Gaudefroyite $Ca_8Mn_6[(BO_3)_6(CO_3)_2O_6]$ Structure: A3B2C4D3E18_hP60_176_h_e_ch_g_2h2i-001

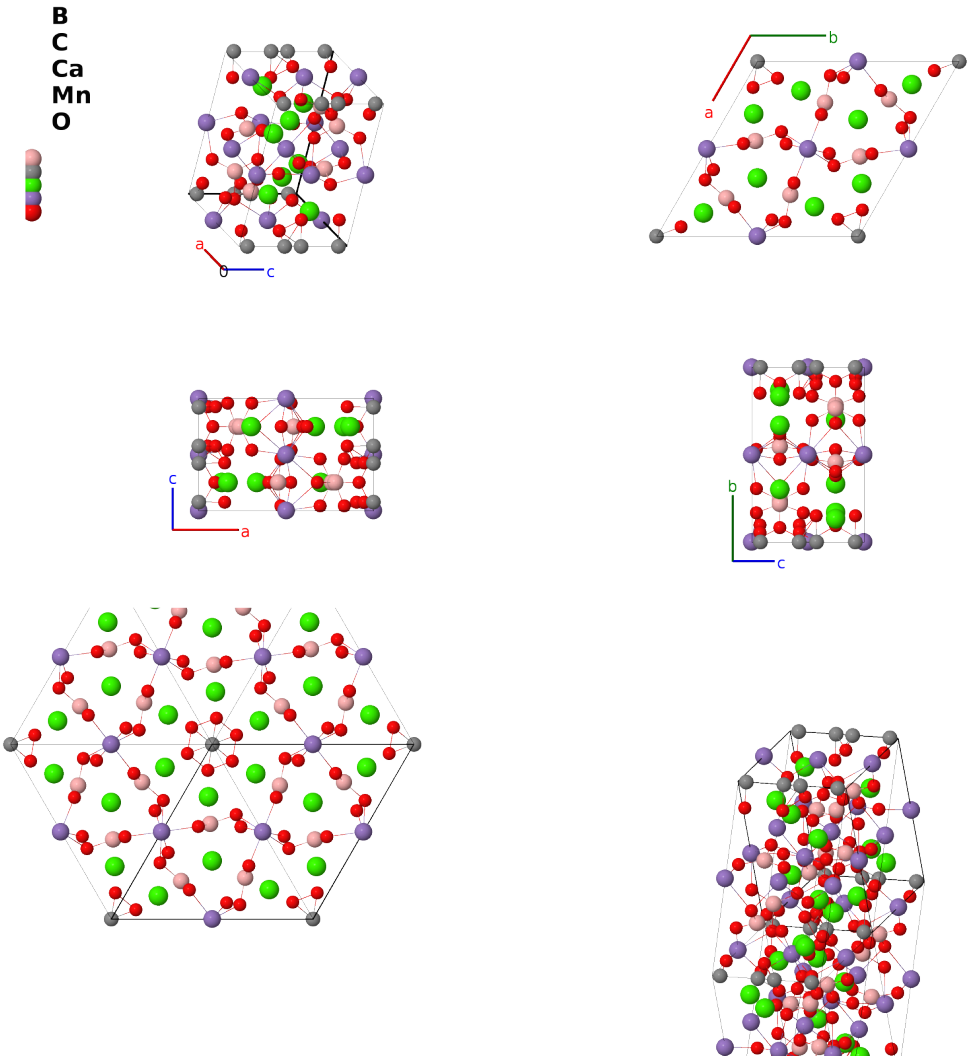
Cite this page as:

- 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/8PYB

https://aflow.org/prototype-encyclopedia/A3B2C4D3E18_hP60_176_h_e_ch_g_2h2i-001



Prototype	$B_3CCa_4Mn_3O_{15}$
AFLOW prototype label	A3B2C4D3E18_hP60_176_h_e_ch_g_2h2i-001
Mineral name	gaudefroyite
ICSD	159983
CCDC	1676402

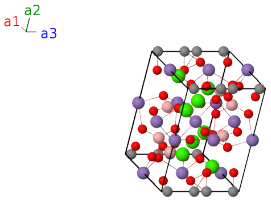
Pearson symbol	hP60
Space group number	176
Space group symbol	$P6_3/m$
AFLOW prototype command	`aflow --proto=A3B2C4D3E18_hP60_176_h_e_ch_g_2h2i-001 --params=`$a, c/a, z_2, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, x_8, y_8, z_8, x_9, y_9, z_9$

Other compounds with this structure
$Ca_3B_4Al_3GdO_{15}$, $Ca_3B_4Al_3YO_{15}$, $Ca_3B_4Cr_3YO_{15}$, $Ca_3B_4Ga_3TbO_{15}$, $Ca_3B_4Ga_3YO_{15}$, $Ca_3B_4Gd_3YO_{15}$, $Ca_3B_4Mn_3YO_{15}$

- The C I (4e) site and the O IV (12i) site are only half occupied, giving the observed stochiometry. We could average the carbon atoms z-coordinates, setting $z_2 = 0$, which would put them on a fully occupied (2b) site. A similar trick, setting $z_9 = 1/4$, would move the O IV atoms to the (6h) site, but this involves moving those atoms by about 1Å, twice as far as the carbon atoms would have to move.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Ca I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Ca I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B_4}$	=	$\left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B_5}$	=	$-z_2\,\mathbf{a}_3$	=	$-cz_2\,\hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B_6}$	=	$-\left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	Mn I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	Mn I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(6g)	Mn I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Mn I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Mn I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Mn I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_{14}}$	=	$-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_{15}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_{16}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_{17}}$	=	$y_4\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_4 + 2y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_{18}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	B I

$\mathbf{B_{19}}$	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 + y_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\;\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ca II
$\mathbf{B_{20}}$	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\;\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ca II
$\mathbf{B_{21}}$	$-(x_5 - y_5)\;\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ca II
$\mathbf{B_{22}}$	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 + y_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ca II
$\mathbf{B_{23}}$	$y_5\,\mathbf{a}_1 - (x_5 - y_5)\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5 + 2y_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ca II
$\mathbf{B_{24}}$	$(x_5 - y_5)\;\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5 - y_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ca II
$\mathbf{B_{25}}$	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\;\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{26}}$	$-y_6\,\mathbf{a}_1 + (x_6 - y_6)\;\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{27}}$	$-(x_6 - y_6)\;\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{28}}$	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 + y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{29}}$	$y_6\,\mathbf{a}_1 - (x_6 - y_6)\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_6 + 2y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{30}}$	$(x_6 - y_6)\;\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_6 - y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{31}}$	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 + y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\;\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{32}}$	$-y_7\,\mathbf{a}_1 + (x_7 - y_7)\;\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - 2y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{33}}$	$-(x_7 - y_7)\;\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_7 - y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{34}}$	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 + y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{35}}$	$y_7\,\mathbf{a}_1 - (x_7 - y_7)\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_7 + 2y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{36}}$	$(x_7 - y_7)\;\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_7 - y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{37}}$	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 + y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_8 - y_8)\;\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{38}}$	$-y_8\,\mathbf{a}_1 + (x_8 - y_8)\;\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - 2y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{39}}$	$-(x_8 - y_8)\;\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_8 - y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{40}}$	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\;\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 + y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_8 - y_8)\;\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{41}}$	$y_8\,\mathbf{a}_1 - (x_8 - y_8)\;\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_8 + 2y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{42}}$	$(x_8 - y_8)\;\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_8 - y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{43}}$	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_8 + y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_8 - y_8)\;\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{44}}$	$y_8\,\mathbf{a}_1 - (x_8 - y_8)\;\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_8 + 2y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{45}}$	$(x_8 - y_8)\;\mathbf{a}_1 + x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_8 - y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{46}}$	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 + y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_8 - y_8)\;\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{47}}$	$-y_8\,\mathbf{a}_1 + (x_8 - y_8)\;\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - 2y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{48}}$	$-(x_8 - y_8)\;\mathbf{a}_1 - x_8\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\;\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_8 - y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{49}}$	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_9 + y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_9 - y_9)\;\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{50}}$	$-y_9\,\mathbf{a}_1 + (x_9 - y_9)\;\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_9 - 2y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{51}}$	$-(x_9 - y_9)\;\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_9 - y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{52}}$	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\;\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_9 + y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_9 - y_9)\;\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{53}}$	$y_9\,\mathbf{a}_1 - (x_9 - y_9)\;\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_9 + 2y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{54}}$	$(x_9 - y_9)\;\mathbf{a}_1 + x_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\;\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_9 - y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{55}}$	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_9 + y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_9 - y_9)\;\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{56}}$	$y_9\,\mathbf{a}_1 - (x_9 - y_9)\;\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_9 + 2y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(12i)	O IV

$\mathbf{B_{57}}$	=	$(x_9 - y_9)\ \mathbf{a}_1 + x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_9 - y_9)\ \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{58}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right)\ \mathbf{a}_3$	=	$\frac{1}{2}a\,(x_9 + y_9)\ \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_9 - y_9)\ \hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right)\ \hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{59}}$	=	$-y_9\,\mathbf{a}_1 + (x_9 - y_9)\ \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right)\ \mathbf{a}_3$	=	$\frac{1}{2}a\,(x_9 - 2y_9)\ \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right)\ \hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{60}}$	=	$-(x_9 - y_9)\ \mathbf{a}_1 - x_9\,\mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right)\ \mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_9 - y_9)\ \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right)\ \hat{\mathbf{z}}$	(12i)	O IV

References

[1] S. M. Antao and I. Hassan, *Gaudefroyite, $Ca_8Mn_6^{3+}[(BO_3)_6(CO_3)_2O_6]$: High-Temperature Crystal Structure*, Can. Mineral. **46**, 183–193 (2008), doi:10.3749/canmin.46.1.183.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

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).