HYDROGEN SULFIDE 109

## 4. CHEMICAL AND PHYSICAL INFORMATION

## 4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of hydrogen 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 is located in Table 4-2.

Hydrogen sulfide (H<sub>2</sub>S) is a heavier-than-air, colorless gas with a sweetish taste and characteristic odor of rotten eggs (HSDB 2006). 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 ppm) can paralyze the olfactory nerve, odor may not be a reliable indicator of the presence of this gas (HSDB 2006).

Table 4-1. Chemical Identity of Hydrogen Sulfide<sup>a</sup>

Characteristic	Information
Chemical name	Hydrogen sulfide
Synonyms/trade names	Hydrosulfuric acid; hydrogen sulphide, sewer gas, stink damp; sulfur hydride; sulfurated hydrogen; dihydrogen monosulfide; dihydrogen sulfide, sulfuretted hydrogen, hepatic acid, sour gas
Chemical formula	$H_2S$
Chemical structure	H_S_H
Identification numbers:	
CAS registry	7783-06-4
NIOSH/RTECS	MX1225000 <sup>b</sup>
EPA hazardous waste	U135
DOT/UN/NA/IMCO shipping	UN1053; IMO 2.1
HSDB	576
EINECS	231-977-3
NCI	No data

 $<sup>^{\</sup>rm a}$  All information obtained from HSDB 2006 ,ChemID 2006, and ChemFinder 2006, except where noted.  $^{\rm b}$  NIOSH 2006

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 Identity of Hydrogen Sulfide<sup>a</sup>

Property	Information
Molecular weight	34.08
Color	Colorless
Taste	Sweetish taste
Physical state	Gas (under normal ambient condition)
Melting point	-85.49 °C
Boiling point	-60.33 °C
Density in Air	1.19 (air=1.00) <sup>b</sup>
Density at 0 °C, 760 mmHg	1.5392 g/L
Odor	Rotten eggs
Odor threshold:	
Water	0.000029 ppm <sup>c</sup>
Air	0.0005–0.3 ppm <sup>d,e</sup>
Solubility:	
Water	5.3 g/L at 10 °C; 4.1 g/L at 20 °C; 3.2 g/L at 30 °C <sup>b</sup>
Other solvent(s)	Soluble in glycerol, gasoline, kerosene, carbon disulfide, crude oil
Partition coefficients:	
Log K <sub>ow</sub>	Not applicable
Log K <sub>oc</sub>	Not applicable
Vapor pressure at 25 °C	15,600 mm Hg
Acid dissociation:	$\implies$ H+(aq) + HS-(aq) (1); HS-(aq) $\implies$ H+(aq) + S <sup>2-</sup> (aq) (2)
pK <sub>a</sub> (1)	$[HS^{-}(aa)][H^{+}(aa)]$
	$Ka_{1} = \frac{[HS^{-}(aq)][H^{+}(aq)]}{[H_{2}S(aq)]}$
16 (0)	
pK <sub>a</sub> (2)	11.96 <sup>b</sup> $Ka_2 = \frac{[S^{2-}(aq)][H^+(aq)]}{[HS^-(aq)]}$
	$[HS^{-}(aq)]$
Henry's law constant:	
at 20 °C	468 atm/mole fraction <sup>f</sup>
at 30 °C	600 atm/mole fraction <sup>f</sup>
at 40 °C	729 atm/mole fraction <sup>f</sup>
Autoignition temperature	500 °F (260 °C)
Conversion factors	1 ppm = $1.40 \text{ mg/m}^{3 \text{ g}}$
Explosive limits	Upper, 45.5%; lower, 4.3% (by volume in air)

<sup>&</sup>lt;sup>a</sup>All information obtained from HSDB 2006, except where noted. <sup>b</sup>O'Neil et al. 2001

<sup>&</sup>lt;sup>c</sup>Amoore and Hautala 1983 <sup>d</sup>Ruth 1986

<sup>&</sup>lt;sup>e</sup>Guidotti 1994

<sup>&</sup>lt;sup>f</sup>Daubert and Danner 1989

<sup>&</sup>lt;sup>g</sup>Al-Haddad et al. 1989