Substance Profile for The Challenge
Dodecamethylcyclohexasiloxane (D6)
CAS No. 540-97-6

Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) required the Minister of Health and Minister of the Environment to categorize the approximately 23,000 substances on the Domestic Substances List (DSL). Categorization involved identifying those substances on the DSL that are a) considered to be persistent (P) and/or bioaccumulative (B), based on criteria set out in the *Persistence and Bioaccumulation Regulations* (Government of Canada, 2000), and "inherently toxic" (iT) to humans or other organisms, or b) that present, to individuals in Canada, the greatest potential for exposure (GPE).

Further to this activity, the Act requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that meet the categorization criteria. A screening assessment involves a scientific evaluation of available information for a substance to determine whether the substance meets the criteria set out in section 64 of CEPA 1999. Based on the results of a screening assessment, the Ministers can propose taking no further action with respect to the substance, adding the substance to the Priority Substances List (PSL) for further assessment or recommending the addition of the substance to the List of Toxic Substances in Schedule 1 of CEPA 1999 and, where applicable, the implementation of virtual elimination of releases to the environment.

A number of substances have been identified by the Ministers as high priorities for action based on the information obtained through the categorization process. This includes substances:

- that were found to meet all of the ecological categorization criteria, including persistence, bioaccumulation potential and inherent toxicity to aquatic organisms (PBiT), and that are known to be in commerce, or of commercial interest, in Canada, and/or
- that were found either to meet the categorization criteria for GPE or to present an intermediate potential for exposure (IPE), and were identified as posing a high hazard to human health based on available evidence on carcinogenicity, mutagenicity, developmental toxicity or reproductive toxicity.

Based on a consideration of the ecological and/or human health concerns associated with these substances, and the requirement under section 76.1 of CEPA 1999 for the Ministers to apply a weight of evidence approach and the precautionary principle when conducting and interpreting the results of an assessment, sufficient data are currently available to conclude whether these substances meet the criteria under section 64 of CEPA 1999.

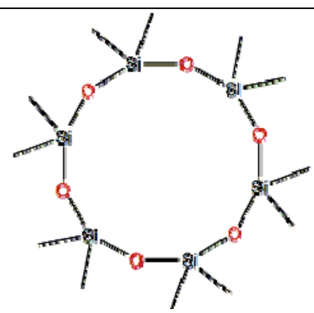
As such, the Ministers have issued a Challenge to industry and other interested stakeholders through publication in Canada Gazette Part I December 9, 2006 to submit, within the timelines stated in the Challenge section of this document, specific information that may be used to inform risk assessment and to develop and benchmark best practices for risk management and product stewardship.

Dodecamethylcyclohexasiloxane (D6) was identified as a high priority for action as it was found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and is believed to be in commerce in Canada. The technical human health and ecological information that formed the basis for concern associated with this substance is contained in Appendices I and II, respectively.

Substance Identity

For the purposes of this document, dodecamethylcyclotetrasiloxane will be referred to as D6, an abbreviated name derived from the General Electric's siloxane notation (Hurd 1946).

D6 belongs to a group of cyclic volatile methyl-siloxanes (VMS) with relatively low molecular weight (< 600) and high vapour pressure. These cyclic VMS are volatile, low-viscosity silicone fluids consisting of three to six $-(CH_3)_2SiO-$ structure units in a cyclic configuration. D6 consists of six of these $-(CH_3)_2SiO-$ structure units as shown in the chemical structure below.

CAS Registry Number	540-97-6
Inventory names	Cyclohexasiloxane, dodecamethyl-; Dodecamethylcyclohexasiloxane (English, French); Dodecamethylcyclohexasiloxan (German); dodecametilciclohexasiloxano (Spanish)
Other names	D6; DC 246; Dodecamethylhexacyclosiloxane; Dow Corning 246; Dow Corning 246 Fluid;
Chemical group	Discrete organics
Chemical sub-group	Cyclic Volatile Methyl Siloxanes (VMS)
Chemical formula	C12H36O6Si6
Chemical structure	
SMILES	C[Si]1(O[Si](O[Si](O[Si](O[Si](C)(C)O[Si](O1)(C)C)(C)C)(C)C)(C)C)C
Molecular mass	444.93 g/mol

Based on information submitted in response to a legal Notice published in 2006 under section 71 of CEPA 1999 (Environment Canada 2006a), D6 was not manufactured in Canada in 2005 in a quantity meeting the 100 kg reporting threshold. In total, seventeen companies reported import of this substance into Canada in 2005, with eight companies in the 100-1,000 kg range, eight companies in the 1,001 – 100,000 kg range and one company in the >100,000 kg range.

D6 is used in a variety of industry activities in Canada such as rubber products; manufacture of pharmaceuticals, cleaning compounds, polishes, and toiletries; and paints, coating, and adhesives (Environment Canada 2006a). In other countries, uses include cosmetics and personal care products; polishes; paint, lacquers and varnishes; and as an ingredient in pesticides (SPIN 2007).

THE CHALLENGE

Respecting direction under section 76.1 of CEPA 1999, and in the absence of additional relevant information as a result of this Challenge, the Ministers are predisposed to conclude, based on a screening assessment, that this substance satisfies the definition of toxic under section 64 of CEPA 1999. As such, the Ministers are prepared to then recommend to the Governor in Council that this substance be added to the List of Toxic Substances in Schedule 1 of CEPA 1999, with the intent of initiating the development of risk management measures taking into account socio-economic considerations.

If it is determined that the substance meets the virtual elimination criteria in subsection 77(4) of CEPA 1999, then subsequent risk management activities will be based on the objective of eliminating the release of any measurable quantity of the substance to the environment. In the absence of further information on existing management practices for a substance, actions would be proposed based on the assumption of worst-case practices. The management actions being considered for such substances at this time include prohibition through regulations, of the manufacture, use, sale, offer for sale and import of this substance, except for those activities controlled under the *Pest Control Products Act* and/or the *Food and Drugs Act.*

Exceptionally, should no information be identified to indicate that this substance is in commerce in Canada, the Ministers will conclude, based on a screening assessment, that this substance does not satisfy the definition of toxic under section 64 of CEPA 1999. However, given the properties of this substance, there is concern that new activities for the substance that have not been identified or assessed under CEPA 1999 could lead to the substance meeting the criteria set out in section 64 of the Act. Therefore it would be recommended that this substance be subject to the Significant New Activity provisions specified under subsection 81(3) of the Act, to ensure that any new manufacture, import or use of this substance in quantities greater than 100 kg/year is notified, and that ecological and human health risk assessments are conducted as specified in section 83 of the Act prior to the substance being introduced into Canada.

Section 71 Notice

Under the Challenge, information deemed necessary for improved decision making may be gathered by the Minister of Environment using section 71 of CEPA 1999. This information may be used for the purpose of assessing whether a substance is toxic or is capable of becoming toxic as defined under section 64 of CEPA 1999, or for the purpose of assessing whether to control, or the manner in which to control a substance.

The information mandated through the notices may relate to, among other things; quantity of the substance imported, manufactured, used, or released, concentrations, suppliers, customers, as well as types of uses of the substance.

Copies of the section 71 notice and guidance on how to comply with it are available from the Government of Canada Chemicals Portal (www.chemicalsubstanceschimiques.gc.ca), or from the contact provided below.

Opportunity to Submit Additional Information to Inform Screening Assessment

The Ministers of Health and Environment are inviting the submission of additional information for consideration during screening assessment of this substance. Data of the types described in the following paragraphs are considered most relevant, although other submitted information will be considered.

Data on the persistence, bioaccumulation, and potential for toxicity of the substance to organisms in different environmental media – Through the categorization exercise, available experimental data were collected up to December 2005. Where acceptable experimental data were not available, Quantitative Structure Activity Relationships (QSARs) or read across data were used to fill the data gaps. Since experimental data are preferred, interested parties have an opportunity to provide new or additional relevant experimental study information on the persistence, bioaccumulation, and potential for toxicity of this substance to organisms in different environmental media (air, water, sediment, soil). Efforts should focus on providing data for the endpoints for which quality experimental data does not already exist, as demonstrated by the information summarized in Appendix II of this document. As submitted data will be evaluated for completeness and robustness, it is recommended that stakeholders follow the guidance for test protocols and alternative approaches for test data, as described in Section 8 of the "Guidelines for the Notification and Testing of New Substances: Chemicals & Polymers".[1]

Data on the toxicity of the substance to human health - Through the categorization exercise, the high health priorities for action were those substances identified by various agencies as representing a high health hazard on the basis of potential to induce cancer, and/or adversely affect reproduction and development, two critical determinants of the health of Canadians of all ages. The hazard classifications used were those developed by national or international agencies in which large numbers of substances have been classified for endpoint-specific hazard based on original review and critical evaluation of data, assessments of weight of evidence and extensive peer review. Interested parties have an opportunity to provide new or additional relevant experimental study information on the toxicity of the substance to human health which could inform the screening assessment.

Responses to this part of the challenge for this substance should be received at the address provided below by November 13, 2007.

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[1] "Guidelines for the Notification and Testing of New Substances: Chemicals & Polymers (version 2005)", Government of Canada, Available from http://www.ec.gc.ca/substances/nsb/eng/cp_guidance_e.shtml

Opportunity to Submit Additional Information on Current Uses and Existing Control Measures to Inform the Risk Management Approach for this Substance

The Ministers of Health and Environment are inviting the submission of additional information that is deemed beneficial by interested stakeholders, relating to the extent and nature of the management/stewardship of substances listed under the Challenge.

Organizations that may be interested in submitting additional information in response to this invitation include those that manufacture, import, export or use this substance whether alone, in a mixture or in a product, including manufactured items.

Additional information is being invited in the following areas:

- Import, manufacture and use quantities
- Substance and product use details
- Releases to the environment and spill management
- Current and potential risk management and product stewardship actions
- Existing legislative or regulatory programs controlling/managing the substance
- Information to support the development of a regulatory impact assessment.

A questionnaire is available which provides a detailed template as an example for the submission of this information. Guidance on how to respond to the challenge questionnaire is also available. Interested stakeholders are invited to provide available additional information, recognizing that not all questions in the questionnaire may be relevant to a particular substance, use, or industrial sector.

Copies of the questionnaire and associated guidance are available from the Government of Canada Chemicals Portal (www.chemicalsubstanceschimiques.gc.ca)**,** or from the contact provided below.

Responses to this part of the challenge for this substance should be received at the address provided below by November 13, 2007.

Request for Documents and Submission of Information

Documents and instructions may be requested from the following contact. Information in response to the above Challenge must be submitted to this address:

DSL Surveys Coordinator
Place Vincent Massey, 20th Floor
351 Saint Joseph Boulevard
Gatineau QC K1A 0H3
Tel: 1-888-228-0530/819-956-9313
Fax: 1-800-410-4314 / 819-953-4936
Email: DSL.surveyco@ec.gc.ca

Appendix I
Human Health Information
to Support the Challenge for
Dodecamethylcyclohexasiloxane (D6)
CAS No. 540-97-6

Introduction

Under the *Canadian Environmental Protection Act, 1999* (CEPA 1999), Health Canada undertook to categorize substances on the Domestic Substances List (DSL) to identify those representing the greatest potential for human exposure (GPE) and those among a subset of substances considered persistent (P) and/or bioaccumulative (B) by Environment Canada that are also considered to be "inherently toxic" to humans.

In order to efficiently identify substances that represent the highest priorities for screening assessment from a human health perspective, Health Canada developed and applied a Simple Exposure Tool (SimET) to the DSL to identify those substances that meet the criteria for GPE, Intermediate Potential for Exposure (IPE) or Low Potential for Exposure (LPE), and a Simple Hazard Tool (SimHaz) to identify those substances that pose a high or low hazard.

Dodecamethylcyclohexasiloxane (D6) (CAS No. 540-97-6)is considered to meet the criteria for IPE under SimET and does not meet the criteria for high hazard under SimHaz. This document summarizes the currently available information on which the SimET and SimHaz results are based.

Exposure Information from Health Related Components of DSL Categorization

SimET was developed and used to identify substances on the DSL considered to represent GPE. This approach was based on three lines of evidence: 1) the quantity in commerce in Canada, 2) the number of companies involved in commercial activities in Canada (i.e., number of notifiers), and 3) the consideration by experts of the potential for human exposure based on various use codes. The proposed approach was released for public comment in November 2003 and also enabled designation of substances as presenting an IPE or LPE, based on criteria for quantity and nature of use (Health Canada 2003).

Results of the Application of SimET

D6 has been determined to be IPE based on a consideration of the DSL nomination information listed below.

Nomination Information for DSL

Quantity in Commerce

The quantity reported to be manufactured, imported or in commerce in Canada during the calendar year 1986 was 110,000 kg.

Number of Notifiers

The number of notifiers for the calendar years 1984-1986 was fewer than four.

Use Codes and Description

The following DSL use codes have been identified for the substance:

21 Formulation component
60 Cosmetics
76 Organic Chemicals, Industrial
85 Pigment, Dye and Printing Ink
86 Plastics

Potential Uses in Canada

Potential uses in Canada are provided in Appendix II.

Hazard Information from Health Related Components of DSL Categorization

Simple Hazard Tool (SimHaz)

SimHaz is a tool that has been used to identify, among all of the approximately 23,000 substances on the DSL, those considered to present either high or low hazard to human health based on formalized weight of evidence criteria and/or peer review/consensus of experts. This tool has been developed through extensive compilation of hazard classifications of Health Canada and other agencies and consideration of their robustness based on availability of transparent documentation of both process and criteria (Health Canada 2005).

Results of the Application of SimHaz

D6 has not been classified for hazard by any of the agencies considered under the SimHaz tool and therefore does not meet the criteria for high hazard under SimHaz.

Uncertainties

SimET and SimHaz have been developed as robust tools for effectively identifying substances from the DSL considered to be human health priorities for further consideration. It is recognized that they do not include a number of elements normally considered in a human health risk assessment such as a comprehensive characterization of exposure and hazard, a comparison of exposure metrics to hazard metrics and a detailed analysis of uncertainties.

References

Health Canada. 2003. Proposal for Priority Setting for Existing Substances on the Domestic Substances List under the Canadian Environmental Protection Act, 1999: Greatest Potential for Human Exposure. http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/existsub/exposure/greatest_potential_human_exposure-risque_exposition_humaine_e.pdf

Health Canada. 2005. Proposed Integrated Framework for the Health-Related Components of Categorization of the Domestic Substances List under CEPA 1999. http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/contaminants/existsub/framework-int-cadre_e.pdf

Appendix II
Ecological Information
to Support The Challenge for
Dodecamethylcyclohexasiloxane (D6)
CAS No. 540-97-6

The information in this document will form the basis of a screening assessment under section 74 of CEPA, 1999. Data relevant to an ecological screening assessment were identified in original literature, review documents, commercial and government databases prior to December 2005. Properties and characteristics may also have been estimated using Quantitative Structure Activity Relationship (QSAR) models. In addition, an industry survey was conducted for the year 2005 through a Canada Gazette Notice issued pursuant to section 71 of CEPA 1999 (Environment Canada 2006b). This Notice requested data on the Canadian manufacture and import of the substance.

Physical and chemical properties

Table 1 contains experimental and modelled physical-chemical properties of D6 which are relevant to its environmental fate.

Table 1. Physical and chemical properties for D6

Property	Type	Value	Temperature ºC	Reference
log K_{ow} (Octanol-water partition coefficient)	Modelled	6.33		Kowwin v.1.67
Boiling point ºC	Experimental	245.00		SRC PHYSPROP Database 2003
Boiling point ºC	Modelled	226.77		MPBPWIN v1.41
Melting point ºC	Experimental	-3.00		SRC PHYSPROP Database 2003
Melting point ºC	Modelled	-8.69		MPBPWIN v1.41
Vapour Pressure (Pa)	Modelled	4.73 (0.0355 mm Hg)	25	MPBPWIN v1.41
Henry's Law Constant ($Pa{\cdot}m^3/mol$)	Modelled	16212 (0.16 atm-m^3/mol)	25	HenryWin v3.10
log K_{oc} (Organic carbon-water partition coefficient)	Modelled	6.07		PCKOCWIN v1.66
Water solubility (mg/L)	Modelled	0.005	25	WSKOWWIN v1.41

Manufacture, Importation, and Uses

Manufacture and Importation

In Canada, no manufacture of D6 was reported in response to a CEPA section 71 survey notice for the 2005 calendar year in a quantity meeting the 100 kg reporting threshold (Environment Canada 2006a). However, there were seventeen companies reporting the import of D6 into Canada in 2005 (Environment Canada 2006a), with eight companies in the 100-1,000 kg/year range, eight companies in the 1,001 – to 100,000 kg/yr range, and one company in the >100,000 kg/year range (See Appendix I for the quantity of D6 reported in commerce in Canada during the calendar year 1986).

Elsewhere, D6 has been identified as a High Production Volume (HPV) chemical by the Organisation for Economic Co-operation and Development (OECD), the US Environmental Protection Agency (EPA), and the International Congress & Convention Association (ICCA). According to information from the US EPA, the import/production of D6 in the United States was in the range of 4.5 – 225 tonnes in 1986, increasing to 450 – 4,500 tonnes in 1990, 1994, and 1998, and then increasing again to 4,500 – 45,000 tonnes in 2002.

In Europe, D6 has been identified as a Low Production Volume (LPV) chemical, with Dow Corning Limited of the UK as the only producer/importer of D6 (ECB 2007). In Nordic countries, the SPIN database indicated its registered consumption was less than 10 tons per year during 2000 – 2004, although Norway and Finland did not specify its use quantity (SPIN 2007).

Uses

In response to a CEPA section 71 survey notice for the 2005 calendar year, companies importing D6 identified their business activity as (Environment Canada 2006a): the retail trade of cosmetics, beauty supplies, perfumes, personal care products, pharmaceuticals and drug products; wholesale trade/distribution of chemical (except agricultural) and allied products, pharmaceuticals, toiletries and cosmetics; manufacture of paper bags and treated paper products, rubber products, medical equipment and supplies, pharmaceuticals, medicines, sanitation goods (like soap cleaning compounds and polishes) and toiletries (which could include perfumes, shaving, hair or face lotion preparations); other chemical products, other foods (which could include perishable prepared foods like salads, fresh pizza / pasta), paints, coating, adhesives and other miscellaneous items.

The above industrial activities identified through the CEPA section 71 Notice are based on the North American Industry Classification System (NAICS) codes. These codes define the company's sectors and business lines, but do not describe the use of the substance or product within the company. This differs from the DSL Nomination Functional Use Codes utilized during categorization and listed in Appendix I. Use Codes indicate specific applications or uses for the substance or products containing the substance. NAICS has currently defined over 3000 NAICS codes. The Functional Use Codes were defined for the purposes of the DSL Nomination.

The number of industrial activities identified as using D6 in 2005 is considerably greater than the number of DSL Use Codes for this substance identified in 1986. A NAICS defines the activities of a company rather then a substance, so the broad number of activities identified may only be distantly relevant to the substance. As well, there were an increased number of notifiers importing or manufacturing the substance as well as an increase in the amount of this substance being manufactured or imported into Canada.

The following use patterns have been identified worldwide (SPIN 2007 unless otherwise specified):

- Raw materials or intermediates for the production of cosmetics and hygienic articles
- Paint, lacquers and varnishes
- Surface treatment and polishing agents for motor vehicles and other plastic materials

Similar uses are expected in Canada based on the use/activity codes reported by industry during the section 71 survey (as listed previously), and those reported to the DSL during the calendar year 1986 in Canada (see Appendix I). In Canada, it is also used as an inert ingredient in pesticide formulations (PMRA 2005).

Since D6 belongs to a group of substances used in various industry applications and in consumer products such as personal care, surface treatment agents, etc., it may be released to the environment in a dispersive manner.

Releases, Fate, and Presence in the Environment

Releases

D6 is not naturally produced in the environment. Measured data concerning the environmental releases of this substance from uses in Canada were not collected as part of the s. 71 survey. Its dispersive use pattern suggests possible release to air, sewage treatment plants (STPs) and landfills. D6 may enter the environment through evaporation due to its high volatility. When released to STPs, its high log K_{ow} and log K_{oc} values indicate partitioning of the compound to the active sludge that may then be applied to agricultural soil as fertilizer or landfilled. Disposal of consumer and industrial products containing D6 can also lead to the release of D6 to landfills. Agricultural, landfill, and STP releases may lead to groundwater, soil, and sediment exposure

Fate

D6 is expected to partition into air based on its high vapour pressure and Henry's law constant. The high log K_{ow} and log K_{oc} values indicate that this substance will likely partition to soil and sediments. Indeed, the results of the Level III Fugacity modelling indicates that if this substance is released equally to the three major environmental compartments (air, water, and soil), it will partition in all compartments including air, water, soil, and sediments, with the latter two compartments being predominant (Table 2).

Table 2. Results of the Level III fugacity modelling for D6 (EPIWIN v3.12)

Receiving media	% in Air	% in Water	% in Soil	% in Sediment
Air (100%)	93.10	0.02	6.36	0.48
Water (100%)	0.23	3.32	0.02	96.40
Soil (100%)	0.22	0	99.70	0.07
Air, water, soil (33.3% each)	0.88	2.11	35.90	61.10

If D6 is released solely to air, a vapour pressure of 4.73 Pa and Henry's Law constant of 16212 Pa·m^3/mole indicates it will mainly remain in air. A small amount of D6 will partition to soil and other environmental compartments (< 7 %, Table 2).

If released to water, D6 is expected to strongly adsorb to suspended solids and sediment based upon an extremely high estimated log K_{oc} value (> 6). Although volatilization from water surfaces is also expected based upon the Henry's Law constant for this compound, its high adsorptivity to sediment may reduce the potential for volatilization. Thus, if water is the receiving medium, D6 is expected to partition mainly to sediments and, to some extent, air (< 4 %, Table 2).

If released to soil, volatilization from dry or moist soil to the atmosphere is expected based on its vapour pressure. The high log K_{oc} value for D6 indicates that this substance is expected to adsorb strongly to soil (i.e., expected to be immobile), which may reduce the potential for volatilization. Thus, if released to soil, D6 will mainly remain in soil, which is illustrated by the results of the Level III fugacity modelling (Table 2).

Presence in the Environment

Once released into the environment, D6 appears to be relatively persistent in the environment. No monitoring data relating to the presence of the substance in Canadian environmental media (air, water, soil, sediment) have yet been identified.

Elsewhere, an environmental monitoring program of volatile methylated siloxanes initiated by Nordic countries found that D6 was present in all sampled media except soil. It was suggested that this substance was distributed in the Nordic environment mainly in urban areas and near or within STPs through its dispersive uses (Norden 2005). The Swedish National Screening Programme in 2004 found D6 present in air, water and STP sludge. D6 was also found in two sediment samples, but was not reported in any fish muscles (Kaj et al. 2005).

In Air

D6 was found in air in Nordic and Swedish environment during 2003 - 2005. In the Nordic Screening Programme, D6 was measured in all air samples, with concentrations generally ranging from 0.02-0.87 $\mu g/cm^3$ in urban areas, landfills and other sampling sites; one sample taken inside an STP was higher (2.1 $\mu g/cm^3$) (Norden 2005). Concentrations of D6 in Sweden ranged from not detected to 0.08 $\mu g/cm^3$ (Kaj et al. 2005).

Sweden also conducted indoor air measurements in 400 households in children's bedroom. D6 was detected in 142 homes at concentrations of 0.6 – 164 $\mu g/m^3$ (personal communication, Norbert Schmidbauer, Norweigian Institute for Air Research, 2005, as cited in Kaj et al. 2005). D6 was also detected in the United States in five air samples from office buildings located in 2 cities, at concentrations ranging from 0.4 to 16.5 $\mu g/m^3$ (VOC data base 1990, as cited in USEPA 1992).

In Water

D6 was not detected in Nordic water samples collected at background or urban sites (detection limit <0.1 µg/L). However, D6 was detected in STP influents and effluents, as well as water from landfills and industrial wastewater (0.12 – 3.8 µg/L) (Norden 2005). In Sweden, D6 was detected in one surface water sample near industrialized area as part of the National Programme, and in eight samples (including one landfill) from the Regional Programme. Concentrations of D6 ranged from below detection to 0.27 µg/L (Kaj et al. 2005). In the United States, D6 was detected in drinking water concentrates from two cities, New Orleans, LA and Cincinnati, OH (Lucas 1984, as cited in USEPA 1992).

In Soil

D6 was not detected (detection limit < 4 ng/g dry weight) in soil samples taken from two landfills from the Faroe Islands (Norden 2005).

In Sediments

D6 was detected in sediments in both the Nordic and Swedish screening programmes, generally in urban areas. Typically, concentrations were <25 ng/g dw (Norden 2005); however, one sample from the Nordic programme was 170 ng/g dw (Norden 2005) and two samples from the Swedish programme were 51 and 196 ng/g dw, respectively (Kaj et al. 2005).

In STPs

D6 was found in all but one STP sludge sample in Sweden. The concentration of D6 was generally below 4,000 ng/g dw in the Nordic programme, but reached a concentration of 11,000 ng/g dw in one sample (Norden 2005). In Sweden, D6 was detected in 53 of 54 sludge samples. Concentrations ranged from 37 to 8,400 ng/g dw, with an average of approximately 1,500 ng/g dw (Kaj et al. 2005).

In Aquatic Organisms
In the Nordic environment, D6 was detected in livers of marine fish but not freshwater fish, and mainly from areas representing urban or diffuse sources. Concentrations generally ranged from <5 to 10 ng/g ww, except for one sample with extremely high siloxane concentrations which had 74 ng/g ww D6. The concentrations varied with species, gender, and age. Among marine mammals monitored, D6 was detected in seal blubber in Denmark at the level of 7.9 ng/g ww (Norden 2005).

As concentrations of D6 in Nordic waters were < 5 µg/L, the detection of D6 in biota indicates that D6 has the potential to bioaccumulate (Norden 2005).

Rationale for P, B and iT status

Environmental Persistence

Once released in the environment, D6 appears to be relatively persistent in all environmental compartments. The Level III Fugacity model indicates that D6 will partition to air, where it is expected to be oxidized by the gas-phase reaction with photochemically produced hydroxyl radicals. The atmospheric oxidation half-life for D6 is predicted to be ~ 6 days (Table 3), indicating that this substance is persistent in air (half-life > 2 days). D6 is not expected to react, or react appreciably, with other photo oxidative species in the atmosphere, such as O_3 and NO_3, nor is it likely to degrade via direct photolysis (Atkinson, 1991). Therefore, it is expected that reactions with hydroxyl radicals will be the most important fate process in the atmosphere for the substance.

Table 3. Modelled persistence data for D6

Medium	Fate Process	Degradation Value	Degradation Endpoint	Model
Air	atm-oxidation	5.96	half-life (days)	AOPWIN v1.91
Water/soil	Biodegradation	60	half-life (days)	BIOWIN v4.02, Ultimate survey
Water/soil	Biodegradation	0	probability	BIOWIN v4.02, MITI Linear Probability
Water/soil	Biodegradation	0	probability	BIOWIN v4.02, MITI Non-linear Probability

Empirical biodegradation data for water, sediment and soil are not available for D6. Therefore, a weight-of-evidence approach (ESD 2006a) was applied by reading across data from similar chemicals and applying model predictions as shown in Table 3.

D6 is structurally similar to, and a close analogue of, both D3 (hexamethylcyclo-trisiloxane, CAS No. 541-05-9) and D4 (octamethylcyclotetrasiloxane, CAS No. 556-67-2) such that it is expected that D6 will exhibit similar biodegradation potential as D3 and D4. Experimental data show no biodegradation of D3 over 28 days in a ready-biodegradation test (SEHSC 2005), suggesting that it is persistent in water, sediment and soil. As well, no biodegradation of D4 was observed in an aerobic water/sediment system (Silicones Health Council 1991, as cited in HSDB 2006). These data are further supported by two of the models in Table 3 which indicate that the probability of biodegradation of D6 occurring in water or soils is effectively zero. Therefore, D6 is expected to behave similarly and be persistent in water, sediment and soils.

The long-range transport potential (LRTP) of D6 from its point of release to air is estimated to be moderate according to the model prediction presented in Table 4. The TaPL3 model was used to estimate Characteristic Travel Distance (CTD), defined as the maximum distance traveled by 63% of a substance; or in other words, the distance that 37% of the substance may travel beyond. Beyer et al. (2000) have proposed CTD's of >2,000 km as representing high LRTP, 700-2,000 km as moderate, and <700 km as low. Based on the result shown in Table 4, D6 is expected to be able to reach areas far from its emission sources, but unlikely to be found in the Arctic.

Table 4. Model Predicted Characteristic Travel Distance (CTD) for D6

Characteristic Travel Distance	Model (Reference)
1,481 Km	TaPL3 (CEMC 2003)

Based on the model (Table 3) and read-across data, it is concluded that D6 meets the persistence criteria (half-lives in air > 2 days; in soil and water ≥ 182 days; in sediments ≥365 days) as set out in the *Persistence and Bioaccumulation Regulations* (Government of Canada 2000).

Potential for Bioaccumulation

The modelled log K_{ow} value for D6 (Table 1) suggests that this substance has the potential to bioaccumulate in the environment. This is supported by the Nordic environmental monitoring data which detected D6 in marine fish livers and marine mammals despite low water concentrations (Norden 2005). Empirical bioaccumulation data are not available for this substance. The Modified GOBAS BAF middle trophic level model produced a BAF of 1,148,154 L/kg wet weight, indicating that this substance has the potential to bioconcentrate and biomagnify. The three BCF models, which all yield estimates that are >5,000 L/kg, also provide evidence supporting the bioconcentration potential of this substance.

Table 5. Modelled bioaccumulation data for D6

Test Organism	Endpoint	Value wet wt	Reference
Fish	BAF	1,148,154 L/kg	Gobas BAF T2MTL (Arnot and Gobas 2003)
Fish	BCF	38,019 L/Kg	Gobas BCF T2LTL (Arnot and Gobas 2003)
Fish	BCF	67,608 L/kg	OASIS 2005
Fish	BCF	14,791 L/kg	BCFWIN v2.15

The modelled bioaccumulation values do not take into account the metabolic potential of the substance. However, an experimental BCF study with a close analogue, D4, indicates that metabolism is not likely significant (Fackler et al. 1995). Therefore, D6 is likewise not expected to exhibit significant metabolism based on the similarity in structure of D4 and D6.

The weight of evidence indicates that this substance meets the bioaccumulation criterion (BCF, BAF ≥ 5,000) as set out in the *Persistence and Bioaccumulation Regulations* (Government of Canada 2000).

Ecological Effects

In the Aquatic Compartment

Empirical ecotoxicity data are not available for D6. However D4, a structurally similar substance and a close analogue to D6, exhibits extremely high short- and long-term toxicity at concentrations in the range of 0.0044 – 0.015 mg/L to fish and daphnia. Similar modes of action and toxicities to aquatic organisms are expected for D6 and D4 based on their similarity in structure and physical-chemical properties.

There is modelled evidence that D6 causes harm to aquatic organisms at relatively low concentrations (e.g., LC50 < 1 mg/L). Table 6 lists those predictions that were considered reliable and were used in the QSAR weight-of-evidence approach (ESD 2006a) for aquatic toxicity used to categorize substances on Canada's DSL. Modelled ecotoxicity data for D6 are in the range of 0.014-0.17 mg/L, which are similar to those for D4.

Table 6. Modelled aquatic toxicity values for D6

Organism	Endpoint	Duration	Concentration (mg/L)	Reference
Fish	LC50	96 h	0.1722	OASIS
Daphnia	EC50	16 d	0.014	ECOSAR v.0.99h
Green Algae	EC50	96 h	0.033	ECOSAR v.0.99h

Both modelled predictions and the category approach indicate D6 is very toxic to aquatic organisms, with extremely high short- and long-term toxicity close to its estimated solubility limit (0.005 mg/L). These results indicate that D6 is highly hazardous to aquatic organisms (i.e., acute LC/EC50 < 1.0 mg/L).

In Other Media

No effects studies for non-aquatic non-mammalian organisms were found for this compound.

Potential to Cause Ecological Harm

Evidence that a substance is highly persistent and bioaccumulative as defined in the Persistence and Bioaccumulation Regulations of CEPA 1999 (Government of Canada 2000) together with evidence of commercial activity provides a significant indication of its potential to be entering the environment under conditions that may have harmful long term ecological effects (ESD 2006b). Substances that are persistent remain in the environment for a long time, increasing the potential magnitude and duration of exposure.

Substances that have long half-lives in mobile media (air and water) and partition into these media in significant proportions have the potential to cause widespread contamination. Releases of small amounts of bioaccumulative substances may lead to high internal concentrations in exposed organisms. Highly bioaccumulative and persistent substances are of special concern, since they may biomagnify in food webs, resulting in very high internal exposures, especially for top predators. Evidence that a substance is both highly persistent and bioaccumulative, when taken together with other information (such as evidence of toxicity at relatively low concentrations, and evidence of uses and releases) may therefore be sufficient to indicate that the substance has the potential to cause ecological harm.

The volume of D6 imported into Canada in 2005 is up to 1000 tonnes. Its large importation volumes and dispersive use, especially its wide application in household products, along with its volatile nature indicate potential for releases into the Canadian environment. Once released in the environment, because of its resistance to degradation, D6 will remain in air, water, sediment and soil for long times, and may be transported relatively long distances. As it persists in the environment, it will likely bioaccumulate and may be biomagnified in trophic food chains. It has also been demonstrated to have very high toxicity. This information suggests that D6 has the potential to cause ecological harm in Canada.

Uncertainties

Uncertainties exist in the conclusions reached in this document because all P, B, iT evaluations were based either on modelled data, or read-across from a structurally similar substance.

Information on environmental concentrations or monitoring data in Canada, and on long-term low level exposure to D6, is also lacking. Very little monitoring data from the United States were found, and that which was available is from 1980-1990. The environmental monitoring data from the Swedish National Screening Programme and Nordic countries indicate that D6 concentrations in surface waters did not reach levels that have been estimated to cause significant adverse effects to aquatic organisms. However, the use volume in Sweden and Nordic countries are relatively small compared to that in Canada and the United States.

Regarding toxicity, based on the predicted partitioning behaviour of this substance, the significance of soil and sediments as important media of exposure is not well addressed by the available effects data.

Predicted concentrations, associated with the inherent toxicity to aquatic organisms, may have an additional source of uncertainty in some situations, e.g., where these concentrations exceed the solubility of the chemical in water. Given that concentrations for both toxicity and water solubility often vary considerably (up to several orders of magnitude), it is acknowledged that these uncertainties exist.

There is also uncertainty associated with basing the overall conclusion that D6 may be causing ecological harm, solely on information relating to its persistence, bioaccumulation, relative toxicity and use pattern. Typically, quantitative risk estimates (i.e., risk quotients or probabilistic analyses) are important lines of evidence when evaluating a substance's potential to cause environmental harm. However, when risks for persistent and bioaccumulative substances such as this cyclosiloxane are estimated using such quantitative methods, they are highly uncertain and are likely to be underestimated (ESD 2006b). Given that the long term risks associated with persistent and bioaccumulative substances cannot at present be reliably predicted, quantitative risk estimates have limited relevance. Furthermore, since accumulations of such substances may be widespread and are difficult to reverse, a conservative response to uncertainty (that avoids underestimation of risks) is justified.

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