Aminosilanes Testing Package

CAS Nos. 919-30-2 and 1760-24-3

Aminosilanes Test Plan
Aminosilanes Category Justification
Robust Summaries for CAS No. 919-30-2
Robust Summaries for CAS No. 1760-24-3

March 16, 2000

Submitted to EPA under the HPV Challenge Program by:

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Aminosilanes
Category Test Plan

CAS Nos. 919-30-2 and 1760-24-3

Silicones Environmental, Health and Safety Council
March 16, 2000

Chemical	Physical-Chemical				
	Melting Point	**Boiling Point**	**Vapor Pressure**	**Partition Coefficient**	**Water Solubility**
919-30-2 1-Propanamine, 3-(triethoxysilyl)-	NR[1]	A	A	NA[3]	NA[3]
1760-24-3 1,2-Ethanediamine, N-[3-(trimethoxysilyl)propyl]-	NR[2]	A	A	NA[3]	NA[3]

Chemical	Environmental Fate			
	Photo-degradation	**Stability in Water**	**Transport/ Distribution**	**Biodegradation**
919-30-2 1-Propanamine, 3-(triethoxysilyl)-	NA[3]	Test	NA[3]	A
1760-24-3 1,2-Ethanediamine, N-[3-(trimethoxysilyl)propyl]-	NA[3]	Test	NA[3]	A

Chemical	Ecotoxicity		
	Acute Toxicity to Fish	**Acute Toxicity to Aquatic Plants (e.g., Algae)**	**Acute Toxicity to Aquatic Invertebrates (e.g., Daphnia)**
919-30-2 1-Propanamine, 3-(triethoxysilyl)-	A	A	A
1760-24-3 1,2-Ethanediamine, N-[3-(trimethoxysilyl)propyl]-	A	A	A

Chemical	Toxicity					
	Acute Toxicity	**Genetic Toxicity *In Vitro***	**Genetic Toxicity *In Vivo***	**Repeat Dose Toxicity**	**Repro-ductive Toxicity**	**Develop-mental Toxicity**
919-30-2 1-Propanamine, 3-(triethoxysilyl)-	A	A	A	Test	Test	A
1760-24-3 1,2-Ethanediamine, N-[3-(trimethoxysilyl)propyl]-	A	A	R	R	R	R

[1] Endpoint is not required because the melting point for this liquid is less 0°C. (a) Melting point <-70°C. Material Safety Data Sheet. CAS No. 919-30-2. Union Carbide Chemicals and Plastics Company, Inc. Effective date 22 October 1992. (b) Melting point <-70°C. Material Safety Data Sheet. CAS No. 919-30-2. OSi Specialties, Inc. Effective date 6 March 1995.

[2] Endpoint is not required because the melting point for this liquid is below O°C. (a) Melting point <-50°C. Material Safety Data Sheet. CAS No. 1760-24-3. Wacker Chemie GmbH. Effective date 29 June 1999.

[3] Endpoints are not applicable because the chemicals are hydrolytically unstable.

Legend

Symbol	Description
R	Endpoint requirement fulfilled using category approach, SAR
Test	Endpoint requirements to be fulfilled with testing
Calc	Endpoint requirement fulfilled based on calculated data
A	Endpoint requirement fulfilled with adequate existing data
NR	Not required per the OECD SIDS guidance
NA	Not applicable due to physical/chemical properties
O	Other

Date Work Plan Available for Comment: (Q1, 2000)

Date Work Plan Complete: (quarter, year)

Aminosilanes
Category Justification

CAS Nos. 919-30-2 and 1760-24-3

Silicones Environmental, Health and Safety Council
March 16, 2000

Introduction

A provision for the use of structure activity relationships (SAR) to reduce testing needs is included under EPA's HPV Challenge Program. Specifically, categories may be formed based on structural similarity, through analogy, or through a combination of category and analogy for use with single chemicals. The benefits of using a category approach are numerous and include (1) accelerated release of hazard information to the public, as category analysis and testing is proposed to be initiated within the first two years of the HPV Program; (2) reduction in the number of animals used for testing; and (3) an economic savings as a result of a reduced testing program.

Two aminosilane materials proposed to be categorized based on structural similarity are:

- 1-Propanamine, 3-(triethoxysilyl)- (CAS No. 919-30-2)
- 1,2-Ethanediamine, *N*-[3-(trimethoxysilyl) propyl]- (CAS No. 1760-24-3).

Both of these aminosilanes are listed as HPV Challenge Program chemicals. The development of this aminosilane category follows current EPA guidance[1].

Background Information: Aminosilane Manufacturing and Commercial Applications

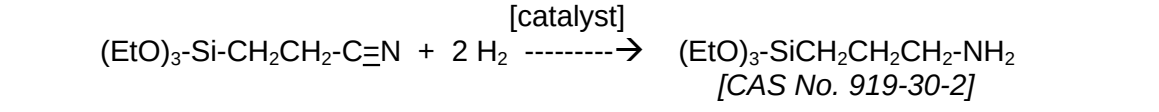
Manufacturing

Two different routes are used to manufacture these aminosilane materials. Both processes are conducted in highly engineered, closed systems that comply with all applicable environmental laws and regulations.

[1] US EPA, Office of Pollution Prevention and Toxics. Development of Chemical Categories, Chemical Right-to-Know Initiative. http://www.epa.gov/opptintr/chemrtk/categuid.htm

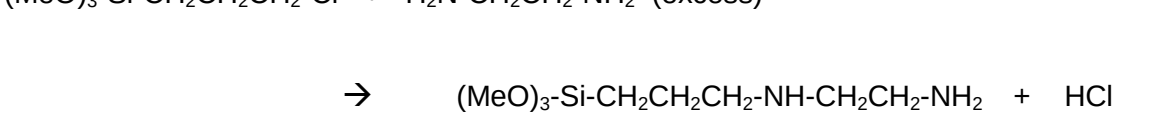
The typical manufacturing procedure of CAS No. 919-30-2 involves the catalyzed hydrogenation of the corresponding nitrile (2-cyanoethyltriethoxysilane) to produce the primary amino-functional silane. Vacuum distillation provides the highest quality version. See Figure 1.

Figure 1. Synthesis of CAS No. 919-30-2



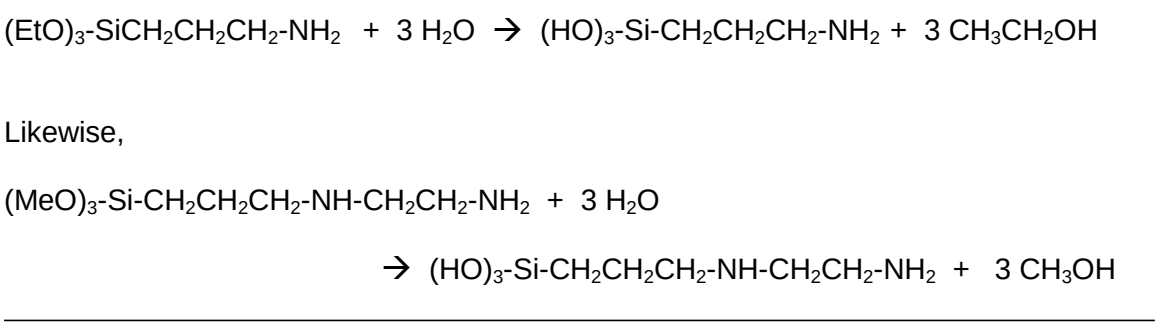
The second aminosilane material, CAS No. 1760-24-3, is typically produced via the non-catalyzed substitution reaction of the corresponding chloroalkylsilane with excess ethylenediamine. High vacuum distillation of the resulting product is optional depending upon quality needs. See Figure 2.

Figure 2. Synthesis of CAS No. 1760-24-3



Aminofunctional silanes, such as the aforementioned candidates, are highly susceptible to hydrolysis. In fact, the amine groups enhance water solubility, as well as catalyze the rapid hydrolysis reaction to produce trisilanol derivatives of the substances in minutes. The corresponding alcohols are generated as by-products of hydrolysis. Both of these alcohols are included in the HPV Challenge Program. See Figure 3.

Figure 3. Hydrolysis of CAS Nos. 919-30-2 and 1760-24-3



The reactive nature of aminosilanes requires handling in closed systems that exclude moisture. This involves inert blanketing and purging during transfers and in container filling. The manufacturers of aminosilanes provide technical assistance and guidelines to customers to ensure safe, hydrolysis-free handling practices.

Commercial Applications

The commercial uses of these two aminofunctional silanes are numerous and include various applications as coupling agents and adhesion promoters in fiberglass, adhesives and sealants, foundry resins, and in pre-treatment for coatings. Aminosilanes are not sold in consumer markets.

As coupling agents and adhesion promoters, aminosilanes are intentionally converted by hydrolysis to the trisilanols, which then bond molecularly to inorganic substrates. During hydrolysis, the alkoxy (methoxy- or ethoxy-) groups are liberated as the corresponding alcohol. The silane-modified surfaces of these inorganic substrates become incorporated within polymeric resins by a chemical reaction with the amine group. This completes the coupling process. Since the amino-functional silane is converted and bound within the substrate by polymer coupling, free silane is not present within the final products. Thus, any toxicological effects originating from the alkoxysilane or amine groups of the silane are eliminated as a result of this coupling process.

Human or environmental exposure to these materials is limited to accidental acute exposures. Acute exposure of the general population following an accidental release is possible from the alcohol liberated following hydrolysis. Because of the reactive nature and the necessary engineering controls in the use of these aminosilanes in industry, such exposures are minimal. The alcohols liberated from hydrolysis of these aminosilanes include methanol and ethanol, which are already included as separate materials under the HPV Challenge Program.

Development of the Aminosilane Category

EPA has described a stepwise process for developing categories. These steps include:

- Grouping a series of like chemicals, including the definition of criteria for the group.
- Gathering data on physicochemical properties, environmental fate and effects, and health effects for each member of the category.
- Evaluating the data for adequacy.
- Constructing a matrix of available and unavailable data.
- Determining whether a correlation exists among category members and gathered data.

Definition of the Aminosilane Category

As defined by EPA under the HPV Program, a chemical category is “a group of chemicals whose physicochemical and toxicological properties are likely to be similar or follow a regular pattern as a result of structural similarity.” The similarities should be based on a common functional group, common precursors or breakdown products (resulting in structurally similar chemicals), and an incremental and constant change across the category. The goal of developing a chemical category is to use interpolation and/or extrapolation to assess chemicals rather than conducting additional testing.

The aminosilanes listed in the current HPV Challenge Program have three carbon atoms linked to a silicon (Si) molecule with an alkoxy group (an alkoxysilane) at one end, and an amine group or groups at the other end of the three carbon chain, as illustrated in Figure 4.

Figure 4. Aminosilane Structural Definition

$(XO)_3$-Si-$CH_2CH_2CH_2$-$(NH_2)_y$

Where: $(XO)_3$ = alkoxy group (methyl, ethyl, etc)
and
y = number of amine groups

Structurally, both aminosilane materials contain a silicon atom at one end of the molecule, each with a different alkoxy group (ethoxy- or methoxy-) (see Figure 5). These materials each contain three carbon atoms, one with a single amine and the other with two amines. Because these materials are aliphatic amines they are very basic and have typical amine reactions. The molecular weights are similar for the two aminosilanes. The molecular weight of CAS No. 919-30-2 is 221.3 grams/mole; the molecular weight of CAS No. 1760-24-3 is 222.1 grams/mole.

Figure 5. Aminosilane Structures

$(EtO)_3$-Si-$CH_2CH_2CH_2$-NH_2 *[CAS No. 919-30-2]*

$(MeO)_3$-Si-$CH_2CH_2CH_2$-NH-CH_2CH_2-NH_2 *[CAS No. 1760-24-3]*

As described below, these materials hydrolyze within minutes to form the corresponding alcohol, and the remaining trisilanol compounds (Figure 6) are even more clearly recognizable as structurally similar. These trisilanols are highly reactive, both in unintended reactions with themselves and with intentional substrates, which forms the basis for their commercial applications. The hydrolysis rate of the aminosilanes is very rapid (within minutes), and is expected to be similar for the two materials discussed herein.

Figure 6. Corresponding Trisilanols Resulting from Hydrolysis of Aminosilanes

$(HO)_3$-Si-$CH_2CH_2CH_2$-NH_2 *[for CAS No. 919-30-2]*

$(HO)_3$-Si-$CH_2CH_2CH_2$-NH-CH_2CH_2-NH_2 *[for CAS No. 1760-24-3]*

Matrix of SIDS Endpoints

In order to construct a matrix of SIDS endpoints for the members of the aminosilane category, the data on physicochemical properties, environmental fate and effects, and health effects for each member of the category were collected and evaluated for adequacy. The results of these activities are presented in Table 1.

Table 1

Matrix of Available and Adequate Data on Aminosilane Category Members		
Test	**CAS No. 919-30-2**	**CAS No. 1760-24-3**
	Physicochemical Properties	
Melting Point	NA	NA
Vapor Pressure	√	√
Boiling Point	√	√
Partition Coefficient	-	-
Water Solubility	-	-
Hydrolysis	-	-
Environmental Fate	-	-
Biodegradation	√	√
Environmental Transport	-	-
Test	**CAS No. 919-30-2**	**CAS No. 1760-24-3**
	Ecotoxicity	
Acute Fish	√	√
Acute Daphnid	√	√
Algae	√	√
Terrestrial	-	-
Test	**CAS No. 919-30-2**	**CAS No. 1760-24-3**
	Heath Effects	
Acute Oral	√	√
Acute Inhalation	-	-
Acute Dermal	√	√
Repeated Dose	-	-
Genotoxicity (*in vitro* -bacteria)	√	√
Genotoxicity (*in vitro* - nonbacterial)	√	√
Genotoxicity (*in vivo*)	√	-
Repro/Developmental	√	-
(√) = Data available and considered adequate; (NA) = Not applicable due to chemical/physical properties; (-) No data available, or data considered inadequate		

Correlation within the Aminosilane Category

The matrix data patterns for physicochemical properties, environmental fate, ecotoxicity, and health effects were evaluated for CAS Nos. 919-30-2 and 1760-24-3. A description of the results of this evaluation follows.

- **Correlation of Physicochemical Properties**

The physical and chemical property data available for the two aminosilane materials are in good agreement. Boiling points for CAS Nos. 919-30-2 and 1760-24-3 are 223°C and 264°C, respectively. Melting points for CAS Nos. 919-30-2 and 1760-24-3 are <–70°C and <–50°C, respectively. The measured vapor pressure at 121°C is 3.3 kPa (29 mm Hg) for CAS No. 919-30-2 and 0.67 kPa (5 mm Hg) for CAS No. 1760-24-3. Similarly, the vapor pressures extrapolated to 20°C are 2 Pa (0.015 mm Hg) and 0.4 Pa (0.003 mm Hg) for CAS Nos. 919-30-2 and 1760-24-3, respectively. Data for octanol/water partition coefficient and water solubility are not available for either material. Moreover, the octanol/water partition coefficient and water solubility are not appropriate because these materials hydrolyze so rapidly.

- **Correlation of Environmental Fate**

Available data indicate that both materials are <u>not</u> "readily biodegradable." Degradation of CAS Nos. 919-30-2 and 1760-24-3 was 67% and 39%, respectively, after 28 days. The hydrolysis rate of CAS No. 1760-24-3 has been measured. The half-life is 24.1 minutes at 25° C. The half-life for hydrolysis of CAS No. 919-30-2 is predicted to be similar based on the trimethoxy analog. Data on photodegradation and transport/distribution are not available for either material, as these materials hydrolyze rapidly. Moreover, these endpoints are not considered appropriate because the materials are hydrolytically unstable.

- **Correlation of Ecotoxicity**

Available data indicate that CAS Nos. 919-30-2 and 1760-24-3 are practically non-toxic (96-h LC_{50} > 100 mg/L) to freshwater fish. Similarly, CAS No. 919-30-2 is practically non-toxic to the water flea (*Daphnia magna)* and freshwater green algae (*Scenedesmus subspicatus*). In contrast, CAS No. 1760-24-3 is moderately toxic (1 mg/L < EC_{50} < 10 mg/L) to the water flea and freshwater green algae *Selenastrum capricornutum* (green algae), and practically non-toxic to bluegreen algae (*Anabaena flos-aquae*).

- **Correlation of Health Effects**

Acute oral and dermal toxicity of the two aminosilanes are comparable as predicted by the structural similarity of the materials. Both materials exhibit a very low order of acute toxicity (LD_{50} > 2000 mg/kg) by either the oral or the dermal route of exposure.

The genotoxicity profile of these two materials also reflects the similarity of the structures. Both materials were negative in multiple bacterial mutagenicity assays, as well as *in vitro* mammalian cell gene mutation studies (CHO/HGPRT). Both aminosilanes lacked significant DNA damaging activity in the Sister Chromatid Exchange Assay. CAS No. 919-30-2 was negative in an *in vitro* chromosome aberration test with Chinese Hamster fibroblasts. CAS No. 919-30-2 was not clastogenic in an *in vivo* mouse micronucleus assay.

Aminosilanes
Robust Summaries
CAS No. 919-30-2

Silicones Environmental, Health and Safety Council
March 16, 2000

Contents

Boiling Point

Test Substance

Identity: 3-aminopropyl-triethoxysilane (CAS No. 919-30-2)

Remarks Field for Test Substance

Purity of test substance not identified.

Method

Method/guideline followed:	Calculated
GLP (Y/N):	No
Year (study performed):	1975

Remarks Field for Test Conditions

This robust summary is based upon a manuscript published in a Russian journal. The English translation of the abstract for the manuscript indicates that the temperature dependence of vapor pressure for the test substance (CAS No. 919-30-2) was determined by isoteniscopic and ebullioscopic methods. Test conditions were not specified.

Results

Boiling point value (°C):	223
Pressure:	101.3
Pressure unit:	kPa
Decomposition (yes/no/ambiguous):	ambiguous

Remarks Field for Results

The Antoine vapor pressure correlation coefficients used to calculate the boiling point (equation provided in the abstract) were obtained by regression of measured data. However, the translated abstract does not provide the data used to derive the Antoine coefficients and does not identify the temperature range over which vapor pressures were measured. The following table summarizes the vapor pressure data available in the published literature and compares the measured values to the values calculated using the Antoine vapor pressure correlation.

Temp. (°C)	Vapor Pressure (mm Hg)		Deviation (%)	Reference
	measured	calculated		
55.0	1	0	52	Albarino et. al., (1973)
110.5	10	16	-56	Belyakova et al. (1972)
115.0	19	19	-2	Speier et al. (1971)
120.5	29	25	14	Klyuchnikov et al. (1970)
122.0	28	27	4	Fialova et al. (1973)

Conclusions

Remarks Field with Ability to Identify Source of Comment

Vapor pressures calculated using the Antoine equation used to generate the boiling point of the test substance (CAS No. 919-30-2) are generally in good agreement with independently measured data. However, serious error may result if the Antoine vapor pressure correlation is used for extrapolations outside the limits of measured data. Hence, significant error may be associated with the reported boiling point for the test substance (CAS 919-30-2). Nonetheless, the result is comparable to values obtained from the literature and other studies (see Supporting Data).

Data Quality

Reliabilities (Klimisch Code):

Remarks Field for Data Reliability

This robust summary is based upon an English translation of an abstract for a manuscript published in a Russian journal. The abstract provides the Antoine vapor pressure correlation. However, the vapor pressure data used to generate the Antoine coefficients and the methods used to obtain the data are not provided. Consequently, the reliability of the data or the calculated boiling point cannot be determined.

References

Key Study: Bragin, G.P.; Karapet'yants, M.K. 1975. Temperature dependence of the saturated vapor pressure of some silicone-germanium-, and tin-containing compounds and mixed organometalic compounds. *Tr. Khim. Khim. Tekhnol.* 4:76-77.

Cited Documents:

- Albarino, R.V. and H. Schonhorn. 1973. Retention of antioxidants in polyethylene by silane coupling agents. *J. Appl. Polym. Sci.* 17(11):3323-3335.
- Belyakova, Z.V., V.N. Bochkarev, S.A. Golubtsov, Z.V. Belikova, M.S. Yamova, A.A. Ainshtein, G.G. Baranova, L.A. Efremova, and K.K. Popkov. 1972. Reaction of triethoxysilane with allylamine in the presence of catalysts. *Zh. Obshch. Khim.* 42(4):858-862.

- Fialova, V.; V. Bazant, and V. Chvalovsky. 1973. Organosilicon compounds. Effect of structure on the basicity of silylalkylamines. *Collect. Czech. Chem. Commun.* 38(12):3837-3844.
- Klimisch, H.J., M. Andreae, and U. Tillman. 1997. A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data. *Regul. Toxicol. Pharmacol.:* 25:1-5.
- Klyuchnikov, N.G., F.I. Karabadzhak, and V.B. Losev. 1970. Inhibiting properties of some organosilazanes and organosilicon amines. *Zh. Prikl. Khim. (Leningrad)* 43(12):2763-2765.
- Speier, J.L., C.A. Roth, and J.W. Ryan. 1971. Syntheses of (3-aminoalkyl) silicon compounds. *J. Org. Chem.* 36(21):3120-3126.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Remarks Field for General Remarks

Supporting Data:

- Extrapolated boiling point of 220°C @ 101.3 kPa. Ditsent, V.E., I.I. Skorokhodov, N.A. Terent'eva, M.N. Zolotareva, Z.V. Belyakova, and Z.V. Belikova. 1976. Saturated vapor pressure of gamma-aminopropyltriethoxysilane. *Zh. Fiz. Khim.* 50(7):1905-1906.
- Reported boiling point of 217°C @ 101.3 kPa. *Dictionary of Organic Compounds, 5th Ed.* 1982. Buckingham, J.; Editor. Chapman and Hall, New York, N. Y., USA. 7840 pp.
- Reported boiling point of 221°C @ 101.3 kPa. *Handbook of Organosilicon Compounds: Advances Since 1961, Vol. 2.* 1973. Bazant, V., V. Chvalovsky; and J. Rathousky, Editors. Dekker, New York, N. Y., USA. 619 pp.
- Reported boiling point of 220°C @ 101.3 kPa. General Electric, physical properties database.
- Reported boiling point of 262°C @ 101.3 kPa. Dow Corning Corporation, physical properties database.

Vapour Pressure

Test Substance

Identity: 3-aminopropyl-triethoxysilane (CAS No. 919-30-2)

Remarks Field for Test Substance

Purity of test substance not identified.

Method

Method/guideline followed:	Calculated
GLP (Y/N):	No
Year (study performed):	1975

Remarks Field for Test Conditions

This robust summary is based upon a manuscript published in a Russian journal. The English translation of the abstract for the manuscript indicates that the temperature dependence of vapor pressure for the test substance (CAS No. 919-30-2) was determined by isoteniscopic and ebullioscopic methods. Test conditions were not specified.

Results

Vapor pressure value:	2 Pa
Temperature (°C):	20
Decomposition (yes/no/ambiguous):	ambiguous

Remarks Field for Results

The Antoine vapor pressure correlation coefficients used to calculate the vapor pressure at 20°C (equation provided in the abstract) were obtained by regression of measured data. However, the translated abstract does not provide the data used to derive the Antoine coefficients and does not identify the temperature range over which the vapor pressures were measured. The following table summarizes the vapor pressure data available in the published literature and compares the measured values to values calculated using the Antoine vapor pressure correlation.

Temp. (°C)	Vapor Pressure (Pa)		Deviation (%)	Reference
	measured	calculated		
55.0	133	64	52	Albarino et. al., (1973)
110.5	1333	2074	-56	Belyakova et al. (1972)
115.0	2533	2581	-2	Speier et al. (1971)
120.5	3866	3336	14	Klyuchnikov et al. (1970)
122.0	3732	3574	4	Fialova et al. (1973)

Conclusions

Remarks Field with Ability to Identify Source of Comment

Vapor pressures of the test substance (CAS No. 919-30-2) calculated using the Antoine equation are generally in agreement with independently measured data. However, serious error may result if the Antoine vapor pressure correlation is used for extrapolations outside the limits of measured data. Hence, significant error may be associated with the reported vapor pressure of the test substance (CAS No. 919-30-2) at 20°C. Nonetheless, the result is comparable to values obtained from the literature (see Supporting Data).

Data Quality

Reliabilities (Klimisch Code):

Remarks Field for Data Reliability

This robust summary is based upon an English translation of an abstract for a manuscript published in a Russian journal. The abstract provides the Antoine vapor pressure correlation. However, the vapor pressure data used to generate the Antoine coefficients and the methods used to obtain the data are not provided. Consequently, the reliability of the data or the calculated vapor pressure at 20°C cannot be determined.

References

Key Study: Bragin, G.P.; Karapet'yants, M.K. 1975. Temperature dependence of the saturated vapor pressure of some silicone-germanium-, and tin-containing compounds and mixed organometalic compounds. *Tr. Khim. Khim. Tekhnol.* 4:76-77.

Cited Documents:

- Albarino, R.V. and H. Schonhorn. 1973. Retention of antioxidants in polyethylene by silane coupling agents. *J. Appl. Polym. Sci.* 17(11):3323-3335.

- Belyakova, Z.V., V.N. Bochkarev, S.A. Golubtsov, Z.V. Belikova, M.S. Yamova, A.A. Ainshtein, G.G. Baranova, L.A. Efremova, and K.K. Popkov. 1972. Reaction of triethoxysilane with allylamine in the presence of catalysts. *Zh. Obshch. Khim.* 42(4):858-862.
- Fialova, V.; V. Bazant, and V. Chvalovsky. 1973. Organosilicon compounds. Effect of structure on the basicity of silylalkylamines. *Collect. Czech. Chem. Commun.* 38(12):3837-3844.
- Klimisch, H.J., M. Andreae, and U. Tillman. 1997. A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data. *Regul. Toxicol. Pharmacol.:* 25:1-5.
- Klyuchnikov, N.G., F.I. Karabadzhak, and V.B. Losev. 1970. Inhibiting properties of some organosilazanes and organosilicon amines. *Zh. Prikl. Khim. (Leningrad)* 43(12):2763-2765.
- Speier, J.L., C.A. Roth, and J.W. Ryan. 1971. Syntheses of (3-aminoalkyl) silicon compounds. *J. Org. Chem.* 36(21):3120-3126.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Remarks Field for General Remarks

Supporting Data:

- Extrapolated vapor pressure of 8 Pa @ 20°C. Ditsent, V.E., I.I. Skorokhodov, N.A. Terent'eva, M.N. Zolotareva, Z.V. Belyakova, and Z.V. Belikova. 1976. Saturated vapor pressure of gamma-aminopropyltriethoxysilane. *Zh. Fiz. Khim.* 50(7):1905-1906.

  The following table summarizes the vapor pressure data available in the published literature and compares the measured values to values calculated using temperature-vapor pressure correlation provided in the abstract.

Temp. (°C)	Vapor Pressure (Pa)		Deviation (%)	Reference
	measured	calculated		
55.0	133	118	12	Albarino et. al., (1973)
110.5	1333	2522	-89	Belyakova et al. (1972)
115.0	2533	3091	-22	Speier et al. (1971)
120.5	3866	3932	-2	Klyuchnikov et al. (1970)
122.0	3732	4193	-12	Fialova et al. (1973)

Biodegradation

Test Substance

Identity: 3-aminopropyl-triethoxysilane (CAS No. 919-30-2)

Remarks Field for Test Substance

- **Material tested:** DYNALYLAN AMEO
- **Purity/components:** 99.0 fluid % CAS No. 919-30-2

Method

Method/guideline followed:	DOC-DIE AWAY TEST (EWG Guideline 79/831/EWG, Appendix V, Part C (updated edition dated July 1990), Method C.4-A
Test Type (test type/aerobic/anaerobic):	Aerobic
GLP (Y/N):	Yes
Year (study performed):	1993
Contact time (units):	28 days
Innoculum:	Biological culture from a primarily communal sewage treatment plant (Marl - East)

Results

Degradation % after time: Duplicates run with test article. Flask 1: Percent degradation after 0, 7, 14, 21, 27 and 28 days was 0, 63, 67, 69, 76, and 68%, respectively. Flask 2: Percent degradation after 0, 7, 14, 21, 27 and 28 days was 0, 64, 65, 67, 82, and 65%, respectively.

Results: Mean percent degradation for test article: 0, 63, 66, 68, 79 and 67% after days 0, 7, 14, 21, 27 and 28 days, respectively.

Kinetic (for sample, positive and negative controls): For each time period %, sample % degradation for each time period noted above. For positive control, sodium benzoate, $\leq$ 96% degradation was reported for each time period in both duplicate samples. For the negative control, % degradation was not calculated, but raw data indicates no degradation at any of the time periods measured.

Breakdown products (yes/no): Not analytically verified. However, the test material is known to be hydrolytically unstable. When added to water, the test material rapidly hydrolyzes, generating ethanol and transient silanetriol derivatives which will crosslink.

Data Quality

Reliabilities (Klimish Code):

Conclusions

Remarks Field with the Ability to Identify Source of Comment

Author: DYNASYLAN AMEO (99.0 fluid % CAS No. 919-30-2) achieved a breakdown rate of 67%(DOC reduction) within 28 days. Based on these findings, DYNASYLAN AMEO was determined to be "not readily biodegradable". The control substance, sodium benzoate, achieved a breakdown rate of 98% within 10 days and 100% degradation after 28 days demonstrating acceptable activity of the biologic culture.

References

Hüls AG. Testing Institute for Biology, Final Report DDA 51. Determination of the biodegradability of DYNASYLAN AMEO in DOC-DIE AWAY TEST. February 2, 1994.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Acute Toxicity to Fish

Test Substance

Identity: 3-aminopropyl-triethoxysilane (CAS No. 919-30-2)

Remarks Field for Test Substance

- **Material tested:** DYNALYLAN AMEO
- **Purity/components:** 99.0 weight % CAS No. 919-30-2
- **Comment:** Hydrolytically unstable material (half-life in water < 5 hr)

Method

Method/guideline followed:	DIN 38412 Part 1; EG Guideline 92/69 C.1; OECD Guideline 203, 1984
Type (test type):	Acute toxicity to fish under semi-static conditions using water-filtered initial concentration
GLP (Y/N):	Yes
Year (study performed):	1993
Species/Strain/Supplier:	Fish/*Brachydanio rerio*, West Aquarium, Bad Lauterberg (Germany)
Analytical monitoring:	Analytical control of test substance concentrations was performed using carbon determination on a TOC-500 Infrared Analyzer.
Exposure period:	96 hours
Statistical methods:	NA. No mortalities or adverse biological effects were observed during the study (highest mean measured exposure concentration of 934 mg/L).

Results

Nominal concentrations (as mg/L):	1000 mg/L
Measured concentrations (as mg/L):	880 at 0 h; 922/947 at 24 h; 1024 at 48 h; 885 at 72; Average value of 943 mg/L (water-filtered initial solution)
Unit (results expressed in what unit):	mg/L

Element value (e.g. LC_{50}, LC_0, LL_{50}, or LL_0 at 48, 72 and 96 hours, etc., based on measured or nominal concentrations):	96 hour $LC_0 \geq$ 934 mg/L (mean measured concentration)
Statistical results, as appropriate:	NA. No mortalities or adverse biological effects were observed during the study (highest mean measured exposure concentration of 934 mg/L). Therefore, endpoints such as the LC_{50} could not be calculated.

Remarks Field for Results

- **Biological observations:** None reported
- **Table showing cumulative mortality:** No mortality in treated or control fish
- **Lowest test substance concentration causing 100% mortality:** NA
- **Mortality of controls:** 0%
- **Abnormal responses:** None reported
- **Any observations, such as precipitation that might cause a difference between measured and nominal values:** When the results are interpreted, one must consider that DYNASYLAN AMEO (99.0 fluid % CAS No. 919-30-2) is sensitive to hydrolysis, and that it hydrolyzes either during preparation of the initial batch or during the testing interval.

Conclusions

Remarks Field with the Ability to Identify Source of Comment

Author: 96 hour $LC_0 \geq$ 934 mg/L (all concentrations are with respect to the material).

Data Quality

Reliabilities (Klimish Code):

References

Hüls AG, Testing Institute for Biology. Final Report FK 1254. Determination of the acute effects of DYNASYLAN AMEO on Fish (in accordance with EG 92/69 C.1). January 4, 1994.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Toxicity to Aquatic Plants (e.g., Algae)

Test Substance

Identity: 3-aminopropyl-triethoxysilane (CAS No. 919-30-2)

Remarks Field for Test Substance

- **Material tested:** DYNALYLAN AMEO
- **Purity/components:** 99.0 fluid % CAS No. 919-30-2
- **Comment:** Hydrolytically unstable material (half-life in water < 5 hr)

Method

Method/guideline followed:	EC Guideline 92/69/EWG; 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
Test type (static/other):	Algae growth test per 92/69/EWG. Analysis was conducted only at the beginning of testing because of the imminent conversion to the new EG Guideline.
GLP (Y/N):	Yes
Year (study performed):	1993
Species/strain # and source:	*Scenedesmus subspicatus*/ CHODAT (86.81 SAG) from the Institute for Water, Ground, and Air Hygiene, Berlin (Germany); followed by cultivation of existing cultures.
Element basis (i.e. number of cells/ml, area under the curve, growth rate, etc.):	Cell count/ml, area under the curve, and growth rate
Exposure period, date of start and end of the test [Duration]:	72 hours: Main test 2: 8/10-8/13/93 and Main test 4: 12/14-12/17/93
Analytical monitoring:	The TOC content was determined using a TOC-500 Infrared Analyzer in order to establish the content of the substance in the hydrous, filtered initial solution. Analysis was conducted at the Testing Institute for Biology.
Statistical methods:	t-test; probit analysis

Remarks Field for Test Conditions

- **Method of calculating mean measured concentrations (i.e. arithmetic mean, geometric mean, etc.):** The TOC content was determined in the hydrous, filtered initial solution. The TOC content (mg/L) and the substance content (mg/L) in the hydrous, filtered initial solution in Main Test 2 were reported to be 543 mg/L and 1111 mg/L, respectively. The concentrations used in Main Test 2 were calculated from TOC content and included 33, 67, 133, 278, 556, and 1000 mg/L. The TOC content (mg/L) and the substance content (mg/L) in the hydrous, filtered initial solution in Main Test 4 were reported to be 309 mg/L and 632 mg/L, respectively. The concentrations used in Main Test were calculated from TOC content and included 1.3, 2.5, 5.1, and 10.1 mg/L.

Results

Nominal concentrations in mg/L in Main test 2:	0, 33, 67, 133, 278, 556, and 1000 mg/L.
Nominal concentrations in mg/L in Main test 4:	1.3, 2.5, 5.1, and 10.1.
Measured concentrations in mg/L:	Not measured
Unit [results expressed in what unit]:	mg/L
Element value (e.g. ErC_{50}, ErL_{50}, EbC_{50}, EbL_{50}, EC_{10}-CD, EL_{10}-CD, EC_{50}-CD, EL_{50}-CD, EL_{90}-CD, EC_{90}-CD, EC_0, or EL_0 at 24, 48, 72 or 96 hours) Note whether cells removed prior to measurement:	The following effective concentrations were reported: • 72 hour E_bC_{50} = 603 mg/L (on the basis of cell growth); • A 10% suppression of cell growth (72 hour E_bC_{10}) = 38 mg/L; • (0-72 hour)E_rC_{10} = 76 mg/L (on the basis of growth rate)
NOEC, LOEC, or NOEL, LOEL:	NOEC = 1.3 mg/L (on the basis of cell growth) This value is from Main test 4 since an NOEC value was not established in Main test 2. All concentrations are with respect to the material.
Was control response satisfactory (yes/no/unknown):	Yes
Statistical results, as appropriate	

Remarks Field for Results

Biological observations:

- **Cell density at each flask at each measuring point:**

Main Test 2				
Concentration (mg/L)	Cell count (*10^4 cells/ml) Test interval (h)			
	0 h	24 h	48 h	72 h
Control	**2**	**7**	**35**	**115**
33	2	6	27	106
67	2	6	27	111
133	2	6	25	105
278	2	5	20	82
556	2	5	15	51
1000	2	5	16	50

*No median values. All concentrations are with respect to the material. Five each and eight each parallels, respectively, were examined. (After 0 h, the theoretical cell concentration was evaluated).

Main Test 4				
Concentration (mg/L)	Cell count (*10^4 cells/ml) Test interval (h)			
	0 h	24 h	48 h	72 h
Control	**2**	**6**	**23**	**97**
1.3	2	5	23	89
2.5	2	4	18	85
5.1	2	5	19	87
10.1	2	5	19	88

*No median values. All concentrations are with respect to the material.

- **Growth curves:** The EC values are calculated by regression analysis based on [Probit] transformation of the percentage suppression values. These values then serve as the basis for the subsequent [Probit] analysis in accordance with Cavalli-Sforza (1972). The results are presented below.

Effective Concentrations on the Basis of Cell Growth (E_bC)	
Parameter	mg/L (substance)
(72 h) E_bC_{50}	603
(72 h) E_bC_{10}	38
(72 h) E_bC_{90}	*

* lies above the highest tested concentration

Effective Concentrations on the Basis of Specific Growth Rate μ(E_rC)	
Parameter	mg/L (substance)
(72 h) E_bC_{50}	*
(72 h) E_bC_{10}	321
(72 h) E_bC_{90}	*

* lies above the highest tested concentration

- **Percent biomass/growth rate inhibition per concentration:**

Main Test 2

Areas under growth curves, growth rates, corresponding percentage suppression rates, and pH values with respect to test concentrations. (All concentrations are with respect to the material.)

Method		(mg/L) Blind	33	67	133	278	556	1000
Area Under Growth Curve	Area	94.5	81	83.5	78.5	61	40.5	41
	% suppression		14.3	11.6	16.9	35.4	57.1	56.6
Growth Rate μ (0-72 h)	μ	1.351	1.323	1.339	1.32	1.238	1.08	1.073
	% suppression		2.1	0.9	2.3	8.4	20.1	20.6
pH values	After 0 h	7.9	8.3	8.4	8.7	8.9	9.1	9.2
	After 72 h	8.6	8.8	9.1	8.8	8.5	8.3	8.4

Main Test 4

Areas under growth curves, growth rates, corresponding percentage suppression rates, and pH values with respect to test concentrations. (All concentrations are with respect to the material.)

Method		(mg/L) Blind	1.3	2.5	5.1	10.1
Area Under Growth Curve	Area	72.5	67.5	59.5	52.5	63
	% suppression		6.9	17.9	13.8	13.1
Growth Rate μ (0-72 h)	μ	1.294	1.265	1.25	1.258	1.261
	% suppression		2.2	3.4	2.8	2.6
pH values	After 0 h	7.5	7.8	7.8	7.9	8.1
	After 72 h	9.0	8.8	8.7	8.7	8.6

- **Comment:** When the results are interpreted, one must consider that DYNASYLAN AMEO (99.0 fluid % CAS No. 919-30-2) is sensitive to hydrolysis, and that it hydrolyzes either during preparation of the initial batch or during the testing interval.

Conclusions

Remarks Field with the Ability to Identify Source of Comment

Author: The following effective concentrations were reported: On the basis of cell growth, a median concentration is calculated of 72 hour E_bC_{50} = 603 mg/L and a 10% suppression of cell growth was achieved at 72 hour E_bC_{10} = 38 mg/L; On the basis of growth rate, a 10% suppression of cell growth was achieved at (0-72 hour)E_rC_{10} = 321 mg/L; The NOEC value was 1.3 mg/L (on the basis of cell growth). All concentrations are with respect to the material.

Data Quality

Reliabilities (Klimisch Code):

References

Hüls AG, Testing Institute for Biology, Final Report AW-325. Determination of the acute effects of DYNASYLAN AMEO on the growth of *Scendesmus subspicatus* 86.81.SAG (Algae growth test per Guideline 92/69/EWG). March 21, 1994.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Acute Toxicity to Aquatic Invertebrates (e.g., Daphnia)

Test Substance

Identity: 3-aminopropyl-triethoxysilane (CAS No. 919-30-2)

Remarks Field for Test Substance

- **Material tested:** DYNALYLAN AMEO
- **Purity/components:** 99.0 fluid % CAS No. 919-30-2
- **Comment:** Hydrolytically unstable material (half-life in water < 5 hr)

Method

Method/guideline followed:	DIN 38412 Part 1; EG Guideline 92/69/EWG; OECD Guideline 202, Part 1, 1984
Test type:	Acute toxicity, 48 hours, EC_{50} (immobilization) under static test conditions
GLP (Y/N):	Yes
Year (study performed):	1993
Analytical procedures:	Not reported
Species/Strain:	*Daphnia magna*/*Straus* clone 5
Test details (static, semi-static, dosing rate, flow-through rate, etc.):	Static
Statistical methods:	

Results

Nominal concentrations in mg/L:	0, 8.7, 16.4, 28.4, 54.7, 94.0, 174.9, 306.0, 546.5, and 983.7 mg/L
Measured concentrations in mg/L:	NA
Unit [results expressed in what unit]:	mg/L
EC50, EL50, LC0, LL0, at 24, 48 hours:	24 hour EC_{50} = 592 mg/L (349 - 1003 mg/L); 48 hour EC_{50} = 331 mg/L (249 - 441 mg/L). After 48 hours exposure, the highest concentration for which no immobilization occurred ($\leq$ 10%) was 94 mg/L. After 48 hours exposure, the lowest

	concentration for which 100% immobilization occurred was 984 mg/L.
Statistical results, as appropriate	

Remarks Field for Results

Biological observations:

- **Number immobilized as compared to the number exposed:** At concentrations 0, 8.7, 16.4, 28.4, 54.7, 94.0, 174.9, 306.0, 546.5, and 983.7 mg/L, the following % of immobilized individuals was reported at 24 hours: 0, 0, 5, 0, 0, 5, 19, 45, 40, and 62%, respectively, and the following % of immobilized individuals was reported at 48 hours: 0, 0, 5, 0, 0, 0, 10, 19, 50, 60, and 100%.
- **Concentration response with 95% confidence limits:** 24 hour EC_{50} values = 592 mg/L (95% confidence limits: 349-1003 mg/L); 48 hour EC_{50} = 331 mg/L (95% confidence limits: 249-441 mg/L)
- **Cumulative immobilization:** After 48 hours, the highest concentration for which no immobilization occurred (≤ 10%) was 94 mg/L. After 48 hours, the lowest concentration for which 100% immobilization occurred was 983.7 mg/L.
- **Was control response satisfactory (yes/no/unknown):** Yes

When the results are interpreted, one must consider that DYNASYLAN AMEO (99.0 fluid % CAS No. 919-30-2) is sensitive to hydrolysis, and that it hydrolyzes either during preparation of the initial batch or during the testing interval.

Conclusions

Remarks Field with the Ability to Identify Source of Comment

Author: 24 hour EC_{50} values = 592 mg/L (95% confidence limits: 349-1003 mg/L); 48 hour EC_{50} = 331 mg/L (95% confidence limits: 249-441 mg/L). All concentrations are with respect to the material.

Data Quality

Reliabilities (Klimisch Code):

References

Hüls AG, Testing Institute for Biology. Final Report DK 569. Determination of the acute effects of DYNASYLAN AMEO on the swimming behavior of *Daphnia magna* (in accordance with EG 92/69/EWG). August 13, 1993

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Acute Oral Toxicity

Test Substance

Identity: 1-Propanamine, 3-(triethoxysilyl); CAS No. 919-30-2

Remarks Field for Test Substance

- purity ≥99%

Method

Method/guideline followed:	EPA TSCA Guideline 798.1175
Type (test type):	Acute oral toxicity
GLP (Y/N):	Y
Year (study performed):	1989
Species/Strain:	Sprague-Dawley albino rats
Sex:	male and female
No. of animals per sex per dose:	5/sex/dose
Vehicle:	none
Route of administration (if inhalation - aerosol, vapor, gas, particulate):	peroral intubation

Remarks Field for Test Conditions

- No significant protocol deviations.
- **Doses (OECD guidelines 401 and 425 do not provide dose levels, so these must be described in detail):** males were dosed with 4, 2, and 1 g/kg; females were dosed with 2, 1.41 and 1 g/kg.
- **Doses per time period:** one
- **Post dose observation period:** 14 days

Results

Value [LD50 or LC50] with confidence limits if calculated:

- **males:** LD_{50} with 95% confidence limits = 2.83 (1.61 to 4.98) g/kg
- **females:** LD_{50} with 95% confidence limits = 1.57 (1.34 to 1.85) g/kg

Number of deaths at each dose level:

Sex	Dose level (g/kg)	No. Deaths	Days to Death
Males	4	4/5	1,2,2,2
	2	1/5	2
	1	0/5	-
Females	2	5/5	2,3,3,3,4
	1.41	1/5	1
	1	0/5	-

Remarks Field for Results

- **Time of death (provide individual animal time if less than 24 hours after dosing)**: See table above.
- **Description, severity, time of onset and duration of clinical signs at each dose level:** Signs of toxicity included sluggishness, lacrimation, kyphosis, an unkempt appearance, piloerection (in one), yellow stains on the perigenital fur (positive for blood by HEMASTIX®), red crust on the perinasal and/or periocular fur, brown stain on the perigenital fur, closed eyelids (in one), emaciation (in one), and diarrhea. Survivors recovered at 2 to 9 days.
- **Necropsy findings, included doses affected, severity and number of animals affected:** Victims had dark red or mottled lungs, dark red or white stomachs (glandular portion), yellow intestines, stomachs and intestines filled with gas and/or yellow to brown liquid, discolored kidneys (dark red, brown or mottled) and one mottled dark red spleen. No remarkable gross lesions in survivors. Acute tubular necrosis (involving the cortical tubules) and mineralization of the tubular epithelium evident for males (4 g/kg) and females (2 g/kg). Hyperplasia involving the renal tubule epithelium was apparent in 1 of 2 males examined at 2 g/kg. Focal area of epithelial necrosis in the urinary bladder in one male rat (4 g/kg).
- **Potential target organs (if identified in the report):** kidney
- **If both sexes tested, results should be compared:** See above.

Conclusions

Remarks Field with the Ability to Identify Source of Comment

Although no GLP Statement is provided in this report, it is assumed that this study was conducted under GLP. Bushy Run Research Center was a certified GLP laboratory during the conduct of this study. This material is a slight to very low acute peroral toxicant in the rat.

Data Quality

Reliabilities (Klimisch Code):

References

Key Study: Silane A-1100: Acute Toxicity and Primary Irritancy Studies. R.C. Myers and S.M. Christopher; Bushy Run Research Center. Project report number 52-43. April 18, 1989.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Remarks Field for General Remarks

Supporting Data: An additional study confirms the very low acute peroral toxicity of CAS No. 919-30-2.

- *Unpublished Report 1976, DeGussa-Huls AG Nr. 76-0043-FKT*. An additional study (test guideline: FDA Handbook, 1959, p. 47) conducted with the same material indicates an acute peroral LD_{50} in rats >3.65 g/kg.

Acute Dermal Toxicity

Test Substance

Identity: 1-Propanamine, 3-(triethoxysilyl); CAS No. 919-30-2

Remarks Field for Test Substance

- purity ≥99%

Method

Method/guideline followed:	EPA TSCA Guideline 798-1100
Type (test type):	Acute dermal toxicity
GLP (Y/N):	Y
Year (study performed):	1989
Species/Strain:	New Zealand white rabbits
Sex:	male and female
No. of animals per sex per dose:	5/sex/dose
Vehicle:	none
Route of administration (if inhalation - aerosol, vapor, gas, particulate):	dermal application

Remarks Field for Test Conditions

- No significant protocol deviations.
- **Doses (OECD guidelines 401 and 425 do not provide dose levels, so these must be described in detail):** males and females were dosed with 8, 4, 2, and 1 g/kg
- **Doses per time period:** one
- **Post dose observation period:** 14 days

Results

Value [LD50 or LC50] with confidence limits if calculated:

- **males and females:** LD_{50} with 95% confidence limits = 4.29 (2.90 to 6.34) g/kg.

Number of deaths at each dose level:

Sex	Dose level (g/kg)	No. Deaths	Days to Death
Males	8	5/5	1,1,1,2,2
	4	2/5	2,3
	2	0/5	-
	1	0/5	-
Females	8	5/5	2,2,2,2,2
	4	2/5	2,3
	2	0/5	-
	1	0/5	-

Remarks Field for Results

- **Time of death (provide individual animal time if less than 24 hours after dosing):** See table above.
- **Description, severity, time of onset and duration of clinical signs at each dose level:** Local cutaneous effects included erythema, edema, ecchymosis, necrosis, desquamation, fissuring, ulceration, alopecia and scabs. Blood in rectal and urogenital areas apparent in several animals (especially at 4 g/kg). Hemorrhaging under the skin evident at 4 g/kg. Other signs of toxicity included sluggishness, salivation (in one), unsteady gait (in 2), prostration, and diarrhea (in one). Survivors recovered at 2 to 4 days.
- **Necropsy findings, included doses affected, severity and number of animals affected:** gross pathologic findings included discolored lungs (red, pink, or mottled), lungs of with dark red foci (in one), mottled tan livers, stomachs with dark areas of hemorrhages, stomach with black foci (in one), tan or hemorrhaged kidneys, ureters and urethra with hemorrhages (in one), bladders filled with red liquid (1 with a dark red clot) and the untreated skin of 2 animals stained red.
- **Potential target organs (if identified in the report):** kidney
- **If both sexes tested, results should be compared:** See above.

Conclusions

Remarks Field with the Ability to Identify Source of Comment

Although no GLP Statement is provided in this report, it is assumed that this study was conducted under GLP. Bushy Run Research Center was a certified GLP laboratory during the conduct of this study. This material is a very low acute dermal toxicant in the rabbit.

Data Quality

Reliabilities (Klimisch Code):

References

Key Study: Silane A-1100: Acute Toxicity and Primary Irritancy Studies. R.C. Myers and S.M. Christopher; Bushy Run Research Center. Project report number 52-43. April 18, 1989.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Remarks Field for General Remarks

Supporting Data: Additional studies indicate CAS No. 919-30-2 has acute nephrotoxic potential following cutaneous administration.

- *Organofunctional Silane A-1100 Acute Nephrotoxicity Potential Following Cutaneous Administration to Rabbits. R.C. Myers, S.M. Christopher, E.H. Fowler and D.A. Neptun. Bushy Run Research Center. Project Report 52-108. April 10, 1990.* This GLP study followed applicable OECD and EPA guidelines. A single (24-hour) cutaneous application of 2.0 g/kg or more of CAS No. 919-30-2 (98.9% pure) to the skin of male New Zealand White rabbits resulted in kidney and urinary bladder injury. These effects appeared to develop within one or 2 days after contact and subside thereafter, possibly indicating a capacity for renal repair.

Genetic Toxicity *In Vivo* (Chromosomal Aberrations)

Test Substance

Identity: 1-Propanamine, 3-(triethoxysilyl); CAS No. 919-30-2

Remarks Field for Test Substance

- purity 99.4%

Method

Method/guideline followed:	EPA Health Effects Test Guidelines, EPA Report 560/6-83-001; Schlegel and MacGregor, Mutation Research 104 (367-369) 1982.
Type (test type):	Mouse micronucleus
GLP (Y/N):	Y
Year (study performed):	1987 - 1988
Species:	mice
Strain:	Swiss-Webster
Sex:	male and female
Route of administration (if inhalation - aerosol, vapor, gas, particulate):	intraperitoneal (i.p.)
Doses/concentration levels: toxicity study:	160, 128 and 102 mg/kg; micronucleus study: 90, 56 and 28 mg/kg.
Exposure period:	single dose
Statistical methods:	LD_{50} calculated using the probit method; Fisher's Exact test used to compare for significant differences from vehicle control micronuclei frequencies.

Remarks Field for Test Conditions

- **Age at study initiation:** 5 weeks old
- **No. of animals per dose:** 5/sex
- **Vehicle:** corn oil
- **Duration of test:** single dose, blood smears prepared at 30, 48 and 72 hours post-dosing.
- **Frequency of treatment:** single dose

- **Sampling times and number of samples:** blood smears prepared at 30, 48 and 72 hours post-dosing.
- **Control groups and treatment:** 5/sex, blood smears prepared at 30 hours post-dosing.
- **Criteria for evaluating results (for example, cell types examined, number of cells counted in a mouse micronucleus test):** Chromosome damage was measured by quantifying the incidence of micronuclei in peripheral blood polychromatic erythrocytes (PCE). A minimum of 1000 PCEs was examined microscopically for each animal/sample time, unless cytotoxicity prevented this goal. The PCE: normochromatic erythrocyte (NCE) ratio for approximately 1000 total cells was calculated as an estimate of cytotoxicity.
- **Criteria for selection of M.T.D.:** Three dose levels of approximately 80, 50 and 25% of the LD_{50} value were evaluated for effects on the incidence of micronuclei.

Results

Effect on mitotic index or PCE/NCE ratio by dose level by sex:	Toxicity study: the PCE/NCE ratio of the vehicle control and the highest dose level with more than 3 survivors was quantified and compared to determine possible bone marrow toxicity at 48 hours. The PCE/NCE ratio was not reduced in male or female mice in comparison to control values. It was not necessary to assess bone marrow toxicity at 72 hours post-dosing. Micronucleus study: No statistically significant decreases in the PCE/NCE ratio relative to the control values were observed at any of the three sample periods. Female mice sampled at the 48-hour period had moderate decrease in the PCE/NCE ratio relative to control value. Analysis of Variance testing showed that these decreases were not significantly different.
Genotoxic effects (positive, negative, unconfirmed, dose-response, equivocal):	negative
NOAEL(NOEL) (C)/LOAEL(LOEL) (C):	NA
Statistical results, as appropriate:	See Remarks Field for Results.

Remarks Field for Results

- **Mortality at each dose level by sex:**

Dose (mg/kg)	Sex	No. Dead	% Mortality
65	M	0/5	0
82	M	0/5	0
102	M	0/5	0
128	M	3/5	60
160	M	5/5	100
65	F	0/5	0

82	F	0/5	0
102	F	3/5	60
128	F	5/5	100
160	F	5/5	100
Control	M	0/5	0
Control	F	0/5	0

- **Mutant/aberration/mPCE/polyploidy frequency, as appropriate:**

Toxicity Test

Dose (mg/kg)	Sex	Mean PCE/1000 NCE +/- (S.D.)	%Control
102	M	32.6 (12.1)	111.6%
Control	M	29.2 (5.1)	
82	F	44.2 (11.2)	120.8%
Control	F	36.6 (6.7)	

Micronucleus Test (30 hour sample)

Dose (mg/kg)	Sex	#PCE Observed	#mPCE	%mPCE
control	combined	10,000	18	0.18
28	combined	10,000	29	0.29
56	combined	10,000	19	0.19
90	combined	10,000	17	0.17
+ control	combined	10,000	245	2.45 (a)

Micronucleus Test (48 hour sample)

Dose (mg/kg)	Sex	#PCE Observed	#mPCE	%mPCE
control	M	5000	15	0.30
control	F	5000	3	0.06
28	M	5000	23	0.46
28	F	5000	10	0.20(b)
56	M	5000	13	0.26
56	F	5000	11	0.22(b)
90	M	5000	15	0.30
90	F	5000	10	0.20(b)

Micronucleus test (72 hour sample)

Dose (mg/kg)	Sex	#PCE Observed	#mPCE	%mPCE
control	M	5000	15	0.30
control	F	5000	8	0.16
28	M	5000	14	0.28
28	F	5000	1	0.02
56	M	5000	6	0.12
56	F	5000	3	0.06
90	M	5000	12	0.24
90	F	5000	5	0.10

(a) = statistically significant increase above control, $p < 0.001$

(b) = statistically significant increase above control, $0.05 > p > 0.01$

Conclusions

Remarks Field with the Ability to Identify Source of Comment

CAS No. 919-30-2 was not an active agent in producing treatment related increases in numbers of micronuclei in PCEs in Swiss-Webster mice. Relatively high dose levels of CAS No. 919-30-2 were tested up to 80% of the LD_{50} with no indication of a positive induction of micronuclei. CAS No. 919-30-2 was considered to be inactive as a clastogenic agent under the statistical criteria used.

Data Quality

Reliabilities (Klimisch Code):

Remarks Field for Data Reliability

Statistically significant increases were observed with the female mice sampled at the 48-hour sample period. However, these statistical increases were the result of the unusually low spontaneous incidence of the concurrent vehicle control group. There was no evidence of a treatment-related increase in the micronucleus frequency and the micronucleus responses for the treated mice were within the historical range of variability for this test system. The statistically significant increases observed for the female mice at the 48-hour sample period were not considered biologically significant.

References

Key Study: Organofunctional Silane A-1100 *In Vivo* Mouse Micronucleus Study. Bushy Run Research Center. BRRC Report 51-33. April 12, 1988.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Remarks Field for General Remarks

Supporting Data: Additional studies indicate CAS No. 919-30-2 was not mutagenic in mammalian cell assays.

- *Unpublished Report 1999, DeGussa-Huls AG Nr. 99-0033-DGM.* In a GLP study, which followed test guideline OECD 473, CAS No. 919-30-2 was tested for the ability to induce chromosome aberrations in Chinese hamster V79 cells. CAS No. 919-30-2 was not clastogenic.
- *Kakenkyo test number 94-060-0117-J. In Vitro Chromosome aberration test with KBE-903.* A chromosome aberration test (based on the Japanese guidelines for testing of chemicals) was conducted with CAS No. 919-30-2 using Chinese Hamster fibroblast cells with and without metabolic activation. DMSO was used as the solvent. Mitotic indices were nearly 100% at

2300 ug/ml in the 24-hour treatment group and the 48-hour treatment group with or without metabolic activation. No increase in frequency of the cells with structural or numerical chromosome aberrations was observed under any condition tested. CAS No. 919-30-2 did not induce any chromosome aberrations under the conditions of this test.

- *Organofunctional Silane A-1100 In Vitro Genotoxicity Studies: Sister Chromatid Exchange Assay. Bushy Run Research Center. BRRC Report 51-13. February 17, 1988.* In this GLP study (EPA Health Effects Test Guidelines report No. 560/6-83-001, October 1983, HG-DNA-Sister Chrom. In Vitro. Fed Reg. 50 (#188) Sept. 27, 1985, amend. Fed Reg. 51 9# 9(January 14, 1986), CAS No. 919-30-2 did not produce dose-related, or statistically significant increases in the incidence of SCEs in CHO cells in tests with and without metabolic activation. No remarkable effects upon the progression of the cells through the mitotic cycle were evident in determinations of numbers of cells at the first vs. second stage of mitosis. CAS No. 919-30-2 was concluded to lack significant DNA damage activity under the conditions of the SCE test system.

Genetic Toxicity *In Vitro* (Gene Mutations)

Test Substance

Identity: 1-Propanamine, 3-(triethoxysilyl); CAS No. 919-30-2

Remarks Field for Test Substance

- purity ≥99%

Method

Method/guideline followed:	EPA Health Effects Test Guideline, HG-Gene Muta - *S. typhimurium*, EPA report No. 560/6-84-002, October 1984.
Type:	*S. typhimurium* reverse mutation assay
System of testing [bacterial, non bacterial]:	bacterial
GLP (Y/N):	Y
Year (study performed):	1988
Species/Strain or cell type and or cell line, bacterial or non-bacterial:	bacterial - *S. typhimurium* TA98, TA100, TA1535, TA1537 and TA1538
Metabolic activation:	Aroclor-1254 induced, Sprague-Dawley male rat-liver homogenate • **Species and cell type:** rat liver • **Quantity:** 40 ul • **Induced or not induced:** Aroclor-1254 induced
Concentrations tested:	0.03, 0.1, 0.3, 1 and 3 mg per plate
Statistical Methods:	Stored in archives

Remarks Field for Test Conditions

Test Design:

- **Number of replicates:** triplicate
- **Frequency of Dosing:** once
- **Positive and negative control groups and treatment:** solvent (DMSO) and positive controls (TA98 and TA1538: 4-Nitro-o-phenylenediamine; TA100 and TA1535: Sodium azide; TA1537: 9-Aminoacridine)

- **Solvent:** DMSO
- **Criteria for evaluating results (e.g. cell evaluated per dose group):** Spontaneous reversion for the solvent control must be within the laboratory's historical range. The positive control must demonstrate that the test systems are responsive with known mutagens. A test article is considered to be a bacterial mutagen if the number of revertant colonies is at least twice the solvent control for at least one dose level and there is evidence of a dose-related increase in the number of revertant colonies. If a test article produces a marginal or weak response that con not be reproduced in a second test, the test result will be considered negative. If there is no evidence of a dose-related increase in the number of revertant colonies and the umber of revertant colonies is not twice the solvent control, then the test article is not considered a bacterial mutagen.

Results

Result:	not a bacterial mutagen
Cytotoxic concentration:	• **With metabolic activation:** ≥5 ug/plate • **Without metabolic activation:** 5 ug/plate
Genotoxic effects (e.g. positive, negative, unconfirmed, dose-response, equivocal):	negative • **With metabolic activation:** 0.1 to 5 ug/plate • **Without metabolic activation:** 0.03 to 3 ug/plate
Statistical results, as appropriate:	NA

Remarks Field for Results

- **Precipitation concentration, if applicable:** No precipitate observed.

Conclusions

Remarks Field with the Ability to Identify Source of Comment

CAS No. 919-30-2 did not produce a dose-dependent mutagenic effect in any of the *Salmonella typhimurium* strains tested with or without a metabolic activation system.

Data Quality

Reliabilities (Klimisch Code):

References

Key Study: Silane A-1100: Salmonella/Microsome (Ames) Bacterial Mutagenicity Assay. Bushy Run Research Center. BRRC Project Number 88-15-18201, Project report 52-44. April 28, 1989.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field)

Remarks Field for General Remarks

Supporting Data: Additional studies indicate CAS No. 919-30-2 was not mutagenic in bacterial mutagenicity assays or *in vitro* mammalian mutagenicity assays.

- *Organofunctional Silane A-1100 Salmonella/Microsome (Ames) Bacterial Mutagenicity Assay. Bushy Run Research center. BRRC Report 50-140. November 3, 1987.* CAS no. 919-30-2 was tested for potential mutagenic activity using the *Salmonella* (strains TA98, TA100, TA1535, TA1537, and TA1538)/microsome bacterial mutagenicity assay (Ames test) conducted under GLP. A range of doses from 0.3 to 3 mg/plate were tested with metabolic activation; doses from 0.1 to 5 mg/plate were tested without metabolic activation. Positive increases in the numbers of mutant colonies of any strain tested were not seen with or without metabolic activation.
- *Unpublished Report 1998, DeGussa-Huls Nr. 98-0111-DGM.* In a GLP study, which followed test guideline OECD 471, CAS No. 919-30-2 was tested with four strains of S. typhimurium. The material was not mutagenic in this bacterial mutagenicity assay.
- *Kakenkyo test number 94-036-0107-J. Bacterial mutagenicity test with KBE-903.* A bacterial mutagenicity test (based on the Japanese guidelines for testing of chemicals) was conducted with CAS No. 919-30-2 in *Salmonella typhimurium* strains TA100, TA1535, TA98, and TA1537 and E. coli strain WP2uvrA with and without metabolic activation. DMSO was used as the solvent. Bacterial toxicity was observed at 5000 ug/plate in all strains without metabolic activation and in TA100, TA1537, and WP2uvrA with metabolic activation. There was no increase in the number of revertant colonies in comparison with the solvent control at any concentration (from 313 to 5000 ug/plate) with or without metabolic activation.
- *Hatano Research test number 77-015-0107-J. Bacterial mutagenicity test with KBE-903.* A bacterial mutagenicity test was conducted with CAS No. 919-30-2 with and without metabolic activation. Bacterial toxicity was observed at 100 ug/plate in all strains with or without metabolic activation. There was no increase in the number of revertant colonies at any concentration (from 0.1 to 10 ug/plate) with or without metabolic activation. CAS No. 919-30-2 was non-mutagenic in this bacterial mutation assay under the test conditions employed.

- *Unpublished Report 1999, DeGussa-Huls AG Nr. 99-0035-DGM.* In a GLP study, which followed test guideline OECD 476, CAS No. 919-30-2 was tested for the ability to induce gene mutations in Chinese hamster ovary cells. CAS No. 919-30-2 was not mutagenic.
- *Organofunctional Silane A-1100 In Vitro Genotoxicity Studies: CHO/HGPRT Gene Mutation Test. Bushy Run Research Center. BRRC Report 51-13. February 17, 1988.* In this GLP study (EPA Health Effects Test Guidelines report No. 560/6-83-001, October 1983, HG-Gene-Muta-Somatic cells), CAS No. 919-30-2 did not produce dose-related increases in the incidence of mutations of CHO cells at concentrations between 0.3 to 2.5 mg/ml in tests without metabolic activation. CAS No. 919-30-2 was concluded to lack significant genotoxic potential under conditions of the CHO mutation cell test system.

Developmental Toxicity/Teratogenicity

Test Substance

Identity: 1-Propanamine, 3-(triethoxysilyl); CAS No. 919-30-2

Remarks Field for Test Substance

- purity 99.5%

Method

Method/guideline followed:	Health Effects Testing Guidelines (TSCA) September 1985.
GLP (Y/N):	Y
Year (study performed):	1996 to 1997
Species:	rat
Strain:	Charles River Crl:CD® VAF/Plus®
Route of administration - oral (gavage, drinking water, feed), dermal, inhalation (aerosol, vapor, gas, particulate), other:	Oral (gavage)
Doses/concentration levels:	20, 100 or 600 mg/kg/day
Sex:	F
Exposure period:	day 6 of gestation through day 20 of gestation
Frequency of treatment:	once per day
Control group and treatment:	vehicle, once per day, day 6 of gestation through day 20 of gestation
Duration of test:	Through day 20 of gestation
Statistical methods:	One-way analysis of variance (ANOVA) was used to analyze mean maternal gestation body weights, body weight changes, and food consumption, mean number of corpora lutea, implantation sites, live fetuses(male and female), postimplantation losses, resorptions (early and late), mean fetal weights (male and female), gravid uterine weights, carcass weights, and net weight change from day 0. If the ANOVA was significant, pairwise comparisons to the vehicle control were performed using Dunnett's test. A Kruskal-

	Wallis test was used to analyze mean percent preimplantation losses and live fetuses (male and female) per animal, mean percent postimplantation losses, dead fetuses, and resorptions (early and late) expressed as percentages of implantations per animal, mean percent affected fetuses per litter for external, visceral, and skeletal malformations and developmental variations, and mean percent affected fetuses per liter for external, visceral, and skeletal malformations and developmental variations. If the Kruskal-Wallis test was significant, pairwise comparisons to the vehicle control were made using a Mann-Whitney U test. A Pearson chi-square test was used to analyze fetal and litter incidence of fetal external, visceral and skeletal malformations and developmental variations, as well as litter incidence of total fetal external, visceral and skeletal malformations and developmental variations. If the chi-square test was significant, pairwise comparisons to the vehicle control were performed using a Fischer's exact test.

Remarks Field for Test Conditions

- **Number of animals per dose per sex:** 30
- **Vehicle:** peanut oil
- **Clinical observations performed and frequency:** cageside observations performed twice per day; detailed clinical observations daily.
- **Mating procedures (M/F ratios per cage, length of cohabitation, proof of pregnancy):** One male and one female per cage; proof of pregnancy was an *in situ* copulatory plug or vaginal smear for sperm.
- **Parameters assessed during study (maternal and fetal):** maternal parameters – clinical signs, body weight, food consumption, laparohysterectomic exam, location of viable and nonviable fetuses, early and late resorptions, number of total implantations and corpora lutea, necropsy; fetal parameters – weight, sex, external malformations and variations, soft-tissue defects, skeletal exam.

Results

NOAEL (NOEL) and LOAEL (LOEL) maternal toxicity:	NOAEL 100 mg/kg/day; LOAEL 600 mg/kg/day
NOAEL (NOEL) and LOAEL (LOEL) developmental toxicity:	NOAEL 100 mg/kg/day; LOAEL 600 mg/kg/day
Actual dose received by dose level by sex if available	NA
Maternal data with dose level (with NOAEL value). Provide at a minimum	Increased incidence of mortality and clinical observations as well as slight decreases in body weight gain and food

qualitative descriptions of responses where dose related effects were seen:	consumption observed at 600 mg/kg/day. No significant maternal effects at 100 or 20 mg/kg/day.
Fetal data with dose level (with NOAEL value). Provide at a minimum qualitative descriptions of responses where dose related effects were seen.	Slight fetal toxicity, as exhibited by a statistically significant increase in the incidences of minor skeletal variations, 27 presacral vertebrae and sternebra unossified at 600 mg/kg/day. No significant developmental effects at 100 or 20 mg/kg/day.
Statistical results, as appropriate:	Fetal effects exhibited as a statistically significant increase in the incidences of minor skeletal variations, 27 presacral vertebrae and sternebra unossified at 600 mg/kg/day. No statistically significant developmental effects at 100 or 20 mg/kg/day.

Remarks Field for Results

- **Mortality and day of death:**

Dose (mg/kg/day)	No. Dead	Day of Death (gestation day)
0	0/30	-
20	0/30	-
100	0/30	-
600	5/30	7,7,13,15,17

- **Number pregnant per dose level:**

Dose (mg/kg/day)	No. Pregnant
0	29/30
20	25/30
100	26/30
600	22/30

- **Number aborting:** none

- **Number of resorptions, early/late if available:**

Dose (mg/kg/day)	No. Resorptions (early + late)
0	34
20	25
100	38
600	25

- **Number of implantations:**

Dose (mg/kg/day)	No. Implantations
0	437
20	368
100	361
600	358

- **Pre and post implantation loss, if available:**

Dose (mg/kg/day)	Preimplantation loss	Postimplantation loss
0	50	34
20	67	25
100	74	38
600	60	25

- **Number of corpora lutea (recommended):**

Dose (mg/kg/day)	No. Corpora lutea
0	487
20	435
100	435
600	418

- **Duration of Pregnancy:** 20 days

- **Body weight:** No significant body weight effects at any dose level. Slight decrease in body weight gain observed gd 6 through 9 at 600 mg/kg/day considered treatment related. This decrease was not statistically significant but was consistent with significant decreases in food consumption.

Dose (mg/kg/day)	Mean body weight, grams (gd 20)
0	404.7
20	405.1
100	390.4
600	407.4

- **Food/water consumption:** A statistically significant decrease in food consumption was observed gd 6 through 9 at 600 mg/kg/day. No other significant treatment related effects on food consumption observed at any dose level during the treatment period.
- **Description, severity, time of onset and duration of clinical signs:** An increased incidence of the following clinical signs were observed in the 600 mg/kg/day group: decreased activity, cold to touch, body surface stained, and material around the nose and eye. Respiratory signs including labored breathing, gasping, and rales observed in the 600 mg/kg/day group. Most of these signs were observed in moribund animals.
- **Gross pathology incidence and severity:** No significant findings at any dose level.
- **Organ weight changes, particularly effects on total uterine weight:** No significant effect on gravid uterine weights at any dose level.
- **Histopathology incidence and severity:** No significant findings at any dose level.

- **Fetal data, provide at a minimum qualitative descriptions of responses where dose related effects were seen:**
  - **Litter size and weights:** No significant treatment related effect at any dose level.
  - **Number viable (number alive and number dead)**: No significant treatment related effect at any dose level.
  - **Sex ratio:** No significant treatment related effect at any dose level.
  - **Grossly visible abnormalities, external, soft tissue and skeletal abnormalities:** No significant effects on fetal external or visceral malformations or developmental variations at any dose level. Statistically significant increases in the incidences of the variations 27 presacral vertebrae and sternebra unossified were observed at 600 mg/kg/day were attributed to treatment and considered manifestations of slight fetal toxicity.

Conclusions

Remarks Field with the Ability to Identify Source of Comment

Increased incidences of mortality and clinical observations, as well as slight decreases in body weight gain and food consumption were observed at 600 mg/kg/day. The occurrence of maternal toxicity at 600 mg/kg/day was accompanied by slight fetal toxicity, as exhibited by 27 presacral vertebrae and sternebra unossified. No significant maternal or developmental effects were observed at 20 or 100 mg/kg/day. Therefore, the maternal and developmental NOAEL was 100 mg/kg/day.

Data Quality

Reliabilities (Klimisch Code):

References

Key Study: Developmental Toxicity Study in Rats (Silquest A-1100). W.J. Breslin, MPI Research Study Identification No. 742-006. April 8, 1998.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Aminosilanes
Robust Summaries
CAS No. 1760-24-3

Silicones Environmental, Health and Safety Council
March 16, 2000

Contents

Boiling Point

Test Substance

- **Identity:** N-(2-aminoethyl)-3-aminopropyltrimethoxysilane (CAS No. 1760-24-3)

Remarks Field for Test Substance

Purity of test substance not identified.

Method

Method/guideline followed:	Calculated
GLP (Y/N):	No
Year (study performed):	1986

Remarks Field for Test Conditions

The best-fitting Halm-Stiel vapor pressure equation was used to extrapolate boiling point from vapor pressures measured at temperatures ranging from 121-194°C.

Results

Boiling point value (°C):	264
Pressure:	101.3
Pressure unit:	kPa
Decomposition (yes/no/ambiguous):	ambiguous

Remarks Field for Results

Coefficients for the Halm-Stiel equation were derived from regression of the following measured vapor pressure data (Menzie 1958):

T (°C)	P (mm Hg)	P (Pa)
121.0	5	667
137.0	10	1333
145.7	15	2000
159.2	25	3333
162.8	30	3999
170.9	40	5332
175.6	50	6665

180.6	60	7998
186.6	70	9331
190.9	80	10664
193.9	90	11997

Conclusions

Remarks Field with the Ability to Identify Source of Comment

Although the Halm-Stiel equation is 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 (CAS No. 1760-24-3). Nonetheless, the result is comparable to values obtained from the literature and other studies (see Supporting Data).

Data Quality

Reliabilities (Klimisch Code):

Remarks Field for Data Reliability

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 (CAS No. 1760-24-3). 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

References

Key Study: Smith, A.L. 1986. Dow Corning Corporation, Report No. 1986-I0032-53.

Cited Documents:

- Klimisch, H.J., M. Andreae, and U. Tillman. 1997. A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data. *Regulatory Toxicology and Pharmacology* 25:1-5.
- Menzie, G.K. 1958. Dow Corning Corporation, Report No. 1958-I0030-1625.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Remarks Field for General Remarks

Supporting Data:

- Reported boiling point of 259°C @ 101.3 kPa. Spivack, J.L., E.R. Pohl, and P. Kochs. 1997. Organoalkoxysilanes, organosilanols, and organosiloxanols, in G. Chandra (ed.), The Handbook of Environmental Chemistry, Vol. 3, Part H, Organosilicon Materials. Springer-Verlag, Berlin, p 105.
- Extrapolated boiling point (Antoine equation) of 275°C @ 101.3 kPa. Flaningam O.L. and A.L. Smith. 1994. Dow Corning Corporation, Report No. 1994-I0000-39053.
- Reported boiling point of 264°C @ 101.3 kPa. Dow Corning Corporation, physical properties database.
- Reported boiling point of 260°C @ 101.3 kPa. General Electric, physical properties database.

Vapour Pressure

Test Substance

Identity: N-(2-aminoethyl)-3-aminopropyltrimethoxysilane (CAS No. 1760-24-3)

Remarks Field for Test Substance

Purity of test substance not identified.

Method

Method/guideline followed:	Not identified
GLP (Y/N):	No
Year (study performed):	1958

Remarks Field for Test Conditions

The Halm-Stiel and Antoine equations were used to extrapolate vapor pressure at 20°C from vapor pressures measured at elevated temperatures ranging from 121-194°C.

Results

Vapor Pressure value:	0.4 Pa
Temperature (°C):	20
Decomposition (yes/no/ambiguous):	ambiguous

Remarks Field for Results

- **Measured vapor pressure and temperature data:**

T (°C)	P (mm Hg)	P (Pa)
121.0	5	667
137.0	10	1333
145.7	15	2000
159.2	25	3333
162.8	30	3999
170.9	40	5332
175.6	50	6665
180.6	60	7998
186.6	70	9331

190.9	80	10664
193.9	90	11997

The extrapolated vapor pressure of the test substance at 20°C was 0.4 Pa and 0.3 Pa, based on the Halm-Stiel equation (Smith 1986) and the Antoine equation (Flaningam and Smith 1994), respectively.

Conclusions

Remarks Field with Ability to Identify Source of Comment

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 (CAS No. 1760-24-3) at 20°C. Nonetheless, measured vapor pressures obtained at elevated temperatures are comparable to values obtained from other studies (see Supporting Data).

Data Quality

Reliabilities (Klimisch Code):

Remarks Field for Data Reliability

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 (CAS No. 1760-24-3). 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 121-194°C.

References

Key Study: Menzie, G.K. 1958. Dow Corning Corporation, Report No. 1958-I0030-1625.

Cited Documents:

- Flaningam, O.L. and A.L. Smith. 1994. Dow Corning Corporation, Report No. 1994-I0000-39053.
- Klimisch, H.J., M. Andreae, and U. Tillman. 1997. A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data. *Regulatory Toxicology and Pharmacology* 25:1-5.
- Smith, A.L. 1986. Dow Corning Corporation, Report No. 1986-I0032-53.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Remarks Field for General Remarks

Supporting Data:

- Measured vapor pressures of 533 Pa and 2000 Pa at 120°C and 141°C, respectively. Speier, J.L. and G.K. Menzie. 1958. Dow Corning Corporation, Report No. 1958-I0030-1713.
- Estimated vapor pressure of 0.04 Pa at 20°C. Dow Corning Corporation, physical properties database.
- Estimated vapor pressure of 4 Pa at 20°C. General Electric, physical properties database.

Biodegradation

Test Substance

Identity: N-(2-aminoethyl)-3-aminopropyltrimethoxysilane (CAS No. 1760-24-3)

Remarks Field for Test Substance

Material tested: DYNASYLAN DAMO-T
Purity/components: 96.0 fluid % CAS No. 1760-24-3

Method

Method/guideline followed:	DOC-DIE AWAY TEST (EWG Guideline 79/831/EWG, Appendix V, Part C (updated edition dated July 1990), Method C.4-A.
Test Type (test type/aerobic/anaerobic):	Aerobic
GLP (Y/N):	Yes
Year (study performed):	1994
Contact time (units):	28 days
Innoculum:	Biological culture from a primarily communal sewage treatment plant (Marl - East)

Remarks Field for Test Conditions

Analytical method used to measure biodegradation: DOC analyses were in the form of a double determination of oxygen-enriched and de-gassed samples (removal of inorganic carbon), previously centrifuged at 3000 RPM for 15 minutes. The DOC analysis was performed using two-point calibration in a carbon analyzer (Shimadzu).

Results

Degradation % after time: Duplicates run with test article: Flask 1: Percent degradation after 0 and 3 hours, and days 7, 14, 21, 27 and 28 was 0, 0, 47.59, 45.81, 48.98, 48.10, and 41.75%, respectively. Flask 2: Percent degradation after 0 and 3 hours, and days 7, 4, 21, 27 and 28 was 0, 0, 45.74, 49.25, 49.50, 51.75, and 35.84%, respectively.

Results: Mean percent degradation for test article: 0, 0, 47, 48, 49, 50, and 39% for 0 and 3 hours, and days 7, 14, 21, 27, and 28 days, respectively.

Kinetic (for sample, positive and negative controls): For each time period %, sample % degradation for each time period noted above. For positive control, sodium benzoate, $\leq$ 98% degradation was reported for each time period in both duplicate samples. For the negative control, % degradation was not calculated, but raw data indicates no degradation at any of the time periods measured.

Breakdown products (yes/no): Not analytically available. However, the test material is known to be hydrolytically unstable. When added to water, the test material rapidly hydrolyzes, generating ethanol and transient silanetriol derivatives which will crosslink.

Conclusions

Remarks Field with the Ability to Identify Source of Comment

Author: DYNASYLAN DAMO-T (96.0 fluid % CAS No. 1760-24-3) achieved a breakdown rate of 39%(DOC reduction) within 28 days. Based on these findings, DYNASYLAN DAMO-T was determined to be "not readily biodegradable". The control substance, sodium benzoate, achieved a breakdown rate of 98.5% (DOC reduction) within 10 days and > 99% within 28 days. This leads to the conclusion that the culture used possessed adequate biological activity.

Data Quality

Reliabilities (Klimisch Code):

References

Hüls AG, Testing Institute for Biology. Final Report DDA 85. Determination of the biodegradability of DYNASYLAN DAMO-T in DOC-DIE AWAY TEST. November 3, 1994

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Acute Toxicity to Fish

Test Substance

Identity: N-(2-aminoethyl)-3-aminopropyltrimethoxysilane (CAS No. 1760-24-3)

Remarks Field for Test Substance

Purity of the test substance was measured by gas chromatography and reported as 96%. The test substance is not stable in water and rapidly hydrolyzes to methanol and aminoethylaminopropylsilanetriol ($R\text{-}Si(OH)_3$ where $R = -(CH_2)_3NH(CH_2)_2NH_2$). The hydrolysis half-life for the test substance is estimated to be < 10 min at pH 7 (Blum et. al., 1991; Wilkinson 1997).

Method

Method/guideline followed:	EPA-660/3-75-009 (USEPA 1975).
Type (test type):	Static acute toxicity (lethality) to freshwater fish.
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain/Supplier:	Bluegill sunfish (*Lepomis macrochirus*) obtained from Fenders Fish Hatchery, Baltic, Ohio (USA).
Analytical monitoring:	None
Element basis:	mortality (lack of movement when prodded)
Exposure period:	96 hours
Statistical methods:	Probit analysis (Finney, 1952)

Remarks Field for Test Conditions

- **design:** static exposure, no solution renewal
- **dilution water:** reconstituted soft-water prepared from glass-distilled water, EPA-660/3-75-009 (USEPA 1975)
- **water chemistry:** not documented (except for pH and dissolved oxygen)
- **test substance stability:** test substance not stable in aqueous solutions; estimated hydrolysis half-life < 10 min at pH 7
- **exposure vessel:** polyethylene-lined vessels containing 10 L of dilution water; vessels aerated prior to study initiation but not during study
- **dosing solutions:** no dosing solutions used; test substance (CAS No. 1760-24-3) added directly to exposure vessels; 4.2 mL of methanol was added to controls because methanol is released on hydrolysis of test substance

- **carrier solvent:** none
- **exposure concentrations:** nominal - 0, 10, 100, 180, 320, 560, 1000 mg/L; measured - concentrations not analytically verified
- **replication:** duplicate controls and single exposure concentrations
- **test system:** juvenile bluegill sunfish having a mean total length of 3.4 cm (range 2.8-4.2 cm); fish were acclimated to laboratory conditions a minimum of two weeks before testing; loading rate of 10 fish per exposure vessel; total of 80 fish
- **observations:** 0, 24, 48, 72, 96 h after study initiation
- **photo-period:** not specified
- **temperature:** 22°C in water bath (mean and ranges not documented)
- **dissolved oxygen:** initiation (t = 0 h): mean 13.4 mg/L (range 13.0-13.5 mg/L); termination (t = 96 h): mean 8.4 mg/L (range 8.0-8.5 mg/L)
- **pH:** initiation (t = 0 h): mean 7.2 (range 7.2-7.3); 48 h observation: mean 8.5 (range 7.4-9.6)

Results

(mg/L nominal concentrations)

- 96-h NOEC = 100
- 96-h LOEC = 180
- 100% mortality = 320
- 96-h LC_{10} = 127 (65-161; 95% CI)
- 96-h LC_{50} = 200 (157-258; 95% CI)
- 96-h LC_{90} = 315 (247-632; 95% CI)

Remarks Field for Results

No mortality observed in controls. The one mortality observed in the 100 mg/L exposure (NOEC) at 24-h observation was not considered dose related (no additional mortality was observed and results were identical to the 180 mg/L exposure). Sublethal effects, if any, were not recorded.

	Cumulative Mortality (%)				
Concentration (mg/L)	0 Hours	24 Hours	48 Hours	72 Hours	96 Hours
0	0	0	0	0	0
10	0	0	0	0	0
100	0	10	10	10	10
180	0	10	10	10	10
320	0	80	90	90	100
560	0	100	100	100	100
1000	0	100	100	100	100

Conclusions

Remarks Field with the Ability to Identify Source of Comment

Based on results from the study (NOEC = 100 mg/L, LOEC = 180 mg/L, and LC_{50} = 200 mg/L), the test substance and hydrolytic degradation products are considered practically non-toxic (LC_{50} > 100 mg/L) to

bluegill sunfish under the described conditions of exposure. The NOEC, LOEC, and LC_{50} obtained from this study are nearly identical to those for rainbow trout (see Supporting Data).

Data Quality

Reliability (Klimisch Code):

Remarks Field for Data Reliability

This study was not conducted in full compliance with OECD 203. However, the study design, documentation of data, and results are scientifically defensible and adequate for assessing the acute toxicity of the test substance (CAS No. 1760-24-3) to freshwater fish. The study is considered to be reliable with the following restrictions:

- study was not conducted under GLP
- exposure concentrations were not analytical verified
- exposure concentrations were not replicated
- temperature not documented for the entire study
- sublethal effects were not documented

References

Key Study: Annelin, R.B. and C.D. McKinney. 1978. Dow Corning Corporation, Report No. 1978-I0005-0589.

Cited Documents:

- Blum, F.D., W. Meesiri, H.J. Kang, and J.E. Gambogi. 1991. Hydrolysis, adsorption, and dynamics of silane coupling agents on silica surfaces. *J. Adhesion Sci. Technol.* 5:479-496.
- Finney, D.J. 1952. *Statistical Method in Biological Assay*. New York, Hafner, 661 p.
- Klimisch, H.J., M. Andreae, and U. Tillman. 1997. A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data. *Regul. Toxicol. Pharmacol.* 25:1-5.
- USEPA. 1975. Methods for acute toxicity tests with fish, macroinvertebrates, and amphibians. United States Environmental Protection Agency, EPA-660/3-75-009.
- Wilkinson, T.J. 1997. Dow Corning Corporation, Report No. 1997-I0000-42725.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Remarks Field for General Remarks

Supporting Data: Annelin, R.B. and C.D. McKinney. 1978. Dow Corning Corporation, Report No. 1978-I0005-0589. The static acute toxicity of the test substance (CAS No. 1760-24-3; purity reported as

96%) to rainbow trout (*Oncorhynchus mykiss*) was determined in reconstituted soft water following guideline EPA-660/3-75-009 (USEPA 1975). Juvenile rainbow trout (size not documented) were exposed in single replicates (loading rate of 10 fish per vessel) to nominal concentrations of 0, 56, 180, 320, 560, and 1000 mg/L. The test substance was added directly to the exposure vessels (polyethylene-lined containers with 10 L of dilution water), a carrier solvent was not used. The non-GLP study was conducted at 12°C. Exposure concentrations were not analytically verified. Mean dissolved oxygen was 11.6 mg/L (range 11.5-12.0 mg/L) at test initiation and 6.4 mg/L (range 4.5-7.5 mg/L) at test termination. Mean pH was 7.4 (range 7.4-7.5) at test initiation and 8.4 (range 7.3-10.0) at test termination. Results from the study were reported as follows (mg/L, nominal concentrations):

- 96-h NOEC = 56
- 96-h LOEC = 180
- 100% mortality = 560
- 96-h LC_{10} = 142 (49-182; 95% CI)
- 96-h LC_{50} = 213 (151-270; 95% CI)
- 96-h LC_{90} = 318 (255-734; 95% CI)

Based on results from the study (NOEC = 56 mg/L, LOEC = 180 mg/L, and LC_{50} = 213 mg/L), the test substance and hydrolytic degradation products are considered practically non-toxic (LC_{50} > 100 mg/L) to rainbow trout under the described conditions of exposure. The NOEC, LOEC, and LC_{50} obtained from this study are nearly identical to those for bluegill sunfish (see Key Study).

This study was not conducted in full compliance with OECD 203. However, the study design, documentation of data, and results are considered scientifically defensible and adequate for assessing the acute toxicity of the test substance (CAS No. 1760-24-3) to freshwater fish. The study is considered to be reliable with the following restrictions:

- study was not conducted under GLP
- exposure concentrations were not analytical verified
- exposure concentrations were not replicated
- temperature not documented for the entire study
- sublethal effects were not documented

Toxicity to Aquatic Plants (e.g., Algae)

Test Substance

Identity: N-(2-aminoethyl)-3-aminopropyltrimethoxysilane (CAS No. 1760-24-3)

Remarks Field for Test Substance

Purity of the test substance was measured by gas chromatography and reported as 96%. The test substance is not stable in water and rapidly hydrolyzes to methanol and aminoethylaminopropylsilanetriol ($R\text{-}Si(OH)_3$ where $R = -(CH_2)_3NH(CH_2)_2NH_2$). The hydrolysis half-life for the test substance is estimated to be < 10 min at pH 7 (Blum et. al., 1991; Wilkinson 1997).

Method

Method/guideline followed:	EPA-670/4-73-00 (USEPA 1973)
Type (test type):	Static acute toxicity (growth inhibition and final yield) to freshwater green algae.
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain/Supplier:	Green algae (*Selenastrum capricornutum*), laboratory culture (source of original culture not documented)
Element basis:	cells/mL (direct counts, in duplicate, using a hemocytometer) and growth rate
Exposure period, date of start and end of the test:	7 days, 11-18 August 1978
Analytical monitoring:	No
Statistical methods:	Probit analysis (Finney, 1952); calculations as described by Stein (1973)

Remarks Field for Test Conditions

- **Test design:** static exposure, no solution renewal
- **Growth medium:** sterile algal broth prepared from glass-distilled water and powdered nutrient media (Difco® Laboratories); source of dilution water not documented
- **Water chemistry:** not documented
- **Test substance stability:** test substance not stable in aqueous solutions; estimated hydrolysis half-life < 10 min at pH 7

- **Exposure vessel:** 125-mL polycarbonate Erlenmeyer flasks containing 40 mL of sterile algal broth; aseptic technique used throughout study
- **Dosing solutions:** 0.1% solution of test material in dilution water used to dose exposure vessels
- **Carrier solvent:** none
- **Exposure concentrations:** nominal - 0, 1, 10, 18, 25, 50 mg/L
  measured - concentrations not analytically verified
- **Replication:** triplicate controls and exposure concentrations
- **Test system:** *Selenastrum capricornutum*, 5.00×10^4 cells/mL at test initiation; laboratory culture (original source and method of cultivation not documented)
- **Observations:** 0, 3, 4, 5, 6, 7 d after study initiation
- **Photo-period:** 24-h light/0-h dark; 600 foot-candle
- **Temperature:** 23 ± 1°C in environmental chamber
- **pH:** not documented

Results

Final Yield (mg/L nominal concentrations)

- 7-d NOEC = 0
- 7-d LOEC = 1
- 7-d EC_{10} = 0.2 (0.1-0.3; 95% CI)
- 7-d EC_{50} = 1.5 (1.0-2.1; 95% CI)
- 7-d EC_{90} = 15 (11-23; 95% CI)

Growth Inhibition (mg/L nominal concentrations)

- 7-d NOEC = 0
- 7-d LOEC = 1
- 7-d EC_{10} = 3.1 (1.5-4.7; 95% CI)
- 7-d EC_{50} = 31 (23-48; 95% CI)
- 7-d EC_{90} = 302 (143-1184; 95% CI)

Remarks Field for Results

Response of the controls was acceptable with exponential growth demonstrated (cell concentration in the controls increased by a factor of 34 over the 7-day study).

	Final Yield ($\times 10^5$ cells/mL)					
Concentration (mg/L)	0 Days	3 Days	4 Days	5 Days	6 Days	7 Days
0	0.50	3.18	5.83	8.58	10.2	17.0
1	0.50	2.00	2.88	6.08	7.00	10.2
10	0.50	0.76	0.81	1.05	1.73	2.52
18	0.50	0.57	0.66	0.82	1.09	1.57
25	0.50	0.59	0.46	0.73	0.74	0.83
50	0.50	0.34	0.39	0.41	0.40	0.37

	Growth Inhibition (%)					
Concentration (mg/L)	0 Days	3 Days	4 Days	5 Days	6 Days	7 Days
0	0	0	0	0	0	0
1	0	37	51	29	31	40

10	0	76	86	88	83	85
18	0	82	89	90	89	91
25	0	82	92	91	93	95
50	0	89	93	95	96	98

Conclusions

Remarks Field with the Ability to Identify Source of Comment

Based on results from the study for final yield (NOEC = 0 mg/L, LOEC = 1 mg/L, and EC_{50} = 1.5 mg/L) and growth inhibition (NOEC = 0 mg/L, LOEC = 1 mg/L, and EC_{50} = 31 mg/L), the test substance and hydrolytic degradation products are considered moderately toxic (1 mg/L < LC_{50} < 10 mg/L) to *Selenastrum capricornutum* (green algae) under the described conditions of exposure. The test substance is considerably less toxic to bluegreen algae (see Supporting Data).

Data Quality

Reliability (Klimisch Code):

Remarks Field for Data Reliability

This study was not conducted in full compliance with OECD 201. However, the study design, documentation of data, and results are scientifically defensible and adequate for assessing the acute toxicity of the test substance (CAS No. 1760-24-3) to freshwater green algae. The study is considered to be reliable with the following restrictions:

- study was not conducted under GLP
- original supplier of the test system not documented
- cultivation methods for laboratory culture not documented
- source of dilution water not documented
- water chemistry not documented
- exposure concentrations not analytically verified

References

Key Study: Annelin, R.B. and C.D. McKinney. 1978. Dow Corning Corporation, Report No. 1978-I0005-0589.

Cited Documents:

- Finney, D.J. 1952. *Statistical Method in Biological Assay*. New York, Hafner, 661 p.
- Klimisch, H.J., M. Andreae, and U. Tillman. 1997. A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data. *Regul. Toxicol. Pharmacol.* 25:1-5.
- Stein, J. 1973. *Handbook of Phycological Methods, Culture Methods and Growth Measurements.* J. Stein (ed.), Cambridge Press, pp 220-229.

- USEPA. 1973. Biological field and laboratory methods. The algal assay proceedure: bottle test. United States Environmental Protection Agency, EPA-670/4-73-00.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Remarks Field for General Remarks

Supporting Data: Annelin, R.B. and C.D. McKinney. 1978. Dow Corning Corporation, Report No. 1978-I0005-0589. The static acute toxicity of the test substance (CAS No. 1760-24-3; purity reported as 96%) to blue-green algae (*Anabaena flos-aquae)* was determined in sterile algal broth prepared from glass-distilled water and powdered nutrient media (Difco® Laboratories), following guideline EPA-670/4-73-00 (USEPA 1973). Blue-green algae (laboratory culture, original source and method of cultivation not documented) were exposed in triplicate replicates (cell density of 1.00×10^4 cells/mL at test initiation) to nominal concentrations of 0, 125, 150, 175, 200 mg/L. The test substance was added directly to the exposure vessels (125-mL polycarbonate Erlenmeyer flasks containing 40 mL of sterile algal broth), a carrier solvent was not used. The non-GLP study was conducted under continuous lighting (600 foot-candle) in an environmental chamber maintained at 23 ± 1°C. Exposure concentrations were not analytically verified and water chemistry parameters, including pH, were not documented. Response of the controls was acceptable with exponential growth demonstrated (cell concentration in the controls increased by a factor of 11 during the 7-day study). Results from the study were reported as follows (mg/L, nominal concentrations):

Final Yield (mg/L nominal concentrations)

- 7-d NOEC = 0
- 7-d LOEC = 125
- 7-d EC_{10} = 72 (34-95; 95% CI)
- 7-d EC_{50} = 173 (159-196; 95% CI)
- 7-d EC_{90} = 412 (300-1014; 95% CI)

Growth Inhibition (mg/L nominal concentrations)

- 7-d NOEC = 0
- 7-d LOEC = 125
- 7-d EC_{10} = 82 (49-101; 95% CI)
- 7-d EC_{50} = 175 (163-196; 95% CI)
- 7-d EC_{90} = 374 (288-710; 95% CI)

Based on results from the study for final yield (NOEC = 0 mg/L, LOEC = 125 mg/L, and EC_{50} = 173 mg/L) and growth inhibition (NOEC = 0 mg/L, LOEC = 125 mg/L, and EC_{50} = 175 mg/L), the test substance and hydrolytic degradation products are considered practically non-toxic (LC_{50} > 100 mg/L) to *Anabaena flos-aquae* (bluegreen algae) under the described conditions of exposure. The test substance is considerably more toxic to green algae (see Key Study).

This study was not conducted in full compliance with OECD 201. However, the study design, documentation of data, and results are considered scientifically defensible and adequate for assessing the

acute toxicity of the test substance (CAS No. 1760-24-3) to freshwater algae. The study is considered to be reliable with the following restrictions:

- study was not conducted under GLP
- original supplier of the test system not documented
- cultivation methods for laboratory culture not documented
- source of dilution water not documented
- water chemistry not documented
- exposure concentrations not analytically verified

Acute Toxicity to Aquatic Invertebrates (e.g., Daphnia)

Test Substance

Identity: N-(2-aminoethyl)-3-aminopropyltrimethoxysilane (CAS No. 1760-24-3)

Remarks Field for Test Substance

Purity of the test substance was measured by gas chromatography and reported as 96%. The test substance is not stable in water and rapidly hydrolyzes to methanol and aminoethylaminopropylsilanetriol ($R\text{-}Si(OH)_3$ where $R = -(CH_2)_3NH(CH_2)_2NH_2$). The hydrolysis half-life for the test substance is estimated to be < 10 min at pH 7 (Blum et. al., 1991; Wilkinson 1997).

Method

Method/guideline followed:	EPA-660/3-75-009 (USEPA 1975).
Type (test type):	Static acute toxicity (immobility) to freshwater macroinvertebrate.
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain/Supplier:	*Daphnia magna*, laboratory culture (source of original culture not documented)
Analytical monitoring:	No
Element basis:	immobilization (no movement after gentle agitation of test chamber)
Exposure period:	48 hours
Statistical methods:	Probit analysis (Finney, 1952)

Remarks Field for Test Conditions

- **test design:** static exposure, no solution renewal
- **dilution water:** reconstituted hard-water; glass-distilled water reconstituted with 192 mg/L $NaHCO_3$, 120 mg/L $CaSO_4$, 120 mg/L $MgSO_4$, and 8 mg/L KCl (pH adjusted to 7.5 with NaOH)
- **water chemistry:** not documented
- **test substance stability:** test substance not stable in aqueous solutions; estimated hydrolysis half-life < 10 min at pH 7
- **exposure vessel:** 250-mL glass beakers containing 200 mL of dilution water; vessels aerated prior to but not after study initiation; vessels covered with Saran Wrap® during exposure
- **dosing solutions:** no dosing solutions used; neat test material added directly to exposure vessels

- **carrier solvent:** none
- **exposure concentrations:** nominal - 0, 10, 100, 1000, 10,000 mg/L; measured - concentrations not analytically verified
- **replication:** duplicate controls and exposure concentrations
- **test system:** *Daphnia magna* neonates (age not documented) from laboratory cultures (original source not documented) maintained under testing conditions; loading rate of 10 organisms per exposure vessel; total of 100 organisms
- **observations:** 0, 24, 48 h after study initiation
- **photo-period:** 18-h light/6-h dark; 600 foot-candle
- **temperature:** 23 ± 1°C in environmental chamber
- **dissolved oxygen:** not documented
- **pH:** not documented

Results

(mg/L nominal concentrations)

- 48-h NOEC = 0
- 48-h LOEC = 10
- 100% Immobilization = 1000
- 48-h EC_{10} = 4 (1-11; 95% CI)
- 48-h EC_{50} = 37 (16-75; 95% CI)
- 48-h EC_{90} = 319 (142-1717; 95% CI)

Remarks Field for Results

One immobilization (5%) observed in controls at 24 and 48 hours. Sublethal effects, if any, were not documented.

	Cumulative Mortality (%)		
Concentration (mg/L)	0 Hours	24 Hours	48 Hours
0	0	5	5
10	0	15	25
100	0	45	65
1000	0	100	100
10,000	0	100	100

Conclusions

Remarks Field with the Ability to Identify Source of Comment

The exposure concentrations were based on a exponential series and spaced too far apart to allow an accurate assessment of the test substance toxicity, including the NOEC and LOEC. Nonetheless, results from the study (NOEC = 0 mg/L, LOEC = 10 mg/L, and EC_{50} = 37 mg/L) suggest that the test substance (CAS No. 1760-24-3) and hydrolytic degradation products are slightly toxic (10 mg/L < LC_{50} < 100 mg/L) to *Daphnia magna* under the described conditions of exposure.

Data Quality

Reliability (Klimisch Code):

Remarks Field for Data Reliability

This study was not conducted in full compliance with OECD 202. However, the study design, documentation of data, and results are scientifically defensible and appear adequate for assessing the acute toxicity of the test substance (CAS No. 1760-24-3) to freshwater macroinvertebrates. The study is considered to be reliable with the following restrictions:

- study was not conducted under GLP
- exponential series of exposure concentrations
- exposure concentrations were not analytical verified
- age of neonates was not documented
- sublethal effects were not documented
- water chemistry, including pH and dissolved oxygen, was not documented

References

Key Study: Annelin, R.B. and C.D. McKinney. 1978. Dow Corning Corporation, Report No. 1978-I0005-0589.

Cited Documents:

- Blum, F.D., W. Meesiri, H.J. Kang, and J.E. Gambogi. 1991. Hydrolysis, adsorption, and dynamics of silane coupling agents on silica surfaces. *J. Adhesion Sci. Technol.* 5:479-496.
- Finney, D.J. 1952. *Statistical Method in Biological Assay*. New York, Hafner, 661 p.
- Klimisch, H.J., M. Andreae, and U. Tillman. 1997. A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data. *Regul. Toxicol. Pharmacol.* 25:1-5.
- USEPA. 1975. Methods for acute toxicity tests with fish, macroinvertebrates, and amphibians. United States Environmental Protection Agency, EPA-660/3-75-009.
- Wilkinson, T.J. 1997. Dow Corning Corporation, Report No. 1997-I0000-42725.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Acute Oral Toxicity

Test Substance

Identity: 1, 2-Ethanediamine, N-[3-(trimethoxysilyl)propyl]- CAS No. 1760-24-3

Method

Method/guideline followed:	OECD 401, EEC 67/548 1967)-79/831 (1979) – 84/449 – Annex V – method B1 (1984) – 91/325 (1991)
Type (test type):	Acute oral LD_{50}
GLP (Y/N):	Y
Year (study performed):	1992
Species/Strain:	Sprague-Dawley Ico rat
Sex:	5 males and 5 females per dose
No. of animals per sex per dose:	5 males and 5 females per dose
Vehicle:	none (neat)
Route of administration (if inhalation - aerosol, vapor, gas, particulate):	oral (gavage)

Remarks Field for Test Conditions

- **Doses (OECD guidelines 401 and 425 do not provide dose levels, so these must be described in detail):** 0, 2009, 2519, 3162 mg/kg
- **Doses per time period:** 1
- **Volume administered or concentration:** neat, controls received 3.10 ml/kg purified water
- **Post dose observation period:** Fifteen minutes after dosing, at 1, 2, 4 hours post-dosing, daily for 14 days. Animals were weighed Day –1, Day of dosing (Day 1), Day 8, and Day 15 and at time of death.

Results

Value [LD50 or LC50] with confidence limits if calculated:	2413 mg/kg (2154-2702 mg/kg) by Bliss' method; 2451 mg/kg (2147 – 2798 mg/kg) by Litchfield & Wilcoxon's method
Number of deaths at each dose level:	See Remarks Field for Results.

Remarks Field for Results

- **Time of death (provide individual animal time if less than 24 hours after dosing):** No deaths were observed among the control animals. One male animal died on Day 2 in the 2009 mg/kg dose group. Three males died on Day 2 and an additional male died on Day 4 in the 2519 mg/kg dose group, while 1 female died on Day 1 and 3 females in this group died on Day 2. Three males and 1 female died on Day 1 in the 3162 mg/kg dose group, with an additional male and 3 additional females dying on Day 2.
- **Description, severity, time of onset and duration of clinical signs at each dose level:**
  - At 2009 mg/kg subdued behavior was noted in all animals at 4 hours. Surviving animals were normal on Day 2.
  - At 2519 mg/kg subdued behavior was noted on Day 1. In some cases subdued behavior, tremors, and diarrhea were noted between Days 2 and 4. All surviving animals were normal by Day 4.
  - At 3162 mg/kg All animals showed subdued behavior on Day 1. All surviving animals were normal on Day 2.
- **Necropsy findings, included doses affected, severity and number of animals affected:** Animals which died prematurely showed lung congestion, autolysis of the alimentary canal, and pale livers. No abnormalities were noted in animals surviving to the end of the study.
- **Potential target organs (if identified in the report):** none

Conclusions

Remarks Field with the Ability to Identify Source of Comment

LD_{50} approximately 2400 mg/kg, according to the EEC directive 91/325, no risk symbol or sentence is required. CAS No. 1760-24-3 is a very low acute peroral toxicant in rats.

Data Quality

Reliabilities (Klimisch Code):

Remarks Field for Data Reliability

GLP study in compliance with guidelines.

References

Key Study: Test to Evaluate the Acute Toxicity Following a Single Oral Administration (LD_{50}) in the Rat. Report No. 203308, Marc Lheritier, Hazelton France. Study conducted for Wacker Chemie, GmbH, 4 August, 1992.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Remarks Field for General Remarks

Supporting Data: These findings are supported by an oral LD_{50} study conducted for Shin-Etsu (2250 mg/kg).

- *Teijin Institute Test Number 76-003-0101-J. Acute Oral Toxicity in Wistar Rats.* The oral LD_{50} with a 95% confidence limit was calculated to be 2.25 (1.91 to 2.66) ml/kg body weight in males and 1.68 (1.52 to 1.86) ml/kg body weight in females.

Acute Dermal Toxicity

Test Substance

Identity: 1, 2-Ethanediamine, N-[3-(trimethoxysilyl)propyl]- CAS No. 1760-24-3

Method

Method/guideline followed:	OECD 402 (1987), EEC 67/548 1967)-79/831 (1979) – 83/467 (1983) -84/449 (1984) EPA Guideline 798.100 (1985) – MAFF Guideline 4200 (1985)
Type (test type):	Acute dermal LD_{50}
GLP (Y/N):	Y
Year (study performed):	1992
Species/Strain:	Sprague-Dawley Ico rat
Sex:	5 males and 5 females per dose
No. of animals per sex per dose:	5 males and 5 females per dose
Vehicle:	none (neat)
Route of administration (if inhalation - aerosol, vapor, gas, particulate):	dermal

Remarks field for Test Conditions

- **Doses (OECD guidelines 401 and 425 do not provide dose levels, so these must be described in detail):** 2009 mg/kg
- **Doses per time period:** 1
- **Volume administered or concentration:** neat
- **Post dose observation period:** Fifteen minutes after dosing, at 1, 2, 4 hours post-dosing, daily for 14 days. Animals were weighed Day –1, Day of dosing (Day 1), Day 8, and Day 15 and at time of death.

Results

Value [LD50 or LC50] with confidence limits if calculated:	> 2009 mg/kg
Number of deaths at each dose level:	No mortality was observed

Conclusions

Remarks Field with the Ability to Identify Source of Comment

LD_{50} greater than the highest dose tested, 2009 mg/kg, according to the EEC directive 83/467, no risk symbol or sentence is required. CAS No. 1760-24-3 is a very low acute percutaneous toxicant in rats.

Data Quality

Reliabilities (Klimisch Code):

References

Key Study: Test to Evaluate the Acute Toxicity Following a Single Cutaneous Application (Limit Test) in the Rat. Report No. 202313, Author: Marc Lheritier, Hazelton France. Study conducted for Wacker Chemie, GmbH, 10 September, 1992.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Genetic Toxicity *In Vivo* (Chromosomal Aberrations)

Test Substance

Identity: 1, 2-Ethanediamine, N-[3-(trimethoxysilyl)propyl]- CAS # 1760-24-3

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Remarks Field for General Remarks

Supporting Data: An additional study indicates CAS No. 1760-24-3 was not mutagenic in an *in vitro* mammalian cell assay.

- *Organofunctional Silane A-1120 In Vitro Genotoxicity Studies: Sister Chromatid Exchange Assay. Bushy Run Research Center. BRRC Report 51-51. August 15, 1988.* In this GLP study (EPA Health Effects Test Guidelines, EPA Report 560/6-83-001, October 1983, HG-DNA-Sister Chrom. In Vitro Fed. Reg. 50 (#188) September 27, 1985, amend. Fed. Reg. 51 9# 9) January 14, 1986.)) CAS No. 1760-24-3 did not produce dose-related, or statistically significant increases in the incidence of SCEs in CHO cells in tests with and without metabolic activation. Several of the dose levels in each test produced increases in SCEs which were statistically greater than the incidence of SCEs in the vehicle controls. The low level of the increases and absence of a dose-related trend in the SCE data indicated that the statistical differences did not represent a chemical-related effect. CAS No. 1760-24-3 was concluded to lack genotoxic potential under the conditions of the SCE test system.

Genetic Toxicity *In Vitro* (Gene Mutations)

Test Substance

Identity: 1, 2-Ethanediamine, N-[3-(trimethoxysilyl)propyl]- CAS No. 1760-24-3

Method

Method/guideline followed:	OECD 471 (1983) – EEC 84/449 – annex V – method B14 (1984)
Type (e.g. reverse mutation assay, gene mutation study, cytogenetic assay, mammalian cell gene mutation assay, cytogenetic assay, etc.):	*Salmonella Typhimurium* incorporation assay (Ames test)
System of testing [bacterial, non bacterial]:	bacterial (*Salmonella*)
GLP (Y/N):	Y
Year (study performed):	1992
Species/Strain or cell type and or cell line, bacterial or non-bacterial:	*Salmonella typhimurium* TA98, TA 100, TA1535, TA1537, TA1538
Metabolic activation:	• **Species and cell type**: rat liver microsomes • **Quantity:** • **Induced or not induced:**
Concentrations tested:	0, 0.1, 0.5, 1.0, 2.5, 5 mg/plate, tested in triplicate
Statistical methods:	NA

Results

Result:	No mutagenic potential was observed in any strain at any dose concentration
Cytotoxic concentration:	• **With metabolic activation:** slight cytotoxicity in all strains at 2.5 and 5 mg/plate • **Without metabolic activation:** slight cytotoxicity in all strains at 2.5 and 5 mg/plate

Genotoxic effects (e.g. positive, negative, unconfirmed, dose-response, equivocal):	• **With metabolic activation:** No mutagenic potential was observed in any strain at any dose concentration • **Without metabolic activation:** No mutagenic potential was observed in any strain at any dose concentration
Statistical results, as appropriate:	NA

Conclusions

Remarks Field with the Ability to Identify Source of Comment

1, 2-ethanediamine, N-[3-(trimethoxysilyl)propyl]- (CAS No. 1760-24-3) is not mutagenic with or without metabolic activation.

Data Quality

Reliabilities (Klimisch Code)

References

Salmonella typhimurium/Mammalian microsome Plate Incorporation Assay (Ames Test), Report number 203301, A. Forichon, Hazelton France. Conducted for Wacker Chemie GmbH, 18 August, 1992.

Other

Last changed (administrative field for updating):

Order number for sorting (administrative field):

Remarks Field for General Remarks

Supporting Data: Additional studies indicate that CAS No. 1760-24-3 was not mutagenic in bacterial or *in vitro* mammalian mutagenicity assays.

- *Organofunctional Silane A-1120 In vitro Genotoxicity Studies: CHO/HGPRT Gene Mutation Test. Bushy Run Research Center. Project Report 51-51. August 15, 1988.* CAS No. 1760-24-3 was evaluated for potential genotoxic activity using the Chinese Hamster Ovary (CHO) Mutation test (EPA Health Effects Test Guidelines, HG-Gene-Muta-Somatic cells. EPA Report No. 560/6-83-001, October 1983). CAS No. 1760-24-3 did not produce any statistically significant increases in incidence of mutations of CHO cells within a range of cytotoxic-to-non-cytotoxic concentrations between 2.5 to 4.0 mg/ml in test without a metabolic activation system. With metabolic activation, there was no reproducible increase in mutant incidence. No dose related trend in mutant values was

observed in the test with or without metabolic activation, indicating CAS No. 1760-24-3 lacks significant genotoxic potential in the CHO/HGPRT system.

- *Unpublished Report 1988, DeGussa-Huls AG Nr. 88-0299-FGM.* In a GLP study [test guideline published in *Mutation Research 31*, 347-364 (1975)] CAS No. 1760-24-3 was tested with four strains of *Salmonella typhimurium*. The material was not mutagenic in this bacterial mutagenicity assay.
- *Kakenkyo. Bacterial mutagenicity test.* A bacterial mutagenicity test (based on Japanese guidelines for testing of chemicals) was conducted with CAS No. 1760-24-3 in *Salmonella typhimurium* strains TA100, TA1535, TA98 and TA1537 and *E. coli* strain WP2uvrA with and without metabolic activation. There was no increase in the number of revertant colonies in comparison with the solvent control at any concentration with or without metabolic activation.