

α -U (A20) Structure: A_oC4_63_c-001

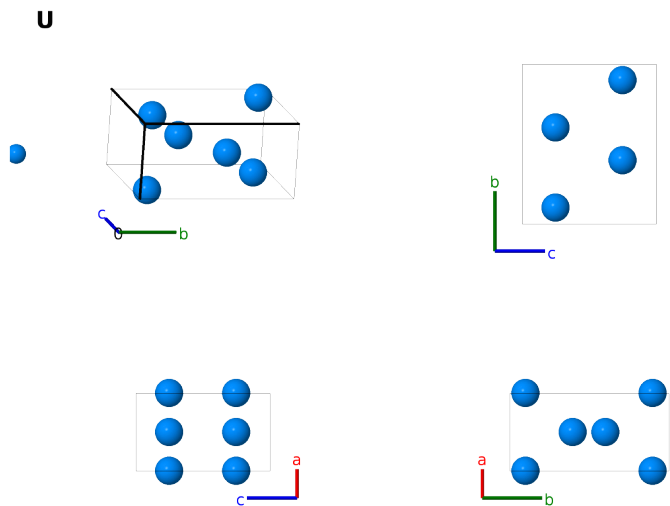
This structure previously used the label(s) **A_oC4_63_c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/AFG5>

https://aflow.org/prototype-encyclopedia/A_oC4_63_c-001



Prototype	U
AFLOW prototype label	A_oC4_63_c-001
<i>Strukturbericht</i> designation	A20
ICSD	106205
CCDC	1664048
Pearson symbol	oC4
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=A_oC4_63_c-001 --params=a, b/a, c/a, y₁</code>

Other compounds with this structure

Bk, Ce, Cf, Cm, Dy, Ge (metastable), Tb, γ -Ti, AgCd (random alloy)

- Uranium has two temperature-driven structural phase transitions (Donohue, 1974):

- Below 662°C it is in the ground state α -U structure ($A20$). (this structure)
- In the range 662-772°C it is in the β -U structure (A_b).
- Above 772°C to the melting point at 1135°C it is in the body-centered cubic structure ($A2$).
- We show the α -U structure at 4.2K.
- (Vohra, 2001) showed that at pressures above 116 GPa titanium transforms from the hexagonal omega ($C32$) phase to this phase.
- This structure was studied by (Wentzcovitch, 1987) as a possible pathway for the pressure-induced transformation of magnesium from the hcp ($A3$) to the bcc ($A2$) phase.
- Much like the trigonal omega phase ($C6$), we can generate several high-symmetry structures from this phase with the appropriate choice of parameters:

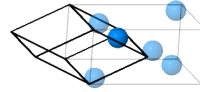
Lattice Parameter	hcp	bcc	fcc	Simple Cubic
a	a_{hcp}	a_{bcc}	a_{fcc}	$\sqrt{2}a_{sc}$
b	$\sqrt{3}a_{hcp}$	$\sqrt{2}a_{bcc}$	a_{fcc}	$\sqrt{2}a_{sc}$
c	c_{hcp}	$\sqrt{2}a_{bcc}$	a	$2a_{sc}$
y	$\frac{1}{6}$	$\frac{1}{4}$	$\frac{1}{4}$	0
Strukturbericht	$A3$	$A2$	$A1$	A_h
Pearson Symbol	hP2	cI2	cF4	cP1
Space group	$P6_3/mmc$	$Im\bar{3}m$	$Fm\bar{3}m$	$Pm\bar{3}m$
Number	194	229	225	221

(This corrects the values of a and b for the simple cubic structure published in (Mehl, 2017).)

Base-centered Orthorhombic primitive vectors

a_1, a_2, a_3

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	U I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	U I

References

- [1] C. S. Barrett, M. H. Mueller, and R. L. Hitterman, *Crystal Structure Variations in Alpha Uranium at Low Temperatures*, Phys. Rev. **129**, 625–629 (1963), doi:10.1103/PhysRev.129.625.
- [2] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).
- [3] Y. K. Vohra and P. T. Spencer, *Novel γ -Phase of Titanium Metal at Megabar Pressures*, Phys. Rev. Lett. **86**, 3068–3071 (2001), doi:10.1103/PhysRevLett.86.3068.
- [4] R. M. Wentzcovitch and M. L. Cohen, *Theoretical model for the hcp-bcc transition in Mg*, Phys. Rev. B **37**, 5571–5576 (1988), doi:10.1103/PhysRevB.37.5571.

- [5] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW library of crystallographic prototypes: part 1*, Comput. Mater. Sci. **136**, S1–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.

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