

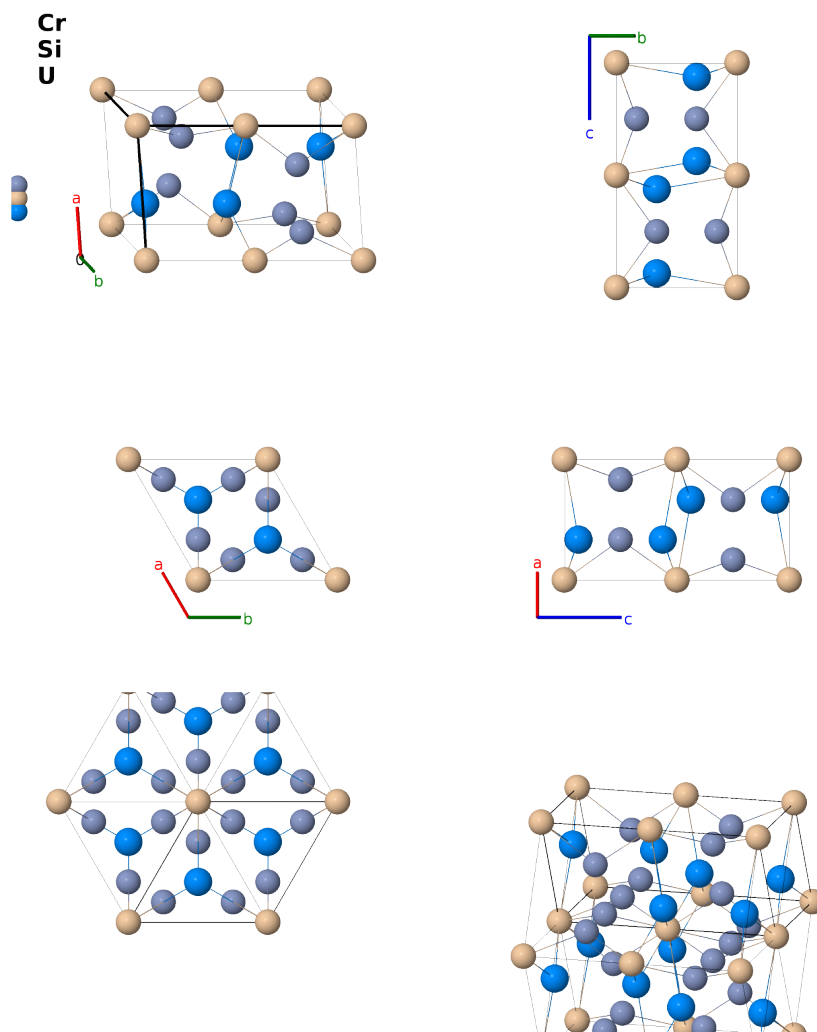
U₂Cr₃Si Structure: A3BC2_hP12_194_h_a_f-002

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<https://aflow.org/prototype-encyclopedia/FW8N>

https://aflow.org/prototype-encyclopedia/A3BC2_hP12_194_h_a_f-002



Prototype	Cr ₃ SiU ₂
AFLOW prototype label	A3BC2_hP12_194_h_a_f-002
ICSD	626830
CCDC	1752198
Pearson symbol	hP12
Space group number	194

Space group symbol $P6_3/mmc$

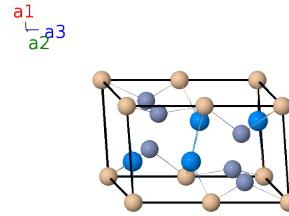
AFLOW prototype command `aflow --proto=A3BC2_hP12_194_h_a_f-002`
`--params=a, c/a, z2, x3`

Other compounds with this structure

Dy₂Al₃Co, Co₂Nb₃Si, Er₂Al₃Co, Eu₂Ga₃Ir, Lu₂Al₃Co, Mg₂Cu₃Si, Mg₂Ir₃Si, Mn₂Co₃Ge, Mo₂Co₃Si, Nb₂Ni₃Si, Pd₂Ga₃U, Ru₂Al₃Sc, Sc₂Fe₃Si, Ta₂Cr₃Cu, Ta₂Ni₃Si, Ti₂Ni₃Si, U₂Al₃Cu, U₂Mn₃Ge, W₂Co₃Si, Zr₂Fe₃Ga, Zr₂Fe₃Ge, Zr₂V₃Ru

- This is a ternary form of the *C14* hexagonal Laves structure. The ICSD lists the prototype as *C14*/MgZn₂, so we chose U₂Cr₃Si as the prototype, as it has a readily available reference.
- U₂Cr₃Si, AFLOW label A3BC2_hP12_194_h_a_f-002, and Ba_xPt₃B₂, A2BC3_hP12_194_f_a_h, occupy the same Wyckoff positions in space group *P6₃/mmc* # 194. They differ in the *c/a* ratio, with U₂Cr₃Si having *c/a* $\approx$ 1.6 and Ba_xPt₃B₂ *c/a* $\approx$ 0.85.

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	(2a)	Si I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2a)	Si I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4f)	U I
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	U I
$\mathbf{B}_5$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4f)	U I
$\mathbf{B}_6$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	U I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cr I
$\mathbf{B}_8$	$= -2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cr I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cr I
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cr I
$\mathbf{B}_{11}$	$= 2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cr I
$\mathbf{B}_{12}$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cr I

References

- [1] J. B. Kusma and H. Nowotny, *Die Kristallstruktur von U₂Cr₃Si, U₄Mn₅Si₃ und U₂Co₃Si*, Monat. Chemie **95**, 1219–1224 (1964), doi:10.1007/BF00904717.

Found in

[1] *Inorganic Crystal Structure Database*. Entry 626830 [U₂Cr₃Si].

First cited in

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