4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identities of hydrogen sulfide and carbonyl sulfide is located in Table 4-1. This information includes synonyms, chemical formula and structure, and identification numbers.

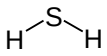
4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of hydrogen sulfide and carbonyl sulfide is located in Table 4-2.

Hydrogen Sulfide. Hydrogen sulfide is a heavier-than-air, colorless gas with a sweetish taste and characteristic odor of rotten eggs (HSDB 2013). The odor threshold for hydrogen sulfide is variable and various ranges have been reported. Ruth (1986) reviewed odor thresholds of several hundred chemicals (including hydrogen sulfide) from the industrial hygiene literature and other compilations of odor threshold data; an odor threshold range of 0.0005–0.010 ppm was reported. Guidotti (1994) reported an odor threshold range of 0.01–0.3 ppm. Since high concentrations of hydrogen sulfide (150–200 ppm) can paralyze the olfactory nerve, odor may not be a reliable indicator of the presence of this gas (Beauchamp et al. 1984).

Carbonyl Sulfide. Carbonyl sulfide is also a colorless gas with a typical sulfide odor, except when it is free from impurities (EPA 1994c; Lewis 2007). An odor threshold of 135 µg/m^3 (0.055 ppm) has been reported (Texas Commission on Environmental Quality 2008).

Table 4-1. Chemical Identity of Hydrogen Sulfide and Carbonyl Sulfide

Characteristic	Hydrogen sulfide[a]	Carbonyl sulfide[b]
Synonyms/trade names	Hydrosulfuric acid; hydrogen sulphide; stink damp; sewer gas; sulfur hydride; dihydrogen monosulfide; dihydrogen sulfide; sulfureted hydrogen; hydrogen sulfuric acid; acide sulfhydrique [French]; acide sulphhydrique; hydrogen sulfure [French]; hydrogene sulfure [French]; idrogeno solforato [Italian]; schwefelwasserstoff [German]; siarkowodor [Polish]; zwavelwaterstof [Dutch]	Carbon monoxide monosulfide; carbon oxide sulfide; carbon oxysulfide; oxycarbon sulfide; carbon oxide sulfide (9CI); carbon oxide sulfide (COS); carbonyl sulphide
Chemical formula	H_2S	COS
Chemical structure		
Identification numbers:		
CAS registry	7783-06-4	463-58-1
NIOSH/RTECS	MX1225000[c]	No data
EPA hazardous waste	U135	D003
DOT/UN/NA/IMCO shipping	UN1053; IMO 2.3	UN2204; IMO 2.3
HSDB	576	6127
EINECS	231-977-3	207-340-0
NCI	No data	No data

[a]All information obtained from HSDB 2013 and ChemID 2013 except where noted.
[b]All information obtained from HSDB 2007 and ChemID 2013.
[c]NIOSH 2011

CAS = Chemical Abstract Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EINECS = European Inventory of Existing Commercial Substances; EPA = Environmental Protection Agency; HSDB = Hazardous Substance 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. Physical and Chemical Properties of Hydrogen Sulfide and Carbonyl Sulfide

Property	Hydrogen sulfide	Carbonyl sulfide
Molecular weight	34.081[a]	60.075[b]
Color	Colorless[a]	Colorless[c]
Taste	Sweetish taste[a]	
Physical state	Gas[a]	Gas[c]
Melting point	-85.49°C[a]	-138.8°C[c]
Boiling point	-60.33°C[a]	-50.2°C[c]
Density in Air	1.189 (air=1.00)[c]	2.1 (air=1.00)[c]
Density at 0°C, 760 mmHg	1.5392 g/L[a]	
Odor	Strong odor of rotten eggs; offensive odor[a]	Typical sulfide odor except when pure[c]; odorless when pure, sulfur odor when it contains impurities[d]
Odor threshold:		
Water	0.000029 ppm[e]	
Air	0.0005–0.3 ppm[f,g]	135 µg/m^3[h]
Solubility:		
Water	3.98 g/L at 20°C[a]; 5.3 g/L at 10°C, 4.1 g/L at 20°C, 3.2 g/L at 30°C[i]	1.22 g/L at 25°C[b]
Other solvent(s)	Soluble in glycerol, gasoline, kerosene, carbon disulfide, crude oil; certain polar organic solvents, notably methanol, acetone, propylene carbonate, sulfolane, tributyl phosphate, various glycols, and glycol ethers[a]	Soluble in alcohol[c]; very soluble in potassium hydroxide, carbon disulfide[i]; soluble in toluene[b]
Partition coefficients:		
Log K_{ow}	Not applicable	
Log K_{oc}	Not applicable	
Vapor pressure at 25°C	13,600 mmHg at 20°C[a]	9412 mmHg[j]
pK_a (1)	7.04[a]	
pK_a (2)	11.96[a]	
Henry's law constant:		
at 20°C	468 atm/mole fraction[j]	
at 25°C	0.0098 atm-m^3/mole[a]	
at 30°C	600 atm/mole fraction[j]	
at 40°C	729 atm/mole fraction[j]	

Table 4-2. Physical and Chemical Properties of Hydrogen Sulfide and Carbonyl Sulfide

Property	Hydrogen sulfide	Carbonyl sulfide
Autoignition temperature	500°F (260°C)[c]	
Incompatibilities		Oxidizing agents (i.e., perchlorates, peroxides, permanganates, chlorates, nitrates, chlorine, bromine, fluorine); may react with water and moist air[k]
Conversion factors	1 ppm=1.40 mg/m^3[l]	1 mg/m^3=0.41 ppm[m]
Explosive limits	Upper, 46%; lower, 4.3% (by volume in air)[a]	Upper, 28.5%; lower, 12%[c]

[a]HSDB 2013
[b]HSDB 2007
[c]Lewis 2007
[d]EPA 1994c
[e]Amoore and Hautala 1983
[f]Ruth 1986
[g]Guidotti 1994
[h]Texas Commission on Environmental Quality 2008
[i]O'Neil et al. 2001
[j]Daubert and Danner 1989
[k]NJDEP 2009
[l]Al-Haddad et al. 1989
[m]EPA 1994a