RuU_2 Structure: AB2_mC12_12_i_aci-001

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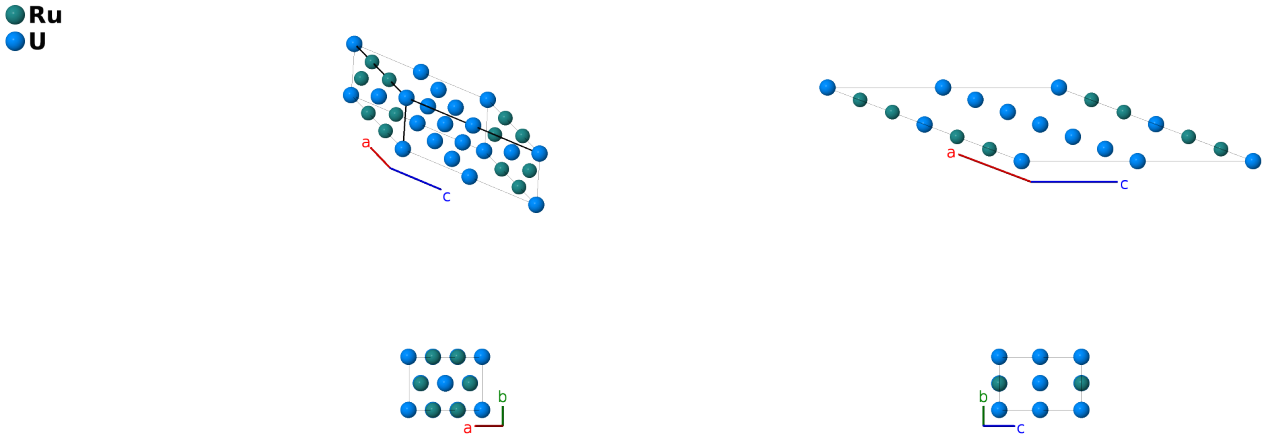
https://aflow.org/p/6TPG

https://aflow.org/p/AB2_mC12_12_i_aci-001

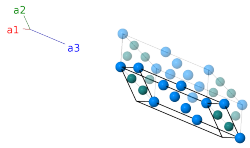


Prototype	RuU_2
AFLOW prototype label	AB2_mC12_12_i_aci-001
ICSD	none
Pearson symbol	mC12
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=AB2_mC12_12_i_aci-001 --params=`$a, b/a, c/a, \beta, x_3, z_3, x_4, z_4$

- (Berndt, 1961) gives the lattice parameters for the unit cell of RuU_2, 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



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.