4. CHEMICAL, PHYSICAL, AND RADIOLOGICAL INFORMATION

4.1 CHEMICAL IDENTITY

Iodine is a nonmetallic element belonging to the halogen family in Group VIIA of the periodic table. Iodine is found in nature as iodide (i.e., I^-) in brines or in molecular compounds with other elements (e.g., iodate or IO_3^-). The chemical information for elemental iodine and some of its compounds is listed in Table 4-1. Radioactive isotopes of iodine (e.g., see Section 4.2) are an additional cause of concern with regard to human health (see Chapter 3).

4.2 PHYSICAL, CHEMICAL, AND RADIOLOGICAL PROPERTIES

The physical properties of iodine and selected iodine compounds are listed in Table 4-2. The percent occurrence of iodine isotopes and radiological properties of iodine isotopes is listed in Table 4-3.

Iodine can exist in several oxidation states: -1, 0, +1, +3, +5, and +7. Under normal environmental conditions, the -1, 0, and +5 oxidation states are the most important. There are 36 isotopes of iodine having masses between 108 and 143 (Chu et al. 1999); 14 of these yield significant radiation. The only naturally-occurring isotopes of iodine are ^{127}I and ^{129}I, which are stable and radioactive, respectively. Isotopes of mass less than 127 are produced in particle accelerators (common examples are ^{123}I and ^{125}I), while those >127 are formed in neutron generators such as nuclear reactors and atomic bombs (common examples are ^{129}I and ^{131}I). A total of 72% of uranium fissions and 75% of plutonium fissions leads directly or by beta decay of precursors, to iodine isotopes. For example, 2.89% of ^{235}U and 3.86% of ^{239}Pu fission atoms lead to the formation of a series of isobar 131 isotopes, including ^{131}In, ^{131}Sn, ^{131}Sb, ^{131}Te, ^{131}I, and ^{131}Xe. Each isotope can be formed as an initial fission product and, once formed, each isotope decays by beta-ray emission to the right on the sequence, through ^{131}I, and with stable ^{131}Xe. The process can be displayed as:

$$^{235}U + {}^{1}n \dashrightarrow {}^{131}In \xrightarrow{0.28\ s} {}^{131}Sn \xrightarrow{56\ s} {}^{131}Sb \xrightarrow{23.0\ m} {}^{131}Te \xrightarrow{25.0\ m} {}^{131}I \xrightarrow{8.02\ d} {}^{131}Xe$$

Table 4-1. Chemical Identity of Iodine and Iodine Compounds

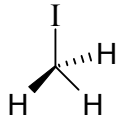
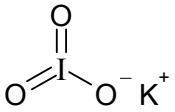
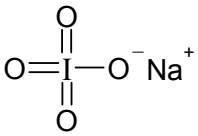
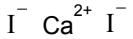
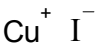
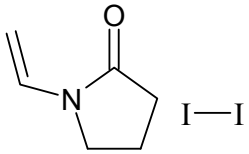
Property	Iodine	Hydrogen iodide	Sodium iodide	Potassium iodide	Methyl iodide	Cesium iodide
Chemical formula	I_2	HI	NaI	KI	CH_3I	CsI
Chemical structure						
Synonyms	Actomar; diiodine; eranol; iodine-127; molecular iodine	Hydroiodic acid	Sodium monoiodide; sodium Iodine	Hydroiodic acid, potassium salt; PIMA; SSK; iodide of potash	Monoiodo-methane; iodomethane	No data
Trade names	None	None	None	None	Halon 10001	No data
Identification numbers						
CAS registry	7553-56-2	10034-85-2	7681-82-5	7681-11-0	74-88-4	7789-17-5
NIOSH RTECS	NN1575000	MW3760000	WB6475000	TT2975000	PA9450000	No data
EPA hazardous waste	None	None	None	None	U138	None
OHM/TADS	None	None	None	None	None	None
DOT/UN/NA/ IMO shipping	UN 1759; UN 1760	UN 2197; UN 1787 Corrosive material/ IMO 8.0; IMO 2.0	None	None	UN 2644 Poison/ IMO 6.1	None
HSDB	34	2155	750	5040	1336	None
NCI	42355	None	None	77362	9366	None
STCC	None	None	None	None	None	None

Table 4-1. Chemical Identity of Iodine and Iodine Compounds

Property	Potassium iodate	Sodium periodate	Calcium iodide	Copper (I) iodide	Povidone iodine
Chemical formula	KIO3	NaIO4	CaI_2	CuI	$C_6H_9I_2NO$
Chemical structure					
Synonyms	Iodic acid, potassium salt	Sodium metaperiodate	Calcium diiodide; calcium iodide hydrate	Copper monoiodide; natural marshite; cuprous iodide	Poly(1-(2-oxo-1-pyrrolidinyl)-ethylene)iodine complex; betadine; efodine; Iodopoly(vinyl pyrrolidinone); isobetadyne; isodine; poly(vinylpyrrolidinone) iodide; ultradine
Trade names	None	None	None	None	None
Identification numbers					
CAS registry	7758-05-6	7790-28-5	10102-68-8	7681-65-4	25655-41-8
NIOSH RTECS	NN1350000	None	None	None	TR1579600
EPA hazardous waste	None	None	None	None	None
OHM/TADS	None	None	None	None	None
DOT/UN/NA/ IMO shipping		None	None	None	None
HSDB	1231	None	None	271	6831
NCI		None	None	None	26245
STCC	None	None	None	None	None

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; 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; STCC = Standard Transportation Commercial Code

Source: HSDB 2001; Lide 2000

Table 4-2. Physical and Chemical Properties of Iodine and Iodine Compoundsa

Property	Iodine	Hydrogen iodide	Sodium iodide	Potassium iodide
Molecular weight, g/mole	253.809[a]	127.91[a]	149.89[a]	166.02[a]
Color	Bluish-black[a]	Colorless[a]	White	Colorless or white[a]
Physical state	Solid; scales or plates[a]	Gas[a]	Solid; crystals or granules	Solid; crystals, granules, or powder[a]
Melting point	113.60 EC[a]	-50.8 EC[a]	651 EC[a]	680 EC[a]
Boiling point	185.24 EC[a]	-35.1 EC[a]	1,304 EC[d]	1,323 EC[d]
Density, g/cm^3 (25 EC)	4.93[a]	5.23[a]	3.67[a]	3.12[a]
Odor	Characteristic[a]	No data	Odorless[a]	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility (25 EC):				
Water	330 mg/L[a]	2,340 g/L (10 EC)[a]	2,000 g/L[a]	1,429 g/L[a]
Organic solvents(s)	141 g/kg benzene[a]	Soluble[a]	500 g/L alcohol[a]	13 g/L acetone[a]
Partition coefficients:				
Log K_{ow}	2.49[b]	No data	No data	No data
Log K_{oc}	No data	No data	No data	No data
Vapor pressure (25 EC)	0.305 mm Hg[a]	5,940 mm Hg[c]	1 mm Hg (767 EC)[c]	No data
Henry's Law constant	No data	No data	No data	No data
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	Non-flammable	No data	No data
Explosive limits	No data	No data	No data	No data

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

Property	Methyl iodide	Cesium iodide	Potassium iodate	Sodium periodate
Molecular weight, g/mole	141.94[a]	259.81[a]	214.02[a]	213.892[d]
Color	Colorless[a]	Colorless[d]	White[a]	White[d]
Physical state	Liquid[a]	Solid; crystals, or powder[a]	Solid, crystals[a]	Solid; crystals[d]
Melting point	-66.5 EC[a]	621 EC[a]	560 EC[a]	Decomposes ~300 EC
Boiling point	42.5 EC[a]	ca. 1,280 EC[a]	No data	No data
Density, g/cm^3 (25 EC)	2.28 (20 EC)[a]	4.5[a]	3.98[c]	3.86[d]
Odor	Pungent, ether-like[c]	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility (25 EC):				
Water	13.9 g/L (20 EC)[c]	Miscible[a]	9.16 g/100 g[c]	Soluble[d]
Organic solvents(s)	Miscible[a]	Soluble in alcohol; insoluble in acetone[a]	No data	No data
Partition coefficients:				
Log K_{ow}	1.51[c]	No data	No data	No data
Log K_{oc}	No data	No data	No data	No data
Vapor pressure (25 EC)	405 mm Hg	No data	No data	No data
Henry's Law constant	0.00526 atm-cu m/mole	No data	No data	No data
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Explosive limits	No data	No data	No data	No data

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

Property	Calcium iodide	Copper (I) iodide	Povidone iodine
Molecular weight, g/mole	293.89[a]	190.45[a]	364.95[c]
Color	Yellow[a]	Red-brown[a]	Yellow-brown[c]
Physical state	Solid; lumps or powder[a]	Solid; powder or crystals[a]	Solid; powder[c]
Melting point	740 EC	588–606 EC[a]	300 EC[e]
Boiling point	1,100 EC	~1,290 EC[a]	No data
Density, g/cm^3 (25 EC)		5.63[a]	
Odor	No data	No data	Slight characteristic[c]
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility (25 EC)			
Water	Very soluble[a]	80 mg/L (18 EC)[c]	Soluble[c]
Organic solvents(s)	Very soluble in alcohol, acetone[a]	Insoluble[a]	Insoluble[c]
Partition coefficients:			
Log K_{ow}	No data	No data	No data
Log K_{oc}	No data	No data	No data
Vapor pressure	No data	No data	No data
Henry's Law constant	No data	No data	No data
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits	No data	No data	No data
Explosive limits	No data	No data	No data

[a]Budavari et al. 1998
[b]Hansch and Leo 1995
[c]HSDB 2000
[d]Lide 2000

Source: Chemfinder 2001, unless otherwise specified

Table 4-3. Percent Natural Occurrence and Radioactive Properties of Isotopes of Iodine

Isotope	CAS registry number	Natural abundance (%)	Beta energies, MeV[a] (intensity)	Gamma energies, keV[a]	Half-life	Activity, Ci/gram[c]
^{123}I	15715-08-9	No data	1.08 (97.0%)	158.97	13.3 hours	1.92×10^{6}
^{124}I	14158-30-6	No data	EC[b]	602.7 722.8 1691.0	4.18 days	2.52×10^{5}
^{125}I	14158-31-7	No data	EC[b]	35.5	59.4 days	1.76×10^{4}
^{126}I	14158-32-8	No data	EC[b]	388.6 666.3 753.8	13.11 days	7.91×10^{4}
^{127}I	7553-56-2	<100	No data	No data	Stable	No data
^{129}I	15046-84-1	1×10^{-13} to 1×10^{-10}	0.154	29.5 29.8 33.6	1.57×10^{7} years	1.77×10^{-4}
^{131}I	10043-66-0	No data	0.334 (7.3%) 0.606 (89.9%)	284.3 364.5	8.04 days[d]	1.24×10^{5}
^{132}I	14683-16-0	No data	0.74 (13.0%) 0.96 (8.2%) 1.18 (18.8%) 1.61 (12.6%) 2.14 (19.0%)	667.7 772.6 954.6	2.30 hours	1.03×10^{7}
^{133}I	14834-67-4	No data	0.54 (87.0%) 0.88 (4.5%)	529.9 875.3	20.8 hours	1.13×10^{6}
^{134}I	14914-27-3	No data	1.31 (30.4%) 1.59 (16.2%) 1.82 (11.0%) 2.44 (12.5%)	847.0 884.1	52.5 minutes	2.67×10^{7}
^{135}I	14834-68-5	No data	679.7 (8.0%) 856.8 (8.8%) 969.9 (21.9%) 1,082.7 (8.0%) 1,387.6 (23.8%)	546.6 836.8 1,038.8 1,131.5	6.57 hours	3.53×10^{6}

[a]Not all gamma and beta energies are included in summary; see Chu et al. (1999) for a complete listing
[b]EC = electron capture decay
[c]Activity = $(N_A \ln 2)/(M_w t_{½})$
[d]Lide 2000

Source: Chu et al. 1999

The same process occurs for ^{129}I ($t_{½}$=1.6x107 years) and includes mass 129 isobars beginning with ^{129}Cd and ending with ^{129}Xe. Iodine isotopes above ^{127}I decay by emitting beta and gamma radiation, whose combined energies are unique to each iodine isotope. ^{131}I, for example, decays by beta particle emission, and 0.96 MeV of energy is shared between the beta particle and the gamma ray. At least seven possible beta/gamma combinations occur. In 90.4% of the decays, a 0.61 MeV beta particle is emitted. The remaining excess energy is emitted as either a 0.364 MeV gamma ray for 85.3% of the time, or a pair of 0.284 and 0.080 MeV gamma rays for the other 5.1% of the time. The following is the decay scheme for ^{131}I (Cember 1996):

$$^{131}I \dashrightarrow {}^{131}Xe\ (\text{stable}) + \beta^- (0.61\ \text{MeV}; 85.3\%) + \gamma (0.36\ \text{MeV})$$
$$+ \beta^- (0.61\ \text{MeV}; 5.1\%) + \gamma (0.284\ \text{MeV}) + \gamma (0.080\ \text{MeV})$$
$$+ \beta^- (0.81\ \text{MeV}; 0.6\%) + \gamma (0.16\ \text{MeV})$$
$$+ \beta^- (0.47\ \text{MeV}; 0.3\%) + \gamma (0.50\ \text{MeV})$$
$$+ \beta^- (0.47\ \text{MeV}; 0.2\%) + \gamma (0.33\ \text{MeV}) + \gamma (0.2\ \text{MeV})$$
$$+ \beta^- (0.33\ \text{MeV}; 6.9\%) + \gamma (0.64\ \text{MeV})$$
$$+ \beta^- (0.25\ \text{MeV}; 1.6\%) + \gamma (0.72\ \text{MeV})$$

Isotopic masses of iodine <127 can be produced using a beam of high energy protons generated using a linear accelerator. Proton beams tuned at fixed energies up to 30 MeV produce isotopes, such as ^{123}I, by interaction of the proton beam with a target of high atomic mass.