

Al₄U (*D*1_b) Structure: A4B_oI20_74_aeh_e-001

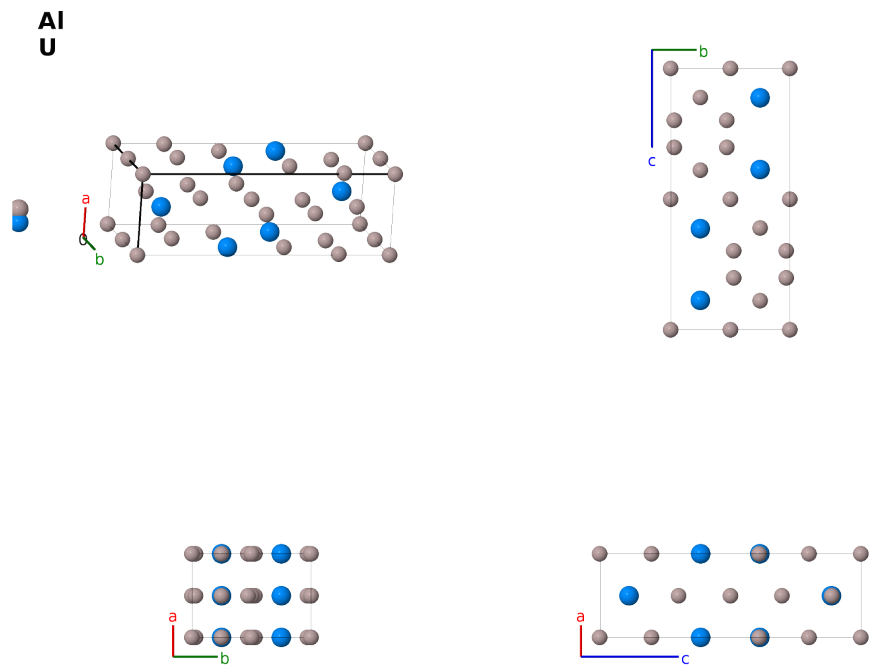
This structure previously used the label(s) **A4B_oI20_74_beh_e**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/FNF2>

https://aflow.org/prototype-encyclopedia/A4B_oI20_74_aeh_e-001



Prototype	Al ₄ U
AFLOW prototype label	A4B_oI20_74_aeh_e-001
<i>Strukturbericht</i> designation	<i>D</i> 1 _b
ICSD	240127
CCDC	1710876
Pearson symbol	oI20
Space group number	74
Space group symbol	<i>Imma</i>
AFLOW prototype command	<code>aflow --proto=A4B_oI20_74_aeh_e-001 --params=a, b/a, c/a, z₂, z₃, y₄, z₄</code>

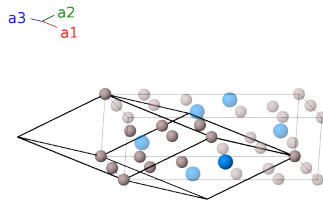
Other compounds with this structure

Al₄Gd, Al₄Np, Al₄Pu, Ga₄Pu

- We replaced the rather obscure (Borgstedt, 1989) reference by the modern work of (Tougait, 2004).

Body-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(4a) Al I
$\mathbf{B}_2$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}b\hat{\mathbf{y}}$	(4a) Al I
$\mathbf{B}_3$	=	$(z_2 + \frac{1}{4})\mathbf{a}_1 + z_2\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{4}b\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(4e) Al II
$\mathbf{B}_4$	=	$-(z_2 - \frac{3}{4})\mathbf{a}_1 - z_2\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{3}{4}b\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(4e) Al II
$\mathbf{B}_5$	=	$(z_3 + \frac{1}{4})\mathbf{a}_1 + z_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{4}b\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(4e) U I
$\mathbf{B}_6$	=	$-(z_3 - \frac{3}{4})\mathbf{a}_1 - z_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{3}{4}b\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$	(4e) U I
$\mathbf{B}_7$	=	$(y_4 + z_4)\mathbf{a}_1 + z_4\mathbf{a}_2 + y_4\mathbf{a}_3$	=	$by_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(8h) Al III
$\mathbf{B}_8$	=	$(-y_4 + z_4 + \frac{1}{2})\mathbf{a}_1 + z_4\mathbf{a}_2 - (y_4 - \frac{1}{2})\mathbf{a}_3$	=	$-b(y_4 - \frac{1}{2})\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(8h) Al III
$\mathbf{B}_9$	=	$(y_4 - z_4 + \frac{1}{2})\mathbf{a}_1 - z_4\mathbf{a}_2 + (y_4 + \frac{1}{2})\mathbf{a}_3$	=	$b(y_4 + \frac{1}{2})\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(8h) Al III
$\mathbf{B}_{10}$	=	$-(y_4 + z_4)\mathbf{a}_1 - z_4\mathbf{a}_2 - y_4\mathbf{a}_3$	=	$-by_4\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(8h) Al III

References

- [1] O. Tougait and H. Noël, *Stoichiometry of UAl₄*, Intermetallics **12**, 219–223 (2004), doi:10.1016/j.intermet.2003.09.012.
- [2] H. U. Borgstedt and H. Wedemeyer, *Gmelin Handbook of Inorganic Chemistry* (Springer-Verlag, Berlin Heidelberg, 1989), vol. Supplement B 2, chap. 3, p. 144.

First cited in

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