Tetranitromethane
CAS No. 509-14-8

Reasonably anticipated to be a human carcinogen
First listed in the Seventh Annual Report on Carcinogens (1994)

Carcinogenicity
Tetranitromethane is reasonably anticipated to be a human carcinogen based on sufficient evidence of carcinogenicity from studies in experimental animals.

Cancer Studies in Experimental Animals
Exposure to tetranitromethane by inhalation caused lung tumors in rats and mice. In rats and mice of both sexes, it caused benign and malignant lung tumors (alveolar/bronchiolar adenoma and carcinoma); the tumors were predominantly malignant, and many of them metastasized, to a variety of organs. Exposure to tetranitromethane also caused a rare form of lung cancer (squamous-cell carcinoma) in rats of both sexes; at the time of the study, squamous-cell carcinoma had not been observed in unexposed female historical controls (~1,600) and had been observed in only 3 of 1,600 unexposed male controls (NTP 1990, Bucher et al. 1991).

Cancer Studies in Humans
No epidemiological studies were identified that evaluated the relationship between human cancer and exposure specifically to tetranitromethane.

Properties
Tetranitromethane is a nitroalkane compound that is a pale-yellow liquid with a biting, acrid odor at room temperature (IARC 1996, HSDB 2009). It is soluble in alcoholic potassium hydroxide, ethanol, and diethyl ether, and insoluble in water. Tetranitromethane is highly explosive when subjected to heat or shock and forms sensitive and powerful explosives when mixed with certain oxygen-deficient explosives or hydrocarbons (IARC 1996). Physical and chemical properties of tetranitromethane are listed in the following table.

<table>
<thead>
<tr>
<th>Property</th>
<th>Information</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>196.0 g/mol</td>
</tr>
<tr>
<td>Specific gravity</td>
<td>1.6229 at 20°C/4°C</td>
</tr>
<tr>
<td>Melting point</td>
<td>13.8°C</td>
</tr>
<tr>
<td>Boiling point</td>
<td>126°C at 760 mm Hg</td>
</tr>
<tr>
<td>Log K_w</td>
<td>-0.791</td>
</tr>
<tr>
<td>Water solubility</td>
<td>85 g/L at 25°C</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td>8.42 mm Hg at 25°C</td>
</tr>
<tr>
<td>Vapor density relative to air</td>
<td>0.8</td>
</tr>
</tbody>
</table>


Use
Tetranitromethane is used as an oxidizer in rocket propellants, in the manufacture of liquid explosives, and as an additive to increase the cetane number of diesel fuel (NTP 1990, IARC 1996, OSHA 2007). It is also used as a reagent for detecting the presence of double bonds in organic compounds and as a mild nitrating reagent, reacting with tyrosine in proteins and peptides. It was proposed as a surface disinfectant against viruses (Singh et al. 1994), based on data suggesting that it was useful against enveloped and nonenveloped viruses and many other microbial infective agents.

Production
In Germany during World War II, attempts were made to synthesize large amounts of tetranitromethane for use as a substitute for nitric acid in rocket fuel. The method, which involved the nitration of acetic anhydride with nitric acid, allowed a production rate of up to 10 tons within a “few weeks,” but the process was costly. By the end of the war, a less expensive method using acetylene and nitric acid was devised, with a reported production capacity of 10 kg/day (NTP 1990). No current estimates of commercial production of tetranitromethane were found. In 2009, tetranitromethane was available from six suppliers worldwide, including four U.S. suppliers (ChemSources 2009).

Exposure
The routes of potential human exposure to tetranitromethane are inhalation, ingestion, and eye or skin contact (OSHA 2007). Tetranitromethane may be released into the environment during its manufacture and use as a rocket fuel, diesel fuel booster, organic reagent, or explosive in mixture with toluene (HSDB 2009). It was reported to be an air pollutant emitted as a by-product of production of explosives in U.S. government factories; the estimated worst-case tetranitromethane level in the vicinity of the factories was 20 mg/m³ (approximately 2.5 ppm). Occupational exposure to tetranitromethane presumably occurred during the manufacture and use of trinitrotoluene (TNT) (NTP 1990). During the early part of World War I, a high incidence of “TNT intoxication” occurred in U.S. and British facilities involved in TNT production; an additional step involving washing the crude material with a sodium sulfite solution to hydrolyze the tetranitromethane was introduced to alleviate this problem (NTP 1990). The National Occupational Exposure Survey (conducted from 1981 to 1983) estimated that 1,445 workers, including 230 women, potentially were exposed to tetranitromethane (NIOSH 1990).

Regulations

Department of Transportation (DOT)
Tetranitromethane is considered a hazardous material, and special requirements have been set for marking, labeling, and transporting this material.

Environmental Protection Agency (EPA)

Clean Air Act
Prevention of Accidental Release: Threshold quantity (TQ) = 10,000 lb.
Comprehensive Environmental Response, Compensation, and Liability Act
Reportable quantity (RQ) = 10 lb.
Emergency Planning and Community Right-To-Know Act
Toxics Release Inventory: Listed substance subject to reporting requirements.
Reportable quantity (RQ) = 10 lb.
Threshold planning quantity (TPQ) = 500 lb.
Resource Conservation and Recovery Act
Listed Hazardous Waste: Waste code for which the listing is based wholly or partly on the presence of tetranitromethane = P112.
Listed as a hazardous constituent of waste.

Occupational Safety and Health Administration (OSHA)
While this section accurately identifies OSHA’s legally enforceable PELs for this substance in 2010, specific PELs may not reflect the more current studies and may not adequately protect workers. Permissible exposure limit (PEL) = 1 ppm (8 mg/m³).

Guidelines

American Conference of Governmental Industrial Hygienists (ACGIH)
Threshold limit value – time-weighted average (TLV-TWA) = 0.005 ppm.

National Institute for Occupational Safety and Health (NIOSH)
Recommended exposure limit (REL) = 1 ppm (8 mg/m³).
Immediately dangerous to life and health (IDLH) limit = 4 ppm.

References


