Mo_2As_3 Structure: A3B2_mC20_12_3i_2i-001

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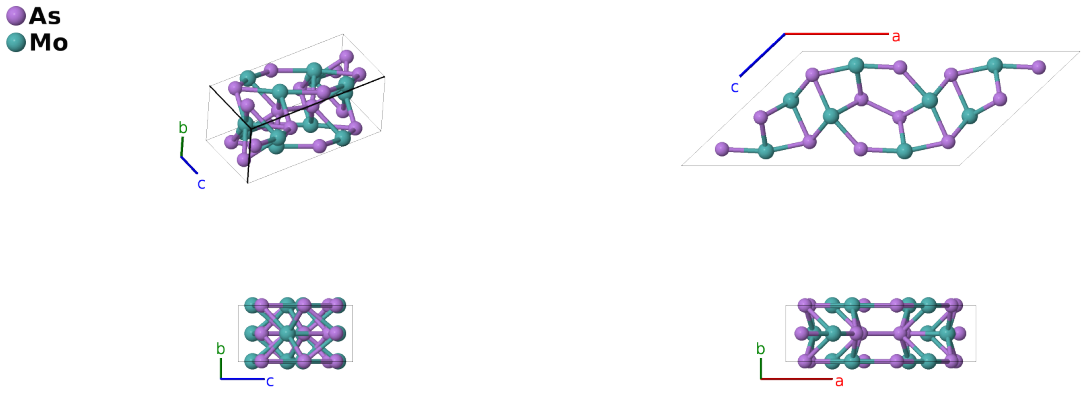
https://aflow.org/p/8QA4

https://aflow.org/p/A3B2_mC20_12_3i_2i-001



Prototype	As_3Mo_2
AFLOW prototype label	A3B2_mC20_12_3i_2i-001
ICSD	43184
Pearson symbol	mC20
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A3B2_mC20_12_3i_2i-001 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5$

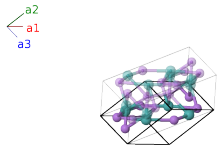
Other compounds with this structure
Nb_2Te_3, W_2As_3

- There are numerous structures with the AFLOW prototype label A2B3_mC20_12_2i_3i or A3B2_mC20_12_3i_2i. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- We have identified the following structures as sufficiently different to warrant their own prototypes:
- Prototypes with the label A2B3_mC20_12_2i_3i:
  - β-Ga_2O_3
  - α-As_2Te_3
- Prototypes with the label A3B2_mC20_12_3i_2i:
  - Mo_2As_3 (this structure)

– Gd_2Cl_3

Base-centered Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	As I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	As I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	As II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	As II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	As III
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	As III
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Mo I
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Mo I
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Mo II
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Mo II

References

[1] P. Jensen, A. Kjekshus, and T. Skansen, *The Crystal Structures of Mo_2As_3 and W_2As_3*, Acta Chem. Scand. **20**, 1003–1015 (1966), doi:10.3891/acta.chem.scand.20-1003.