$Mg_3Cr_2Al_{18}$ Structure: A18B2C3_cF184_227_fg_d_ac-001

This structure previously used the label(s) `A18B2C3_cF184_227_fg_d_ac`. Calls to these addresses will be redirected here.

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- 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.

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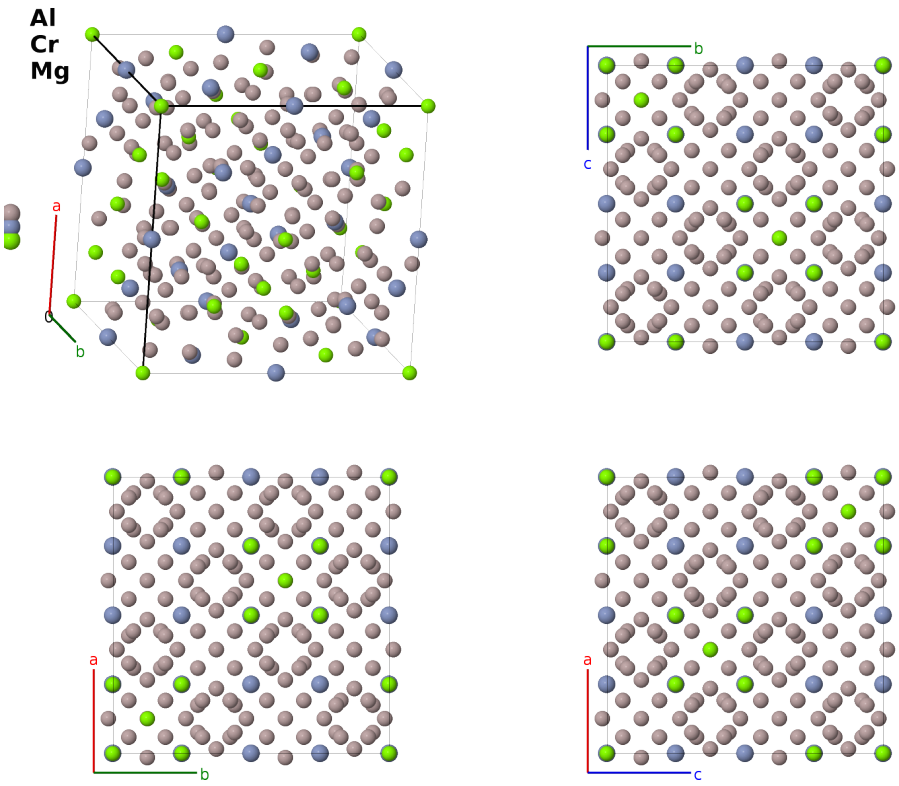
https://aflow.org/prototype-encyclopedia/3DEV

https://aflow.org/prototype-encyclopedia/A18B2C3_cF184_227_fg_d_ac-001



Prototype	$Al_{18}Cr_2Mg_3$
AFLOW prototype label	A18B2C3_cF184_227_fg_d_ac-001
ICSD	57659
CCDC	1621707
Pearson symbol	cF184
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A18B2C3_cF184_227_fg_d_ac-001 --params=`a, x_4, x_5, z_5

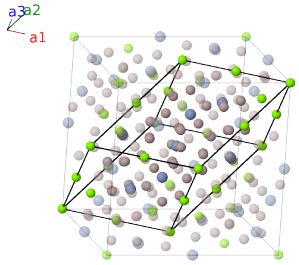
Other compounds with this structure

$Mg_3Mn_2Al_{18}$, $Mg_3Mo_2Al_{18}$, $Mg_3Ta_2Al_{18}$, $Mg_3Ti_2Al_{18}$, $Mg_3V_2Al_{18}$, $Mg_3W_2Al_{18}$, $CaCr_2Al_{20}$, $CeCr_2Al_{20}$, $CeIr_2Zn_{20}$, $CeNi_2Cd_{20}$, $CePd_2Cd_{20}$, $CePt_2Cd_{20}$, $CeTi_2Al_{20}$, CeV_2Al_{20}, $DyCr_2Al_{20}$, $DyRu_2Zn_{20}$, $ErCr_2Al_{20}$, ErV_2Al_{20}, $EuCr_2Al_{20}$, $EuTa_2Al_{20}$, $EuTi_2Al_{20}$, EuV_2Al_{20}, $GdCr_2Al_{20}$, $GdCr_2Cd_{20}$, $GdCo_2Zn_{20}$, $GdNi_2Cd_{20}$, GdV_2Al_{20}, $HfRu_2Zn_{20}$, $HoCr_2Al_{20}$, $LaCr_2Al_{20}$, $LaNi_2Cd_{20}$, $LaPt_2Cd_{20}$, $LaTi_2Al_{20}$, LaV_2Al_{20}, LuV_2Al_{20}, $NbFe_2Zn_{20}$, $NdCr_2Al_{20}$, $NdNi_2Cd_{20}$, $NdPt_2Cd_{20}$, $PrCr_2Al_{20}$, $PrNi_2Cd_{20}$, $PrPd_2Cd_{20}$, $PrPt_2Cd_{20}$, $PrTi_2Al_{20}$, PrV_2Al_{20}, ScV_2Al_{20}, $SmCr_2Al_{20}$, $SmNi_2Cd_{20}$, $SmPd_2Cd_{20}$, $SmPt_2Cd_{20}$, $SmTi_2Al_{20}$, SmV_2Al_{20}, $TbFe_2Zn_{20}$, $TbNb_2Cd_{20}$, ThV_2Al_{20}, UCo_2Zn_{20}, UCr_2Al_{20}, UFe_2Zn_{20}, UIr_2Zn_{20}, UNb_2Al_{20}, UOs_2Zn_{20}, UPd_2Cd_{20}, URh_2Zn_{20}, URu_2Zn_{20}, UV_2Al_{20}, YCr_2Al_{20}, YNi_2Cd_{20}, YRu_2Zn_{20}, YV_2Al_{20}, $YbCr_2Al_{20}$, $YbTi_2Al_{20}$, $ZrCo_2Zn_{20}$, $ZrCu_2Zn_{20}$, $ZrFe_2Zn_{20}$, $ZrNi_2Zn_{20}$

- (Samson, 1958) gives the atomic coordinates in terms of Setting 1 of space group $F\bar{4}dm$ #227. We have shifted this to the standard Setting 2, where the inversion site of the lattice is at the origin.
- If the (8a), (16c) and (16d) sites are occupied by the same type of atom this becomes the $Zn_{22}Zr$ structure.
- In the ternary compounds $LnMX_{20}$, the rare earth (Ln) metal occupies the (8a) site, the transition metal (M) the (16d) site, and X=Al,Cd,Zn occupies the (16c), (48gf) and (96g) sites. These compounds are sometimes listed under the $CeCr_2Al_{20}$ prototype.

Face-centered Cubic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	Mg I
$\mathbf{B_2}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$	(8a)	Mg I
$\mathbf{B_3}$	=	0	=	0	(16c)	Mg II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(16c)	Mg II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Mg II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Mg II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(16d)	Cr I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(16d)	Cr I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16d)	Cr I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16d)	Cr I
$\mathbf{B_{11}}$	=	$-\left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Al I
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Al I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Al I
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Al I

$$\mathbf{B_{15}} = x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(x_4 - \tfrac{1}{4}\right)\,\mathbf{a}_3 = \tfrac{1}{8}a\,\hat{\mathbf{x}} + \tfrac{1}{8}a\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}} \quad (48f) \quad \text{Al I}$$

$$\mathbf{B_{16}} = -\left(x_4 - \tfrac{1}{4}\right)\,\mathbf{a}_1 - \left(x_4 - \tfrac{1}{4}\right)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3 = \tfrac{1}{8}a\,\hat{\mathbf{x}} + \tfrac{1}{8}a\,\hat{\mathbf{y}} - a\left(x_4 - \tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (48f) \quad \text{Al I}$$

$$\mathbf{B_{17}} = \left(x_4 + \tfrac{3}{4}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(x_4 + \tfrac{3}{4}\right)\,\mathbf{a}_3 = \tfrac{3}{8}a\,\hat{\mathbf{x}} + a\left(x_4 + \tfrac{3}{4}\right)\,\hat{\mathbf{y}} + \tfrac{3}{8}a\,\hat{\mathbf{z}} \quad (48f) \quad \text{Al I}$$

$$\mathbf{B_{18}} = -x_4\,\mathbf{a}_1 + \left(x_4 + \tfrac{3}{4}\right)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3 = \tfrac{3}{8}a\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + \tfrac{3}{8}a\,\hat{\mathbf{z}} \quad (48f) \quad \text{Al I}$$

$$\mathbf{B_{19}} = -x_4\,\mathbf{a}_1 + \left(x_4 + \tfrac{3}{4}\right)\,\mathbf{a}_2 + \left(x_4 + \tfrac{3}{4}\right)\,\mathbf{a}_3 = a\left(x_4 + \tfrac{3}{4}\right)\,\hat{\mathbf{x}} + \tfrac{3}{8}a\,\hat{\mathbf{y}} + \tfrac{3}{8}a\,\hat{\mathbf{z}} \quad (48f) \quad \text{Al I}$$

$$\mathbf{B_{20}} = \left(x_4 + \tfrac{3}{4}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} + \tfrac{3}{8}a\,\hat{\mathbf{y}} + \tfrac{3}{8}a\,\hat{\mathbf{z}} \quad (48f) \quad \text{Al I}$$

$$\mathbf{B_{21}} = -x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(x_4 + \tfrac{3}{4}\right)\,\mathbf{a}_3 = \tfrac{3}{8}a\,\hat{\mathbf{x}} + \tfrac{3}{8}a\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}} \quad (48f) \quad \text{Al I}$$

$$\mathbf{B_{22}} = \left(x_4 + \tfrac{3}{4}\right)\,\mathbf{a}_1 + \left(x_4 + \tfrac{3}{4}\right)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3 = \tfrac{3}{8}a\,\hat{\mathbf{x}} + \tfrac{3}{8}a\,\hat{\mathbf{y}} + a\left(x_4 + \tfrac{3}{4}\right)\,\hat{\mathbf{z}} \quad (48f) \quad \text{Al I}$$

$$\mathbf{B_{23}} = z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + (2x_5 - z_5)\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{24}} = z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - \left(2x_5 + z_5 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{25}} = (2x_5 - z_5)\,\mathbf{a}_1 - \left(2x_5 + z_5 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = -a\left(x_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - a\left(z_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{26}} = -\left(2x_5 + z_5 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + (2x_5 - z_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} - a\left(x_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(z_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{27}} = (2x_5 - z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{28}} = -\left(2x_5 + z_5 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = az_5\,\hat{\mathbf{x}} - a\left(x_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{29}} = z_5\,\mathbf{a}_1 + (2x_5 - z_5)\,\mathbf{a}_2 - \left(2x_5 + z_5 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(z_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{30}} = z_5\,\mathbf{a}_1 - \left(2x_5 + z_5 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + (2x_5 - z_5)\,\mathbf{a}_3 = -a\left(z_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - a\left(x_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{31}} = z_5\,\mathbf{a}_1 + (2x_5 - z_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{32}} = z_5\,\mathbf{a}_1 - \left(2x_5 + z_5 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = -a\left(x_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} - a\left(x_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{33}} = -\left(2x_5 + z_5 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + (2x_5 - z_5)\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} - a\left(z_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{34}} = (2x_5 - z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - \left(2x_5 + z_5 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(z_5 - \tfrac{1}{4}\right)\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{35}} = -z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + \left(2x_5 + z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(x_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{36}} = -z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - (2x_5 - z_5)\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{37}} = -(2x_5 - z_5)\,\mathbf{a}_1 + \left(2x_5 + z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = a\left(x_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + a\left(z_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{38}} = \left(2x_5 + z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - (2x_5 - z_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(z_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{39}} = -(2x_5 - z_5)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + \left(2x_5 + z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(x_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(z_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{40}} = \left(2x_5 + z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - (2x_5 - z_5)\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} + a\left(z_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{41}} = -z_5\,\mathbf{a}_1 - (2x_5 - z_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{42}} = -z_5\,\mathbf{a}_1 + \left(2x_5 + z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = a\left(x_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} + a\left(x_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$$\mathbf{B_{43}} = -z_5\,\mathbf{a}_1 - (2x_5 - z_5)\,\mathbf{a}_2 + \left(2x_5 + z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(z_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_5 + \tfrac{1}{4}\right)\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}} \quad (96g) \quad \text{Al II}$$

$\mathbf{B_{44}}$	=	$-z_5\,\mathbf{a}_1 + \left(2x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(2x_5 - z_5\right)\,\mathbf{a}_3$	=	$a\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{45}}$	=	$\left(2x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{46}}$	=	$-\left(2x_5 - z_5\right)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(96g)	Al II

References

[1] S. Samson, *The Crystal Structure of the Intermetallic Compound $Mg_3Cr_2Al_{18}$*, Acta Cryst. **11** (1958), doi:10.1107/S0365110X58002425.

Found in

[1] S. Samson, *The Crystal Structure of the Intermetallic Compound $ZrZn_{22}$*, Acta Cryst. **14** (1961), doi:10.1107/S0365110X61003600.

First cited in

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.