

RuU₂ Structure:

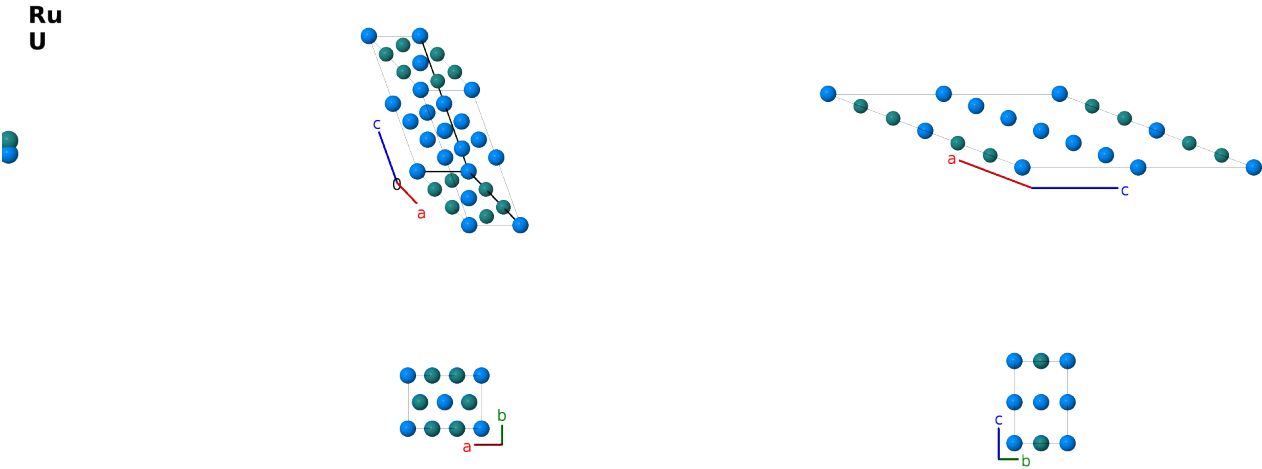
AB2_mC12_12_i_aci-001

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<https://aflow.org/prototype-encyclopedia/6TPG>

https://aflow.org/prototype-encyclopedia/AB2_mC12_12_i_aci-001

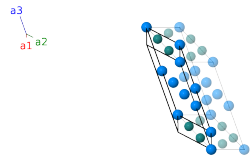


Prototype	RuU ₂
AFLOW prototype label	AB2_mC12_12_i_aci-001
Pearson symbol	mC12
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<code>aflow --proto=AB2_mC12_12_i_aci-001 --params=a, b/a, c/a, β, x_3, z_3, x_4, z_4</code>

- (Berndt, 1961) gives the lattice parameters for the unit cell of RuU₂, but only gives approximate positions for the atoms, and states that the space group is either $P2/m$ #10 or $P2_1/m$ #11.
- We follow Villars and assume that atoms are evenly spaced as shown in Berndt's Figure 2, in which case the space group becomes $C2/m$ #12. To our knowledge there has been no further refinement of this structure.

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) U I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} c \cos \beta \hat{\mathbf{x}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(2c) U II
$\mathbf{B}_3$	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Ru I
$\mathbf{B}_4$	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Ru I
$\mathbf{B}_5$	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) U III
$\mathbf{B}_6$	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) U III

References

- [1] A. F. Berndt, *The unit cell of U_2Ru* , Acta Cryst. **14**, 1301–1302 (1961), doi:10.1107/S0365110X61003879.

Found in

- [1] P. Villars, ed., *PAULING FILE in: Inorganic Solid Phases (online database)* (Springer Materials, Heidelberg, 2016). Cs_4Sb_2 (Cs_2Sb) Crystal Structure.

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