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/m³ (0.055 ppm) has been reported (Texas Commission on Environmental Quality 2008).
Table 4-1. Chemical Identity of Hydrogen Sulfide and Carbonyl Sulfide

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Hydrogen sulfide(^a)</th>
<th>Carbonyl sulfide(^b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Synonyms/trade names</td>
<td>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]; hydrogen sulfure [French]; idrogeno solforato [Italian]; schwefelwasserstoff [German]; siarkowodor [Polish]; zwavelwaterstof [Dutch]</td>
<td>Carbon monoxide monosulfide; carbon oxide sulfide; carbon oxysulfide; oxycarbon sulfide; carbon oxide sulfide (9CI); carbon oxide sulfide (COS); carbonyl sulphide</td>
</tr>
<tr>
<td>Chemical formula</td>
<td>H(_2)S</td>
<td>COS</td>
</tr>
</tbody>
</table>
| Chemical structure       | \[\begin{array}{c}
\text{H} \\
\text{S} \\
\text{H}
\end{array}\]                                                                           | \[\text{COS}\]                                                                         |
| 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
### Table 4-2. Physical and Chemical Properties of Hydrogen Sulfide and Carbonyl Sulfide

<table>
<thead>
<tr>
<th>Property</th>
<th>Hydrogen sulfide</th>
<th>Carbonyl sulfide</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>34.081&lt;sup&gt;a&lt;/sup&gt;</td>
<td>60.075&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Color</td>
<td>Colorless&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Colorless&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td>Taste</td>
<td>Sweetish taste&lt;sup&gt;a&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>Physical state</td>
<td>Gas&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Gas&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td>Melting point</td>
<td>-85.49°C&lt;sup&gt;a&lt;/sup&gt;</td>
<td>-138.8°C&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td>Boiling point</td>
<td>-60.33°C&lt;sup&gt;a&lt;/sup&gt;</td>
<td>-50.2°C&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td>Density in Air</td>
<td>1.189 (air=1.00)&lt;sup&gt;c&lt;/sup&gt;</td>
<td>2.1 (air=1.00)&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
<tr>
<td>Density at 0°C, 760 mmHg</td>
<td>1.5392 g/L&lt;sup&gt;a&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>Odor</td>
<td>Strong odor of rotten eggs; offensive odor&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Typical sulfide odor except when pure&lt;sup&gt;c&lt;/sup&gt;; odorless when pure, sulfur odor when it contains impurities&lt;sup&gt;d&lt;/sup&gt;</td>
</tr>
<tr>
<td>Odor threshold:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>0.000029 ppm&lt;sup&gt;e&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>Air</td>
<td>0.0005–0.3 ppm&lt;sup&gt;f,g&lt;/sup&gt;</td>
<td>135 µg/m&lt;sup&gt;3h&lt;/sup&gt;</td>
</tr>
<tr>
<td>Solubility:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>3.98 g/L at 20°C&lt;sup&gt;a&lt;/sup&gt;; 5.3 g/L at 10°C, 4.1 g/L at 20°C, 3.2 g/L at 30°C&lt;sup&gt;i&lt;/sup&gt;</td>
<td>1.22 g/L at 25°C&lt;sup&gt;i&lt;/sup&gt;</td>
</tr>
<tr>
<td>Other solvent(s)</td>
<td>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&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Soluble in alcohol&lt;sup&gt;c&lt;/sup&gt;; very soluble in potassium hydroxide, carbon disulfide&lt;sup&gt;i&lt;/sup&gt;; soluble in toluene&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Partition coefficients:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Log K&lt;sub&gt;ow&lt;/sub&gt;</td>
<td>Not applicable</td>
<td></td>
</tr>
<tr>
<td>Log K&lt;sub&gt;oc&lt;/sub&gt;</td>
<td>Not applicable</td>
<td></td>
</tr>
<tr>
<td>Vapor pressure at 25°C</td>
<td>13,600 mmHg at 20°C&lt;sup&gt;a&lt;/sup&gt;</td>
<td>9412 mmHg&lt;sup&gt;i&lt;/sup&gt;</td>
</tr>
<tr>
<td>pK&lt;sub&gt;a&lt;/sub&gt; (1)</td>
<td>7.04&lt;sup&gt;a&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>pK&lt;sub&gt;a&lt;/sub&gt; (2)</td>
<td>11.96&lt;sup&gt;a&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>Henry's law constant:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>at 20°C</td>
<td>468 atm/mole fraction&lt;sup&gt;i&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>at 25°C</td>
<td>0.0098 atm-m&lt;sup&gt;3&lt;/sup&gt;/mole&lt;sup&gt;a&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>at 30°C</td>
<td>600 atm/mole fraction&lt;sup&gt;i&lt;/sup&gt;</td>
<td></td>
</tr>
<tr>
<td>at 40°C</td>
<td>729 atm/mole fraction&lt;sup&gt;i&lt;/sup&gt;</td>
<td></td>
</tr>
</tbody>
</table>
### Table 4-2. Physical and Chemical Properties of Hydrogen Sulfide and Carbonyl Sulfide

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

\(^a\) 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