

# $\zeta$ -Nb<sub>2</sub>O<sub>5</sub> (B-Nb<sub>2</sub>O<sub>5</sub>) Structure: A2B5\_mC28\_15\_f\_e2f-003

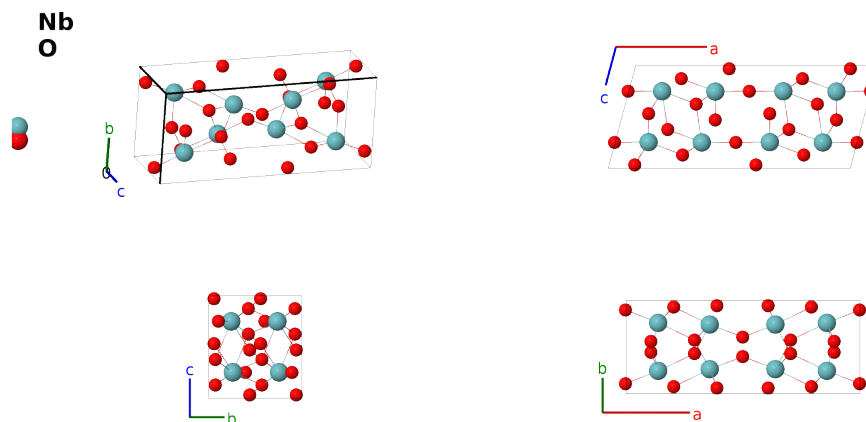
This structure previously used the label(s) **A2B5\_mC28\_15\_f\_e2f.Nb2O5**. Calls to these addresses will be redirected here.

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- 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/S3CP>

[https://aflow.org/prototype-encyclopedia/A2B5\\_mC28\\_15\\_f\\_e2f-003](https://aflow.org/prototype-encyclopedia/A2B5_mC28_15_f_e2f-003)



|                         |                                                                                                                                                                                                                                                                                                |
|-------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype               | Nb <sub>2</sub> O <sub>5</sub>                                                                                                                                                                                                                                                                 |
| AFLOW prototype label   | A2B5_mC28_15_f_e2f-003                                                                                                                                                                                                                                                                         |
| ICSD                    | 71317                                                                                                                                                                                                                                                                                          |
| CCDC                    | 1632216                                                                                                                                                                                                                                                                                        |
| Pearson symbol          | mC28                                                                                                                                                                                                                                                                                           |
| Space group number      | 15                                                                                                                                                                                                                                                                                             |
| Space group symbol      | <i>C</i> 2/ <i>c</i>                                                                                                                                                                                                                                                                           |
| AFLOW prototype command | <code>aflow --proto=A2B5_mC28_15_f_e2f-003</code><br><code>--params=a, b/a, c/a, <math>\beta</math>, <math>y_1</math>, <math>x_2</math>, <math>y_2</math>, <math>z_2</math>, <math>x_3</math>, <math>y_3</math>, <math>z_3</math>, <math>x_4</math>, <math>y_4</math>, <math>z_4</math></code> |

## Other compounds with this structure

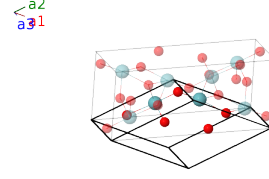
Sb<sub>2</sub>O<sub>5</sub>

- This structure is referred to as both  $\zeta$ -Nb<sub>2</sub>O<sub>5</sub> and B-Nb<sub>2</sub>O<sub>5</sub>.
- Nb<sub>2</sub>O<sub>5</sub> and B<sub>2</sub>Pd<sub>5</sub> share the same AFLOW prototype label, A2B5\_mC28\_15\_f\_e2f, but have substantially different environments around each atom. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Previously (Hicks, 2021) we inadvertently set  $y_1 = 0.6465$ . The correct value is 0.8965.

- The ICSD uses  $\text{Sb}_2\text{O}_5$  as the prototype for this structure.

## Base-centered Monoclinic primitive vectors

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



## Basis vectors

|                   | Lattice coordinates                                                                         |     | Cartesian coordinates                                                                                                                   | Wyckoff position | Atom type |
|-------------------|---------------------------------------------------------------------------------------------|-----|-----------------------------------------------------------------------------------------------------------------------------------------|------------------|-----------|
| $\mathbf{B}_1$    | $= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$                         | $=$ | $\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$                           | (4e)             | O I       |
| $\mathbf{B}_2$    | $= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$                          | $=$ | $\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$                           | (4e)             | O I       |
| $\mathbf{B}_3$    | $= (x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$                  | $=$ | $(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$                                  | (8f)             | Nb I      |
| $\mathbf{B}_4$    | $= -(x_2 + y_2) \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (8f)             | Nb I      |
| $\mathbf{B}_5$    | $= -(x_2 - y_2) \mathbf{a}_1 - (x_2 + y_2) \mathbf{a}_2 - z_2 \mathbf{a}_3$                 | $=$ | $-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$                                 | (8f)             | Nb I      |
| $\mathbf{B}_6$    | $= (x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$  | (8f)             | Nb I      |
| $\mathbf{B}_7$    | $= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$                  | $=$ | $(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$                                  | (8f)             | O II      |
| $\mathbf{B}_8$    | $= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (8f)             | O II      |
| $\mathbf{B}_9$    | $= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$                 | $=$ | $-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$                                 | (8f)             | O II      |
| $\mathbf{B}_{10}$ | $= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$  | (8f)             | O II      |
| $\mathbf{B}_{11}$ | $= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$                  | $=$ | $(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$                                  | (8f)             | O III     |
| $\mathbf{B}_{12}$ | $= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (8f)             | O III     |
| $\mathbf{B}_{13}$ | $= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$                 | $=$ | $-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$                                 | (8f)             | O III     |
| $\mathbf{B}_{14}$ | $= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$  | (8f)             | O III     |

## References

- [1] T. S. Ercit, *Refinement of the structure of  $\zeta\text{-Nb}_2\text{O}_5$  and its relationship to the rutile and thoreaulite structures*, Mineral. Petrol. **43**, 217–223 (1991), doi:10.1007/BF01166893.
- [2] D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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.

## First cited in

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