

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

The common synonyms and other information for fluorine, hydrogen fluoride, sodium fluoride, fluorosilicic acid, and sodium fluorosilicate are listed in Table 4-1. The terms “fluorine” and “fluoride” are often used interchangeably in the literature as generic terms. In this document, we will use “fluoride” as a general term to refer to all combined forms of fluorine unless the particular compound or form is known and there is a reason for referring to it. The term “fluorine gas” will sometimes be used to emphasize the fact that we are referring to the elemental form of fluorine rather than a combined form. In general, the differentiation between different ionic and molecular or gaseous and particulate forms of fluorine-containing substances is uncertain and may also be unnecessary.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Fluorine is the lightest member of Group 17 (VIIA) of the periodic table. This group, the halogens, also includes chloride, bromine, and iodine. As with the other halogens, fluorine occurs as a diatomic molecule, F_2 , in its elemental form. It has only one stable isotope and its valence in all compounds is -1. Fluorine is the most reactive of all the elements, which may be attributed to its large electronegativity (estimated standard potential +2.85 V). It reacts at room temperature or elevated temperatures with all elements other than nitrogen, oxygen, and the lighter noble gases. Fluorine is also notable for its small size; large numbers of fluorine atoms fit around atoms of another element. This, along with its electronegativity, allows the formation of many simple and complex fluorides in which the other element is in its highest oxidation state. Important physical and chemical properties of fluorine, hydrogen fluoride, sodium fluoride, fluorosilicic acid, and sodium fluorosilicate are presented in Table 4-2. It should be noted that fluorosilicic acid only exists in aqueous solution, and not in the anhydrous state. Its properties will depend on its concentration and temperature (Aigueperse et al. 1988).

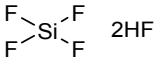
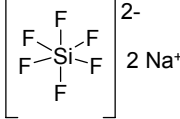
4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-1. Chemical Identity of Fluorine, Hydrogen Fluoride, Sodium Fluoride, Fluosilicic Acid, and Sodium Silicofluoride^a

Characteristic	Fluorine	Hydrogen fluoride	Sodium fluoride
Synonym(s)	Fluorine-19	Hydrofluoric acid; hydrofluoride	Monosodium fluoride ^b
Registered trade name(s)	No data	No data	Alcoa sodium fluoride ^b
Chemical formula	F ₂	FH	FNa
Chemical structure	F-F	H-F	Na-F
Identification numbers:			
CAS registry	7782-41-4	7664-39-3	7681-49-4
NIOSH RTECS	NIOSH/LM64750000	NIOSH/MW7890000	NIOSH/WB0350000
EPA hazardous waste	P056	U134	No data
OHM/TADS	No data	7216750	7216897
DOT/UN/NA/IMO shipping	UN1045; fluorine	UN1790; hydrofluoric acid solution UN1052; anhydrous hydrogen fluoride	UN1690; sodium fluoride
HSDB	541	546	1766
EINECS	231-954-8	231-634-8	231-667-8
NCI	No data	No data	C55221

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-1. Chemical Identity of Fluorine, Hydrogen Fluoride, Sodium Fluoride, Fluosilicic Acid, and Sodium Silicofluoride^a

Characteristic	Fluorosilicic acid	Sodium fluorosilicate
Synonym(s) ^c	Dihydrogen hexafluorosilicate; hexafluorosilicic acid; fluosilicic acid; hexafluosilicic acid; hydrofluorosilicic acid; hydrogen hexafluorosilicate; hydrosilicofluoric acid; silicofluoric acid; silicon hexafluoride dihydride	Disodium hexafluorosilicate; disodium silicofluoride; silicon sodium fluoride; sodium silicofluoride; sodium fluosilicate; sodium hexafluorosilicate; sodium hexafluosilicate; sodium silicon fluoride
Registered trade name(s) ^c	FKS	Prodan; Salufer
Chemical formula	H ₂ SiF ₆	Na ₂ SiF ₆
Chemical structure		
Identification numbers:		
CAS registry	16961-83-4	16893-85-9
NIOSH RTECS	NIOSH/VV8410000	NIOSH/VV8225000
EPA hazardous waste	No data	No data
OHM/TADS	No data	No data
DOT/UN/NA/IMO shipping	UN 2674; sodium silicofluoride	UN 1778; fluosilicic acid
HSDB	770	2018
EINECS	241-034-8	240-934-8
NCI	No data	No data

^aAll information obtained from HSDB 2003 and ChemID 2001 except where noted.

^bSodium fluoride is an ingredient in many dental care products and rodenticides. Since it is not the only component in these products, they cannot properly be considered trade names or synonyms. Some of these products are: Floridine, Antibulit, Cavi-trol, Chemifluor, Credo, Duraphat, F1-tabs, Florocid, Flozenges, Fluoral, Fluorident, Fluorigard, Fluorineed, Fluorinse, Fluoritab, Fluorocid, Fluor-o-kote, Fluorol, Fluoros, Flura, Flura drops, Flura-gel, Flura-Loz, Flurcare, Flursol, Fungol B, Gel II, Gelution, Gleem, Iradicav, Karidium, Karigel, Kari-rinse, Lea-Cov, Lemoflur, Luride, Luride Lozi-tabs, Luride-SF, Nafeen, Nafpak, Na Frinse, Nufluor, Ossalin, Ossin, Osteofluor, Pediaflor, Pedident, Pennwhite, Pergantene, Phos-flur, Point Two, Preident, Rafluor, Rescue Squad, Roach salt, So-flo, Stay-flo, Studafluor, Super-dent, T-fluoride, Thera-flur, Thera-Flur-N, Villiaumite, and Zymafluor. Another compound of sodium and fluorine is sodium bifluoride (also called sodium hydrofluoride and sodium hydrofluoride), NaF·HF or NaHF₂, which is not discussed here.

^cIARC 1982

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Organization 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

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Physical and Chemical Properties of Fluorine, Hydrogen Fluoride, Sodium Fluoride, Fluosilicic Acid, and Sodium Silicofluoride^a

Property	Fluorine	Hydrogen fluoride	Sodium fluoride
Molecular weight	37.997	20.006	42.00
Color	Pale yellow	Colorless	Colorless
Physical state	Gas	Gas	Cubic or tetragonal crystals
Molecular formula	F ₂	FH	FNa
Melting point, °C	-219.61	-83.36	993
Boiling point, °C	-188.13	19.51b	1,704
Density, g/cm ³	1.5127 at -188.13 °C	0.991 at 19.54 °C	2.78
Odor	Pungent, irritating odor	Strong, irritating odor	Odorless
Odor threshold:			
Water	Not relevant	No data	No data
Air	0.035 ppm	0.5–3 ppm	No data
Solubility:			
Water	1.69 mg/L	Miscible	43 g/L at 25 °C
Organic solvents	No data	Benzene (2.54); toluene (1.80); ethanol (very soluble); <i>m</i> -xylene in ethanol (1.28); tetraline (0.27) ^b	Very slightly soluble
Partition coefficients:			
Log K _{ow}	Not relevant	No data	No data
Log K _{oc}	Not relevant	Not relevant	No data
Vapor pressure	0.4 kPa (3 mmHg) at 55 °K ^c ; 12.3 kPa (92.3 mmHg) at 70 °K	400 mmHg at 2.5 °C	1 mmHg at 1,077 °C
Henry's Law constant at 20 °C	No data	0.104 at m-L/mole ^e	No data
Autoignition temperature	No data	No data	No data
Flashpoint	Not flammable	Not flammable	Not flammable
Flammability limits	No data	No data	No data
Conversion factors	1 mg/m ³ = 1.554 ppm ^d 1 ppm = 0.64 mg/m ³	1 mg/m ³ = 1.223 ppm ^d 1 ppm = 0.82 mg/m ³	Not applicable
Explosive limits	No data	No data	No data

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Physical and Chemical Properties of Fluorine, Hydrogen Fluoride, Sodium Fluoride, Fluosilicic Acid, and Sodium Silicofluoride^a

Property	Fluorosilicic Acid	Sodium Fluorosilicate
Molecular weight	144.1	188.1
Color	Colorless, fuming liquid	white
Physical state	liquid	granular powder
Molecular formula	H ₂ SiF ₆	Na ₂ SiF ₆
Melting point, °C	60-70% solution solidifies at about 19 °C, forming a crystalline dihydrate	decomposes at red heat ^b
Boiling point, °C	decomposes	decomposes at red heat ^b
Density, g/cm ³	1.4634 (60.97% solution) at 25 °C: 17.5/17.5 1.2742 (30% solution) ^f	2.679 ^f
Odor	Sour, pungent odor ^b	No data
Odor threshold:		
Water	No data	No data
Air	No data	No data
Solubility:		
Water	No data	0.76 g/100 g water at 25 °C ^g
Organic solvents	No data	No data
Partition coefficients:		
Log K _{ow}	No data	No data
Log K _{oc}	No data	No data
Vapor pressure	No data	No data
Henry's Law constant at 20 °C	No data	No data
Autoignition temperature	No data	No data
Flashpoint	No data	No data
Flammability limits	No data	No data
Conversion factors	Not applicable	Not applicable
Explosive limits	No data	No data

^aAll information obtained from HSDB 2003 except where noted^bBudavari 2001^cLide 1992^dNAS 1971a^eBetterton 1992; apparent Henry's law constant (ratio of the gas phase concentration to that of the total dissolved solute)^fIARC 1982^gAigueperse et al. 1988

