

Trigonal MoS₂ Structure: AB2_hP12_143_ad_bc2d-001

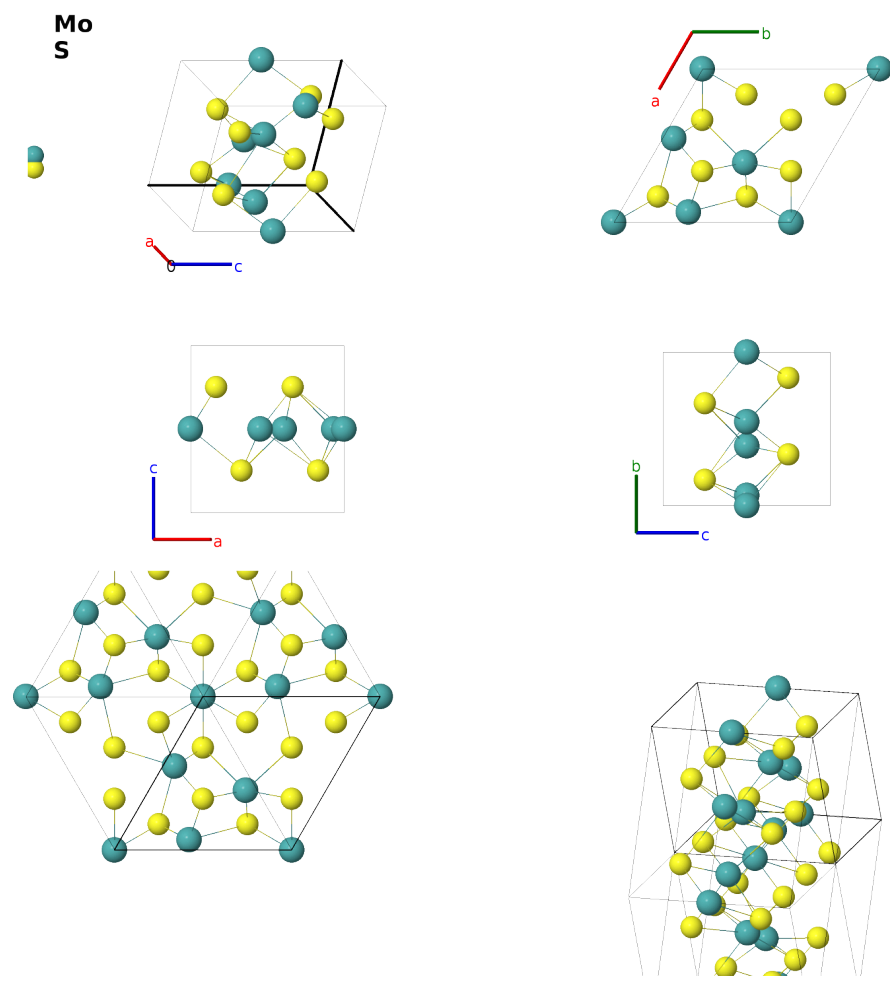
This structure previously used the label(s) **AB2_hP12_143_cd_ab2d**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/1G0H>

https://aflow.org/prototype-encyclopedia/AB2_hP12_143_ad_bc2d-001



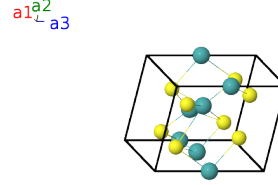
Prototype	MoS ₂
AFLOW prototype label	AB2_hP12_143_ad_bc2d-001
Pearson symbol	hP12
Space group number	143
Space group symbol	<i>P</i> 3

AFLOW prototype command `aflow --proto=AB2_hP12_143_ad_bc2d-001`
 `--params=a, c/a, z1, z2, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6`

- MoS₂ exists naturally in two forms: a rhombohedral structure and the hexagonal structure, molybdenite, *Strukturbericht* C7. The two structures differ due to the stacking of the MoS₂ layers.
- Depending on the preparation method, MoS₂ can exist in other forms, including this trigonal structure.
- Space group *P*3 # 143 allows an arbitrary choice of the origin of the z-axis. Here we choose $z_1 = 1/2$ for the Mo I site.

Trigonal (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
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(1a)	Mo I
$\mathbf{B}_2$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(1b)	S I
$\mathbf{B}_3$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(1c)	S II
$\mathbf{B}_4$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(3d)	Mo II
$\mathbf{B}_5$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(3d)	Mo II
$\mathbf{B}_6$	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(3d)	Mo II
$\mathbf{B}_7$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(3d)	S III
$\mathbf{B}_8$	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(3d)	S III
$\mathbf{B}_9$	$= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(3d)	S III
$\mathbf{B}_{10}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_6 - y_6) \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(3d)	S IV
$\mathbf{B}_{11}$	$= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(3d)	S IV
$\mathbf{B}_{12}$	$= -(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(3d)	S IV

References

- [1] K. E. Dungey, M. D. Curtis, and J. E. Penner-Hahn, *Structural Characterization and Thermal Stability of MoS₂ Intercalation Compounds*, Chem. Mater. **10**, 2152–2161 (1998), doi:10.1021/cm980034u.

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