V_2MoO_8 Structure: AB8C2_oC22_35_a_ab3d_d-002

This structure previously used the label(s) `AB8C2_oC22_35_a_ab3e_e`. Calls to these addresses will be redirected here.

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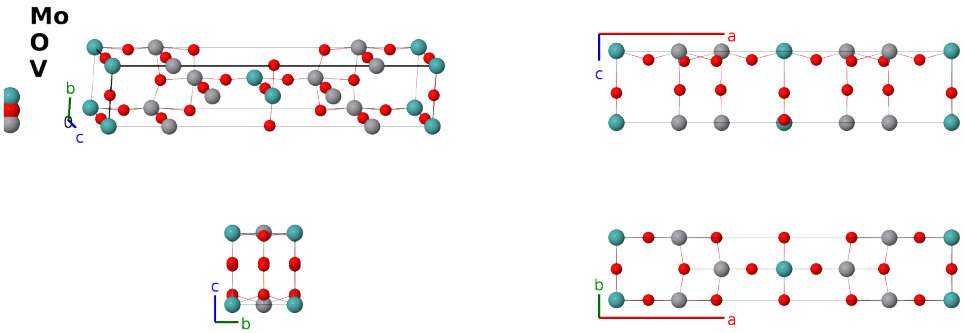
https://aflow.org/prototype-encyclopedia/8B57

https://aflow.org/prototype-encyclopedia/AB8C2_oC22_35_a_ab3d_d-002

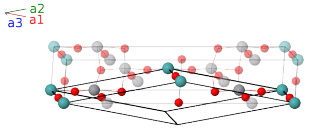


Prototype	MoO_8V_2
AFLOW prototype label	AB8C2_oC22_35_a_ab3d_d-002
ICSD	25378
CCDC	1601121
Pearson symbol	oC22
Space group number	35
Space group symbol	$Cmm2$
AFLOW prototype command	`aflow --proto=AB8C2_oC22_35_a_ab3d_d-002 --params=`$a, b/a, c/a, z_1, z_2, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7$

- Our previous report of this structure (Hicks, 2019) transposed the primitive vectors, leading to a structure with the oxygen atoms too close together. This is the corrected structure.
- AFLOW rotates the (Mahe-Pailleret, 1970) structure by 90° around the z-axis.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Mo I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B_5}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B_6}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(4d)	O IV
$\mathbf{B_7}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(4d)	O IV
$\mathbf{B_8}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(4d)	O V
$\mathbf{B_9}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(4d)	O V
$\mathbf{B_{10}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(4d)	V I
$\mathbf{B_{11}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(4d)	V I

References

[1] P. Mahe-Pailleret, *Contribution a l'etude chimique et structurale des composes AB_2O_8 rencontres dans les systemes Mo-V-O, U-V-O et U-Mo-O*, Rev. Chim. Minerale **7**, 807–846 (1970).

[2] D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

Found in

[1] P. Villars, *V_2MoO_8 orth Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043