β-UH_3 Structure: A3B_cP32_223_k_ac-001

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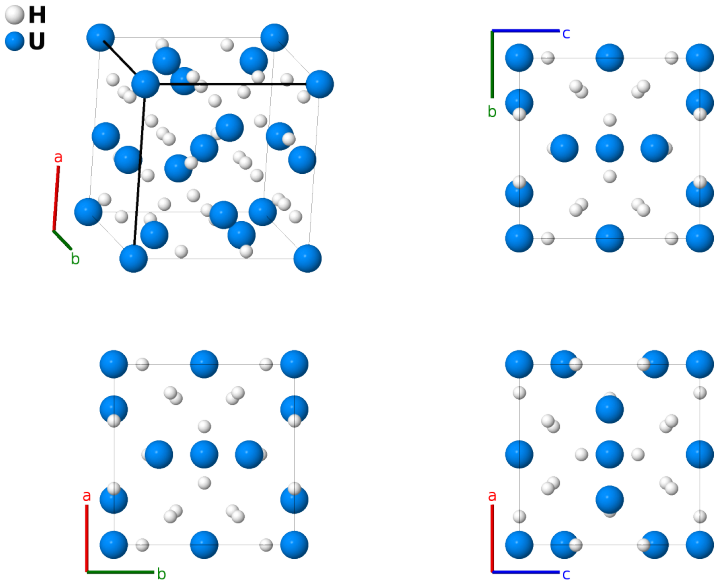
https://aflow.org/p/4UMV

https://aflow.org/p/A3B_cP32_223_k_ac-001



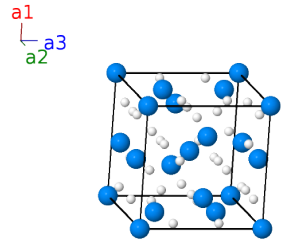
Prototype	H_3U
AFLOW prototype label	A3B_cP32_223_k_ac-001
ICSD	none
Pearson symbol	cP32
Space group number	223
Space group symbol	$Pm\bar{3}n$
AFLOW prototype command	`aflow --proto=A3B_cP32_223_k_ac-001 --params=`a, y_3, z_3

Other compounds with this structure
Zn_3Au

- UH_3 exists in two different structures, both with space group $Pm\bar{3}n$ #223 (Halevy, 2004).
- α-UH_3 forms in the Cr_3Si ($A15$) structure, but rapidly transforms into the ground state β-UH_3 structure shown here.
- In this case, all of the uranium atoms sit on the sites of the $A15$ structure, with the hydrogens in the interstitials.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	U I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(2a)	U I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6c)	U II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6c)	U II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(6c)	U II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$	(6c)	U II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(6c)	U II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(6c)	U II
$\mathbf{B_9}$	=	$y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{10}}$	=	$-y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{11}}$	=	$y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{12}}$	=	$-y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{13}}$	=	$z_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{14}}$	=	$z_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{15}}$	=	$-z_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{16}}$	=	$-z_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{17}}$	=	$y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}}$	(24k)	H I
$\mathbf{B_{18}}$	=	$-y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$-ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}}$	(24k)	H I
$\mathbf{B_{19}}$	=	$y_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}}$	(24k)	H I
$\mathbf{B_{20}}$	=	$-y_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}}$	(24k)	H I
$\mathbf{B_{21}}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{22}}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{23}}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + a\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{24}}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + a\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{25}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + a\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{26}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + a\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	H I
$\mathbf{B_{27}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - a\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	H I

$$\mathbf{B_{28}} = \tfrac{1}{2}\,\mathbf{a}_1 - \left(z_3 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,\hat{\mathbf{x}} - a\left(z_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(y_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (24k) \quad \text{H I}$$

$$\mathbf{B_{29}} = \left(z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = a\left(z_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad (24k) \quad \text{H I}$$

$$\mathbf{B_{30}} = \left(z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = a\left(z_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad (24k) \quad \text{H I}$$

$$\mathbf{B_{31}} = -\left(z_3 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = -a\left(z_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad (24k) \quad \text{H I}$$

$$\mathbf{B_{32}} = -\left(z_3 - \tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = -a\left(z_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad (24k) \quad \text{H I}$$

References

[1] I. Halevy, S. Salhov, S. Zalkind, M. Brill, and I. Yaar, *High pressure study of β-UH_3 crystallographic and electronic structure*, J. Alloys Compd. **370**, 59–64 (2004), doi:10.1016/j.jallcom.2003.09.124.