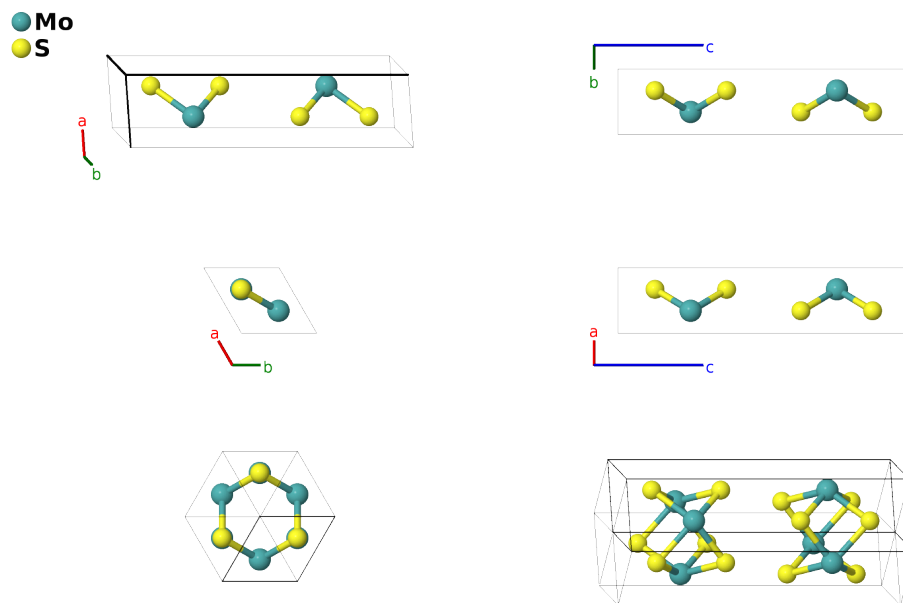# Molybdenite (MoS$_2$, $C7$) Structure: AB2_hP6_194_c_f-001

This structure originally had the label `AB2_hP6_194_c_f`. Calls to that address will be redirected here.

https://aflow.org/p/A8HJ

https://aflow.org/p/AB2_hP6_194_c_f-001

Prototype	MoS$_2$
AFLOW prototype label	AB2_hP6_194_c_f-001
***Strukturbericht* designation**	$C7$
Mineral name	molybdenite
ICSD	105091
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=$a, c/a, z_2$

Other compounds with this structure

BPt$_2$, MoSe$_2$, MoTe$_2$, NbS$_2$, NbSe$_2$, ReS$_2$, TaS$_2$, TaSe$_2$, WS$_2$, WSe$_2$, WTe$_2$

- MoS$_2$ 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 MoS$_2$ layers.

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- Depending on the preparation method, MoS$_2$ can exist in other forms, including a trigonal structure.

- Note that the stacking here is B**A**BAB**A**, where the layers in bold text are the Mo atoms.

Hexagonal primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
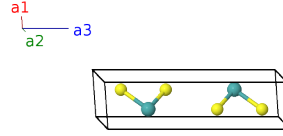
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Mo I
$\mathbf{B_2}$	=	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Mo I
$\mathbf{B_3}$	=	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + z_2\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4f)	S I
$\mathbf{B_4}$	=	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \left(z_2 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	S I
$\mathbf{B_5}$	=	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} - z_2\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4f)	S I
$\mathbf{B_6}$	=	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} - \left(z_2 - \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_2 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(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-MoS$_2$*, 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).