_{103} =$	$x_{52} \mathbf{a}_1 + y_{52} \mathbf{a}_2 + z_{52} \mathbf{a}_3$	$=$	$(ax_{52} + cz_{52} \cos \beta) \hat{\mathbf{x}} + by_{52} \hat{\mathbf{y}} + cz_{52} \sin \beta \hat{\mathbf{z}}$	(2a)	O XXXVI
$\mathbf{B}_{104} =$	$x_{52} \mathbf{a}_1 - y_{52} \mathbf{a}_2 + (z_{52} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{52} + c(z_{52} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{52} \hat{\mathbf{y}} +$ $c(z_{52} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O XXXVI
$\mathbf{B}_{105} =$	$x_{53} \mathbf{a}_1 + y_{53} \mathbf{a}_2 + z_{53} \mathbf{a}_3$	$=$	$(ax_{53} + cz_{53} \cos \beta) \hat{\mathbf{x}} + by_{53} \hat{\mathbf{y}} + cz_{53} \sin \beta \hat{\mathbf{z}}$	(2a)	O XXXVII
$\mathbf{B}_{106} =$	$x_{53} \mathbf{a}_1 - y_{53} \mathbf{a}_2 + (z_{53} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{53} + c(z_{53} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{53} \hat{\mathbf{y}} +$ $c(z_{53} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O XXXVII
$\mathbf{B}_{107} =$	$x_{54} \mathbf{a}_1 + y_{54} \mathbf{a}_2 + z_{54} \mathbf{a}_3$	$=$	$(ax_{54} + cz_{54} \cos \beta) \hat{\mathbf{x}} + by_{54} \hat{\mathbf{y}} + cz_{54} \sin \beta \hat{\mathbf{z}}$	(2a)	O XXXVIII
$\mathbf{B}_{108} =$	$x_{54} \mathbf{a}_1 - y_{54} \mathbf{a}_2 + (z_{54} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{54} + c(z_{54} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{54} \hat{\mathbf{y}} +$ $c(z_{54} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O XXXVIII
$\mathbf{B}_{109} =$	$x_{55} \mathbf{a}_1 + y_{55} \mathbf{a}_2 + z_{55} \mathbf{a}_3$	$=$	$(ax_{55} + cz_{55} \cos \beta) \hat{\mathbf{x}} + by_{55} \hat{\mathbf{y}} + cz_{55} \sin \beta \hat{\mathbf{z}}$	(2a)	O XXXIX
$\mathbf{B}_{110} =$	$x_{55} \mathbf{a}_1 - y_{55} \mathbf{a}_2 + (z_{55} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{55} + c(z_{55} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{55} \hat{\mathbf{y}} +$ $c(z_{55} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O XXXIX
$\mathbf{B}_{111} =$	$x_{56} \mathbf{a}_1 + y_{56} \mathbf{a}_2 + z_{56} \mathbf{a}_3$	$=$	$(ax_{56} + cz_{56} \cos \beta) \hat{\mathbf{x}} + by_{56} \hat{\mathbf{y}} + cz_{56} \sin \beta \hat{\mathbf{z}}$	(2a)	O XL
$\mathbf{B}_{112} =$	$x_{56} \mathbf{a}_1 - y_{56} \mathbf{a}_2 + (z_{56} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{56} + c(z_{56} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{56} \hat{\mathbf{y}} +$ $c(z_{56} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O XL
$\mathbf{B}_{113} =$	$x_{57} \mathbf{a}_1 + y_{57} \mathbf{a}_2 + z_{57} \mathbf{a}_3$	$=$	$(ax_{57} + cz_{57} \cos \beta) \hat{\mathbf{x}} + by_{57} \hat{\mathbf{y}} + cz_{57} \sin \beta \hat{\mathbf{z}}$	(2a)	O XLI
$\mathbf{B}_{114} =$	$x_{57} \mathbf{a}_1 - y_{57} \mathbf{a}_2 + (z_{57} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{57} + c(z_{57} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{57} \hat{\mathbf{y}} +$ $c(z_{57} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O XLI
$\mathbf{B}_{115} =$	$x_{58} \mathbf{a}_1 + y_{58} \mathbf{a}_2 + z_{58} \mathbf{a}_3$	$=$	$(ax_{58} + cz_{58} \cos \beta) \hat{\mathbf{x}} + by_{58} \hat{\mathbf{y}} + cz_{58} \sin \beta \hat{\mathbf{z}}$	(2a)	O XLII
$\mathbf{B}_{116} =$	$x_{58} \mathbf{a}_1 - y_{58} \mathbf{a}_2 + (z_{58} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{58} + c(z_{58} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{58} \hat{\mathbf{y}} +$ $c(z_{58} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O XLII
$\mathbf{B}_{117} =$	$x_{59} \mathbf{a}_1 + y_{59} \mathbf{a}_2 + z_{59} \mathbf{a}_3$	$=$	$(ax_{59} + cz_{59} \cos \beta) \hat{\mathbf{x}} + by_{59} \hat{\mathbf{y}} + cz_{59} \sin \beta \hat{\mathbf{z}}$	(2a)	O XLIII
$\mathbf{B}_{118} =$	$x_{59} \mathbf{a}_1 - y_{59} \mathbf{a}_2 + (z_{59} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{59} + c(z_{59} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{59} \hat{\mathbf{y}} +$ $c(z_{59} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O XLIII
$\mathbf{B}_{119} =$	$x_{60} \mathbf{a}_1 + y_{60} \mathbf{a}_2 + z_{60} \mathbf{a}_3$	$=$	$(ax_{60} + cz_{60} \cos \beta) \hat{\mathbf{x}} + by_{60} \hat{\mathbf{y}} + cz_{60} \sin \beta \hat{\mathbf{z}}$	(2a)	O XLIV
$\mathbf{B}_{120} =$	$x_{60} \mathbf{a}_1 - y_{60} \mathbf{a}_2 + (z_{60} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{60} + c(z_{60} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{60} \hat{\mathbf{y}} +$ $c(z_{60} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O XLIV
$\mathbf{B}_{121} =$	$x_{61} \mathbf{a}_1 + y_{61} \mathbf{a}_2 + z_{61} \mathbf{a}_3$	$=$	$(ax_{61} + cz_{61} \cos \beta) \hat{\mathbf{x}} + by_{61} \hat{\mathbf{y}} + cz_{61} \sin \beta \hat{\mathbf{z}}$	(2a)	O XLV
$\mathbf{B}_{122} =$	$x_{61} \mathbf{a}_1 - y_{61} \mathbf{a}_2 + (z_{61} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{61} + c(z_{61} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{61} \hat{\mathbf{y}} +$ $c(z_{61} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O XLV
$\mathbf{B}_{123} =$	$x_{62} \mathbf{a}_1 + y_{62} \mathbf{a}_2 + z_{62} \mathbf{a}_3$	$=$	$(ax_{62} + cz_{62} \cos \beta) \hat{\mathbf{x}} + by_{62} \hat{\mathbf{y}} + cz_{62} \sin \beta \hat{\mathbf{z}}$	(2a)	O XLVI
$\mathbf{B}_{124} =$	$x_{62} \mathbf{a}_1 - y_{62} \mathbf{a}_2 + (z_{62} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{62} + c(z_{62} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{62} \hat{\mathbf{y}} +$ $c(z_{62} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O XLVI

References

- [1] H. Fujishita, M. Sato, S. Sato, and S. Hoshino, *Structure Determination of low-dimensional conductor Mo_8O_{23}* , J. Solid State Chem. **60**, 40–46 (1987), doi:10.1016/0022-4596(87)90218-0.

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