T-50 B (A_g) Structure: A_tP50_134_a2m2n-001

This structure originally had the label `A_tP50_134_b2m2n`. Calls to that address will be redirected here.

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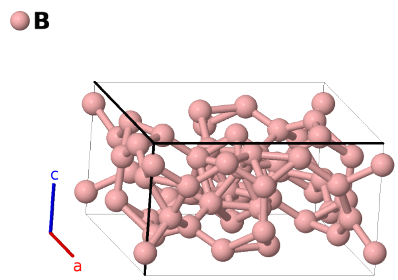
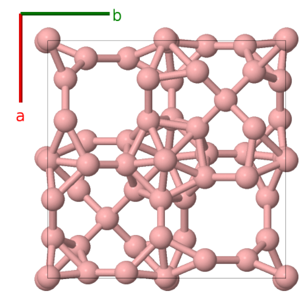
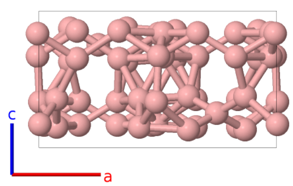
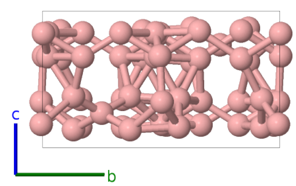
https://aflow.org/p/R7N6

https://aflow.org/p/A_tP50_134_a2m2n-001







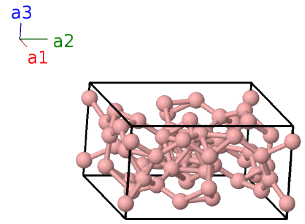


Prototype	B
AFLOW prototype label	A_tP50_134_a2m2n-001
***Strukturbericht* designation**	A_g
ICSD	26636
Pearson symbol	tP50
Space group number	134
Space group symbol	$P4_2/nnm$
AFLOW prototype command	`aflow --proto=A_tP50_134_a2m2n-001` `--params=`$a, c/a, x_2, z_2, x_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

- This is apparently the most common form of boron. At least it is listed first in (Donohue, 1982).
- The basic building block is a slightly distorted icosahedron. This icosahedron also appears in α-B (hR12) and β-B (hR105).

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
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2a)	B I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2a)	B I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8m)	B II
$\mathbf{B_4}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8m)	B II
$\mathbf{B_5}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8m)	B II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8m)	B II
$\mathbf{B_7}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8m)	B II
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8m)	B II
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8m)	B II
$\mathbf{B_{10}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8m)	B II
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8m)	B III
$\mathbf{B_{12}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8m)	B III
$\mathbf{B_{13}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8m)	B III
$\mathbf{B_{14}}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8m)	B III
$\mathbf{B_{15}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8m)	B III
$\mathbf{B_{16}}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8m)	B III
$\mathbf{B_{17}}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8m)	B III
$\mathbf{B_{18}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8m)	B III
$\mathbf{B_{19}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{20}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{21}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{22}}$	=	$y_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B IV

$\mathbf{B_{23}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1+y_4\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ay_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{24}}$	=	$x_4\,\mathbf{a}_1-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{25}}$	=	$y_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{26}}$	=	$-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{27}}$	=	$-x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{28}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{29}}$	=	$\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_1-x_4\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{30}}$	=	$-y_4\,\mathbf{a}_1+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{31}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1-y_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{32}}$	=	$-x_4\,\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{33}}$	=	$-y_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{34}}$	=	$\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(16n)	B IV
$\mathbf{B_{35}}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{36}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{37}}$	=	$-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{38}}$	=	$y_5\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{39}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1+y_5\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{40}}$	=	$x_5\,\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{41}}$	=	$y_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{42}}$	=	$-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{43}}$	=	$-x_5\,\mathbf{a}_1-y_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{44}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{45}}$	=	$\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_1-x_5\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{46}}$	=	$-y_5\,\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{47}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1-y_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{48}}$	=	$-x_5\,\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}+a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{49}}$	=	$-y_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16n)	B V
$\mathbf{B_{50}}$	=	$\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16n)	B V

References

[1] J. L. Hoard, R. E. Hughes, and D. E. Sands, *The Structure of Tetragonal Boron*, J. Am. Chem. Soc. **80**, 4507–4515 (1958), doi:10.1021/ja01550a019.

Found in

[1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).