V_2MoO_8 Structure: AB8C2_oC22_35_a_ab3d_d-002

This structure originally had the label `AB8C2_oC22_35_a_ab3e_e`. Calls to that address will be redirected here.

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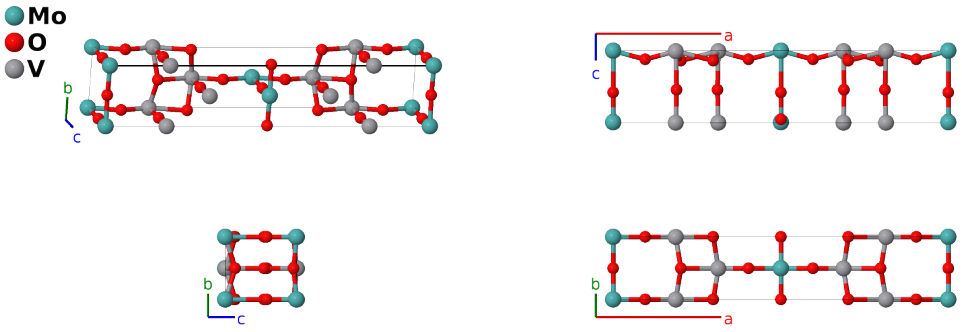
https://aflow.org/p/8B57

https://aflow.org/p/AB8C2_oC22_35_a_ab3d_d-002

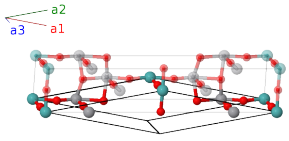


Prototype	MoO_8V_2
AFLOW prototype label	AB8C2_oC22_35_a_ab3d_d-002
ICSD	25378
Pearson symbol	oC22
Space group number	35
Space group symbol	$Cmm2$
AFLOW prototype command	`aflow --proto=AB8C2_oC22_35_a_ab3d_d-002 --params=`$a, b/a, c/a, z_1, z_2, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7$

- 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.