# Simpsonite ($Ta_3Al_4O_{13}[OH]$) Structure: A4B14C3_hP21_143_ad_bc4d_d-001

This structure previously used the label(s) `A4B14C3_hP21_143_bd_ac4d_d`. Calls to these addresses will be redirected here.

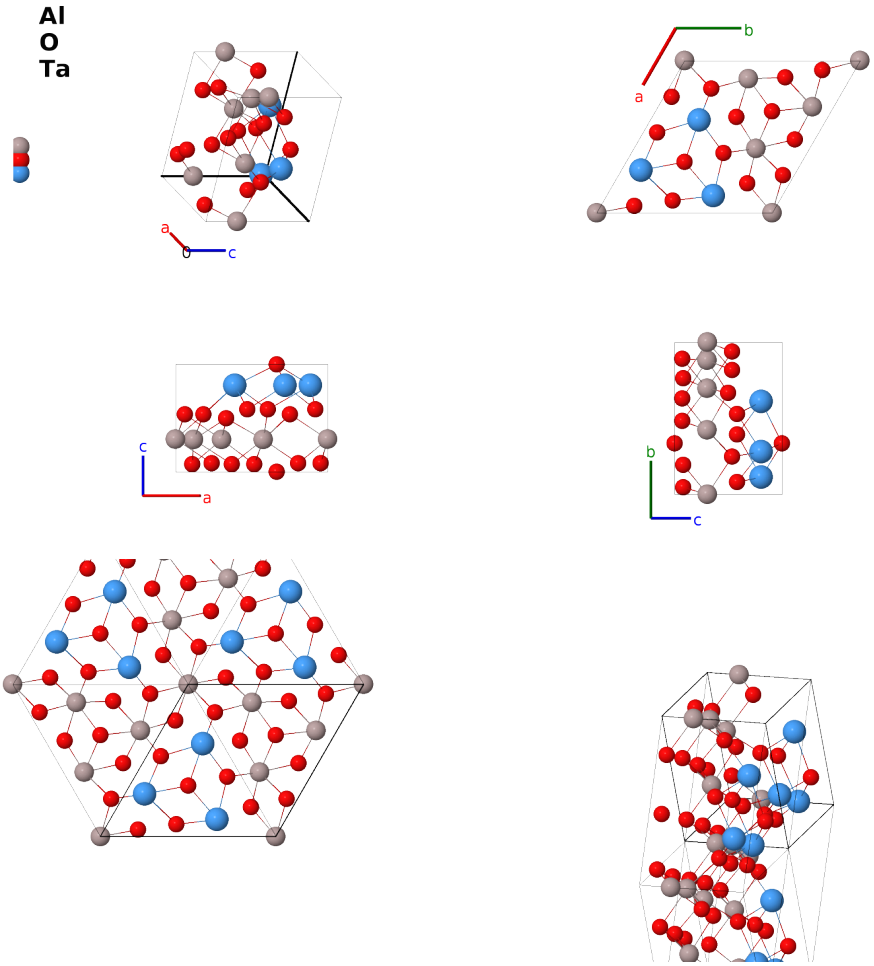
Cite this page as:

- 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/TY99

https://aflow.org/prototype-encyclopedia/A4B14C3_hP21_143_ad_bc4d_d-001




| | |
|---|---|
| **Prototype** | $Al_4O_{14}Ta_3$ |
| **AFLOW prototype label** | A4B14C3_hP21_143_ad_bc4d_d-001 |
| **Mineral name** | simpsonite |
| **ICSD** | 67673 |
| **CCDC** | 1629650 |
| **Pearson symbol** | hP21 |

| | |
|---|---|
| **Space group number** | 143 |
| **Space group symbol** | $P3$ |
| **AFLOW prototype command** | `aflow --proto=A4B14C3_hP21_143_ad_bc4d_d-001 --params=`$a, c/a, z_1, z_2, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$ |

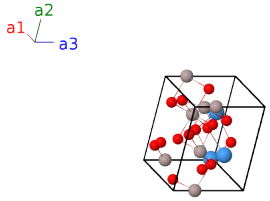
---

- The OH molecule is centered on the (1c) site, however it is only listed as O in this prototype.
- Space group $P3$ #143 allows an arbitary origin for the $z$-axis, here we set it so the $z_1 = 0$ for the O-I atom.

---

**Trigonal (Hexagonal) primitive vectors**

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$




---

**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $z_1\,\mathbf{a}_3$ | = | $cz_1\,\hat{\mathbf{z}}$ | (1a) | Al I |
| $\mathbf{B_2}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (1b) | O I |
| $\mathbf{B_3}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (1c) | O II |
| $\mathbf{B_4}$ | = | $x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (3d) | Al II |
| $\mathbf{B_5}$ | = | $-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (3d) | Al II |
| $\mathbf{B_6}$ | = | $-(x_4 - y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (3d) | Al II |
| $\mathbf{B_7}$ | = | $x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (3d) | O III |
| $\mathbf{B_8}$ | = | $-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (3d) | O III |
| $\mathbf{B_9}$ | = | $-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (3d) | O III |
| $\mathbf{B_{10}}$ | = | $x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (3d) | O IV |
| $\mathbf{B_{11}}$ | = | $-y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (3d) | O IV |
| $\mathbf{B_{12}}$ | = | $-(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (3d) | O IV |
| $\mathbf{B_{13}}$ | = | $x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (3d) | O V |
| $\mathbf{B_{14}}$ | = | $-y_7\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (3d) | O V |
| $\mathbf{B_{15}}$ | = | $-(x_7 - y_7)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (3d) | O V |
| $\mathbf{B_{16}}$ | = | $x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_8 + y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_8 - y_8)\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$ | (3d) | O VI |
| $\mathbf{B_{17}}$ | = | $-y_8\,\mathbf{a}_1 + (x_8 - y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_8 - 2y_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$ | (3d) | O VI |
| $\mathbf{B_{18}}$ | = | $-(x_8 - y_8)\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_8 - y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$ | (3d) | O VI |
| $\mathbf{B_{19}}$ | = | $x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_9 + y_9)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_9 - y_9)\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$ | (3d) | Ta I |
| $\mathbf{B_{20}}$ | = | $-y_9\,\mathbf{a}_1 + (x_9 - y_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_9 - 2y_9)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$ | (3d) | Ta I |
| $\mathbf{B_{21}}$ | = | $-(x_9 - y_9)\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_9 - y_9)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$ | (3d) | Ta I |

## References

[1] T. S. Ercit, P. Černý, and F. C. Hawthorne, *The Crystal Chemistry of Simpsonite*, Can. Mineral. **30**, 663–671 (1992).

## 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