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TOXICOLOGICAL EVALUATIONS

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TOXICOLOGICAL EVALUATION

last updated: 06/2000

Sulfuryl chloride

No. 179

CAS No. 7791-25-5

BG Chemie
Berufsgenossenschaft der chemischen Industrie

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Sulfuryl chloride

This Toxicological Evaluation replaces a previously published version in volume 5.

1 Summary and assessment

Sulfuryl chloride reacts with water to form hydrochloric acid and sulphuric acid. This reaction explains the extremely irritant and corrosive action of the compound on the skin and mucous membranes.

Sulfuryl chloride is toxic upon single inhalation (LC_{50} rat, 4 hours 878 mg/m³; LC_{50} rat, 1 hour 330 mg/m³ and 723 mg/m³ (males) and 1336 mg/m³ (females)). In rats, subacute inhalation of sulfuryl chloride at concentrations of 0 (controls), 3, 10 and 30/20 ppm (equivalent to 0, 16.6, 55.2 and 165.6/110.4 mg/m³) for 2 weeks caused deaths and retardation of body weight gain at the high concentration levels, and at concentrations of 10 ppm and above concentration-dependent increases in red blood cell counts, haemoglobin levels and relative lung weights were seen. Histological examination revealed fibrinonecrotic bronchopneumonia in the mid and top concentration groups and in addition fibrinopurulent rhinitis in the top concentration group. According to the authors the only finding observed in the animals of the 3-ppm group was an increase in normally occurring murine pneumonitis.

In a Salmonella/microsome assay conducted in *Salmonella typhimurium* strain TA 100 with and without metabolic activation, sulfuryl chloride caused a concentration-dependent increase in revertant count in the absence of metabolic activation. This positive result was not confirmed by two further Salmonella/microsome tests in strain TA 100 in the presence and absence of metabolic activation.

On accidental local and inhalation exposure, sulfuryl chloride was found to cause lower-leg corrosions and respiratory tract irritation in one employee.

2 Name of substance

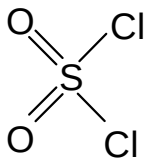
2.1	Usual name	Sulfuryl chloride
2.2	IUPAC name	Sulfuryl chloride
2.3	CAS No.	7791-25-5
2.4	EINECS No.	232-245-6

3 Synonyms, common and trade names

Sulfonyl chloride
Sulfonyl dichloride
Sulfur chloride oxide
Sulfuric dichloride
Sulfuric oxychloride
Sulfur oxychloride
Sulfurylchlorid
Sulphonyl chloride
Sulphuric oxychloride
Sulphur oxychloride

4 Structural and molecular formulae

4.1 Structural formula



4.2 Molecular formula SO_2Cl_2

5 Physical and chemical properties

5.1	Molecular mass, g/mol	134.96	
5.2	Melting point, °C	–54	(EC, 1996; Falbe and Regitz, 1992; Lauss and Steffens, 1994)
		–54.1	(Budavari et al., 1989)

5.3	Boiling point, °C	69 (at 1013 hPa) (EC, 1996; Falbe and Regitz, 1992) 69.1 (at 1013 hPa) (Lauss and Steffens, 1994) 69.3 (Budavari et al., 1989)
5.4	Vapour pressure, hPa	127 (at 18 °C) (Lauss and Steffens, 1994) 148 (at 20 °C) (EC, 1996) 511 (at 50 °C) (EC, 1996)
5.5	Density, g/cm³	1.6570 (at 25 °C) (Lauss and Steffens, 1994) 1.667 (at 20 °C) (Bayer, 1997) 1.6674 (at 20 °C) (Budavari et al., 1989) 1.67 (at 20 °C) (EC, 1996)
5.6	Solubility in water	Reacts with water to form hydrochloric acid and sulphuric acid (Falbe and Regitz, 1992; Lauss and Steffens, 1994)
5.7	Solubility in organic solvents	Miscible with benzene, toluene, ether, glacial acetic acid and other organic solvents (Budavari et al., 1989; Falbe and Regitz, 1992)
5.8	Solubility in fat	–
5.9	pH value	–
5.10	Conversion factor	1 ml/m³ (ppm) ≙ 5.52 mg/m³ 1 mg/m³ ≙ 0.18 ml/m³ (ppm) (at 1013 hPa and 25 °C)

6 Uses

Chlorinating and sulfonating or chlorosulfonating agent in organic syntheses, e. g. in the production of chlorophenol and chlorothymol. The chemical has been used in war gas formulations (Budavari et al., 1989).

Used as a dehydrating agent, for chlorination of organic compounds and for introducing the SO_2 group into carbon compounds, e. g. in the manufacture of sulfonyl chlorides, sulfonic acids and sulfonates, as cathode material and in lithium batteries (Falbe and Regitz, 1992).

7 Experimental results

7.1 Toxicokinetics and metabolism

No information available.

7.2 Acute and subacute toxicity

The LC_{50} of sulfuryl chloride (approx. 100% pure) in male Sprague-Dawley rats (10 animals/group) exposed to a single 4-hour inhalation (nose only) was found to be 159 ppm (equivalent to 878 mg/m³). All exposed animals displayed red nasal and ocular discharge. The survivors showed body weight loss for 1 to 2 days after the exposure. No macroscopic findings were reported (Du Pont, 1982; Kelly and Stula, 1983).

Further LC_{50} values reported for male and female rats were 131 ppm (equivalent to 723 mg/m³) and 242 ppm (equivalent to 1336 mg/m³), respectively. The duration of exposure was one hour (no further details; Bayer, 1987).

In male and female rats (10 animals/group), an LC_{50} value of 330 mg/m³ was calculated after a one-hour exposure to sulfuryl chloride (approx. 100% pure). All test concentrations produced salivation and dyspnoea, the severity of which was concentration-dependent. Locally, lacrimation and chemosis with erythema of the skin around the ears and nose were observed. Necropsy of the surviving and the deceased animals revealed haemorrhagic lungs. In the deceased animals, severe erythema in the gastrointestinal tract was seen in addition (Stauffer, 1970).

In a subacute study, Sprague-Dawley rats underwent daily exposure to sulfuryl chloride at concentration levels of 0 (controls), 3, 10 and 30 ppm (equivalent to 0, 16.6, 55.2 and 165.6 mg/m³, respectively) for 6 hours per day on 5 days per week for 2 weeks. The high concentration (30 ppm) was reduced to 20 ppm (equivalent to 110.4 mg/m³) after the second exposure due to considerable weight loss. Exposure at this level was terminated after 8 exposures due to the death of two of the animals. Immediately after exposure, there was a dose-dependent increase in erythrocyte count, haemoglobin level and the relative lung weights in the rats of the intermediate and high-dose groups. Histologically, these animals were found to have a fibrinonecrotic bronchopneumonia, and in addition the high-level rats exhibited

fibrinopurulent rhinitis. After an observation period of 2 weeks, the findings as well as the observed retardation of body weight gain were clearly reversible. In the 3-ppm group, the only effect observed was an exacerbation of normally occurring murine pneumonitis (no further details; Kelly and Stula, 1983).

7.3 Skin and mucous membrane effects

Liquid sulfuryl chloride and its vapours were described as severely corrosive to the skin and mucous membranes (no further details; Bayer, 1987).

7.4 Sensitisation

No information available.

7.5 Subchronic and chronic toxicity

No information available.

7.6 Genotoxicity

7.6.1 In vitro

Sulfuryl chloride (no indication of purity; solvent: ethylene glycol dimethyl ether) was tested in the Salmonella/microsome assay using *Salmonella typhimurium* strains TA 98, TA 100, TA 1535 and TA 1537 with and without metabolic activation (S-9 mix from Aroclor 1254-induced rat liver). The concentrations of test substance ranged from 10 up to 5000 µg/plate. A concentration of 5000 µg/plate was toxic to all strains tested, while 3333.3 µg/plate was toxic to strains TA 98 and TA 100. A concentration-dependent increase in the number of revertants was seen in strain TA 100 in the absence of metabolic activation. Sulfuryl chloride was thus shown in this study to induce point mutations in strain TA 100 (CCR, 1989).

In an attempt to confirm the positive result obtained in *Salmonella typhimurium* strain TA 100, additional Salmonella/microsome assays were carried out in the same strain, one as a standard-plate incorporation test with ex-

posure to sulfuryl chloride (no indication of purity) at concentration levels ranging from 15 to 5000 µg/plate, and another as a preincubation test at concentration levels ranging from 15 to 250 µg/plate with and without metabolic activation (S-9 mix from Aroclor 1254-induced rat liver). Ethylene glycol dimethyl ether served as the solvent. The result was negative. A bacteriotoxic effect was detectable at levels from 100 up to 500 µg/plate (BASF, 1991).

In a Salmonella/microsome assay – conducted as a standard-plate incorporation test in *Salmonella typhimurium* strain TA 100 with and without metabolic activation (S-9 mix from Aroclor 1254-induced rat liver) – sulfuryl chloride (99.8% pure, dissolved in ethylene glycol dimethyl ether) was tested at concentration levels ranging from 6.4 to 4000 µg/plate. As sulfuryl chloride undergoes gradual hydrolysis to hydrochloric acid and sulfuric acid (in a molar ratio of 2 : 1) in water, an equimolar mixture of hydrochloric acid and sulfuric acid (solvent: ethylene glycol dimethyl ether) was also tested in parallel. At the higher concentration levels, a weak bacteriotoxic effect was seen, but levels up to 4000 µg/plate could still be evaluated. Comparable bacteriotoxic effects were observed for the hydrochloric/sulfuric acid mixture. Neither in the absence nor in the presence of metabolic activation was sulfuryl chloride observed to induce point mutations in strain TA 100. Moreover, the mixture of hydrochloric and sulfuric acid also proved negative (Bayer, 1993).

7.6.2 In vivo

No information available.

7.7 Carcinogenicity

Sulfuryl chloride which was contaminated with 0.19 to 0.41 mg benzo(a)pyrene/kg was tested in mice (F1, $C_{57}B_1$xCBA) for its carcinogenic potential, together with a number of other compounds. The chemical was applied chronically to the animals' skin as a 4-percent solution. In addition, one group was given a single exposure to benzo(a)pyrene followed by dermal application of sulfuryl chloride (no further details). In total, 2 sebaceous gland adenomas and 1 squamous epithelial carcinoma occurred (no indication of which group was affected). The authors interpreted these results as confirmation that sulfuryl chloride presents a carcinogenic health risk. In

addition, a test was carried out in mice to assess sebaceous gland loss. A decrease in the number of sebaceous glands was reported after short-term dermal application of sulfuryl chloride (no further details in the English abstract; Yanisheva et al., 1982). With essential information on the conduct and the results of the study lacking, e. g. regarding the frequency of the observed tumours in the various study groups, and the test substance being contaminated with benzo(a)pyrene, a known carcinogen, the cited publication is unsuitable for the assessment of the carcinogenic potential of sulfuryl chloride.

7.8 Reproductive toxicity

No information available.

7.9 Effects on the immune system

No information available.

7.10 Neurotoxicity

No information available.

7.11 Other effects

No information available.

8 Experience in humans

According to one report, human exposure to a sulfuryl chloride concentration of 10 ppm (56 mg/m³) for one minute caused marked toxic effects, while exposure to 4 ppm (22 mg/m³) for longer periods gave rise to symptoms of illness, which were not further specified (tabular presentation; no further details; Goldblatt, 1955).

Contact with sulfuryl chloride led to severe irritation of the eyes, skin, mucous membranes and the entire respiratory tract in humans (no further details; Grant, 1974; Reichel, 1984).

On accidental local and inhalation exposure during an industrial accident, sulfuryl chloride was found to cause lower-leg corrosions and respiratory tract irritation in one employee (BASF, 1992).

An earlier publication reports the development of lung oedema subsequent to sulfuryl chloride exposure (no further details; Gerbis, 1931).

9 Classifications and threshold limit values

No information available.

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