

β -UH₃ Structure:

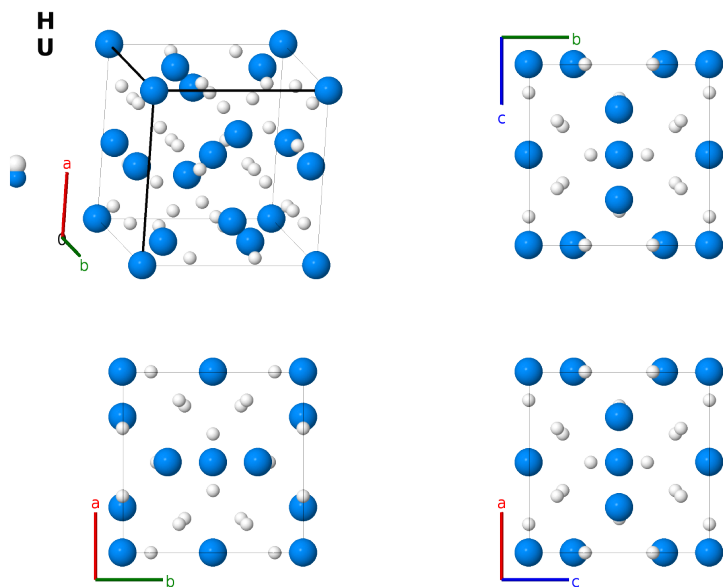
A3B_cP32_223_k_ac-001

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<https://aflow.org/prototype-encyclopedia/4UMV>

https://aflow.org/prototype-encyclopedia/A3B_cP32_223_k_ac-001



Prototype	H ₃ U
AFLOW prototype label	A3B_cP32_223_k_ac-001
Pearson symbol	cP32
Space group number	223
Space group symbol	$Pm\bar{3}n$
AFLOW prototype command	<code>aflow --proto=A3B_cP32_223_k_ac-001</code> <code>--params=a, y₃, z₃</code>

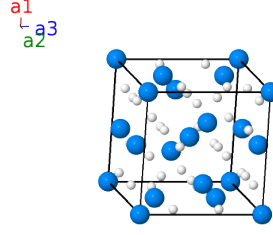
Other compounds with this structure

Zn₃Au

- UH₃ exists in two different structures, both with space group $Pm\bar{3}n$ #223 (Halevy, 2004).
- α -UH₃ forms in the Cr₃Si (A15) structure, but rapidly transforms into the ground state β -UH₃ 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

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) U I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(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
$\mathbf{B}_{21}$	$=$	$(y_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - a (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k) H I
$\mathbf{B}_{22}$	$=$	$-(y_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - a (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k) H I
$\mathbf{B}_{23}$	$=$	$(y_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + a (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k) H I
$\mathbf{B}_{24}$	$=$	$-(y_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + a (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k) H I
$\mathbf{B}_{25}$	$=$	$\frac{1}{2} \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_2 - (y_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + a (z_3 + \frac{1}{2}) \hat{\mathbf{y}} - a (y_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k) H I
$\mathbf{B}_{26}$	$=$	$\frac{1}{2} \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_2 + (y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + a (z_3 + \frac{1}{2}) \hat{\mathbf{y}} + a (y_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k) H I
$\mathbf{B}_{27}$	$=$	$\frac{1}{2} \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_2 - (y_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - a (z_3 - \frac{1}{2}) \hat{\mathbf{y}} - a (y_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k) H I

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

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

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

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

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

References

- [1] I. Halevy, S. Salhov, S. Zalkind, M. Brill, and I. Yaar, *High pressure study of β -UH₃ crystallographic and electronic structure*, J. Alloys Compd. **370**, 59–64 (2004), doi:10.1016/j.jallcom.2003.09.124.

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