FOREWORD INTRODUCTION

ETHYLTRIACETOXYSILANE

CAS N°: 17689-77-9

SIDS Initial Assessment Report

For

SIAM 21

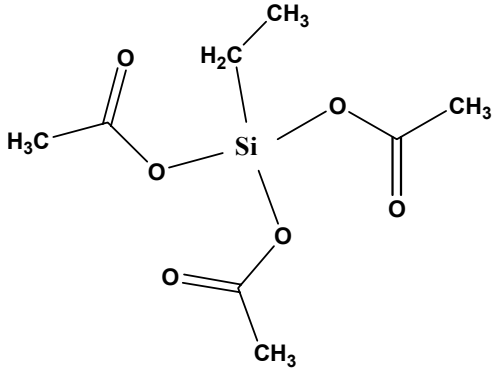
Washington, DC, 18-21 October 2005

1. Chemical Name:	Ethyltriacetoxysilane
2. CAS Number:	17689-77-9
3. Sponsor Country:	United States
	Oscar Hernandez Director, Risk Assessment Division (7403M) U.S. Environmental Protection Agency 1200 Pennsylvania Ave, N.W. Washington, DC 20460 Phone: 202-564-7641
4. Shared Partnership with:	Silicones Environmental Health and Safety Council (SEHSC): Clariant LSM (Florida), Inc. Degussa Corporation Dow Corning Corporation GE Silicones Rhodia Inc. Shin-Etsu Silicones of America Wacker Silicones, A Division of Wacker Chemical Corporation
5. Roles/Responsibilities of the Partners:	
• Name of industry sponsor /consortium	Silicones Environmental Health and Safety Council Contact point: Tracy Hill SEHSC 703-904-4322 thill@sehsc.com
• Process used	The SEHSC produced the documents; EPA reviewed the documents and provided additional information where there were data gaps.
6. Sponsorship History	
• How was the chemical or category brought into the SIDS Program?	Documents were prepared and reviewed by industry prior to submission to sponsor country. Sponsor country conducted reviews of submitted data and offered comments to industry. Industry prepared and resubmitted documents for consideration at SIAM 21. no testing (X)

testing ( )

7. Review Process Prior to the SIAM:	The U.S. EPA reviewed this case.
8. Quality check process:	Literature searches were conducted by sponsor country to determine if all relevant data have been included in this submission.
9. Date of Submission:	December 2004
10. Comments:	1. Acetic acid is currently sponsored by the Czech Republic. 2. Acetic acid and its salts were sponsored by the American Chemistry Council Acetic Acid and Salts Panel under the USEPA HPV Challenge Program. 3. Data from the structural analogue, vinyltriacetoxysilane, is considered to be representative of acetic acid, due to the rapid hydrolysis rate of this material.

SIDS INITIAL ASSESSMENT PROFILE

CAS No.	17689-77-9
Chemical Name	Ethyltriacetoxysilane
Structural Formula	

SUMMARY CONCLUSIONS OF THE SIAR

Analogue Justification

Ethyltriacetoxysilane undergoes rapid hydrolysis in moist/aqueous environments (t1/2 is less than 13 seconds) to acetic acid and the corresponding trisilanol, thus observed toxicity is likely due primarily to acetic acid. Abiotic hydrolysis products of the test substance undergo continuous condensation reactions to produce higher molecular weight cyclic and linear siloxanes (the number-average and weight-average molecular weights were 633 and 809 with 22 area % of the chromatogram higher than 1000 molecular weight at the1-hr reaction time; at the 4-hr reaction time, the number-average and weight-average molecular weights increased to 750 and 1085 with 38 area % of the chromatogram higher than 1000 molecular weight, respectively). The alkyl silanols condense to siloxane oligomers; this condensation of silanols is affected by both concentration and pH, and since both change over time it is not feasible to isolate specific silanols for analysis. While the hydrolysis of ethyltriacetoxysilane is rapid, the polymerization products, while not volatile, are in a molecular weight range small enough to be considered, at least in part, biologically available. The structural analogue methyltriacetoxysilane (CAS number 4253-34-3) has been used for in vitro bacterial gene mutation and chromosomal aberrations endpoints. The hydrolysis product, acetic acid (CAS number 64-19-7) and its salts [calcium acetate (CAS number 62-54-4), potassium acetate (CAS number 127-08-2) and sodium acetate (CAS number 127-09-3)]), have been used to assess the acute aquatic toxicity (fish, aquatic invertebrate and algae), repeated dose toxicity, fertility and developmental toxicity endpoints. Acetic acid and its salts are grouped together because of their close structural relationships and the salts are the neutralized form of the acid that can be more easily administered, their natural occurrence in plants and animals, and their fundamental role in cell metabolism, particularly in the tricarboxylic acid cycle (also known as the citric acid or Kreb's cycle), which is where humans get their energy. In addition the structural analogue vinyltriacetoxysilane (CAS number 4130-08-9) has been used to support the acute aquatic toxicity endpoints. Data from both ethyltriacetoxysilane and vinyltriacetoxysilane are representative of acetic acid, based on the rapid hydrolysis of these materials.

Human Health

The acute toxicity of ethyltriacetoxysilane is described by an LD50 rat (oral) = 1462 mg/kg. Clinical signs included decreased activity; lethargy; lacrimation; salivation; irregular gait; hunched posture; decreased body weight, food consumption and fecal volume; red urine; red staining of the snout, eyes and extremities; and labored respiration. Although acute toxicity data for the inhalation or dermal routes of exposure are not available for ethyltriacetoxysilane, these exposures will likely result in local site of contact effects from acetic acid. Ethyltriacetoxysilane is severely irritating and corrosive to the skin, is expected to be severely irritating to the eyes of animals, and is likely to be a respiratory irritant based on production of acetic acid following hydrolysis.

In a 7-day oral range-finding study (gavage) rats were treated with undiluted ethyltriacetoxysilane (dose levels of

0, 17 (males), 23 (females), 100, 500 and 1000 mg/kg/d). Ethyltriacetoxysilane rapidly hydrolyzes (in seconds) to acetic acid and a trisilanol (3:1). The silanol generated is insignificant in both quantity and toxicity relative to the production of acetic acid and its associated toxicity. Animals from the 17 (males), 23 (females) and 100 mg/kg/day dose groups survived to day 7. Animals from the 500 and 1000 mg/kg/day dose groups were sacrificed after the third dose as a consequence of two deaths (one from each group), marked body weight loss, and severity of lesions (ulceration and erosion of stomach and esophagus) observed in necropsied animals. The stomach lesions observed resembled irritation from acetic acid production. This 7-day range-finder study indicated that a maximum dose level of less than 20 mg/kg/day would be required for a longer duration repeated dose study in order to avoid death or obvious suffering due to the corrosivity of the hydrolysis product, acetic acid. Based on the findings of the 7-day range-finder, a longer duration study will present technical difficulty questioning dosing accuracy and a very low nominal systemic dose. Additional testing (repeated dose, reproductive effects or developmental toxicity) with ethyltriacetoxysilane has not been conducted. Toxicity is represented by an irritative mechanism following single or repeated dosing, likely due to production of acetic acid during hydrolysis. NOAELs following repeated exposure to acetic acid and its salts range from 210 mg/kg bw/day (2-4 month acetic acid drinking water study; systemic toxicity) to 3600 mg/kg bw/day (acetic acid, sodium salt, 4 week dietary study; no effects reported). Signs of irritation/corrosion at the site of contact as well as systemic toxicity have been reported. Prolonged inhalation exposure to acetic acid results in muscle imbalance, increase in blood cholinesterase activity, decreases in albumins and decreased growth at concentrations greater than 0.01 mg/m^3/day.

Groups of 20 mice/sex were given 0.025% sodium acetate in the drinking water (about 60 mg/kg bw/day) for 1 week before breeding, during a 9-day breeding period and (females only) throughout pregnancy, lactation and until the offspring were weaned at 3 weeks of age. The male offspring were given the same solution until they were 5-7 weeks old and were then examined in a 24-hour activity test. No effects on fertility were observed. Examination of the litters revealed no overt deformities, and pup weights were normal at day 1 and day 21. The activity of offspring of the treated group was lower than that of controls during the first 12 hours but was similar during the second 12 hours. It is unknown if the decreased activity observed in the sodium acetate treated group to was a result of exposure in utero and/or post-weaning, since the pups were exposed during both time periods. Acetic acid had no effects on implantation or on maternal or fetal survival in rats, mice or rabbits dosed via gavage on days 6-19 to doses up to 1600 mg/kg/day. The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring in the controls. Sodium acetate had no effect on parents or offspring when mice were administered 1000 mg/kg bw, by gavage on days 8-12 of gestation.

In vitro, ethyltriacetoxysilane and methyltriacetoxysilane were negative in bacterial mutagenicity assays Methyltriacetoxysilane did not induce chromosomal aberrations in CHO cells.

Environment

The melting point of ethyltriacetoxysilane is 8.4°C and the boiling point is 227 °C at 1013 hPa. The vapor pressure is 0.05 hPa at 20 deg C. The estimated water solubility of ethyltriacetoxysilane is 42 g/L; the estimated log Kow is 0.74. The water solubility and log Kow values may not be reliable because the chemical is hydrolytically unstable. The overall reaction half-life in air is estimated to be less than 3 minutes because of rapid hydrolysis of the material with moisture in the atmosphere. Photodegradation as a mode of removal is therefore unlikely because ethyltriacetoxysilane is hydrolytically unstable in this medium. In addition, photodegradation of the parent silane is not expected to be a significant degradation process in the aquatic environment due to the rapid rate of hydrolysis. Although, the vapor pressure indicates that ethyltriacetoxysilane resides in the atmosphere and may undergo photodegradation due to ozone and/or hydroxyl radicals, due to extremely rapid hydrolysis, the substance is not expected to reside in the air compartment and the vapor pressure of the substance may not be relevant.
Ethyltriacetoxysilane is hydrolytically unstable ($t_{1/2}$ < 13 seconds) over a range of environmentally relevant pH and temperature conditions. At pH 7, the half-life is = <13 seconds. Rapid hydrolysis of this material produces acetic acid and trisilanols.
Level III Fugacity modeling, using loading rates for Air, Soil, and Water of 1000 kg/h for each medium, shows the following percent distribution: Air = 47.3%; Soil = 47.4%; Water = 5.3%; Sediment = 0.0. However, ethyltriacetoxysilane is unlikely to be found in the environment, as this material is hydrolytically unstable. Ethyltriacetoxysilane is readily biodegradable; however this material rapidly hydrolyzes and generates 3 moles of acetic acid for every mole of parent material. Thus, the biodegradation observed is likely reflective of the hydrolysis product, acetic acid. The biodegradation rate for acetic acid after 14 days under aerobic conditions is 74%. Bioaccumulation is not anticipated since this material is hydrolytically unstable.

Ethyltriacetoxysilane undergoes rapid hydrolysis in aquatic media, and thus the exposures to

ethyltriacetoxysilane are likely to be transient. Limited data are available for ethyltriacetoxysilane, therefore, data from a structural analog, vinyltriacetoxysilane, as well as the primary hydrolysis product, acetic acid are used to address the acute aquatic toxicity endpoints. The 96-hour LC50 of ethyltriacetoxysilane for *Brachydanio rerio* is 251 mg/L (the test media was not neutralized). Studies have been conducted on a structural analog, vinyltriacetoxysilane, as well as the primary hydrolysis product, acetic acid. The 96-hour LC50 of vinyltriacetoxysilane for *Oncorhyncus mykiss* is 51 mg/L and for *Lepomis macrochirus* is 68 mg/L (in both cases the test media was not neutralized).. The 72 hour LC50s for acetic acid are 75, 79-88 (pH $\leq$5.9) and 251 mg/L (several species of fish). The 48 hour EC50 for ethyltriacetoxysilane is 62 mg/L for *Daphnia magna*. The 48 hour EC50 of vinyltriacetoxysilane is 100 mg/L for *Daphnia magna* (the test media was not neutralized. Under static conditions, the 48 hour EC50 for acetic acid is 65 mg/L for aquatic invertebrates (the test media was not neutralized). When the test solutions are neutralized, the static EC50 for acetic acid is 6000 mg/L. In renewal systems with aquatic invertebrates, 48 hour EC50s for acetic acid are 100 mg/L and 180 mg/L Ethyltriacetoxysilane toxicity to *Scenedesmus subspicatus* provided a 72 hour EC50 of 73 and 76 mg/L for biomass and growth rate, respectively (the test media was not neutralized). When results are expressed on the basis of the amount of acetic acid generated from the hydrolysis reaction, the toxicity of the parent material is comparable to the reported toxicity of acetic acid (EC_{50} = 50-450 mg/L, depending on test species). Studies have been performed with a silanol monomer, trimethylsilanol (CAS No. 1066-40-6). Although this silanol is not expected to be produced following hydrolysis of methyltriacetoxysilane. A semistatic 96h study with trimethylsilanol and rainbow trout (*Oncorhynchus mykiss*) resulted in a No Observed Effect Concentration (NOEC) of 128 mg/L and an LC_{50} of 271 mg/L.

Exposure

The commercial use of this material is almost exclusively as a cross linker for silicone sealants and adhesives. The final formulated sealant and adhesive is sold in consumer, industrial and construction markets. In production, this material is mostly handled in closed systems. Necessary engineering controls during production include proper ventilation, containment, safety equipment and actual hardware designed to minimize exposure, through splashing, or exposure to the air. Transfer of this material is in closed pipe, drums, or tanks rather than in open systems to minimize loss of this material (through hydrolysis). Ethyltriacetoxysilane is transported from the production site as the parent silane to sealant formulators. The parent silane partially reacts during sealant formulation and then completely reacts during curing of the sealant into the polymer matrix and is no longer available for consumer or worker exposure. Ethyltriacetoxysilane does not volatilize during cure of sealants. Instead this material hydrolyzes and condenses, releasing acetic acid. Therefore, there is no human exposure to ethyltriacetoxysilane from use in silicones sealants. Generally, ethyltriacetoxysilane is used as a cross linker at 3% to 5%. As ethyltriacetoxysilane is compounded into a consumer or industrial sealant or adhesive, it reacts with the silicone. After curing the parent silane becomes crosslinked into the silicone rubber matrix and no longer exists, this greatly reduces the potential for consumer or worker exposure. Any toxicological effects of the silane are greatly reduced as a result of this crosslinking process. The production volume of ethyltriacetoxysilane in the sponsor country was 891 tonnes in 2001.

The reactive nature of this material destroys the parent material in any moisture-containing environment, thus limiting environmental exposure to the parent silane. In a spill situation, the parent material is hydrolyzed; the rapid hydrolysis means that the parent silane is unlikely to be found in the environment. If ethyltriacetoxysilane monomer is slowly released into the environment such that resulting concentrations of the parent compound are low, it is less likely that polymerization will occur and more likely that free triol or short-chain oligomers will result. The spectrum of by-products will depend upon the initial concentration of the parent compound.

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

Human Health: The chemical possesses properties indicating a hazard for human health (severe irritation and corrosivity caused by acetic acid). Due to the extremely rapid hydrolysis to acetic acid and the corresponding trisilanol and based on exposure data presented by the Sponsor country, the parent material will not be available for exposure, and therefore this chemical is currently of low priority for further work. The identified hazards should nevertheless be noted by chemical safety professionals and users.

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 currently of low priority for further work for the environment because of its rapid hydrolysis and its limited potential for bioaccumulation.

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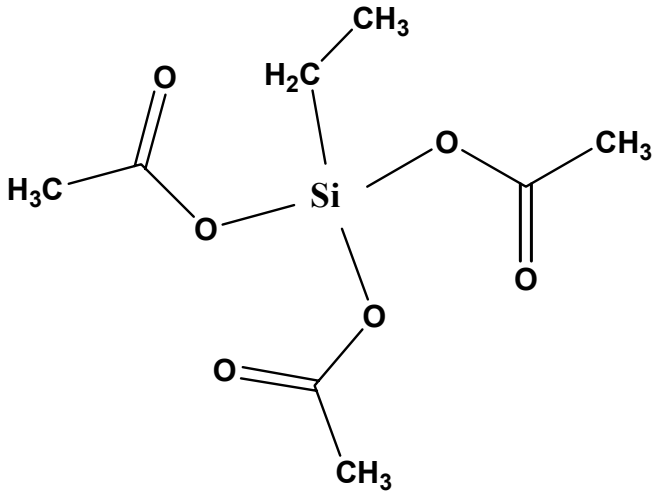
1 IDENTITY

1.1 Identification of the Substance

CAS Number: 17689-77-9
IUPAC Name: Ethyltriacetoxysilane
Molecular Formula: C8H14O6Si
Structural Formula:



Molecular Weight: 234.28
Synonyms: Ethylsilanetriol, triacetate
Ethyltriacetoxysilane
Silanetriol, ethyl-, triacetate
Triacetoxyethylsilane
Tris(acetyloxy)ethylsilane

1.2 Purity/Impurities/Additives

Purity: >95-100%
Impurities: Acetic acid (CAS number 64-19-7) <5%

1.3 Physico-Chemical properties

Table 1 Summary of physico-chemical properties

Property	Value	Comment
Physical state	Liquid	
Melting point	8.4°C	Principe (2000) Other reported values: 5 °C, Dow Corning (1964).
Boiling point	227 °C at 1013 hPa	Smith, A.L. (1988) Other reported values: 201 at 1013 hPa (Hobbs, 1971), 220 °C at 1013 hPa (General Electric, 2000)
Relative density	1.1437 at 20 °C	Smith (1988)
Vapour pressure	.05 hPa at 20 °C	Smith (1988) Other reported values: .025 hPa at 20 °C, Dow Corning (2001) Additional vapor pressures at higher temperatures are provided in the dossier.
Water solubility	41.6 g/L at 25°C	USEPA (2000) Estimated. This value may not be applicable because the material is hydrolytically unstable
Partition coefficient n-octanol/water (log value)	0.74	USEPA (2000) Estimated. This value may not be applicable because the material is hydrolytically unstable Additional value: -1.87 (methylsilanetriol) USEPA(2000)
Henry's law constant	Not available	

1.4 Analogue Justification

Ethyltriacetoxysilane undergoes rapid hydrolysis (t1/2 is less than 13 seconds). The primary hydrolysis products are known to be acetic acid and the corresponding trisilanols. The structural analogue, methyltriacetoxysilane (CAS number 4253-34-3) has been used for in vitro bacterial gene mutation and chromosomal aberrations endpoints. The hydrolysis product, acetic acid (CAS number 64-19-7) and its salts [calcium acetate (CAS number 62-54-4), potassium acetate (CAS number 127-08-2) and sodium acetate (CAS number 127-09-3) salts]), have also been used to assess the acute aquatic toxicity (fish, aquatic invertebrate and algae), the repeated dose toxicity, and fertility and developmental toxicity endpoints. Acetic acid and its salts are grouped together because of their close structural relationships and the salts are the neutralized form of the acid that can be more easily administered, their natural occurrence in plants and animals, and their fundamental role in cell metabolism, particularly in the tricarboxylic acid cycle (also known as the citric acid or Kreb's cycle), which is where humans get their energy. In addition, the structural analogue, vinyltriacetoxysilane (CAS number 4130-08-9) has been used to support the acute aquatic toxicity endpoints. Data from both ethyltriacetoxysilane and vinylacetoxysilane are representative of acetic acid based on the rapid hydrolysis of these materials.

2 GENERAL INFORMATION ON EXPOSURE

In production, this material is mostly handled in closed systems. Necessary engineering controls during production include proper ventilation, containment, safety equipment and actual hardware designed to minimize exposure, through splashing, or exposure to the air. Transfer of this material is in closed pipe, drums, or tanks rather than in open systems to minimize loss of this material (hydrolysis). Ethyltriacetoxysilane is transported from the production site as the parent silane to sealant formulators. The parent silane partially reacts during sealant formulation and then completely reacts during curing of the sealant into the polymer matrix and is no longer available for consumer or worker exposure. Ethyltriacetoxysilane does not volatilize during cure of sealants. Instead this material hydrolyzes and condenses, releasing acetic acid. Therefore, there is no human exposure to ethyltriacetoxysilane from use in silicones sealants.

Ethyltriacetoxysilane undergoes rapid hydrolysis, which occurs during testing, such that observed toxicity is likely due primarily to the hydrolysis products acetic acid, with some potential exposure to trisilanols, and silanol oligomers. Abiotic hydrolysis studies show that hydrolysis products from the test substance undergo continuous, condensation reactions to produce higher molecular weight cyclic and linear siloxanes (the number-average and weight-average molecular weights were 633 and 809 with 22 area % of the chromatogram higher than 1000 molecular weight at the1-hr reaction time; at the 4-hr reaction time, the number-average and weight-average molecular weights increased to 750 and 1085 with 38 area % of the chromatogram higher than 1000 molecular weight, respectively) (Sun, Y. et al., 2002). The alkyl silanols condense to siloxane oligomers; this condensation of silanols is affected by both concentration and pH, and since both change over time it is not feasible to isolate specific silanols for analysis (the structures continue to evolve until they either reach equilibrium or precipitate out of solution). While the hydrolysis of ethyltriacetoxysilane is rapid, the polymerization products, while not volatile, are in a molecular weight range small enough to be considered, at least in part, biologically available.

2.1 Production Volumes and Use Pattern

In the Sponsor Country, production volume in 2001 was 891 tonnes. Ethyltriacetoxysilane is produced in North America, Europe and Asia.

In order to prevent the rapid hydrolysis and subsequent loss of this material in production, it is mostly handled in closed systems. Necessary engineering controls during production include proper ventilation, containment, safety equipment and actual hardware designed to minimize exposure through splashing, or exposure to the air. Transfer of this material is in closed pipes or closed containers rather than in open systems to minimize loss of this material (hydrolysis) although some customers may transfer the material in open systems. Ethyltriacetoxysilane is transported from the production site as the parent silane to formulators. Generally, ethyltriacetoxysilane is used as a cross linker at 3% to 5%. As ethyltriacetoxysilane is compounded into a consumer or industrial sealant or adhesive, it reacts with the silicone. After curing the parent silane becomes cross-linked into the silicone rubber matrix and no longer exists, this greatly reduces the potential for consumer or worker exposure.

The commercial use of this material is almost exclusively as a cross linker for silicone sealants and adhesives. The final formulated sealants and adhesives are sold in consumer, industrial and construction markets.

During curing of the silicone sealant or adhesive the ethyltriacetoxysilane hydrolyzes as it reacts with silanol polymers and atmospheric moisture to form a cross-linked rubber. Since the acetoxy-functional silane is converted and bound within the substrate by polymer coupling, free silane is not present within the final products.

2.2 Environmental Exposure and Fate

2.2.1 Sources of Environmental Exposure

The reactive nature of this material destroys the parent material in any moisture-containing environment, thus limiting environmental exposure to the silane. Ethyltriacetoxysilane hydrolyzes rapidly (half-life of less than 13 seconds, depending on the aqueous solution temperature, pH and concentration of buffer). Hydrolysis of ethyltriacetoxysilane results in the formation of silanetriols which can then condense to form highly cross-linked, high molecular weight polymers, further reducing the potential for exposure. In the environment, at lower concentrations of the parent compound (and thus lower concentrations of the hydrolysis products), exposure to unpolymerized silanetriols may occur.

2.2.2 Photodegradation

Ethyltriacetoxysilane in air is not expected to undergo direct photolysis, but may undergo indirect photolysis through hydroxyl radical oxidation. The hydroxyl radicals reaction was calculated using EpiWin version 3.10. The overall OH rate constant is 1.32E-12 cm3/molecule-sec with an estimated half-life of 12 days with a hydroxyl radical concentration of 5E-5 molecule/cm3. Photodegradation as a mode of removal is unlikely as ethyltriacetoxysilane is hydrolytically unstable. Ethyltriacetoxysilane is highly reactive and hydrolytically unstable, such that acetic acid and ethylsilanetriol are rapidly generated upon contact with water or water vapor. Consequently, reaction with water vapor is likely the predominant degradation process for ethyltriacetoxysilane in air and the overall reaction half-life in air should include both the oxidation half-life and the hydrolytic half-life. The overall reaction half-life in air is estimated to be less than 3 minutes because of rapid hydrolysis of the material with moisture in the atmosphere. The ethylsilanetriol resulting from hydrolysis in the atmosphere is expected to further react with hydroxyl radicals.

2.2.3 Stability in Water

Ethyltriacetoxysilane is hydrolytically unstable ($t_{1/2}$ < 13 seconds) over a range of environmentally relevant pH and temperature conditions (Sun and Taylor, 2001):

Table 2 Summary of stability in water

	Half life (seconds)		
pH	at 10 deg C	at 24.7 deg C	at 37 deg C
4.0	*	<13	*
7.0	*	<13	*
9.0	*	<11	*

* In all experiments, test substance was completely hydrolyzed by the time the first 1H-NMR spectrum was acquired and remained unchanged thereafter. Initial spectra were acquired after 77-100 seconds and 7-8 spectra were subsequently acquired at 15 seconds intervals. Since the hydrolysis is so rapid, there are no data to determine the rate constants (k1, k2, and k3) for the hydrolysis reactions by regression modeling. Rate constants and half-lives could not be determined quantitatively, although the data are certainly adequate for estimating the upper limit of t1/2.

Rapid hydrolysis of this material produces acetic acid and trisilanols. The Si-C bond will not undergo further hydrolysis. The Si-C bond is hydrolytically stable. Only the acetoxy groups will be hydrolyzed. The transient silanol groups will condense with other silanols to yield:

$Et\text{-}Si(OAc)_3 + 3H_2O \rightarrow Et\text{-}Si(OH)_3 + 3HOAc \rightarrow Et\text{-}Si(OR)_3$

where R = H or $EtSi(OR)_2$

As a result, ethyl siloxane resins are generated.

2.2.4 Transport between Environmental Compartments

The EQC Level III Fugacity model (USEPA, 2000) was used to evaluate the fate, transport and distribution of ethyltriacetoxysilane between environmental matrices. Level III Fugacity modelling, using loading rates for Air, Soil, and Water of 1000 kg/h for each media, shows the following percent distribution: Air = 47.3%; Soil = 47.4%; Water = 5.3%; Sediment = 0.0% (Powell, D.E., 2003). However, ethyltriacetoxysilane is unlikely to be found in the environment, as this material is hydrolytically unstable.

2.2.5 Biodegradation

Available data (Degussa Huls AG, 1995a) indicate that ethyltriacetoxysilane is "readily biodegradable" with degradation being 74% after 21 days. However, ethyltriacetoxysilane rapidly hydrolyzes and generates 3 moles of acetic acid for every mole of parent material. Thus, the biodegradation observed is likely reflective of the hydrolysis product, acetic acid. . Acetic acid (CAS number 64-19-7) is readily degraded (74% after 14 days) under aerobic conditions (National Institute of Technology and Evaluation, 1993). Under anaerobic conditions, acetic acid is degraded 99% after 7 days under anaerobic conditions (Kameya T. et al., 1995; http://www.epa.gov/chemrtk/acetisalt/c13102rr.pdf).

Table 3 Summary of the biodegradation of ethyltriacetoxysilane and acetic acid

Ethyltriacetoxysilane	Reliability	Acetic Acid	Reliability
74 % after 21 days (Degussa-Huls, 1995a)	(1) valid without restriction	74% after 14 days (National Institute of Technology and Evaluation, 1993)	(2) valid with restrictions
		99% biodegradation in 7 days (Kameya et al., 1995)	(2) valid with restrictions

2.2.6 Bioaccumulation

Bioaccumulation is not anticipated since this material is hydrolytically unstable. Rapid hydrolysis of this material produces acetic acid and trisilanols. The Si-C bond will not undergo further hydrolysis. That bond is hydrolytically stable. Only the acetoxy groups will be hydrolyzed. The transient silanol groups will condense with other silanols to yield:

$Et\text{-}Si(OR)_3$ type resins where R=H or $-Si(Et)(OR)_2$

As a result silanol-functional resins are generated.

If the silane is slowly released such that the concentration of the resulting silanetriol is not high enough to result in polymerization, the trisilanol will exist largely as a monomer. The monomer is known to be water soluble by virtue of the three hydroxy groups on the silicon. It is expected that this silanetriol will have a low Kow (predicted value is -1.87) because of these hydroxy groups and so is not expected to bioaccumulate. The water solubility of the silanetriol cannot be measured because of the tendency to condense at concentrations greater than 500 ppm. It is known however

that the silanetriol and small condensation products will only precipitate out of water due to formation of larger, water insoluble polymeric resins.

2.3 Human Exposure

Ethyltriacetoxysilane is used as a crosslinker in silicone sealants, converting it from a paste consistency to a rubber. It is compounded into the sealant during manufacture and immediately reacts with the silanol groups of the silicone polymer, thus there is little or no free acetoxysilane once compounding is completed. When the sealant is applied the remaining acetoxy groups react with moisture in the air to crosslink and release acetic acid (by product). Touching the curing sealant could expose the person to acetic acid or possibly to acetoxy groups already anchored to the silicone polymer.

2.3.1 Occupational Exposure

In order to prevent the rapid hydrolysis and subsequent loss of this material, in production, it is mostly handled in closed systems. Necessary engineering controls during production include proper ventilation, containment, safety equipment and actual hardware designed to minimize exposure, through splashing, or exposure to the air. Transfer of this material is in closed pipes or containers rather than in open systems to minimize loss of this material (hydrolysis) although some customers may transfer the material using open systems. The material is shipped via air, road, and marine in returnable intermediate bulk containers (IBCs), drums, (plastic and steel) pails, cans, and non-returnable IBCs.

A worker may be exposed during compounding of sealant or adhesive to low levels (generally <5%) of the silane. Potential routes of exposure for workers include dermal contact, although the MSDS properly warns against contact with the skin. There is no known production process that involves aerosolized material or sprayed material. The vapour pressure of this material is low enough that vapour inhalation is not considered a potential route of exposure.

During professional or consumer use the packaging recommends wearing gloves to prevent dermal contact. It is unlikely that there is any exposure to the acetoxysilane itself (it is already covalently bonded to the silanol polymer and continuing to react into the matrix) as demonstrated by analysis of the headspace above the curing sealant, no acetoxysilane was detected (100 ppb detection limit). While dermal contact is discouraged (for uncured sealant), contact would expose the person principally to silicone polymer and acetic acid (from the hydrolyzing acetoxysilane attached to the silicone polymer).

2.3.2 Consumer Exposure

The use of ethyltriacetoxysilane into the consumer market is limited to use as a cross linker in sealants and adhesives. The substance is used at generally <5% in these formulations and reacts with silanol polymers in the formulation during compounding and then further reacts during exposure to atmospheric moisture. After curing the parent silane is consumed into the polymer matrix and no longer exists, greatly reducing the potential for consumer exposure. The curing time is generally less than 24 hours at room temperature and ambient humidity. In addition, a series of experiments was conducted to evaluate the potential for any exposure to ethyltriacetoxysilane during the curing reaction of RTV compositions (SEHSC, 2001). These compositions develop a cured skin within about 10-30 minutes and are fully cured within 8-16 hours, depending on relative humidity. A mass of two different commercially available RTV compositions was exposed to both humid and dry air under controlled conditions. The atmosphere over the curing RTV compositions was sampled and analyzed for ethyltriacetoxysilane by Gas Chromatography – Mass Spectroscopy

(GC-MS). No ethyltriacetoxysilane or silanetriols were detected in the atmosphere down to 100 ppb, rather the expected cure by-product acetic acid and other volatiles were found. Thus the consumer is not exposed to the acetoxysilane.

3 HUMAN HEALTH HAZARDS

Analogue Justification

Ethyltriacetoxysilane undergoes rapid hydrolysis, which occurs during testing, such that observed toxicity is likely due primarily to acetic acid. Endpoints have been addressed using data from methyltriacetoxysilane (chromosome aberration), and a hydrolysis product, acetic acid and its salts to assess the acute toxicity, repeated dose toxicity, and reproductive and developmental toxicity endpoints. Abiotic hydrolysis studies show that hydrolysis products from ethyltriacetoxysilane undergo continuous, condensation reactions to produce higher molecular weight cyclic and linear siloxanes. The polymerization products of ethyltriacetoxysilane are not volatile.

3.1 Effects on Human Health

3.1.1 Toxicokinetics, Metabolism and Distribution

No data available.

3.1.2 Acute Toxicity

This material has been tested for acute toxicity by the oral route of exposure. Acetic acid has also been tested for acute toxicity by the oral, inhalation and dermal routes of exposure.

Oral

The combined LD50 in male and female rats of ethyltriacetoxysilane is 1462 mg/kg (Huntingdon Life Sciences (2000). The clinical signs observed, delayed deaths, weight losses and gross necropsy findings all indicate an irritative mechanism of toxicity. The range of reported LD50s for acetic acid and its potassium, sodium and calcium salts, and sodium diacetate is 3250 to 5600 mg/kg bw (rat) (BIBRA, 1993; USEPA, 1991; Smyth et al., 1951; Smyth et al., 1969; and Woodward et al., 1941) and 4960 mg/kg bw (mouse) (BIBRA, 1993 and Woodward et al., 1941).

Since ethyltriacetoxysilane hydrolysis produce 3 moles of acetic acid for each mole of silanetriol, this would suggest that the estimated LD50 value for ethyltriacetoxysilane should be about one-third of the LD50 of acetic acid, which is 1083 - 1867 mg/kg bw (rat) and 1650 mg/kg bw (mouse) based on the reported LD50 values for acetic acid. This is in good agreement with the reported LD50 of ethyltriacetoxysilane of 1462 mg/kg bw (rat). The similarity of the predicted and measured acute oral LD50 of this material, as well as the noted findings of an irritative mechanism of toxicity supports the hypothesis that the toxicity of ethyltriacetoxysilane is due to the formation of acetic acid.

Inhalation

The 4-hour LC50 in rats of acetic acid is 11.4 mg/L (BASF, A.G., 1989).

Dermal

The dermal LD50 in rats of sodium diacetate is greater than 2000 mg/kg bw (USEPA, 1991).

Table 4 Summary of the acute toxicity of ethyltriacetoxysilane, acetic acid and its salts

Route	Ethyltriacetoxysilane	Reliability	Acetic Acid and its salts	Reliability
Oral	Rat; LD50 =1462 mg/kg (Huntingdon Life Sciences (2000)	(1) valid without restriction	Rat; LD50 = 4280 mg/kg bw (calcium salt) (Smyth et al., 1951; Smyth et al., 1962)	(2) valid with restrictions.
			Rat; LD50 = 3250 mg/kg bw (potassium salt) (Smyth et al., 1962; Smyth et al., 1969)	(2) valid with restrictions.
			Rat; LD50 = 3530 mg/kg bw (sodium salt) (Food and Agriculture Organization of the United Nations)	(2) valid with restrictions.
			Rat; LD50 = 3250 to 5600 mg/kg bw (includes acetic acid, and its potassium, sodium and calcium salts and sodium diacetate) (BIBRA, 1993)	(2) valid with restrictions.
			Rat; LD50 = 5600 mg/kg bw (sodium diacetate) (USEPA, 1991)	(2) valid with restrictions.
			Mouse; LD50 = 4960 mg/kg (acetic acid) bw (Woodward et al., 1941 and BIBRA, 1993)	(2) valid with restrictions.
Inhalation	No data		Rat; 4-hr LC50 = 11.4 mg/L (acetic acid) (BASF, 1989)	(2) valid with restrictions.
			Rat; 1-hr LC50 > 30000 mg/m3 (acetic acid, sodium salt) (BIOFAX Industrial Bio-Test Laboratories, Inc., 1971)	(2) valid with restrictions.
			Rat; 4-hr LC50 > 16000 ppm (acetic acid) (Smyth et al., 1951)	(2) valid with restrictions.
			Mouse; 1-hr LC50 = 5620 ppm (acetic acid) (Ghiringhelli and Difabio, 1957)	(2) valid with restrictions.
			Guinea pig; 1-hr LC50 > 5000 ppm (acetic acid) (Ghiringhelli, and Difabio., 1957)	(2) valid with restrictions.
Dermal	No data		Rat; LD50 > 2000 mg/kg bw (sodium diacetate) (USEPA, 1991)	(2) valid with restrictions.
			Rabbit; LD50 = 1060 mg/kg bw (acetic acid) Union Carbide, 1963; BIBRA, 1993)	(2) valid with restrictions

Studies in Humans

No data available.

3.1.3 Irritation

Skin Irritation

Semi-occlusive application of 0.5 ml of ethyltriacetoxysilane for 3 minutes produced severe lesions observed at 72 hours with slight reversibility at the day 14 reading in 4 of 6 rabbits (Wacker Chemie GmbH, 1989). Ethyltriacetoxysilane was corrosive under the conditions of this study. The Skin2 ZK-1350 model predicted the corrosivity of ethyltriacetoxysilane, although it appeared to slightly underestimate the degree of corrosivity. CORROSITEX model also predicted ethyltriacetoxysilane as corrosive. However, TER assay did not identify ethyltriacetoxysilane as corrosive (Dow Corning Corporation, 1994).

Eye Irritation

Ethyltriacetoxysilane has not been tested for eye irritation. The result of the skin irritation study adequately represents the potential for severe eye irritation. The severe irritancy of ethyltriacetoxysilane was predicted by Skin2 1200 in vitro model (Dow Corning Corporation, 1994).

Respiratory Tract Irritation

No data available.

Conclusion

The acute toxicity of ethyltriacetoxysilane is described by an LD50 rat (oral) = 1462 mg/kg. Clinical signs included decreased activity; lethargy; lacrimation; salivation; irregular gait; hunched posture; decreased body weight, food consumption and fecal volume; red urine; red staining of the snout, eyes and extremities; and labored respiration. Although acute toxicity data for the inhalation or dermal routes of exposure are not available for ethyltriacetoxysilane, these exposures will likely result in local site of contact effects from acetic acid. Ethyltriacetoxysilane is severely irritating and corrosive to the skin, is predicted to be severely irritating to the eye and is likely to be a respiratory irritant based on production of acetic acid following hydrolysis.

3.1.4 Sensitisation

No data available.

3.1.5 Repeated Dose Toxicity

Oral

In a 7-day oral range-finding study (gavage) rats were treated with undiluted ethyltriacetoxysilane (dose levels of 0, 17 (males), 23 (females), 100, 500 and 1000 mg/kg/d) (DCC, 2004). Animals from the 20 and 100 mg/kg/day dose groups survived to day 7. Animals from the 500 and 1000 mg/kg/day dose groups were sacrificed after the third dose as a consequence of two deaths (one from each group), marked body weight loss, and severity of lesions observed in necropsied animals. Necropsy findings included marked ulceration of stomach and esophagus at 100 mg/kg/d and higher. Stomach erosion was present at 20 mg/kg/day. Ethyltriacetoxysilane rapidly (seconds) hydrolyzes to acetic acid and a trisilanol (3:1). The silanol generated is insignificant in both quantity and toxicity relative to the production of acetic acid and its associated toxicity. In the 7-day range-finding study, stomach lesions were observed at low doses of ethyltriacetoxysilane and resembled acetic acid toxicity. This 7-day range-finder study indicated that a maximum dose level of less than 20 mg/kg/day would be required for a longer duration repeated dose study in order to avoid death or obvious suffering due to the corrosivity of the hydrolysis product, acetic acid. The data provided in this range-finder study indicate a practical and humane dose range for subsequent longer term studies is below the limit of technical practicality and toxicological significance.

In a subchronic study, four groups of 3 to 6 rats were given 0.01, 0.1, 0.25, or 0.5 % acetic acid in drinking water (up to 390 mg/kg bw/day) for periods of nine to 15 weeks. Fluid intake was the same in all groups. At 0.5 % there was immediate, progressive reduction in body weight gain, loss of appetite, and up to a 27 % reduction in food consumption. Mortality was unaffected. None of these effects were seen at the lower doses. (Sollmann, 1921; FAO/WHO, 1974; FASEB, 1977; BIBRA, 1993; and Celanese, 2003). The NOAEL (systemic toxicity) was 210 mg/kg bw. Rats were treated by gavage with 3 ml of a 10% acetic acid solution for 90 days (Wysokinska, 1952 and BIBRA, 1993). The treatment decreased the red blood cell count and hemoglobin concentration. The

LOAEL (systemic toxicity) was 750 mg/kg bw. There were no reported effects in an 8 week dietary study in which rats were given 2% sodium diacetate (about 1000 mg/kg bw) (USEPA, 1991). Groups of three to four rats were given 1800 mg/kg bw/day of free acid intragastrically or 4200 - 4800 mg/kg bw of sodium acetate (J.R. Geigy, 1970). Animals survived to 14 days when given 1800 mg/kg bw/d of free acid intragastrically or 4200 - 4800 mg/kg bw of sodium acetate, but animals survived only three to five days on daily intra-gastric doses of 2400 mg/kg bw of free acid. Animals lost weight and showed blistered paws and reddened noses before death at 14 days. The LOAEL (systemic toxicity) was greater than or equal to 4200-4800 mg/kg bw. Four groups of two young pigs each were fed daily diets containing 0, 240, 720, 960, or 1200 mg acetic acid/kg bw per day for successive 30-day periods to a total of 150 days (Lamb and Evvard, 1919 and FAO/WHO, 1977). There were no significant differences in growth rate, weight gain, early morning urinary ammonia, and terminal blood pH between controls and test groups. The NOAEL (no effects reported) was 1200 mg/kg bw. Rats were exposed to acetic acid, sodium salt, at a dose of 21 mg/kg bw/d in feed (Goldman, 1981) for 3 months. There were indications of altered thyroid function and decreased growth was reported. The NOAEL (systemic toxicity) was 21 mg/kg bw. Rats were fed approximately 4.5 g acetic acid/kg bw daily in the diet for 30 or 325 days; stomach damage was observed (Mori, 1995; BiblioLine, 2004). The LOAEL (irritation) was 4500 mg/kg bw. Rats were given either N-nitrosarcosin ethyl ester (NSEE; a known carcinogen) alone, NSEE with the acetic acid solution, or the acetic acid solution alone, by gavage (Alexandrov, et al, 1989; ACC, 2003). Prolonged administration of acetic acid alone did not induce tumors. All rats, however, did experience hyperplasia in the esophagus and forestomach. The LOAEL (irritation) was approximately 60 mg/kg bw. Thirteen male rats were fed ad libitum a 25% protein, vitamin B12-deficient ration containing approximately 3.6 g/kg bw acetic acid, sodium salt, daily, for 4 weeks (Dryden and Hartman, 1971). There were no effects on growth or survival. The NOAEL (no effects reported) was 3600 mg/kg bw. Four groups of 6 male rats were administered a regimen of 50 or 500 ppm sodium acetate (controls) or 50 or 500 ppm lead acetate in distilled water (Cory-Slechta, 1986). The test material was administered ad libitum for eight months. No significant effects on survival, reinforcement behavior, or body weight gain were observed. The rats treated with acetic acid, sodium salt served as the control for a lead exposure study. Therefore, no separate untreated controls are available for comparison. Groups of three or four rats were given 1800 or 2400 mg/kg bw acetic acid for 14 days (Hemmingway and Sparrow, 1942). All animals in the 1800 mg/kg bw group survived. Administration of 2400 mg/kg bw was lethal after 3-5 days. The NOAEL (mortality) was 1800 mg/kg bw.

Inhalation

Male rats were exposed for 95 days to 0.01, 0.2, or 5.0 mg/m3 acetic acid vapor in air. Rats developed progressive muscle imbalance, increases of blood cholinesterase activity and serum globulins, and decreases of serum albumins in the two higher doses. The highest dose group also had raised white blood cell counts and decreases in ascorbic acid levels (Tracor-Jitco, Inc., 1974). The NOAEL (systemic toxicity) was 0.01 mg/m3. Groups of at least 10 rats and 10 mice were exposed to 11-35 ppm of acetic acid (Savina and Anisimov, 1987). Exposure to 11 ppm for 22 days had no effect on activity, behavior, work capacity, growth, blood, or the weights and microscopic appearance of tissues examined. At 15 ppm (for 22 days) or more, the animals showed decreased activity, behavioral changes and reduced work capacity. At 23-31 ppm (17-35 days), there was decreased growth, increased spleen weight, an increase of the level of iron stored in the spleen, signs of kidney damage and increased kidney weights. The NOAEL (systemic toxicity) was 11 ppm.

Table 5 Summary of the repeated dose toxicity of ethyltriacetoxysilane, acetic acid and its salts

Route	Ethyltriacetoxysilane	Reliability	Acetic Acid and its salts	Reliability
Oral	7-day gavage, rat NOAEL = 17 (male); <23 (female) mg/kg bw (Dow Corning Corporation, 2004)	(2) valid with restrictions	2-4 month drinking water, rat NOAEL (systemic) = 210 mg/kg bw (acetic acid) (Sollmann, 1921, FAO/WHO, 1974, FASEB, 1977, BIBRA, 1993, and Celanese, 2003,)	(2) valid with restrictions
			90 day gavage, rat LOAEL(systemic) = 750 mg/kg bw (acetic acid) (Wysokinska, 1952 and BIBRA, 1993)	(2) valid with restrictions
			8 week dietary, rat NOAEL (single dose study) >1000 mg/kg bw (acetic acid) (US EPA, 1991)	(2) valid with restrictions
			14 day gavage, rat LOAEL (systemic) $\geq$ 4200 - 4800 mg/kg bw (acetic acid or sodium salt) (J.R. Geigy, 1970)	(2) valid with restrictions
			150 day dietary, pig NOAEL(no effects reported) = 1200 mg/kg bw (acetic acid) (Lamb, 1919 and FAO/WHO, 1974)	(2) valid with restrictions
			3 month dietary, rat LOAEL (systemic) = 21 mg/kg bw/d (sodium acetate) (Goldman, 1981)	(2) valid with restrictions
			8 month dietary, rat LOAEL(irritation) = 4500 mg/kg bw (acetic acid) (Mori, 1952 and BiblioLine, 2004)	(2) valid with restrictions
			8 month gavage, rat LOAEL (irritation) = ca. 60 mg/kg bw (acetic acid) (Alexandrov, 1989 and ACC, 2003)	(2) valid with restrictions
			4 week dietary, rat NOAEL (no effects reported) = 3600 mg/kg bw (Sodium acetate) (Dryden and Hartman, 1971)	(2) valid with restrictions
			8 month drinking water, rat LOAEL (no effects reported) = 500 ppm (Sodium acetate) (Cory-Slechta, 1986)	(2) valid with restrictions
			14 day gavage, rat LOAEL (no effects reported) = 1800 mg/kg bw (acetic acid) (Hemmingway and Sparrow, 1942 and BIBRA, 1993)	(2) valid with restrictions
Inhalation	No data	-	95 day inhalation, rat NOAEL (systemic) = 0.01 mg/m3 (acetic acid) (Mori, 1995 and BiblioLine, 2004)	(2) valid with restrictions
			22 day inhalation, rat NOAEL (systemic) = 11 ppm (27 mg/m3); LOAEL = 15 ppm (acetic acid) (Savina. and Anisimov, 1987)	(2) valid with restrictions
Dermal	No data	-	No data	

Conclusion

Observations from a 14 day gavage study of ethyltriacetoxysilane to rats at 100, 500 and 1000 mg/kg for 14 days indicate a practical and humane dose range for subsequent longer term studies is below the limit of technical practicality and toxicological significance. NOAELs following repeated exposure to acetic acid, and its salts range from 210 mg/kg bw/d (2-4 month acetic acid drinking water study) to 3600 mg/kg bw (acetic acid, sodium salt, 4 week dietary study). Signs of irritation/corrosion at the site of contact, as well as systemic toxicity, have been reported. Prolonged inhalation exposure to acetic acid shows effects of toxicity at concentrations greater than .1 mg/m3.

Studies in Humans

No data available.

3.1.6 Mutagenicity

In vivo Studies

No data available.

In vitro Studies

Gene Mutations

The test substance, ethyltriacetoxysilane, did not induce any cytotoxicity or mutagenicity in a bacterial mutagenicity test at doses up to 5000 ug/plate, both with and without metabolic activation. Appropriate concurrent negative and positive controls were included, and the expected responses were observed. Therefore, the test substance was not a bacterial mutagen under the conditions of this assay (Dow Corning Corporation, 1984). Methyltriacetoxysilane did not induce any cytotoxicity or mutagenicity in a bacterial mutagenicity test at doses up to 5000 ug/plate, both with and without metabolic activation. Appropriate concurrent negative and positive controls were included, and the expected responses were observed. Therefore, the test substance was not a bacterial mutagen under the conditions of this assay (BioReliance, 2002a).

Chromosome Aberrations

There are no data available that directly assess the genotoxic activity of ethyltriacetoxysilane using mammalian cells. Methyltriacetoxysilane was tested in a chromosome aberration assay (CHO cells) in which the cells were treated for 4 and 20 hours in a non-activation system and for 4 hours in a metabolic activation system. All the cells were harvested at 20 hours after treatment initiation. Appropriate solvent, positive and negative controls were included. In the absence of substantial toxicity at any dose level in any treatment group, 2200 g/ml was selected as the high dose for microscopic analysis in all three-treatment groups. The next two lower doses were also analyzed in all harvests. Methyltriacetoxysilane was negative for the induction of structural and numerical chromosome aberrations in CHO cells (BioReliance, 2002b).

Conclusion

In vitro bacterial mutation assays with ethyltriacetoxysilane and methyltriacetoxysilane and *in vitro* studies in mammalian cells with methyltriacetoxysilane have not revealed any evidence of genotoxic potential for ethyltriacetoxysilane.

3.1.7 Carcinogenicity

No data available.

3.1.8 Toxicity for Reproduction

Effects on Fertility

In a 7-day oral range-finding study, stomach lesions were observed at low doses of ethyltriacetoxysilane and resembled acetic acid toxicity (DCC, 2004). This 7-day range-finder study indicated that a maximum dose level of less than 20 mg/kg/day would be required for a reproduction study in order to avoid death or obvious suffering due to the corrosivity of the hydrolysis product, acetic acid. Due to the low solubility and rapid hydrolysis of ethyltriacetoxysilane, a suitable vehicle cannot be selected, and all studies would utilize neat dosing. Based on the findings of the 7-day range-finder, less than 5 ul/d dose volumes would be required for a longer duration study, which would present technical difficulties, questions regarding dosing accuracy and a very low nominal systemic dose. The data provided in this range-finder study indicate a practical and humane dose range for reproductive toxicity studies is below the limit of technical practicality and toxicological significance. Additional testing with this material is not warranted.

Groups of 20 mice/sex were given 0.025% sodium acetate in the drinking water (about 60 mg/kg bw/day) for 1 week before breeding, during a 9-day breeding period and (females only) throughout pregnancy, lactation and until the offspring were weaned at 3 weeks of age. The male offspring were given the same solution until they were 5-7 weeks old and were then examined in a 24-hour activity test (BIBRA International, 1993 and Donald, J.M. et al., 1988). Examination of the litters revealed no overt deformities, and pup weights were normal at day 1 and day 21. The activity of offspring of the treated group was lower than that of controls during the first 12 hours but was similar during the second 12 hours (it is unknown if the decreased activity observed in the sodium acetate treated group was a result of in utero and/or post-weaning, since the pups were exposed during both time periods). The NOAEL (fertility) was 60 mg/kg bw.

Table 6 Summary of the effects on fertility of ethyltriacetoxysilane and acetic acid, sodium salt

Route	Ethyl triacetoxysilane	Acetic Acid, Sodium salt	Reliability
Oral	No data	Drinking water, mouse NOAEL = 60 mg/kg bw (Sodium acetate) (BIBRA, 1993 and Donald, et al., 1988)	(2) valid with restrictions
Inhalation	No data	No data	-
Dermal	No data	No data	-

Developmental Toxicity

In a 7-day oral range-finding study, stomach lesions were observed at low doses of ethyltriacetoxysilane and resembled acetic acid toxicity (DCC, 2004). This 7-day range-finder study indicated that a maximum dose level of less than 20 mg/kg/day would be required for a developmental toxicity study in order to avoid death or obvious suffering due to the corrosivity of the hydrolysis product, acetic acid. Due to the low solubility and rapid hydrolysis of ethyltriacetoxysilane, a suitable vehicle cannot be selected, and all studies would utilize neat dosing. Based on the findings of the 7-day range-finder, less than 5 ul/d dose volumes would be required for a longer duration study, which would present technical difficulties, questions regarding dosing accuracy and a very low nominal systemic dose. The data provided in this range-finder study indicate a practical and humane dose range for developmental toxicity studies is below the limit of technical practicality and toxicological significance. Additional testing with this material is not warranted.

Rats were dosed daily with acetic acid at 0, 16, 74, 345, and 1600 mg/kg/day by oral gavage beginning on day 6 of gestation (Food and Drug Research Laboratories, 1974; BIBRA, 1993). Animals were observed daily and body weights recorded. On day 20, Caesarean sections were performed on all dams and the numbers of implantation sites, resorption sites, and live and dead fetuses was recorded. General external and internal examinations were also made of the dams. No effects on implantation or on maternal or fetal survival at doses of acetic acid up to 1600 mg/kg/day. The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring in the controls. The NOAEL (maternal and developmental) for rats was 1600 mg/kg bw. Mice were dosed daily with acetic acid at 0, 16, 74, 345, and 1600 mg/kg/day by oral gavage beginning on day 6 of gestation (Food and Drug Research Laboratories, 1974; BIBRA, 1993). Animals were observed daily and body weights recorded for 10 days. On day 17, Caesarean sections were performed on all dams and the numbers of implantation sites, resorption sites, and live and dead fetuses was recorded. General external and internal examinations were also made of the dams. No effects on implantation or on maternal or fetal survival were observed at doses up to 1600 mg/kg/day. The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring in the controls. The NOAEL (maternal and developmental) for mice was 1600 mg/kg bw. Rabbits were dosed daily with acetic acid at 0, 16, 74, 345, and 1600 mg/kg/day by oral gavage beginning on day 6 of gestation (Food and Drug Research Laboratories, 1974; BIBRA, 1993). Animals were observed daily and body weights recorded. On day 29, Caesarean sections were performed on all does and the numbers of corpora lutea, implantation sites, resorption sites, and live and dead fetuses was recorded. General external and internal examinations were also made of the does. No effects on implantation or on maternal or fetal survival at doses up to 1600 mg/kg bw/day. The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring in the controls. The NOAEL (maternal and developmental) for rabbits was 1600 mg/kg bw. Thirty pregnant mice, approximately 60 days old, were given a single oral dose of 1000 mg/kg bw of acetic acid, sodium salt, by gavage on days 8-12 of gestation (Kavlock, et al, 1987). There were no general parental toxicity effects or effects on the offspring. The NOAEL (maternal and developmental) for mice was 1000 mg/kg bw.

Table 7 Summary of the developmental toxicity of ethyltriacetoxysilane, acetic acid and its sodium salt

Route	Ethyl triacetoxysilane	Acetic Acid and its Sodium Salt	Reliability
Oral	No data	Gavage, mouse NOAEL (maternal and developmental) = 1000 mg/kg bw (Sodium acetate) (Kavlock et al, 1987)	(2) valid with restrictions
	-	Gavage, mouse NOAEL (maternal and developmental) = 1600 mg/kg bw (Acetic acid) (BIBRA, 1993 and Food and Drug Research Laboratories, 1974)	(2) valid with restrictions
	-	Gavage, rabbit NOAEL (maternal and developmental) = 1600 mg/kg bw (Acetic acid) (BIBRA, 1993 and Food and Drug Research Laboratories, 1974)	(2) valid with restrictions
	-	Gavage, rat NOAEL (maternal and developmental) = 1600 mg/kg bw (Acetic acid) (BIBRA, 1993 and Food and Drug Research Laboratories, 1974)	(2) valid with restrictions
Inhalation	No data	No data	
Dermal	No data	No data	

Conclusion

Ethyltriacetoxysilane rapidly (seconds) hydrolyzes to acetic acid and a trisilanol (3:1). The silanol generated is insignificant in both quantity and toxicity relative to the production of acetic acid and its associated toxicity. The silanols condense to siloxane oligomers; this condensation of silanols is affected by both concentration and pH, and since both change over time it is not feasible to isolate specific silanols for analysis (the structures continue to evolve until they either reach equilibrium or precipitate out of solution). The toxicity of ethyltriacetoxysilane is represented by an irritative mechanism of toxicity following single or repeated dosing, likely due to production of acetic acid during hydrolysis; any additional information provided though the conduct of repeated dose, reproduction or developmental toxicity studies with ethyltriacetoxysilane would be limited in order to avoid death or obvious suffering due to the corrosivity of the hydrolysis product, acetic acid.
Acetic acid had no effects on implantation or on maternal or fetal survival in rats, mice or rabbits at doses up to 1600 mg/kg/day. The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring in the controls. Sodium acetate had no effect on reproduction when administered in drinking water at about 60 mg/kg bw in mice.

3.2 Initial Assessment for Human Health

Ethyltriacetoxysilane undergoes rapid hydrolysis in moist/aqueous environments (less than 13 seconds) to acetic acid and silanetriols, thus, observed toxicity is likely due primarily to acetic acid. Abiotic hydrolysis products of the test substance undergo continuous, condensation reactions to produce higher molecular weight cyclic and linear siloxanes (the number-average and weight-average molecular weights were 633 and 809 with 22 area % of the chromatogram higher than 1000 molecular weight at the1-hr reaction time; at the 4-hr reaction time, the number-average and weight-average molecular weights increased to 750 and 1085 with 38 area % of the chromatogram higher than 1000 molecular weight, respectively) (Sun, Y. et al., 2002). The silanols condense to siloxane oligomers; this condensation of silanols is affected by both concentration and pH, and since both change over time it is not feasible to isolate specific silanols for analysis. While the hydrolysis of ethyltriacetoxysilane is rapid, the polymerization products, while not volatile, are in a molecular weight range small enough to be considered, at least in part, biologically available. The structural analogue methyltriacetoxysilane (CAS number 4253-34-3) has been used for in vitro bacterial gene mutation and chromosomal aberrations endpoints. The hydrolysis product, acetic acid (CAS number 64-19-7) and its salts [calcium acetate (CAS number 62-54-4), potassium acetate (CAS number 127-08-2) and sodium acetate (CAS number 127-09-3), have been used to assess the repeated dose toxicity, fertility and developmental toxicity endpoints.

The acute toxicity of ethyltriacetoxysilane is described by an LD50 rat (oral) = 1462 mg/kg, and the indications of the irritative properties of the test substance. Clinical signs included decreased activity; lethargy; lacrimation; salivation; irregular gait; hunched posture; decreased body weight, food consumption and fecal volume; red urine; red staining of the snout, eyes and extremities; and labored respiration. Ethyltriacetoxysilane is severely irritating and corrosive to the skin, and expected to be severely irritating to the eyes of animals.

In a 7-day oral range-finding study (gavage) rats were treated with undiluted ethyltriacetoxysilane (dose levels of 0, 17 (males), 23 (females), 100, 500 and 1000 mg/kg/d). Ethyltriacetoxysilane rapidly (seconds) hydrolyzes to acetic acid and a trisilanol (3:1). The silanol generated is insignificant in both quantity and toxicity relative to the production of acetic acid and its associated toxicity. Animals from the 17 (males), 23 (females), and 100 mg/kg/day dose groups survived to day 7. Animals from the 500 and 1000 mg/kg/day dose groups were sacrificed after the third dose as a consequence of two deaths (one from each group), marked body weight loss, and severity of lesions (ulceration and erosion of stomach and esophagus) observed in necropsied animals. The

stomach lesions observed resembled acetic acid toxicity. This 7-day range-finder study indicated that a maximum dose level of less than 20 mg/kg/day would be required for a longer duration repeated dose study in order to avoid death or obvious suffering due to the corrosivity of the hydrolysis product, acetic acid. Based on the findings of the 7-day range-finder, a longer duration study will present technical difficulty questioning dosing accuracy and a very low nominal systemic dose. Additional testing (repeated dose, reproductive effects or developmental toxicity) with ethyltriacetoxysilane has not been conducted. Toxicity is represented by an irritative mechanism following single or repeated dosing, likely due to production of acetic acid during hydrolysis.

Groups of 20 mice/sex were given 0.025% sodium acetate in the drinking water (about 60 mg/kg bw/day) for 1 week before breeding, during a 9-day breeding period and (females only) throughout pregnancy, lactation and until the offspring were weaned at 3 weeks of age. The male offspring were given the same solution until they were 5-7 weeks old and were then examined in a 24-hour activity test. Examination of the litters revealed no overt deformities, and pup weights were normal at day 1 and day 21. The activity of offspring of the treated group was lower than that of controls during the first 12 hours but was similar during the second 12 hours (the study did not show unequivocally that the decreased activity was maternally-mediated, since the pups were also exposed post-weaning). Acetic acid had no effects on implantation or on maternal or fetal survival in rats, mice or rabbits at doses up to 1600 mg/kg/day. The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring in the controls. Sodium acetate had no effect on parents or offspring when mice were administered 1000 mg/kg bw, by gavage on days 8-12 of gestation.

In vitro, ethyltriacetoxysilane and methyltriacetoxysilane were negative in bacterial mutagenicity assays and did not produce any statistically significant increases in incidence of bacterial mutations. Methyltriacetoxysilane did not induce chromosomal aberrations in CHO cells.

4 HAZARDS TO THE ENVIRONMENT

Analogue Justification

Ethyltriacetoxysilane undergoes rapid hydrolysis, which occurs during testing, such that observed toxicity is likely due primarily to acetic acid. Aquatic toxicity test have been conducted with ethyltriacetoxysilane, and the results are considered to be representative of acetic acid, due to its rapid hydrolysis. Acute toxicity to fish, daphnia and algae endpoints are supported using data from a structural analogue, vinyltriacetoxysilane, as well as for a hydrolysis product, acetic acid. The data for vinyltriacetoxysilane are also considered to be representative of acetic acid, due to its rapid hydrolysis. Abiotic hydrolysis studies show that hydrolysis products from ethyltriacetoxysilane undergo continuous, condensation reactions to produce higher molecular weight cyclic and linear siloxanes.

4.1 Aquatic Effects

Aquatic toxicity data are available for ethyltriacetoxysilane. Data from ethyltriacetoxysilane and a structurally related acetoxysilane, vinyltriacetoxysilane (CAS No. 4130-08-9) show the resulting toxicity to aquatic organisms is due to acetic acid. When results are expressed on the basis of the amount of acetic acid generated from the hydrolysis reaction, the toxicity of ethyltriacetoxysilane and vinyltriacetoxysilane are comparable to the reported toxicity of acetic acid (EC_{50} = 50-450 mg/L, depending on test species):

Table 8 Summary of the reported toxicity of ethyltriacetoxysilane, vinyltriacetoxysilane, and acetic acid to various aquatic organisms

	Reported Toxicity (mg/L)			
Test System	**Ethyltriacetoxy silane**	**Vinyltriacetoxy silane**	**HOAc[a]**	**Acetic Acid**
Fish (96-h EC_{50}; lethality)				
Brachydanio rerio	251 (measured; semi-static)** Degussa-Huls Ag, 1995c		194	
Oncorhyncus mykiss		51 (nominal; static) ** DCC, 1980	40	
Lepomis macrochirus		68 (nominal; static) ** DCC, 1980	53	75 (72 hr LC50; static) US Public Health Service, 1960; USEPA Aquire
Pimephales promelas				88 (72 hr LC50; static) Mattson et al, 1976; USEPA Aquire
Pimephales promelas				79 (72 hr LC50; static) Mattsonet al, 1976; USEPA Aquire
Cyprinus carpio				49 (48 hr LC50; test type not reported) Funasakaet al., 1976; USEPA Aquire
Carassius auratus				100 (flow-through) Ellis, 1937; USEPA Aquire
Ictalurus punctatus				446 (72 hr LC50; static) Clemens and Sneed,, 1959; USEPA Aquire
Gambusia affinis				251 (static) ACC, 2003; et al., 1957; USEPA Aquire
Fish (unspecified)				27792 [b] USEPA, 2000
Invertebrate (48-h EC_{50}; immobility)				
Daphnia magna	62 (nominal; static) ** Degussa-Huls Ag, 1995d		48	
Daphnia magna		100 (nominal; renewal) ** DCC, 1980	78	
Daphnia magna				65 (static) ** Janssen, Espiritu and Persoone, 1993; ACC , 2003
Daphnia magna				6000 (neutralized; pH 8.0, static);

				95 (un-neutralized) Bringmann and Kuhn, 1982; ACC, 2003
Carcinus maenas				180 (renewal) Portmann and Wilson, 1971; USEPA Aquire
Crangon crangon				≥100 (static) Portmann and Wilson, 1971; USEPA Aquire
Daphnia				26099[b] USEPA, 2000
Algae (7-d EC_{50}; growth rate)				
Scenedesmus subspicatus	73 (nominal) ** Degussa-Huls Ag, 1995e		59	
Selenastrum capricornutum		111 (nominal; growth rate), 23 (nominal; biomass) ** DCC, 1980	87	
Anabaena flos-aquae		>100 (nominal; growth rate)**, 57 (nominal; biomass) ** DCC, 1980	78	
Microcystis aeruginosa				90 Bringmann and Kuhn, 1978; USEPA Aquire
Green algae				14617[b] USEPA, 2000

[a] HOAc is the estimated toxicity based on the estimated amount of acetic acid generated from the hydrolysis reaction. The amount of acetic acid generated was estimated using the assumption that 1 mole of test material (ethyl- or vinyl- triacetoxysilane) produces 3 moles of acetic acid.

** Not neutralized

General

Ethyltriacetoxysilane undergoes rapid hydrolysis in aquatic media, and thus the exposures to ethyltriacetoxysilane are likely to be transient. For much of the duration of the tests, the organisms will be exposed to the hydrolysis products, which include acetic acid and trisilanols. The Si-C bond will not undergo further hydrolysis. That bond is hydrolytically stable. Only the acetoxy groups will be hydrolyzed. The transient silanol groups will condense with other silanols to yield:

$Et\text{-}Si(OR)_3$ type resins where R=H or $\text{-}Si(Et)(OR)_2$

As a result silanol-functional resins are generated.

Acute Toxicity Test Results

Ethyltriacetoxysilane undergoes rapid hydrolysis in aquatic media, and thus the exposures to ethyltriacetoxysilane are likely to be transient. For these studies, the test article was dissolved in water and stirred for an 18 hour period. Acetic acid has also been tested for aquatic effects.

The 96-hour LC50 of ethyltriacetoxysilane for a freshwater fish (*Brachydanio rerio*) is 251 mg/L (the test media was not neutralized; Degussa-Huls AG, 1995c). The 96-hour LC50 of vinyltriacetoxysilane for *Oncorhyncus mykiss* is 51 mg/L and for *Lepomis macrochirus* is 68 mg/L (DCC, 1980). In both studies the test media was not neutralized. Ten fish (*Gambusia affinis*) were exposed to acetic acid concentrations of 10, 18, 32, 56 and 100 ppm (first experiment) or between 100 and 1,000 ppm for a period of 96 hours under static conditions (Wallen, Greer, and Lasater, 1957). The temperature, turbidity, and pH of the experimental water were measured after the test substance was added and daily throughout the experiment. Survivor observations were made at 24, 48, 72 and 96 hours. The 96 hour LC50 was 251 mg/L. Fish (*Ictalurus punctatus*) were exposed to acetic acid for a period of 72 hours under static conditions (Clemens, and Sneed, 1959). The 72 hour LC50 was 446 mg/L. Fish (*Lepomis macrochirus*) were exposed to acetic acid for a period of 96 hours under static conditions (US Public Health Service Grant, 1960). The 72 hour LC50 was 75 mg/L. Fish (*Pimephales promelas*) were exposed to acetic acid for a period of 96 hours under static conditions (Mattson, Arthur, and Walbridge, 1976). The 72 hour LC50 was 79 to 88 mg/L. Fish (*Carassius auratus*) were exposed to acetic acid for a period of 48 to 96 hours under flow through conditions (Ellis, 1937). Mortality was observed at 100 mg/L. Fish (*Cyprinus carpio*) were exposed to acetic acid for a period of 48 hours (Funasaka, Ose, and Sato, 1976). The 48 hour LC50 was 49 mg/L. Studies have been performed with a silanol monomer, trimethylsilanol (CAS No. 1066-40-6). Although this silanol is not expected to be produced following hydrolysis of ethyltriacetoxysilane, it has been predicted to be one of the most toxic to aquatic organisms of all the silanols identified to date. A semi-static 96 hour study with trimethylsilanol and rainbow trout (Oncorhynchus mykiss) resulted in a No Observed Effect Concentration (NOEC) of 128 mg/L and an LC50 of 271 mg/L.

The 48 hour EC50 of ethyltriacetoxysilane is 62 mg/L for the water flea (*Daphnia magna*) under static conditions (the test media was not neutralized; (Degussa-Huls AG, 1995d). The 48 hour EC50 of vinyltriacetoxysilane is 100 mg/L for Daphnia magna (the test media was not neutralized; DCC, 1980). When results are expressed on the basis of the amount of acetic acid generated from the hydrolysis reaction, the toxicity of ethyltriacetoxysilane and vinyltriacetoxysilane are comparable to the reported toxicity of acetic acid (EC_{50} = 65-180 mg/L, depending on test species). The 48 hour EC50 of acetic acid is 100 mg/L for the crustacean, *Crangon crangon* in a renewal system (Portmann, and Wilson, 1971). The 24 hour EC50 of acetic acid is 6000 mg/L for the water flea (*Daphnia magna*) under static conditions (Bringmann and Kuhn, 1982). This value of 6000 mg/L pertains to test solutions neutralized (pH 8.0) prior to daphnid exposures. For the un-neutralized test, the 24-hour EC50 was 95 mg/L. The 48 hour EC50 of acetic acid is 65 mg/L to the water flea (*Daphnia magna*) in a static system (Janssen, Espiritu, and Persoone, 1993). The solutions were not neutralized. The 48 hour EC50 of acetic acid is 180 mg/L to *Carcinus maenas* in a renewal system (Portmann, and Wilson, 1971).

In an algae study with ethyltriacetoxysilane, on the basis of cell growth, a median concentration is calculated of 72 hour EbC50 = 73 mg/L; on the basis of growth rate, a median effective concentration was achieved at (0-72 hour) ErC10 = 76 mg/L (the test media was not neutralized; Degussa-Huls AG, 1995e). In a study with vinyltriacetoxysilane, the EC50 for growth rate of *Selenastrum capricornutum* is 111 mg/L, and for *Anabaena flos-aquae* is 100 mg/L (the test media was not neutralized; DCC, 1980). When results are expressed on the basis of the amount of acetic acid generated from the hydrolysis reaction, the toxicity of ethyltriacetoxysilane and vinyltriacetoxysilane are comparable to the reported toxicity of acetic acid (EC_{50} = 90 mg/L). A

change in the number of species groups in a community (i.e. species diversity) was reported at 90 mg/L acetic acid in an 8 day study with *Microcystis aeruginosa* (Bringmann and Kuhn, 1978).

Chronic Toxicity Test Results

No data available.

4.2 Terrestrial Effects

A group of 40 earthworms (*Eisenia fetida*) was exposed for 14 days to a limit concentration of 1000 mg/kg of ethyltriacetoxysilane (Degussa AG, 1995f). There were no deaths recorded for the control group at 7 or 14 days or for the test substance group at 7 days. At 14 days, one animal in the test substance treated group had died. The LC10 was calculated to be greater than 1000 mg/kg.

4.3 Other Environmental Effects

The toxicity of ethyltriacetoxysilane to bacteria was determined by oxygen content where the effective concentration (EC10 and EC100) is measured after 5 hours of incubation with a bacterial suspension (Degussa-Huls AG, 1995b). The EC10 and EC100 were 60-80 mg/L. The pH value decreased with increased test concentration:

10 mg/L pH= 7 , 60 mg/L pH= 5.7, 80 mg/L pH= 5.2.

4.4 Initial Assessment for the Environment

The melting point of ethyltriacetoxysilane is <-2.9°C and the boiling point is 227 °C at 1013 hPa. The vapor pressure is 0.05 hPa at 20 deg C. The estimated water solubility of ethyltriacetoxysilane is 42 g/L; the estimated log Kow is 0.74. The water solubility and log Kow values may not be applicable because the chemical is hydrolytically unstable. The overall reaction half-life in air is estimated to be less than 3 minutes because of rapid hydrolysis of the material with moisture in the atmosphere. However, photodegradation as a mode of removal is unlikely because ethyltriacetoxysilane is hydrolytically unstable. Photodegradation of the parent silane is not expected to be a significant degradation process in the aquatic environment due to the rapid rate of hydrolysis. Although, the vapor pressure indicates that ethyltriacetoxysilane resides in the atmosphere and may undergo photodegradation due to ozone and/or hydroxyl radicals, due to extremely rapid hydrolysis, the substance is not expected to reside in the air compartment and the vapor pressure of the substance may not be relevant.

Ethyltriacetoxysilane is hydrolytically unstable over a range of environmentally relevant pH and temperature conditions. At pH 7, the half-life is <13 seconds. Rapid hydrolysis of this material produces acetic acid and trisilanols. Level III Fugacity modeling, using loading rates for Air, Soil, and Water of 1000 kg/h for each medium, shows the following percent distribution: Air = 47.3%; Soil = 47.4%; Water = 5.3%; Sediment = 0.0. However, ethyltriacetoxysilane is unlikely to be found in the environment, as this material is hydrolytically unstable. Ethyltriacetoxysilane is readily biodegradable; however this material rapidly hydrolyzes and generates 3 moles of acetic acid for every mole of parent material. Thus, the biodegradation observed is likely reflective of the hydrolysis product, acetic acid. The biodegradation rate for acetic acid after 7 days under anaerobic conditions is 99%. The rapid hydrolysis of ethyltriacetoxysilane means that it is unlikely to be present in the environment. Bioaccumulation is not anticipated since this material is hydrolytically unstable.

Ethyltriacetoxysilane undergoes rapid hydrolysis in aquatic media, and thus the exposures to ethyltriacetoxysilane are likely to be transient. The 96-hour LC50 of ethyltriacetoxysilane for

Brachydanio rerio is 251 mg/L. Studies have been conducted on a structural analog, vinyltriacetoxysilane, as well as the primary hydrolysis product, acetic acid. The 96-hour LC50 of vinyltriacetoxysilane for *Oncorhyncus mykiss* is 51 mg/L and for *Lepomis macrochirus* is 68 mg/L. The 96 hour LC50s for acetic acid are 75, 79-88 and 251 mg/L (several species of fish). A semi-static 96 hour study with trimethylsilanol and rainbow trout (Oncorhynchus mykiss) resulted in a No Observed Effect Concentration (NOEC) of 128 mg/L and an LC50 of 271 mg/L. This suggests the silanetriol degradation products are not likely higher than acetic acid alone. The 48 hour EC50 for ethyltriacetoxysilane is 62 mg/L for *Daphnia magna*. The 48 hour EC50 of vinyltriacetoxysilane is 100 mg/L for *Daphnia magna*. Under static conditions, the 48 hour EC50 for acetic acid is 65 mg/L for aquatic invertebrates. When the test solutions are neutralized, the static EC50 for acetic acid is 6000 mg/L. In renewal systems with aquatic invertebrates, 48 hour EC50s for acetic acid are 100 mg/L and 180 mg/L Ethyltriacetoxysilane toxicity to *Scenedesmus subspicatus* provided a 72 hour EC50 of 73 and 76 mg/L for biomass and growth rate, respectively. When results are expressed on the basis of the amount of acetic acid generated from the hydrolysis reaction, the toxicity of the parent material is comparable to the reported toxicity of acetic acid (EC_{50} = 50-450 mg/L, depending on test species).

5 RECOMMENDATIONS

Human Health: The chemical possesses properties indicating a hazard for human health (severe irritation and corrosivity caused by acetic acid). Due to the extremely rapid hydrolysis to acetic acid and the corresponding trisilanol and based on exposure data presented by the Sponsor country, the parent material will not be available for exposure, and therefore this chemical is currently of low priority for further work. The identified hazards should nevertheless be noted by chemical safety professionals and users.

Environment: The chemical has properties indicating a hazard for aquatic toxicity. However the chemical is of low priority for further work for the environment because of its rapid hydrolysis and its limited potential for bioaccumulation.

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S I D S

Dossier

Existing Chemical	:	ID: 17689-77-9
CAS No.	:	17689-77-9
EINECS Name	:	triacetoxyethylsilane
EC No.	:	241-677-4
Molecular Weight	:	234.28
Structural Formula	:	CC[Si](OC(=O)C)(OC(=O)C)OC(=O)C
Molecular Formula	:	C8H14O6Si

Producer related part

Company	:	Epona Associates, LLC
Creation date	:	27.06.2003

Substance related part

Company	:	Epona Associates, LLC
Creation date	:	27.06.2003
Status	:	
Memo	:	SEHSC merged
Printing date	:	01.11.2005
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1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : Analogue Justification

Remark : Ethyltriacetoxysilane undergoes rapid hydrolysis in moist/aqueous environments (t1/2 is less than 13 seconds) to acetic acid and the corresponding trisilanol, thus observed toxicity is likely due primarily to acetic acid. Abiotic hydrolysis products of the test substance undergo continuous condensation reactions to produce higher molecular weight cyclic and linear siloxanes (the number-average and weight-average molecular weights were 633 and 809 with 22 area % of the chromatogram higher than 1000 molecular weight at the1-hr reaction time; at the 4-hr reaction time, the number-average and weight-average molecular weights increased to 750 and 1085 with 38 area % of the chromatogram higher than 1000 molecular weight, respectively). The alkyl silanols condense to siloxane oligomers; this condensation of silanols is affected by both concentration and pH, and since both change over time it is not feasible to isolate specific silanols for analysis. While the hydrolysis of ethyltriacetoxysilane is rapid, the polymerization products, while not volatile, are in a molecular weight range small enough to be considered, at least in part, biologically available. The structural analogue methyltriacetoxysilane (CAS number 4253-34-3) has been used for in vitro bacterial gene mutation and chromosomal aberrations endpoints. The hydrolysis product, acetic acid (CAS number 64-19-7) and its salts [calcium acetate (CAS number 62-54-4), potassium acetate (CAS number 127-08-2) and sodium acetate (CAS number 127-09-3)]), have been used to assess the acute aquatic toxicity (fish, aquatic invertebrate and algae), repeated dose toxicity, fertility and developmental toxicity endpoints. Acetic acid and its salts are grouped together because of their close structural relationships and the salts are the neutralized form of the acid that can be more easily administered, their natural occurrence in plants and animals, and their fundamental role in cell metabolism, particularly in the tricarboxylic acid cycle (also known as the citric acid or Kreb's cycle), which is where humans get their energy. In addition the structural analogue vinyltriacetoxysilane (CAS number 4130-08-9) has been used to support the acute aquatic toxicity endpoints. Data from both ethyltriacetoxysilane and vinyltriacetoxysilane are representative of acetic acid, based on the rapid hydrolysis of these materials.

01.11.2005

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name : Ethyltriacetoxysilane
Smiles Code : O=C(O[Si](OC(=O)C)(OC(=O)C)CC)C
Molecular formula : C8H14O6Si

Molecular weight : 234
Petrol class :

07.12.2004

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type : typical for marketed substance
Substance type : organic
Physical status : liquid
Purity : > 95 - 100 % w/w
Colour : off white
Odour : acetic acid odor

Source : SEHSC
06.12.2004 (35) (45)

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Dow Corning (R) 3-7110

20.04.2004

ethylsilanetriol, triacetate

Source : Degussa AG Duesseldorf
06.05.1996

Ethyltriacetoxysilane

Reliability : (2) valid with restrictions
12.03.2004 (18)

silanetriol, ethyl-, triacetate

Source : Degussa AG Duesseldorf
05.02.2003

Triacetoxyethylsilane

12.03.2004 (18)

Tris(acetyloxy)ethylsilane

02.12.2004 (18)

1.3 IMPURITIES

Purity : typical for marketed substance
CAS-No : 64-19-7
EC-No : 200-580-7

EINECS-Name : acetic acid
Molecular formula : CH3COOH
Value : < 5 % w/w

Source : SEHSC
06.12.2004 (35)

Purity : typical for marketed substance
CAS-No : 108-24-7
EC-No :
EINECS-Name : Acetic anhydride
Molecular formula :
Value : < 3 % w/w

20.04.2004 (35)

Purity : typical for marketed substance
CAS-No : 4253-34-3
EC-No :
EINECS-Name : Methyl triacetoxysilane
Molecular formula :
Value : < 1 % w/w

20.04.2004 (45)

Purity : typical for marketed substance
CAS-No :
EC-No :
EINECS-Name : Impurities
Molecular formula :
Value : 1 - 5 % w/w

20.04.2004 (35)

1.4 ADDITIVES

1.5 TOTAL QUANTITY

Quantity : ca. 891 - tonnes produced in 2001

Remark : Reflects production in the Sponsor country
Source : SEHSC
06.12.2004

Quantity : ca. 6.3 - tonnes imported in 2001

Remark : Reflects importation into the Sponsor country
Source : SEHSC
06.12.2004

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	use
Category	:	
Remark	:	The commercial use of this material is almost exclusively as a cross linker for silicone sealants and adhesives. . The final formulated sealant and adhesive is sold in consumer markets. During curing of the silicone sealant or adhesive the ethyltriacetoxysilane hydrolyzes as it reacts with silanol polymers and atmospheric moisture to form a cross linker rubber. Since the acetoxy-functional silane is converted and bound within the substrate by polymer coupling, free silane is not present within the final products. In production, this material is mostly handled in closed systems. Necessary engineering controls during production include proper ventilation, containment, safety equipment and actual hardware designed to minimize exposure through splashing, or exposure to the air. Transfer of this material is in closed pipes or closed containers rather than in open systems to minimize loss of this material (hydrolysis) although some customers may transfer the material in open systems. Ethyltriacetoxysilane is transported from the production site as the parent silane to formulators. Generally, ethyltriacetoxysilane is used as a cross linker at 3 to 5 %. As ethyltriacetoxysilane is compounded into a consumer or industrial sealant or adhesive, it reacts with the silicone. After curing the parent silane becomes cross linked into the silicone rubber matrix and no longer exists, this greatly reduces the potential for consumer or worker exposure.

17.03.2004

1.7.1 DETAILED USE PATTERN

Industry category	:	15/0 other
Use category	:	55/0 other
Extra details on use category	:	No extra details necessary No extra details necessary
Emission scenario document	:	not available
Product type/subgroup	:	
Tonnage for Application	:	
Year	:	
Fraction of tonnage for application	:	
Fraction of chemical in formulation	:	
Production	:	:
Formulation	:	:
Processing	:	:
Private use	:	

Recovery :

Remark : Industry category: 65% chemical industry; 25% polymer industry; 10% other-sealants
Main category: 91% use resulting in inclusion into or onto matrix; 9% is non-dispersive - not directly sold into the consumer market.
Use categories: 91% cross-linking ingredient; 9% adhesives, bindings, other- sealants
Uses are the same in the Sponsor country (USA), Europe and Japan.

Source : SEHSC
06.12.2004

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

Type : degradation product in air
CAS-No :
EC-No :
EINECS-Name :
IUCLID Chapter :

Remark : The DC732 sealant experiment was run in triplicate with identical results.

Result : The following materials were not detected in the headspace Concentration (PPM) for the Target Silane:
Methyltriacetoxysilane
Ethyltriacetoxysilane
Diacetoxydimethylsilane
Acetoxytrimethylsilane

Methyltriacetoxysilane @ 59% relative humidity
DC732 silicone sealant
GE RTV108 silicone sealant
GE RTV108 with no added water

These materials were detected at >100 ppm headspace concentration for acetic acid/anhydride.

The detection limit for the acetoxysilane target compounds was estimated to be on the order of 100 ppb, based on the typical response factors noted for the siloxanes quantified and the response for neat acetoxysilanes measured as a liquid phase. It was not possible to prepare accurate gas phase standards of the acetoxysilanes without hydrolysis or other reaction rapidly occurring.

Test condition : " Conditions: Sealant samples (2 grams) were extruded in a dry atmosphere into a sealed vessel. Experiments were run with water present, with a 59% relative humidity, and with no additional water. Samples were incubated for 20 minutes at 27 C then headspace samples were taken.
" Controls: Samples of each of the neat silanes were also treated in the same manner as the sealant samples and were used for calibration of the test method.
" Analytical procedures: 200 microliter aliquots were sampled from the headspace of the sealed container and injected into a GC-MS

Test substance : " Commercial silicone sealants which utilize an acetoxy alkylsilane crosslinking reaction were used. Neat samples of the individual silanes were also tested.
Acetoxy-alkylsilanes in room temperature vulcanizing sealants
" Methyltriacetoxysilane CAS # 4253-34-3
" Ethyltriacetoxysilane CAS# 17689-77-9
" GE RTV!08 Sealant Batch AA881
" DC732 Sealant Batch 0000673137

Conclusion : None of the acetoxy alkylsilanes used as crosslinkers volatilize during cure of the sealants. Instead they hydrolyze and condense releasing acetic acid, which was detected. Therefore there is no human exposure to the acetoxy alkylsilanes from their predominant use in silicones sealants.

Reliability : (1) valid without restriction
25.02.2004 (76)

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

Source of exposure : other: human and environment
Exposure to the : Substance

Remark : In production, this material is mostly handled in closed systems. Necessary engineering controls during production include proper ventilation, containment, safety equipment and actual hardware designed to minimize exposure, through splashing,

or exposure to the air. Transfer of this material is in closed pipe, drums, or tanks rather than in open systems to minimize loss of this material (hydrolysis). Ethyltriacetoxysilane is transported from the production site as the parent silane to sealant formulators. The parent silane partially reacts during sealant formulation and then completely reacts during curing of the sealant into the polymer matrix and is no longer available for consumer or worker exposure. Ethyltriacetoxysilane volatilizes during cure of sealants. Instead this material hydrolyzes and condenses, releasing acetic acid. Therefore, there is no human exposure to ethyltriacetoxysilane from use in silicones sealants.

01.11.2005

Source of exposure : other: environment: General
Exposure to the : Substance

Remark : The reactive nature of this material destroys the parent material in any moisture-containing environment, thus limiting environmental exposure to the silane. The rapid hydrolysis means that the parent silane is unlikely to be found in the environment. If ethyltriacetoxysilane monomer is slowly released into the environment such that resulting concentrations of the parent compound are low, it is less likely that polymerisation will occur and more likely that free triol or short-chain oligomers will result. The spectrum of by-products will depend upon the initial concentration of the parent compound.

01.11.2005

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= 8.4 °C
Sublimation	:	no
Method	:	other: ASTM E794-98
Year	:	2000
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	8.4 ºC should be used as the critical value for melting point because a peak at -3.2 ºC was believed to correspond to the MP of ethyltriacetoxysilane. The original study showed a single peak across a temperature range of -2.9 to 8.4 ºC, suggesting that the test material contained an impurity (probably a hydrolysis product) having a low melting point. Ethyltriacetoxysilane readily hydrolyzes in the presence of moisture in the air with the initial formation of acetic acid and ethyldiacetoxysilanol. Initial DSC scan indicated one peak with onset of -2.9C and a maximum at 8.4C. A second scan of the sample indicated the formation of a second material as illustrated by a new peak appearing at -3.2 C and the 8.4 C peak. The new peak is believed to be due to the ethyldiacetoxysilanol formed by hydrolysis of the sample. Review of DSC scans indicate good reliability. MP of ethyltriacetoxysilane varied by less than 0.1C at low hydrolysis levels.
Test condition	:	Melting point determined by DSC. A Dupont 910 DSC instrument was used. Instrument calibrated according to manufacturer's instructions. Dichloroethane and distilled, deionized water used for melting point calibration. Onset of melting of water found to be 0.7C. DSC purged with nitrogen at 50 ml/min. Aliquots (about 10 mg) of sample material were placed in aluminum sample pans and hermetically sealed. Temperature was increased as the rate of 10C/minute from -100C to 30 C.
Test substance	:	Ethyltriacetoxysilane (CAS# 17689-77-9) purity >98%
Conclusion	:	DSC provides unambiguous melting point and provides a qualitative purity confirmation as materials within mixture have distinct DSC peaks. Absolute error in melting point depends on calibration. Calibration value within acceptable limits.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.04.2004 (72)

Value	:	= 5 °C
Sublimation	:	
Method	:	other: unknown
Year	:	1964
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Dow Corning Corporation Midland, MI

06.04.2004 (29)

2.2 BOILING POINT

Value : = 227 °C at 1013.25 hPa
Decomposition : yes
Method : other: Extrapolation of lower, ebulliometric boiling points
Year : 1988
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Observations: Extrapolations of VP for several (OAc)3 compounds were compared. Decomposition noted ca 202 C
The boiling point value selected is an extrapolation of lower, ebulliometric boiling points and is in excellent agreement with measurements reported by individual member companies.

Result : Coefficients for the Halm-Stiel and Antoine equations were derived from regression of the following measured vapor pressure data:

T (deg C)	P (mm Hg)	P (Pa)
87.3	4.2	565
94.8	6.7	888
108.1	12.6	1674
118.8	20.7	2758

Source : Dow Corning Corporation Midland, MI
Test condition : The best-fitting Halm-Stiel and Antoine vapor pressure equations were used to extrapolate boiling point from vapor pressures measured at temperatures ranging from 87-119 C.
Conclusion : Although the Halm-Stiel and Antoine equations are valid for interpolations, serious error may result from extrapolations outside the limits of measured data. Hence, significant error may be associated with the reported boiling point for the test substance. Nonetheless, the result is comparable to values obtained from the literature and other studies
Reliability : (2) valid with restrictions
Review of the study report and raw data indicate that the results are scientifically defensible and adequate for assessing the boiling point of the test substance. The study is considered to be reliable with the following restrictions:
" study was not conducted under GLP
" purity of test substance was not documented
" methods used to generate vapor pressure/temperature data were not documented
" boiling point is extrapolated from vapor pressures measured at elevated temperatures ranging from 87-119 C.
Flag : Critical study for SIDS endpoint
10.07.2003 (34) (78)

Value : = 201 °C at 1013 hPa
Decomposition :
Method : other
Year : 1971
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : Dow Corning Corporation Midland, MI
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Reliability : (2) valid with restrictions
25.02.2004 (34) (54)

Value : = 220 °C at 1013 hPa
Decomposition :
Method : other
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : General Electric
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Reliability : (2) valid with restrictions
25.02.2004 (46)

2.3 DENSITY

Type : relative density
Value : = 1.1437 at 20 °C
Method : other: Densimeter
Year : 1988
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Observations: Density relative to 4 C water density
Source : Dow Corning Corporation Midland, MI
Reliability : (2) valid with restrictions
25.02.2004 (78)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .05 hPa at 20 °C
Decomposition : yes
Method : other (calculated): Smoothed data by fitting it to Halm & Stiel CSP correlation
Year : 1988
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Ebulliometric measurements in DC Lab Book E-7863:19-27, 41, 42 (1988)
Test substance tends to decompose as temperature approaches boiling point (227 C)
Result : Measured vapor pressure and temperature data:

T (deg C)	P (mm Hg)	P (Pa)
87.3	4.2	565
94.8	6.7	888
108.1	12.6	1674
118.8	20.7	2758

The extrapolated vapor pressure of the test substance at 20 deg C was 6.0 Pa and 4.1 Pa, based on the Halm-Stiel equation and the Antoine equation, respectively. The reported vapor pressure of 5.1 Pa at 20 C is the average of the two extrapolated values.
Source : Dow Corning Corporation Midland, MI

Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Conclusion : Although the Halm-Stiel and Antoine equations are valid for interpolations, serious error may result from extrapolations outside the limits of measured data. Hence, significant error may be associated with the estimated vapor pressure of the test substance at 20 degrees C. Nonetheless, measured vapor pressures obtained at elevated temperatures are comparable to values obtained from other studies.
Reliability : (2) valid with restrictions
Review of the study report and raw data indicate that the results are scientifically defensible and adequate for assessing the vapor pressure of the test substance. The study is considered to be reliable with the following restrictions:
" study was not conducted under GLP
" purity of test substance was not documented
" methods used to generate vapor pressure/temperature data were not documented
" vapor pressure at 20 C is extrapolated from vapor pressures measured at elevated temperatures ranging from 87-119 C.
Flag : Critical study for SIDS endpoint
22.03.2004 (78)

Value : = .025 hPa at 20 °C
Decomposition :
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : SEHSC
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Reliability : (2) valid with restrictions
27.06.2003 (34)

Value : = .013 hPa at 65 °C
Decomposition :
Method :
Year : 1975
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : SEHSC
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Reliability : (2) valid with restrictions
10.07.2003 (50)

Value : = .015 hPa at 65 °C
Decomposition :
Method :
Year : 1969
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : Degussa AG Duesseldorf
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Reliability : (2) valid with restrictions
27.06.2003 (51)

Value : = .2 hPa at 80 °C
Decomposition :
Method :
Year : 1959
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : SEHSC
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Reliability : (2) valid with restrictions
27.06.2003 (15)

Value : = .267 hPa at 89 °C
Decomposition :
Method :
Year : 1960
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : SEHSC
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Reliability : (2) valid with restrictions
10.07.2003 (17)

Value : = .533 hPa at 97.5 °C
Decomposition :
Method :
Year : 1961
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : SEHSC
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Reliability : (2) valid with restrictions
10.07.2003 (83)

Value : = .533 hPa at 98 °C
Decomposition :
Method :
Year : 1947
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : SEHSC
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Reliability : (2) valid with restrictions
27.06.2003 (75)

Value : = 1.466 hPa at 98 °C
Decomposition :
Method :
Year : 1987
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : SEHSC
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Reliability : (2) valid with restrictions
27.06.2003 (3)

Value : = .533 hPa at 101 °C
Decomposition :
Method :
Year : 1951
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : SEHSC
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Reliability : (2) valid with restrictions
10.07.2003 (62)

Value : = .533 hPa at 101 °C
Decomposition :
Method :
Year : 1958
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : SEHSC
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Reliability : (2) valid with restrictions
10.07.2003 (63)

Value : = 1.066 hPa at 108 °C
Decomposition :
Method :
Year : 1957
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : SEHSC
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Reliability : (2) valid with restrictions
27.06.2003 (27)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = .74 at 25 °C
pH value :
Method : other (calculated)
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Log Kow of ethyltriacetoxysilane at 25 ºC was estimated using the SAR Model KOWWIN® (version 1.66). This value may not be applicable because the material is hydrolytically unstable.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
01.11.2005 (92)

Partition coefficient : octanol-water
Log pow : -1.87 at 25 °C
pH value :
Method : other (calculated)

Year : 2004
GLP : no
Test substance : other TS

Test substance : Ethylsilanetriol
Reliability : (2) valid with restrictions
01.11.2005 (92)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = 41.6 g/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable : no
Deg. product :
Method : other: estimated
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Water solubility of ethyltriacetoxysilane at 25 ºC was estimated using the SAR Model WSKOWWIN® (version 1.40). This value may not be applicable because the material is hydrolytically unstable.
Reliability : (2) valid with restrictions
27.05.2004 (93)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : = 104 °C
Type :
Method : other: Open Cup
Year : 1971
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : Dow Corning Corporation Midland, MI
Reliability : (2) valid with restrictions
10.07.2003 (30)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

Result : other: N/A

Source : Dow Corning Corporation Midland, MI
26.02.2003

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	500000 molecule/cm³
Rate constant	:	= .0000000000013212 cm³/(molecule*sec)
Degradation	:	= 50 % after 12 day(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Rate constant estimated using the model AOPWIN (ver. 1.90) as provided in the Estimations Program Interface (EPI) Suite (ver. 3.10), which was obtained from the US EPA.
Remark	:	Photodegradation as a mode of removal is unlikely as ethyltriacetoxysilane is hydrolytically unstable. Ethyltriacetoxysilane is highly reactive and hydrolytically unstable, such that acetic acid and ethylsilanetriol are rapidly generated upon contact with water or water vapor. Consequently, reaction with water vapor is likely the predominant degradation process for ethyltriacetoxysilane in air and the overall reaction half life in air should include both the oxidation half life and the hydrolytic half life. The ethylsilanetriol resulting from hydrolysis in the atmosphere is expected to further react with hydroxyl radicals.
Result	:	The overall reaction half life of ethyltriacetoxysilane in air is estimated to be < 3 min because of rapid hydrolysis of the material with moisure in the atmosphere.
Test substance	:	Estimated rate constant was based on the SMILES notation: O=C(O[Si](OC(=O)C)(OC(=O)C)CC)C
Conclusion	:	Ethyltriacetoxysilane in air is not expected to undergo direct photolysis, but may undergo indirect photolysis through hydroxyl radical oxidation. Because ethyltriacetoxysilane is highly reactive and hydrolytically unstable it is expected that reaction with water vapor is likely the predominant degradation process for the material in air.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

19.03.2004 (71)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	< .2 minute(s) at 25 °C
t1/2 pH7	:	< .2 minute(s) at 25 °C
t1/2 pH9	:	< .2 minute(s) at 25 °C
Deg. product	:	yes
Method	:	OECD Guide-line 111 "Hydrolysis as a Function of pH"

Year	:	2001
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	This study was not designed to monitor the subsequent condensation reaction involving silanol hydrolysis product. Values of upper limit on estimated t1/2 (shown above) refer to disappearance of test substance and appearance of acetic acid as a hydrolysis co-product. *In all experiments, test substance was completely hydrolyzed by the time the first 1H-NMR spectrum was acquired and remained unchanged thereafter. *Initial spectra were acquired after 77-100 seconds and 7-8 spectra were subsequently acquired at 15 seconds intervals. *Since the hydrolysis is so rapid, there is no data to determine the rate constants (k1, k2, and k3) for the hydrolysis reactions by regression modeling. *Rate constants and half-lives could not be determined quantitatively, although the data is certainly adequate for estimating the upper limit of t1/2. *First order or pseudo-first order behavior could not be confirmed because: a) unable to measure the decrease of parent peak intensity from test substance or increase of peak intensity of hydrolysis co-product due to a rapid hydrolysis reaction, b) no data obtained during the critical portion of the process (20-70% hydrolyzed), and c) the relationship between k1, k2, and k3 is not known. *Breakdown products from hydrolysis: acetic acid and silanol. For given solution conditions, the degradation product acetic acid was observed to be stable during data collection. Consequently, acetic acid was considered stable. The stability of silanol was not measured, however silanols will undergo condensation reactions to form siloxanes. The stabilities of silanols lie in the order R3SiOH > R2Si(OH)2 > RSi(OH)3, with the bulkier R groups lending more stability to the SiOH function.
Result	:	Estimated t1/2 (seconds) @ ~ 25 C: @pH 4.06 <13 @pH 7.14 <13 @pH 9.13 <11 Nominal: 1x10-3 M (243.28 mg/L) Ethyltriacetoxysilane Measured value (the value with units preferably mg/L): 0 M (0 mg/L) No -CH3 peak of -OC(O)CH3 group from test substance observed at pH 4.06 0 M (0 mg/L) No -CH3 peak of -OC(O)CH3 group from test substance observed at pH 7.14 0 M (0 mg/L) No -CH3 peak of -OC(O)CH3 group from test substance observed at pH 9.13
Source	:	Dow Corning Corporation Midland, MI
Test condition	:	Analytical procedures: o The hydrolysis reaction was followed by monitoring the decrease of peak intensity for the methyl (i.e., -CH3) of acetoxy (i.e., -OC(O)CH3) group from test substance and the increase of peak intensity for the methyl (i.e., -CH3) of acetic acid (i.e., HO-C(O)CH3) from hydrolysis co-product using proton-nuclear magnetic resonance spectroscopy

(1H-NMR).
*A Varian Mercury 300 MHz spectrometer was used and has been verified to be fully operational at 6 month intervals as part of our ISO9001 quality system.
*Samples were run under standard 1-pulse acquisition conditions on the spectrometer in a 5mm H1/BB switchable PFG probe. Samples were spun at 20 Hz and one scan was acquired per experiment utilizing 4 sec acquisition times and 90 degree pulses.
*Buffer solutions were prepared with deuterated water (99.9% of D2O, 0.1% of DOH residual, ISOTEC INC.)
*Samples were locked to D2O and referenced to the residual water peak at ~ 4.7 ppm.
*Verification of the neat test substance was conducted prior to prepare samples for hydrolysis study.
*Constant ionic strength was maintained for samples and buffers (0.5 M) by addition of sodium chloride.
*Temperature: Room temperature (~ 25 oC)
*Replicates: Two at pH 4.06, 7.14, and 9.13
*Vessels: High-density polyethylene bottles of 60-mL capacity with screw caps. Vessels were not sterilized.
*Buffer solutions were not sterilized.
*Co-solvent: None
*Buffer volume for hydrolysis: 50 mL
*Buffers

Target pH	Buffer System	Measured pH (before addition of test subst.)
4.0 F	Formic Acid/Sodium Hydroxide	4.06
7.0	Monobasic Sodium Phosphate /Dibasic Sodium Phosphate	7.14
9.0	Boric Acid/Sodium Hydroxide	9.13

Data treatment: For given solution conditions, the hydrolysis of test substance was followed to completion as indicated by disappearance of -CH3 peak of -OC(O)CH3 group from test substance. The elapsed time between the addition of the test substance to the aqueous buffer solution and the first acquired spectrum was used to estimate an upper limit on t1/2 (seconds) assuming that at least 7 half-lives represents exhaustive hydrolysis (99.2% complete).

Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Ethyltriacetoxysilane (CAS No. 17689-77-9); Gelest Inc., product number SIE 4899.0; purity of 98.5% by GC

Conclusion : According to the definition put forth in the test guidelines, the test substance was found to be hydrolytically unstable (Estimated t½ < 1 year at ~ 25 oC) over the range of environmentally relevant pH values and the temperature tested.

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

22.03.2004 (6) (49) (68) (77) (85)

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product : yes
Method : other: Experimental - no recognized guideline available

Year : 2002
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : The study described above was not designed to monitor the subsequent (> 4 hrs) condensation reactions.
· The estimated hydrolysis half-life for the test substance at pH 4.06 and ~ 25ºC is less than 13 seconds

Result : Value (mg/L) at temperature °C: Quantitation was not conducted. Based on the qualitative analytical results, hydrolysis products from the test substance underwent continuous, condensation reactions to produce higher molecular weight cyclic and linear siloxanes.
Description of solubility (e.g., miscible to soluble to not soluble):Soluble
pH value of the test system and concentration of the test system at temperature °C: pH = 1.29 and 3.4 x 105 (mg/L)(*) of ethyltriacetoxysilane/0.1 N HCl at 37°C

Breakdown products:Yes - Acetic acid and transient silanol materials

(*)= Calculation as following
Density of ethyltriacetoxysilane: 1.143 g/ml (obtained from Gelest Inc. catalog)
0.3 ml (ethyltriacetoxysilane)/1ml (0.1 N HCl) x 1.143 g/ml x 98.5% x 1000 mg/g x 1000 ml/1L(0.1 N HCl) = 3.4 x 105 mg/L

·The GPC chromatograms consisted of one main low molecular weight peak with a high molecular weight shoulder.
·The 4-hr sample had a larger high molecular weight shoulder in comparison to the 1-hr sample when both samples appeared to be completely dissolved in the THF solvent.
·At the 1-hr reaction time, the number-average and weight-average molecular weights of the test substance solution were determined by GPC to be 633 and 809, respectively, with 22% of the chromatogram represented by a MW range higher than 1000.
·At the 4-hr reaction time, the number-average and weight-average molecular weights increased to 750 and 1085, respectively, with 38% of the chromatogram represented by a MW range higher than 1000.
·ESI-MS analyses showed that similar hydrolysis/condensation species were observed in both liquid and gel samples at both reaction times. However, the relative peak intensities of the higher MW species occurred more in the gel than in the liquid. More extensive condensation reactions occurred by the 4-hr reaction time.
·The major component observed by ESI-MS for both 1-hr and 4-hr was T'4 (monocyclic structure) in the liquids and T2T'4 (bicyclic structure) in the gels, where T = CH3CH2SiO3/2 and T' = CH3CH2(Z'O)SiO2/2, Z' = H or Me.
·The NMR results support the findings from the GPC and ESI-MS analyses, indicating that the condensation reactions continued over the period of time.
·In the NMR analysis, a small ratio of CH3CH2Si(OZ)3 [Z = most likely H(2) or can be assigned as OC(O)CH3)] species still existed in the liquid layer for both 1-hr and 4-hr

samples.
·Breakdown products from hydrolysis: acetic acid and silanol. The stabilities of acetic acid and silanol were not measured. However, in general, silanols will undergo condensation reactions to form siloxanes. The stabilities of silanols follow the order R3SiOH > R2Si(OH)2 > RSi(OH)3, with the bulkier R groups lending more stability to the SiOH function.

Test condition : ·Analytical procedures:
o0.1 N HCl solution in water (Lot# 04126DA, Conc. 0.0994 N) was purchased from Sigma-Aldrich company.
o0.6:2 (v/v) of the neat ethyltriacetoxysilane and 0.1 N HCl were mixed in a HDPE bottle inside N2 bag as test solution to simulate gastric conditions.
oThe test solution was immediately aliquot into six HDPE vials followed by hand mixing for ~ 3 sec. and then placed into an Digital Incubator Shaker (innovaTM 4000/4080, New Brunswick Scientific Co., Inc.) which was pre-set at 37 ± 0.2oC and 25 RPM. Three of the sub-samples were allowed to equilibrate in the Incubator for 1 hour ± 10 minutes, and the other three was in there for 4 hours ± 10 minutes prior to analysis.
oTemperature: 37 ± 0.2oC
oReplicates: Single
oVessels: 60-mL High-density polyethylene (HDPE) bottles with screw caps. 20-mL HDPE Scintillation vials with cone-shaped plastic liner screw cap for GPC and NMR sub-samples, and with Teflon septum screw caps for MS sub-samples. Vessels were not sterilized.
oCo-solvent: None
oGel permeation chromatography (GPC) was used to determine the relative molecular weight distribution (MWD) of the hydrolysis and condensation products.
oThe chromatographic equipment consisted of a Waters 600 pump, a Waters 717 autosampler and a Waters 410 differential refractometer. The separation was made with two PLgel 5 um Mixd-C columns (Polymer Laboratories, 300 mm x 7.5 mm, molecular weight separation range of 200 to 2,000,000), preceded by a PLgel 5 um guard column (50 mm x 7.5 mm).
oThe samples were prepared in THF at about 2% w/v solids (using the entire sub-samples), and filtered through a 0.45 µm PTFE syringe filter into glass autosampler vials. All samples appeared to completely dissolve in THF.
oESI-MS spectra were acquired on a Sciex API 350 triple quadrupole mass spectrometer (Sciex, Toronto, Canada) or a Bruker (Bruker Daltonics, Billerica) APEX II 47e Fourier transform ion cyclotron resonance mass spectrometer (FTICR MS).
oThe samples (total of 8) were prepared separately by dissolving approximately 10 ul liquid and 0.01 g gel into ~ 6 ml CH3CN/CHCl3 (1:1) from each sub-sample at 1-hr and 4-hr reaction times.
oA Varian Mercury 300 MHz spectrometer equipped with a switchable probe was used to collect the NMR data for the gels.
oA Varian Mercury 400 MHz FT-NMR spectrometer equipped with 13C/29Si Silicon-free probe was used to collect the NMR data for the liquids.
o 29Si NMR spectra were acquired at the two reaction times for both liquid (in D2O) and gel (in d-DMSO) NMR samples

(total of 8).

·Data treatment:
oFor GPC analysis, molecular weight averages were determined relative to a calibration curve (3rd order) created using polystyrene standards covering the molecular weight range of 580 - 2,300,000. Also, the area percent values were not only relative to the polystyrene standards, but the responses of the higher and lower molecular weight species (assuming equal responses for all species). Data collection and processing was performed using PE Nelson Access*SEC software.
oThe ESI-MS instrument was calibrated with a Hewlett Pakard ES tuning mix with molecular weight spanning a mass range of m/z 118 - m/z 2722. Data acquired in the broadband mode were typically collected using 512 K data points.
oNMR data were acquired and processed using both merc300 and merc400. Data was processed using Varian's VNMR version 6.1. Based on the NMR peak integration and chemical shift, molar ratio of each type of produced species at the two reaction times were determined. Estimated relative error for the gel samples is ±8%.

Test substance : Ethyltriacetoxysilane CH3CH2Si[OC(O)CH3]3; CAS number:17689-77-9; Purity: 98.5% by GC

Conclusion : In general, both NMR and ESI-MS analyses showed that similar hydrolysis/condensation species were observed in both liquid and gel samples at both reaction times. The major component observed by ESI-MS for both 1-hr and 4-hr was T¢4 (monocyclic structure) in the liquids and T2T¢4 (bicyclic structure) in the gels, where T = CH3CH2SiO3/2 and T¢ =? CH3CH2(Z¢O)SiO2/2, Z¢ = H or Me. The number-average and weight-average molecular weights of the ethyltriacetoxysilane solution were determined by GPC to be 633 and 809, respectively, with 22% of the chromatogram represented by a MW range higher than 1000 at the1-hr reaction time. At the 4-hr reaction time, the number-average and weight-average molecular weights increased to 750 and 1085, respectively, with 38% of the chromatogram represented by a MW range higher than 1000. The test substance was found to be hydrolytically unstable at 37oC with 25 RPM slow shaking under the given pH 1.29 condition.

Reliability : (1) valid without restriction
17.03.2004 (84)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : other: Fugacity model Level III

Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: calculated using EQC (equilibrium criterion) model; version 1.01
Year : 2001

Remark : Acetoxysilane materials, including ethyltriacetoxysilane, are highly reactive and hydrolytically unstable. Upon contact with water or water vapor, acetoxysilane materials rapidly generate acetic acid and the corresponding silanol which, depending upon concentration, will condense to form a highly cross-linked polymeric gel. The measured hydrolysis half-life for ethyltriacetoxysilane at pH 7.1 is < 13 seconds at 25 ºC (1). As such, ethyltriacetoxysilane will not exist in the environment but will rapidly hydrolyze to acetic acid and ethylsilanetriol. The fate, transport, and distribution of ethyltriacetoxysilane in the environment were evaluated using the fugacity-based EQC (equilibrium criterion) model

Result : Level-I Simulation: Results from the Level-I simulation indicate that ethyltriacetoxysilane has the tendency to partition almost exclusively into the water compartment, which holds essentially 99% of the total chemical mass. About 1% of the total mass of ethyltriacetoxysilane is equally distributed between the air and soil compartments, with an insignificant amount (< 0.1% of the total mass) found in the sediment compartment.

Environmental distribution of ethyltriacetoxysilane, based on Level-I fugacity modeling.

Environmental Distribution (%)			
Air	Water	Soil	Sediment
0.6	98.9	0.5	0.0

Level-II Simulation: Results from the Level-II simulation show the same environmental distribution characteristics as the Level-I simulation, with 99% of the total mass of ethyltriacetoxysilane found in the water compartment. The results also show that degradation (i.e., hydrolysis) in water is the primary mechanisms of removal for ethyltriacetoxysilane in the local environment. Degradation in air and soil, and advective losses account for < 0.2% of the total mass removed. Output from the model indicates that ethyltriacetoxysilane will have a local persistence of about 0.005 hours (18 sec) and a global persistence of about 0.005 hours (18 sec).

Table 3. Distribution and environmental residence time of ethyltriacetoxysilane, based on Level-II fugacity modeling.

	Environmental Compartment			
	Air	Water	Soil	Sediment
Distribution(%)	0.6	98.9	0.5	0.0
Reaction losses(%)	0.1	99.9	0.1	0.0
Advective losses(%)	0.0	0.0		0.0

Overall residence time(h) 0.005

Reaction residence time(h) 0.005
Advective residence time(h) 955
Level-III Simulation: Results from the Level-III simulations demonstrate that 100% of the total mass of ethyltriacetoxysilane released into an environmental compartment (i.e., air, water, or soil) will be rapidly degraded within that compartment. Emission of ethyltriacetoxysilane directly to air results in 100% of the total chemical mass residing in the air compartment, with degradation in air accounting for >99% of the total mass removed from the local environment. Similar results were obtained when ethyltriacetoxysilane was released directly to soil or water. In all simulations, intermedia exchange of ethyltriacetoxysilane between the other compartments was insignificant. Likewise, advective losses of the total chemical mass removed from the system were insignificant (< 0.1%). Persistence of ethyltriacetoxysilane in the model system was about 0.05 hours (3 min) or less, regardless if the material is emitted to air, soil, or water.

Distribution and environmental residence time of ethyltriacetoxysilane emitted to the the air, soil and water compartments, based on Level III fugacity modeling.

Emission Rates (Kg/h): Air = 1000; Soil = 1000; Water = 1000

	Environmental Compartment			
	Air	Water	Soil	Sediment
Distribution (%)	47.3	5.3	47.4	0.0
Reaction losses (%)	33.3	33.3	33.3	0.0
Advective losses (%)	0.0	o.o	0.0	

Overall residence time (h) .037
Reaction residence time (h) .037
Advective residence time (h) 209

Source : SEHSC

Test condition : (Note 1): Water solubility of ethyltriacetoxysilane at 25 ºC was estimated using the SAR Model WSKOWWIN® (version 1.40). The model was used as received from the United States Environmental Protection Agency (USEPA, 2000). A melting point of 8.4 ºC (Principe, 2000) was used for the estimation.
(Note 2): Vapor pressure of ethyltriacetoxysilane at 25 ºC was extrapolated from a temperature-vapor pressure relationship that was developed using peer-reviewed experimental data measured at temperatures ranging from 87-119 ºC (Smith, 1988).
(Note 3): Log Kow of ethyltriacetoxysilane at 25 ºC was estimated using the SAR Model KOWWIN® (version 1.66). The model was used as received from the United States Environmental Protection Agency (USEPA, 2000).
(Note 4): Hydrolysis is the primary degradation pathway for ethyltriacetoxysilane, which rapidly generates acetic acid and ethylsilanetriol upon contact with water or water vapor. The half-life of ethyltriacetoxysilane in sediment was assumed to be equal to the measured half-life in water. Because of the decreased activity of water in air and soil, the half-life of ethyltriacetoxysilane in these two compartments was assumed to be 10 times longer than the measured half-life in water.

The EQC model (Mackay, D., A. Di Guardo, S. Paterson, C.E. Cowan. 1996) was used for all fugacity calculations as recommended by EPA. All simulations were conducted at a data temperature of 25degC using default values of the model for compartment dimensions and properties. If chemical-specific data required for the simulations were not available, estimated values were obtained using structure activity relationship (SAR) models developed by the EPA Office of Pollution Prevention Toxics and Syracuse Research Corporation, as provided with the EPI Suite™ (version 3.10) package (EPA, 2000). Level-I, -II, and -III fugacity models for a Type-1 chemical (i.e., chemicals that partition into all environmental media) were used for the simulation.

Physical and chemical properties of ethyltriacetoxysilane:
Molecular weight: 234.28
Data temperature (deg C): 25
Water solubility (g/m3): 41,570 (estimated value) (Note 1) (USEPA, 2000)
Vapor pressure (Pa): 5.1 (interpolated from temperature-vapor pressure correlation) (Note 2) (Smith, 1988)
Log Kow: 0.74 (estimated value) (USEPA, 2000)
Melting point (deg C): 8.4 (Principe, 2000)
Half-life in air (h): 0.036 (Assumed to be 10 times longer than the half-life in water) (Note 4)
Half-life in water (h): 0.004 (Measured at pH 7.1 and 25 ºC) (Sun and Taylor, 2001)
Half-life in soil (h): 0.036 (Assumed to be 10 times longer than the half-life in water) (Note 4)
Half-life in sediment (h): 0.004 (Assumed to be equal to the half-life in water) (Note 4)

Conclusion : Results from the multimedia model simulations indicate that ethyltriacetoxysilane will not exist in the environment. Rather, ethyltriacetoxysilane will rapidly degrade (i.e., hydrolyze) to acetic acid and ethylsilanetriol within the environmental compartment (air, water, soil) in which it is released. Because of the rapid rates of degradation, advective losses and intermedia exchange of ethyltriacetoxysilane between environmental compartments is insignificant. However, the fate, transport, and distribution of the hydrolysis product, ethylsilanetriol, will be dependant upon the environmental compartment in which ethyltriacetoxysilane is released. Because of its high solubility and relatively low volatility, ethylsilanetriol is not expected to partition to air, even when the material is produced from ethyltriacetoxysilane emitted directly to the air compartment. Biodegradation in soil and water remove about 90% of total mass of ethylsilanetriol from the local environment, whereas advection in water accounts for about 10%. In contrast, emission of ethyltriacetoxysilane directly to water results in ethylsilanetriol remaining almost exclusively to the water compartment (>99% of the total mass), with biodegradation and advection accounting for 66% and 34%, respectively, of the total mass removed from the model system. Global persistence of ethylsilanetriol in the model system was about 22 days, regardless if

ethyltriacetoxysilane was released directly to air, soil or water. Hence, the environmental compartments of concern for ethyltriacetoxysilane, based on formation of the degradation product ethylsilanetriol (and ignoring the effects of acetic acid), are water and soil.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
01.11.2005 (61) (71) (72) (78) (85) (91)

Type : other
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: calculated
Year : 2001

Remark : The measured hydrolysis half-life for ethyltriacetoxysilane at pH 7.1 is < 13 seconds at 25 ºC. As such, ethyltriacetoxysilane will not exist in the environment but will rapidly hydrolyze to acetic acid and ethylsilanetriol. Hence, the environmental fate, transport, and distribution of ethylsilanetriol were evaluated to provide a more realistic assessment of ethyltriacetoxysilane. The EQC model was used for all fugacity calculations as recommended by EPA. All simulations were conducted at a data temperature of 25*C using default values of the model for compartment dimensions and properties. If chemical-specific data required for the simulations were not available, estimated values were obtained using structure activity relationship (SAR) models developed by the EPA Office of Pollution Prevention Toxics and Syracuse Research Corporation, as provided with the EPI Suite™ (version 3.10) package. The Level-III fugacity model for a Type-1 chemical (i.e., chemicals that partition into all environmental media) was used for the simulations. Results are summarized in Tables 6a-6c.

Physical and chemical properties of ethylsilanetriol (hydrolysis product of ethyltriacetoxysilane):
Molecular weight: 108.17
Data temperature (deg C): 25
Water solubility (g/m3): 4.3 x 10E6 (estimated value) (Note 1) (USEPA, 2000)
Vapor pressure (Pa): 0.039 (estimated value) (Note 2) (USEPA, 2000)
Log Kow: -1.87 (estimated value) (Note 3) (USEPA, 2000)
Melting point (deg C): 36.02 (estimated value) (Note 4) (USEPA, 2000)
Half-life in air (h): 11.1 (estimated value) (Note 5) (USEPA, 2000)
Half-life in water (h): 360 (estimated value) (Note 6) (USEPA, 2000)
Half-life in soil (h): 360 (Assumed to be equal to half-life in water) (Note 6)
Half-life in sediment (h): 1440 (Assumed to be 4 times the half-life in water) (Note 6)

(Note 1): Water solubility of ethylsilanetriol at 25 ºC was estimated using the SAR Model WSKOWWIN® (version 1.40). The model was used as received from the United States Environmental Protection Agency (USEPA, 2000).
(Note 2): Vapor pressure of ethylsilanetriol at 25 ºC was estimated using the SAR Model MPBPWIN® (version 1.40). The model was used as received from the United States Environmental Protection Agency (USEPA, 2000).
(Note 3): Log Kow of ethylsilanetriol at 25 ºC was estimated using the SAR Model KOWWIN® (version 1.66). The model was used as received from the United States Environmental Protection Agency (USEPA, 2000).
(Note 4): Melting point of ethylsilanetriol at 25 ºC was estimated using the SAR Model MPBPWIN® (version 1.40). The model was used as received from the United States Environmental Protection Agency (USEPA, 2000).
(Note 5): Half-life of ethylsilanetriol in air was estimated using the SAR Model AOPWIN® (version 1.90). The model was used as received from the United States Environmental Protection Agency (USEPA, 2000).
(Note 6): Half-life of ethylsilanetriol in water was estimated using the SAR Model BIOWIN® (version 4.00). The model was used as received from the United States Environmental Protection Agency (USEPA, 2000). The BIOWIN result for ultimate biodegradation timeframe (2.9601; "weeks") was converted to an estimated half-life in water (360 days) using the EPA default conversion factors in EPI Suite™ (USEPA, 2000). Similarly, default half-life factors in EPI Suite™ were used to estimate the half-life of ethylsilanetriol in soil (1x the half-life in water) and sediment (4x the half-life in water).

Table 6a. Distribution and environmental residence time of ethylsilanetriol (hydrolysis product of ethyltriacetoxysilane) generated in the atmospheric compartment, based on Level-III fugacity modeling.

Emission Rates (kg/h): Air = 1000; Soil = 0; Water = 0

	Environmental Compartment			
	Air	Water	Soil	Sediment
Distribution (%)	0.0	28.0	71.9	0.0
Reaction losses (%)	0.0		24.5	62.8 0.0
Advective losses (%)	0.0		12.7	0.0

Overall residence time (h)	454
Reaction residence time (h)	520
Advective residence time (h)	3568

Table 6b. Distribution and environmental residence time of ethylsilanetriol (hydrolysis product of ethyltriacetoxysilane) generated in the soil compartment, based on Level-III fugacity modeling.

Emission Rates (kg/h): Air = 0; Soil = 1000; Water = 0

	Environmental Compartment			
	Air	Water	Soil	Sediment
Distribution (%)	0.0	22.2	77.8	0.0
Reaction losses (%)	0.0	19.9	69.8	0.0
Advective losses (%)	0.0	10.3		0.0

Overall residence time (h) 466
Reaction residence time (h) 520
Advective residence time (h) 4514

Table 6c. Distribution and environmental residence time of ethylsilanetriol (hydrolysis product of ethyltriacetoxysilane) generated in the water compartment, based on Level-III fugacity modeling.

Emission Rates (kg/h): Air = 0; Soil = 0; Water = 1000

	Environmental Compartment			
	Air	Water	Soil	Sediment
Distribution (%)	0.0	99.8	0.0	0.2
Reaction losses (%)		0.0	65.8	0.0 0.0
Advective losses (%)		0.0	34.2	0.0

Overall residence time (h) 342
Reaction residence time (h) 520
Advective residence time (h) 1002

Source : Dow Corning Corporation Midland, MI
Test substance : Other: ethylsilanetriol
Reliability : (1) valid without restriction
27.05.2004 (70)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : other: domestic sewage
Concentration : 1086 mg/l related to Test substance
457 mg/l related to DOC (Dissolved Organic Carbon)
Contact time : 21 day(s)
Degradation : = 74 (±) % after 21 day(s)
Result : readily biodegradable
Kinetic of testsubst. : 0 day(s) = 0 - 0 %
7 day(s) = 77.16 - 77.39 %
14 day(s) = 71.28 - 72.27 %
21 day(s) = 72.47 - 76.16 %
%
Control substance : Benzoic acid, sodium salt
Kinetic : 0 day(s) = 0 - 0 %
21 day(s) = 96.63 - 98.33 %
Deg. product : not measured
Method : Directive 84/449/EEC, C.4 "Biotic degradation - modified AFNOR test NF T90/302"
Year : 1995
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : DOC-DIE AWAY TEST (EEC Guideline 79/831/EEC, Appendix V,Part C (updated edition dated July 1990), Method C.4-A.
Remark : Rates of hydrolysis have been determined for

methyltriacetoxysilane and ethyltriacetoxysilane. The hydrolytic half-lives were < .2 minutes for pH 7.1 at 25 ºC. These results confirm that these close structural analogs are hydrolytically unstable and will immediately hydrolyze upon contact with water or watervapor. Methyl- and ethyltriacetoxysilane rapidly hydrolyzeand generate 3 moles of acetic acid for every mole of parent material.
The test material rapidly hydrolyzes to acetic acid and silanetriol.

Test condition : Inoculum was a living slime from a primary communal sewage treatment plant (Marl-East). The test consisted of two flasks with test substance (14.99 mg DOC/l after 3 h) and inoculum; two flasks without test substance with inoculum;and two flasks with sodium benzoate (13.71 mg DOC/l after 3h) and inoculum.

DOC analyses was performed at 0 and 3 hours and on the 7th,14th and 21st days. DOC analyses were in the form of a double determination of oxygen-enriched and de-gassed samples (removal of inorganic carbon). The DOC analysis was performed using two-point calibration in a carbon analyzer.

Test substance : DYANSYLAN ATAC: 99.4% Ethyltriacetoxysilane.

The test substance is susceptible to hydrolysis.

Conclusion : DYNASYLAN ATAC achieved a breakdown rate of 74% (DOC reduction) within 21 days. Since the degree of breakdown within 10 days after an initial exceedance of the 10% breakdown threshold was greater than 70%, the substance may be considered "readily biodegradable".

The control substance achieved a breakdown rate of >70% (DOC reduction) within 14 days. Thus, the sludge specimen used possessed sufficient biological activity.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
02.12.2004 (26)

Type : aerobic
Inoculum : other: activated sludge
Concentration : 100 mg/l related to Test substance
related to
Contact time : 14 day(s)
Degradation : (±) % after
Result : readily biodegradable
Deg. product :
Method : OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year : 1993
GLP : no data
Test substance : other TS

Method : Concentration of Activated Sludge = 30 ppm
MITI-I(OECD TG 301C)
Result : BOD = 74%
Test substance : Acetic acid; 64-19-7
Conclusion : Chemical substance determinated to be ready biodegradable
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
31.10.2005 (67)

Type	:	anaerobic
Inoculum	:	domestic sewage, non-adapted
Concentration	:	30 mg/l related to DOC (Dissolved Organic Carbon) related to
Contact time	:	28 day(s)
Degradation	:	= 99 (±) % after 7 day(s)
Result	:	readily biodegradable
Deg. product	:	
Method	:	other
Year	:	1995
GLP	:	no data
Test substance	:	other TS
Method	:	Medium: Sewage treatment Test procedures were carried out in an enclosed glove box with N2 atmosphere. Oxygen-free water was used. The test period was 4 weeks at 37 °C and with pH adjusted to 7. Biodegradation was determined by analyzing the decrease of DOC.
Remark	:	Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Test substance	:	Acetic acid (64-19-7)
Reliability	:	(2) valid with restrictions

31.10.2005 (2) (58)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Elimination	:	
Method	:	other: estimated
Year	:	2004
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Bioaccumulation is not anticipated since this material is hydrolytically unstable. Rapid hydrolysis of this material produces acetic acid and trisilanols. The Si-C bond will not undergo further hydrolysis. That bond is hydrolytically stable. Only the acetoxy groups will be hydrolyzed. The transient silanol groups will condense with other silanols to yield: Et-Si(OR)3 type resins where R=H or -Si(Et)(OR)2 As a result silanol-functional resins are generated. If the silane is slowly released such that the concentration of the resulting silanetriol is not high enough to result in polymerization, the trisilanol will exist largely as a monomer. The monomer is known to be water soluble by virtue of the three hydroxy groups on the silicon. It is expected

that this silanetriol will have a low Kow because of these hydroxy groups and so is not expected to bioaccumulate. The water solubility of the silanetriol cannot be measured because of the tendency to condense at concentrations greater than 500 ppm. It is known however that the silanetriol and small condensation products will only precipitate out of water due to formation of larger, water insoluble polymeric resins.

Reliability : (2) valid with restrictions
02.12.2004

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Brachydanio rerio (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC0	:	= 180
LC50	:	= 251
LC100	:	= 350
Limit test	:	yes
Analytical monitoring	:	yes
Method	:	Directive 92/69/EEC, C.1
Year	:	1995
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Method : Analytical evaluation of test substance concentrations was performed by TOC determination.

Groups of ten fish per 20 l aquarium were exposed for 96 hours to test substance target concentrations of 0, 100, 180, 350, 550 or 1000 mg/l.

The test solutions were not neutralized.

Remark : Because ethyltriacetoxysilane generates considerable amounts of acetic acid when exposed to water, results from aquatic tests reflect the toxicity of acetic acid rather than the toxicity of the parent triacetoxysilane. Acetoxysilanes are highly reactive and undergo rapid hydrolysis when exposed to moisture. When ethyltriacetoxysilane is added to water, 100% of the parent compound is hydrolyzed in less than 0.2 minutes, producing 3 moles of acetic acid and 1 mole of silanetriol for every mole of parent material. Studies indicate that the observed acute toxicity of ethyltriacetoxysilane (CAS No. 17689-77-9) to aquatic organisms is due to acetic acid. When results are expressed on the basis of the amount of acetic acid generated from the hydrolysis reaction, the toxicity of ethyltriacetoxysilane is comparable to the reported toxicity of acetic acid (EC50 =50-450 mg/L), depending on test species.
Mortality may be attributed to the low pH values in higher concentrations. At 0 hours, the pH of the test solutions at concentrationsof 0, 100, 180, 350, 550, and 1000 mg/L was 7.6, 6.2, 5.6, 4.6, 4.3, and 3.9, respectively. By 24 hours, the pH was 7.5, 6.2, 5.6, and 4.8 in solutions containing 0, 100, 180, and 350 mg/L, respectively (100% mortality in solutions containing 550 and 1000 mg/L). By 48 hours, pH values of 7.6, 6.3, and 5.6 were recorded for solutions of 0, 100, and 180 mg/L, respectively (100% mortality in solution containing 350 mg/L). At 72 hours, pH values of 7.9, 6.8, and 6.2 were recorded for solutions of 0, 100, and 180 mg/L, respectively.
OECD Guideline 203 indicates that the test should be carried out without adjustment of pH. However, if there is evidence of marked change in the pH of the tank water after addition of the test substance, it is advisable that the test be

repeated, adjusting the pH of the stock solution to that of the tank water before addition of the test substance. This pH adjustment should be made in such a way that the stock solution concentration is not changed to any significant extent and that no chemical reaction or precipitation of the test substance is caused.

Result : Measured concentrations after 24 hours deviated < 20% from fresh concentrations. It was assumed that neither the test substance or any hydrolysis products were removed from the test system, and were considered biologically available.

Target Concentrations (mg/l)	Geometric Measured Concentrations (0-24 hrs) (mg/l)
100	115
180	191
350	376
550	568
1000	971

The LC50 values for 24, 48, 72 and 96 hours were 313, 251, 251, and 251, respectively.

Test substance : DYNASYLAN ATAC: 99.4% Ethyltriacetoxysilane.

The test substance is susceptible to hydrolysis.As the test substance has low water solubility, it was dissolved at 1 g/l in VE water and stirred for 18 h and then filtered.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
01.11.2005 (22)

Type : flow through
Species : Carassius auratus (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
mortality : = 100
Method : other
Year : 1937
GLP : no
Test substance : other TS

Method : Age/Life Stage: 60-90 millimeters, 3-5 grams
Water Parameters:
Temperature: 18-23 deg C
Hardness: HARD
Dissolved O2: 6-7 mg/L
pH: 6.8 (mean value)

Exposure Duration: 48-96 hours

Remark : Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
31.10.2005 (38) (89)

Type : other: not reported
Species : Cyprinus carpio (Fish, fresh water)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : = 49
Method : other
Year : 1976
GLP : no data
Test substance : other TS

Method : Age/Life Stage: not reported
Water Parameters:
Temperature:17-18 deg C
pH = 5.8 (minimum value)-7.2 (maximum value)
Remark : Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
31.10.2005 (44) (89)

Type : static
Species : Gambusia affinis (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 251
Limit test :
Analytical monitoring : no data
Method : other
Year : 1957
GLP : no
Test substance : other TS

Method : Age/Life Stage: Adult female
Water Parameters:
Temperature: 16-25 deg C
Alkalinity: <100 mg/l CaCO3 (mean value)
pH: 6.9 (minimum value)-8.7 (maximum value)
Turbidity <= 25 TO 169 mg/l

Ten fish were exposed to test concentrations for a period of 96 hours. The concentrations used for the first experiment were 10, 18, 32, 56 and 100 ppm. When deaths did not occur at these concentrations within 96 hours the same series was run between 100 and 1,000 ppm. The temperature, turbidity, and pH of the experimental water were measured after the test substance was added and daily throughout the experiment. Survivor observations were made at 24, 48, 72 and 96 hours. Test water was maintained at pH 6.9 - 8.7 and 16-25°C.
Remark : Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid

and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : Fish transferred to concentrations between 100 and 1,000 ppm swam frantically and at 100 and 180 ppm returned to normal in 24 hours. At 320 ppm and higher all fish were dead at 24 hours.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
31.10.2005 (2) (89) (95)

Type : static
Species : Ictalurus punctatus (Fish, fresh water)
Exposure period : 72 hour(s)
Unit : mg/l
LC50 : = 446
Method : other
Year : 1959
GLP : no
Test substance : other TS

Method : Age/Life Stage: FINGERLINGS, 2-3 inches
Water Parameters: 25 deg C (mean value)
Remark : Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
03.06.2005 (19) (89)

Type : static
Species : Lepomis macrochirus (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 75
Method : other
Year : 1960
GLP : no
Test substance : other TS

Method : Age/Life Stage: 5.3-7.2 centimeters, 3.5-3.9 grams
Water Parameters:
Temperature: 18-20 deg C
Hardness: 10 mg/l CaCO3 (mean value)
Dissolved O2: 5-9 mg/l
Remark : Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
31.10.2005 (89) (90)

Type : static

Species	:	Lepomis macrochirus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
NOEC	:	= 56
LC50	:	= 68
LC100	:	= 100
LOEC	:	= 100
Limit test	:	
Analytical monitoring	:	no
Method	:	other: Methods for acute toxicity tests with fish, macroinvertebrates, and amphibians. United States Environmental Protection Agency, EPA 660/3 75 009, 1975
Year	:	1980
GLP	:	no
Test substance	:	other TS
Method	:	Test Vessels: Polyethylene-lined containers Test System: Bluegill sunfish (Lepomis macrochirus) - 10 fish/control; 10 fish/exposure concentration. Endpoint: 96-h mortality Statistics: Probit analysis based on Finney's Method (Statistical Methods In Biological Assay, 1952) Exposure Concentrations (product, mg/L) " nominal: 0, 10, 18, 32, 56, 100 Test Procedure and Conditions " exposure period: 96 h "dilution water: reconstituted soft-water "temperature: 22 C "study design: static exposure "carrier solvent: none "observation periods: 0, 24, 48, 72, 96 h The test solutions were not neutralized.
Remark	:	Vinyltriacetoxysilane is a structural analogue for methyltriacetoxysilane (CAS 4253-34-3) and ethyltriacetoxysilane (CAS 17689-77-9)
Result	:	"NOEC = 56 "LC10 = 34 (15-47; 95% CI) "LOEC = 100 "LC50 = 68 (51-103; 95% CI) "LC100 = 100 "LC90 = 133 (92-421; (95% CI) Test substance added directly to each test chamber, a carrier solvent was not used. Dissolved oxygen and pH were measured at test initiation and termination. No mortality observed in controls. One mortality observed in 32 mg/L exposure at 96-h observation-was not considered dose related. No mortality observed in 56 mg/L exposure (NOEC). No mortality observed in 100 mg/L exposure (LOEC and LC100) until 24-h observation (100% mortality).
Test substance	:	Dow Corning Z-6075 Silane Specified composition - not specified; Dow Corning MDMS database indicates that the test material is 93% vinyltriacetoxysilane (CAS 4130-08-9)
Reliability	:	(2) valid with restrictions
31.10.2005		(31)
Type	:	static
Species	:	Oncorhynchus mykiss (Fish, fresh water)

Exposure period	:	96 hour(s)
Unit	:	mg/l
NOEC	:	128
LC0	:	128
LC50	:	271
Limit test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	2004
GLP	:	yes
Test substance	:	other TS

Method :

OECD. 1993. OECD Guidelines for Testing of Chemicals. Guideline 203: Fish, Acute Toxicity Test. Updated Guideline adopted on 17 July 1992.

USEPA. 1996. Fish Acute Toxicity Test, Freshwater and Marine. Series 850 - Ecological Effects Test Guidelines (draft), OPPTS Number 850.1075.

Statistical methods: Binomial Probability, Probit Met
96-Hour Static-Renewal Acute (Daily Renewals)
Test fish: Age 77 Days/Mean Total Length 5.9 cm (Range 5.5 to 6.3 cm)/Wet Weight 1.7 g (Range 1.4 to 2.3 g), Loading 0.58 g/L, Fish were acclimated to laboratory conditions for a minimum of 2 weeks prior to the test.
Test Conditions:
oSemi-Static
oDilution water source: Well Water
oDilution water chemistry: Hardness 122 mg/L as CaCO3, Alkalinity 180 mg/L as CaCO3, Conductivity 270 mhos/cm, pH 8.6
oStock and test solution and how they were prepared: Direct addition of test article to dilution water
oConcentrations dosing rate: Negative Control, 63, 125, 250, 500 and 1000 mg/L in dilution water
oVehicle/solvent and concentrations: No organic solvent
oStability of the test chemical solutions: Not Stable
oExposure vessel type: 38-L or 54-L stainless steel aquaria containing 30-L of test solution
oNumber of replicates, fish per replicate: Two replicates per treatment, 10 Fish per replicate
oWater chemistry in test: DO, pH and temperature measured in each test chamber daily (old and new solutions as appropriate)
Test Temperature Range: 11.3 - 12.2 C
Method of Calculating Mean Arithmetic mean.
Measured Concentrations: Negative Control, 63, 125, 250, 500 and 1000 mg/l.
Measurement of test concentrations in each test chamber at test initiation, on Day 1 (old solutions) and at test termination by GC/FID.

Remark : Acetoxysilanes rapidly hydrolyze to form silanols and acetic acid. The toxicity of trimethylsilanol was determined in this study, as a means to further characterize the toxicity of the parent material.

Result : Measured concentrations (as mg/L):<LOQ, 65, 128, 250, 481 and 949

Statistical results (95% confidence interval), as

appropriate:
24-Hour LC50: >949 mg/L (not calculable)
48-Hour LC50: 523 mg/L (250 - 949)
72-Hour LC50: 476 mg/L (402 - 565)
96-Hour LC50: 271 mg/L (128 - 481 mg/L)
No Mortality Concentration - 128 mg/L
NOEC - 128 mg/L

Biological observations: After 96 hours of exposure, all surviving fish appeared normal.
Table showing cumulative mortality:

Mean Measured Concentration (mg/L)	Number Dead/Number Exposed (hours) 0	24	48	72	96
0	0/20	0/20	0/20	0/20	1/20
65	0/20	0/20	0/20	0/20	0/20
128	0/20	0/20	0/20	0/20	0/20
250	0/20	0/20	0/20	1/20	8/20
481	0/20	0/20	8/20	9/20	20/20
949	0/20	6/20	20/20	20/20	20/20

Lowest test substance concentration causing 100% mortality: 481 mg/L
"Mortality of controls: 5%
"Abnormal responses: Surfacing, loss of equilibrium, erratic swimming and lying on bottom
"Any observations, such as precipitation that might cause a difference between measured and nominal values: All test solutions appeared clear and colorless.

Test substance : Trimethylsilanol (CAS Number 1066-40-6)
Conclusion : The 96-hour LC50 for rainbow trout (Oncorhynchus mykiss) exposed to trimethylsilanol under static-renewal test conditions was 271 mg/L with 95% confidence limits of 128 and 481 mg/L. The no mortality concentration and NOEC were 128 mg/L.
Reliability : (1) valid without restriction
This was a GLP compliant study with measured test concentrations. The study is scientifically defensible because a concentration-effect relationship was demonstrated
Flag : Critical study for SIDS endpoint
31.10.2005 (96)

Type : static
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : = 32
LC50 : = 51
LC100 : = 100
LOEC : = 56
Method : other: Methods for acute toxicity tests with fish, macroinvertebrates, and amphibians. United States Environmental Protection Agency, EPA 660/3 75 009, 1975
Year : 1980
GLP : no
Test substance : other TS

Method : Test Vessels: Polyethylene-lined containers

Test System: Rainbow trout (Oncorhynchus mykiss) - 10 fish/control; 10 fish/exposure concentration
Endpoint: 96-h mortality
Statistics: Probit analysis based on Finney's Method (Statistical Methods In Biological Assay, 1952)

Exposure Concentrations (product, mg/L)
" nominal: 0, 10, 18, 32, 56, 100

Test Procedure and Conditions
" exposure period: 96 h
" dilution water: reconstituted soft-water
"temperature: 12 C
" study design: static exposure
"dissolved oxygen:
" carrier solvent: none
" observation periods: 0, 24, 48, 72, 96 h
The test solutions were not neutralized.

Remark : Vinyltriacetoxysilane (CAS 4130-08-9) is a structural analogue for methyltriacetoxysilane (CAS 4253-34-3) and ethyltriacetoxysilane (CAS 17689-77-9)

Result : "NOEC = 32
"LC10 = 29 (15-18; 95% CI)
"LOEC = 56
"LC50 = 51 (39-67; 95% CI)
"LC100 = 100
"LC90 = 88 (67-175; 95% CI)

Test substance added directly to each test chamber, a carrier solvent was not used. Dissolved oxygen and pH were measured at test initiation and termination. No mortality observed in controls. No mortality observed in 56 mg/L exposure (LOEC) until 48-h observation (30% mortality)-60% mortality observed at 96-h observation. No mortality observed in 100 mg/L exposure (LC100) until 24-h observation (100% mortality).

Test substance : Dow Corning Z-6075 Silane
Specified composition - not specified; Dow Corning MDMS database indicates that the test material is 93% vinyltriacetoxysilane (CAS 4130-08-9)

Reliability : (2) valid with restrictions
31.10.2005 (31)

Type : static
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 79
Method : other
Year : 1976
GLP : no
Test substance : other TS

Method : Age/Life Stage: JUVENILE, 4-8 weeks, 1.1-3.1 centimeters
Water Parameters:
Temperature: 18 - 22 deg C
Dissolved O2: >4.0 mg/L (mean value)
pH: <=5.9 (mean value)

Remark : Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the

parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
03.06.2005 (65) (89)

Type : static
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 88
Method : other
Year : 1976
GLP : no data
Test substance : other TS

Method : Age/Life Stage: JUVENILE, 4-8 weeks, 1.1-3.1 centimeters
Water Parameters:
Temperature: 18 - 22 deg C
Dissolved O2: >4.0 mg/L (mean value)
pH: <=5.9 (mean value)
Remark : Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
03.06.2005 (65) (89)

Type : other
Species :
Exposure period :
Unit :
Method : other: analogy
Year : 2004
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Ethyltriacetoxysilane (CAS No. 17689-77-9) and vinyltriacetoxysilane (CAS No. 4130-08-9) have been tested and the results show the resulting toxicity to aquatic organisms is due to acetic acid. When results are expressed on the basis of the amount of acetic acid generated from the hydrolysis reaction, the toxicity of ethyltriacetoxysilane and vinyltriacetoxysilane are comparable to the reported toxicity of acetic acid (EC50 = 50-450 mg/L, depending on test species):

Reported Toxicity (mg/L) of Ethyltriacetoxysilane, Vinyltriacetoxysilane, HOAc and Acetic Acid to Fish (96-h EC50; lethality):

Brachydanio rerio: 251 (Ethyltriacetoxysilane); 194 (HOAc(1))

Oncorhyncus mykiss: 51 (Vinyltriacetoxysilane); 40 (HOAc)

Lepomis macrochirus: 68 (Vinyltriacetoxysilane); 53 (HOAc); 75 (Acetic acid)

Pimephales promelas: 88, 79 (Acetic acid)

Cyprinus carpio: 49 (Acetic acid)

Carassius auratus: 100 (Acetic acid)

Ictalurus punctatus: 446 (Acetic acid)

Gambusia affinis: 251 (Acetic acid)

(1) = HOAc is the estimated toxicity based on the estimated amount of acetic acid generated from the hydrolysis reaction. The amount of acetic acid generated was estimated using the assumption that 1 mole of test material (ethyl- or vinyl- triacetoxysilane) produces 3 moles of acetic acid.

Source : SEHSC
Reliability : (2) valid with restrictions
20.05.2004

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
NOEC	:	= 43
EC50	:	= 62
EC100	:	= 129
24 hr EC50	:	= 85
Limit Test	:	no
Analytical monitoring	:	yes
Method	:	Directive 92/69/EEC, C.2
Year	:	1995
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Method : The test included seven test substance concentrations (target values of 8.6, 15, 26, 43, 75, 129, and 215 mg/l) and a control. Test substance concentrations were determined using a TOC-500 Infrared Analyzer. Daphnia were observed for immobilization at 24 and 48 hours.

Potassium dichromate was used as a reference substance in order to determine the test specimen's sensitivity.

The test solutions were not neutralized.

Remark : Because ethyltriacetoxysilane generates considerable amounts of acetic acid when exposed to water, results from aquatic tests reflect the toxicity of acetic acid rather than the toxicity of the parent triacetoxysilane. Acetoxysilanes are highly reactive and undergo rapid

hydrolysis when exposed to moisture. When ethyltriacetoxysilane is added to water, 100% of the parent compound is hydrolyzed in less than 0.2 minutes, producing 3 moles of acetic acid and 1 mole of silanetriol for every mole of parent material. Studies indicate that the observed acute toxicity of ethyltriacetoxysilane (CAS No. 17689-77-9) to aquatic organisms is due to acetic acid. When results are expressed on the basis of the amount of acetic acid generated from the hydrolysis reaction, the toxicity of ethyltriacetoxysilane is comparable to the reported toxicity of acetic acid (EC50 =50-450 mg/L), depending on test species.
When the results are interpreted, the hydrolysis of the test substance during the preparation of the initial solution or during the test should be considered.

The pH value decreased with increased test concentration:
control pH=8.7
43 mg/l pH=7.5
75 mg/l pH=5.9
129 mg/l pH=4.7
215 mg/l pH=4.1

Result : The geometric mean of analytical values at 0 and 48 hrs deviated <20% from the nominal concentrations as follows:

Target Concentration (mg/l)	48 hr Measured Concentrations (mg/l)
8.6	9.3
15	13.0
26	25.1
43	41.9
75	75.3
129	131
215	215

Nominal concentrations were assumed for the purposes of the evaluation.

The measured concentrations at 48 hrs deviated <20% (up to 8.6 and 15 mg/l) from the fresh concentrations. It was assumed that neither the test substance nor its hydrolysis products were removed from the test system, and are considered biologically available.

Test substance : DYNASYLAN ATAC: 99.4% Ethyltriacetoxysilane.

The test substance is susceptible to hydrolysis.

As the test substance has low water solubility, it was added to synthetic fresh water at 1 g/l and stirred for 18 h. The solution was filtered and the carbon content was determined.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
01.11.2005 (24)

Type : other: renewal
Species : Crangon crangon (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 100

Method : other
Year : 1971
GLP : no
Test substance : other TS

Method : Age/Life Stage: ADULT
Water Parameters:
Temperature: 15 deg C (mean value)
Remark : Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
03.06.2005 (69) (89)

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 24 hour(s)
Unit : mg/l
EC50 : = 6000
Analytical monitoring : no data
Method : other
Year : 1982
GLP : no data
Test substance : other TS

Method : The stock cultures of test organisms were fed dry algae, but no feeding occurred during the 24-hour exposure. The testing took place in a defined standardized culture medium (artificial fresh water). The endpoint was immobilization. Study temperature was 20°C.
Remark : Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
The stated result was for test solutions neutralized (pH 8.0) prior to daphnid exposures. For the un-neutralized test, the 24-hour EC50 was 95 mg/L. The pH of unneutralized test solutions was not stated. Study temperature was 20°C.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
31.10.2005 (2) (14)

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 65
Method : other
Year : 1993
GLP : no data
Test substance : other TS

Method	:	Daphnia magna were exposed to a series of concentrations of acetic acid. The endpoint was immobilization. The test solutions were not neutralized.
Remark	:	Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material. Test solutions were apparently un-neutralized.
Test substance	:	Acetic acid (64-19-7)
Reliability	:	(2) valid with restrictions
31.10.2005		(2) (57)

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
NOEC	:	= 32
EC50	:	> 100
EC100	:	= 100
LOEC	:	= 100
Analytical monitoring	:	no
Method	:	
Year	:	1980
GLP	:	no
Test substance	:	other TS

Method	:	Test Method: Not specified. Other Daphnid studies in 1980 were conducted according to: Methods for acute toxicity tests with fish, macroinvertebrates, and amphibians. United States Environmental Protection Agency, EPA 660/3 75 009, 1975. Test Vessels: Glass beakers, 250-mL Test System: Daphnid (Daphnia magna) - 20 daphnids/control; 20 daphnids/exposure concentration Replicates: Duplicate controls and duplicate exposure concentrations (10 organisms/replicate) Endpoint: 48-h immobility Statistics: Probit analysis based on Finney's Method (Statistical Methods In Biological Assay, 1952) Exposure Concentrations (product, mg/L) "nominal: 0, 1, 3.2, 10, 32, 100 Test Procedure and Conditions "exposure period: 48 h "photo-period: 18L/6D, 600 foot-candle "dilution water: reconstituted hard-water "temperature: 23 ± 1 C "study design: static exposure "dissolved oxygen: "carrier solvent: none "observation periods: 0, 24, 48 h Test solutions were not neutralized.
Remark	:	Vinyltriacetoxysilane (CAS 4130-08-9) is a structural analogue for methyltriacetoxysilane (CAS 4253-34-3) and ethyltriacetoxysilane (CAS 17689-77-9)
Result	:	"NOEC = 32

"LOEC = 100
"EC50 > 100
"EC100 = >100
Test substance added directly to each test chamber, a carrier solvent was not used. Dissolved oxygen and pH were measured at test initiation and termination. One immobilization in controls at 24-h observation. No immobilization observed in 100 mg/L exposure (LOEC) until 24-h observation (20% immobilized)-20% immobilized at 48-h observation.

Test substance : Dow Corning Z-6075 Silane
Specified composition - not specified; Dow Corning MDMS database indicates that the test material is 93% vinyltriacetoxysilane (CAS 4130-08-9)

Reliability : (2) valid with restrictions
31.10.2005 (31)

Type : other: renewal
Species : other: Carcinus maenas
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 180
Method : other
Year : 1971
GLP : no
Test substance : other TS

Method : Age/Life Stage: ADULT
Water Parameters:
Temperature: 15 deg C (mean value)

Remark : Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Test substance : Acetic acid (64-19-7)

Reliability : (2) valid with restrictions
03.06.2005 (69) (89)

Type : other
Species :
Exposure period :
Unit :
Method : other: analogy
Year : 2004
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Ethyltriacetoxysilane (CAS No. 17689-77-9) and vinyltriacetoxysilane (CAS No. 4130-08-9) have been tested and the results show the resulting toxicity to aquatic organisms is due to acetic acid. When results are expressed on the basis of the amount of acetic acid generated from the hydrolysis reaction, the toxicity of ethyltriacetoxysilane and vinyltriacetoxysilane are comparable to the reported toxicity of acetic acid (EC50 = 65-180 mg/L, depending on test species):

Reported Toxicity (mg/L) of Ethyltriacetoxysilane, Vinyltriacetoxysilane, and Acetic Acid to Aquatic Invertebrates (48-h EC50 Immobility):

Daphnia magna: 62 (Ethyltriactoxysilane); 100 (Vinyltriactoxysilane); 48, 78 (HOAc)(1); 65, 6000 (Acetic acid)

Carcinus maenas: 180 (Acetic acid)

Crangon crangon: 100 (Acetic acid)

(1) = HOAc is the estimated toxicity based on the estimated amount of acetic acid generated from the hydrolysis reaction. The amount of acetic acid generated was estimated using the assumption that 1 mole of test material (ethyl- or vinyl- triacetoxysilane) produces 3 moles of acetic acid.

Source : SEHSC
Reliability : (2) valid with restrictions
20.05.2004

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Scenedesmus subspicatus (Algae)
Endpoint	:	biomass
Exposure period	:	72 hour(s)
Unit	:	mg/l
NOEC	:	= 54 measured/nominal
EC50	:	= 73 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	other: EC Guideline 92/69/EWG
Year	:	1995
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Method : Recommended procedure of the ad-hoc working group of the Federal Environment Bureau for development of ecological and toxicological testing procedures in aquatic systems: Suppression of cell reproduction among green alga Scenedesmus subspicatus 1984; OECD 201.

The test solutions were not neutralized.

Remark : Because ethyltriacetoxysilane generates considerable amounts of acetic acid when exposed to water, results from aquatic tests reflect the toxicity of acetic acid rather than the toxicity of the parent triacetoxysilane. Acetoxysilanes are highly reactive and undergo rapid hydrolysis when exposed to moisture. When ethyltriacetoxysilane is added to water, 100% of the parent compound is hydrolyzed in less than 0.2 minutes, producing 3 moles of acetic acid and 1 mole of silanetriol for every mole of parent material. Studies indicate that the observed acute toxicity of ethyltriacetoxysilane (CAS No. 17689-77-9) to aquatic organisms is due to acetic acid. When results are expressed on the basis of the amount of acetic acid generated from the hydrolysis reaction, the toxicity of ethyltriacetoxysilane is comparable to the reported toxicity

of acetic acid (EC50 =50-450 mg/L), depending on test species.
When the results are interpreted, the hydrolysis of the test substance during the preparation of the initial solution or during the test should be considered.

pH at test start: 4.4-8.1; pH at test end: 4.2-9.2: There was a partial strong increase in pH value in some test solutions. Since the growth was not influenced by this increase, the alteration in pH value was not considered to have an effect on quality.

Result : The following effective concentrations were reported: On the basis of cell growth, a median concentration is calculated of 72 hour EbC50 = 73 mg/L; On the basis of growth rate, a median effective concentration was achieved at (0-72 hour)ErC10 = 76 mg/L; The NOEC value was 54 mg/L (on the basis of cell growth). All concentrations are with respect to the material.

Test condition : As the test substance has low water solubility, it was dissolved at 1 g/l in VE water and agitated for 18 h. The solution was filtered and served as the initial solution for testing.

Algae cell counts were made photometrically at 0, 24, 48 and 72 hrs.

Test substance concentrations were determined using a TOC Infrared Analyzer.

Target test substance concentrations were 0, 6.5, 11, 20, 33, 54 and 98 mg/l. The 72 hr values were 0, 5.3, 8.7, 19, 32, 41 and 95 mg/l. The geometric mean of analytical values at 0 and 72 hrs deviates <20% from that of the nominal concentrations (except at the target concentration of 54 mg/l). Therefore, the nominal concentrations were used for the evaluation.

Test substance : DYANSYLAN ATAC: 99.4% Ethyltriacetoxysilane.

The test substance is susceptible to hydrolysis.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
01.11.2005 (23)

Species : Anabaena flos-aquae (Algae)
Endpoint : other: biomass and growth rate
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : = 10
LOEC : = 32
Limit test :
Analytical monitoring : no
Method : other: Biological field and laboratory methods. The algal assay procedure: bottle test. United States Environmental Protection Agency, EPA 670/4 73 00, 1973
Year : 1980
GLP : no
Test substance : other TS

Method : Test Vessels: Polycarbonate flasks
Test System: Blue-green algae (Anabaena flos-aquae) - 1.00 ×

104 cells/mL at test initiation.
Replicates: triplicate controls, triplicate exposure concentrations
Endpoint: 7-d growth inhibition
7-d final yield
Statistics: Probit analysis based on Finney's Method (Statistical Methods In Biological Assay, 1952).
Calculations conducted as described in the Handbook of Phycological Methods, Culture Methods and Growth Measurements, J. Stein (ed.), Cambridge Press, pp 220-229 (1973).
Exposure Concentrations (product, mg/L)
"nominal: 0, 10, 32, 100
Test Procedure and Conditions
"exposure period: 7 d
"dilution water: sterile algal broth
"study design: static exposure
"carrier solvent: none
"observation periods: 0, 3, 4, 5, 6, 7 d
The test solutions were not neutralized.
The algae study was conducted with vinyltriacetoxysilane in accordance with EPA "Biological Field and Laboratory Methods" (EPA 67014-73-00).
The Anabaena study was conducted for 13-d with cell counts at days 0, 3, 4, 5, 6, 7, 12, and 13. Visual examination of the growth curve for the Anabaena test indicates exponential growth through the initial seven days of the test with the exception of the 100 mg/L dose. At the 100 mg/L dose an initial decline in cell number was observed from days 0-3 followed by exponential growth from days 3-6. The statistical calculations were made using methods described in "Handbook of Phycological Methods" (1973).
No pH data were included in the report and presumably pH was not adjusted.

Remark : Vinyltriacetoxysilane (CAS 4130-08-9) is a structural analogue for methyltriacetoxysilane (CAS 4253-34-3) and ethyltriacetoxysilane (CAS 17689-77-9)

Result : Results - 96 hour Growth Rate (mg/L)
"NOEC = 10
"LOEC = 32
"EC50 > 100
Results - 96 hour Final Yield (mg/L)
"NOEC = 10
"EC10 = 28 (23-34; 95% CI)
"LOEC = 32
"EC50 = 57 (51-65; 95% CI)
"EC90 = 117 (99-146; 95% CI)

Test substance added directly to each test chamber, a carrier solvent was not used. Dissolved oxygen and pH were measured at test initiation and termination. Mean cell density (cells/mL ± S.D.) after 7 days was 15.0 ± 12.0 × 104, 18.7 ± 4.2 × 104, 12.7 ± 9.8 × 104, and 2.4 ± 1.9 × 104 in the control, 10 mg/l, 32 mg/l, and the 100 mg/l exposures, respectively.

Test substance : Dow Corning Z-6075 Silane
Specified composition - not specified; Dow Corning MDMS database indicates that the test material is 93% vinyltriacetoxysilane (CAS 4130-08-9)

Reliability : (2) valid with restrictions
31.10.2005 (31)

Species : Microcystis aeruginosa (Algae, blue, cyanobacteria)

Endpoint : other: biomass
Exposure period : 8 day(s)
Unit : mg/l
Method : other
Year : 1978
GLP : no data
Test substance : other TS

Remark : Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Result : A change in the number of species groups in a community (i.e. biomass) was reported at 90 mg/l.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
31.10.2005 (12) (89)

Species : Scenedesmus quadricauda (Algae)
Endpoint : other: growth inhibition
Exposure period : 8 day(s)
Unit : mg/l
Toxicity Threshold (TT) : = 4000
Method : other
Year : 1980
GLP : no data
Test substance : other TS

Method : Filled culture tubes were maintained at 27 °C and relative humidity of 50%. The concentration of the algal suspension is measured turbidmetrically (while diffused light is screened off) and expressed by the extinction of the primary light of the monochromatic radiation at 578 nm for a layer of 10 mm thickness. The test temperature was 25°C.
Remark : Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Test substance : Acetic acid (64-19-7)
Reliability : (3) invalid
Algae were not in an exponential growth phase over the whole duration of the test
31.10.2005 (2) (13)

Species : Selenastrum capricornutum (Algae)
Endpoint : other: biomass and growth rate
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : = 0
LOEC : = 1
Limit test :
Analytical monitoring : no

Method : other: Biological field and laboratory methods. The algal assay procedure: bottle test. United States Environmental Protection Agency, EPA 670/4 73 00, 1973
Year : 1980
GLP : no
Test substance : other TS

Method : Test Vessels: Polycarbonate flasks
Test System: Green algae (Selenastrum capricornutum) - 1.0 × 104 cells/mL at test initiation
Replicates: triplicate controls, triplicate exposure concentrations
Endpoint: 7-d growth inhibition
7-d final yield
Statistics: Probit analysis based on Finney's Method (Statistical Methods In Biological Assay, 1952).
Calculations conducted as described in the Handbook of Phycological Methods, Culture Methods and Growth Measurements, J. Stein (ed.), Cambridge Press, pp 220-229 (1973).
Exposure Concentrations (product, mg/L)
"nominal:0, 18, 32, 56
Test Procedure and Conditions
"exposure period: 7 d
"dilution water: sterile algal broth
"study design: static exposure
"carrier solvent: none
"observation periods: 0, 3, 4, 5, 6, 7 d

The algae study was conducted with vinyltriacetoxysilane in accordance with EPA "Biological Field and Laboratory Methods" (EPA 67014-73-00). The Selenastrum test was conducted for 10-d with algal cell counts on days 0, 3, 4, 6, 7, and 10. Visual examination of the growth curve for the Selenastrum test shows exponential growth from days 3-7 for the control and 3-6 for the algae exposed to the test material. The statistical calculations were made using methods described in "Handbook of Phycological Methods" (1973). No pH data were included in the report and presumably pH was not adjusted.
Remark : Vinyltriacetoxysilane (CAS 4130-08-9) is a structural analogue for methyltriacetoxysilane (CAS 4253-34-3) and ethyltriacetoxysilane (CAS 17689-77-9)
Result : Results - 96 hour Growth Rate (mg/L)
"NOEC = 0
"EC10 = 19 (9-25; 95% CI)
"LOEC = 1
"EC50 = 111 (72-387; 95% CI)
"EC90 = 651 (238-14343; 95% CI)
Results - 96 hour Final Yield (mg/L)
"NOEC = 0
"EC10 = 4 (1-8; 95% CI)
"LOEC = 1
"EC50 = 23 (16-28; 95% CI)
"EC90 = 136 (84-448; 95% CI)

Test substance added directly to each test chamber, a carrier solvent was not used. Dissolved oxygen and pH were measured at test initiation and termination. Mean cell density (cells/mL ± S.D.) after 7 days was 2.05 ± 0.24 × 106, 1.12 ± 0.36 × 106, 0.93 ± 0.09 × 106, and 0.48 ± 0.61 × 106 in the control, 18 mg/l, 32 mg/l, and the 56 mg/l

exposures, respectively.

Test substance : Dow Corning Z-6075 Silane
Specified composition - not specified; Dow Corning MDMS database indicates that the test material is 93% vinyltriacetoxysilane (CAS 4130-08-9)

Reliability : (2) valid with restrictions
31.10.2005 (31)

Method : other: analogy
Year : 2004
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Ethyltriacetoxysilane (CAS No. 17689-77-9) and vinyltriacetoxysilane (CAS No. 4130-08-9) have been tested and the results show the resulting toxicity to aquatic organisms is due to acetic acid. When results are expressed on the basis of the amount of acetic acid generated from the hydrolysis reaction, the toxicity of ethyltriacetoxysilane and vinyltriacetoxysilane are comparable to the reported toxicity of acetic acid (EC50 = 90 mg/L):

Reported Toxicity (mg/L) of Ethyltriacetoxysilane, Vinyltriacetoxysilane, and Acetic Acid to Aquatic Plants (7-d EC50 growth rate)

Scenedesmus subspicatus: 76 (Ethyltriactoxysilane); 59 (HOAc)(1)

Selenastrum capricornutum: 111 (Vinyltriacetoxysilane); 87 (HOAc)

Anabaena flos-aquae: 100 (Vinyltriacetoxysilane); 78 (HOAc)
Anacystis aeruginosa: 90 (Acetic acid)

(1) = HOAc is the estimated toxicity based on the estimated amount of acetic acid generated from the hydrolysis reaction. The amount of acetic acid generated was estimated using the assumption that 1 mole of test material (ethyl- or vinyl- triacetoxysilane) produces 3 moles of acetic acid.

Source : SEHSC
Reliability : (2) valid with restrictions
20.05.2004

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type : other
Species : Pseudomonas putida (Bacteria)
Exposure period : 5 hour(s)
Unit : mg/l
EC10 : = 60 - 80 calculated
EC100 : = 60 - 80 calculated
Analytical monitoring : no
Method : other: DIN 38412, Part 8
Year : 1995
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : The pH value decreased with increased test concentration:
10 mg/l pH= 7
60 mg/l pH= 5.7
80 mg/l pH= 5.2

Because triacetoxysilanes generate considerable amounts of acetic acid when exposed to water, results from aquatic tests reflect the toxicity of acetic acid rather than the toxicity of the parent triacetoxysilane. Acetoxysilanes are highly reactive and undergo rapid hydrolysis when exposed to moisture. When methyl- or ethyltriacetoxysilane is added to water, 100% of the parent compound is hydrolyzed in less than 0.2 minutes, producing 3 moles of acetic acid and 1 mole of silanetriol for every mole of parent material. Studies indicate that the observed acute toxicity of ethyltriacetoxysilane (CAS No. 17689-77-9) to aquatic organisms is due to acetic acid. When results are expressed on the basis of the amount of acetic acid generated from the hydrolysis reaction, the toxicity of ethyltriacetoxysilane is comparable to the reported toxicity of acetic acid (EC50 =50-450 mg/L), depending on test species.

Test condition : Six 250 ml Erlenmeyer flasks were coated with the culture solution, the bacterial suspension, and the test substance in staged concentrations (10, 20, 40, 60, 80 and 100 mg/l), were sealed without air, and were incubated for 5 to 6 hours at 252 deg C. Three additional flasks were included in parallel for analytical determination. Six control bottles without the test substance were used as reference; four of these contained HgCl2 to determine the final oxygen content. At the end of testing HCl was added to stop biochemical processes.

An emulsifier was added into the test medium due to the lowwater solubility of the test substance. The differential between the oxygen content of the solutions stored in the individual containers at the initial time (0)and after the incubation period reveals the bacterial oxygen consumption. Comparison of the amounts of oxygen consumed in there ference and test preparations provides information regarding the concentration-related influence on oxygen consumption by the test substance.

Test substance : DYANSYLAN ATAC: 99.4% Ethyltriacetoxysilane.

The test substance is susceptible to hydrolysis.

Reliability : (1) valid without restriction
02.12.2004 (21)

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

Type	:	artificial soil
Species	:	Eisenia fetida (Worm (Annelida), soil dwelling)
Endpoint	:	mortality
Exposure period	:	14 day(s)
Unit	:	mg/kg soil dw
LC10	:	> 1000 calculated
Method	:	Directive 87/302/EEC, part C, p. 95 "Toxicity for earthworms: Artificial soil test"
Year	:	1995
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	One group of 40 earthworms was exposed for 14 days to a limit concentration of 1000 mg/kg. A second group of 40 earthworms was also included as a control. Mortality was recorded at 7 and 14 days.
Remark	:	Original report cited the method as 88/302/EEC.
Result	:	There were no deaths recorded for the control group at 7 or 14 days or for the test substance group at 7 days. At 14 days, one animal in the test substance treated group had died.
Test substance	:	DYANSYLAN ATAC: 99.4% Ethyltriacetoxysilane. The test substance is susceptible to hydrolysis.
Reliability	:	(1) valid without restriction

02.12.2004 (25)

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 1462 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	50
Vehicle	:	other: none
Doses	:	300, 600, 1000, 1500 or 2000 mg/kg
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"
Year	:	2000
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Result :

The acute median lethal dose (LD50), calculated by the method of Litchfield and Wilcoxon (probit analysis) was 1462 mg/kg for male and female rats (combined data) with 95% confidence limits of 1269-1683 mg/kg. By sex, the LD50 was 1441 mg/kg for both males and females. (It should be noted that the results from the two lowest dosages where no deaths occurred were excluded from the LD50 calculation.)

There were 0, 0, 0, 3 and 4 deaths among males and 0, 0, 0, 3 and 4 deaths among females at dosages of 300, 600, 1000, 1500 and 2000 mg/kg, respectively. There was a tendency for deaths to be delayed. In the 1500 mg/kg group, there was one death on day 1 (the day of dosing), one on day 2, one on day 3, two on day six and one on day 9. In the 2000 mg/kg group, there was one death on day 2, three on day 3 and one each on days 4, 5, 9 and 10.

Rats in the 300 mg/kg group exhibited few clinical signs and appeared essentially normal throughout the study. Clinical signs seen in the 600, 1000, 1500 and 2000 mg/kg groups in a general dose response pattern included decreased activity, lacrimation, excessive salivation, rales, irregular gait and/or hunched posture, decreased food consumption and fecal volume, red urine, abnormal stool 9watery, unformed, absent), various anogenital stains and red staining of the snout, eyes and extremities. In addition, one-half or more of the rats in the 1500 and 2000 mg/kg groups exhibited lethargy and labored respiration. The majority of the surviving rats in the 600 and 1000 mg/kg groups appeared normal within one week of dosing, while the majority of the surviving rats in the 1500 and 2000 mg/kg groups did not fully return to a clinically normal condition by study termination.

All rats in the 300, 600 and 1000 mg/kg groups (except one 1000 mg/kg female) gained weight during the study, surpassing their prefasted weights. One-half of the six survivors in the 1500 and 2000 mg/kg groups lost weight over the 14-day study period.

Although the majority of rats that died (>60%) were within normal limits at necropsy, several remarkable findings were seen in the stomach/gastrointestinal tract in a dose-responsive pattern. These included discoloration, adhesions and thickened mucosa. Similar but more severe gastric and intestinal findings were seen in nearly all rats that died, including adhesions (often multiple), discoloration (often black), thickened mucosa, enlargement or distention and abnormal contents (usually brown or black).

Source : SEHSC
Test condition : Each rat received a single dose of the test substance. Young adult rats weighing 282 +/- 45 grams (males) and 201 +/- 23 grams (females) were used. The rats were fasted overnight prior to test substance administration and received dosages of 300, 600, 1000, 1500 or 2000 mg/kg body weight of undiluted test substance.. The rats were observed frequently after dosing and at least once daily thereafter for fourteen days. Body weights were recorded prior to fasting, on the day of dosing and weekly thereafter. Gross necropsies were performed on all animals.
Test substance : Ethyltriacetoxysilane (CAS No. 17689-77-9)
Conclusion : There was an excellent dose response on the study, and it was possible to calculate LD50 values for each sex individually, as well as when the data were combined. The test substance was moderately toxic to rats by the oral route of exposure. The clinical signs observed, delayed deaths, weight losses and gross necropsy findings all indicate an irritative mechanism of toxicity.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
22.03.2004 (55)

Type : LD50
Value : = 4280 mg/kg bw
Species : rat
Strain : Wistar
Sex : male
Number of animals : 5
Vehicle : water
Doses : 0.1 g/ml
Method : other
Year : 1951
GLP : no
Test substance : other TS

Method : Range-finding toxicity tests were conducted in which five non-fasted male rats were given a single oral dose by gastric intubation of 100 mg/L (0.1 g/mL) of acetic acid, calcium salt in water. Rats were observed for 14 days and the number of mortalities counted.
Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role.

Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : The 95% confidence limits were 3860-4760 mg/kg.
Test substance : Acetic acid, calcium salt (62-54-4)
Reliability : (2) valid with restrictions
Peer reviewed published information.

07.06.2005 (79) (81)

Type : LD50
Value : = 3250 mg/kg bw
Species : rat
Strain : Wistar
Sex : male
Number of animals : 5
Vehicle : water
Doses : 0.1 g/ml
Method : other
Year : 1962
GLP : no
Test substance : other TS

Method : Range-finding toxicity tests were conducted in which five non-fasted male rats were given a single oral dose by gastric intubation of 100 mg/L (0.1 g/mL) of acetic acid, potassium salt in water. Rats were observed for 14 days and the number of mortalities counted.

Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role.
Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : The 95% confidence limits were 2480-4260 mg/kg.
Test substance : Acetic acid, potassium salt (127-08-2)
Reliability : (2) valid with restrictions
Peer reviewed published information.

07.06.2005 (80) (81)

Type : LD50
Value : = 3530 mg/kg bw
Species : rat
Strain : no data
Sex : no data
Number of animals :
Vehicle :
Doses : no data

Method	:	other
Year	:	
GLP	:	no data
Test substance	:	other TS
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Test substance	:	Acetic acid, sodium salt (127-09-3)
Reliability	:	(2) valid with restrictions Peer reviewed published information.

03.06.2005 (42)

Type	:	LD50
Value	:	3250 - 5600 mg/kg bw
Species	:	rat
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	
Doses	:	no data
Method	:	other
Year	:	
GLP	:	no
Test substance	:	other TS
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Result	:	These values cover acetic acid, its potassium, sodium and calcium salts and sodium diacetate. Doses in the region of the LD50 values caused central nervous system depression in rats (Woodard et al, 1941).
Test substance	:	Acetic Acid, and its potassium and sodium salts, and sodium diacetate.
Reliability	:	(2) valid with restrictions

Peer reviewed published information.

03.06.2005 (8) (79) (80) (88) (97)

Type	:	LD50
Value	:	= 5600 mg/kg bw
Species	:	rat
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	
Doses	:	no data
Method	:	other
Year	:	1991
GLP	:	no data
Test substance	:	other TS
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Test substance	:	Sodium diacetate (126-96-5)
Reliability	:	(2) valid with restrictions Data used in support of a published EPA registration document

03.06.2005 (88)

Type	:	LD50
Value	:	= 4960 mg/kg bw
Species	:	mouse
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	
Doses	:	no data
Method	:	other
Year	:	1941
GLP	:	no
Test substance	:	other TS
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the

parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
Peer reviewed published information.

03.06.2005 (8) (97)

5.1.2 ACUTE INHALATION TOXICITY

Type : LC50
Value : = 11.4 mg/l
Species : rat
Strain : no data
Sex : no data
Number of animals :
Vehicle :
Doses : no data
Exposure time : 4 hour(s)
Method : other
Year : 1989
GLP : no
Test substance : other TS

Method : BASF Test protocol
Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Test substance : Acetic acid (64-19-7)
Purity 96%
Reliability : (2) valid with restrictions
03.06.2005 (5)

Type : LC50
Value : > 30000 mg/m³
Species : rat
Strain : no data
Sex : no data
Number of animals :
Vehicle :
Doses : no data
Exposure time : 1 hour(s)
Method : other
Year : 1971

GLP : no
Test substance : other TS

Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Test substance : Acetic acid, sodium salt (127-09-3)
Reliability : (2) valid with restrictions
Peer reviewed published information.

03.06.2005 (9)

Type : LC50
Value : > 16000 ppm
Species : rat
Strain : no data
Sex : no data
Number of animals :
Vehicle :
Doses : no data
Exposure time : 4 hour(s)
Method : other
Year : 1951
GLP : no
Test substance : other TS

Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Result : Exposure at 16,000 ppm to acetic acid killed one of 6 rats.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
Peer reviewed published information.

03.06.2005 (79)

Type : LC50
Value : = 5620 ppm

Species	:	mouse
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	
Doses	:	no data
Exposure time	:	1 hour(s)
Method	:	other
Year	:	1957
GLP	:	no
Test substance	:	other TS
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Result	:	Mice exposed at 1000 ppm (2500 mg/m3) acetic acid for 1 hr showed ruffled coats, reddening of eyes, ears and nose, and rapid breathing. Inhalation of > 1,000 ppm produced irritation of the conjunctiva and upper respiratory tract. Autopsy of animals exposed to unspecified concentrations (but including 4500 ppm) revealed heart dilation, and congestion (fluid accumulation) in the lungs, kidneys, spleen and liver.
Test substance	:	Acetic acid (64-19-7)
Reliability	:	(2) valid with restrictions Peer reviewed published information.

03.06.2005 (8) (47)

Type	:	other
Value	:	
Species	:	mouse
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	
Doses	:	no data
Exposure time	:	
Method	:	other
Year	:	1987
GLP	:	no data
Test substance	:	other TS
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the

respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : 4-5 hr exposure at 4-12 ppm caused increased activity in mice. Continuous exposure at 360 ppm for 24 hrs produced a marked decrease in spleen weight.
Test substance : Acetic acid (64-19-7)
Reliability : (3) invalid
BIBRA (1993) described this study as doubtful regarding validity.

03.06.2005 (73)

Type : other
Value :
Species : guinea pig
Strain : no data
Sex : no data
Number of animals :
Vehicle :
Doses : no data
Exposure time : 1 hour(s)
Method : other
Year : 1957
GLP : no
Test substance : other TS

Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Result : Guinea pigs exposed to 5000 ppm acetic acid showed mild effects.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
Peer reviewed published information.

03.06.2005 (8) (47)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : > 2000 mg/kg bw

Species	:	rat
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	
Doses	:	no data
Method	:	other
Year	:	1991
GLP	:	no data
Test substance	:	other TS

Method	:	Conditions unspecified
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Test substance	:	Sodium diacetate (126-96-5)
Reliability	:	(2) valid with restrictions Data used in support of a published EPA registration document

03.06.2005 (88)

Type	:	other
Value	:	
Species	:	rat
Strain	:	no data
Sex	:	male
Number of animals	:	5
Vehicle	:	
Doses	:	2 ml
Method	:	other
Year	:	1960
GLP	:	no
Test substance	:	other TS

Method	:	2 ml (approximately 5 g/kg bw) of acetic acid was applied to the skin of five male rats for up to 40 minutes.
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C

and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : Decreased urine production and red blood cell damage, as indicated by the urinary excretion of the red blood cell protein, hemoglobin.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
Reviewed and summarized in BIBRA (1993)

03.06.2005 (74)

Type : LD50
Value : = 1060 mg/kg bw
Species : rabbit
Strain : no data
Sex : no data
Number of animals :
Vehicle :
Doses : no data
Method : other
Year : 1963
GLP : no
Test substance : other TS

Method : Conditions unspecified
Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
Reviewed and summarized in BIBRA (1993)

03.06.2005 (8) (87)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : undiluted
Exposure : Semiocclusive
Exposure time : 3 minute(s)
Number of animals : 6
Vehicle : other: none
PDII : 4.28
Result : corrosive

Classification	:	highly corrosive (causes severe burns)
Method	:	Directive 84/449/EEC, B.4 "Acute toxicity (skin irritation)"
Year	:	1989
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Application of 0.5 ml for 3 minutes produced severe lesions observed at 72 hours with slight reversibility at the day 14 reading in 4 of the 6 rabbits.
Source	:	Wacker Chemie GmbH
Test condition	:	Rabbits were dosed with 0.5 ml of the test substance. The dose was applied to the clipped, intact skin under a gauze patch held in contact with the skin with a semi-occlusive dressing for a contact period of 3 minutes. The animals were kept in individual boxes during the exposure period. The dressings were then removed and the rabbits returned to their individual cages. Cutaneous examinations were performed at 1, 24, 48 and 72 hours after removal of the dressing. Due to the severity of the lesions observed at 72 hours, these readings were repeated at day 7 and day 14.
Test substance	:	Ethyltriacetoxysilane (CAS No. 17689-77-9)
Conclusion	:	The test substance was corrosive under the conditions of the study
Reliability	:	(1) valid without restriction
25.02.2004		(52)

Species	:	other
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Vehicle	:	no data
PDII	:	
Result	:	
Classification	:	
Method	:	other: in vitro
Year	:	1994
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Skin2 ZK-1350 model correctly identified the corrosivity of ethyltriacetoxysilane, although it appeared to slightly underestimate the degree of corrosivity. CORROSITEX model also correctly identified ethyltriacetoxysilane as corrosive. CORROSITEX appeared to be more sensitive than the Skin2 ZK-1350. However, TER assay did not identify ethyltriacetoxysilane as corrosive.
Source	:	Dow Corning Corporation Midland, MI
Conclusion	:	Skin2 ZK-1350 and CORROSITEX models correctly identified the corrosivity of ethyltriacetoxysilane. However, TER assay did not identify ethyltriacetoxysilane and certain other acetoxysilanes as corrosive. Therefore, TER assay may not be suitable for testing corrosivity of the silane compounds. The author proposed that future work should focus on the Skin2 ZK-1350 assay while maintaining a vigilant watch on other emerging in vitro technologies.
Reliability	:	(2) valid with restrictions
02.12.2004		(33)

5.2.2 EYE IRRITATION

Species	:	other
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	
Vehicle	:	none
Result	:	
Classification	:	
Method	:	other: in vitro
Year	:	1994
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	The severe irritancy of ethyltriacetoxysilane was correctly detected by Skin2 1200 in vitro model.
Source	:	Dow Corning Corporation Midland, MI
Conclusion	:	The results described in this report indicate that Skin2 1200 model is useful technique for the in vitro assessment of eye irritation and the model correctly predicted the irritancy potential of ethyltriacetoxysilane. The author proposed that future work should focus on the Skin2 1200 while maintaining a vigilant watch on other emerging in vitro technologies.
Reliability	:	(2) valid with restrictions

02.12.2004 (33)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-chronic
Species	:	rat
Sex	:	no data
Strain	:	no data
Route of admin.	:	drinking water
Exposure period	:	9-15 weeks
Frequency of treatm.	:	continuously
Post exposure period	:	
Doses	:	0.01, 0.1, 0.25, or 0.5 percent (8 to 390 mg/kg bw/day)
Control group	:	
NOAEL	:	= .25 %
LOAEL	:	= .5 %
Method	:	other
Year	:	1921
GLP	:	no
Test substance	:	other TS
Method	:	In a subchronic study four groups of three to six rats were given 0.01, 0.1, 0.25, or 0.5 percent acetic acid in drinking water (up to 390 mg/kg body weight) for periods of nine to 15 weeks.
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical

structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role.
Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : Fluid intake was the same in all groups. Rats at the 0.5 percent level (390 mg/kg bw/day) experienced immediate, progressive reduction in body weight gain, loss of appetite, and up to a 27 percent reduction in food consumption. Mortality was unaffected. None of these effects were seen at the lower doses (8 to 210 mg/kg bw/day). NOAEL (systemic toxicity) = 210 mg/kg bw

Test substance : Acetic acid (64-19-7)

Reliability : (2) valid with restrictions
Data used in support of a published EPA registration document. Peer-reviewed and published information. Reviewed andsummarized in BIBRA (1993).

Flag : Critical study for SIDS endpoint

31.10.2005 (8) (16) (39) (40) (82)

Type : Sub-acute
Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : gavage
Exposure period : 7 days
Frequency of treatm. : Daily for 7 days
Post exposure period : none
Doses : 0, 17 (males only), 23 (females only), 100, 500, 1000 mg/kg/day
Control group : other: concurrent, sham dosed
NOAEL : 17 - 23 mg/kg bw
Method : other
Year : 2004
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : Analysis of variance was performed on the mean body weight, mean body weight gain and food consumption data using Microsoft Excel 9.0.
Test Subjects

Age at study initiation: approximately 9 weeks
No. of animals per sex per dose: Five
Study Design
Vehicle: None
Satellite groups and reasons they were added: None

Individual body weights were recorded on study days one and four prior to dosing, and on study day eight prior to the scheduled necropsy. Feeder weights were recorded on study day 1 prior to dosing and on the days of scheduled

euthanasia, unscheduled euthanasia, or the day that an animal was found dead. Food consumption was calculated from these initial and final feeder weights.

Clinical observations performed and frequency: Once a day and at approximately one hour after dosing. Observations included changes in the skin, fur, eyes, mucous membranes, respiratory, circulatory, autonomic and central nervous systems functions, motor activity, and behavior.

Organs examined at necropsy (macroscopic and microscopic): A detailed gross necropsy was performed and included examination of the external surface of the body, all orifices, and the cranial, thoracic and abdominal cavities and their contents.

Remark : Ethyltriacetoxysilane is sensitive to rapid hydrolysis, which may occur during testing, such that observed toxicity is likely due primarily to acetic acid. Abiotic hydrolysis studies show that hydrolysis products from the test substance undergo continuous, condensation reactions to produce higher molecular weight cyclic and linear siloxanes (the number-average and weight-average molecular weights were 633 and 809 with 22 area % of the chromatogram higher than 1000 molecular weight at the1-hr reaction time; at the 4-hr reaction time, the number-average and weight-average molecular weights increased to 750 and 1085 with 38 area % of the chromatogram higher than 1000 molecular weight, respectively). The alkyl silanols condense to siloxane oligomers; this condensation of silanols is affected by both concentration and pH, and since both change over time it is not feasible to isolate specific silanols for analysis (the structures continue to evolve until they either reach equilibrium or precipitate out of solution). While the hydrolysis of ethyltriacetoxysilane is rapid, the polymerization products, while not volatile, are in a molecular weight range small enough to be considered, at least in part, biologically available.

Result : All animals in the 0, 17, 23, and 100 mg/kg/day dose groups survived to the scheduled necropsy. There were two early deaths (one 500 mg/kg/day dose group female on day 3 and one 1000 mg/kg/day dose group male on day 4). All remaining 500 and 1000 mg/kg/dose group males and females were euthanized on day 4 as a consequence of decreased physical condition, marked body weight loss, and macroscopic findings (stomach/esophagus ulceration) observed during necropsy of the dead and moribund animals. Body weight gain and food consumption were reduced in the 100 mg/kg/day dose group males and females. Body weight, body weight gain, and food consumption for males and females in the low dose groups (17 and 23 mg/kg/day) were not different from control.

Macroscopic findings on day four of the 500 and 1000 mg/kg/day dose group animals revealed severe lesions (ulcerations/erosions in the esophagus and stomach). These lesions were consistent in appearance and location with deposition of a corrosive material. The known moisture sensitivity of this test substance and associated liberation of acetic acid suggests that acetic acid liberation at the site of dose administration is responsible for the lesions. Thickening of the esophagus wall and minor glandular stomach

ulceration were observed in many of the 100 mg/kg/day dose group males and females along with minimal glandular stomach erosion present in two of the 23 mg/kg/day dose group females.

This study was conducted to provide data in support of dose selection for a subsequent repeated-dose toxicity study with screening reproductive and developmental endpoints with ethyltriacetoxysilane (OECD422). The results have provided sufficient information to indicate that conduct of a repeated-dose toxicity study is not warranted. Ethyltriacetoxysilane is a corrosive material producing significant tissue destruction upon contact. Administration of 23 mg/kg bw/day (5 ul of neat material) results in macroscopically observable erosions in the glandular stomach after seven daily administrations. Repeated dosing for even longer durations can reasonably be expected to result in an increase in the proportion of animals with such lesions, as well as to increase the severity of the resulting lesions. Administration of lower dose levels presents the obvious challenges of administering sub-microliter volumes, realizing differentiation of dose levels, and in achieving systemic exposures of any toxicological importance.

The no observable adverse effect level (NOAEL) for ethyltriacetoxysilane in this study was 17 mg/kg/day for male rats. The NOAEL for female rats could not be determined, but was less than 23 mg/kg/day.

Source : Dow Corning Corporation Midland, MI
Test condition : The test substance was administered neat because the moisture sensitivity and hydrophilicity of ethyltriacetoxysilane precluded use of a suitable carrier.
Test substance : Ethyltriacetoxysilane - Test article of >= 94.8% purity was used
Conclusion : Daily oral administration of ethyltriacetoxysilane to male and female rats at 500 and 1000 mg/kg resulted in ulceration of the stomach and/or esophagus. Also, administration of 100 mg/kg test article to male and female rats and 23 mg/kg to female rats produced similar stomach and esophageal lesions as those observed with the higher dose levels. However, no evidence of injury to the stomach or esophagus was observed in male rats at the 17 mg/kg dose level. The NOAEL for ethyltriacetoxysilane in this study was 17 mg/kg/day for male rats. The NOAEL for female rats could not be determined, but was less than 23 mg/kg/day. The data provided in this range-finder study indicate a practical and humane dose range for subsequent longer term studies is below the limit of technical practicality and toxicological significance. The results indicate that conduct of a subsequent repeated dose toxicity study (such as an OECD 422) is not warranted.
Reliability : (2) valid with restrictions
Study was Non-GLP
Flag : Critical study for SIDS endpoint
06.12.2004 (36)

Type : Sub-chronic
Species : rat
Sex : male
Strain : no data

Route of admin.	:	gavage
Exposure period	:	90 days
Frequency of treatm.	:	
Post exposure period	:	
Doses	:	approximately 750 mg/kg bw
Control group	:	
LOAEL	:	= 750 mg/kg bw
Method	:	other
Year	:	1952
GLP	:	no
Test substance	:	other TS

Method : Rats were treated by gavage with 3 ml of a 10% acetic acid solution for 90 days.

Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : The treatment decreased the red blood cell count and hemoglobin concentration. The LOAEL (systemic toxicity) = 750 mg/kg bw.

Test substance : Acetic acid (64-19-7)

Reliability : (2) valid with restrictions
Peer-reviewed and published information. Reviewed and summarized in BIBRA (1993)

31.10.2005 (8) (98)

Type	:	Sub-acute
Species	:	rat
Sex	:	
Strain	:	no data
Route of admin.	:	oral feed
Exposure period	:	8 week
Frequency of treatm.	:	
Post exposure period	:	
Doses	:	2% in diet
Control group	:	
NOAEL	:	> 1000 mg/kg bw
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	other TS

Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven

by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : There were no effects
Test substance : Sodium diacetate (126-96-5)
Reliability : (2) valid with restrictions
Data used in support of a published EPA registration document

16.06.2005 (88)

Type : Sub-acute
Species : rat
Sex : no data
Strain : no data
Route of admin. : gavage
Exposure period : 3-14 days
Frequency of treatm. : daily
Post exposure period :
Doses : 1800 mg/kg bw free acid or 4200 - 4800 mg/kg bw of sodium acetate
Control group :
LOAEL : >= 4200 - 4800 mg/kg bw
Method : other
Year : 1970
GLP : no
Test substance : other TS

Method : Groups of three to four rats were given 1800 mg/kg body weight per day of free acid intragastrically or 4200 - 4800 mg/kg body weight of sodium acetate.

Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : Groups of three to four rats survived for 14 days when given 1800 mg/kg body weight per day of free acid intragastrically or 4200 - 4800 mg/kg body weight of sodium acetate, but survived only three to five days on daily intra-gastric doses of 2400 mg/kg body weight of free acid. Animals lost weight and showed blistered paws and reddened noses before death at fourteen days. No autopsies were done.

LOAEL (systemic toxicity) >/= 4200-4800 mg/kg bw

Test substance : Acetic acid, sodium salt (127-09-3)
Reliability : (2) valid with restrictions

Data used in support of a published EPA registration document

31.10.2005 (56)

Type	:	Sub-chronic
Species	:	pig
Sex	:	no data
Strain	:	no data
Route of admin.	:	oral feed
Exposure period	:	150 days
Frequency of treatm.	:	successive 30 day periods
Post exposure period	:	
Doses	:	0, 240, 720, 960, or 1200 mg/kg bw
Control group	:	yes
NOAEL	:	1200 mg/kg bw
Method	:	other
Year	:	1919
GLP	:	no
Test substance	:	other TS
Method	:	Four groups of two young pigs each were fed daily diets containing 0, 240, 720, 960, or 1200 mg/kg body weight per day for successive 30-day periods to a total of 150 days.
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Result	:	There were no significant differences in growth rate, weight gain, early morning urinary ammonia, and terminal blood pH between controls and test groups. No autopsies were done. NOAEL (no effects reported) - 1200 mg/kg bw.
Test substance	:	Acetic acid (64-19-7)
Reliability	:	(2) valid with restrictions Data used in support of a published EPA registration document

31.10.2005 (39) (60)

Type	:	Sub-chronic
Species	:	rat
Sex	:	no data
Strain	:	no data
Route of admin.	:	oral feed
Exposure period	:	3 months
Frequency of treatm.	:	daily
Post exposure period	:	
Doses	:	21 mg/kg b.w./day
Control group	:	no data specified
LOAEL	:	21 mg/kg bw
Method	:	other

Year	:	1981
GLP	:	no data
Test substance	:	other TS
Method	:	Ten rats were used.
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Result	:	Indications of altered thyroid function and decreased growth were reported. LOAEL (systemic toxicity) = 21 mg/kg bw.
Test substance	:	Acetic acid, sodium salt (127-09-3)
Reliability	:	(2) valid with restrictions Peer reviewed published information. Reviewed and summarized in BIBRA (1993).

31.10.2005 (48)

Type	:	Sub-chronic
Species	:	rat
Sex	:	no data
Strain	:	no data
Route of admin.	:	oral feed
Exposure period	:	8 months
Frequency of treatm.	:	daily
Post exposure period	:	
Doses	:	4500 mg/kg bw
Control group	:	
LOAEL	:	= 4500 mg/kg bw
Method	:	other
Year	:	1952
GLP	:	no
Test substance	:	other TS
Method	:	A small number of rats were fed approximately 4.5 g acetic acid/kg bw daily in the diet for 30 or 325 days.
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole

of (alkyl) triacetoxysilane parent material.

Result : Stomach damage was observed. LOAEL (irritation) = 4500 mg/kg bw.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
Peer-reviewed and published information. Reviewed and summarized in BIBRA (1993)

31.10.2005 (7) (66)

Type : Sub-chronic
Species : rat
Sex : male
Strain : no data
Route of admin. : gavage
Exposure period : 8 months
Frequency of treatm. : 3 times per week
Post exposure period :
Doses : 0.5 ml of 3% water solution of acetic acid (about 60 mg/kg bw/treatment)
Control group :
LOAEL : ca. 60 mg/kg bw
Method : other
Year : 1989
GLP : no data
Test substance : other TS

Method : Nine outbred white male rats weighing approximately 100 gwere used in the acetic acid alone study. Rats were given either N-nitrosarcosin ethyl ester (NSEE; a known carcinogen) alone, NSEE with the acetic acid solution, or the acetic acid solution alone. All doses were given by intubation into the esophagus. Animals were killed by ether inhalation after 8 months of experiments and autopsied.
Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Result : Prolonged administration of acetic acid alone did not induce tumors. All nine of these rats, however, did experience hyperplasia in the esophagus and forestomach. LOAEL (irritation) ~ 60 mg/kg bw.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
Reviewed and summarized in BIBRA (1993)

31.10.2005 (1) (2)

Type : Sub-acute
Species : rat
Sex : male
Strain : Wistar
Route of admin. : oral feed

Exposure period	:	4 weeks
Frequency of treatm.	:	daily
Post exposure period	:	
Doses	:	3.58% of the diet (approx. 3.6 g/kg bw)
Control group	:	
NOAEL	:	3600 mg/kg bw
Method	:	other
Year	:	1971
GLP	:	no
Test substance	:	other TS

Method : Thirteen male Wistar rats were fed ad libitum a 25% protein, vitamin B12-deficient ration. The rats came from mothers who were transferred from a stock ration to a vitamin B12-deficient ration at parturition and continued on the deficient ration during lactation. They were weaned at 25 days old and at 28 days old they were divided into experimental groups.

Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : Growth and survival were normal. NOAEL (no effects reported) = 3600 mg/kg bw.

Test substance : Acetic acid, sodium salt (127-09-3)

Reliability : (2) valid with restrictions
Peer reviewed published information. Reviewed and summarized in BIBRA (1993).

31.10.2005 (37)

Type	:	Sub-chronic
Species	:	rat
Sex	:	male
Strain	:	Long-Evans
Route of admin.	:	drinking water
Exposure period	:	8 months
Frequency of treatm.	:	daily ad libitum
Post exposure period	:	
Doses	:	50 and 500 ppm
Control group	:	
LOAEL	:	500 mg/l
Method	:	other
Year	:	1986
GLP	:	no
Test substance	:	other TS

Method : Two groups of 12 male Long-Evans hooded rats 21 days old and weighing between 32-44 g were each subdivided into groups of equal mean weight. The 4 groups of 6

rats were administered a regimen of 50 or 500 ppm sodium acetate (controls) or 50 or 500 ppm lead acetate in distilled water. The test material was administered ad libitum for eight months.

Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : No significant effects on survival, reinforcement behavior, or body weight gain were observed. The rats treated with acetic acid, sodium salt served as the control for a lead exposure study. Therefore, no separate untreated controls are available for comparison. LOAEL (no effects reported) = 500 ppm.

Test substance : Acetic acid, sodium salt (127-09-3)

Reliability : (2) valid with restrictions
Peer reviewed published information.

31.10.2005 (20)

Type : Sub-chronic
Species : rat
Sex : male
Strain : Wistar
Route of admin. : drinking water
Exposure period : 112 days
Frequency of treatm. : continuous
Post exposure period :
Doses : 100 ppm
Control group : yes
NOAEL : 100 mg/l
Method : other
Year : 1987
GLP : no data
Test substance : other TS

Method : Eight young adult male Wistar rats were exposed to acetic acid, sodium salt in their drinking water beginning at 31 days of age. Training in mazes began on day 112 and lasted until day 157 at which time all animals were sacrificed.

Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the

corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
The rats treated with acetic acid, sodium salt served as the control for a lead exposure study. Therefore, no untreated controls are available for comparison.

Result : No mortality or cognitive impairment was observed. NOAEL (no effects reported) = 100 ppm
Test substance : Acetic acid, sodium salt (127-09-3)
Reliability : (3) Invalid
The ABSTRACT does not contain the same methodological information as the MATERIALS and METHODS section of the published report. It is not possible to determine the exact conduct of the study.

31.10.2005 (64)

Type : Sub-acute
Species : rat
Sex : no data
Strain : no data
Route of admin. : gavage
Exposure period : 14 days
Frequency of treatm. : daily
Post exposure period :
Doses : 1.8 or 2.4 g/kg bw
Control group :
Method : other
Year : 1942
GLP : no
Test substance : other TS

Method : Groups of three or four rats were given 1800 or 2400 mg/kg bw for 14 days.
Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role.
Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Result : All animals in the 1800 mg/kg bw group survived. Administration of 2400 mg/kg bw was lethal after 3-5 days.
Test substance : Acetic acid (64-19-7)
Reliability : (2) valid with restrictions
Peer-reviewed and published information. Reviewed and summarized in BIBRA (1993)

16.06.2005 (8) (53)

Type : Sub-chronic
Species : rat
Sex : no data
Strain : no data

Route of admin.	:	gavage
Exposure period	:	
Frequency of treatm.	:	
Post exposure period	:	
Doses	:	
Control group	:	
Method	:	other
Year	:	1987
GLP	:	no data
Test substance	:	other TS
Method	:	Rats were given about 20 mg sodium acetate/kg bw on days 6, 9, 12 and 18 of age. A second group of eight 21 day old rats were given 4 mg sodium acetate/kg bw in drinking water for 112 days.
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Result	:	No cognitive impairment was observed in either group of rats.
Test substance	:	Sodium diacetate (126-96-5)
Reliability	:	(3) invalid The ABSTRACT does not contain the same methodological information as the MATERIALS and METHODS section of the published report. It is not possible to determine the exact conduct of the study.

16.06.2005 (64)

Type	:	Chronic
Species	:	rabbit
Sex	:	female
Strain	:	no data
Route of admin.	:	drinking water
Exposure period	:	13 months
Frequency of treatm.	:	twice daily
Post exposure period	:	
Doses	:	up to 700 mg/kg bw
Control group	:	
Method	:	other
Year	:	1953
GLP	:	no
Test substance	:	other TS
Method	:	Female rabbits received varying doses, up to 700 mg/kg bw acetic acid twice daily, in drinking water for 13 months during a 16 month period.
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate

behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
BIBRA (1993) indicates there may have been changes in the mammary glands.

Result : Lactation was induced
Test substance : Acetic acid (64-19-7)
Reliability : (3) invalid
Considered an inadequate study in BIBRA (1993)

16.06.2005 (41)

Type : Sub-chronic
Species : rat
Sex : male
Strain : no data
Route of admin. : inhalation
Exposure period : 95 days
Frequency of treatm. :
Post exposure period :
Doses : 0.01, 0.2, or 5.0 mg/m3
Control group :
NOAEL : .01 mg/m³
Method : other
Year : 1974
GLP : no
Test substance : other TS

Method : Male rats exposed for 95 days to 0.01, 0.2, or 5.0 mg/m3 acetic acid vapor in air.
Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Result : Rats developed progressive muscle imbalance, increases of blood cholinesterase activity and serum globulins, and decreases of serum albumins in the two higher doses. The highest dose group also had raised white blood cell counts and decreases in ascorbic acid levels. NOAEL (systemic toxicity) = 0.01 mg/m3.
Test substance : Acetic acid (64-19-7)

Reliability	:	(2) valid with restrictions Peer reviewed published information. Data used in support of a published EPA registration document.

31.10.2005 (86)

Type	:	Sub-acute
Species	:	other: rat and mouse
Sex	:	no data
Strain	:	no data
Route of admin.	:	inhalation
Exposure period	:	3-35 days
Frequency of treatm.	:	continuous
Post exposure period	:	
Doses	:	11-35 ppm
Control group	:	no data specified
NOAEL	:	27 mg/m³
Method	:	other
Year	:	1987
GLP	:	no data
Test substance	:	other TS
Method	:	Groups of at least 10 rats and 10 mice were exposed to 11-35 ppm of acetic acid.
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Result	:	Exposure to 11 ppm for 22 days had no effect on activity, behavior, work capacity, growth, blood, or the weights and microscopic appearance of tissues examined. At 15 ppm (for 22 days) or more, the animals showed decreased activity, behavioral changes and reduced work capacity. At 23-31 ppm (17-35 days), there was decreased growth, increased spleen weight, an increase of the level of iron stored in the spleen, signs of kidney damage and increased kidney weights. NOAEL (systemic effects) = 11 ppm (27 mg/m3). LOAEL (systemic toxicity) = 15 ppm.
Test substance	:	Acetic acid (64-19-7)
Reliability	:	(2) valid with restrictions Peer-reviewed and published information. Reviewed and summarized in BIBRA (1993)

31.10.2005 (73)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Bacterial reverse mutation assay
System of testing	:	Bacterial

Test concentration	:	312.5, 625, 1250 and 5000 ug plate (Plate Incorporation Method)
Cycotoxic concentr.	:	>5000 ug/plate
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: The study was conducted in conformance with Draft OECD Protocol Nos. 419 and 420 and in general conformance with OECD Health Effects Test Guidelines Nos. 471 and 472 (both May 26, 1983).
Year	:	1984
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Statistical Methods: Means and standard deviations were calculated for each treatment. Responses (numbers of revertants) to the test substance were compared to concurrent negative and positive controls, as well as to historical data.
Result	:	The test substance was not mutagenic at any concentration tested, either with or without metabolic activation. The test substance was not cytotoxic at any concentration tested. The highest level tested, 5000 ug/plate, is the maximum required dose for studies of this type.
Source	:	Dow Corning Corporation Midland, MI
Test condition	:	S. typhimurium: TA-97, TA-98, TA-100 and TA-1535; E. coli: WP2 Species and cell type: Rat liver Quantity: 0.5 ml of a commercial S-9 mix was added to approximately 2.06 ml of the plating mixture Induced or Not Induced: Yes, Aroclor 1254 * All treatments were plated in triplicate. * The control and test substances were administered once. * The solvent (negative control) for all treatments/strains was dimethylsulfoxide (DMSO). * Anthracine was the positive control agent for the activation assays (all strains). In the nonactivation assays, the positive control substances were sodium azide (TA-1535 and TA-100), 4-nitroquinolone-N-oxide (TA-97), 2-nitrofluorene (TA-98) and N-methyl-N-nitro-N-nitroquanidine (WP2). All positive control substance treatments were 10 ug/plate. * The plates were incubated for 72 hours at 37 degrees C, then counted. * The number of cells evaluated per dose group was not reported. Revertants per plate for positive control substances ranged from 161-1768, depending on the agent and strai
Test substance	:	Ethyltriacetoxysilane (CAS No. 17689-77-9)
Conclusion	:	The test substance, ethyltriacetoxysilane, did not induce any cytotoxicity or mutagenicity in the tested strains at dosages up to 5000 ug/plate, both with and without metabolic activation. Appropriate concurrent negative and positive controls were included, and the expected responses were observed. Therefore, the test substance was not a bacterial mutagen under the conditions of this assay.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

25.02.2004 (32)

Type	:	Chromosomal aberration test
System of testing	:	Chinese hamster ovary cells
Test concentration	:	275, 550, 1100, 2200 ug/mL
Cycotoxic concentr.	:	With metabolic activation: 15% at 2200 ug/mL
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 473
Year	:	2002
GLP	:	yes
Test substance	:	other TS
Method	:	OECD 473 (1998); Swierenga, Mutation Research (246: 301-322;ICH (1996 and 1997); Evans (1976) The number and type of aberrations found, the percentage of structurally and numerically damaged cells (% aberrant cells) in the total population examined and mean aberrations per cell were calculated for each group. Fisher's exact test was used to compare pairwise the percent aberrant cells of each treatment group with that of the solvent control.
Remark	:	Ethyltriacetoxysilane and methyltriacetoxysilane differ only by a -CH2- group, and thus are close structural analogues. Both materials are unstable and undergo rapid hydrolysis to acetic acid and the corresponding silanetriol. Specifically, the hydrolysis rates of the two materials are <13 and <12 seconds for ethyltriacetoxysilane and methyltriacetoxysilane, respectively.
Result	:	Treatment time: 4 hrs Recovery time: 16 hrs Harvest time: 20 hrs S9: none Toxicity at highest dose scored: none at 2200 ug/plate Mitotic index: none Lowest effective dose (LED) for structural aberrations: none LED for numerical aberrations: none Treatment time: 20 hrs Recovery time: 0 hrs Harvest time: 20 hrs S9: none Toxicity at highest dose scored: none at 2200 ug/plate Mitotic index: none Lowest effective dose (LED) for structural aberrations: none LED for numerical aberrations: none Treatment time: 4 hrs Recovery time: 16 hrs Harvest time: 20 hrs S9: yes Toxicity at highest dose scored: 15% at 2200 ug/plate Mitotic index: 13% Lowest effective dose (LED) for structural aberrations: none LED for numerical aberrations: none
Test condition	:	In the chromosome aberration assay, the cells were treated for 4 and 20 hours in the non-activation system and for 4 hours in the S9 activation system. All the cells were harvested at 20 hours after treatment initiation. The solvent and negative control for all test article dose levels was dimethylsulfoxide (DMSO). Mitomycin was dissolved

in water and used as the positive control in the nonactivated system. Cyclophosphamide was dissolved in water and used as the positive control in the S9 activation system. In the absence of substantial toxicity at any dose level in any treatment group, 2200 g/ml was selected as the high dose for microscopic analysis in all three treatment groups. The next two lower doses were also analyzed in all harvests.

Test substance : Methyltriacetoxysilane CAS No. 4253-34-3; purity > 97%
Conclusion : Methyltriacetoxysilane CAS No. 4253-34-3 was concluded to be negative for the induction of structural and numerical chromosome aberrations in CHO cells.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
06.12.2004 (11)

Type : Bacterial reverse mutation assay
System of testing : Bacterial (Salmonella typhimurium and E. coli)
Test concentration : 100, 333, 1000,3333, and 5000 ug/plate
Cycotoxic concentr. : > 5000 ug/plate
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471
Year : 2002
GLP : yes
Test substance : other TS

Method : Ames, Mutation Research (1975); ICH (1996 and 1997); Maron, Mutation Research (1983). Responses (numbers of revertants) to the test substance were compared to concurrent negative and positive controls, as well as to historical data.
Remark : Ethyltriacetoxysilane and methyltriacetoxysilane differ only by a -CH2- group, and thus are close structural analogues. Both materials are unstable and undergo rapid hydrolysis to acetic acid and the corresponding silanetriol. Specifically, the hydrolysis rates of the two materials are <13 and <12 seconds for ethyltriacetoxysilane and methyltriacetoxysilane, respectively.
Test condition : The control and test substances were administered once. The solvent (negative control) for all treatment and strains was dimethylsulfoxide (DMSO) except for the sodium azide positive control which was diluted in water.

Positive Control Agents and Doses (ug/plate)
With activation:TA-98 - 2-AA (1.0)
TA100 - 2-AA (1.0)
TA1535 - 2-AA (1.0)
TA1537 - 2-AA (1.0)
WP2uvrA - 2-AA (10)

Without Activation:TA98 - NF (1.0)
TA100 - AZ (1.0)
TA1535 - AZ (1.0)
TA1537 - AA (75)
WP2uvrA - MM (1000)

2-AA = 2-Aminoanthracene
NF = Nitrofluorene
AZ = Sodium azide
AA = Aminoacridine

MM = Methyl methanesulfonate

All dose levels of test article, vehicle controls and positive controls were plated in triplicate. The plates were incubated at 37 degrees C for 48-72 hours. Plates that were not counted immediately following the incubation period were stored at 2-8 degrees C until counted.

Test substance : Methyltriacetoxysilane CAS no. 4253-34-3
Conclusion : Methyltriacetoxysilane CAS No. 4253-34-3 did not cause a positive mutagenic response in either the presence or absence of Aroclor-induced rat liver S9.
Reliability : (1) valid without restriction
06.12.2004 (10)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

Type : other
Species : mouse
Sex : male/female
Strain : no data
Route of admin. : drinking water
Exposure period :
Frequency of treatm. : daily
Premating exposure period
Male : 1 week prior to breeding
Female : 1 week prior to breeding
Duration of test :
No. of generation studies :
Doses : 60 mg/kg bw/day
Control group : yes
Method : other
Year : 1988
GLP : no data
Test substance : other TS

Method : Groups of 20 mice of each sex were given 0.025% sodium acetate in the drinking water (about 60 mg/kg bw/day) for 1 week before breeding, during a 9-day breeding period and (females only) throughout pregnancy, lactation and until the offspring were weaned at 3 weeks of age. The male offspring were given the same solution until they were 5-7 weeks old and were then examined in a 24-hour activity test.
Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role.

Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : Examination of the litters revealed no overt deformities, and pup weights were normal at day 1 and day 21. The activity of offspring of the treated group was lower than that of controls during the first 12 hours but was similar during the second 12 hours (the study did not show unequivocally that the decreased activity was maternally-mediated, since the pups were also exposed post-weaning).

Test substance : Acetic acid, sodium salt (127-09-3)

Reliability : (2) valid with restrictions
Peer reviewed published information. Reviewed and summarized in BIBRA (1993)

03.06.2005 (8) (28)

Type :
Species :
Sex :
Strain :
Route of admin. :
Exposure period :
Frequency of treatm. :
Premating exposure period
Male :
Female :
Duration of test :
No. of generation studies :
Doses :
Control group :
Method : other
Year : 2004
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Ethyltriacetoxysilane is sensitive to rapid hydrolysis, which may occur during testing, such that observed toxicity is likely due primarily to acetic acid. Abiotic hydrolysis studies show that hydrolysis products from the test substance undergo continuous, condensation reactions to produce higher molecular weight cyclic and linear siloxanes (the number-average and weight-average molecular weights were 633 and 809 with 22 area % of the chromatogram higher than 1000 molecular weight at the1-hr reaction time; at the 4-hr reaction time, the number-average and weight-average molecular weights increased to 750 and 1085 with 38 area % of the chromatogram higher than 1000 molecular weight, respectively). The alkyl silanols condense to siloxane oligomers; this condensation of silanols is affected by both concentration and pH, and since both change over time it is not feasible to isolate specific silanols for analysis (the structures continue to evolve until they either reach equilibrium or precipitate out of solution). While the hydrolysis of ethyltriacetoxysilane is rapid, the

polymerization products, while not volatile, are in a molecular weight range small enough to be considered, at least in part, biologically available.
In a 7-day range-finding study, stomach lesions were observed at low doses of ethyltriacetoxysilane and resembled acetic acid toxicity. This 7-day range finder study indicated that a maximum dose level of less than 20 mg/kg/day would be required for a reproduction study in order to avoid death or obvious suffering due to the corrosivity of the hydrolysis product, acetic acid. Due to the rapid hydrolysis of this material, a suitable vehicle can not be selected and all studies would utilize neat dosing. Based on the findings of the 7-day range-finder, less than 5 ul/d dose volumes and dose levels of 20 mg/kg bw/d or less would be required for a longer duration study, which would present technical difficulties, questions regarding dosing accuracy and a very low nominal systemic dose.

Reliability : (2) valid with restrictions
Study was Non-GLP

Flag : Critical study for SIDS endpoint

06.12.2004 (36)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	mouse
Sex	:	female
Strain	:	CD-1
Route of admin.	:	gavage
Exposure period	:	5 days (days 8-12 of gestation)
Frequency of treatm.	:	daily
Duration of test	:	three weeks
Doses	:	1,000 mg/kg bw
Control group	:	yes
NOAEL maternal tox.	:	= 1000 mg/kg bw
NOAEL teratogen.	:	= 1000 mg/kg bw
Method	:	other
Year	:	1987
GLP	:	no data
Test substance	:	other TS

Method : 30 pregnant CD-1 mice, approximately 60 days old, were give a single oral dose by gavage on days 8-12 of gestation. Animal quarters were maintained at a temperature of 22 °C, a relative humidity of 40-60%, and a 7 am to 7 pm photoperiod.

Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role.
Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid

and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : General parental toxicity: No effects
Toxicity to offspring: No effects

Test substance : Acetic acid, sodium salt (127-09-3)

Reliability : (2) valid with restrictions
Peer reviewed published information. Reviewed and summarized in BIBRA (1993).

Flag : Critical study for SIDS endpoint

03.06.2005 (59)

Species : rat
Sex :
Strain :
Route of admin. :
Exposure period :
Frequency of treatm. :
Duration of test :
Doses :
Control group :
Method : other: Range-finding study
Year : 2004
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Ethyltriacetoxysilane is sensitive to hydrolysis, which may occur during testing, such that observed toxicity is likely due primarily to the hydrolysis products acetic acid, with some potential exposure to trisilanols, and silanol oligomers. Abiotic hydrolysis studies show that hydrolysis products from the test substance undergo continuous, condensation reactions to produce higher molecular weight cyclic and linear siloxanes (the number-average and weight-average molecular weights were 633 and 809 with 22 area % of the chromatogram higher than 1000 molecular weight at the1-hr reaction time; at the 4-hr reaction time, the number-average and weight-average molecular weights increased to 750 and 1085 with 38 area % of the chromatogram higher than 1000 molecular weight, respectively). The alkyl silanols condense to siloxane oligomers; this condensation of silanols is affected by both concentration and pH, and since both change over time it is not feasible to isolate specific silanols for analysis (the structures continue to evolve until they either reach equilibrium or precipitate out of solution). While the hydrolysis of ethyltriacetoxysilane is rapid, the polymerization products, while not volatile, are in a molecular weight range small enough to be considered, at least in part, biologically available.
In a 7-day range-finding study, stomach lesions were observed at low doses of ethyltriacetoxysilane and resembled acetic acid toxicity. This 7-day range finder study indicated that a maximum dose level of less than 20 mg/kg/day would be required for a reproduction study in order to avoid death or obvious suffering due to the corrosivity of the hydrolysis product, acetic acid. Due to the rapid hydrolysis of this material, a suitable vehicle can not be selected and all studies would utilize neat dosing. Based on the findings of the 7-day range-finder, less than 5 ul/d dose volumes and dose levels of 20 mg/kg

bw/d or less would be required for a longer duration study, which would present technical difficulties, questions regarding dosing accuracy and a very low nominal systemic dose.

Reliability : (2) valid with restrictions
Study was Non-GLP

Flag : Critical study for SIDS endpoint

06.12.2004 (36)

Species : rat
Sex : female
Strain : Wistar
Route of admin. : gavage
Exposure period : 10 days
Frequency of treatm. : daily
Duration of test : 14 days
Doses : 0, 16, 74, 345, and 1600 mg apple cider vinegar/kg bw/day (1600 mg/kg bw/day is equivalent to approximately 100 mg acetic acid/kg bw/day)
Control group : yes, concurrent no treatment
Result : No effects on nidation or on maternal or fetal survival at doses up to 1600 mg/kg bw/day (equal to 100 mg acetic acid/kg bw/day).
Method : other
Year : 1974
GLP : no
Test substance : other TS

Method : Following mating, adult female albino rats (Wistar) were dosed daily with 1.6 g apple cider vinegar (5% acetic acid)/kg bw/d by oral intubation beginning on day 6 and ending on day 18 of gestation. Animals were observed daily and body weights recorded. On day 20, Caesarian sections were performed on all dams and the numbers of implantation sites, resorption sites, and live and dead fetuses was recorded. General external and internal examinations were also made of the dams.

Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role.
Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
Conversion of dose: 1600 mg apple cider vinegar/kg bw/day approximately equal to 100 mg acetic acid/kg bw/day

Result : No effects on nidation or on maternal or fetal survival at doses up to 1600 mg apple cider vingegar/kg bw/day (equal to 100 mg acetic acid/kg bw/day). The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring in the controls.
Test substance : Apple cider vinegar; acetic acid (64-19-7) 5%
Reliability : (2) valid with restrictions
Comparable to a guideline study. Peer-reviewed published

information. Reviewed and summarized in BIBRA (1993).

03.06.2005 (8) (43)

Species	:	mouse
Sex	:	female
Strain	:	no data
Route of admin.	:	gavage
Exposure period	:	10 days
Frequency of treatm.	:	daily
Duration of test	:	17 days
Doses	:	0, 16, 74, 345, and 1600 mg apple cider vinegar/kg bw/day (1600 mg apple cider vinegar/kg bw/day approximately equivalent to 100 mg acetic acid/kg bw/day)
Control group	:	yes, concurrent no treatment
Result	:	No effects on nidation or on maternal or fetal survival were observed at doses up to 1600 mg/kg bw/day (equal to 100 mg acetic acid/kg bw/day).
Method	:	other
Year	:	1974
GLP	:	no
Test substance	:	other TS
Method	:	Following mating, adult female albino CD-1 mice were dosed daily by oral intubation beginning on day 6 of gestation. Animals were observed daily and body weights recorded for 10 days. On day 17, Caesarian sections were performed on all dams and the numbers of implantation sites, resorption sites, and live and dead fetuses was recorded. General external and internal examinations were also made of the dams.
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material. Conversion of dose: 1600 mg apple cider vinegar/kg bw/day approximately equal to 100 mg acetic acid/kg bw/day
Result	:	No effects on nidation or on maternal or fetal survival at doses up to 1600 mg apple cider vinegar/kg bw/day (equal to 100 mg acetic acid/kg bw/day). The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring in the controls.
Test substance	:	Apple cider vinegar; acetic acid (64-19-7) 5%
Reliability	:	(2) valid with restrictions Comparable to a guideline study. Peer-reviewed published information. Reviewed and summarized in BIBRA (1993).

03.06.2005 (2) (43)

Species	:	rabbit
Sex	:	female
Strain	:	no data

Route of admin.	:	gavage
Exposure period	:	13 days
Frequency of treatm.	:	daily
Duration of test	:	23 days
Doses	:	0, 16, 74, 345, and 1600 mg apple cider vinegar/kg bw/day (1600 mg apple cider vinegar/kg bw/day approximately equivalent to 100 mg acetic acid/kg bw/day)
Control group	:	yes, concurrent no treatment
Result	:	No effects on nidation or on maternal or fetal survival were observed at doses up to 1600 mg/kg bw/day (equal to 100 mg acetic acid/kg bw/day).
Method	:	other
Year	:	1974
GLP	:	no
Test substance	:	other TS
Method	:	Following artificial insemination, adult Dutch-belted female rabbits were dosed daily by oral intubation beginning on day 6 of gestation. Animals were observed daily and body weights recorded. On day 29, Caesarian sections were performed onall does and the numbers of of corpora lutea, implantation sites, resorption sites, and live and dead fetuses was recorded. General externaland internal examinations were also made of the does.
Remark	:	Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role. Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material. Conversion of dose: 1600 mg apple cider vinegar/kg bw/day approximately equal to 100 mg acetic acid/kg bw/day
Result	:	No effects on nidation or on maternal or fetal survival at doses up to 1600 mg apple cider vinegar/kg bw/day (equal to 100 mg acetic acid/kg bw/day). The number of abnormalities seen in either soft or skeletal tissues of the test groups did not differ from the number occurring in the controls.
Test substance	:	Apple cider vinegar; acetic acid (64-19-7) 5%
Reliability	:	(2) valid with restrictions Comparable to a guideline study. Peer reviewed published information. Reviewed and summarized in BIBRA (1993)

03.06.2005 (2) (43)

Species	:	other: Fertile single-comb white leghorn chicken eggs
Sex	:	
Strain	:	
Route of admin.	:	other: injection into egg
Exposure period	:	
Frequency of treatm.	:	single injection
Duration of test	:	
Doses	:	maximum 10.0 mg/egg
Control group	:	yes

Method : other
Year : 1980
GLP : no data
Test substance : other TS

Method : Fertile eggs from single-comb white leghorn chickens were used. The test substance in water was administered by two routes, injection via the yolk and via the air cell. For each injection route, eggs were treated at two stages of incubation: preincubation (0 hrs) and on the fourth day (96 hrs). At least 100 embryos per each of four dose levels were treated. After treatment, all eggs were candled daily and nonviable embryos were removed. Surviving embryos were allowed to hatch.
Remark : Acetic acid and its salts include acetic acid, calcium acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role.
Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.
The LD50 is for the test condition in which the injection was made to the yolk sac at 0 hrs.
Result : LD50: 4.58 mg/egg
NOAEL teratogenicity: 10.0 mg/egg
No teratogenic response under any of the four test conditions was observed at the highest concentration injected.
Test substance : Acetic acid, sodium salt (127-09-3)
Reliability : (2) valid with restrictions
Peer reviewed published information.

03.06.2005 (94)

Species : rat
Sex : female
Strain : no data
Route of admin. : drinking water
Exposure period : 18 days
Frequency of treatm. : daily
Duration of test : 44 days
Doses : .03% (100 mg/kg bw)
Control group :
NOAEL maternal tox. : = .03 - %
Method : other
Year : 1982
GLP : no data
Test substance : other TS

Method : Rats suckling from birth for 18 days from mothers exposed to 0.03% acetic acid in drinking water.
Remark : Acetic acid and its salts include acetic acid, calcium

acetate, potassium acetate and sodium acetate. The chemical structures, physical-chemical properties, environmental fate behavior, and aquatic and mammalian toxicity of these compounds are similar. Acetic acid and its salts undergo dissociation in aqueous media into the acetate anion and the respective cations. The toxicity of each compound is driven by acetate, with the cations playing a minor role.
Acetoxysilanes are not stable when exposed to moisture and undergo rapid hydrolysis. When added to water, 100% of the parent material is hydrolyzed to acetic acid and the corresponding silanetriol in less than 0.2 minutes at 25°C and pH 7.1. This hydrolysis produces 3 moles of acetic acid and 1 mole of alkyl substituted silanetriol for every mole of (alkyl) triacetoxysilane parent material.

Result : Increased body weights and a decreased activity by 44 days after birth. No effect on dams.
Test substance : Acetic acid (64-19-7)
Reliability : (3) invalid
Does not meet important criteria of a guideline study.
Considered limited in BIBRA (1993)

03.06.2005 (4)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

Type of experience : other: Volatile Species from Sealants Containing Acetoxysilanes

Result : Methyltriacetoxysilane was not detected in the headspace. > 100 ppm acetic acid was detected in the headspace. The same results were obtained when the study was conducted with commercial samples (DC732 silicone sealant, GE RTV108 silicone sealant or GE RTV108 with no added water).
The detection limit for the acetoxysilane target compounds was estimated to be on the order of 100 ppb, based on the typical response factors noted for the siloxanes quantified and the response for neat acetoxysilanes measured as a liquid phase. It was not possible to prepare accurate gas phase standards of the acetoxysilanes without hydrolysis or other reaction rapidly occurring.
Source : GE Silicones
Test condition : -Conditions: Sealant samples (2 grams) were extruded in a dry atmosphere into a sealed vessel. Experiments were run with water present, with a 59% relative humidity, and with no additional water. Samples were incubated for 20 minutes at 27 C then headspace samples were taken.

-Controls: Samples of each of the neat silanes were also treated in the same manner as the sealant samples and were used for calibration of the test method.

-Analytical procedures: 200 microliter aliquots were sampled from the headspace of the sealed container and

injected into a GC-MSThe DC732 sealant experiment was run in triplicate with identical results.

Test substance : Methyltriacetoxysilane
Ethyltriacetoxysilane
Diacetoxydimethylsilane
Acetoxytrimethylsilane
Methyltriacetoxysilane @ 59% relative humidity
DC732 silicone sealant
GE RTV108 silicone sealant
GE RTV108 with no added water

Commercial silicone sealants which utilize an acetoxy alkylsilane crosslinking reaction were used. Neat samples of the individual silanes were also tested.

Conclusion : None of the acetoxy alkylsilanes used as crosslinkers volatilize during cure of the sealants. Instead they hydrolyze and condense releasing acetic acid, which was detected. Therefore there is no human exposure to the acetoxy alkylsilanes from their predominant use in silicones sealants.

Reliability : (1) valid without restriction
02.12.2004 (70)

5.11 ADDITIONAL REMARKS

Type : other

Remark : Ethyltriacetoxysilane is sensitive to rapid hydrolysis, which may occur during testing, such that observed toxicity is likely due primarily to acetic acid. Abiotic hydrolysis studies show that hydrolysis products from the test substance undergo continuous, condensation reactions to produce higher molecular weight cyclic and linear siloxanes (the number-average and weight-average molecular weights were 633 and 809 with 22 area % of the chromatogram higher than 1000 molecular weight at the1-hr reaction time; at the 4-hr reaction time, the number-average and weight-average molecular weights increased to 750 and 1085 with 38 area % of the chromatogram higher than 1000 molecular weight, respectively). The alkyl silanols condense to siloxane oligomers; this condensation of silanols is affected by both concentration and pH, and since both change over time it is not feasible to isolate specific silanols for analysis (the structures continue to evolve until they either reach equilibrium or precipitate out of solution). While the hydrolysis of ethyltriacetoxysilane is rapid, the polymerization products, while not volatile, are in a molecular weight range small enough to be considered, at least in part, biologically available.

Source : Epona Associates, LLC
20.05.2004

Type : other: GRAS

Remark : "Both acetic acid and sodium diacetate are considered by the Food and Drug Administration to be Generally Recognized as Safe (GRAS) (21 CFR 184.1005 and 184.1754) for use in food."

"EPA has also briefly discussed above sodium diacetate's chemistry relative to sodium acetate and acetate as well as chemical and metabolic properties of these individual compounds. Given these compounds' low toxicities, natural occurrence, and inherent functions in the metabolic pathways of humans and domestic animals EPA is not concerned about the negligible human dietary exposure or risk from the use of sodium diacetate. The Agency is therefore not requiring any human health studies for sodium diacetate."

31.05.2005 (88)

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