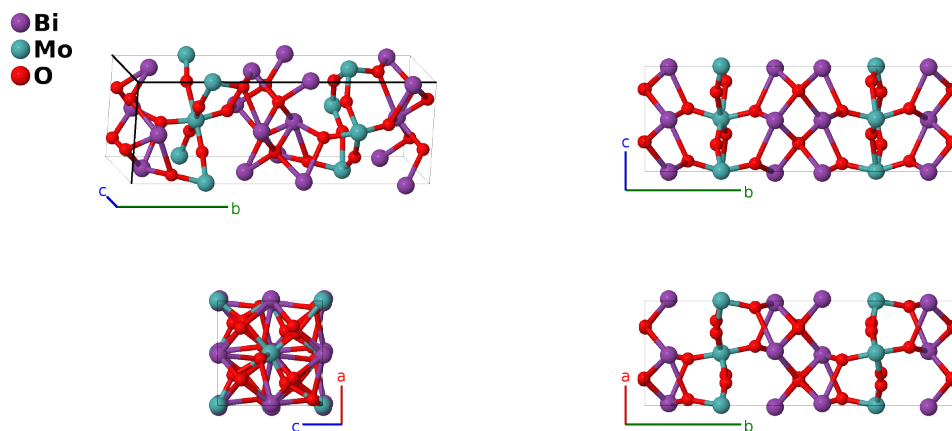


Koechlinite (Room temperature Bi_2MoO_6) Structure: A2BC6_oP36_29_2a_a_6a-001

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<https://aflow.org/p/UQQ3>

https://aflow.org/p/A2BC6_oP36_29_2a_a_6a-001



Prototype	Bi_2MoO_6
AFLOW prototype label	A2BC6_oP36_29_2a_a_6a-001
Mineral name	koechlinite
ICSD	47139
Pearson symbol	oP36
Space group number	29
Space group symbol	$Pca2_1$
AFLOW prototype command	<pre>aflow --proto=A2BC6_oP36_29_2a_a_6a-001 --params=a, b/a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9</pre>

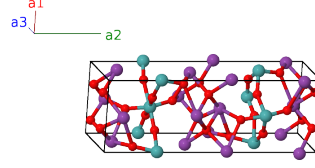
Other compounds with this structure

Bi_2WO_6 (russelite)

- This is the room temperature structure of Bi_2MoO_6 . Above 896°C it transforms to the high-temperature monoclinic Bi_2MoO_6 structure (Villars, 2018).
- (Teller, 1984) state that $\gamma\text{-Bi}_2\text{MoO}_6$ is in the $Pna2_1$ #33 space group, but the symmetry operations they give are for $Pca2_1$ #29, and interatomic distances they give are consistent with this space group. The ICSD, (Villars, 2018), and others are in agreement with this assessment.
- Space group $Pca2_1$ does not specify the origin of the z -axis. We follow (Teller, 1984) and chose it so that the molybdenum atom has $z_3 = 0$.

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(4a)	Bi I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} + c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Bi I
\mathbf{B}_3	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a (x_1 + \frac{1}{2}) \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(4a)	Bi I
\mathbf{B}_4	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_1 - \frac{1}{2}) \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} + c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Bi I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(4a)	Bi II
\mathbf{B}_6	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Bi II
\mathbf{B}_7	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(4a)	Bi II
\mathbf{B}_8	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Bi II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4a)	Mo I
\mathbf{B}_{10}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Mo I
\mathbf{B}_{11}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4a)	Mo I
\mathbf{B}_{12}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Mo I
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_{14}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_{15}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_{16}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{18}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{19}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a (x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{20}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{21}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} + b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{22}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_6 \hat{\mathbf{x}} - b y_6 \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{23}	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a (x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{24}	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b y_6 \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{25}	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$a x_7 \hat{\mathbf{x}} + b y_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(4a)	O IV
\mathbf{B}_{26}	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_7 \hat{\mathbf{x}} - b y_7 \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O IV
\mathbf{B}_{27}	$= (x_7 + \frac{1}{2}) \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$a (x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b y_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(4a)	O IV

$$\begin{aligned}
\mathbf{B}_{28} &= \begin{matrix} -(x_7 - \frac{1}{2}) \mathbf{a}_1 + y_7 \mathbf{a}_2 + \\ (z_7 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O IV} \\
\mathbf{B}_{29} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{30} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{31} &= (x_8 + \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{32} &= \begin{matrix} -(x_8 - \frac{1}{2}) \mathbf{a}_1 + y_8 \mathbf{a}_2 + \\ (z_8 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{33} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{34} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 = -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{35} &= (x_9 + \frac{1}{2}) \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{36} &= \begin{matrix} -(x_9 - \frac{1}{2}) \mathbf{a}_1 + y_9 \mathbf{a}_2 + \\ (z_9 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O VI}
\end{aligned}$$

References

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