α-$Gd_2(MoO_4)_3$ Structure: A2B3C12_mC68_15_f_ef_6f-001

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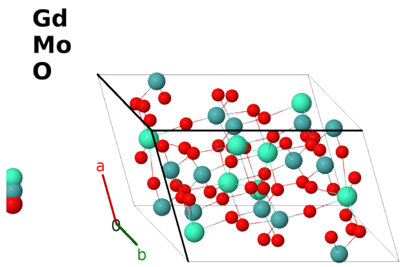
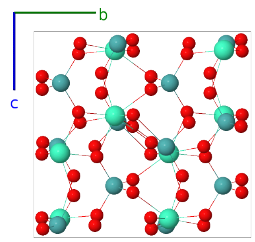
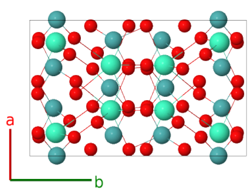
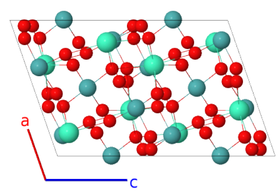
https://aflow.org/prototype-encyclopedia/B6G4

https://aflow.org/prototype-encyclopedia/A2B3C12_mC68_15_f_ef_6f-001









Prototype	$Gd_2Mo_3O_{12}$
AFLOW prototype label	A2B3C12_mC68_15_f_ef_6f-001
ICSD	251703
CCDC	1717207
Pearson symbol	mC68
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=A2B3C12_mC68_15_f_ef_6f-001 --params=`$a, b/a, c/a, \beta, y_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

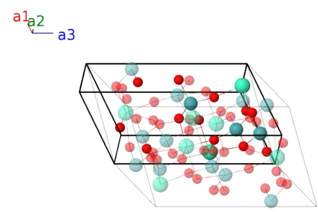
Other compounds with this structure

$Eu_2(MoO_4)_3$, $Eu_2(WO_4)_3$, $Sm_2(MoO_4)_3$

- $Gd_2Mo_3O_{12}$ 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. (Shown here)
  - Above 850°C it is in the tetragonal β-$Gd_2(MoO_4)_3$ structure.
- (Morozov, 2014) took the data for this compound at 293K.
- The ICSD lists $Eu_2(WO_4)_3$ as the prototype for this structure, but we prefer to use $Eu_2(MoO_4)_3$ to keep these related compounds together.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} - \tfrac{1}{2}b\,\mathbf{\hat{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} + \tfrac{1}{2}b\,\mathbf{\hat{y}} \\
\mathbf{a_3} &= c\cos\beta\,\mathbf{\hat{x}} + c\sin\beta\,\mathbf{\hat{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\mathbf{\hat{x}} + by_1\,\mathbf{\hat{y}} + \frac{1}{4}c\sin\beta\,\mathbf{\hat{z}}$	(4e)	Mo I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\mathbf{\hat{x}} - by_1\,\mathbf{\hat{y}} + \frac{3}{4}c\sin\beta\,\mathbf{\hat{z}}$	(4e)	Mo I
$\mathbf{B_3}$	=	$(x_2 - y_2)\,\mathbf{a}_1 + (x_2 + y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\mathbf{\hat{x}} + by_2\,\mathbf{\hat{y}} + cz_2\sin\beta\,\mathbf{\hat{z}}$	(8f)	Gd I
$\mathbf{B_4}$	=	$-(x_2 + y_2)\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_2\,\mathbf{\hat{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	Gd I
$\mathbf{B_5}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - (x_2 + y_2)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\mathbf{\hat{x}} - by_2\,\mathbf{\hat{y}} - cz_2\sin\beta\,\mathbf{\hat{z}}$	(8f)	Gd I
$\mathbf{B_6}$	=	$(x_2 + y_2)\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_2\,\mathbf{\hat{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	Gd I
$\mathbf{B_7}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\mathbf{\hat{x}} + by_3\,\mathbf{\hat{y}} + cz_3\sin\beta\,\mathbf{\hat{z}}$	(8f)	Mo II
$\mathbf{B_8}$	=	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_3\,\mathbf{\hat{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	Mo II
$\mathbf{B_9}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\mathbf{\hat{x}} - by_3\,\mathbf{\hat{y}} - cz_3\sin\beta\,\mathbf{\hat{z}}$	(8f)	Mo II
$\mathbf{B_{10}}$	=	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_3\,\mathbf{\hat{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	Mo II
$\mathbf{B_{11}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} + cz_4\sin\beta\,\mathbf{\hat{z}}$	(8f)	O I
$\mathbf{B_{12}}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O I
$\mathbf{B_{13}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} - cz_4\sin\beta\,\mathbf{\hat{z}}$	(8f)	O I

$$\mathbf{B_{14}} = \left(x_4+y_4\right)\,\mathbf{a}_1 + \left(x_4-y_4\right)\,\mathbf{a}_2 + \left(z_4+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(a x_4 + c\left(z_4+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b y_4\,\hat{\mathbf{y}} + c\left(z_4+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O I}$$

$$\mathbf{B_{15}} = \left(x_5-y_5\right)\,\mathbf{a}_1 + \left(x_5+y_5\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = \left(a x_5 + c z_5\cos\beta\right)\,\hat{\mathbf{x}} + b y_5\,\hat{\mathbf{y}} + c z_5\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O II}$$

$$\mathbf{B_{16}} = -\left(x_5+y_5\right)\,\mathbf{a}_1 - \left(x_5-y_5\right)\,\mathbf{a}_2 - \left(z_5-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(a x_5 + c\left(z_5-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b y_5\,\hat{\mathbf{y}} - c\left(z_5-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O II}$$

$$\mathbf{B_{17}} = -\left(x_5-y_5\right)\,\mathbf{a}_1 - \left(x_5+y_5\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = -\left(a x_5 + c z_5\cos\beta\right)\,\hat{\mathbf{x}} - b y_5\,\hat{\mathbf{y}} - c z_5\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O II}$$

$$\mathbf{B_{18}} = \left(x_5+y_5\right)\,\mathbf{a}_1 + \left(x_5-y_5\right)\,\mathbf{a}_2 + \left(z_5+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(a x_5 + c\left(z_5+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b y_5\,\hat{\mathbf{y}} + c\left(z_5+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O II}$$

$$\mathbf{B_{19}} = \left(x_6-y_6\right)\,\mathbf{a}_1 + \left(x_6+y_6\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = \left(a x_6 + c z_6\cos\beta\right)\,\hat{\mathbf{x}} + b y_6\,\hat{\mathbf{y}} + c z_6\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O III}$$

$$\mathbf{B_{20}} = -\left(x_6+y_6\right)\,\mathbf{a}_1 - \left(x_6-y_6\right)\,\mathbf{a}_2 - \left(z_6-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(a x_6 + c\left(z_6-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b y_6\,\hat{\mathbf{y}} - c\left(z_6-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O III}$$

$$\mathbf{B_{21}} = -\left(x_6-y_6\right)\,\mathbf{a}_1 - \left(x_6+y_6\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -\left(a x_6 + c z_6\cos\beta\right)\,\hat{\mathbf{x}} - b y_6\,\hat{\mathbf{y}} - c z_6\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O III}$$

$$\mathbf{B_{22}} = \left(x_6+y_6\right)\,\mathbf{a}_1 + \left(x_6-y_6\right)\,\mathbf{a}_2 + \left(z_6+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(a x_6 + c\left(z_6+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b y_6\,\hat{\mathbf{y}} + c\left(z_6+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O III}$$

$$\mathbf{B_{23}} = \left(x_7-y_7\right)\,\mathbf{a}_1 + \left(x_7+y_7\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \left(a x_7 + c z_7\cos\beta\right)\,\hat{\mathbf{x}} + b y_7\,\hat{\mathbf{y}} + c z_7\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O IV}$$

$$\mathbf{B_{24}} = -\left(x_7+y_7\right)\,\mathbf{a}_1 - \left(x_7-y_7\right)\,\mathbf{a}_2 - \left(z_7-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(a x_7 + c\left(z_7-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b y_7\,\hat{\mathbf{y}} - c\left(z_7-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O IV}$$

$$\mathbf{B_{25}} = -\left(x_7-y_7\right)\,\mathbf{a}_1 - \left(x_7+y_7\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -\left(a x_7 + c z_7\cos\beta\right)\,\hat{\mathbf{x}} - b y_7\,\hat{\mathbf{y}} - c z_7\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O IV}$$

$$\mathbf{B_{26}} = \left(x_7+y_7\right)\,\mathbf{a}_1 + \left(x_7-y_7\right)\,\mathbf{a}_2 + \left(z_7+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(a x_7 + c\left(z_7+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b y_7\,\hat{\mathbf{y}} + c\left(z_7+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O IV}$$

$$\mathbf{B_{27}} = \left(x_8-y_8\right)\,\mathbf{a}_1 + \left(x_8+y_8\right)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = \left(a x_8 + c z_8\cos\beta\right)\,\hat{\mathbf{x}} + b y_8\,\hat{\mathbf{y}} + c z_8\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O V}$$

$$\mathbf{B_{28}} = -\left(x_8+y_8\right)\,\mathbf{a}_1 - \left(x_8-y_8\right)\,\mathbf{a}_2 - \left(z_8-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(a x_8 + c\left(z_8-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b y_8\,\hat{\mathbf{y}} - c\left(z_8-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O V}$$

$$\mathbf{B_{29}} = -\left(x_8-y_8\right)\,\mathbf{a}_1 - \left(x_8+y_8\right)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = -\left(a x_8 + c z_8\cos\beta\right)\,\hat{\mathbf{x}} - b y_8\,\hat{\mathbf{y}} - c z_8\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O V}$$

$$\mathbf{B_{30}} = \left(x_8+y_8\right)\,\mathbf{a}_1 + \left(x_8-y_8\right)\,\mathbf{a}_2 + \left(z_8+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(a x_8 + c\left(z_8+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b y_8\,\hat{\mathbf{y}} + c\left(z_8+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O V}$$

$$\mathbf{B_{31}} = \left(x_9-y_9\right)\,\mathbf{a}_1 + \left(x_9+y_9\right)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = \left(a x_9 + c z_9\cos\beta\right)\,\hat{\mathbf{x}} + b y_9\,\hat{\mathbf{y}} + c z_9\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O VI}$$

$$\mathbf{B_{32}} = -\left(x_9+y_9\right)\,\mathbf{a}_1 - \left(x_9-y_9\right)\,\mathbf{a}_2 - \left(z_9-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(a x_9 + c\left(z_9-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b y_9\,\hat{\mathbf{y}} - c\left(z_9-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O VI}$$

$$\mathbf{B_{33}} = -\left(x_9-y_9\right)\,\mathbf{a}_1 - \left(x_9+y_9\right)\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = -\left(a x_9 + c z_9\cos\beta\right)\,\hat{\mathbf{x}} - b y_9\,\hat{\mathbf{y}} - c z_9\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O VI}$$

$$\mathbf{B_{34}} = \left(x_9+y_9\right)\,\mathbf{a}_1 + \left(x_9-y_9\right)\,\mathbf{a}_2 + \left(z_9+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(a x_9 + c\left(z_9+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b y_9\,\hat{\mathbf{y}} + c\left(z_9+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (8f) \qquad \text{O VI}$$

References

[1] V. A. Morozov, M. V. Raskina, B. I. Lazoryak, K. W. Meert, K. Korthout, P. F. Smet, D. Poelman, N. Gauquelin, J. Verbeeck, A. M. Abakumov, and J. Hadermann, *Crystal Structure and Luminescent Properties of $R_{2-x}Eu_x(MoO_4)_3$ (R = Gd, Sm) Red Phosphors*, Chem. Mater. **26**, 7124–7136 (2014), doi:10.1021/cm503720s.

Found in

[1] *Inorganic Crystal Structure Database*. Entry 251703 (Gd2(MoO4)3).

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