4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of nitrate and nitrite is provided in Table 4-1 and information regarding the chemical identity of selected inorganic nitrate and nitrite compounds is provided in Table 4-2. Information regarding ammonia and urea is provided in Table 4-3.

Inorganic nitrate and nitrite are naturally occurring ionic species that are part of the earth's nitrogen cycle (see Figure 5-1). These anions are the products formed via the fixation of nitrogen and oxygen. Chemical processes, biological processes, and microbial processes in the environment convert nitrogen compounds to nitrite and nitrate via nitrogen fixation and nitrification. Compounds such as urea are converted via hydrolysis to ammonia, protonation of ammonia to ammonium (cation), followed by oxidation of ammonium to form nitrite, and then oxidation to form nitrate. Nitrate and nitrite are not neutral compounds, but rather the ionic (anionic; negatively charged) portions of compounds, commonly found in commerce as organic and inorganic salts. As used in this profile, the word "ion" is implied and not used, unless added for clarity.

Nitrate and nitrite typically exist in the environment as highly water-soluble inorganic salts, often bound when not solubilized to metal cations such as sodium or potassium. The nitrate ion is the more stable form as it is chemically unreactive in aqueous solution; however, it may be reduced through biotic processes with nitrate reductase to the nitrite ion. The nitrite ion is readily oxidized back to the nitrate ion via *Nitrobacter* (a genus of proteobacteria), or conversely, the nitrite ion may be reduced to various compounds (IARC 2010; WHO 2011b).

Under certain conditions, nitrite may be converted to a class of compounds called N-nitrosamines. In foods, endogenous production of N-nitrosamines occurs when nitrite reacts with secondary amines or amides. Several factors, including the presence of antioxidants, such as vitamin C, affect the rate of formation. N-nitrosamines are a class of chemical compounds that have a nitroso (N=O) group bonded to an amine (-N(R)R') with a general chemical structure of RN(R')-N=O (IARC 94).

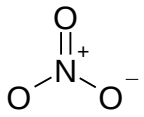
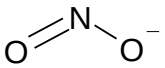
There is a wide range of both organic and inorganic nitrate and nitrite compounds. Common nitrate and nitrite salts include potassium nitrate, potassium nitrite, sodium nitrate, sodium nitrite, and ammonium nitrate; these salts are highly soluble in water, dissociate under environmental conditions, and exist as

ions (WHO 1978, 2011b). Common inorganic fertilizers that contribute to environmental concentrations of nitrate and nitrite include ammonia and urea.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of selected inorganic nitrate and nitrite compounds is provided in Table 4-4 and information regarding the physical and chemical properties of ammonia and urea is provided in Table 4-5.

Table 4-1. Chemical Identity of Nitrate and Nitrite Ions[a]

Characteristic	Nitrate ion	Nitrite ion
Synonym(s)	Nitrate ion; nitrate(1-); nitrate ion (NO_3^-); nitrate ion(1-); nitrato; nitric acid, ion (1-)	Nitrite ion; nitrite (1-); nitrite anion; nitrite ion (NO_2^-); nitrite ion (1-); nitrogen dioxide(1-); nitrogen peroxide ion (1-); nitrous acid, ion (1-)
Registered trade name(s)	No data	No data
Chemical formula	NO_3^-	NO_2^-
Chemical structure[b]		
Ionic weight	62.005	45.995
Identification numbers:		
CAS registry	14797-55-8	14797-65-0
NIOSH RTECS	No data	No data
EPA hazardous waste	No data	No data
DOT/UN/NA/IMDG shipping[c]	UN3218; UN1447	No data
HSDB	Not applicable	Not applicable
NCI	No data	No data
EPA Pesticide Chemical Code	No data	No data

[a]All information obtained from IARC (2010), except where noted.
[b]HSDB 2007.
[c]ChemIDplus 2014.

CAS = Chemical Abstracts Service; DOT/UN/NA/IMDG = 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; RTECS = Registry of Toxic Effects of Chemical Substances

Table 4-2. Chemical Identity of Selected Inorganic Nitrate and Nitrite Compounds[a]

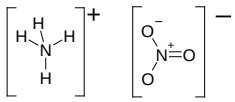
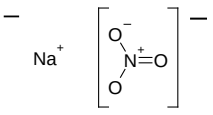
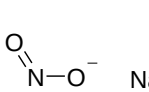
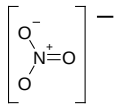
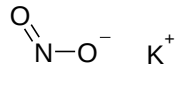
Characteristic	Ammonium nitrate	Sodium nitrate	Sodium nitrite	Potassium nitrate	Potassium nitrite
Synonym(s)	Nitric acid, ammonium salt; ammonium nitrate (NH_4NO_3); Emulite; EXP 200; German saltpeter; Norge saltpeter; Norway saltpeter; Norwegian saltpeter; Plenco 12203; Varioform I; ZhVK	Nitric acid, sodium salt; Chile saltpeter; niter; nitric acid sodium salt(1:1); saltpeter; soda niter; nitrate of soda; cubic niter; nitratine	Nitrous acid, sodium salt; nitrous acid soda; nitrous acid sodium salt (1:1)	Nitric acid, potassium salt; niter; nitre; nitric acid potassium salt (1:1); saltpeter; saltpetre; nitrate of potash	Nitrous acid, potassium salt; Chile saltpeter; niter; nitric acid sodium salt (1:1); salpeter; soda niter
Registered trade name(s)	No data	No data	No data	No data	No data
Chemical formula	NH_4NO_3	$NaNO_3$	$NaNO_2$	KNO_3	KNO_2
Chemical structure	Trigonal $NH_4^+NO_3^-$ 	$Na^+NO_3^-$ 	Trigonal $Na^+NO_2^-$ 	Orthorhombic $K^+NO_3^-$ 	$K^+NO_2^-$ 
Identification numbers:					
CAS registry	6484-52-2	7631-99-4	7632-00-0	7757-79-1	7758-09-0
NIOSH RTECS	BR9050000	WC5600000	RA1225000	TT3700000	TT3750000
EPA hazardous waste	No data	No data	No data	No data	No data
DOT/UN/NA/IMDG shipping	UN 2426; UN 0223; UN 1942; UN 2067; UN 2068; UN 2069; UN 2070; UN 2071; UN 2072; UN 0222 IMO 5.1; NA 1942; IMO 1.1; IMO 9.0	UN 1498; IMO 5.1	UN 1500; IMO 5.1	UN 1486; IMO 5.1	UN 1488; IMO 5.1
HSDB	475	726	757	1227	1216
NCI	No data	No data	No data	No data	No data
NFPA instability hazard[b]	3	No data	No data	No data	No data

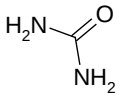
Table 4-2. Chemical Identity of Selected Inorganic Nitrate and Nitrite Compounds[a]

Characteristic	Ammonium nitrate	Sodium nitrate	Sodium nitrite	Potassium nitrate	Potassium nitrite
EPA Pesticide Chemical Code	076101[c]	076104[c]	076204[c]	076103[c]	076203[c]

[a]All information obtained from IARC 2010 and HSDB 2007, except where noted.
[b]NFPA 2002; instability hazard 3 = materials that in themselves are capable of detonation or explosive decomposition or explosive reaction, but that require a strong initiating source or that must be heated under confinement before initiation.
[c]EPA 2014f.

CAS = Chemical Abstracts Service; DOT/UN/NA/IMDG = 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; NFPA = National Fire Protection Association; NIOSH = National Institute for Occupational Safety and Health; RTECS = Registry of Toxic Effects of Chemical Substances

Table 4-3. Chemical Identity of Ammonia[a] and Urea[b]

Characteristic	Ammonia	Urea
Synonym(s)	Anhydrous ammonia, ammonia gas; aqua ammonia; liquid ammonia	Alphahydrate; carbamide; carbonyl diamide; carbonyldiamine; isourea
Registered trade name(s)	BCMW; BUSAN 1215	UAL-37; N-Dure; UF-Concentrate-85; Ureacin-20
Chemical formula	NH_3	CH_4N_2O
Chemical structure		
Ionic weight	17.03	60.06
Identification numbers:		
CAS registry	7664-41-7	57-13-6
NIOSH RTECS	No data	No data
EPA hazardous waste	No data	No data
DOT/UN/NA/IMDG shipping	UN 1005; UN 3318; UN 2672; UN 2073	No data
HSDB	162	163
NCI	No data	No data
EPA Pesticide Chemical Code	005302	085702

[a]HSDB 2012.
[b]HSDB 2003.

CAS = Chemical Abstracts Service; DOT/UN/NA/IMDG = 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; RTECS = Registry of Toxic Effects of Chemical Substances

Table 4-4. Physical and Chemical Properties of Selected Inorganic Nitrate and Nitrite Compounds[a]

Characteristic	Ammonium nitrate	Sodium nitrate	Sodium nitrite	Potassium nitrate	Potassium nitrite
CAS	6484-52-2	7631-99-4	7632-00-0	7757-79-1	7758-09-0
Molecular weight	80.043	84.995	68.985	101.103	85.093
Color	White; colorless (pure); gray or brown (fertilizer grade)	White; colorless	White to pale yellow	Colorless	Pale yellow
Physical state	Solid	Solid	Solid	Solid	Solid
Melting point	169.7°C	306°C; 308°C	271°C	334°C; 337°C	440°C
Boiling point	Decomposes at ~210°C (200–260°C)	380°C; decomposes	320°C; decomposes	400°C; decomposes	537°C; explodes
Density: at 20°C/4°C	1.725 g/cm^3	2.26 g/cm^3	2.17 g/cm^3	2.11 g/cm^3	1.915 g/cm^3
Odor	Odorless	Odorless[b]	No data	Odorless	No data
Odor threshold:	No data	No data	No data	No data	No data
Taste threshold	No data	No data	No data	No data	No data
Solubility:					
Water at 25°C	213 g/100 g	91.2[c] g/100 g	84.8 g/100 g	38.3 g/100 g	312 g/100 g
Organic solvent(s)	Acetone, ammonia, ethanol, isopropanol, methanol	Ammonia, hydrazine, ethanol, methanol, acetone, glycerol	Ammonia, ethanol, methanol	Ammonia; glycerol; sl sol ethanol	Ammonia; alcohol
Partition coefficients	Not available	Not available	Not available	Not available	Not available
Vapor pressure	Not available	Not available	Not available	Not available	Not available
Henry's law constant	Not available	Not available	Not available	Not available	Not available
Flashpoint	Not available	Flames up when heated to 540°C	498ºC; May explode above 530°C	Not flammable	Not flammable
Flammability limits	Not available	Not available	Not available	Not available	Not available
Explosive limits	Not available	Not available	>1,000°C	Not available	Not available

[a]All information obtained from HSDB 2007, unless otherwise noted.
[b]Lewis 2002.
[c]Lide 2013.

CAS = Chemical Abstracts Service; HSDB = Hazardous Substances Data Bank

Table 4-5. Physical and Chemical Properties of Ammonia[a] and Urea[b]

Characteristic	Ammonia	Urea
CAS	7664-41-7	57-13-6
Molecular weight	17.03	60.06
Color	Colorless	White
Physical state	Gas	Crystal/powder
Melting point	-77.7°C	132.70°C
Boiling point	-33.35 °C at 760 mm Hg	Decomposes
Density:		
at 20°C/4°C	0.696 g/L (liquid)	1.3230
Odor	Sharp, pungent, irritating	Slight odor of ammonia; odorless
Odor threshold:	Water: 1.5 mg/L; Air: 5.2 µL/L	No data
Taste threshold	No data	No data
Solubility:		
Water	4.82×10^5 mg/L at 24°C	5.45×10^5 mg/L at 25°C
Organic solvent(s)	Alcohol, chloroform, ether	Alcohol; acetic acid; pyrimidine
Partition coefficients	No data	-2.11
Vapor pressure at 25°C	7.51×10^3 mm Hg	1.2×10^{-5} mm Hg
Henry's law constant	1.61×10^{-5} atm m^3/mole at 25°C	No data
Flashpoint	No data	No data
Flammability limits	No data	No data
Explosive limits	No data	No data

[a]HSDB 2012
[b]HSDB 2003

CAS = Chemical Abstracts Service; HSDB = Hazardous Substances Data Bank

Nitrate is the most oxidized form of nitrogen present in the environment (oxidation state of nitrogen +5). It accounts for the majority of the total available nitrogen in surface waters (Environment Canada 2012), perhaps due to its formation by converting the ammonium ion (e.g., from fertilizer and manure) through a 2-step oxidation process, first to nitrite and then to nitrate. In compounds, nitrate and nitrite typically exist in an oxidation state of 1^-. Nitrate is the conjugate base of nitric acid (HNO_3), a strong acid with pKa of -1.38 at 25°C (Dean 1985). Nitric acid and salts of nitric acid completely dissociate in aqueous solutions, except for nitrates of mercury and bismuth (Environment Canada 2012; WHO 1978). Nitrite is the conjugate base of nitrous acid (HNO_2), a weak acid with a pKa of 3.14 at 25°C (Dean 1985); nitrite readily decomposes to yield water and dinitrogen trioxide (N_2O_3), or nitric acid, nitric oxide (NO), and water (H_2O) (WHO 1978, 2011b).