β-U (A_b) Structure: A_tP30_136_af2ij-001

This structure originally had the label `A_tP30_136_bf2ij`. Calls to that address will be redirected here.

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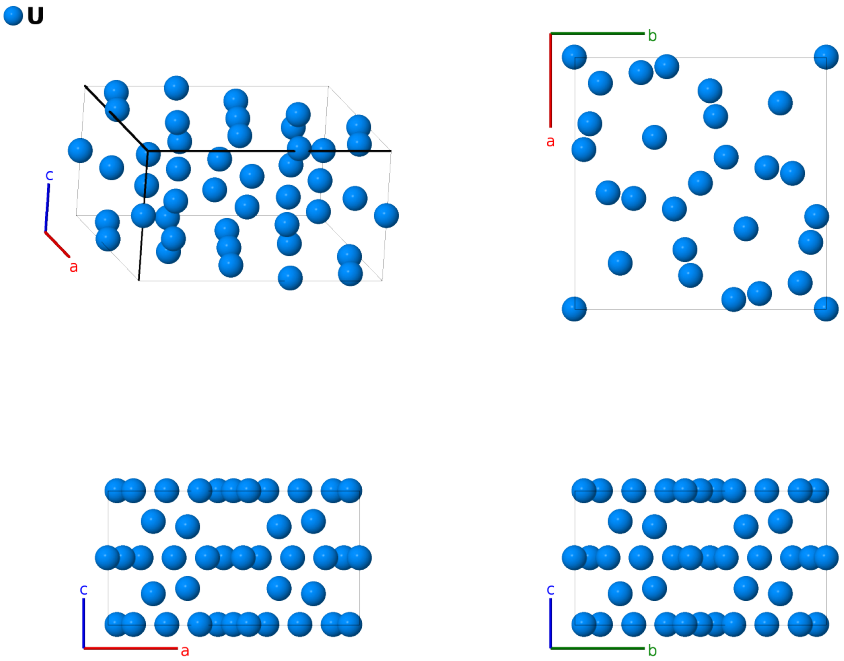
https://aflow.org/p/5T44

https://aflow.org/p/A_tP30_136_af2ij-001



Prototype	U
AFLOW prototype label	A_tP30_136_af2ij-001
***Strukturbericht* designation**	A_b
ICSD	76166
Pearson symbol	tP30
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	`aflow --proto=A_tP30_136_af2ij-001 --params=`$a, c/a, x_2, x_3, y_3, x_4, y_4, x_5, z_5$

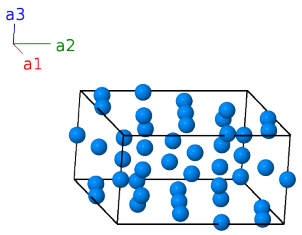
- Uranium has two structural phase transitions with temperature (Donohue, 1974):
  - Below 662°C it is in the ground state α-U structure ($A20$).

- 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. Except for a shift of the origin, this structure is isostructural with σ-CrFe ($D8_b$).

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= a\,\hat{\mathbf{x}}\\ \mathbf{a_2} &= a\,\hat{\mathbf{y}}\\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	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
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1+x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}}+ax_2\,\hat{\mathbf{y}}$	(4f)	U II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1-x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}}-ax_2\,\hat{\mathbf{y}}$	(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
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1+y_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}}+ay_3\,\hat{\mathbf{y}}$	(8i)	U III
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1-y_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}-ay_3\,\hat{\mathbf{y}}$	(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
$\mathbf{B_{13}}$	=	$y_3\,\mathbf{a}_1+x_3\,\mathbf{a}_2$	=	$ay_3\,\hat{\mathbf{x}}+ax_3\,\hat{\mathbf{y}}$	(8i)	U III
$\mathbf{B_{14}}$	=	$-y_3\,\mathbf{a}_1-x_3\,\mathbf{a}_2$	=	$-ay_3\,\hat{\mathbf{x}}-ax_3\,\hat{\mathbf{y}}$	(8i)	U III
$\mathbf{B_{15}}$	=	$x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}}+ay_4\,\hat{\mathbf{y}}$	(8i)	U IV
$\mathbf{B_{16}}$	=	$-x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{y}}$	(8i)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	U V

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).