# $\alpha$-U ($A20$) Structure: A_oC4_63_c-001

This structure originally had the label `A_oC4_63_c`. Calls to that address will be redirected here.

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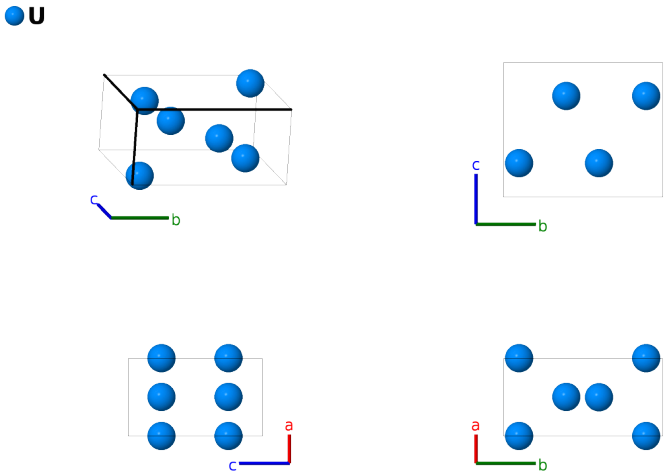
https://aflow.org/p/AFG5

https://aflow.org/p/A_oC4_63_c-001




| | |
|---|---|
| **Prototype** | U |
| **AFLOW prototype label** | A_oC4_63_c-001 |
| ***Strukturbericht* designation** | $A20$ |
| **ICSD** | 106205 |
| **Pearson symbol** | oC4 |
| **Space group number** | 63 |
| **Space group symbol** | $Cmcm$ |
| **AFLOW prototype command** | `aflow --proto=A_oC4_63_c-001 --params=`$a, b/a, c/a, y_1$ |

**Other compounds with this structure**
Bk, Ce, Cf, Cm, Dy, Ge (metastable), Tb, $\gamma$-Ti, AgCd (random alloy)

- Uranium has two structural phase transitions with temperature (Donohue, 1974):
  - Below 662°C it is in the ground state $\alpha$-U structure ($A20$). (this structure)
  - In the range 662-772°C it is in the $\beta$-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 $\alpha$-U structure at 4.2K.

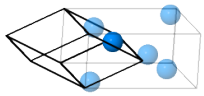
- (Vohra, 2001) showed that at pressures above 116 GPa titanium transforms from the hexagonal omega ($C32$) phase to this phase.
- This structure was studied by (Wentzcovitch, 1987) as a possible pathway for the pressure-induced transformation of magnesium from the hcp ($A3$) to the bcc ($A2$) phase.
- 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**


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



**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**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[3] Y. K. Vohra and P. T. Spencer, *Novel $\gamma$-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.