$CsPr(MoO_4)_2$ Structure: AB2C8D_oP24_49_e_q_2qr_f-001

This structure originally had the label `AB2C8D_oP24_49_g_q_2qr_e`. Calls to that address will be redirected here.

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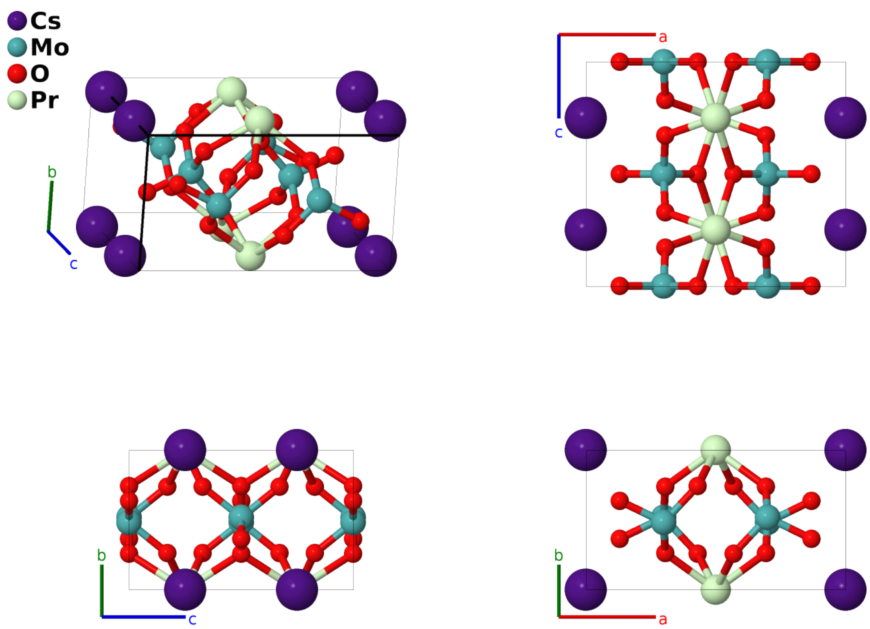
https://aflow.org/p/M8U7

https://aflow.org/p/AB2C8D_oP24_49_e_q_2qr_f-001



Prototype	$CsMo_2O_8Pr$
AFLOW prototype label	AB2C8D_oP24_49_e_q_2qr_f-001
ICSD	9374
Pearson symbol	oP24
Space group number	49
Space group symbol	$Pccm$
AFLOW prototype command	`aflow --proto=AB2C8D_oP24_49_e_q_2qr_f-001` `--params=`$a, b/a, c/a, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, z_6$

Other compounds with this structure

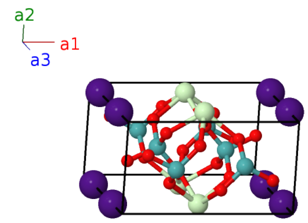
$CsDy(MoO_4)_2$, $CsEu(MoO_4)_2$, $CsGd(MoO_4)_2$, α-$CsLu(MoO_4)_2$, $CsNd(MoO_4)_2$, $CsSm(MoO_4)_2$, $CsTh(MoO_4)_2$, α-$CsTm(MoO_4)_2$, $CsY(MoO_4)_2$, α-$CsYb(MoO_4)_2$

- Our previous version of this page (Hicks, 2019) inadvertantly used the data from $RbPr(MoO_4)_2$. We have been able to obtain the correct reference (Klevtsova, 1972) and present the results here.

- We have shifted the origin by 1/2 $a\hat{x}$ from that given in (Klevtsova, 1972).

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(2e)	Cs I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(2e)	Cs I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2f)	Pr I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2f)	Pr I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}}$	(4q)	Mo I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}}$	(4q)	Mo I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4q)	Mo I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4q)	Mo I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}}$	(4q)	O I
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}}$	(4q)	O I
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4q)	O I
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4q)	O I
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}}$	(4q)	O II
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}}$	(4q)	O II
$\mathbf{B_{15}}$	=	$-x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4q)	O II
$\mathbf{B_{16}}$	=	$x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4q)	O II
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B_{19}}$	=	$-x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B_{20}}$	=	$x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B_{21}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B_{22}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B_{23}}$	=	$x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8r)	O III
$\mathbf{B_{24}}$	=	$-x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8r)	O III

References

[1] R. F. Klevstova, V. A. Vinokurov, and P. V. Klevtsov, *Crystal structure and thermal stability of cesium praseodymium molybdate, $CsPr(MoO_4)_2$*, Kristallografiya **17**, 284–288 (1972). In Russian.

[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] *Inorganic Crystal Structure Database*. Entry 9374 (CsMo2O8Pr).