substance: boron compounds, general properties
property: α-tetragonal boron structure group

The 50 atoms of the idealized unit cell of α-tetragonal boron are arranged in four B_{12} icosahedra at 4(c) positions and two single B atoms in 2(b) positions (Wyckoff notation). One of the five-fold axes of the icosahedra is arranged parallel to the *c axis* (Fig. 1). In the isostructural borides the 2(b) positions and an additional interstitial void position at 2(a) are completely or partly occupied by foreign, preferably metal atoms.

Representatives of the α-tetragonal boron structure group

Chemical formula (idealized)	Structural formula		
	binary compound	ternary compounds	
B (α-tetragonal modification)	$(B_{12})_4B_2$		77M1
compounds		$(B_{12})_4X_2Y_2$	
$B_{12}Be$	$(B_{12})_4\,Be_4$		87L1, 60B, 87H2
$B_{24}BeAl$		$(B_{12})_4Be_2Al_2$	87L1, 68B
$B_{24.2}\,AlBe_{0.8}$			85H1
$B_{48.7}\,Be_{1.6}\,Al_2$		$(B_{12})_4B_{0.7}\,Be_{1.6}Al_2$	87L2, 72K
β-AlB_{12}	$(B_{12})_4Al_4$		64P1
$C_2Al_3B_{48}$[2])		$(B_{12})_4C_2Al_4$[3])	70E, 77M2
filled and distorted variant			96H
$C_2Al_3\,B_{48}$			87L1, 73K
$B_{51}C$	$(B_{12})_4B_3C$		87H1
$B_{25}C$	$(B_{12})_4B_2C_2$		74W, 87L1
$B_{25}N$	$(B_{12})_4B_2N_2$		74W, 87L1
$B_{25}Ni$	$(B_{12})_4B_2Ni_2$		87L1, 64D
$Al_{1.00}Cu_{0.79}B_{25}$		$(B_{12})_4B_2Al_2Cu_{1.58}$	85H2
$(B_{25}Al_{1.00}Cu_{0.79})$		$(B_{12})_4Al_2Cu_2$[1])	86H
			87L1
$B_{48}B_2Ti_{1.3–2.0}$			87L1, 75A, 76P
$B_{48}C_2Ti_{1.86}$			87L1, 80A
$B_{48}C_2V_{1.29}$			87L1, 80A
$B_{48}B_2Zn_2$			87L1, 64P2

[1]) Metal sites incompletely occupied.
[2]) The attribution of $C_2Al_3B_{48}$ to the α-tetragonal boron structure group was argued to be incorrect in [65M] because only the high-temperature phase could be attributed to this structure group, while at low temperatures two crystallographically related twinned orthorhombic phase were assumed. For a more detailed information on this and closely related boron compounds, see below at $C_2Al_3B_{48}$.
[3]) 3 of 4 Al sites are statistically occupied.

B_8C	$((B_{12})_4C_6)_{4\text{ or }8}$	74P1,

In consequence of the additional C atoms the structure becomes disproportionately distorted and is no more tetragonal but orthorhombic.

So far as electronic properties of representatives of the α-tetragonal boron structure group have become known, they indicate semiconducting or insulating behavior.

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Fig. 1.

α-tetragonal boron structure group. Unit cell of α-tetragonal boron containing B_{12} icosahedra and two single B atoms in 2(b) positions (Wyckoff notation). In the isostructural borides the 2(b) positions and the additional interstitial void position at 2(a) are completely or partly occupied by foreign, preferably metal atoms.