

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Boron appears in Group 13 (IIIA) of the periodic table and is the only nonmetal of this group (Jansen 2003). Table 4-1 lists common synonyms, trade names, and other pertinent information to identify boron and selected compounds.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Boron is a nonmetal and is typically found in nature bound to oxygen. It is never found as the free element (Cotton et al. 1999). Boron has two stable isotopes, ^{10}B and ^{11}B , which are naturally present at 19.10–20.31 and 79.69–80.90%, respectively (Jansen 2003). There are ten other known non-radioactive isotopes of boron (Lide 2008). Elemental boron exists in several allotropic forms (Jansen 2003). In addition to being an amorphous powder, boron has four crystalline forms: α -rhombohedral, β -rhombohedral, α -tetragonal, and β -tetragonal (Jansen 2003).

The chemical properties of boron are more similar to carbon and silicon than elements of its own group, although boron is more electron deficient. Boron has a high affinity for oxygen-forming borates, and reacts with water at temperatures above 100 °C to form boric acid and other boron compounds. The electron deficiency of boron does not allow conventional two-electron bonds, but rather multicenter bonds that are exclusively covalent (Jansen 2003; Schubert and Brotherton 2006). Boron hydrides consequently have structures quite different from hydrocarbons (Jansen 2003). The multi-center nature of boron allows the formation of a diverse array of covalent networks, rings, cages, and clusters. Boron forms strong covalent bonds with electronegative elements such as fluorine and oxygen (Schubert and Brotherton 2006).

Table 4-2 lists important physical and chemical properties of boron and selected compounds.

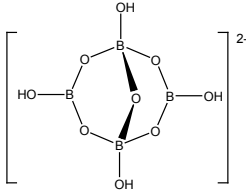
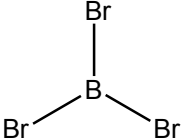
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Table 4-1. Chemical Identity of Boron and Selected Boron Compounds^a

Characteristic	Boron	Boron oxide	Boric acid
Synonym(s)	Boron, metallic	Boric anhydride; boric acid, anhydride; boron sesquioxide; boron trioxide; diboron trioxide; fused boric acid	Orthoboric acid; boron hydroxide; boron trihydroxide
Registered trade name(s)	No data	No data	Optibor ^b
Chemical formula	B	B ₂ O ₃	B(OH) ₃
Chemical structure	Amorphous powder, as well as four crystalline forms: α -rhombohedral, β -rhombohedral, α -tetragonal, and β -tetragonal ^c	Randomly oriented B ₃ O ₃ rings with bridging oxygen atoms ^d	Planar BO ₃ ³⁻ units linked by asymmetrical hydrogen bonds ^d
Identification numbers:			
CAS registry	7440-42-8	1303-86-2	10043-35-3
NIOSH RTECS ^e	ED7350000	ED7900000	ED4550000
EPA hazardous waste	No data	No data	No data
EPA/OPP pesticide Code	128945	011002	011001
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMDG shipping	No data	No data	No data
HSDB	4482	1609	1432
EINECS	231-151-2	215-125-8	233-139-2
NCI	No data	No data	C56417

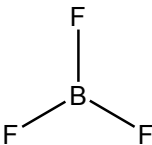
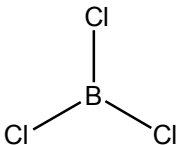
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Table 4-1. Chemical Identity of Boron and Selected Boron Compounds^a

Characteristic	Borax	Sodium tetraborate	Boron tribromide
Synonym(s)	Sodium borate; sodium tetraborate; borax decahydrate; disodium tetraborate decahydrate	Sodium borate; sodium borate anhydrous; disodium tetraborate; sodium baborate; sodium pyroborate; boric acid, disodium salt	Boron bromide; tribromoborane; tribromoboron
Registered trade name(s)	Jaikin, Pyrobor, Three Elephant, V-Bor ^b	Dehybor 65 ^b	No data
Chemical formula	B ₄ Na ₂ O ₇ •10H ₂ O	Na ₂ B ₄ O ₇	BBr ₃
Chemical structure	 <p style="text-align: center;">Tetraborate anion in solution^d</p>	Anhydrous borates have polymeric assemblies of planar BO ₃ and/or tetrahedral BO ₄ units linked by shared oxygen atoms ^d	
Identification numbers:			
CAS registry	1303-96-4	1330-43-4	10294-33-4
NIOSH RTECS ^e	VZ2275000	ED4588000	ED7400000
EPA hazardous waste	No data	No data	No data
EPA/OPP Pesticide Code	029601	011112	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMDG shipping	No data	No data	UN 2692; IMDG 8.1
HSDB	328	5025	327
EINECS	233-139-2	215-540-4	233-657-9
NCI	No data	No data	No data

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Table 4-1. Chemical Identity of Boron and Selected Boron Compounds^a

Characteristic	Boron trifluoride	Boron trichloride
Synonym(s)	Anca 1040; boron fluoride; trifluoroborane	Trichloroborane; trichloroboron
Registered trade name(s)	No data	No data
Chemical formula	BF ₃	BCl ₃
Chemical structure		
Identification numbers:		
CAS registry	7637-07-2	10294-34-5
NIOSH RTECS ^e	ED2275000	ED1925000
EPA hazardous waste	No data	No data
EPA/OPP Pesticide Code	No data	No data
OHM/TADS	No data	No data
DOT/UN/NA/IMDG shipping	UN 1008; IMDG 6.1 (boron trifluoride); UN 2851; IMDG 8.2 (boron trifluoride dihydrate)	UN 1741; IMDG 2.2
HSDB	325	326
EINECS	231-569-5	233-658-4
NCI	No data	No data

^aAll information obtained from HSDB 2009 and ChemIDplus 2009, except where noted.

^bNIOSH 2005

^cJansen 2003

^dCotton et al. 1999

^eRTECS 2007

CAS = Chemical Abstracts Service; DOT/UN/NA/IMDG = Department of Transportation/United Nations/North America/Intergovernmental Maritime Dangerous Goods Code; EINECS = European Inventory of Existing Chemical Substances; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

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Table 4-2. Physical and Chemical Properties of Boron and Selected Boron Compounds^a

Property	Boron	Boron oxide	Boric acid
Molecular weight	10.811	69.620	61.833
Physical description	Black or dark brown powder (amorphous form); clear red crystals (α -rhombohedral form); black, opaque crystals with metallic luster (α -tetragonal form); black (β -rhombohedral form)	Colorless, glassy or hexagonal crystals, hygroscopic	Colorless, transparent crystals; white granules or powder
Melting point	2,075 °C	450 °C (crystal)	170.9 °C
Boiling point	4,000 °C	1,500 °C (crystal)	No data
Density	2.350 g/cm ³ (amorphous); 2.46 g/cm ³ (α -rhombohedral); 2.31 g/cm ³ (α -tetragonal); 2.35 g/cm ³ (β -rhombohedral)	1.8 g/cm ³ (amorphous); 2.46 g/cm ³ (crystal)	1.435 g/cm ³ at 15 °C
Odor	No data	Odorless	Odorless
Solubility:			
Water	Insoluble	4.0% at 20 °C	50 g/L at 25 °C
Organic solvent(s)	Insoluble alcohol, ether	Soluble in alcohol, glycerol	17.5% in glycerol; 18.5% in ethylene glycol; 173.9 g/L in methanol; 94.4 g/L in ethanol; 0.6% in acetone; 1.5% in ethyl acetate (all at 25 °C)
Other	Soluble in concentrated nitric and sulfuric acids	No data	No data
pK _a	No data	No data	9.42
Log K _{ow}	No data	No data	0.175
Vapor pressure	0.0119 mm Hg at 2,140 °C	Negligible at 20 °C	Negligible at 20 °C
Autoignition temperature	580 °C	No data	No data
Flashpoint	No data	No data	No data
Flammability limits in air	Dust ignites spontaneously in air	Noncombustible	Not flammable
Conversion factors	No data	No data	No data
Explosive limits	No data	No data	No data

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Table 4-2. Physical and Chemical Properties of Boron and Selected Boron Compounds^a

Property	Borax	Sodium tetraborate	Boron tribromide
Molecular weight	381.373	201.220	250.52
Physical Description	White, monoclinic crystals	Colorless glassy solid; hygroscopic	Colorless, fuming liquid
Melting point	75 °C (decomposes)	743 °C	-46.0 °C
Boiling point	No data	1,575 °C (decomposes)	90 °C
Density	1.73 g/cm ³	2.367 g/cm ³	2.698 g/cm ³ at 0 °C
Odor	Odorless	Odorless	Sharp, irritating odor, pungent
Solubility:			
Water	59.3 g/L at 25 °C	3.1% at 25 °C	Decomposes in water
Organic solvents	1 g/1 mL in glycerol; insoluble in alcohol	16.7% in methanol; 30% in ethylene glycol; 40.6 g/L in formamide (all at 25 °C)	Decomposes in alcohol; soluble in carbon tetrachloride, sulfur dioxide (liquid), carbon disulfide
Other	Insoluble in acid	No data	No data
pK _a	No data	No data	No data
Log K _{ow}	No data	No data	No data
Vapor pressure	Negligible	Negligible at 20 °C	100 mm Hg at 33.5 °C
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits in air	Not flammable	Noncombustible	Nonflammable
Conversion factors	No data	No data	1 ppm=10.25 mg/m ^{3b}
Explosive limits	No data	No data	No data

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Table 4-2. Physical and Chemical Properties of Boron and Selected Boron Compounds^a

Property	Boron trifluoride	Boron trichloride
Molecular weight	67.81	117.17
Physical Description	Colorless gas	Colorless fuming liquid at low temperature
Melting point	-126.8 °C	-107 °C
Boiling point	-101 °C	12.5 °C
Density	3.07666 g/L at 1 atm, 0 °C	1.3728 g/cm ³ at 0 °C
Odor	Pungent, suffocating odor, irritating ^c	Pungent, suffocating odor, irritating, sharp
Solubility:		
Water	332 g/100 g water at 0 °C with some hydrolysis forming fluoboric and boric acids	Decomposes in water, hydrolyzed easily
Organic solvents	Soluble in benzene, dichlorobenzene, chloroform, carbon tetrachloride, carbon sulfide; soluble in most saturated and halogenated hydrocarbons and in aromatic compounds	Decomposes in alcohol
Other	1.94 g/100 g in anhydrous sulfuric acid, soluble in concentrated nitric acid	No data
pK _a	No data	No data
Log K _{ow}	No data	No data
Vapor pressure	3.656x10 ⁴ mm Hg at -13.2 °C	1 mm Hg at 25 °C (extrapolated)
Autoignition temperature	No data	No data
Flashpoint	No data	No data
Flammability limits in air	Nonflammable	Nonflammable
Conversion factors	1 ppm=2.77 mg/m ^{3b}	No data
Explosive limits	No data	No data

^aAll information from HSDB 2009, except where noted.

^bNIOSH 2009

^cOdor threshold 4.50 mg/m³ (Ruth 1986)