URe_2 Structure: A2B_oC24_63_acg_f-001

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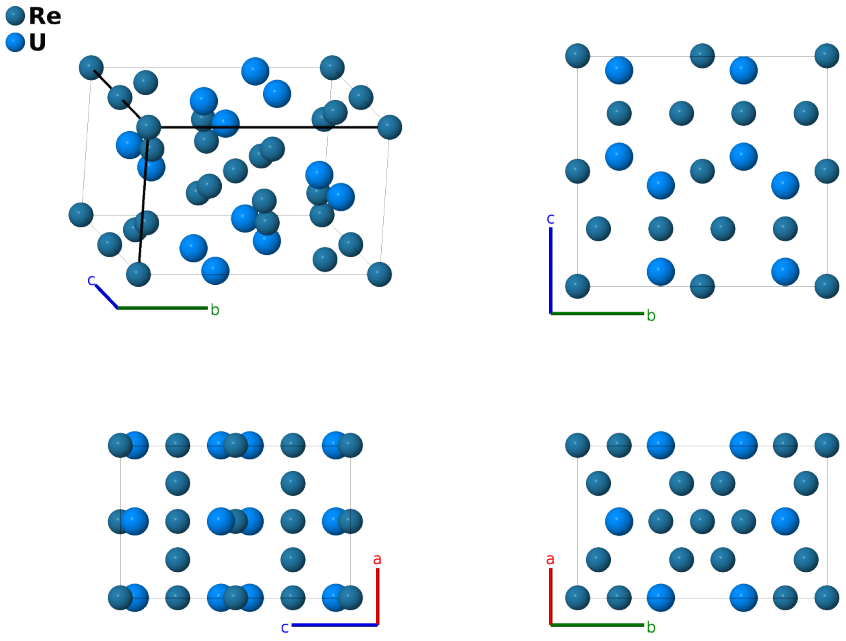
https://aflow.org/p/RKF7

https://aflow.org/p/A2B_oC24_63_acg_f-001

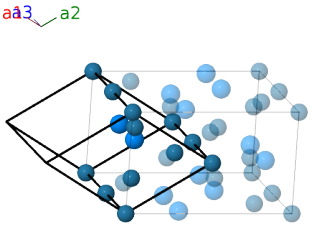


Prototype	Re_2U
AFLOW prototype label	A2B_oC24_63_acg_f-001
ICSD	105898
Pearson symbol	oC24
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=A2B_oC24_63_acg_f-001 --params=`$a, b/a, c/a, y_2, y_3, z_3, x_4, y_4$

- Above 180°C URe_2 transforms from this structure to the $C14$ 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

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



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
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	U I
$\mathbf{B_7}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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.

Found in

[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.