

Molybdenite (MoS_2 , $C7$) Structure: AB2_hP6_194_c_f-001

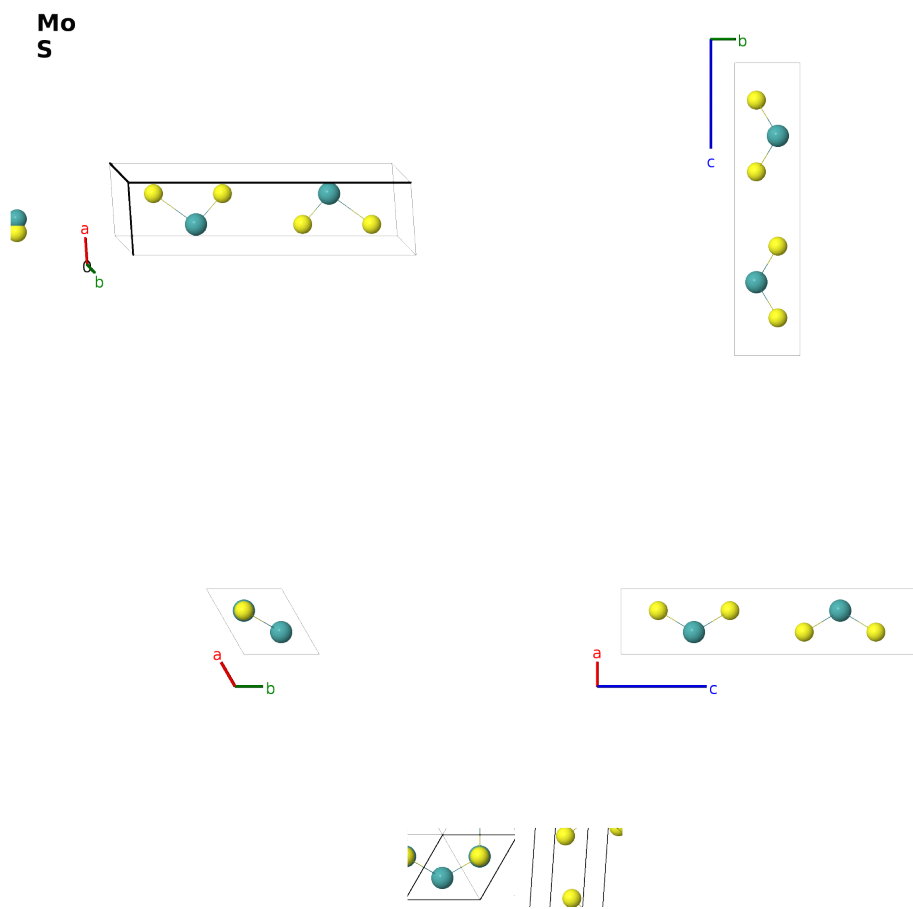
This structure previously used the label(s) **AB2_hP6_194_c_f**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/A8HJ>

https://aflow.org/prototype-encyclopedia/AB2_hP6_194_c_f-001



Prototype	MoS_2
AFLOW prototype label	AB2_hP6_194_c_f-001
<i>Strukturbericht</i> designation	$C7$
Mineral name	molybdenite
ICSD	105091
CCDC	1662990
Pearson symbol	hP6

Space group number 194

Space group symbol $P6_3/mmc$

AFLOW prototype command `aflow --proto=AB2_hP6_194_c_f-001
--params=a, c/a, z2`

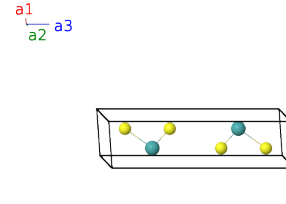
Other compounds with this structure

BPt₂, MoSe₂, MoTe₂, NbS₂, NbSe₂, ReS₂, TaS₂, TaSe₂, WS₂, WSe₂, WTe₂

- MoS₂ exists naturally in two forms: a rhombohedral structure and this 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 a trigonal structure.
 - Note that the stacking here is **BABABA**, where the layers in bold text are the Mo atoms.
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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
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Mo I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Mo I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4f)	S I
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	S I
$\mathbf{B}_5$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4f)	S I
$\mathbf{B}_6$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	S I

References

- [1] B. Schönfeld, J. J. Huang, and S. C. Moss, *Anisotropic Mean-Square Displacements (MSD) in single Crystals of 2H- and 3R-MoS₂*, Acta Crystallogr. Sect. B **39**, 404–407 (1983), doi:10.1107/S0108768183002645.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017