

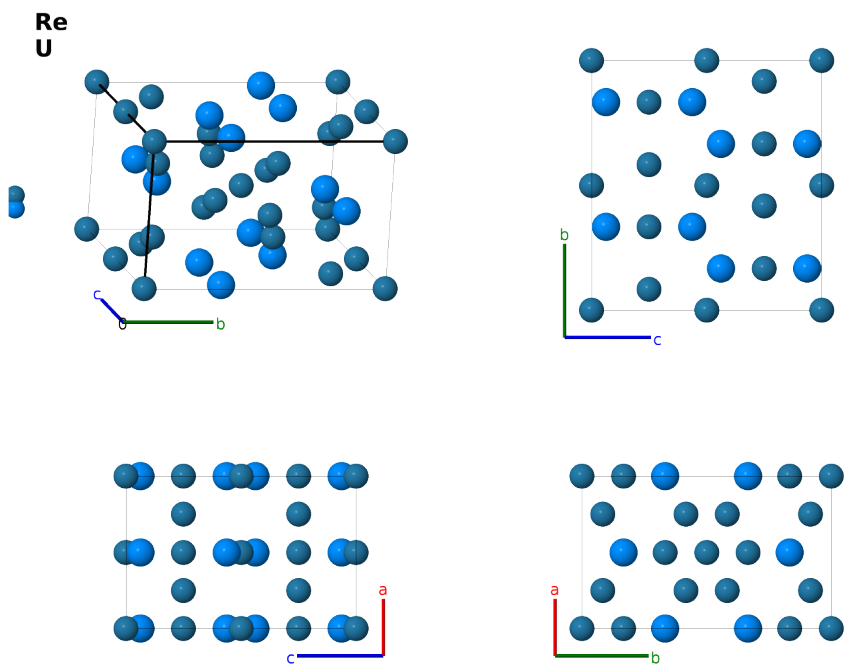
URe₂ Structure: A2B_oC24_63_acg_f-001

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<https://aflow.org/prototype-encyclopedia/RKF7>

https://aflow.org/prototype-encyclopedia/A2B_oC24_63_acg_f-001



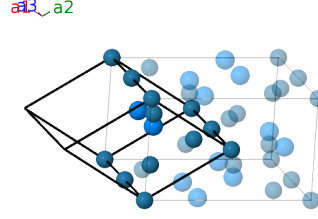
Prototype	Re ₂ U
AFLOW prototype label	A2B_oC24_63_acg_f-001
ICSD	105898
CCDC	1663765
Pearson symbol	oC24
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=A2B_oC24_63_acg_f-001 --params=a, b/a, c/a, y₂, y₃, z₃, x₄, y₄</code>

- Above 180°C URe₂ transforms from this structure to the *C*14 Hexagonal Laves structure. We use the data from (Hatt, 1961) taken at 20°C.

- Although the abstract of (Hatt, 1961) gives the space group as $Cmca$, the text of the paper correctly identifies it as $Cmcm$.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(4a) Re I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(4a) Re I
$\mathbf{B}_3$	$=$	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c) Re II
$\mathbf{B}_4$	$=$	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c) Re II
$\mathbf{B}_5$	$=$	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8f) U I
$\mathbf{B}_6$	$=$	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f) U I
$\mathbf{B}_7$	$=$	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f) U I
$\mathbf{B}_8$	$=$	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8f) U I
$\mathbf{B}_9$	$=$	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g) Re III
$\mathbf{B}_{10}$	$=$	$-(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g) Re III
$\mathbf{B}_{11}$	$=$	$-(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g) Re III
$\mathbf{B}_{12}$	$=$	$(x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g) Re III

References

- [1] B. A. Hatt, *The crystal structure of URe_2* , Acta Cryst. **14**, 119–123 (1961), doi:10.1107/S0365110X61000516.

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- [1] A. Jain, S. Ping, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013), doi:10.1063/1.4812323.

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