

Na₂Tl Structure:

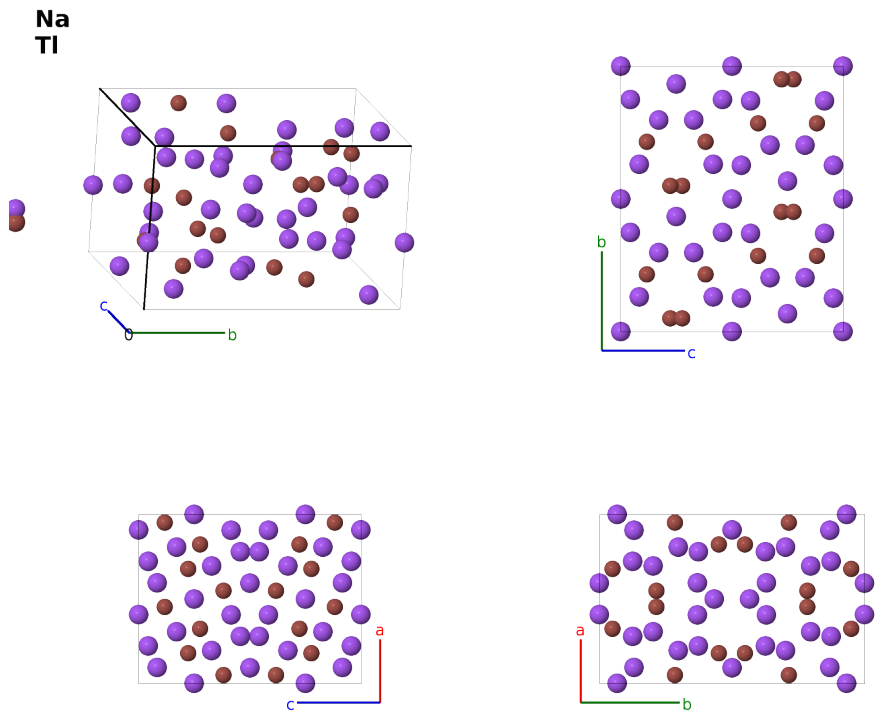
A2B_oC48_20_ab3c_2c-001

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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/PRYE>

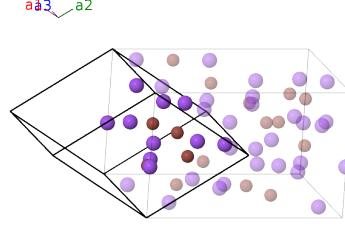
https://aflow.org/prototype-encyclopedia/A2B_oC48_20_ab3c_2c-001



Prototype	Na ₂ Tl
AFLOW prototype label	A2B_oC48_20_ab3c_2c-001
ICSD	105171
CCDC	1663062
Pearson symbol	oC48
Space group number	20
Space group symbol	$C222_1$
AFLOW prototype command	<pre>aflow --proto=A2B_oC48_20_ab3c_2c-001 --params=a, b/a, c/a, x₁, y₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇</pre>

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 =$		$ax_1 \hat{\mathbf{x}}$	(4a)	Na I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$		$-ax_1 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 =$		$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4b)	Na II
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 =$		$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4b)	Na II
$\mathbf{B}_5$	$= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3 =$		$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	Na III
$\mathbf{B}_6$	$= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3 =$		$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Na III
$\mathbf{B}_7$	$= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3 =$		$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Na III
$\mathbf{B}_8$	$= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3 =$		$ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8c)	Na III
$\mathbf{B}_9$	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3 =$		$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8c)	Na IV
$\mathbf{B}_{10}$	$= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3 =$		$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Na IV
$\mathbf{B}_{11}$	$= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3 =$		$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Na IV
$\mathbf{B}_{12}$	$= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3 =$		$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8c)	Na IV
$\mathbf{B}_{13}$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 =$		$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8c)	Na V
$\mathbf{B}_{14}$	$= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3 =$		$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Na V
$\mathbf{B}_{15}$	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3 =$		$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Na V
$\mathbf{B}_{16}$	$= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3 =$		$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8c)	Na V
$\mathbf{B}_{17}$	$= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3 =$		$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8c)	Tl I
$\mathbf{B}_{18}$	$= -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 =$		$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Tl I

$$\begin{aligned}
\mathbf{B}_{19} &= \begin{matrix} -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - \\ (z_6 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Tl I} \\
\mathbf{B}_{20} &= \begin{matrix} (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - \\ z_6 \mathbf{a}_3 \end{matrix} = ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8c) & \text{Tl I} \\
\mathbf{B}_{21} &= \begin{matrix} (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + \\ z_7 \mathbf{a}_3 \end{matrix} = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8c) & \text{Tl II} \\
\mathbf{B}_{22} &= \begin{matrix} -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 + \\ (z_7 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Tl II} \\
\mathbf{B}_{23} &= \begin{matrix} -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - \\ (z_7 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Tl II} \\
\mathbf{B}_{24} &= \begin{matrix} (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - \\ z_7 \mathbf{a}_3 \end{matrix} = ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (8c) & \text{Tl II}
\end{aligned}$$

References

- [1] D. A. Hansen, *Crystal structures of Na₂Tl and Li₉Al₄ and a bonding model for Na₂Tl* (1966). Retrospective Theses and Dissertations, Iowa State University.
- [2] D. A. Hansen and J. F. Smith, *Structure and Bonding Model for Na₂Tl*, Acta Cryst. **22**, 836–845 (1967), doi:10.1107/S0365110X67001653.

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