4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Barium is an alkaline earth metal with an atomic number of 56 and is classified in Group IIA of the periodic table of elements. Its outer shell of electrons has a $6s^2$ configuration. Because barium is highly reactive, it exists in the environment in the +2 oxidation state, which is its only oxidation state.

Barium forms useful alloys with aluminum and magnesium, which are used as getters in electronic tubes to remove residual gases (Genter 2001). Barium is also used as a deoxidizer for steel and other metals (Boffito 2002).

Barium reacts with several other elements to form commercially-important compounds. Of these, eight barium compounds are covered in this chapter: barium acetate, barium carbonate, barium chloride, barium cyanide, barium, hydroxide, barium oxide, barium sulfate, and barium sulfide. Their chemical formulas, structures, synonyms, and identification numbers, in addition to those for barium metal, are listed in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Metallic barium is a silvery-white soft metal, but takes on a silver-yellow color when exposed to air (Boffito 2002; Genter 2001). Like other alkaline earth metals, barium decomposes in water, evolving hydrogen gas. Barium oxidizes readily in moist air. In powdered form, barium reacts violently with air. Because of its high reactivity, barium does not exist as the metal in the environment; it exists in a combined state with other elements.

The barium compounds, barium acetate, barium chloride, barium cyanide, barium hydroxide, and barium oxide, are quite soluble in water. Barium carbonate and sulfate are poorly soluble in water. Barium oxide reacts rapidly with carbon dioxide in water to form barium hydroxide and barium carbonate (Dibello et al. 2003). Barium sulfide slowly decomposes in water, forming barium hydroxide and barium hydrosulfide. Barium sulfide is also known to undergo slow oxidation in solution to form elemental sulfur and various oxidized sulfur species including the sulfite, thiosulfate, polythionates, and sulfate. The water solubility of barium compounds increases with decreasing pH (IPCS 1991).

Table 4-1. Chemical Identity of Barium and Barium Compounds[a]

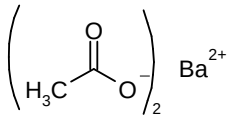
Characteristic	Barium	Barium acetate	Barium carbonate
Synonyms	No data	Acetic acid, barium salt; barium diacetate	Carbonic acid, barium salt; barium monocarbonate; Pigment White 10; BW-C3; BW-P
Trade names	No data	No data	No data
Chemical formula	Ba	$Ba(C_2H_3O_2)_2$	$BaCO_3$
Chemical structure	Ba		$[Ba^{2+}]\ [CO_3^{2-}]$
Identification numbers:			
CAS registry	7440-39-3	543-80-6	513-77-9
NIOSH RTECS	CQ8370000[b]	AF4550000[b]	CQ8600000[b]
EPA hazardous waste	D005	No data	D005
DOT/UN/NA/IMCO shipping	UN1440/IMO 4.3	No data	UN 1564/IMO 6.1
HSDB	4481	No data	950
EINECS	231-149-1	208-849-0	208-167-3
NCI	No data	No data	No data

Table 4-1. Chemical Identity of Barium and Barium Compounds[a]

Characteristic	Barium chloride	Barium cyanide	Barium hydroxide
Synonyms	Barium dichloride; NCI-C61074; SBa 0108E	Barium dicyanide	Barium dihydroxide; barium hydroxide lime; caustic baryta
Trade names	No data	No data	No data
Chemical formula	$BaCl_2$	$Ba(CN)_2$	$Ba(OH)_2$
Chemical structure	$[Ba^{2+}]\ [Cl^-]_2$	$[Ba^{2+}]\ [CN^-]_2$	$[Ba^{2+}]\ [OH^-]_2$
Identification numbers:			
CAS registry	10361-37-2	542-62-1	17194-00-2
NIOSH RTECS	CQ8750000[b]	CQ8785000[b]	CQ9200000[b]
EPA hazardous waste	D005	PO13/D003/D005	D005
DOT/UN/NA/IMCO shipping	UN 1564/IMO 6.1	UN 1565/IMO 6.1	UN 1564/IMO 6.1
HSDB	2633	403	1605
EINECS	233-788-1	208-822-3	241-234-5
NCI	No data	No data	No data

Table 4-1. Chemical Identity of Barium and Barium Compounds[a]

Characteristic	Barium oxide	Barium sulfate	Barium sulfide
Synonyms	Barium monoxide; barium protoxide; baryta; calcined baryta	Artificial heavy spar; artificial barite; baridol; barytes; blanc fixe; C.I. Pigment White 21; Citobaryum; Enamel White; E-Z-Paque; Solbar; precipitated barium sulphate; sulfuric acid, barium salt[f]	Barium suphide
Trade names	No data	No data	No data
Chemical formula	BaO	$BaSO_4$	BaS
Chemical structure	$[Ba^{2+}]$ $[O^{2-}]$	$[Ba^{2+}]$ $[SO_4{}^{2-}]$	$[Ba^{2+}]$ $[S^{2-}]$
Identification numbers:			
CAS registry	1304-28-5	7727-43-7	21109-95-5
NIOSH RTECS	CQ9800000[b]	CR0600000[b]	CR0660000[b]
EPA hazardous waste	No data	D005	No data
DOT/UN/NA/IMCO shipping	UN1884	UN1564/IMO6.1	UN1564/IMDG6.1[c]
EINECS	215-127-9	231-784-4	244-214-4
HSDB	No data	5041	No data
NCI	No data	No data	No data

[a]All information obtained from HSDB 2007 and ChemIDplus 2007 except where noted
[b]RTECS 2007
[c]Kresse et al. 2007

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

4. CHEMICAL AND PHYSICAL INFORMATION

Information regarding the physical and chemical properties of barium and barium compounds is located in Table 4-2.

Table 4-2. Physical and Chemical Properties of Barium and Barium Compounds[a]

Property	Barium	Barium acetate	Barium carbonate
Molecular weight	137.327	255.416 (anhydrous) 273.431 (monohydrate)	197.336
Physical description	Silvery-yellow metal; cubic	White powder (anhydrous); white crystals (monohydrate)	White orthorhombic crystals
Melting point	727 °C	Decomposes at 110 °C (monohydrate)	1,555 °C
Boling point	1,897 °C	No data	No data
Density	3.62 g/cm^3	2.47 g/cm^3 (anhydrous); 2.19 g/cm^3 (monohydrate)	4.2865 g/cm^3
Specific gravity	No data	2.02 (below 24.7 °C)[b]	No data
Odor	No data	No data	Odorless[c]
Odor threshold	No data	No data	No data
Solubility:			
Water	Reacts with water	79.2 g/100 g water at 25 °C	0.0014 g/100 g water at 20 °C; soluble in dilute HCl, HNO_3, and acetic acid[d]; soluble in NH_4Cl and NH_4NO_3 solutions[d]
Organic solvents	Slightly soluble in ethanol	Slightly soluble in ethanol (monohydrate)	Insoluble in alcohol[e]
Partition coefficients	No data	No data	No data
Vapor pressure	6.65x10^{-4} mmHg (at 630 °C)[f]; 0.998 mmHg (at 1,050 °C)[f]	No data	Essentially zero[g]
Henry's law coefficients	No data	No data	No data
Autoignition temperature	No data	No data	Nonflammable[c]
Flashpoint	No data	No data	Nonflammable[c]
Flammability limits	Explosion hazard if exposed to moist air[d]	No data	Nonflammable[c]
Conversion factors	No data	No data	No data
Explosive limits	No data	No data	No data

Table 4-2. Physical and Chemical Properties of Barium and Barium Compounds[a]

Property	Barium chloride	Barium cyanide	Barium hydroxide
Molecular weight	208.232 (anhydrous); 244.263 (dihydrate)[e]	189.361	171.342 (anhydrous); 189.357 (monohydrate); 315.464 (octahydrate)
Physical description	White hygroscopic orthorhombic crystals (anhydrous); white monoclinic crystals (dihydrate)	White crystalline powder	White powder (anhydrous, monohydrate); white monoclinic crystals (octahydrate)
Melting point	962 °C (anhydrous); decomposes at approximately 120 °C (dihydrate)	No data	408 °C (anhydrous); decomposes at 78 °C (octahydrate)
Boling point	1,560 °C (anhydrous)	No data	No data
Density	3.9 g/cm^3 (anhydrous); 3.097 g/cm^3 (dihydrate)	No data	3.743 g/cm^3 (monohydrate); 2.18 g/cm^3 (octahydrate)
Specific gravity	No data	No data	4.495 (anhydrous)[h]
Odor	Odorless[g]	No data	No data
Odor threshold	No data	No data	No data
Solubility:			
Water	37.0 g/100 g water at 25 °C	800 g/L (at 14 °C)[e]	4.91 g/100 g water at 25 °C
Organic solvents	Insoluble in ethanol (dehydrate)	180 g/L (in 70% alcohol at 14 °C)[e]	Soluble in methanol[d]
Partition coefficients	No data	No data	No data
Vapor pressure	Essentially zero[g]	No data	0 mm Hg at 15 °C (monohydrate)[i]; 11.4 mm Hg at 15 °C (water vapor pressure of octahydrate)[i]
Henry's law coefficients	No data	No data	No data
Autoignition temperature	No data	Nonflammable[c]	No data
Flashpoint	No data	Nonflammable[c]	No data
Flammability limits	No data	Nonflammable[c]	No data
Conversion factors	No data	No data	No data
Explosive limits	No data	No data	Explosive >216 °C[j]

Table 4-2. Physical and Chemical Properties of Barium and Barium Compounds[a]

Property	Barium oxide	Barium sulfate	Barium sulfide
Molecular weight	153.326	233.391	169.393
Physical description	White-yellow powder; cubic and hexagonal crystals	White orthorhombic crystals	Colorless cubic crystals or gray powder
Melting point	1,972 °C	1,580 °C	2,229 °C
Boling point	No data	No data	No data
Density	5.72 g/cm^3 (cubic)	4.49 g/cm^3	4.3 g/cm^3
Specific gravity	5.32 (hexagonal)[b]	4.50[b]	No data
Odor	Odorless[g]	Odorless[d]	Sulfurous
Odor threshold	No data	No data	No data
Solubility:			
Water	1.5 g/100 g water at 20 °C	00.00031 g/100 g water at 20 °C	8.94 g/100 g water at 25 °C
Organic solvents	Soluble in ethanol; insoluble in acetone	Insoluble in ethanol	No data
Partition coefficients	No data	No data	No data
Vapor pressure	Essentially zero[g]	No data	No data
Henry's law coefficients	No data	No data	No data
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits	Produces heat on contact with water or steam[k]	Noncombustible[k]	Flammable by spontaneous chemical reactions[k]
Conversion factors	No data	No data	No data
Explosive limits	Contact with CO_2 may cause explosion[k]	Heating with aluminum may cause violent explosions[k]	Air, moisture, or acid fumes may cause it to ignite[k]

[a]All information obtained from Lide 2005 except where noted
[b]Dibello et al. 2003
[c]DOT 2005
[d]Budavari et al. 2001
[e]Weast 1989
[f]Boffito 2002
[g]NIOSH/OSHA 1978
[h]Perry and Chilton 1973
[i]Preisman and Davis 1948
[j]HSDB 2007
[k]Lewis 2000