

MICHIGAN DEPARTMENT OF ENVIRONMENTAL QUALITY

INTEROFFICE COMMUNICATION

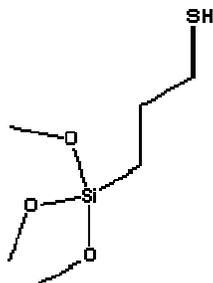
October 22, 2004

TO: File for 3-mercaptopropyltrimethoxysilane (CAS #4420-87-0)  
FROM: Anne Kim, Air Quality Division, Toxics Unit  
SUBJECT: Screening Level Derivation

**The initial threshold screening level (ITSL) for 3-mercaptopropyltrimethoxysilane is 2.40  $\mu\text{g}/\text{m}^3$  based on an annual averaging time.**

The following references or databases were searched to identify data to determine the screening level: U.S. Environmental Protection Agency (EPA) Integrated Risk Information System, Registry for Toxic Effects of Chemical Substances, American Conference of Governmental and Industrial Hygienists Threshold Limit Values, National Institute for Occupational Safety and Health Pocket Guide to Hazardous Chemicals, Environmental Protection Bureau Library, International Agency for Research on Cancer Monographs, Chemical Abstract Service (CAS) - Online (1967 – 2004), National Library of Medicine, Health Effects Assessment Summary Tables, and National Toxicology Program Status Report. The EPA has not established a reference concentration or reference dose for 3-mercaptopropyltrimethoxysilane. The molecular weight of 3-mercaptopropyltrimethoxysilane is 196.3 g. The molecular structure of 3-mercaptopropyltrimethoxysilane is shown in Figure 1.

Figure 1



After a thorough literature search, only two references listing LD50 values were readily available. Other potentially valid studies have been ordered (and have yet to be received to be reviewed), but the study titles do not clarify if the studies may or may not be useful for screening level development. Therefore, the initial threshold screening level (ITSL) is based on the information at hand. It will be re-evaluated when other studies are received and reviewed.

An acute toxicity test was done using Carworth-Wistar rats weighing 90 to 120 g (Smyth et al., 1969). A single oral dose was given to groups of 5 male rats and, at times, to female rats. Mortality rates were determined 14 days after dosing. The presented LD50 (and confidence interval) in mL/kg was 2.83 (1.61-4.98).

Another LD50 was listed in the Registry for Toxic Effects of Chemical Substances (RTECS) from the *Journal of Toxicology, Cutaneous and Ocular Toxicology* (1996). It was noted, however, that "details of toxic effects [were] not reported other than [the] lethal dose value". The oral LD50 in rats was 730 uL/kg.

### Derivations of Screening Level

The following equation is from Rule 232(1)(h):

$$ITSL = \frac{1}{500} \times \frac{1}{40} \times \frac{1}{100} \times \frac{LD50 \text{ (mg/kg)} \times W_A}{0.167 \times I_A}$$

$W_A$  = Body weight of experimental animal in kilograms (kg)

$I_A$  = Daily inhalation rate of experimental animal in m<sup>3</sup>/day

### Using Smyth et al.'s value of 2.83 mL/kg:

#### Conversion of concentration from mL/kg to mg/kg:

$$X \text{ mg/kg} = \text{mL/kg} \times \text{density g/mL} \times 1000 \text{ mg/g}$$

$$X \text{ mg/kg} = 2.83 \text{ mL/kg} \times 1.039 \text{ g/mL} \times 1000 \text{ mg/g}$$

$$X \text{ mg/kg} = 2940.4 \text{ mg/kg}$$

$W_A$  = mean value of the weights 0.090 kg and 0.120 kg (Smyth et al., 1969)

$$W_A = \frac{0.090 + 0.120}{2}$$

$$W_A = 0.105 \text{ kg}$$

$$I_A = 0.8W_A^{0.8206} \text{ (EPA, 1988)}$$

$$I_A = 0.8(0.105)^{0.8206}$$

$$I_A = 0.126 \text{ m}^3/\text{day}$$

$$ITSL = \frac{1}{500} \times \frac{1}{40} \times \frac{1}{100} \times \frac{2940.4 \times 0.105}{0.167 \times 0.126}$$

$$ITSL = .00734 \text{ mg/m}^3 = 7.34 \text{ ug/m}^3$$


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Using RTECS's value of 730 uL/kg:

Conversion of concentration from uL/kg to mg/kg:

$$X \text{ mg/kg} = \text{uL/kg} \times \text{mL}/1000 \text{ uL} \times \text{density g/mL} \times 1000 \text{ mg/g}$$

$$X \text{ mg/kg} = 730 \text{ uL/kg} \times 1 \text{ mL}/1000 \text{ uL} \times 1.039 \text{ g/mL} \times 1000 \text{ mg/g}$$

$$X \text{ mg/kg} = 758.5 \text{ mg/kg}$$

$W_A$  = using default value for body weight of rat (EPA, 1988)

$W_A$  = mean value of male weight of 0.470 kg and female weight of 0.319 kg

$$W_A = \frac{0.470 + 0.319}{2}$$

$$W_A = 0.395 \text{ kg}$$

$$I_A = 0.8W_A^{0.8206}$$

$$I_A = 0.8(0.395)^{0.8206}$$

$$I_A = 0.373 \text{ m}^3/\text{day}$$

$$\text{ITSL} = \frac{1}{500} \times \frac{1}{40} \times \frac{1}{100} \times \frac{758.5 \times 0.395}{0.167 \times 0.373}$$

$$\text{ITSL} = 0.00240 \text{ mg/m}^3 = \mathbf{2.40 \text{ ug/m}^3}$$

The most conservative value calculated is 2.40 ug/m<sup>3</sup> using RTECS LD50 value. Therefore, the ITSL for 3-mercaptopropyltrimethoxysilane is 2.40 ug/m<sup>3</sup> based on an annual averaging time.

## References

EPA. (1988) Recommendation for and documentation of biological values for use in risk assessment. PB 88-179874.

Smyth, H.F., Carpenter, C.P., Weil, C.S., Pozzani, U.C., Striegel, J.A., and Nycum, J.S. (1969) Range-Finding Toxicity Data: List VII. *American Industrial Hygiene Association Journal*. 30(5): 470 – 476.

Dekker, M. (1996) Cutaneous and Ocular Toxicology. *Journal of Toxicology*. Vol 15, pg 261.