

URu₃B₂ Structure:

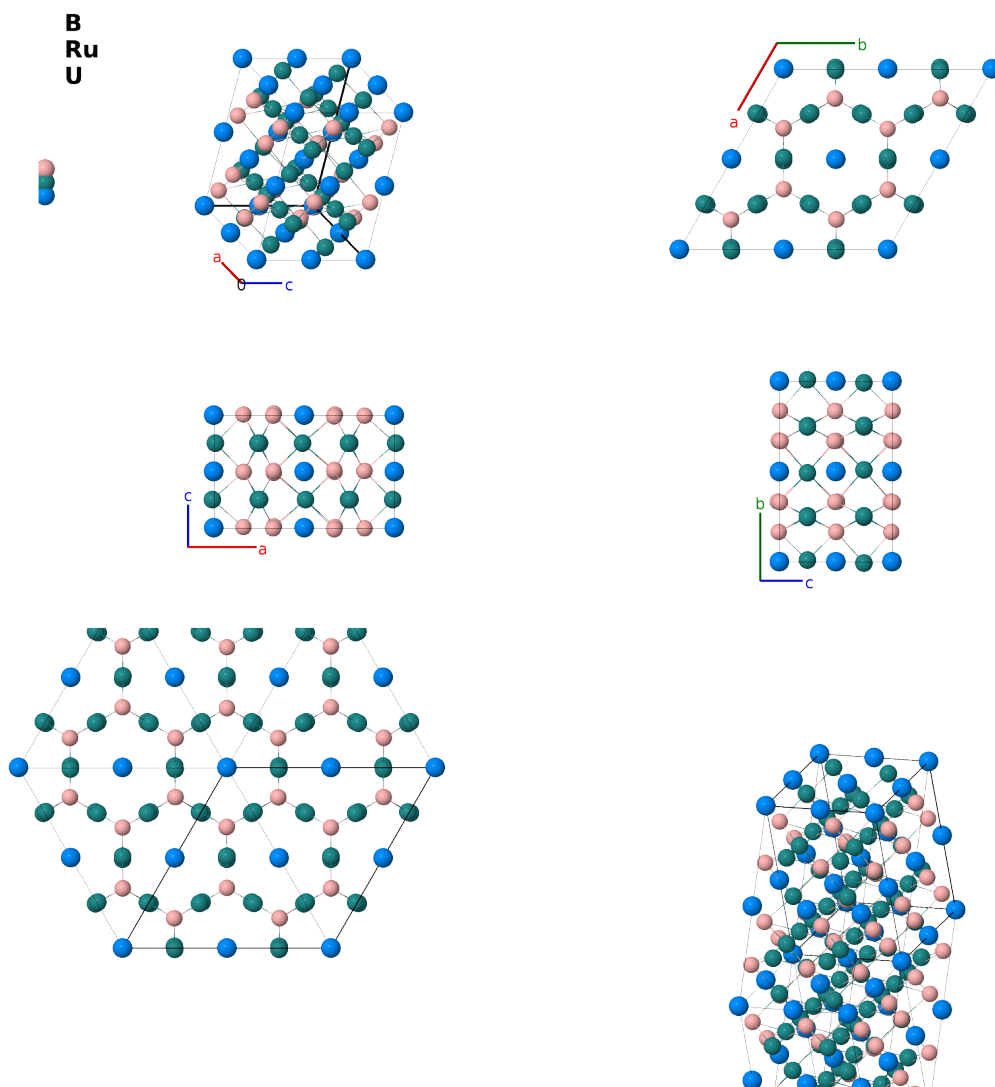
A2B3C_hP48_147_2d2g_4g_abef-001

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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.

<https://aflow.org/prototype-encyclopedia/B1DH>

https://aflow.org/prototype-encyclopedia/A2B3C_hP48_147_2d2g_4g_abef-001



Prototype	B ₂ Ru ₃ U
AFLOW prototype label	A2B3C_hP48_147_2d2g_4g_abef-001
ICSD	44578
CCDC	1613950
Pearson symbol	hP48

Space group number 147

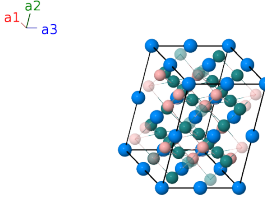
Space group symbol $P\bar{3}$

AFLOW prototype command `aflow --proto=A2B3C_hP48_147_2d2g_4g_abef-001`
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Other compounds with this structure

UOs₃B₂

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(1a)	U I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(1b)	U II
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2d)	B I
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(2d)	B I
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2d)	B II
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(2d)	B II
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(3e)	U III
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(3e)	U III
$\mathbf{B}_9$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	(3e)	U III
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3f)	U IV
$\mathbf{B}_{11}$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3f)	U IV
$\mathbf{B}_{12}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3f)	U IV
$\mathbf{B}_{13}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_7 - y_7) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(6g)	B III
$\mathbf{B}_{14}$	$= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(6g)	B III
$\mathbf{B}_{15}$	$= -(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(6g)	B III
$\mathbf{B}_{16}$	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_7 + y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_7 - y_7) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(6g)	B III
$\mathbf{B}_{17}$	$= y_7 \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_7 + 2y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(6g)	B III
$\mathbf{B}_{18}$	$= (x_7 - y_7) \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_7 - y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(6g)	B III
$\mathbf{B}_{19}$	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_8 + y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_8 - y_8) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(6g)	B IV
$\mathbf{B}_{20}$	$= -y_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_8 - 2y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(6g)	B IV
$\mathbf{B}_{21}$	$= -(x_8 - y_8) \mathbf{a}_1 - x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(6g)	B IV
$\mathbf{B}_{22}$	$= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_8 + y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_8 - y_8) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(6g)	B IV
$\mathbf{B}_{23}$	$= y_8 \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_8 + 2y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(6g)	B IV

$$\begin{aligned}
\mathbf{B}_{24} &= (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}} & (6g) & \text{B IV} \\
\mathbf{B}_{25} &= 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}} & (6g) & \text{Ru I} \\
\mathbf{B}_{26} &= -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}} & (6g) & \text{Ru I} \\
\mathbf{B}_{27} &= -(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}} & (6g) & \text{Ru I} \\
\mathbf{B}_{28} &= -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}} & (6g) & \text{Ru I} \\
\mathbf{B}_{29} &= 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}} & (6g) & \text{Ru I} \\
\mathbf{B}_{30} &= (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}} & (6g) & \text{Ru I} \\
\mathbf{B}_{31} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (6g) & \text{Ru II} \\
\mathbf{B}_{32} &= -y_{10} \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \frac{1}{2}a(x_{10} - 2y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (6g) & \text{Ru II} \\
\mathbf{B}_{33} &= -(x_{10} - y_{10}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = -\frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (6g) & \text{Ru II} \\
\mathbf{B}_{34} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 = -\frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (6g) & \text{Ru II} \\
\mathbf{B}_{35} &= y_{10} \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 = \frac{1}{2}a(-x_{10} + 2y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (6g) & \text{Ru II} \\
\mathbf{B}_{36} &= (x_{10} - y_{10}) \mathbf{a}_1 + x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 = \frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (6g) & \text{Ru II} \\
\mathbf{B}_{37} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = \frac{1}{2}a(x_{11} + y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{11} - y_{11}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (6g) & \text{Ru III} \\
\mathbf{B}_{38} &= -y_{11} \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3 = \frac{1}{2}a(x_{11} - 2y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (6g) & \text{Ru III} \\
\mathbf{B}_{39} &= -(x_{11} - y_{11}) \mathbf{a}_1 - x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = -\frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (6g) & \text{Ru III} \\
\mathbf{B}_{40} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 = -\frac{1}{2}a(x_{11} + y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{11} - y_{11}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (6g) & \text{Ru III} \\
\mathbf{B}_{41} &= y_{11} \mathbf{a}_1 - (x_{11} - y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3 = \frac{1}{2}a(-x_{11} + 2y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (6g) & \text{Ru III} \\
\mathbf{B}_{42} &= (x_{11} - y_{11}) \mathbf{a}_1 + x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 = \frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (6g) & \text{Ru III} \\
\mathbf{B}_{43} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \frac{1}{2}a(x_{12} + y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{12} - y_{12}) \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (6g) & \text{Ru IV} \\
\mathbf{B}_{44} &= -y_{12} \mathbf{a}_1 + (x_{12} - y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \frac{1}{2}a(x_{12} - 2y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (6g) & \text{Ru IV} \\
\mathbf{B}_{45} &= -(x_{12} - y_{12}) \mathbf{a}_1 - x_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = -\frac{1}{2}a(2x_{12} - y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (6g) & \text{Ru IV} \\
\mathbf{B}_{46} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 = -\frac{1}{2}a(x_{12} + y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{12} - y_{12}) \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (6g) & \text{Ru IV} \\
\mathbf{B}_{47} &= y_{12} \mathbf{a}_1 - (x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3 = \frac{1}{2}a(-x_{12} + 2y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (6g) & \text{Ru IV} \\
\mathbf{B}_{48} &= (x_{12} - y_{12}) \mathbf{a}_1 + x_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 = \frac{1}{2}a(2x_{12} - y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (6g) & \text{Ru IV}
\end{aligned}$$

References

[1] P. Rogl, *The crystal structure of URu₃B₂*, J. Nucl. Mater. **92**, 292–298 (1980), doi:10.1016/0022-3115(80)90113-0.

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