

ThBC Structure: ABC_tP24_95_d_d_d-001

This structure previously used the label(s) **ABC_tP24_95_d_d_d**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/8RZF>

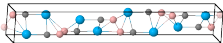
https://aflow.org/prototype-encyclopedia/ABC_tP24_95_d_d_d-001

Prototype	BCTh
AFLOW prototype label	ABC_tP24_95_d_d_d-001
ICSD	2368
CCDC	1592270
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

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8d) B I

$\mathbf{B}_2$	$=$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B}_3$	$=$	$-y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(z_1 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B}_4$	$=$	$y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_6$	$=$	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B}_7$	$=$	$y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - \left(z_1 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B}_8$	$=$	$-y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - \left(z_1 - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{3}{4}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{10}$	$=$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	C I
$\mathbf{B}_{11}$	$=$	$-y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(z_2 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(8d)	C I
$\mathbf{B}_{12}$	$=$	$y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$=$	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	C I
$\mathbf{B}_{15}$	$=$	$y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8d)	C I
$\mathbf{B}_{16}$	$=$	$-y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - \left(z_2 - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{3}{4}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{18}$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	Th I
$\mathbf{B}_{19}$	$=$	$-y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(z_3 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(8d)	Th I
$\mathbf{B}_{20}$	$=$	$y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{22}$	$=$	$x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	Th I
$\mathbf{B}_{23}$	$=$	$y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8d)	Th I
$\mathbf{B}_{24}$	$=$	$-y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - \left(z_3 - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{3}{4}\right) \hat{\mathbf{z}}$	(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.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

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