

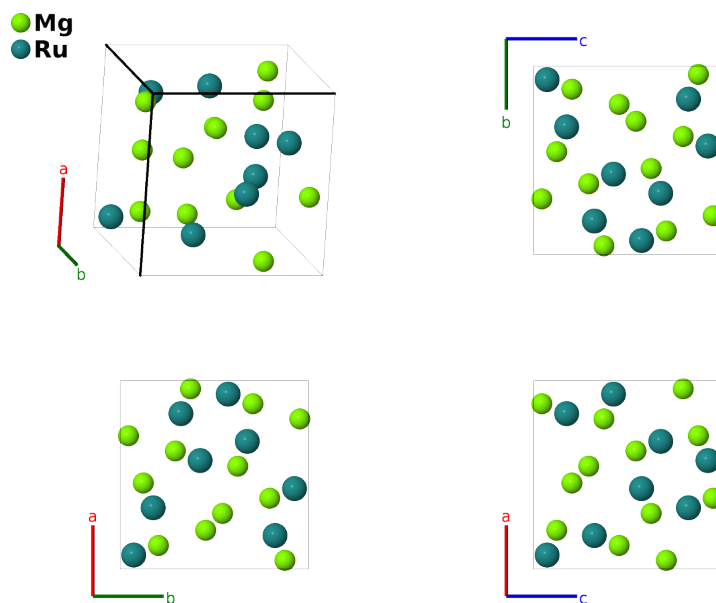
Mg₃Ru₂ Structure: A3B2_cP20_213_d_c-001

This structure originally had the label A3B2_cP20_213_d_c. Calls to that address will be redirected here.

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<https://afLOW.org/p/6QE7>

https://afLOW.org/p/A3B2_cP20_213_d_c-001

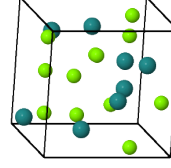


Prototype	Mg ₃ Ru ₂
AFLOW prototype label	A3B2_cP20_213_d_c-001
ICSD	260022
Pearson symbol	cP20
Space group number	213
Space group symbol	<i>P</i> 4 ₁ 32
AFLOW prototype command	<code>afLOW --proto=A3B2_cP20_213_d_c-001 --params=<i>a</i>, <i>x</i>₁, <i>y</i>₂</code>

- This is the binary form of the β -Mn (*A13*) structure.
- This structure may also be found in the enantiomorphic space group *P*4₃32 #212.

Simple Cubic primitive vectors

a1
a2
a3



$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$

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	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 - x_1 \mathbf{a}_2 + (x_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Ru I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 - (x_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Ru I
\mathbf{B}_4	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(8c)	Ru I
\mathbf{B}_5	$= (x_1 + \frac{3}{4}) \mathbf{a}_1 + (x_1 + \frac{1}{4}) \mathbf{a}_2 - (x_1 - \frac{1}{4}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{3}{4}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{z}}$	(8c)	Ru I
\mathbf{B}_6	$= -(x_1 - \frac{3}{4}) \mathbf{a}_1 - (x_1 - \frac{3}{4}) \mathbf{a}_2 - (x_1 - \frac{3}{4}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{3}{4}) \hat{\mathbf{x}} - a(x_1 - \frac{3}{4}) \hat{\mathbf{y}} - a(x_1 - \frac{3}{4}) \hat{\mathbf{z}}$	(8c)	Ru I
\mathbf{B}_7	$= (x_1 + \frac{1}{4}) \mathbf{a}_1 - (x_1 - \frac{1}{4}) \mathbf{a}_2 + (x_1 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_1 + \frac{3}{4}) \hat{\mathbf{z}}$	(8c)	Ru I
\mathbf{B}_8	$= -(x_1 - \frac{1}{4}) \mathbf{a}_1 + (x_1 + \frac{3}{4}) \mathbf{a}_2 + (x_1 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_1 + \frac{3}{4}) \hat{\mathbf{y}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(8c)	Ru I
\mathbf{B}_9	$= \frac{1}{8} \mathbf{a}_1 + y_2 \mathbf{a}_2 + (y_2 + \frac{1}{4}) \mathbf{a}_3$	$=$	$\frac{1}{8} a \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + a(y_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(12d)	Mg I
\mathbf{B}_{10}	$= \frac{3}{8} \mathbf{a}_1 - y_2 \mathbf{a}_2 + (y_2 + \frac{3}{4}) \mathbf{a}_3$	$=$	$\frac{3}{8} a \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + a(y_2 + \frac{3}{4}) \hat{\mathbf{z}}$	(12d)	Mg I
\mathbf{B}_{11}	$= \frac{7}{8} \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (y_2 - \frac{1}{4}) \mathbf{a}_3$	$=$	$\frac{7}{8} a \hat{\mathbf{x}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(12d)	Mg I
\mathbf{B}_{12}	$= \frac{5}{8} \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 - (y_2 - \frac{3}{4}) \mathbf{a}_3$	$=$	$\frac{5}{8} a \hat{\mathbf{x}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - a(y_2 - \frac{3}{4}) \hat{\mathbf{z}}$	(12d)	Mg I
\mathbf{B}_{13}	$= (y_2 + \frac{1}{4}) \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + y_2 \mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}}$	(12d)	Mg I
\mathbf{B}_{14}	$= (y_2 + \frac{3}{4}) \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 - y_2 \mathbf{a}_3$	$=$	$a(y_2 + \frac{3}{4}) \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}}$	(12d)	Mg I
\mathbf{B}_{15}	$= -(y_2 - \frac{1}{4}) \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + (y_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{7}{8} a \hat{\mathbf{y}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	Mg I
\mathbf{B}_{16}	$= -(y_2 - \frac{3}{4}) \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 - (y_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_2 - \frac{3}{4}) \hat{\mathbf{x}} + \frac{5}{8} a \hat{\mathbf{y}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	Mg I
\mathbf{B}_{17}	$= y_2 \mathbf{a}_1 + (y_2 + \frac{1}{4}) \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} + a(y_2 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}}$	(12d)	Mg I
\mathbf{B}_{18}	$= -y_2 \mathbf{a}_1 + (y_2 + \frac{3}{4}) \mathbf{a}_2 + \frac{3}{8} \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} + a(y_2 + \frac{3}{4}) \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}}$	(12d)	Mg I
\mathbf{B}_{19}	$= (y_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{4}) \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{7}{8} a \hat{\mathbf{z}}$	(12d)	Mg I
\mathbf{B}_{20}	$= -(y_2 - \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{3}{4}) \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_2 - \frac{3}{4}) \hat{\mathbf{y}} + \frac{5}{8} a \hat{\mathbf{z}}$	(12d)	Mg I

References

- [1] R. Pöttgen, V. Hlukhyy, A. Baranov, and Y. Grin, *Crystal Structure and Chemical Bonding of Mg₃Ru₂*, *Inorg. Chem.* **47**, 6051–6055 (2008), doi:10.1021/ic800387a.