La_3TiSb_5: A3B5C_hP18_193_g_dg_b-001

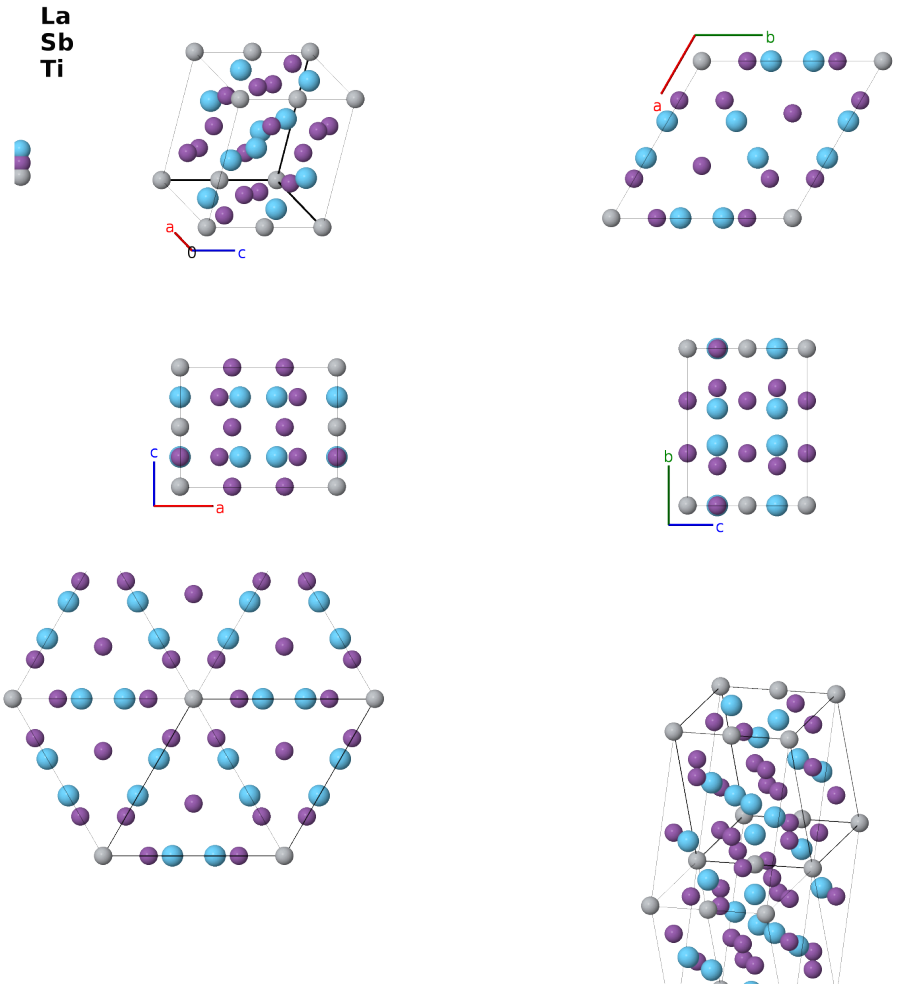
Cite this page as:

- 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/6LTC

https://aflow.org/prototype-encyclopedia/A3B5C_hP18_193_g_dg_b-001



Prototype	La_3Sb_5Ti
AFLOW prototype label	A3B5C_hP18_193_g_dg_b-001
ICSD	80907
CCDC	1641084
Pearson symbol	hP18
Space group number	193
Space group symbol	$P6_3/mcm$

AFLOW prototype command `aflow --proto=A3B5C_hP18_193_g_dg_b-001 --params=`$a, c/a, x_3, x_4$

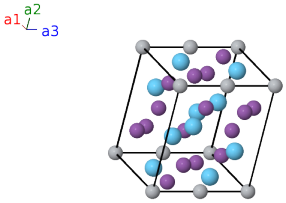
Other compounds with this structure

Al_3NHf_5, Ba_3ScTe_5, Bi_3BrBa_5, Bi_3BrCa_5, Bi_3BrLa_5, Bi_3ClBa_5, Bi_3ClCa_5, Bi_3CuCe_5, Bi_3CuGd_5, Bi_3CuLa_5, Bi_3CuNd_5, Bi_3CuPr_5, Bi_3CuTb_5, Bi_3CuZr_5, Ce_3HfSb_5, Ce_3MnBi_5, Ce_3NbSb_5, Ce_3TiBi_5, Ce_3TiSb_5, Ce_3ZrSb_5, Ge_3CrLa_5, In_3AgZr_5, In_3BrLa_5, In_3CuSc_5, In_3CuZr_5, La_3CrAs_5, La_3HfBi_5, La_3HfSb_5, La_3MgBi_5, La_3MnBi_5, La_3NbSb_5, La_3ScBi_5, La_3TiAs_5, La_3TiBi_5, La_3TiP_5, La_3TiSb_5, La_3ZrBi_5, La_3ZrSb_5, Nd_3HfSb_5, Nd_3MnBi_5, Nd_3NbSb_5, Nd_3TiSb_5, Nd_3ZrSb_5, P_3NV_5, Pb_3AgCe_5, Pb_3AgLa_5, Pb_3AgZr_5, Pb_3AlZr_5, Pb_3AsLa_5, Pb_3AsZr_5, Pb_3CdZr_5, Pb_3CeLa_5, Pb_3CoLa_5, Pb_3CoZr_5, Pb_3CrLa_5, Pb_3CuCe_5, Pb_3CuHf_5, Pb_3CuLa_5, Pb_3CuY_5, Pb_3CuZr_5, Pb_3FeCa_5, Pb_3FeLa_5, Pb_3FeZr_5, Pb_3GaZr_5, Pb_3GeZr_5, Pb_3ILa_5, Pb_3InZr_5, Pb_3MnLa_5, Pb_3NiDy_5, Pb_3NiEr_5, Pb_3NiHo_5, Pb_3NiLa_5, Pb_3NiLu_5, Pb_3NiPr_5, Pb_3NiTb_5, Pb_3NiTm_5, Pb_3NiZr_5, Pb_3PLa_5, Pb_3PZr_5, Pb_3RuLa_5, Pb_3SLa_5, Pb_3SZr_5, Pb_3SbLa_5, Pb_3SbZr_5, Pb_3SeLa_5, Pb_3SeZr_5, Pb_3SiZr_5, Pb_3SnZr_5, Pb_3TeZr_5, Pb_3ZnLa_5, Pb_3ZnZr_5, Pr_3HfSb_5, Pr_3MnBi_5, Pr_3NbSb_5, Pr_3TiSb_5, Pr_3ZrSb_5, Sb_3AgZr_5, Sb_3AlZr_5, Sb_3AsZr_5, Sb_3BrBa_5, Sb_3BrLa_5, Sb_3ClBa_5, Sb_3ClCa_5, Sb_3ClSr_5, Sb_3CoZr_5, Sb_3CuHf_5, Sb_3CuTi_5, Sb_3CuZr_5, Sb_3FeZr_5, Sb_3GeZr_5, Sb_3NiHf_5, Sb_3NiZr_5, Sb_3PZr_5, Sb_3RuZr_5, Sb_3SZr_5, Sb_3SeZr_5, Sb_3SiZr_5, Sb_3ZnHf_5, Sb_3ZnZr_5, Si_3DTi_5, Si_3PNb_5, Sm_3HfSb_5, Sm_3NbSb_5, Sm_3TiSb_5, Sm_3ZrBi_5, Sm_3ZrSb_5, Sn_3AgCe_5, Sn_3AlZr_5, Sn_3AsZr_5, Sn_3BrLa_5, Sn_3ClLa_5, Sn_3CuCe_5, Sn_3CuYb_5, Sn_3CuZr_5, Sn_3GaZr_5, Sn_3GeZr_5, Sn_3HfGa_5, Sn_3ILa_5, Sn_3LiTb_5, Sn_3NZr_5, Sn_3NiHf_5, Sn_3PZr_5, Sn_3SZr_5, Sn_3SeZr_5, Sn_3SiZr_5, Sn_3ZnZr_5, U_3CrSb_5, U_3HfSb_5, U_3MnSb_5, U_3NbSb_5, U_3ScSb_5, U_3TiGe_5, U_3TiSb_5, U_3VSb_5, U_3ZrSb_5

- This is a ternary form of the Ti_5Ga_4 structure.

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
$\mathbf{B_1}$	=	0	=	0	(2b)	Ti I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Ti I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(4d)	Sb I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4d)	Sb I
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(4d)	Sb I
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4d)	Sb I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	La I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	La I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	La I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	La I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	La I
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	La I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	Sb II
$\mathbf{B_{14}}$	=	$x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	Sb II

$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	Sb II
$\mathbf{B_{16}}$	=	$-x_4\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	Sb II
$\mathbf{B_{17}}$	=	$-x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	Sb II
$\mathbf{B_{18}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	Sb II

References

[1] G. Bolloré, M. J. Ferguson, R. W. Hushagen, and A. Mar, *New Ternary Rare-Earth Transition-Metal Antimonides RE_3MSb_5 (RE = La, Ce, Pr, Nd, Sm; M = Ti, Zr, Hf, Nb)*, Chem. Mater. **7**, 2229–2231 (1995), doi:10.1021/cm00060a005.

Found in

[1] M. Matin, R. Kulkarni, A. Thamizhavel, S. K. Dhar, A. Provino, and P. Manfrinetti, *Probing the magnetic ground state of single crystalline Ce_3TiSb_5*, J. Phys.: Condens. Matter **29**, 145601 (2017), doi:10.1088/1361-648X/aa57c0.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5.* Submitted to Computational Materials Science (2026).