ThBC Structure: ABC_tP24_91_d_d_d-001

This structure originally had the label `ABC_tP24_91_d_d_d`. Calls to that address will be redirected here.

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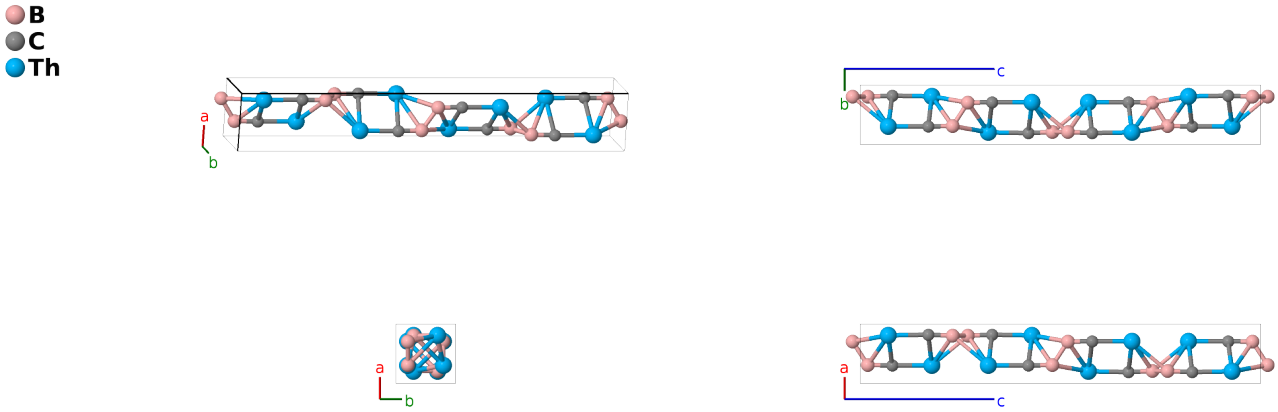
https://aflow.org/p/S6UF

https://aflow.org/p/ABC_tP24_91_d_d_d-001

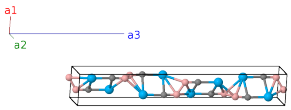


Prototype	BCTh
AFLOW prototype label	ABC_tP24_91_d_d_d-001
ICSD	2368
Pearson symbol	tP24
Space group number	91
Space group symbol	$P4_122$
AFLOW prototype command	`aflow --proto=ABC_tP24_91_d_d_d-001 --params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

- This structure can also be found in the enantiomorphic space group $P4_322$ #95.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ay_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(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
$\mathbf{B_3}$	=	$-y_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B_4}$	=	$y_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(z_1 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + ay_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(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
$\mathbf{B_7}$	=	$y_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 - \left(z_1 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - c\left(z_1 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B_8}$	=	$-y_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - \left(z_1 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{11}}$	=	$-y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8d)	C I
$\mathbf{B_{12}}$	=	$y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8d)	C I
$\mathbf{B_{13}}$	=	$-x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{15}}$	=	$y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8d)	C I
$\mathbf{B_{16}}$	=	$-y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8d)	C I
$\mathbf{B_{17}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{19}}$	=	$-y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8d)	Th I
$\mathbf{B_{20}}$	=	$y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(z_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8d)	Th I
$\mathbf{B_{21}}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{23}}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8d)	Th I
$\mathbf{B_{24}}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8d)	Th I

References

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

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.