Al_4U ($D1_b$) Structure: A4B_oI20_74_aeh_e-001

This structure originally had the label `A4B_oI20_74_beh_e`. Calls to that address will be redirected here.

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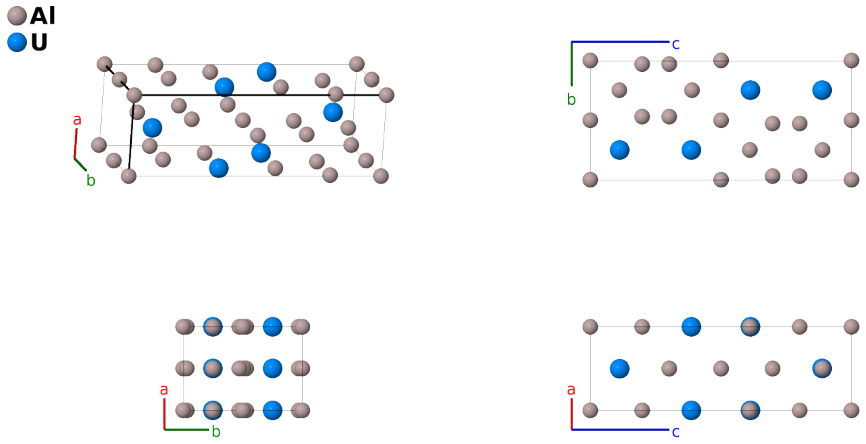
https://aflow.org/p/FNF2

https://aflow.org/p/A4B_oI20_74_aeh_e-001



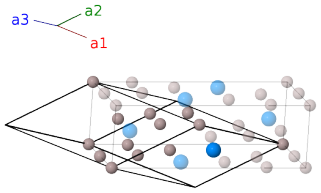
Prototype	Al_4U
AFLOW prototype label	A4B_oI20_74_aeh_e-001
***Strukturbericht* designation**	$D1_b$
ICSD	240127
Pearson symbol	oI20
Space group number	74
Space group symbol	$Imma$
AFLOW prototype command	`aflow --proto=A4B_oI20_74_aeh_e-001 --params=`$a, b/a, c/a, z_2, z_3, y_4, z_4$

Other compounds with this structure
Al_4Gd, Al_4Np, Al_4Pu, Ga_4Pu

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

Body-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_3}$	=	$\left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4e)	Al II
$\mathbf{B_4}$	=	$-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4e)	Al II
$\mathbf{B_5}$	=	$\left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	U I
$\mathbf{B_6}$	=	$-\left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(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
$\mathbf{B_8}$	=	$\left(-y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8h)	Al III
$\mathbf{B_9}$	=	$\left(y_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8h)	Al III
$\mathbf{B_{10}}$	=	$-\left(y_4 + z_4\right)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8h)	Al III

References

[1] O. Tougait and H. Noël, *Stoichiometry of UAl_4*, 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.