

β -U (A_b) Structure: A_tP30_136_af2ij-001

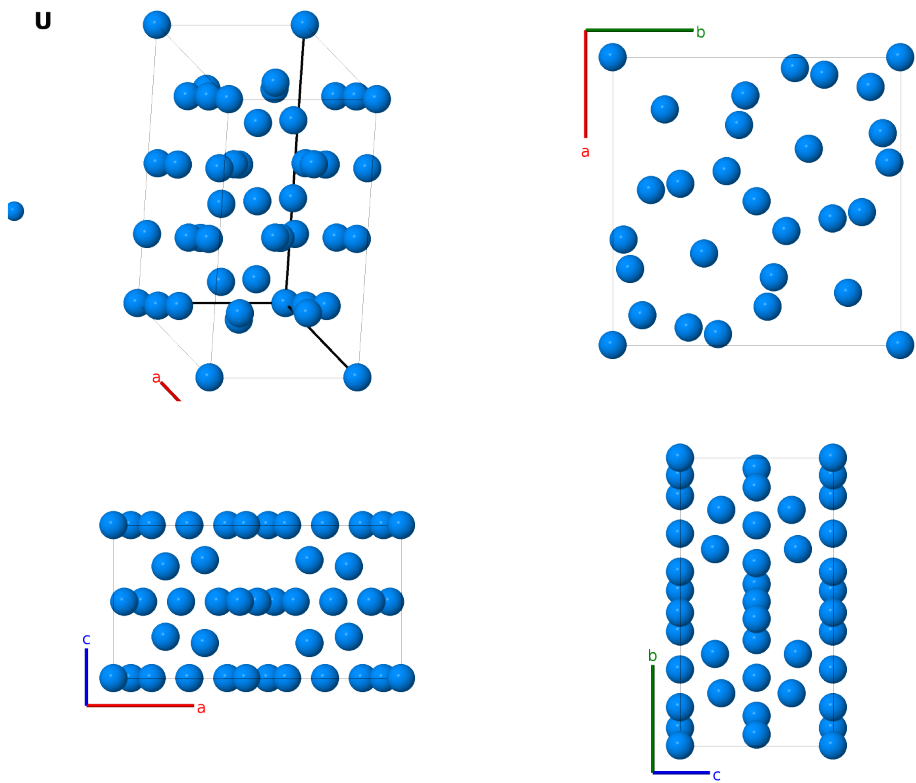
This structure previously used the label(s) **A.tP30_136_bf2ij**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/5T44>

https://aflow.org/prototype-encyclopedia/A_tP30_136_af2ij-001

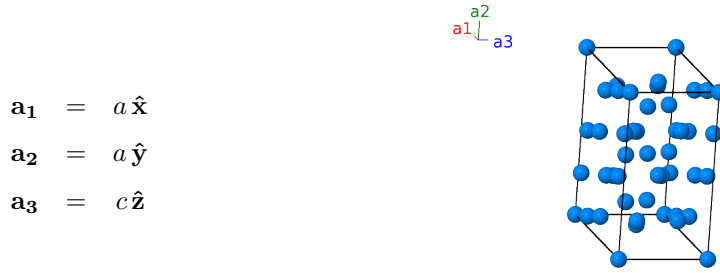


Prototype	U
AFLOW prototype label	A_tP30_136_af2ij-001
<i>Strukturbericht</i> designation	A_b
ICSD	76166
CCDC	1636783
Pearson symbol	tP30
Space group number	136
Space group symbol	$P4_2/mnm$

AFLOW prototype command `aflow --proto=A_tP30_136_af2ij-001`
 `--params=a, c/a, x2, x3, y3, x4, y4, x5, z5`

- Uranium has two temperature-driven structural phase transitions (Donohue, 1974):
 - Below 662°C it is in the ground state α -U structure ($A20$).
 - In the range 662-772°C it is in the β -U structure (A_b). (this structure)
 - Above 772°C to the melting point at 1135°C it is in the body-centered cubic structure ($A2$).
- According to (Donohue, 1982) there are three possible space groups which fit the diffraction data for β -U. This is the highest symmetry space group of the three.
- The AFLOW prototype labeling scheme moves the origin so that the U I atom is on the (2a) site. Then it is easily seen that β -U is isostructural with σ -CrFe ($D8_b$).

Simple Tetragonal primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	U I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	U I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$a x_2 \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}}$	(4f)	U II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-a x_2 \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}}$	(4f)	U II
$\mathbf{B}_5$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	U II
$\mathbf{B}_6$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	U II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$a x_3 \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}}$	(8i)	U III
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-a x_3 \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}}$	(8i)	U III
$\mathbf{B}_9$	$= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	U III
$\mathbf{B}_{10}$	$= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	U III
$\mathbf{B}_{11}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	U III
$\mathbf{B}_{12}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8i)	U III
$\mathbf{B}_{13}$	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$a y_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}}$	(8i)	U III
$\mathbf{B}_{14}$	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-a y_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}}$	(8i)	U III
$\mathbf{B}_{15}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$a x_4 \hat{\mathbf{x}} + a y_4 \hat{\mathbf{y}}$	(8i)	U IV

$$\begin{aligned}
\mathbf{B}_{16} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 &= -ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} & (8i) & \text{U IV} \\
\mathbf{B}_{17} &= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (8i) & \text{U IV} \\
\mathbf{B}_{18} &= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (8i) & \text{U IV} \\
\mathbf{B}_{19} &= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (8i) & \text{U IV} \\
\mathbf{B}_{20} &= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (8i) & \text{U IV} \\
\mathbf{B}_{21} &= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 &= ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} & (8i) & \text{U IV} \\
\mathbf{B}_{22} &= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 &= -ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} & (8i) & \text{U IV} \\
\mathbf{B}_{23} &= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (8j) & \text{U V} \\
\mathbf{B}_{24} &= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= -ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (8j) & \text{U V} \\
\mathbf{B}_{25} &= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8j) & \text{U V} \\
\mathbf{B}_{26} &= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8j) & \text{U V} \\
\mathbf{B}_{27} &= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8j) & \text{U V} \\
\mathbf{B}_{28} &= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8j) & \text{U V} \\
\mathbf{B}_{29} &= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (8j) & \text{U V} \\
\mathbf{B}_{30} &= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (8j) & \text{U V}
\end{aligned}$$

References

- [1] J. C. W. Tucker and P. Senio, *An improved determination of the crystal structure of β -uranium*, Acta Cryst. **6**, 753–760 (1953), doi:10.1107/S0365110X53002167.

Found in

- [1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).

First cited in

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