

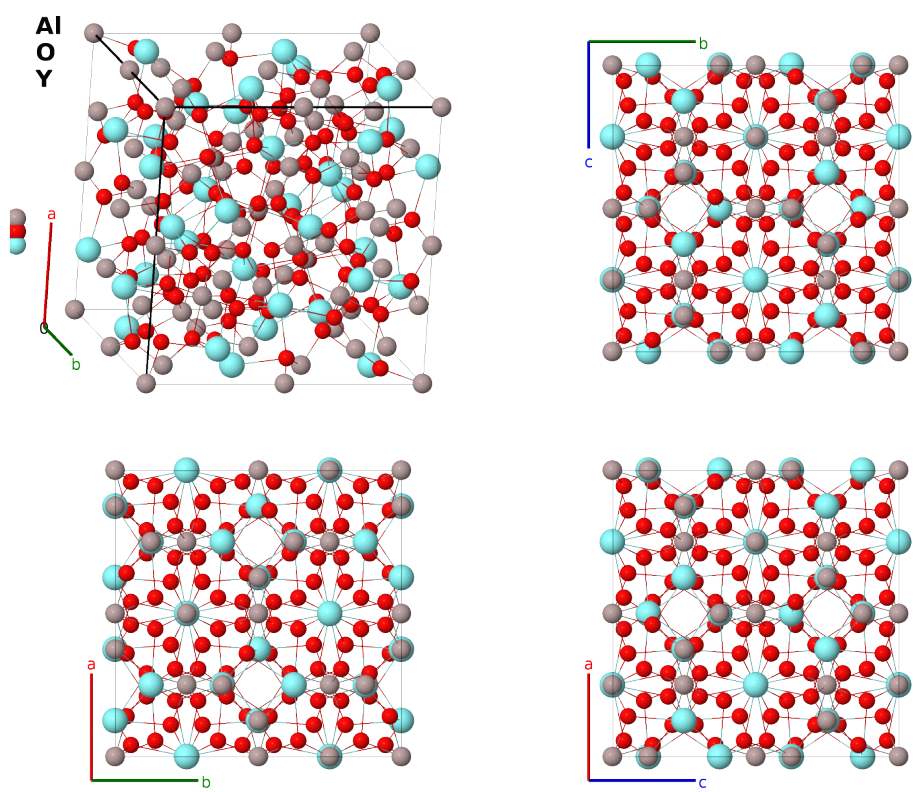
Y₃Al₅O₁₂ Garnet (YAG) Structure: A5B12C3_cI160_230_ad_h_c-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/TX22>

https://aflow.org/prototype-encyclopedia/A5B12C3_cI160_230_ad_h_c-001



Prototype	Al ₅ O ₁₂ Y ₃
AFLOW prototype label	A5B12C3_cI160_230_ad_h_c-001
ICSD	138300
CCDC	2122342
Pearson symbol	cI160
Space group number	230
Space group symbol	Ia $\bar{3}d$
AFLOW prototype command	<code>aflow --proto=A5B12C3_cI160_230_ad_h_c-001 --params=a, x₄, y₄, z₄</code>

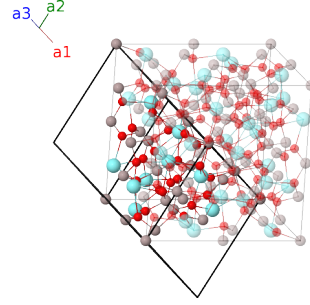
Other compounds with this structure

Er₃Al₅O₁₂, Eu₃Al₅O₁₂, Eu₃Fe₅O₁₂, Gd₃Al₅O₁₂, Gd₃Fe₅O₁₂, Gd₃Ga₅O₁₂, Ho₃Al₅O₁₂, Ho₃Fe₅O₁₂, Ho₃Ga₅O₁₂, Lu₃Al₅O₁₂, Lu₃Fe₅O₁₂, Lu₃Ga₅O₁₂, Nd₃Fe₅O₁₂, Nd₃Ga₅O₁₂, Tb₃Al₅O₁₂, Yb₃Al₅O₁₂

- This is the ternary form of garnet. As with other forms of garnet there are frequent substitutions on all sites.
- In the measured sample, 1.3% of the yttrium is replaced by dysprosium.

Body-centered Cubic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}a\hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(16a) Al I
$\mathbf{B}_2$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}}$	(16a) Al I
$\mathbf{B}_3$	$=$	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}}$	(16a) Al I
$\mathbf{B}_4$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{2}a\hat{\mathbf{z}}$	(16a) Al I
$\mathbf{B}_5$	$=$	$\frac{1}{2}\mathbf{a}_1$	$=$	$-\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16a) Al I
$\mathbf{B}_6$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16a) Al I
$\mathbf{B}_7$	$=$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - \frac{1}{4}a\hat{\mathbf{z}}$	(16a) Al I
$\mathbf{B}_8$	$=$	$\frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16a) Al I
$\mathbf{B}_9$	$=$	$\frac{1}{4}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c) Y I
$\mathbf{B}_{10}$	$=$	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	$=$	$-\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c) Y I
$\mathbf{B}_{11}$	$=$	$\frac{1}{8}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}}$	(24c) Y I
$\mathbf{B}_{12}$	$=$	$\frac{3}{8}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24c) Y I
$\mathbf{B}_{13}$	$=$	$\frac{3}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(24c) Y I
$\mathbf{B}_{14}$	$=$	$\frac{1}{8}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - \frac{1}{8}a\hat{\mathbf{z}}$	(24c) Y I
$\mathbf{B}_{15}$	$=$	$\frac{3}{4}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c) Y I
$\mathbf{B}_{16}$	$=$	$\frac{1}{4}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3$	$=$	$\frac{5}{8}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c) Y I
$\mathbf{B}_{17}$	$=$	$\frac{7}{8}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24c) Y I
$\mathbf{B}_{18}$	$=$	$\frac{5}{8}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{5}{8}a\hat{\mathbf{y}}$	(24c) Y I
$\mathbf{B}_{19}$	$=$	$\frac{5}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(24c) Y I
$\mathbf{B}_{20}$	$=$	$\frac{7}{8}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{5}{8}a\hat{\mathbf{z}}$	(24c) Y I
$\mathbf{B}_{21}$	$=$	$\frac{1}{4}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d) Al II
$\mathbf{B}_{22}$	$=$	$\frac{3}{4}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{z}}$	(24d) Al II

$\mathbf{B}_{23} =$	$\frac{3}{8} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}}$	(24d)	Al II
$\mathbf{B}_{24} =$	$\frac{1}{8} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}}$	(24d)	Al II
$\mathbf{B}_{25} =$	$\frac{5}{8} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}}$	(24d)	Al II
$\mathbf{B}_{26} =$	$\frac{7}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}}$	(24d)	Al II
$\mathbf{B}_{27} =$	$\frac{5}{8} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{8} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(24d)	Al II
$\mathbf{B}_{28} =$	$\frac{7}{8} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3$	$=$	$-\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(24d)	Al II
$\mathbf{B}_{29} =$	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3$	$=$	$\frac{1}{8} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24d)	Al II
$\mathbf{B}_{30} =$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3$	$=$	$\frac{3}{8} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{4} a \hat{\mathbf{z}}$	(24d)	Al II
$\mathbf{B}_{31} =$	$\frac{1}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}}$	(24d)	Al II
$\mathbf{B}_{32} =$	$\frac{3}{8} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}}$	(24d)	Al II
$\mathbf{B}_{33} =$	$(y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 +$ $(x_4 + y_4) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{34} =$	$(-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 -$ $(x_4 - z_4) \mathbf{a}_2 - (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{35} =$	$(y_4 - z_4) \mathbf{a}_1 - (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 +$ $(-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{36} =$	$-(y_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 +$ $(x_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{37} =$	$(x_4 + y_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 +$ $(x_4 + z_4) \mathbf{a}_3$	$=$	$az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{38} =$	$-(x_4 + y_4 - \frac{1}{2}) \mathbf{a}_1 +$ $(-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - z_4) \mathbf{a}_3$	$=$	$az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{39} =$	$(-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_1 +$ $(y_4 - z_4) \mathbf{a}_2 - (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-az_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{40} =$	$(x_4 - y_4) \mathbf{a}_1 - (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 +$ $(x_4 - z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(z_4 - \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{41} =$	$(x_4 + z_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 +$ $(y_4 + z_4) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{42} =$	$-(x_4 - z_4) \mathbf{a}_1 -$ $(x_4 + y_4 - \frac{1}{2}) \mathbf{a}_2 +$ $(-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{43} =$	$-(x_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 +$ $(-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 - z_4) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{44} =$	$(x_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 +$ $(x_4 - y_4) \mathbf{a}_2 - (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{45} =$	$(x_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 +$ $(y_4 - z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$	$=$	$a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_4 - \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{46} =$	$-(x_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 -$ $(y_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 -$ $(x_4 + y_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} - a(z_4 - \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{47} =$	$-(x_4 - z_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 +$ $(-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(z_4 - \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{48} =$	$(x_4 + z_4) \mathbf{a}_1 +$ $(-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	O I
$\mathbf{B}_{49} =$	$(-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 +$ $(x_4 - y_4) \mathbf{a}_2 + (x_4 + z_4) \mathbf{a}_3$	$=$	$a(x_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_4 - \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	O I

$$\begin{aligned}
\mathbf{B}_{50} &= (y_4 + z_4) \mathbf{a}_1 + (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - z_4) \mathbf{a}_3 &= -a(x_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(z_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(y_4 + \frac{1}{4}) \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{51} &= -(y_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_2 - (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_3 &= -a(x_4 - \frac{1}{4}) \hat{\mathbf{x}} - a(z_4 - \frac{1}{4}) \hat{\mathbf{y}} - a(y_4 - \frac{1}{4}) \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{52} &= (y_4 - z_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_3 &= a(x_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(y_4 - \frac{1}{4}) \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{53} &= (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3 &= a(z_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{54} &= (x_4 - y_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 &= a(z_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_4 - \frac{1}{4}) \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{55} &= (x_4 + y_4) \mathbf{a}_1 + (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 - z_4) \mathbf{a}_3 &= -a(z_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(y_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{56} &= -(x_4 + y_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 - (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_3 &= -a(z_4 - \frac{1}{4}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{4}) \hat{\mathbf{y}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{57} &= -(y_4 + z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3 &= -ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{58} &= (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 &= ax_4 \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{59} &= -(y_4 - z_4) \mathbf{a}_1 + (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 &= a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{60} &= (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3 &= -ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + a(z_4 + \frac{1}{2}) \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{61} &= -(x_4 + y_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 - (x_4 + z_4) \mathbf{a}_3 &= -az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{62} &= (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - z_4) \mathbf{a}_3 &= -az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{63} &= (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - z_4) \mathbf{a}_2 + (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 &= az_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{64} &= -(x_4 - y_4) \mathbf{a}_1 + (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 &= a(z_4 + \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{65} &= -(x_4 + z_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - (y_4 + z_4) \mathbf{a}_3 &= -ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{66} &= (x_4 - z_4) \mathbf{a}_1 + (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_3 &= a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{67} &= (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3 &= -ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{68} &= (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 &= ay_4 \hat{\mathbf{x}} + a(z_4 + \frac{1}{2}) \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{69} &= (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3 &= -a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{z}} &(96h) &\quad \text{O I} \\
\mathbf{B}_{70} &= (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 &= a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{z}} &(96h) &\quad \text{O I}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{71} &= \begin{pmatrix} (x_4 - z_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(y_4 - \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{72} &= \begin{pmatrix} -(x_4 + z_4) \mathbf{a}_1 + \\ (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3 \end{pmatrix} = a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(z_4 - \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{73} &= \begin{pmatrix} (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_4 - y_4) \mathbf{a}_2 - (x_4 + z_4) \mathbf{a}_3 \end{pmatrix} = -a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(z_4 - \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{74} &= \begin{pmatrix} -(y_4 + z_4) \mathbf{a}_1 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - z_4) \mathbf{a}_3 \end{pmatrix} = a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(y_4 - \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{75} &= \begin{pmatrix} (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{76} &= \begin{pmatrix} -(y_4 - z_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 + \\ (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_4 - \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{77} &= \begin{pmatrix} (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 - z_4) \mathbf{a}_2 - (y_4 + z_4) \mathbf{a}_3 \end{pmatrix} = -a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(y_4 - \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{78} &= \begin{pmatrix} -(x_4 - y_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 + \\ (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(z_4 - \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{79} &= \begin{pmatrix} -(x_4 + y_4) \mathbf{a}_1 + \\ (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3 \end{pmatrix} = a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(x_4 - \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{80} &= \begin{pmatrix} (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I}
\end{aligned}$$

References

- [1] S. Singh, A. P. Simantilleke, and D. Singh, *Crystal structure and photoluminescence investigations of $Y_3Al_5O_{12}:Dy^{3+}$ nanocrystalline phosphors for WLEDs*, Chem. Phys. Lett. **765**, 138300 (2021), doi:10.1016/j.cplett.2020.138300.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).