

UCoC₂ Structure:

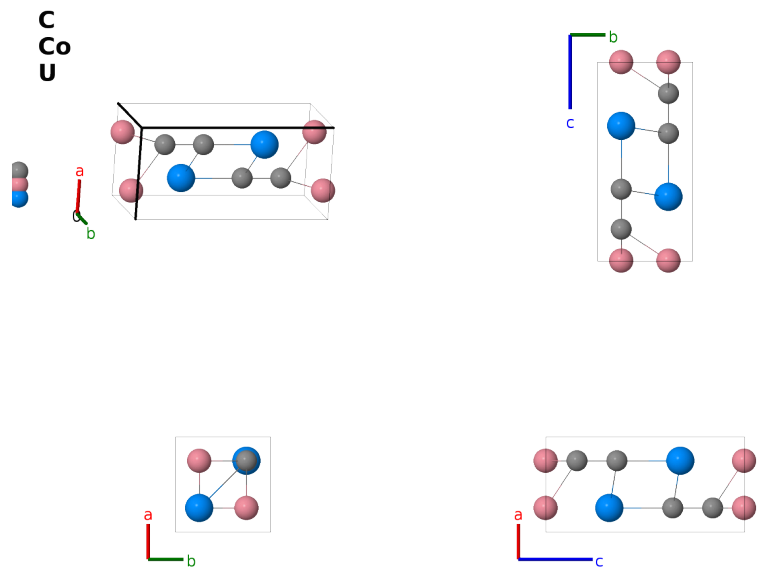
A2BC_tP8_129_2c_a_c-002

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<https://aflow.org/prototype-encyclopedia/K32Y>

https://aflow.org/prototype-encyclopedia/A2BC_tP8_129_2c_a_c-002



Prototype	C ₂ CoU
AFLOW prototype label	A2BC_tP8_129_2c_a_c-002
ICSD	63622
CCDC	1626706
Pearson symbol	tP8
Space group number	129
Space group symbol	<i>P4/nmm</i>
AFLOW prototype command	<code>aflow --proto=A2BC_tP8_129_2c_a_c-002 --params=a, c/a, z₂, z₃, z₄</code>

Other compounds with this structure

PuFeC₂, ScCoC₂, ScNiC₂, ScFeC₂, UFeC₂, UNiC₂

- (Gem's, 1986) found a small concentration of vacancies on the carbon and cobalt sites: 0.3% on Co (2a), 2% on C-I (2c), and 3% on C-II (2c).

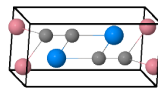
Simple Tetragonal primitive vectors



$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(2a)	Co I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(2a)	Co I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2c)	C I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2c)	C I
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2c)	C II
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(2c)	C II
$\mathbf{B}_7$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2c)	U I
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(2c)	U I

References

- [1] M. H. Gerss and W. Jeitschko, *The crystal structures of ternary actinoid iron (cobalt, nickel) carbides with composition 1:1:2*, Mater. Res. Bull. **21**, 209–216 (1986), doi:10.1016/0025-5408(86)90208-4.

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