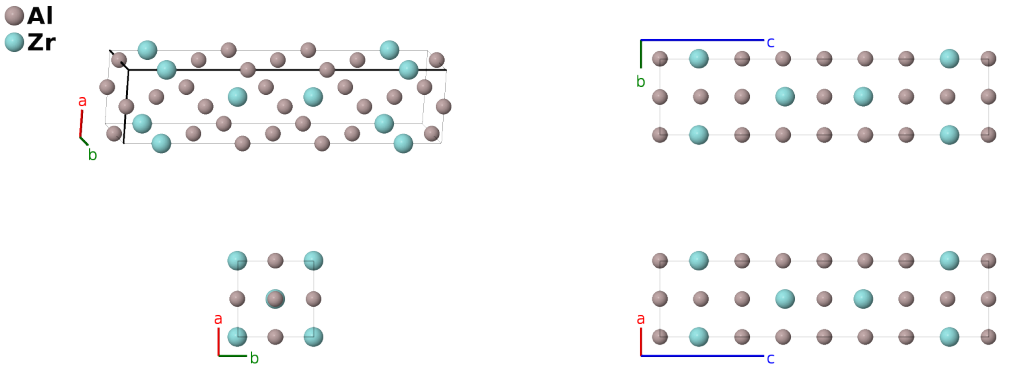
# $Al_3Zr$ ($D0_{23}$) Structure: A3B_tI16_139_cde_e-001

This structure originally had the label `A3B_tI16_139_cde_e`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/CSTH

https://aflow.org/p/A3B_tI16_139_cde_e-001



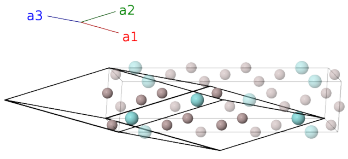

| | |
|---|---|
| **Prototype** | $Al_3Zr$ |
| **AFLOW prototype label** | A3B_tI16_139_cde_e-001 |
| ***Strukturbericht* designation** | $D0_{23}$ |
| **ICSD** | 107130 |
| **Pearson symbol** | tI16 |
| **Space group number** | 139 |
| **Space group symbol** | $I4/mmm$ |
| **AFLOW prototype command** | `aflow --proto=A3B_tI16_139_cde_e-001 --params=`$a, c/a, z_3, z_4$ |

**Other compounds with this structure**
$Al_3Hf$, $Ga_3Zr$

- When c=4a, $z_3$=3/8 and $z_4$=1/8 the atoms are on the sites of a face-centered cubic lattice. This phase can also be described as a set of alternating $L1_2$ and $D0_{22}$ lattices.

**Body-centered Tetragonal primitive vectors**

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



**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}}$ | (4c) | Al I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}}$ | (4c) | Al I |
| $\mathbf{B_3}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4d) | Al II |
| $\mathbf{B_4}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4d) | Al II |
| $\mathbf{B_5}$ | = | $z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$ | = | $cz_3\,\hat{\mathbf{z}}$ | (4e) | Al III |
| $\mathbf{B_6}$ | = | $-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$ | = | $-cz_3\,\hat{\mathbf{z}}$ | (4e) | Al III |
| $\mathbf{B_7}$ | = | $z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$ | = | $cz_4\,\hat{\mathbf{z}}$ | (4e) | Zr I |
| $\mathbf{B_8}$ | = | $-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$ | = | $-cz_4\,\hat{\mathbf{z}}$ | (4e) | Zr I |

**References**


[1] Y. Ma, C. Romming, B. Lebech, J. Gjonnes, and J. Tafto, *Structure Refinement of AI3Zr using Single-Crystal X-ray Diffraction, Powder Neutron Diffraction and CBED*, Acta Crystallogr. Sect. B **48**, 11–16 (1992), doi:10.1107/S0108768191010467.


**Found in**


[1] G. Ghosh and M. Asta, *First-principles calculation of structural energetics of Al-TM (TM = Ti, Zr, Hf) intermetallics*, Acta Mater. **53**, 3225–3252 (2005), doi:10.1016/j.actamat.2005.03.028.