

ThBC Structure: ABC_tP24_95_d_d_d-001

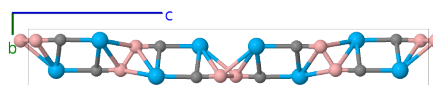
This structure originally had the label `ABC_tP24_95_d_d_d`. Calls to that address will be redirected here.

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<https://aflow.org/p/8RZF>

https://aflow.org/p/ABC_tP24_95_d_d_d-001

● B
● C
● Th



Prototype	BCTh
AFLOW prototype label	ABC_tP24_95_d_d_d-001
ICSD	2368
Pearson symbol	tP24
Space group number	95
Space group symbol	$P4_322$
AFLOW prototype command	<code>aflow --proto=ABC_tP24_95_d_d_d-001 --params=a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3</code>

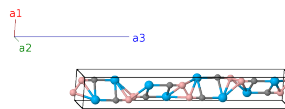
- This structure is identical to ThBC in the enantiomorphic space group $P4_122$ #91. It was generated from that structure by reflecting the atomic coordinates through the $z = 0$ plane. The ICSD entry is written for space group #91.

Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{x}$$

$$\mathbf{a}_2 = a \hat{y}$$

$$\mathbf{a}_3 = c \hat{z}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates		Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	$(8d)$		B I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	$(8d)$		B I
\mathbf{B}_3	$= -y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + (z_1 + \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{3}{4}) \hat{\mathbf{z}}$	$(8d)$		B I
\mathbf{B}_4	$= y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + (z_1 + \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{4}) \hat{\mathbf{z}}$	$(8d)$		B I
\mathbf{B}_5	$= -x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	$(8d)$		B I
\mathbf{B}_6	$= x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	$(8d)$		B I
\mathbf{B}_7	$= y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - (z_1 - \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - c(z_1 - \frac{1}{4}) \hat{\mathbf{z}}$	$(8d)$		B I
\mathbf{B}_8	$= -y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - (z_1 - \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - c(z_1 - \frac{3}{4}) \hat{\mathbf{z}}$	$(8d)$		B I
\mathbf{B}_9	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	$(8d)$		C I
\mathbf{B}_{10}	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	$(8d)$		C I
\mathbf{B}_{11}	$= -y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + (z_2 + \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{3}{4}) \hat{\mathbf{z}}$	$(8d)$		C I
\mathbf{B}_{12}	$= y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	$(8d)$		C I
\mathbf{B}_{13}	$= -x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	$(8d)$		C I
\mathbf{B}_{14}	$= x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	$(8d)$		C I
\mathbf{B}_{15}	$= y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - (z_2 - \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{4}) \hat{\mathbf{z}}$	$(8d)$		C I
\mathbf{B}_{16}	$= -y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - (z_2 - \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - c(z_2 - \frac{3}{4}) \hat{\mathbf{z}}$	$(8d)$		C I
\mathbf{B}_{17}	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	$(8d)$		Th I
\mathbf{B}_{18}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	$(8d)$		Th I
\mathbf{B}_{19}	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{3}{4}) \hat{\mathbf{z}}$	$(8d)$		Th I
\mathbf{B}_{20}	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	$(8d)$		Th I
\mathbf{B}_{21}	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	$(8d)$		Th I
\mathbf{B}_{22}	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	$(8d)$		Th I
\mathbf{B}_{23}	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - (z_3 - \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}}$	$(8d)$		Th I
\mathbf{B}_{24}	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - c(z_3 - \frac{3}{4}) \hat{\mathbf{z}}$	$(8d)$		Th I

References

- [1] P. Rogl, *The Crystal Structure of ThBC*, J. Nucl. Mat. **73**, 198–203 (1978), doi:10.1016/0022-3115(78)90560-3.