Ta_3B_4 ($D7_b$) Structure: A4B3_oI14_71_ef_af-001

This structure previously used the label(s) `A4B3_oI14_71_gh_cg`. Calls to these addresses will be redirected here.

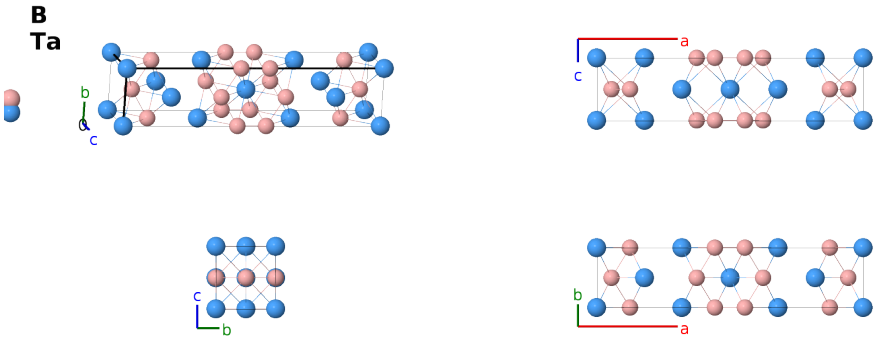
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/3XYE

https://aflow.org/prototype-encyclopedia/A4B3_oI14_71_ef_af-001



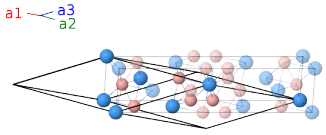
Prototype	B_4Ta_3
AFLOW prototype label	A4B3_oI14_71_ef_af-001
***Strukturbericht* designation**	$D7_b$
ICSD	44589
CCDC	1613959
Pearson symbol	oI14
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	`aflow --proto=A4B3_oI14_71_ef_af-001 --params=`$a, b/a, c/a, x_2, x_3, x_4$

Other compounds with this structure

B_4Cr_3, B_4Mn_3, B_4Mo_2Ni, B_4Nb_3, B_4Ta_3, B_4V_3, B_4CoMo_2, B_4FeMo_2

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ta I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}$	(4e)	B I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}$	(4e)	B I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	B II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	B II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	Ta II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	Ta II

References

[1] R. Kiessling, *The Borides of Tantalum*, Acta Chem. Scand. **3**, 603–615 (1949), doi:10.1021/cm00015a035.

Found in

[1] R. Minyaev and R. Hoffmann, *Transition-metal borides with the tantalum boride (Ta_3B_4) crystal structure: their electronic and bonding properties*, Chem. Mater. **3**, 547–557 (1991), doi:10.1021/cm00015a035.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043