β-Ta_2O_5 Structure: A5B2_oP14_49_cehq_ab-001

This structure previously used the label(s) `A5B2_oP14_49_dehq_ab`. Calls to these addresses will be redirected here.

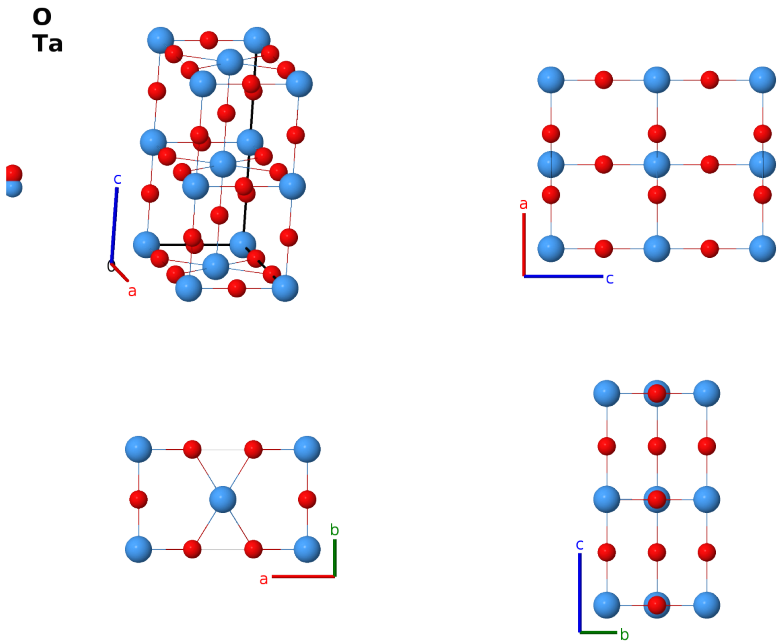
Cite this page as:

- 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/XVUH

https://aflow.org/prototype-encyclopedia/A5B2_oP14_49_cehq_ab-001



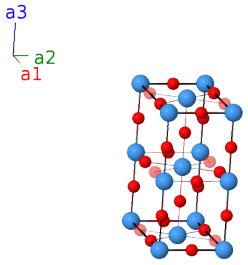
Prototype	O_5Ta_2
AFLOW prototype label	A5B2_oP14_49_cehq_ab-001
ICSD	95462
CCDC	1654862
Pearson symbol	oP14
Space group number	49
Space group symbol	*Pccm*
AFLOW prototype command	`aflow --proto=A5B2_oP14_49_cehq_ab-001 --params=`$a, b/a, c/a, x_6, y_6$

- (Aleshina, 2002) place this structure in space group *Pccm* #49, while AFLOW's (and VASP's) default tolerance halves the size of the c-axis and places the system in space group *Pmmm* #47. The reported structure can be recovered using

- aflow --proto=A5B2_oP14_49_cehq_ab:O:Ta --params=a,b/a,c/a,x_6,y_6 --tolerance=0.001 .
- It is likely that first-principles calculations starting from this point will relax to produce a structure equivalent to the smaller *Pmmm* unit cell.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ta I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Ta I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(2b)	Ta II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Ta II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(2c)	O I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_7}$	=	$\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(2e)	O II
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(2e)	O II
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2h)	O III
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2h)	O III
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}}$	(4q)	O IV
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}}$	(4q)	O IV
$\mathbf{B_{13}}$	=	$-x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4q)	O IV
$\mathbf{B_{14}}$	=	$x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4q)	O IV

References

[1] L. A. Aleshina and S. V. Loginova, *Rietveld analysis of X-ray diffraction pattern from beta-Ta_2O_5 oxide*, Crystallogr. Rep. **47**, 415–419 (2002), doi:10.1134/1.1481927. Translated from Kristallografiya **47**, 460-464 (2002).

[2] H. T. Stokes and D. M. Hatch, FINDSYM*: program for identifying the space-group symmetry of a crystal*, Appl. Crystallogr. **38**, 237–238 (2005), doi:10.1107/S0021889804031528.

[3] D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy, and S. Curtarolo, *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*, Acta Crystallogr. Sect. A **74**, 184–203 (2018), doi:10.1107/S2053273318003066.

[4] A. L. Speck, *Single-crystal structure validation with the program PLATON*, Appl. Crystallogr. **36**, 7–13 (2003), doi:10.1107/S0021889802022112.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

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