

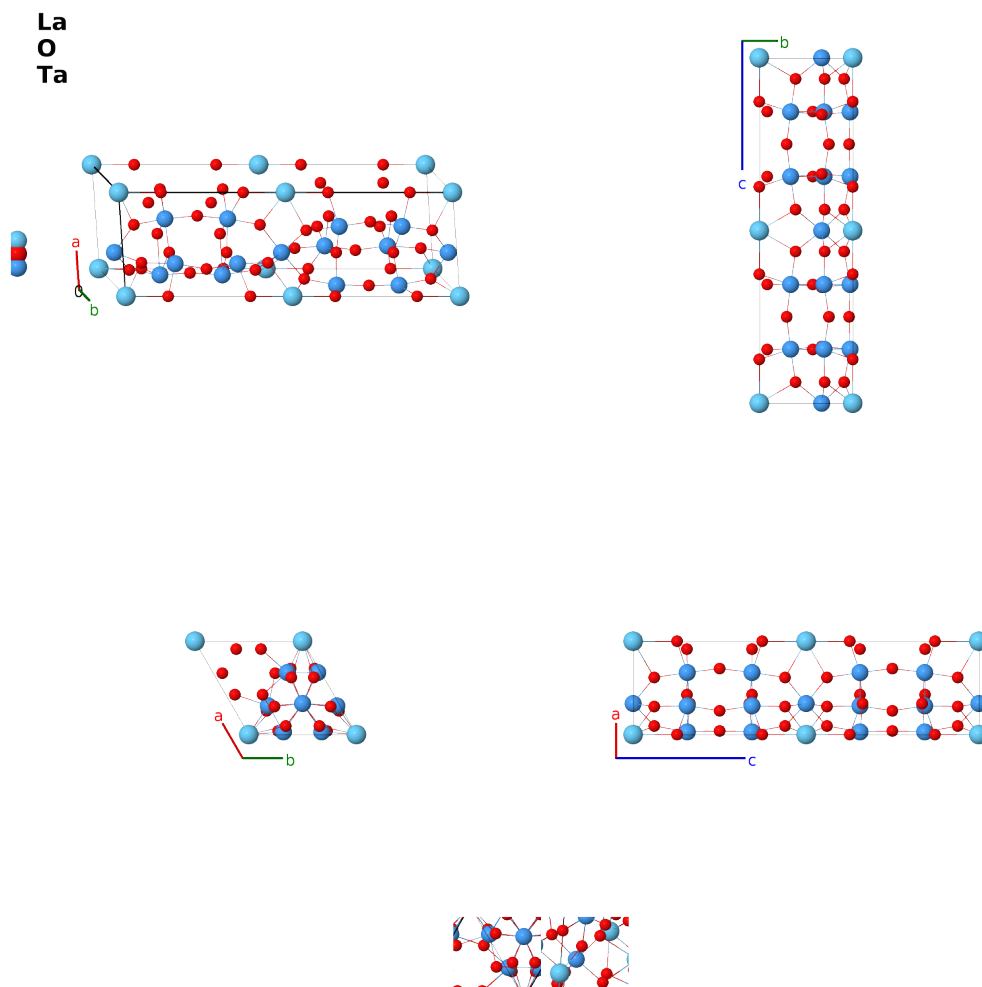
LaTa₇O₁₉ Structure: AB19C7_hP54_188_a_ghk2l.cl-001

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/7DPB>

https://aflow.org/prototype-encyclopedia/AB19C7_hP54_188_a_ghk2l.cl-001



Prototype	LaO ₁₉ Ta ₇
AFLOW prototype label	AB19C7_hP54_188_a_ghk2l.cl-001
ICSD	60837
CCDC	1624400
Pearson symbol	hP54
Space group number	188
Space group symbol	$P\bar{6}c2$

AFLOW prototype command `afLOW --proto=AB19C7_hP54_188_a_ghk21_c1-001`
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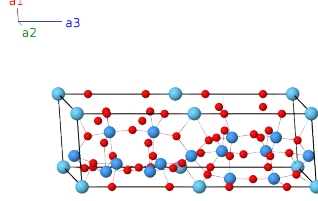
Other compounds with this structure

BiTa₇O₁₉, DyTa₇O₁₉, GdTa₇O₁₉, HoTa₇O₁₉, NdTa₇O₁₉, PrTa₇O₁₉, SmTa₇O₁₉

- Applying the AFLOW standard label protocol moves the La I atoms from the published (2c) site to the (2a) site.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	La I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2a)	La I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}}$	(2c)	Ta I
$\mathbf{B}_4$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2c)	Ta I
$\mathbf{B}_5$	$= z_3 \mathbf{a}_3$	$=$	$cz_3 \hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B}_6$	$= -\left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B}_7$	$= \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B}_8$	$= -z_3 \mathbf{a}_3$	$=$	$-cz_3 \hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B}_9$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B}_{10}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B}_{11}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B}_{12}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6k)	O III
$\mathbf{B}_{14}$	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6k)	O III
$\mathbf{B}_{15}$	$= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6k)	O III
$\mathbf{B}_{16}$	$= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6k)	O III
$\mathbf{B}_{17}$	$= -(x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6k)	O III
$\mathbf{B}_{18}$	$= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6k)	O III
$\mathbf{B}_{19}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(12l)	O IV
$\mathbf{B}_{20}$	$= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(12l)	O IV
$\mathbf{B}_{21}$	$= -(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(12l)	O IV

$\mathbf{B}_{22} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(121)	O IV
$\mathbf{B}_{23} =$	$-y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(121)	O IV
$\mathbf{B}_{24} =$	$-(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(121)	O IV
$\mathbf{B}_{25} =$	$-y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(121)	O IV
$\mathbf{B}_{26} =$	$-(x_6 - y_6) \mathbf{a}_1 + y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(121)	O IV
$\mathbf{B}_{27} =$	$x_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(121)	O IV
$\mathbf{B}_{28} =$	$-y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(121)	O IV
$\mathbf{B}_{29} =$	$-(x_6 - y_6) \mathbf{a}_1 + y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(121)	O IV
$\mathbf{B}_{30} =$	$x_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(121)	O IV
$\mathbf{B}_{31} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(121)	O V
$\mathbf{B}_{32} =$	$-y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(121)	O V
$\mathbf{B}_{33} =$	$-(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(121)	O V
$\mathbf{B}_{34} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(121)	O V
$\mathbf{B}_{35} =$	$-y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(121)	O V
$\mathbf{B}_{36} =$	$-(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(121)	O V
$\mathbf{B}_{37} =$	$-y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(121)	O V
$\mathbf{B}_{38} =$	$-(x_7 - y_7) \mathbf{a}_1 + y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_7 + 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(121)	O V
$\mathbf{B}_{39} =$	$x_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(121)	O V
$\mathbf{B}_{40} =$	$-y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(121)	O V
$\mathbf{B}_{41} =$	$-(x_7 - y_7) \mathbf{a}_1 + y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_7 + 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(121)	O V
$\mathbf{B}_{42} =$	$x_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(121)	O V
$\mathbf{B}_{43} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 + y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_8 - y_8) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(121)	Ta II
$\mathbf{B}_{44} =$	$-y_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 - 2y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(121)	Ta II
$\mathbf{B}_{45} =$	$-(x_8 - y_8) \mathbf{a}_1 - x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(121)	Ta II
$\mathbf{B}_{46} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a$				

$$\mathbf{B}_{52} = -y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 = -\frac{1}{2}a(x_8 + y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_8 - y_8) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} \quad (121) \quad \text{Ta II}$$

$$\mathbf{B}_{53} = -(x_8 - y_8) \mathbf{a}_1 + y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 = \frac{1}{2}a(-x_8 + 2y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} \quad (121) \quad \text{Ta II}$$

$$\mathbf{B}_{54} = x_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3 = \frac{1}{2}a(2x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} \quad (121) \quad \text{Ta II}$$

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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).