Na$_2$Tl Structure:
A2B_oC48_20_ab3c_2c-001

https://aflow.org/p/PRYE

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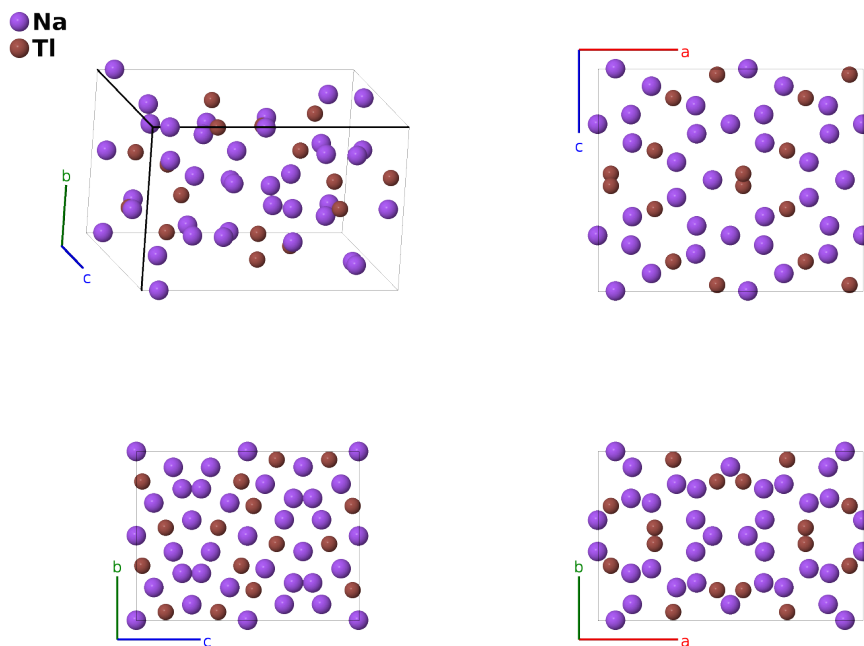
Prototype	Na$_2$Tl
AFLOW prototype label	A2B_oC48_20_ab3c_2c-001
ICSD	105171
Pearson symbol	oC48
Space group number	20
Space group symbol	$C222_1$
AFLOW prototype command	aflow --proto=A2B_oC48_20_ab3c_2c-001 --params=$a, b/a, c/a, x_1, y_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
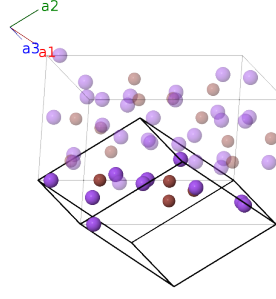
Basis vectors

		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
$\mathbf{B_2}$	$=$	$-x_1\,\mathbf{a_1} - x_1\,\mathbf{a_2} + \tfrac{1}{2}\,\mathbf{a_3}$	$=$	$-ax_1\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_3}$	$=$	$-y_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$by_2\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	Na II
$\mathbf{B_4}$	$=$	$y_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$-by_2\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_6}$	$=$	$-(x_3 - y_3)\,\mathbf{a_1} - (x_3 + y_3)\,\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Na III
$\mathbf{B_7}$	$=$	$-(x_3 + y_3)\,\mathbf{a_1} - (x_3 - y_3)\,\mathbf{a_2} - \left(z_3 - \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{10}}$	$=$	$-(x_4 - y_4)\,\mathbf{a_1} - (x_4 + y_4)\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Na IV
$\mathbf{B_{11}}$	$=$	$-(x_4 + y_4)\,\mathbf{a_1} - (x_4 - y_4)\,\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{14}}$	$=$	$-(x_5 - y_5)\,\mathbf{a_1} - (x_5 + y_5)\,\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Na V
$\mathbf{B_{15}}$	$=$	$-(x_5 + y_5)\,\mathbf{a_1} - (x_5 - y_5)\,\mathbf{a_2} - \left(z_5 - \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{18}}$	$=$	$-(x_6 - y_6)\,\mathbf{a_1} - (x_6 + y_6)\,\mathbf{a_2} + \left(z_6 + \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Tl I
$\mathbf{B_{19}}$	$=$	$-(x_6 + y_6)\,\mathbf{a_1} - (x_6 - y_6)\,\mathbf{a_2} - \left(z_6 - \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Tl I

$$\mathbf{B_{20}} = (x_6 + y_6)\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 \qquad = \qquad ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \qquad\qquad \text{(8c)} \qquad \text{Tl I}$$

$$\mathbf{B_{21}} = (x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 \qquad = \qquad ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad\qquad \text{(8c)} \qquad \text{Tl II}$$

$$\mathbf{B_{22}} = -(x_7 - y_7)\,\mathbf{a}_1 - (x_7 + y_7)\,\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad -ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(8c)} \qquad \text{Tl II}$$

$$\mathbf{B_{23}} = -(x_7 + y_7)\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad -ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(8c)} \qquad \text{Tl II}$$

$$\mathbf{B_{24}} = (x_7 + y_7)\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 \qquad = \qquad ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad\qquad \text{(8c)} \qquad \text{Tl II}$$

References

[1] D. A. Hansen, *Crystal structures of Na$_2$Tl and Li$_9$Al$_4$ and a bonding model for Na$_2$Tl* (1966). Retrospective Theses and Dissertations, Iowa State University.

[2] D. A. Hansen and J. F. Smith, *Structure and Bonding Model for Na$_2$Tl*, Acta Cryst. **22**, 836–845 (1967), doi:10.1107/S0365110X67001653.