Mg_3Ru_2 Structure: A3B2_cP20_213_d_c-001

This structure previously used the label(s) `A3B2_cP20_213_d_c`. Calls to these addresses will be redirected here.

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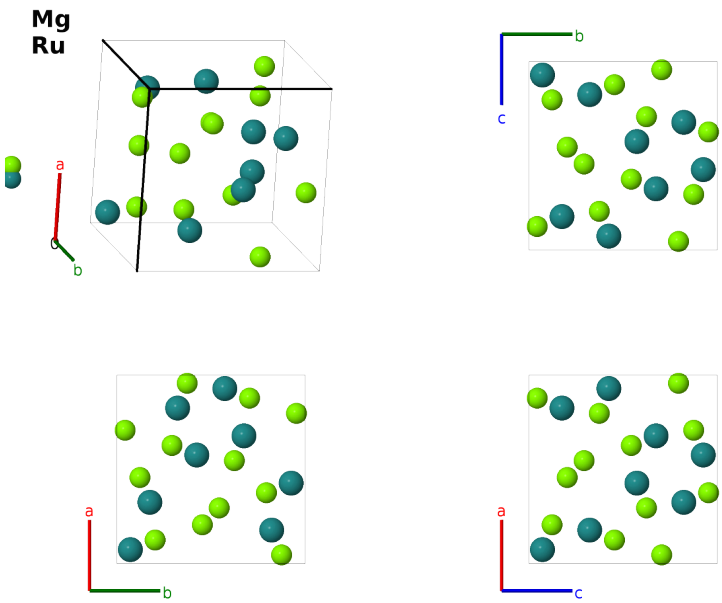
https://aflow.org/prototype-encyclopedia/6QE7

https://aflow.org/prototype-encyclopedia/A3B2_cP20_213_d_c-001

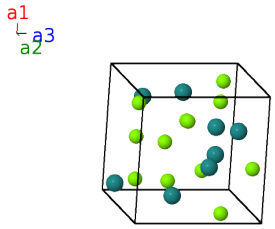


Prototype	Mg_3Ru_2
AFLOW prototype label	A3B2_cP20_213_d_c-001
ICSD	260022
CCDC	1718052
Pearson symbol	cP20
Space group number	213
Space group symbol	$P4_132$
AFLOW prototype command	`aflow --proto=A3B2_cP20_213_d_c-001 --params=`a, x_1, y_2

- This is the binary form of the β-Mn ($A13$) structure.
- This structure may also be found in the enantiomorphic space group $P4_332$ #212.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(8c)	Ru I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ru I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ru I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(8c)	Ru I
$\mathbf{B_5}$	=	$\left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Ru I
$\mathbf{B_6}$	=	$-\left(x_1 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{3}{4}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{3}{4}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{3}{4}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Ru I
$\mathbf{B_7}$	=	$\left(x_1 + \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_1 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Ru I
$\mathbf{B_8}$	=	$-\left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8c)	Ru I
$\mathbf{B_9}$	=	$\frac{1}{8}\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} + a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(12d)	Mg I
$\mathbf{B_{10}}$	=	$\frac{3}{8}\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} + a\left(y_2 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(12d)	Mg I
$\mathbf{B_{11}}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(12d)	Mg I
$\mathbf{B_{12}}$	=	$\frac{5}{8}\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{5}{8}a\,\hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_2 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(12d)	Mg I
$\mathbf{B_{13}}$	=	$\left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}}$	(12d)	Mg I
$\mathbf{B_{14}}$	=	$\left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}}$	(12d)	Mg I
$\mathbf{B_{15}}$	=	$-\left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Mg I
$\mathbf{B_{16}}$	=	$-\left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{5}{8}a\,\hat{\mathbf{y}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Mg I
$\mathbf{B_{17}}$	=	$y_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(12d)	Mg I
$\mathbf{B_{18}}$	=	$-y_2\,\mathbf{a}_1 + \left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + a\left(y_2 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(12d)	Mg I
$\mathbf{B_{19}}$	=	$\left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$	(12d)	Mg I
$\mathbf{B_{20}}$	=	$-\left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_2 - \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{5}{8}a\,\hat{\mathbf{z}}$	(12d)	Mg I

References

[1] R. Pöttgen, V. Hlukhyy, A. Baranov, and Y. Grin, *Crystal Structure and Chemical Bonding of Mg_3Ru_2*, Inorg. Chem. **47**, 6051–6055 (2008), doi:10.1021/ic800387a.

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