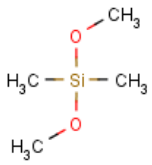
SIDS INITIAL ASSESSMENT PROFILE

CAS No.	1112-39-6
Chemical Name	Dimethoxydimethylsilane
Structural Formula	

SUMMARY CONCLUSIONS OF THE SIAR

Reduced Testing Rationale

Testing for water solubility, partition coefficient and biodegradation was not conducted because dimethoxydimethylsilane (DMDMS) undergoes rapid hydrolysis in the presence of water with the half life of<0.6 hours at pH 7 and 25°C. The hydrolysis products, methanol (CAS No. 67-56-1) and dimethylsilanediol (CAS 1066-42-8), are expected based on the chemical structure of DMDMS at an equal ratio of 2 moles methanol to 1 mole dimethylsilanediol. Nonetheless, modeled data are provided for the water solubility and partition coefficient endpoints for DMDMS; as it provides valuable information on substance behavior. Biodegradation data are available and provided for the hydrolysis products, methanol and dimethylsilanediol. In aqueous solutions, exposure to DMDMS is likely to be transient and observed aquatic toxicity is likely due primarily to the hydrolysis products, methanol and dimethylsilanediol. Dimethylsilanediol has been shown to be stable at environmentally relevant temperature and pH for 96 hours. As such, data from the hydrolysis products (methanol and dimethylsilanediol) are used to address the acute toxicity to fish and toxicity to aquatic plants for DMDMS. Data from the hydrolysis product methanol have been presented and agreed upon at SIAM 19 (sponsored by the United States; documents are available at http://www.oecd.org/document/63/0,3343,en_2649_34379_1897983_1_1_1_1,00.html).

Physical-Chemical Properties

The EPISuite program (v 4.0) developed by the U.S. Environmental Protection Agency and Syracuse Research Corporation has not been validated for chemicals that contain silanes in their molecular structure (although some measured data are included in the training data set); therefore, there is uncertainty associated with the calculated values and they should be used with caution whenever they are reported.

Dimethoxydimethylsilane (DMDMS) is a liquid with a melting point of -80.2 °C, a boiling point of 81.5 °C at 1010.9 hPa and a measured vapour pressure of 113.68 hPa at 25°C. The calculated octanol-water partition coefficient (log K_{ow}) is 0.585, and the calculated water solubility is 6800 mg/L at 25 °C. The water solubility and log K_{ow} values are not applicable because the chemical is hydrolytically unstable.

Human Health

No toxicokinetics data are available on the parent substance; however, rapid hydrolysis of this material is expected to produce 2 moles of methanol and 1 mole of dimethylsilanediol. *In vitro* percutaneous penetration of ^{14}C-labeled dimethylsilanediol (^{14}C-DMSD) was evaluated when applied in aqueous solution to human skin for 24 hours [OECD TG 428]. At the end of the assay, 59.5% of ^{14}C-DMSD volatilized from the skin surface (captured in the charcoal baskets placed above the exposure site), 18.3% was on the skin surface, 2.5% remained in the skin after washing and tape stripping, and 13.9% of the applied dose was absorbed; 82.1% of the absorbed dose penetrated

through the skin.

The oral (gavage) LD_{50} in male and female rats of DMDMS was 4235 mg/kg bw [OECD TG 401]. Central nervous system effects were the predominant clinical sign of toxicity. No experimental data are available for irritation or skin sensitization in animals.

In a combined repeated-dose/reproductive/developmental toxicity screening test [OECD TG 422], DMDMS was administered via gavage to 10 rats/sex/dose at 0 (corn oil), 50, 250 and 1000 mg/kg bw/day. Males were treated during pre-mating and mating periods. Males and toxicity group females were sacrificed after they had been treated for 29 or 28 days, respectively. Clinical signs included soiling of the chin and/or urogenital area in both sexes dosed at 1000 mg/kg bw/day; soiling of the muzzle was also noted in females at 1000 mg/kg bw/day. There were no statistically significant treatment-related differences between controls and treatment groups in mean body weight, body weight gain, food consumption, FOB tests and motor activity parameters, hematological, prothrombin and/or clinical chemistry parameters during the study. At 1000 mg/kg bw/day, statistically significantly decreased absolute and relative adrenal gland, thymus and testes weights and statistically significantly decreased absolute epididymides, prostate gland and seminal vesicle weights were observed in males; statistically significantly decreased absolute and relative spleen weight were observed in females. Statistically significantly increased absolute and relative liver weights were observed in males and females at 250 and 1000 mg/kg bw/day. Histopathological examination showed adverse changes at 1000 mg/kg bw/day in the liver of male rats (centrilobular hepatocyte hypertrophy, hepatocellular vacuolation and protoporphyria), adrenal glands (adrenal cortical atrophy), male kidneys, testes and epididymides of male rats (degeneration of spermatocytes, seminiferous tubular degeneration) and in the liver of female rats (centrilobular and panlobular hepatocyte hypertrophy). Follicular cell hypertrophy was observed in the thyroid gland of all males and females at 1000 mg/kg bw/day. This is considered as an adaptive secondary effect (related to up-regulation of hepatic microsomal enzymes) and adverse for the rat, but that the mechanism is generally not applicable to species with significant levels of thyroid binding globulin. The NOAEL for systemic toxicity was 250 mg/kg bw/day with a LOAEL of 1000 mg/kg bw/day.

DMDMS did not induce gene mutations in bacterial cells (*Salmonella typhimurium* TA98, TA100, TA102, TA1535 and TA1537) *in vitro* [OECD TG 471] or chromosomal aberrations in Chinese hamster ovary cells [OECD TG 473; tested at the limit dose of 10 mM]. Based on these results, DMDMS is not considered to be genotoxic *in vitro*.

No data are available for the carcinogenicity of DMDMS.

The reproductive toxicity of DMDMS has been investigated in a repeated-dose/reproductive/developmental toxicity screening test in rats [OECD TG 422]. DMDMS was administered via gavage to 10 rats/sex/dose at 0 (corn oil), 50, 250, and 1000 mg/kg bw/day. Males were treated for at least 29 days (14 days prior to mating and through the mating period) and females were treated for 14 days prior to mating, during mating and gestation periods and through post-partum day 3. There was a decrease in body weight gain for females at 1000 mg/kg bw/d (during gestational week 3 and during the 4 day post-partum period). Based on observations at 1000 mg/kg bw/day (an increase in days of gestation and a decrease in live pups), the NOAEL for effects on fertility was 250 mg/kg bw/day. No gross abnormalities were found for any of the pups. Based on observations at 1000 mg/kg bw/day (an increase in post-implantation loss, a significant decrease in the total number of viable pups and the ratio of number of viable pups/total, a decrease in final litter weight, a decrease in final average pup weight and an increase in the percentage of post-natal loss) the NOAEL for maternal and developmental toxicity was 250 mg/kg bw/day.

DMDMS may present a hazard for human health (repeated-dose (liver, adrenal gland, kidney, testes and epididymides), reproductive and developmental toxicity). Adequate screening-level data are available to characterize the human health hazard for the purposes of the OECD HPV Chemicals Programme.

Environment

Testing for water solubility, partition coefficient and biodegradation was not conducted because dimethoxydimethylsilane (DMDMS) undergoes rapid hydrolysis in the presence of water with the half life of <0.6 hours at pH 7 and 25°C.

The measured hydrolysis half-life for DMDMS at pH 7 and 25^{o}C is <0.6 hrs. In the atmosphere, indirect photo-oxidation by reaction with hydroxyl radicals is predicted to occur with a half-life of 5.5 days with an overall OH rate constant of 1.96 x 10^{-12} cm^3/molecule-sec. The biodegradation of DMDMS has not been determined due to its

rapid hydrolysis. Based on the rapid hydrolysis of this material, any potential for biodegradation is likely to be of the hydrolysis products. Consequently, the only substances remaining in the test system will be methanol and dimethylsilanediol. Methanol is readily biodegradable based on the results of standard tests that show 76 – 82 % and 95 % removal in standard ready tests after 5 and 20 days, respectively. Dimethylsilanediol has been shown to biodegrade in soils at rates between 0.9 to 6.4% per month based on $^{14}CO_2$ production and is not expected to be readily biodegradable.

A level III fugacity model calculation with equal and continuous distributions to air, water and soil compartments suggests that DMDMS will distribute mainly to the soil (58.3%), water (25.8%) and air (15.8%) compartments with minor distribution to the sediment compartment (<1%). However, DMDMS is unlikely to be found in the environment, as this material is hydrolytically unstable. A calculated Henry's Law constant of 1.20 x 10^2Pa-m3/mole (1.18 x 10^{-3} atm-m3/mole) suggests that volatilization from the water phase for DMDMS is expected to be high.

(these two paragraph differ only slightly; one should be deleted; believe the first paragraph is correct)

Bioaccumulation is not anticipated since the parent compound, DMDMS, is hydrolytically unstable. The estimated BCF for the hydrolysis product dimethylsilanediol is low (3.16). However, as the model is not validated for this compound a final conclusion on bioaccumulation of dimethylsilanediol cannot be drawn with accuracy. Experimental BCFs of < 10 in fish species, including *Cyprinus carpio* and *Leuciscus idus*, have been measured for methanol.

Bioaccumulation is not anticipated since the parent substance DMDMS, is hydrolytically unstable. The estimated BCF for the hydrolysis product dimethylsilanediol is low (3.16). However, as the model is not validated for compounds containing silane in their structure a final conclusion on bioaccumulation of dimethylsilanediol cannot be drawn with accuracy. Experimental BCFs of < 10 in fish species, including *Cyprinus carpio* and *Leuciscus idus*, have been measured for methanol.

DMDMS reacts to form methanol and dimethylsilanediol through hydrolysis. The bioaccumulation potential for dimethylsilanediol cannot be predicted accurately, but is expected to be low (calculated BCF = 3.16). Methanol is not likely to bioaccumulate (measured BCF<10). Furthermore, due to these properties, current estimation models are not capable of calculating physicochemical or environmental fate values of dimethylsilanediol with a known degree of accuracy. The adsorption of dimethylsilanediol onto surfaces and its tendency to polymerize itself are important properties of this chemical. In the environment, dimethylsilanediol is expected to be found in water and air and to be adsorbed by soil and sediment, but is still subject to hydrolysis. Unbound dimethylsilanediol in air, water, and soil is expected to degrade photolytically to silica and carbon dioxide.

Due to the rapid hydrolysis of DMDMS, aquatic organisms are likely exposed to the parent and its hydrolysis products, methanol and dimethylsilanediol. Acute aquatic toxicity to invertebrates has been investigated for DMDMS. Data for the hydrolysis products, methanol and dimethylsilanediol, are provided for acute toxicity to fish, aquatic invertebrates and aquatic plants.

The following acute toxicity test results have been determined for aquatic species:

DMDMS

Fish: no data
Invertebrate [*Daphnia magna*]: 48 h EC_{50} > 100 mg/L (static; nominal)
Algae: no data

Methanol

Fish [*Lepomis macrochirus*]: 96 h LC_{50} = 15,400 mg/L (flow-through)
Fish [*Salmo gairdneri*]: 96 h LC_{50} = 20,100 mg/L (flow-through)
Fish [*Pimephales promelas*]: 96 h LC_{50} = 28,100 mg/L (flow-through)
Invertebrate [*Daphnia magna*]: 48 h EC_{50} = 10,000 mg/L (no details located)
Algae [*Scenedesmus quadricauda*]: 10-14 d EC_{50} =28,400 (no details located)

Dimethylsilanediol

Fish [*Oncorhynchus mykiss*]: 96 h LC_{50} > 126 mg/L (static, measured)
Invertebrate [*Daphnia magna*]: 48 h EC_{50} > 117 mg/L (static; measured)
Algae [*Pseudokirchneriella subcapitata*]: 72 hr E_yC_{50}, EC_{50} >118 (static; measured)

Algae [*Pseudokirchneriella subcapitata*] NOEC = 118 mg/L (static; measured)

DMDMS does not present a hazard for the environment based on its low hazard profile and the low hazard profile of its hydrolysis products. DMDMS is not expected to be readily biodegradable. Adequate screening-level data are available to characterize the environmental hazard for the purposes of the OECD HPV Chemicals Programme.

Exposure

DMDMS was produced and/or imported in the United States at a volume between 454 and < 4,540 tonnes (1 million and < 10 million pounds) during 2005. This material is also produced in Japan (< 45 tonnes in 2005). The substance is used as a chemical intermediate, an intermediate for silicone polymer/oligomers, rubber additive, water repellent; and in automotive products. Percent use in the final product is 0.02-100% with no parent substance remaining after end use.

DMDMS is manufactured in closed systems. Engineering controls include ventilation devices and related equipment; closed sampling loops; grounding. Personal protective equipment includes safety glasses, respirator, gloves (impermeable chemical resistant), fire resistant clothing, safety shoes, and hard hat. No exposure is anticipated under routine operations. Potential routes of exposure during routine operations include dermal and inhalation.

The industrial consumers use DMDMS in closed systems; potential non-accidental exposure is not ruled out because additional information could not be obtained. Engineering controls include grounding and ventilation. Personal protective equipment includes gloves, safety glasses, and respirator. Potential routes of non-accidental exposure include inhalation and dermal.

DMDMS is used in consumer automotive products at <1%; dermal exposure is possible.

There are no intentional releases to the environment. The reactive nature of this material destroys the parent material in water, thus limiting environmental exposure to DMDMS.