$Mg_3Cr_2Al_{18}$ Structure: A18B2C3_cF184_227_fg_d_ac-001

This structure originally had the label `A18B2C3_cF184_227_fg_d_ac`. Calls to that address will be redirected here.

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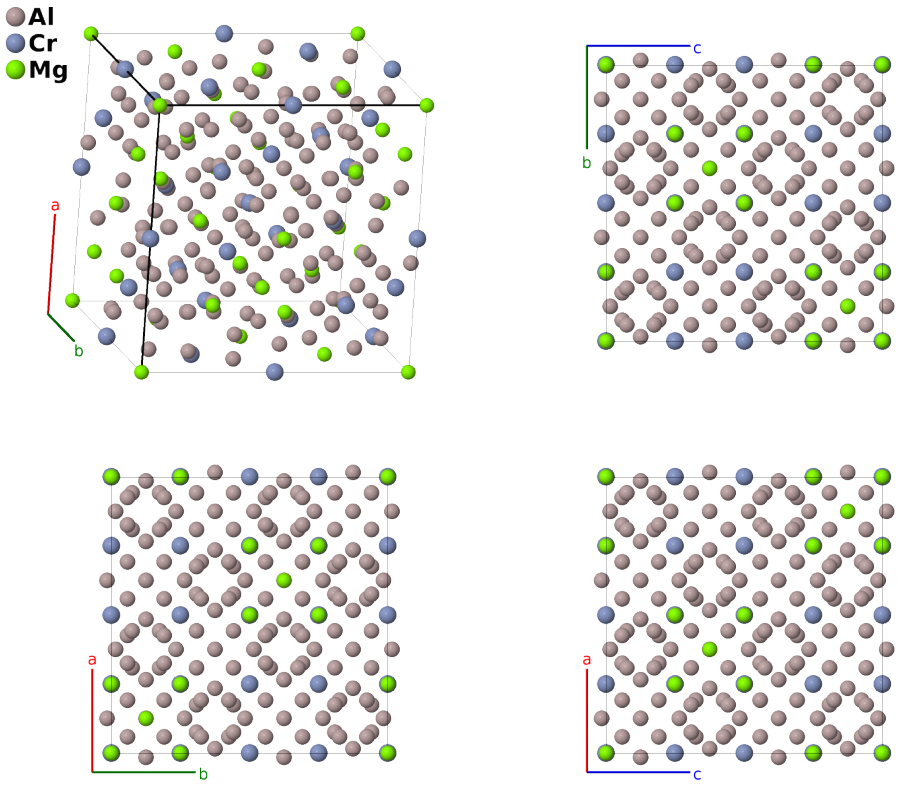
https://aflow.org/p/3DEV

https://aflow.org/p/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
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

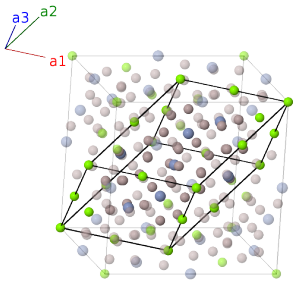
Other compounds with this structure

$LaCr_2Al_{20}$, $CeCr_2Al_{20}$, $PrCr_2Al_{20}$, $SmCr_2Al_{20}$, $YbCr_2Al_{20}$, $CeTi_2Al_{20}$, $PrTi_2Al_{20}$, $SmTi_2Al_{20}$, $YbTi_2Al_{20}$, CeV_2Al_{20}, GdV_2Al_{20}, LaV_2Al_{20}, PrV_2Al_{20}, SmV_2Al_{20}, $CeNi_2Cd_{20}$, $GdNi_2Cd_{20}$, $LaNi_2Cd_{20}$, $NdNi_2Cd_{20}$, $PrNi_2Cd_{20}$, $SmNi_2Cd_{20}$, YNi_2Cd_{20}, $CePd_2Cd_{20}$, $PrPd_2Cd_{20}$, $SmPd_2Cd_{20}$, UOs_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

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



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
$\mathbf{B_{15}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(48f)	Al I
$\mathbf{B_{16}}$	=	$-\left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48f)	Al I
$\mathbf{B_{17}}$	=	$\left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + a\left(x_4 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Al I
$\mathbf{B_{18}}$	=	$-x_4\,\mathbf{a}_1 + \left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Al I
$\mathbf{B_{19}}$	=	$-x_4\,\mathbf{a}_1 + \left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Al I
$\mathbf{B_{20}}$	=	$\left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Al I

$\mathbf{B_{21}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(48f)	Al I
$\mathbf{B_{22}}$	=	$\left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + a\left(x_4 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(48f)	Al I
$\mathbf{B_{23}}$	=	$z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + (2x_5 - z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{24}}$	=	$z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - \left(2x_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{25}}$	=	$(2x_5 - z_5)\,\mathbf{a}_1 - \left(2x_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - a\left(z_5 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{26}}$	=	$-\left(2x_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + (2x_5 - z_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(z_5 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{27}}$	=	$(2x_5 - z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{28}}$	=	$-\left(2x_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{29}}$	=	$z_5\,\mathbf{a}_1 + (2x_5 - z_5)\,\mathbf{a}_2 - \left(2x_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(z_5 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{30}}$	=	$z_5\,\mathbf{a}_1 - \left(2x_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + (2x_5 - z_5)\,\mathbf{a}_3$	=	$-a\left(z_5 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{31}}$	=	$z_5\,\mathbf{a}_1 + (2x_5 - z_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{32}}$	=	$z_5\,\mathbf{a}_1 - \left(2x_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} - a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{33}}$	=	$-\left(2x_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + (2x_5 - z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - a\left(z_5 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{34}}$	=	$(2x_5 - z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - \left(2x_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(z_5 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{35}}$	=	$-z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + \left(2x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{36}}$	=	$-z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - (2x_5 - z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{37}}$	=	$-(2x_5 - z_5)\,\mathbf{a}_1 + \left(2x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + a\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{38}}$	=	$\left(2x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - (2x_5 - z_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{39}}$	=	$-(2x_5 - z_5)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + \left(2x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{40}}$	=	$\left(2x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - (2x_5 - z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + a\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{41}}$	=	$-z_5\,\mathbf{a}_1 - (2x_5 - z_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{42}}$	=	$-z_5\,\mathbf{a}_1 + \left(2x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} + a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{43}}$	=	$-z_5\,\mathbf{a}_1 - (2x_5 - z_5)\,\mathbf{a}_2 + \left(2x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(96g)	Al II
$\mathbf{B_{44}}$	=	$-z_5\,\mathbf{a}_1 + \left(2x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - (2x_5 - z_5)\,\mathbf{a}_3$	=	$a\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{46}}$	=	$-(2x_5 - z_5)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(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.