

U₆Mn (*D*2_{*c*}) Structure: AB6_tI28_140_a_hk-001

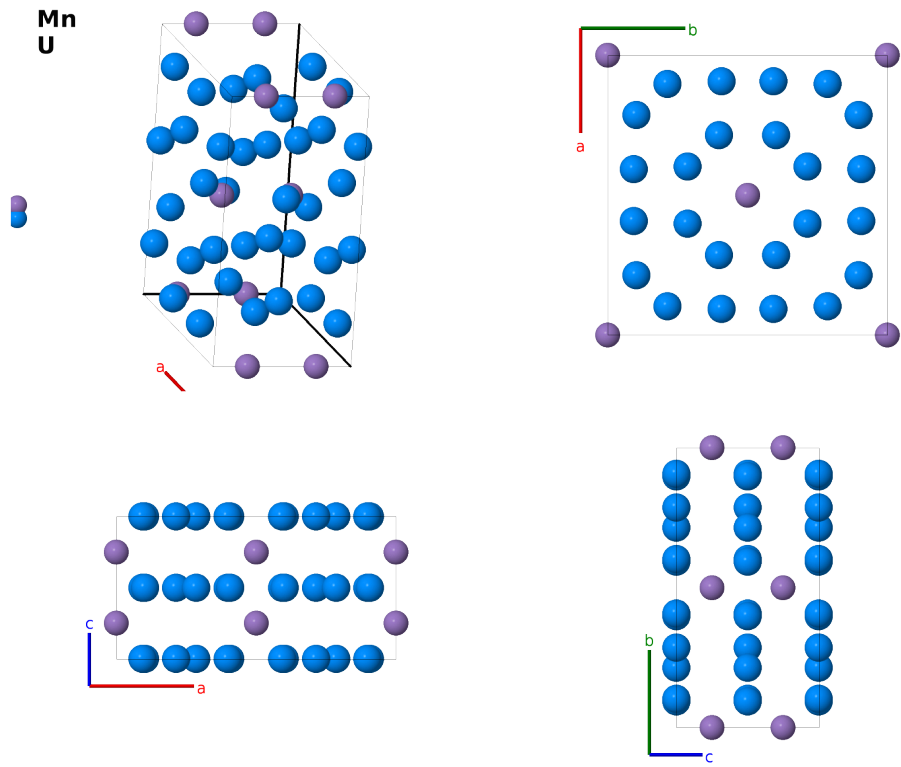
This structure previously used the label(s) **AB6-tI28_140_a_hk**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/1Q6T>

https://aflow.org/prototype-encyclopedia/AB6_tI28_140_a_hk-001



Prototype	MnU ₆
AFLOW prototype label	AB6_tI28_140_a_hk-001
<i>Strukturbericht</i> designation	<i>D</i> 2 _{<i>c</i>}
ICSD	150486
CCDC	1667654
Pearson symbol	tI28
Space group number	140
Space group symbol	<i>I</i> 4/ <i>mcm</i>
AFLOW prototype command	<code>aflow --proto=AB6_tI28_140_a_hk-001 --params=a, c/a, x₂, x₃, y₃</code>

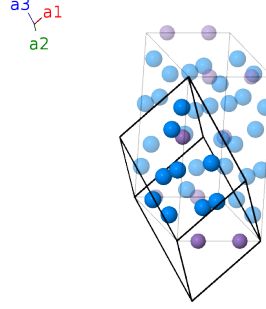
Other compounds with this structure

Pu₆Co, Pu₆Fe, U₆Co, U₆Fe, U₆Ni, U₆Np

- This structure is closely related to the V₄SiSb₂ structure. This can also be identified as a defected version of the $D8_m$ W₅Si₃ structure.

Body-centered Tetragonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(4a)	Mn I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(4a)	Mn I
$\mathbf{B}_3$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 + (2x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	U I
$\mathbf{B}_4$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 - (2x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	U I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(8h)	U I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(8h)	U I
$\mathbf{B}_7$	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}}$	(16k)	U II
$\mathbf{B}_8$	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}}$	(16k)	U II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(16k)	U II
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(16k)	U II
$\mathbf{B}_{11}$	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(16k)	U II
$\mathbf{B}_{12}$	$= -(y_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(16k)	U II
$\mathbf{B}_{13}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(16k)	U II
$\mathbf{B}_{14}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(16k)	U II

References

- [1] N. C. Baenziger, R. E. Rundle, A. I. Snow, and A. S. Wilson, *Compounds of uranium with the transition metals of the first long period*, Acta Cryst. **3**, 34–40 (1950), doi:10.1107/S0365110X50000082.

Found in

[1] P. Villars, *PAULING FILE* (2016). In: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg.

First cited in

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