Rhombohedral MoS_2 Structure: AB2_hR3_160_a_2a-001

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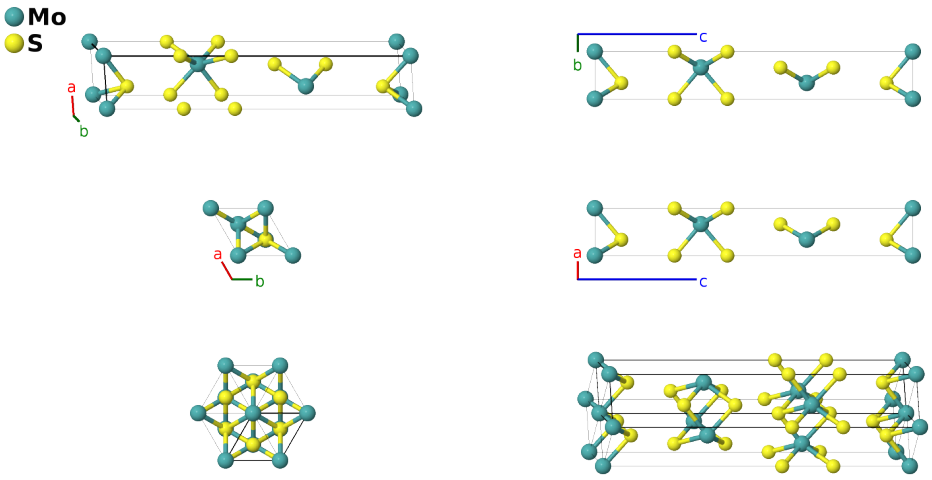
https://aflow.org/p/EW06

https://aflow.org/p/AB2_hR3_160_a_2a-001



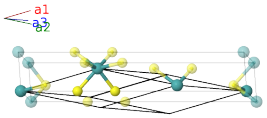
Prototype	MoS_2
AFLOW prototype label	AB2_hR3_160_a_2a-001
ICSD	43695
Pearson symbol	hR3
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=AB2_hR3_160_a_2a-001 --params=`$a, c/a, x_1, x_2, x_3$

Other compounds with this structure
MoN_2, NbS_2, $NbSe_2$, TaS_2, $TaSe_2$, WS_2

- MoS_2 exists naturally in two forms: this rhombohedral structure, and the 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 a trigonal structure.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(1a)	Mo I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(1a)	S I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(1a)	S II

References

[1] F. Jellinek, G. Brauer, and H. Müller, *Molybdenum and Niobium Sulphides*, Nature **185**, 376–377 (1960), doi:10.1038/185376a0.