β-$Gd_2(MoO_4)_3$ Structure: A2B3C12_tP34_113_e_ae_2e2f-001

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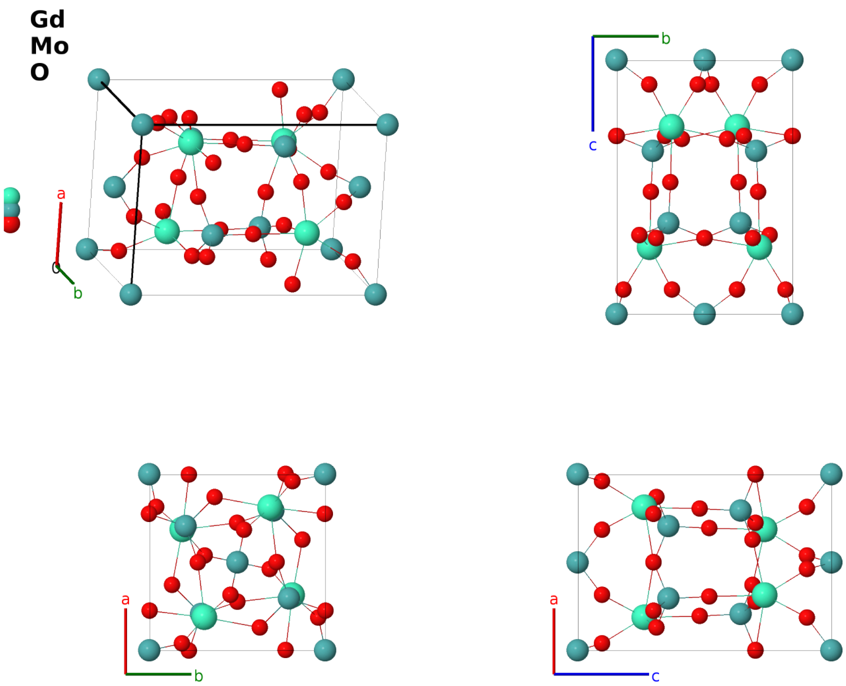
https://aflow.org/prototype-encyclopedia/53TN

https://aflow.org/prototype-encyclopedia/A2B3C12_tP34_113_e_ae_2e2f-001



Prototype	$Gd_2Mo_3O_{12}$
AFLOW prototype label	A2B3C12_tP34_113_e_ae_2e2f-001
ICSD	2708
CCDC	1592520
Pearson symbol	tP34
Space group number	113
Space group symbol	$P\bar{4}2_1m$
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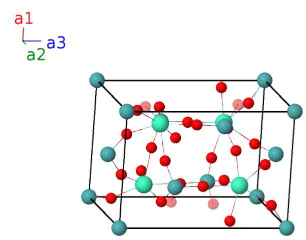
Other compounds with this structure

$Dy_2(MoO_4)_3$, $Eu_2(MoO_4)_3$, $Gd_2(MoO_4)_3$, $Nd_2(MoO_4)_3$, $Pr_2(MoO_4)_3$, $Sm_2(MoO_4)_3$, $Tb_2(MoO_4)_3$

- $Gd_2Mo_3O_{12}$ takes on several different forms with changing temperature (Yuan, 2001):
  - below 159°C it is in the orthorhombic ground state β'-$Gd_2(MoO_4)_3$ structure.
  - In the range 159-850°C it is in the monoclinic α-$Gd_2(MoO_4)_3$ structure.
  - Above 850°C it is in the tetragonal β-$Gd_2(MoO_4)_3$ structure. (Shown here)
- The ICSD entry for (Jeitschko, 1972) gives the structural information in the $C\bar{4}m2_1$ setting of space group #113 rather than the standard $P\bar{4}2_1m$ setting. This doubled unit cell is nearly cubic. If a_1, a_2, and a_3 are the primitive vectors of $P\bar{4}2_1m$ cell, then the primitive vectors of the $C\bar{4}m2_1$ cell are:
- $a_1' = a_1 - a_2$
- $a_2' = a_1 + a_2$
- $a_3' = a_3$
- The data was taken at 183°C. If the phase diagram from (Yaun, 2001) is correct, β-$Gd_2(MoO_4)_3$ is metastable at this temperature. (Jeitschko, 1972) only gives data for the β and β' phases.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Mo I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(2a)	Mo I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4e)	Gd I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4e)	Gd I
$\mathbf{B_5}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4e)	Gd I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4e)	Gd I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	Mo II
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	Mo II
$\mathbf{B_9}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	Mo II
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	Mo II
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_{13}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_{15}}$	=	$x_5\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{16}}$	=	$-x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4e)	O II

$\mathbf{B_{17}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{18}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{19}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{20}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{21}}$	=	$y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{22}}$	=	$-y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{23}}$	=	$-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{24}}$	=	$\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{25}}$	=	$-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_6-\frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{26}}$	=	$\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_6+\frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{27}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{28}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{29}}$	=	$y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{30}}$	=	$-y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{31}}$	=	$-\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_7+\frac{1}{2}\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{32}}$	=	$\left(x_7+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_7-\frac{1}{2}\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{33}}$	=	$-\left(y_7-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_7-\frac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{34}}$	=	$\left(y_7+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_7+\frac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$a\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8f)	O IV

References

[1] W. Jeitschko, *A comprehensive X-ray study of the ferroelectric-ferroelastic and paraelectric-paraelastic phases of* $Gd_2(MoO_4)_3$, Acta Crystallogr. Sect. B **28**, 60–76 (1972), doi:10.1107/S0567740872001876.

[2] Q. Yuan, C. Zhao, W. Luo, X. Yin, J. Xu, and S. Pan, *Crystal growth of β'-*$Gd_2(MoO_4)_3$ *and in situ observation of its domain structure by the microscope and the synchrotron X-ray topography*, J. Cryst. Growth **233**, 717–722 (2001), doi:10.1016/S0022-0248(01)01594-9.

Found in

[1] *Inorganic Crystal Structure Database.* Entry 2708 (Gd2(MoO4)3).

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