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

This structure originally had the label `A4B14C3_hP21_143_bd_ac4d_d`. Calls to that address will be redirected here.

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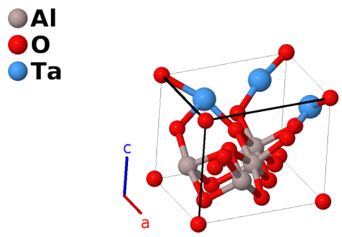
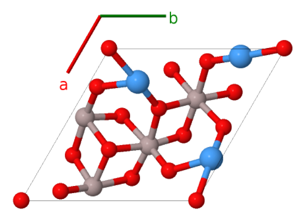
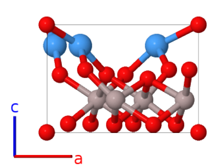
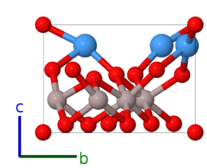
https://aflow.org/p/TY99

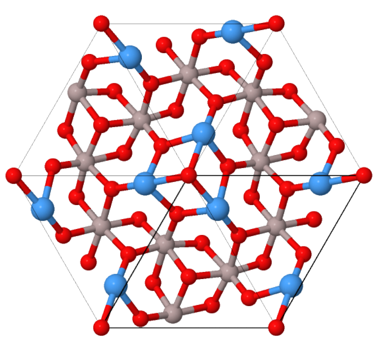
https://aflow.org/p/A4B14C3_hP21_143_ad_bc4d_d-001

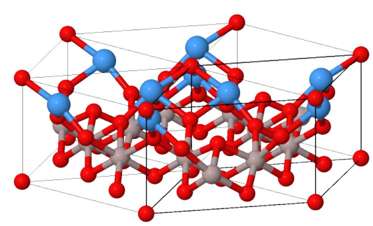










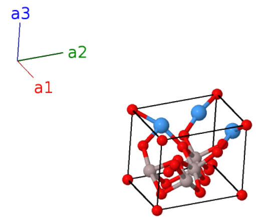


Prototype	$Al_4O_{14}Ta_3$
AFLOW prototype label	A4B14C3_hP21_143_ad_bc4d_d-001
Mineral name	simpsonite
ICSD	67673
Pearson symbol	hP21
Space group number	143
Space group symbol	$P3$
AFLOW prototype command	`aflow --proto=A4B14C3_hP21_143_ad_bc4d_d-001` `--params=`$a, c/a, z_1, z_2, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

- 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.