SIDS INITIAL ASSESSMENT PROFILE

CAS No.	141-79-7
Chemical Name	Mesityl Oxide
Structural Formula	CH3 –CO-CH=C(CH3)2

Human Health

Mesityl oxide exhibits slight toxicity in acute mammalian studies. The acute oral toxicity has been examined in the rat, guinea pig, rabbit and mouse, and the median lethal dose in those species ranges from approximately 600 to 1100 mg/kg. The acute inhalation LC_{50} of mesityl oxide in the rat, mouse, and guinea pig has been estimated at from 4400 to 9000 mg/m^3. Mesityl oxide was irritating to the rabbit skin when tested under an occlusive patch.

A combined repeated dose and reproductive/developmental toxicity study by inhalation in rats gave a LOAEL of 124 mg/m^3 with no unusual findings. In this 49-day inhalation study conducted at levels up to 1212 mg/m^3, effects were transient and reversible and were attributed to the irritative property of the chemical. No neurotoxicity was observed. The NOEL for reproductive toxicity from this study was 412 mg/m^3 and no developmental toxicity was noted at any exposure concentration.

Ames/Salmonella reverse mutation and mouse micronucleus studies were negative.

Environment

Mesityl oxide has limited persistence in water, soil or air. The predicted soil absorption coefficient is low. It is readily biodegradable and has a low potential to bioconcentrate. Loss from water or soil will primarily be by volatilization to the air. Once airborne, mesityl oxide is reactive, with an overall OH rate constant of 79.48 x 10-12 cm3/molecule-sec and a predicted half-life of 1.615 hours.

Mesityl oxide has moderate acute toxicity toward aquatic invertebrate species and freshwater vertebrates as well as a variety of bacterial species. Acute toxicity data calculated using the US EPA QSAR computer program, ECOSAR, generally are in the range 50 to 500 mg/l for fresh- and saltwater organisms. Laboratory-derived data for several aquatic organisms including fish, invertebrates, algae, and bacteria were conducted in open systems. Acute toxicity values for aquatic species ranged from over 1000 mg/L for *Daphnia magna* to 71 mg/L for *Salmo gairdneri*, the rainbow trout. Mesityl oxide has low toxicity toward a variety of bacterial species and has been shown experimentally to be stimulatory to the germination of two species.

Effects on terrestrial plants range from inhibition of germination (lettuce) to a slight growth stimulating effect (bean plants). Mesityl oxide was slightly toxic to spider mites and caused an increase in alarm behavior in several species of ants.

Exposure

Estimated total U.S. production of mesityl oxide is 20,700 metric tons. However, a 1999 search of the SRI Chemical Economics Handbook (CEH) and of the journal, Chemical Marketing Reporter, for mesityl oxide & ketone production statistics and chemical production statistics in general indicated that mesityl oxide is no longer produced as an isolated product in the U.S. for sale. Mesityl oxide is a non-isolated or site-limited intermediate used in the manufacture of methyl isobutyl ketone (MIBK) and during manufacture one pound of mesityl oxide yields one pound of MIBK. Based on the previously mentioned 1999 search, the 1999 U.S. demand for MIBK was estimated to be 180,000,000 pounds and production capacity for U.S. facilities was 210,000,000 pounds. Therefore, similar amounts of mesityl oxide would be produced and consumed as an intermediate in MIBK manufacture.

Mesityl oxide is manufactured by the aldol condensation of acetone within a closed, continuous, process. Nearly all mesityl oxide formed is reacted further as an intermediate to the manufacture of MIBK. In some cases, the mesityl oxide is not isolated but is immediately converted to MIBK. In other cases, the mesityl oxide may be stored

temporarily on site for subsequent conversion to MIBK. Any mesityl oxide isolated might be purified by distillation; otherwise, only the final product (MIBK) is purified by distillation.

In cases where mesityl oxide is manufactured as a non-isolated intermediate and is formed only in low concentrations in a reaction mixture and reacted further, all in closed equipment, fugitive emissions are expected to be low. Economic considerations also motivate to minimize emissions in order to maintain process efficiency. Environmental concentrations are expected to be low due to mesityl oxide's use as an industrial intermediate and its rapid aquatic and atmospheric degradability. Use as a pesticide inert may cause seasonal short-term higher concentrations in areas of pesticide application.
Few workers are occupationally exposed to mesityl oxide. Potential exposures would occur only during sample collection and maintenance of equipment.

RECOMMENDATIONS AND RATIONALE FOR THE RECOMMENDATION AND NATURE OF FURTHER WORK RECOMMENDED

Human Health: The chemical possesses properties indicating low hazards for human health. Based on data provided by the sponsor country, appropriate risk management measures are being applied (engineering controls, occupational standards, drinking water standards, Material Safety Data Sheets, and other US regulations). Countries may desire to check their own risk management measures to find out whether there is need for additional measures. Therefore the chemical is of a low priority for further work.

Environment: The chemical has properties indicating a hazard for the environment (acute aquatic EC/LC50 values between 1 and 100 mg/l). However the chemical is of low priority for further work for the environment because of its rapid biodegradation and its limited potential for bioaccumulation.