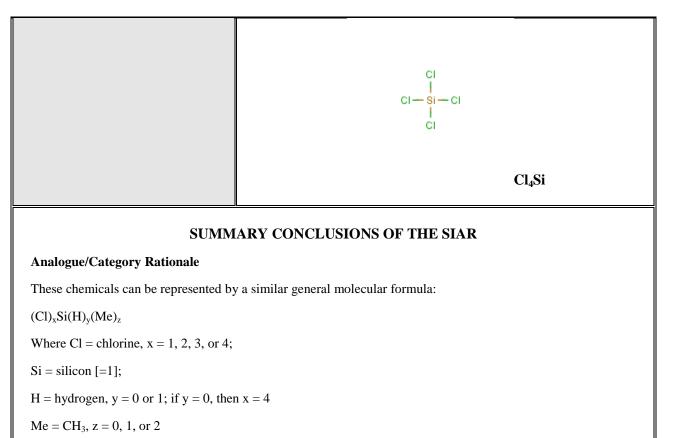
Category Name	Monomeric Chlorosilanes		
CAS No(s).	1066-35-9 75-54-7 10025-78-2 10026-04-7		
Chemical Name(s)	Chlorodimethylsilane ( <b>ClMe<sub>2</sub>SiH</b> ) Dichloromethylsilane ( <b>Cl<sub>2</sub>MeSiH</b> ) Trichlorosilane ( <b>Cl<sub>3</sub>SiH</b> ) Tetrachlorosilane ( <b>Cl<sub>4</sub>Si</b> )		
Structural Formula(s)	$\mathbf{C}_{\mathbf{H}_{3}\mathbf{C}}^{C_{1}} \mathbf{C}_{\mathbf{H}_{3}}^{C_{3}} \mathbf{C}_{\mathbf{H}_{2}}^{C_{3}} \mathbf{C}_{\mathbf{H}_{2}}^{C_{3}} \mathbf{C}_{\mathbf{H}_{3}}^{C_{2}} \mathbf{C}_{\mathbf{H}_{3}}^{C_{2}} \mathbf{C}_{\mathbf{H}_{3}}^{C_{2}} \mathbf{C}_{\mathbf{H}_{3}}^{C_{3}} \mathbf{C}_{\mathbf{H}_{3}}$		

# SIDS INITIAL ASSESSMENT PROFILE

(Cl<sub>3</sub>MS).



Chlorosilanes react rapidly when exposed to moisture or polar reagents (those that contain a dissociable  $H^+$ ), producing hydrogen chloride (HCl; CAS No. 7647-01-0) and the corresponding silanols (in general, siloxane oligomers and polymers). The half lives of the monomeric chlorosilanes are expected to be < 1 minute based on data from the structurally similar chlorosilanes dichloro(dimethyl)silane (Cl<sub>2</sub>DMS) and trichloro(methyl)silane

Data are not available on the hydrolysis of these compounds. However, the following is expected:

- **CIMe<sub>2</sub>SiH** is expected to hydrolyze to form one mole each of HCl and dimethylsilanol (note that dimethylsilanol can hydrolyze to form dimethylsilanediol (DMSD) ultimately through hydrolysis of the SiH bond, which is pH dependent and occurs most rapidly under alkaline conditions).
- **Cl<sub>2</sub>MeSiH** is expected to hydrolyze to form two moles of HCl and one mole of methylsilanediol (note that methylsilanediol can hydrolyze to form methylsilanetriol (MST) ultimately through hydrolysis of the SiH bond).
- **Cl<sub>3</sub>SiH** is expected to hydrolyze to form three moles of HCl and one mole of silanetriol (note that silanetriol can hydrolyze to form silaneterol ultimately through hydrolysis of the SiH bond).
- **Cl<sub>4</sub>Si** is expected to hydrolyze to four moles of HCl and one mole of silanetetrol, which rapidly precipitates to insoluble silica (SiO<sub>2</sub>) when the concentration is sufficiently high.

As noted, the silanols resulting from initial hydrolysis can condense spontaneously to form highly cross-linked polymeric gels in uncontrolled environments at concentrations greater than 500 mg/L. Because of these properties, they cannot be readily isolated without spontaneously forming highly cross-linked polymeric gels in uncontrolled environments and as such cannot be tested.

*Hydrolysis Analogues*. It is appropriate to use other chlorosilane data to estimate hydrolysis of the sponsored substances. Structurally similar chlorosilanes used for hydrolysis are dichloro(dimethyl)silane (Cl<sub>2</sub>DMS) and trichloro(methyl)silane (Cl<sub>3</sub>MS). These two analogous chlorosilanes were selected based on a hydrolysis study of

six chlorosilanes with varying substitutions. Despite the differences in substitution of these chlorosilanes, all the half-lives were < 17 seconds.

*Human Health and Aquatic Toxicity Analogues.* (1) All category members are expected to hydrolyze rapidly to form hydrogen chloride (HCl) as one of the products. Therefore, data for HCl can be used to represent the toxicity of the monomeric chlorosilanes.

(2) Trimethoxysilane rapidly hydrolyzes at pH 7 with  $t_{1/2} < 0.3$  minutes at 2 °C to silanetriol as well as methanol. In aqueous environments, exposures to trimethoxysilane are likely to be transient and observed toxicity is likely due primarily to the hydrolysis products methanol, silanetriol, and condensed silanetriol materials. **Cl<sub>3</sub>SiH** is expected to form the same silanol (silanetriol) upon hydrolysis. Therefore trimethoxysilane is used as a supporting substance, along with HCl. Reproductive toxicity data are not available for trimethoxysilane.

(3) Another previously assessed alkoxysilane, tetraethylorthosilicate (TEOS), rapidly hydrolyzes to ethanol and silanetetrol at pH 4, 7 and 9 with  $t_{1/2} = 0.1$ , 4.4 and 0.2 hrs, respectively. In aqueous environments, exposures to TEOS are likely to be transient and observed toxicity is likely due primarily to the hydrolysis products ethanol, silanetetrol, and condensed silanol materials. Since TEOS hydrolyzes to the same silanol, it can be used as a supporting substance for **Cl<sub>4</sub>Si**, along with HCl.

(4) A previously assessed alkylsilane, methyltrimethoxysilane (MTMS), rapidly hydrolyzes to methanol and methylsilanetriol at pH 4, 7 and 9 with  $t_{1/2} = 0$ , 2.2 and 0.1 hrs, respectively. In aqueous environments, exposures to MTMS are likely to be transient and observed toxicity is likely due primarily to the hydrolysis products methanol, methylsilanetriol, and condensed silanetriol materials (high molecular weight polymers). Given the structural similarity between silanetriol and the supporting substance hydrolysis product methylsilanetriol, MTMS can be used as a supporting substance for  $Cl_2MeSiH$  and  $Cl_3SiH$ , along with HCl.

(5) For the supporting substances trimethoxysilane, TEOS, and MTMS, toxicity due to hydrolysis to methanol or ethanol is expected to be negligible.

(6) For the chromosome aberrations endpoint, data for supporting chlorosilane substance dichlorodimethylsilane ( $Cl_2DMS$ ) are provided because this supporting substance hydrolyzes to the same silanol (and HCl) as sponsored substance,  $Cl_2MeSiH$ .

(7) A structurally similar silanol, dimethylsilanediol (DMSD) is stable, isolatable and as such has been tested in mammalian and aquatic systems. DMSD is closely related structurally to methylsilanediol (replacement of -H with -CH<sub>3</sub>) and both substances have expected similar physicochemical properties, therefore the toxicological properties are expected to be similar and DMSD can be used as a supporting substance for  $Cl_2MeSiH$ , along with HCl.

(8) A structurally similar silanol, trimethylsilanol (TMS) is stable, isolatable and as such has been tested in mammalian and aquatic systems. TMS is closely related structurally to dimethylsilanol (replacement of -H with -  $CH_3$ ) and both substances have similar physicochemical properties, therefore the toxicological properties are expected to be similar. This structural similarity suggests TMS can be used as a supporting substance for **CIMe<sub>2</sub>SiH**, along with HCl.

HCl, trimethoxysilane, MTMS, TEOS,  $Cl_2DMS$ , and  $Cl_3MS$  were all presented and agreed under the OECD HPV Chemicals Programme (<u>http://www.oecd.org/env/hazard/data</u>). TMS and DMSD have both been used as analogues in the OECD HPV Chemicals Programme, most recently for chloroalkylchlorosilanes at CoCAM 3. Data for all can be found at <u>http://www.oecd.org/env/hazard/data</u>.

The read-across strategy follows:

	Environmental fate	Mammalian toxicity			Environmental effects
Substance	Hydrolysis	Eye irritation	Mutagenicity	Repeated dose toxicity, Reproductive toxicity	Acute aquatic toxicity

ClMe <sub>2</sub> SiH	Cl <sub>2</sub> DMS	HCl	Cl <sub>2</sub> DMS, <b>Cl<sub>4</sub>Si,</b> HCl	TMS, HCl	TMS, DMSD, HCl
 Cl <sub>2</sub> Me	Cl <sub>2</sub> DMS	HCl	$Cl_2DMS, Cl_4Si,$	DMSD, MTMS, HCl	DMSD, HCl
SiH			HCl		
Cl₃SiH	Cl <sub>3</sub> MS	HCl	Cl₄Si, HCl	Trimethoxysilane <sup>(1)</sup> , MTMS, HCl	Trimethoxysilan e, HCl
Cl <sub>4</sub> Si	Cl <sub>3</sub> MS	HCl	Cl₄Si, HCl	TEOS, HCl	TEOS, HCl

(1) Read across for repeated dose (inhalation) endpoint only

The toxicity of the category will be described by the most toxic category member or supporting chemical.

TMS and DMSD are not reactive like other supporting substances or HCl. Therefore, the data from TMS and DMSD should be evaluated along with data on HCl or other structurally similar/reactive compounds for a more complete understanding of the toxicity of the sponsored monomeric chlorosilanes.

#### **Physical-chemical Properties**

Not all programs within EPI Suite have been validated for chemicals that contain the element Si, but recent upgrades to the Kow module, found in the current version of EPI Suite (v4.10), may improve estimates for silanes and siloxanes for this endpoint. However, there is still uncertainty associated with the calculated values and they should be used with caution whenever they are reported. Inorganic substances ( $Cl_3SiH$  and  $Cl_4Si$ ) are outside the applicability domain of EPI Suite.

The sponsored substances are liquids with measured melting points of -126.5 °C ( $Cl_3SiH$ ) to -68.9 °C ( $Cl_4Si$ ), measured boiling points of 31.5 °C ( $Cl_3SiH$ ) to 56.9 °C ( $Cl_4Si$ ) at 1013 hPa and vapour pressures of 292 hPa ( $Cl_4Si$ ) to 721.8 hPa ( $Cl_3SiH$ ) at 20°C. The calculated octanol-water partition coefficients (log K<sub>ow</sub>) range from 1.46 ( $Cl_3SiH$ ) to 1.93 ( $ClMe_2SiH$ ), and the calculated water solubilities range from 3274 mg/L ( $ClMe_2SiH$ ) to 9951 mg/L ( $Cl_3SiH$ ) at 25 °C. The calculated water solubility and log K<sub>ow</sub> values may not be accurate because the substances are hydrolytically unstable.

## Human Health

No data are available on the toxicokinetics, metabolism and distribution of the monomeric chlorosilanes. However, these substances rapidly hydrolyze on contact with moisture. Dimethylsilanol, but not the remaining three silanol hydrolysis products (methylsilanediol, silanetriol, silanetetrol), may be absorbed across the skin or respiratory epithelium; as the size of the silanol hydrolysis products increase, absorption by the respiratory tract decreases and retention by respiratory mucus is expected to increase. Damage to membranes caused by the corrosive nature of HCl might enhance the uptake of the sponsored substances or the silanol hydrolysis products. Hydrogen and chloride ions will enter the body's natural homeostatic processes. HCl will rapidly dissociate and its effects are thought to be a result of pH change (local deposition of  $H^+$ ). The low molecular weight and water solubility of the silanols suggest elimination via the kidneys in urine.

The attached Annex provides a summary of the read across values for mammalian toxicity.

The acute inhalation toxicity of the monomeric chlorosilanes is well characterized by the effects of HCl and is expected to result from HCl exposure. The 1-hour acute inhalation  $LC_{50}$ s (OECD 403) with rats for the monomeric chlorosilanes range from 8.4 (**Cl<sub>2</sub>MeSiH**; nominal) to 17.3 mg/L (**ClMe<sub>2</sub>SiH**; nominal). The acute inhalation hazard posed by a chlorosilane, as defined by an  $LC_{50}$  value, is directly proportional to its chlorine content and subsequently to the HCl that is liberated during hydrolysis. The principal clinical signs are expected to be indicative of respiratory and ocular effects resulting from HCl exposure. The acute inhalation  $LC_{50}$  of the supporting substance trimethoxysilane was ca. 0.3 mg/L. A 6-hour inhalation  $LC_{50}$  of >42 mg/L was reported for the supporting substance MTMS. Inhalation  $LC_{50}$  values for HCl were determined to be 4.2-4.7 mg/L for 1-hour exposures to rats. Dermal toxicity data were not located for the monomeric chlorosilanes. The oral  $LD_{50}$ s for the monomeric chlorosilanes when dosed diluted in oil were 3141 mg/kg bw (**Cl<sub>2</sub>MeSiH**), 1030 mg/kg bw (**Cl<sub>3</sub>SiH**) and 238 mg/kg bw (**Cl<sub>4</sub>Si**). When dosed undiluted, **Cl<sub>2</sub>MeSiH** resulted in an LD50 of <278 mg/kg-bw. Oral LD<sub>50</sub> values of HCl were determined to be 238-277 mg/kg-bw for female rats.

The monomeric chlorosilanes rapidly hydrolyze to HCl and the associated silanol. Two of the sponsored

substances have been tested ( $Cl_2MeSiH$  and  $ClMe_2SiH$ ) and are considered corrosive to the skin. Based on findings from acute oral and inhalation studies, the sponsored substances are expected to be respiratory and GI tract irritants. Eye irritation data are not available for the sponsored substances. HCl is corrosive and highly irritating to the skin, eyes and respiratory tract with no data reported to suggest as a sensitizer. Based on HCl formation, monomeric chlorosilanes possess properties indicating possible hazards for acute inhalation toxicity, skin, eye, and respiratory tract irritation.

No data regarding sensitization are available on the monomeric chlorosilanes.

Limited repeated dose toxicity data are available for the monomeric chlorosilanes with Cl<sub>3</sub>SiH as the only tested material. Groups of rats (5/sex/concentration) were exposed in a nose-only exposure system to target concentrations of ca. 0.06 and 0.18 mg/L of Cl<sub>3</sub>SiH or ca. 0.016 and 0.05 mg/L of HCl. Rats were exposed six hours per day, five days per week, for two weeks. There were no deaths, clinical signs, effects on body or organ weights and no findings at gross necropsy. Microscopic examination of animals exposed to Cl<sub>3</sub>SiH showed mineralization in the kidneys of females; no other apparent treatment-related effects were observed. Data from supporting substances, trimethoxysilane, MTMS and TEOS, supporting hydrolysis products TMS and DMSD and hydrolysis product HCl are used to fill the repeated-dose toxicity endpoint for the monomeric chlorosilanes. Systemic effects following inhalation of TMS, trimethoxysilane, or MTMS (trimethoxysilane, and MTMS exposure likely as a mixture with silanol hydrolysis products) are well characterized. In the absence of adverse effects, in an OECD 422 study the NOAEC for TMS was ca. 2.2 mg/L (the highest concentration tested) in rats exposed for at least 28 days. Repeated inhalation exposure of rats to trimethoxysilane for 28 days at ca. 0.025 or 0.050 mg/L was lethal, with death likely a consequence of respiratory tract injury. Based on the body weight, organ weight, clinical pathology, histopathologic observations, and deaths, the NOAEC from this study appeared to be ca. 0.0025 mg/L. Exposure of rats to trimethoxysilane vapor ca. 0.0001, 0.0005, or 0.0025 mg/L for 90 days, followed by a 4-week recovery period produced no exposure-related effects in the biologic parameters monitored during this study. The NOEC for trimethoxysilane in a 90-day inhalation study with rats was determined to be at least ca. 0.0025 mg/L. Based on the increased incidence of grossly observed urinary bladder calculi along with the kidney dilation at the 2.2 mg/L/day exposure level, the NOAEC for repeated inhalation exposure (OECD 413) for MTMS was 0.56 mg/L and the LOAEC was 2.2 mg/L/day. By the inhalation route, during repeated dose toxicity studies, the local effects of irritation of HCl were observed in the groups of 0.015 mg/L and above in the 90-day inhalation study. The NOAEC for systemic toxicity for HCl, excluding the local effects of irritation, has been determined to be 0.030 mg/L for rats and mice.

Based on the observation of tubular nephropathy and associated clinical chemistry changes in male rats at 50 mg/kg-bw/day, the NOAEL for repeated oral exposure (at least 4 weeks) to TEOS was 10 mg/kg-bw/day and 50 mg/kg-bw/day in male and female rats, respectively (OECD 422). The NOAEL for repeated oral exposure (28 days) to TMS was 250 mg/kg-bw/day based on clinical signs, growth retardation, and changes in the liver (bile ducts) at 750 mg/kg-bw/day (OECD 407). The NOAEL for DMSD following repeated oral exposure (at least 28 days) was 250 mg/kg-bw/day based on liver porphyria in male rats and liver vacuolation in female rats (OECD 422). Based on liver effects (females), increased prothrombin time (males) and thyroid effects (both sexes), the NOAEL for repeated oral exposure (at least four weeks in an OECD TG 422 study) to MTMS was 50 mg/kg bw/day with a LOAEL of 250 mg/kg bw/day.

The sponsored substances did not induce gene mutations in *Salmonella typhimurium* bacterial cells (TA98, TA100, TA1535 and TA1537 for **ClMe<sub>3</sub>SiH**, **Cl<sub>3</sub>SiH**, or **Cl<sub>4</sub>Si**, and TA1538 for **Cl<sub>3</sub>SiH** and **Cl<sub>4</sub>Si**) *in vitro* (OECD 471). The sponsored substance **Cl<sub>4</sub>Si** did not cause chromosomal aberrations *in vitro* (OECD 476). The hydrolysis product HCl did not induce gene mutations in bacterial cells. Positive results in the *in vitro* chromosome aberration test with HCl were considered to be the effect of low pH. In *in vitro* chromosome aberration tests using mouse lymphoma cells **Cl<sub>2</sub>DMS** was negative. Based on the available data, the monomeric chlorosilanes are not expected to be genotoxic.

No data are available for the carcinogenicity of the monomeric chlorosilanes.

No data are available on the reproductive toxicity of the monomeric chlorosilanes; data are available for the supporting substances MTMS, TEOS, TMS, and DMSD, and the hydrolysis product HCl. In a combined repeated-dose/reproductive/developmental toxicity screening test (OECD TG 422), TMS was administered via whole body vapor inhalation to 3 groups of rats, at nominal concentrations of 0, 60, 300 or 600 ppm (ca. 0, 0.22,

1.1, and 2.2 mg/L) for 6 hours/day, 7 days/week; each group consisted of 10 males, 10 toxicity phase females and 10 reproductive phase females. The NOAEC for reproductive, systemic and neonatal toxicity of TMS was ca. 2.2 mg/L when administered via whole-body inhalation exposure to rats. In a combined repeateddose/reproductive/developmental toxicity screening test (OECD TG 422), rats (10/sex/dose) were administered DMSD at 0 (corn oil), 50, 250 or 500 mg/kg-bw/kg-bw/day via oral gavage. No test article-related effects were observed in any of the effects on fertility or developmental parameters evaluated. The NOAEL for maternal toxicity is 250 mg/kg bw; the NOAEL for effects on fertility and developmental toxicity of DMSD in rats was 500 mg/kg-bw/day (highest dose tested). The reproductive and developmental toxicity of MTMS has been investigated in a reproductive and developmental toxicity screening test in rats [OECD TG 422]. In this study, MTMS was administered via gavage to 10 rats/sex/dose at 0 (corn oil), 50, 250, and 1000 mg/kg-bw/day, for at least 28 days (males) and up to PND 4 (females). No adverse effects on reproductive or developmental parameters were observed up to the highest dose tested. Based on no adverse effects the NOAEL for reproductive and developmental toxicity was considered to be 1000 mg/kg-bw/day. In an OECD TG 422 with TEOS, no adverse effects on reproduction or development of rats were observed up to the highest dose tested. The NOAEL for fertility/developmental toxicity for TEOS was 100 mg/kg-bw/day in rats. The NOAEL for maternal toxicity was 50 mg/kg-bw/day. No reliable studies have been reported regarding toxicity to reproduction and development in animals after oral, dermal or inhalation exposure to hydrogen chloride/hydrochloric acid. Because proton and chloride ions are the normal constituents in the body fluid of animal species, lower concentration of hydrogen chloride gas/mist or solution does not seem to cause adverse effects to animals. In fact, the cells of gastric glands secretes hydrochloric acid into the cavity of stomach and orally administered sulfuric acid, which results in pH change as well, did not cause developmental toxicity to laboratory animals. These facts indicate that hydrogen chloride/hydrochloric acid is not expected to have developmental toxicity. In addition, no effects on the gonads were observed in a 90-day inhalation repeated-dose study up to concentrations of 0.073 mg/L. Based on data for the supporting substances, structurally similar silanols and the hydrolysis product, HCl, the monomeric chlorosilanes are not expected to be reproductive or developmental toxicants.

The monomeric chlorosilanes possess properties indicating a hazard for human health (lethality from acute oral and inhalation), corrosive and highly irritating to the skin, eyes (based on HCl), GI and respiratory tracts, repeated dose toxicity). Adequate screening-level data are available to characterize the human health hazard for the purposes of the OECD Cooperative Chemicals Assessment Programme.

## Environment

Not all programs within EPI Suite have been validated for chemicals that contain the element Si, but recent upgrades to the Kow module, found in the current version of EPI Suite (v4.10), may improve estimates for silanes and siloxanes for this endpoint. However, there is still uncertainty associated with the calculated values and they should be used with caution whenever they are reported.

The chlorine group is the most active functional group of these molecules and determines many aspects of the behaviour of the category members. The monomeric chlorosilanes are expected to undergo rapid hydrolysis in the presence of water to form one to three moles of HCl and one mole of mono-, di- or tri- silanol, depending on the parent substance. Hydrolysis is the primary reaction in aqueous systems. Hydrolysis studies were not conducted on the monomeric chlorosilanes. The momeric chlorosilanes hydrolyze rapidly; the half-lives are expected to be <1 minute based on data from two analogous substances, dichloro(dimethyl)silane (CAS No. 75-78-5) and trichloro(methyl)silane (CAS No. 75-79-6). Observed rates of hydrolysis were so rapid in all cases that it was not possible to distinguish among the different pH conditions.

The overall rate constants for reaction with OH radicals in the atmosphere due to indirect photolysis are 0.2992 x  $10^{-12}$  and 0.1496 x  $10^{-12}$  cm<sup>3</sup>/molecule-sec for **CIMe<sub>2</sub>SiH** and **Cl<sub>2</sub>MeSiH**, respectively. The resulting half-lives due to indirect photolysis are 35.8 and 71.5 days for **CIMe<sub>2</sub>SiH** and **Cl<sub>2</sub>MeSiH**, respectively. **Cl<sub>3</sub>SiH** and **Cl<sub>4</sub>Si** are considered to be inorganic according to EPI Suite, and very few inorganic compounds were included in the training set for the methodology utilized in several EPI Suite programs. Therefore, inorganic compounds are considered to be outside the estimation domain. Any potential for photodegradation might be superseded by hydrolysis of the parent compound depending on the concentration of water vapor in the air. Biodegradation tests were not located for the sponsored substances. In an OECD 310, supporting hydrolysis product TMS showed 0% biodegradation over 28 days and based on studies of DMSD (<sup>14</sup>C-dimethylsilanediol) in four soils at 25 °C, the substance is not rapidly biodegradable. HCl is an inorganic compound and biodegradation tests are not applicable. Based on this information, **CIMe<sub>2</sub>SiH** and **Cl<sub>2</sub>MeSiH** are not expected to be readily biodegradable. **Cl<sub>3</sub>SiH** and

 $Cl_4Si$  are considered to be inorganic compounds and biodegradation tests are not applicable. Due to rapid hydrolysis of the sponsored substances, any potential for biodegradation is likely to be of the hydrolysis products. Consequently, the only biodegradable materials in the test system will be silanols, and condensed silanol materials (high molecular weight polymers). At high concentrations, the silanols will condense to form highly cross linked, high molecular weight polymers that are water insoluble and effectively nonbiodegradable.

Fugacity modeling for inorganic substances ( $Cl_3SiH$  and  $Cl_4Si$ ) is outside the applicability domain of EPI Suite. Fugacity modeling of HCl is not applicable. A Level III fugacity model calculation with equal and continuous distributions to air, water and soil compartments suggests that the monomeric chlorosilanes will distribute mainly to the air (47.6 – 49%) and soil (ca. 46.2 - 47.6%) compartments, with minor distribution to water (ca. 5%) and negligible distribution to sediments (<0.1). Since the parent materials are not expected to be released to soil or water based on their uses and handling, a scenario of 100% emission to air is more realistic. When the monomeric chlorosilanes are released to air exclusively, the fugacity model predicts that 99.8% is reacted. The unreacted 0.2% remains in air (100%). The modeling results show that the environmental fate of the monomeric chlorosilanes is controlled by their high reactivity with water in all compartments. Level III fugacity modeling using equal loading rates of 1000 kg/h each for air, soil and water predicts that the hydrolysis products will distribute mainly to soil (62.8 – 75.2 %), with a smaller fraction to water (ca. 24.5 – 31.8 %) and negligible amounts to sediment and air. Based on the more realistic scenario of 100% release to air, the model predicts that dimethylsilanol will be distributed mainly in air (83.3%) and water (11.7%), and that the remaining three silanol hydrolysis products will be distributed mainly in soil (ca. 85-88%) and water (ca. 9-11%).

The bioaccumulation potential of the monomeric chlorosilanes was not measured due to rapid hydrolysis. The estimated BCF using the BCFBAF Program (v3.01) range from 4.3 L/kg wet-wt ( $Cl_3SiH$ ) to 8.8 L/kg wet-wt ( $ClMe_2SiH$ ), indicating the monomeric chlorosilanes are not expected to bioaccumulate. For the hydrolysis products, the estimated BCFs were all 3.2 L/kg wet-wt.

Acute aquatic toxicity data are not available for the monomeric chlorosilanes. The monomeric chlorosilanes are expected to undergo rapid hydrolysis, which occurs during testing; exposure to parent chlorosilane is likely to be transient and observed toxicity is likely due to its hydrolysis products, HCl and the respective silanol hydrolysis products. [The silanol hydrolysis product of  $ClMe_2SiH$  is structurally similar to both TMS and DMSD. The silanol hydrolysis product of  $Cl_2MeSiH$  is structurally similar to DMSD. The silanol hydrolysis product of  $Cl_3SiH$  is the same as the hydrolysis product of trimethoxysilane. The silanol hydrolysis product of  $Cl_4Si$  is the same as the hydrolysis product of TEOS.]

Test substance	Species	Result (mg/L)	Guideline; Test type
Fish, acute toxicity	7		
Supporting hydrol	ysis product for ClMe <sub>2</sub>	SiH	
TMS	Oncorhynchus	96-hr $LC_{50} = 271$	OECD TG 203; semi-static
1066-40-6	mykiss	(measured)	
Supporting hydrol	ysis product for ClMe <sub>2</sub>	SiH, Cl <sub>2</sub> MeSiH	
DMSD	Oncorhynchus	96-hr $LC_{50} > 126$	OECD TG 203; static
1066-42-8	mykiss	(measured)	
Supporting substa	nce for Cl <sub>3</sub> SiH		
Trimethoxysilan	Oncorhynchus	96-hr $LC_{50} > 100$	OECD TG 203; static
e	mykiss	(nomimal)	
2487-90-3			
Supporting substa	nce for Cl₄Si		
TEOS	Danio rerio	96-hr LC <sub>50</sub> > 245	Directive 92/69/EEC, C.1;
78-10-4		(measured) semi-static	
Hydrolysis produc	t for all category memb	oers	
HCl	Cyprinus carpio	96-hr $LC_{50} = pH$	OECD TG 203
7647-01-0		4.3 (4.92 mg/L)	
Aquatic invertebra	ates, acute toxicity		
Supporting hydrol	ysis product for ClMe <sub>2</sub>	SiH	
TMS	Daphnia magna	48-hr $EC_{50} = 124$	OECD TG 202; semi-static
1066-40-6		(measured)	
Supporting hydrol	ysis product for ClMe <sub>2</sub>	SiH, Cl <sub>2</sub> MeSiH	

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DMSD	Daphnia magna	48-hr EC <sub>50</sub> > 117	OECD TG 202; static
1066-42-8	1 0	(measured)	
Supporting substan	nce for Cl <sub>3</sub> SiH	, , , , , , , , , , , , , , , , , , ,	
Trimethoxysilan	Daphnia magna	48-hr $EC_{50} > 100$	OECD TG 202; static
e	1 U	(nominal)	
2487-90-3		<b>`</b>	
Supporting substan	nce for Cl <sub>4</sub> Si		
TEOS	Daphnia magna	48-hr $EC_{50} > 75$	OECD TG 202; flow-through
78-10-4		(measured)	-
Hydrolysis product	t for all category memb	ers	
HCl	Daphnia magna	48-hr $EC_{50} = pH$	OECD TG 202
7647-01-0		5.3 (0.492 mg/L)	
Aquatic plants toxi	icity		
Supporting hydrol	ysis product for ClMe <sub>2</sub> S	SiH	
TMS	Pseudokirchnerie	72-hr $EC_{50} > 750$	OECD TG 201
1066-40-6	lla subcapitata	(measured)	
Supporting hydrol	ysis product for ClMe <sub>2</sub> S	SiH, Cl₂MeSiH	
DMSD	Pseudokirchnerie	72-hr E <sub>r</sub> C <sub>50</sub> and	OECD TG 201
1066-42-8	lla subcapitata	$E_b C_{50} > 118$	
		(measured)	
Supporting substan	nce for Cl <sub>3</sub> SiH		
Trimethoxysilan	Pseudokirchnerie	72-hr $E_rC_{50}$ and	OECD TG 201
e	lla subcapitata	$E_b C_{50} > 100$	
2487-90-3			
Supporting substan	nce for Cl <sub>4</sub> Si		
TEOS	Pseudokirchnerie	72-hr E <sub>r</sub> C <sub>50</sub> and	OECD TG 201
78-10-4	lla subcapitata	$E_b C_{50} > 100$	
	Î.	(nominal)	
	Scenedesmus	$E_bC_{50} = 889.2;$	Directive 87/302/EEC, part C,
	subspicatus	$E_bC_{50} > 1039.3$	p. 89
Hydrolysis product	t for all category membe		
HCl	Selenastrum	$72-hr E_r C_{50} = pH$	OECD TG 201; static
7647-01-0	capricornutum	5.3 (0.492 mg/L)	

The hazard of hydrochloric acid for the environment is caused by the proton (pH) effect. For this reason the effect of hydrogen chloride on the organisms depends on the buffer capacity of the aquatic ecosystem. Also the variation in acute toxicity for aquatic organisms can be explained to a significant extent by the variation in buffer capacity of the test medium. For example,  $LC_{50}$  values of acute fish toxicity tests varied from 4.92 to 282 mg/L. The toxicity values to *Selenastrum capricornutum* 72h-EC<sub>50</sub> is 0.780 mg/L at pH 5.1 for biomass, 0.492 mg/L at pH 5.3 for growth rate, and the 72h-NOEC is 0.097 mg/L at pH 6.0 for biomass and growth rate. The 48h-EC50 for *Daphnia magna* is 0.492 mg/L at pH 5.3 based on immobilization.

Based on the properties of the hydrolysis product, HCl, the monomeric chlorosilanes possess properties indicating a hazard for the environment (acute toxicity to fish between 1 and 100 mg/L, acute toxicity to aquatic invertebrates and toxicity to algae < 1 mg/L). Toxic effects are expected primarily from the hydrolysis products (in particular hydrogen chloride, and depend on the buffering capacity of a particular aquatic environment. Therefore, the stated effect levels pertain to unbuffered systems and can be viewed as conservative). The monomeric chlorosilanes and their hydrolysis products are not expected to be readily biodegradable or to bioaccumulate. Adequate screening-level data are available to characterize the hazard for the environment for the purposes of the OECD HPV Programme.

#### Exposure

The estimated annual production volumes for the category members are:

Substance	Estimated United States 2010 Production (metric tonnes)	Estimated European 2010 production (metric tonnes)	Estimated Japanese 2010 production (metric tonnes)	
ClMe <sub>2</sub> SiH	2268 - 68,039	2268 - 68,039	113 (purchased)	
Cl <sub>2</sub> MeSiH	5359 - 362,874	5359 - 362,874	454 - 4536	
Cl <sub>3</sub> SiH	45,359 - 362,874	11,340 – 113,398 (a)	22,680 - 204,117	
Cl <sub>4</sub> Si	45,359 - 362,874	11340 - 90719 (b)	0	

(a) Note: 88% of the reported volume produced in Europe is from 2008 data. The remaining 12% is from 2010 data.)

(b) Note: 64% of the reported volume produced in Europe is from 2008 data. The remaining 36% is from 2010 data.

100% of the monomeric chlorosilanes, by volume, are used as intermediates in the manufacture of commercial organosiloxanes. The monomeric chlorosilanes are reacted during use and lose their chemical identities.

The monomeric chlorosilanes are expected to be primarily produced and processed in closed systems. Due to the dynamic and exothermic nature of the processes incorporating chlorosilanes, many engineering controls are recommended to prevent occupational exposure such as local and general ventilation; ventilation system tied into scrubbers with nitrogen padding; ambient temperature; closed loop unloading; dry break connections; specific worker training; use of air emission abatement equipment such as incinerators, scrubbers and fabric filters is applicable as a best practice; treatment of effluent in waste water treatment plant. Production facility employees involved in chlorosilane production and application are required by the manufacturing facility to use personal protective equipment (PPE) such as respirators with organic vapor cartridges, full-face respirator with ABEK-filter; face shield and self-contained, positive pressure breathing apparatus (for prolonged or high exposure), slicker suit, rubber boots, Viton gloves/gauntlets (5-layer laminate of PE and EVOH (4H) or Butyl and Viton types recommended; nitrile gloves may also be used for short durations). For any situation (e.g. equipment maintenance and repair) where potential exposure to chlorosilanes is expected, the use of acid resistant protective equipment, respiratory equipment and face shield is recommended by the manufacturing facility because of their irritating or corrosive properties. Environmental exposure is expected to be low.

There are no consumer uses of the monomeric chlorosilanes.

ANNEX Summary of Mammalian Toxicity Data Read Across Approach

Substance	Acute Toxicity (oral) (mg/kg)	Acute Toxicity (inhalation) (LC <sub>50</sub> = mg/L)	Repeated Dose (oral) (mg/kg)	Repeated Dose (inhalation)	Gene Mutation in vitro	Chromosome Aberration in vitro	Effects on Fertility and Reproductive Organs (oral = mg/kg bw/day) (inhalation = mg/L)	Developmental Toxicity (oral = mg/kg bw/day) (inhalation = mg/L)
ClMe <sub>2</sub> SiH	238 (RA)	17.3 (60 min; nominal)	NOAEL (systemic) = 250 (RA)	NOAEC = 0.03 (RA)	Negative	Negative (RA)	NOAEC (inh) = 0.073 (RA)	NOAEC (inh) = 2.2 (RA)
Supporting S	ubstances			•				
Trimethyls ilanol (TMS)	No used for read across	Not used for read across	NOAEL (systemic) = 250	NOAEC = ca. 2.2 (hct)	Not used for read across	Not used for read across	NOAEC (inh) = 2.2 (hct)	NOAEC (inh)= 2.2 (hct)
Cl <sub>2</sub> DMS	Not used for read across	Not used for read across	Not used for read across	Not used for read across	Not used for read across	Negative	Not used for read across	Not used for read across
Cl₂MeSiH	< 278 (undilute d)	8.4 (60 min; nominal)	NOAEL (systemic) = 250 (RA)	NOAEC = 0.03 (RA)	Negative (RA)	Negative (RA)	NOAEC (inh) = 0.073 (RA) NOAEL (oral) = 500 (RA)	NOAEL (oral) = 500 (RA)
Supporting S	ubstances							
DMSD	Not used for read across	Not used for read across	NOAEL (systemic) = 250	Not used for read across	Not used for read across	Not used for read across	NOAEL (oral) = 500	NOAEL (oral) = 500
MTMS	Not used for read across	Not used for read across	Not used for read across	NOAEC = ca. 0.56 LOAEC = ca. 2.2	Not used for read across	Not used for read across	NOAEL (oral) = 1000	NOAEL (oral) = 1000
Cl <sub>2</sub> DMS	Not used for read across	Not used for read across	Not used for read across	Not used for read across	Not used for read across	Negative	Not used for read across	Not used for read across
Cl <sub>3</sub> SiH	1030 (10% dilution/ male)	15.0 (60 min; measured)	NOAEL (systemic) = 50(RA)	NOAEC = ca. 0.0025 (RA)	Negative	Negative (RA)	NOAEC (inh) = 0.073 (RA) NOAEL (oral) = 1000 (RA)	NOAEL (oral) = 1000 (RA)
Supporting S					•		· · ·	
Trimethox ysilane	Not used for read across	Not used for read across	No data	NOAEC = ca. 0.0025	Not used for read across	Not used for read across	Not used for read across	Not used for read across
MTMS	Not used for read across	Not used for read across	NOAEL (systemic) = 50	NOAEC = ca. 0.56 LOAEC = ca. 2.2	Not used for read across	Not used for read across	NOAEL (oral) = 1000	NOAEL (oral) = 1000
Cl <sub>4</sub> Si	238 (diluted)	9.1 (60 min; nominal)	NOAEL (systemic) = 10 (males); 50 (females) (RA)	NOAEC = 0.030 (RA)	Negative	Negative	NOAEC (inh) = 0.073 (RA) NOAEL (oral) = 100 (RA)	NOAEL (oral) = 100 (RA)
Supporting S	Substances					1		
TEOS	Not used for read across	Not used for read across	NOAEL = 10 (males) = 50 (females)	Not used for read across	Not used for read across	Not used for read across	NOAEL (oral) = 100	NOAEL (oral) = 100
Supporting substance for all category members								
HCI	238-277 mg/kg (female)	4.2-4.7 (60 min)	No data	NOAEC = 0.030	Negative	Positive (pH effect)	NOAEC (inh) = 0.073	Not used for read across

RA = Read Across; hct = highest concentration tested