Trigonal MoS_2 Structure: AB2_hP12_143_ad_bc2d-001

This structure originally had the label `AB2_hP12_143_cd_ab2d`. Calls to that address will be redirected here.

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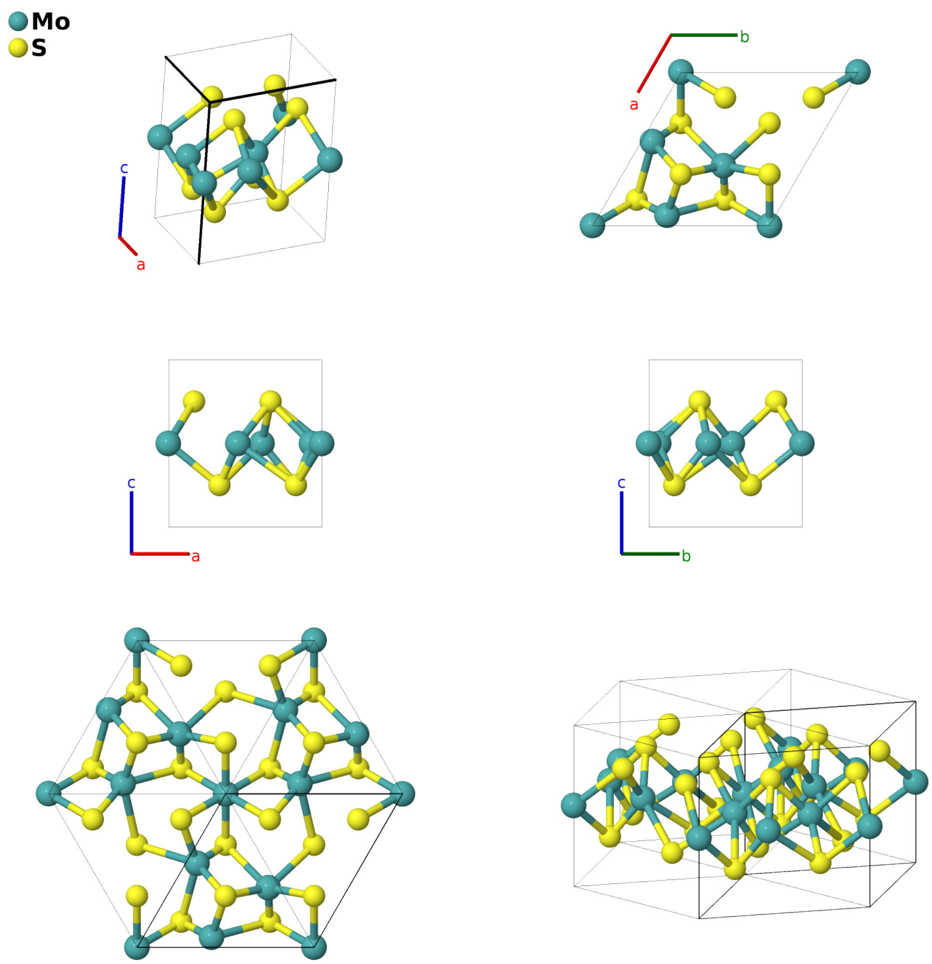
https://aflow.org/p/1G0H

https://aflow.org/p/AB2_hP12_143_ad_bc2d-001

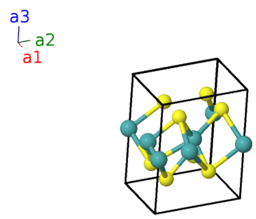


Prototype	MoS_2
AFLOW prototype label	AB2_hP12_143_ad_bc2d-001
ICSD	none
Pearson symbol	hP12
Space group number	143
Space group symbol	$P3$
AFLOW prototype command	`aflow --proto=AB2_hP12_143_ad_bc2d-001` `--params=`$a, c/a, z_1, z_2, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- MoS_2 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 MoS_2 layers.
- Depending on the preparation method, MoS_2 can exist in other forms, including this trigonal structure.
- Space group $P3$ # 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

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(1a)	Mo I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(1b)	S I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(1c)	S II
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(3d)	Mo II
$\mathbf{B_5}$	=	$-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(3d)	Mo II
$\mathbf{B_6}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(3d)	Mo II
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(3d)	S III
$\mathbf{B_8}$	=	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(3d)	S III
$\mathbf{B_9}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(3d)	S III
$\mathbf{B_{10}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(3d)	S IV
$\mathbf{B_{11}}$	=	$-y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(3d)	S IV
$\mathbf{B_{12}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(3d)	S IV

References

[1] K. E. Dungey, M. D. Curtis, and J. E. Penner-Hahn, *Structural Characterization and Thermal Stability of MoS_2 Intercalation Compounds*, Chem. Mater. **10**, 2152–2161 (1998), doi:10.1021/cm980034u.