Substance Profile for The Challenge
(3,3,5-trimethylcyclohexylidene)bis[(1,1-dimethylethyl)peroxide]
CAS No. 6731-36-8

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 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.

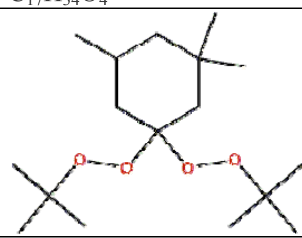
Based on a consideration of the ecological and/or human health concerns associated with these substances, and the requirement under section 76.1 of CEPA 1999 for the Ministers to apply a weight of evidence approach and the precautionary principle when conducting and interpreting the results of an assessment, sufficient data are currently available to consider these substances as meeting 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 the document, below, specific information that may be used to develop and benchmark best practices for risk management and product stewardship.

The substance (3,3,5-trimethylcyclohexylidene)bis[(1,1-dimethylethyl)peroxide] 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 report, this substance will be referred to as DBTMC, which has been derived from the inventory name 1,1-Di-tert-butylperoxy-3,3,5-trimethylcyclohexane.

CAS Registry Number	6731-36-8
Inventory names	Peroxide, (3,3,5-trimethylcyclohexylidene)bis[(1,1-dimethylethyl); di-tert-butyl 3,3,5-trimethylcyclohexylidene diperoxide; 1,1-Bis(tert-butyldioxy)-3,3,5-trimethylcyclohexane; 1,1-Di-tert-butylperoxy-3,3,5-trimethylcyclohexane
Other names	1,1-Bis(tert-butylperoxy)-3,5,5-trimethylcyclohexane; 1,1-Di(t-butylperoxy)-3,3,5-trimethylcyclohexane; 3,3,5-Trimethyl-1,1-bis(tert-butylperoxy)cyclohexane; Interox TMCH 401C, Link-Cup TMCH, Luperco 231G, 231G40, 231XL, 231XLP; Luperox 231, 231-50, 231XL; Lupersol 230XL, 231, L 231; Perhexa 3M, 3M40, Sanperox CY 1.1; Trigonox 29, 29-40B-PD, 29/40, 29/40MB, 29A, 29B50, 29B75, 29B90, 29C75, Tx 29, 29B50, Varox 231XL
Chemical group	Discrete organics
Chemical sub-group	Diperoxyketal
Chemical formula	$C_{17}H_{34}O_4$
Chemical structure	
SMILES	O(OC(C)(C)C)C(OOC(C)(C)C)(CC(CC1(C)C)C)C1
Molecular mass	302.46 g/mol

Based on information submitted in response to a legal Notice published in 2006 under section 71 of CEPA 1999, DBTMC was not manufactured in Canada in 2005 in a quantity meeting the 100 kg reporting thresholds. Six companies reported importing up to 100,000 kg into Canada in 2005 for activities described as motor vehicle manufacturing, rubber product manufacturing (tires and hoses), basic chemical manufacturing, other chemical product and preparation manufacturing (which could include printing, inks and cartridges) and wholesale trade/distribution of chemical (except agricultural) and allied products. DBTMC is suitable to be used as an initiator for the polymerization of monomers as well as for the hardening of polyester resins and the cross-linking of polymers. It can be used as a polymerisation initiator for plastics and in rubber processing for the production of window seals and automotive seals, hoses, and soles of shoes. It may also be used for the curing of some resins for applications ranging from boat hulls and swimming pools to bodywork parts.

THE CHALLENGE

Based on the information presented in Appendix II of this document, it is expected that the screening assessment of this substance will conclude that it satisfies the definition of toxic under section 64 of CEPA 1999 in that it "may enter the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity". The substance will then be proposed for addition to the List of Toxic Substances in Schedule I of the Act and proposed for virtual elimination of releases to the environment.

Subsequent risk management activities will be based on the objective of eliminating the release of a measurable quantity of a PBiT substance to the environment. In the absence of further information on existing handling practices for these substances, proposed actions would be based on realistic worst case assumptions. At this time, prohibition is being considering 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.*

Opportunity to Submit Information on P, B and iT Properties

Through the categorization exercise, available experimental aquatic toxicity information as well as experimental data on the potential for a substance to persist or bioaccumulate in the environment were collected prior 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 the categorization outcome on P, B, and iT form the basis for prioritizing this substance for action, and experimental data are preferred, interested parties have an opportunity to provide relevant experimental study information on the persistence, bioaccumulation, and inherent toxicity to aquatic organisms for this substance.

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]

Responses to this part of the challenge for this substance should be received at the address provided below by June 5, 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

Section 71 Notice

Information needed for improved decision-making with regard to risk assessment and management of this substance is being gathered using section 71 of CEPA 1999. This notice applies to any person who reported pursuant to the *Canadian Environmental Protection Act*, 1999 section 71 Notice with Respect to Selected Substances Identified as Priority for Action, published in the Canada Gazette, Part I, on March 4, 2006.

The 2006 information mandated through the notice relates to, among other things, quantity of the substance imported, manufactured or used, types of uses of the substance, and releases of the substance to the environment.

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.

Responses to the section 71 notice must be received at the address provided below by June 5, 2007.

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, in a product or in a manufactured item.

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 June 5, 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
(3,3,5-trimethylcyclohexylidene)bis[(1,1-dimethylethyl)peroxide]
(DBTMC)
CAS No. 6731-36-8

Introduction

Under the *Canadian Environmental Protection Act, 1999* (CEPA, 1999), Health Canada undertook to categorize all 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 persistant (P) and/or bioaccumulative (B) that are also considered to be "inherently toxic" to humans.

In order to efficiently identify substances that represent the highest priorities for screening assessment, 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.

DBTMC is considered to meet the criteria for LPE 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

As mentioned above, 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

DBTMC has been determined to be LPE 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 20,200 kg.

Number of Notifiers

The number of notifiers for the calendar years 1984-1986 was 4.

Use Codes and Description

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

8	Catalyst/accelerator/initiator/activator
21	Formulation component
37	Polymer, crosslinking agent
77	Organic Chemicals, Specialty
86	Plastics
87	Plastics and Synthetic Resins
92	Rubber Products

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

DBTMC 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 related 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
(3,3,5-trimethylcyclohexylidene)bis[(1,1-dimethylethyl)peroxide]
(DBTMC)
CAS No. 6731-36-8

Introduction

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, 2006). 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 DBTMC which are relevant to its environmental fate.

Table 1. Physical and chemical properties for DBTMC.

Property	Type	Value	Temperature (°C)	Reference
Boiling Point	Modelled	306.87°C		MPBPWIN v1.41
Melting Point	Modelled	86.3°C		MPBPWIN v1.41
Melting Point	Experimental	-20°C		Acros Organics MSDS, 2004
log Kow	Modelled	7.56	25	Kowwin v.1.67
log Koc	Modelled	5.53		PCKOCWIN v.1.66
Vapour Pressure	Modelled	0.09Pa		MPBPWIN v1.41
Vapour Pressure	Modelled	0.000653 mm Hg		MPBPWIN v1.41
Henry's Law Constant	Modelled	0.001507 atm-m^3/mol	25	HenryWin v3.10
Water solubility	Modelled	0.004118 mg/L	25	WSKOWWIN v1.41

Manufacture, Importation and Uses

Manufacture and Importation

Work was carried out under contract in 2002 by ChemInfo to determine the use of initiators in polymer resin manufacturing and processing in Canada. From this activity, it was determined that organic peroxide initiators were not manufactured in Canada in 2000. The 2002 investigation also determined that peroxyketals make up the smallest class of organic peroxides that were used in the polymer resin manufacturing process in Canada. Approximately 100,000 kg of peroxyketals and other organic peroxides were used in the Canadian polymer resin manufacturing process in 2000.

Under the CEPA section 71 Notice with respect to Selected Substances Identified as Priority for Action, Canadian companies who manufactured or imported (in 2005) greater than 100 kg of a substance listed in the notice were required to provide specific data regarding the substance to Environment Canada. Information gathered from this survey notice indicates that DBTMC was not manufactured in Canada in 2005 in a quantity meeting the 100kg reporting threshold.

In total, six companies reported import of this substance with three companies in the 100-1,000 kg/year range and three companies in the 1,001 – 100,000 kg/year range. The importing companies identified their business activities as: motor vehicle manufacturing, rubber product manufacturing (tires and hoses), basic chemical manufacturing, other chemical product and preparation manufacturing (which could include printing, inks and cartridges) and wholesale trade/distribution of chemical (except agricultural) and allied products. In addition, five Canadian companies and one American company identified themselves as having a stakeholder interest in the substance.

Elsewhere, DBTMC was reported to the US Environmental Protection Agency under the Inventory Update Rule for use between 4.5 and 225 tonnes from 1990 to 1998 which increased to 225 to 455 tonnes in 2002. DBTMC is an European Union (EU) Low Production Volume Chemical, indicating that production within the EU is estimated to be in the order of 10 tonnes per year. The database for Substances in Preparations in Nordic Countries indicates that it was used in Sweden, Norway and Denmark from 1999-2004 (SPIN Database). In Japan, it was found that 108 tonnes of DBTMC were manufactured or imported in 2004. Results from their 2001 Ministry of Economy, Trade and Industry survey show that 100 to 1000 tonnes were manufactured or imported (NITE website).

Uses

DBTMC is suitable as an initiator for the polymerization of monomers as well as for the hardening of insatiated polyester resins and the cross-linking of polymers. It can be used as a polymerisation initiator for plastics and in rubber processing for the production of window seals and automotive seals, hoses, and soles of shoes. It may also be used for the curing of some resins for applications ranging from boat hulls and swimming pools to bodywork parts (Arkema).

Releases, Fate and Presence in the Environment

Releases

DBTMC is not naturally produced in the environment. Releases from anthropogenic sources have not been reported. However, due to the potentially explosive nature of peroxides when they dry, it is anticipated that waste material and container residues are commonly rinsed down the drain.

Fate

The high log Kow and Koc values indicate that this substance will likely partition to soil and sediments. Indeed, the results of the Level III Fugacity modelling indicates that if the chemical is released equally into the three major environmental compartments (air, water and soil), it will mainly partition into soil and sediments (Table 2), where the chemical has been indicated to persist (Table 3).

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

	Fraction of Substance Partitioning to Each Medium (%)			
Substance Released to:	**Air**	**Water**	**Soil**	**Sediment**
Air (100%)	37.2	0.636	13.3	48.8
Water (100%)	0.00328	1.29	0.00117	98.7
Soil (100%)	5.79×10^{-5}	0.00242	99.8	0.186
Air, water, soil (33.3% each)	0.0973	0.773	39.8	59.3

A vapour pressure of 0.09Pa and Henry's Law Constant of 1.5×10^{-3} atm-m^3/mol indicate that DBTMC is relatively volatile. Therefore, if released solely to air, it should remain in this compartment. However, the high Koc gives it a high affinity for particulate matter causing it to sorb to particulate matter and partition to soil and sediment (~60%).

If released to water, DBTMC is expected to strongly sorb to suspended solids and sediment based on its extremely high log Koc value. Although volatilization from water surfaces may occur based on the Henry's Law Constant, it is predicted that when released to water, the chemical partitions mainly to sediment.

If released to soil, DBTMC is expected to have extremely high adsorptivity to soil (i.e. expected to be immobile) based on an estimated log Koc of ~5 where it is expected to persist (Table 3). The vapour pressure and Henry's Law Constant indicate that volatilization may occur in dry and moist soil surfaces, however due to the extremely high adsorptivity to soil particles, volatilization is not expected to be significant. Therefore, if released to soil, DBTMC will remain in this compartment, which can be illustrated by the results of the Level III fugacity modelling (Table 2).

Presence in the Environment
No monitoring data relating to the presence of this substance in environmental media (air, water, soil, sediment) have yet been identified.

Evaluation of P, B and iT Properties

Environmental Persistence

Once released in the environment, models predict that DBTMC will persist in water, soil and sediments. Experimental persistence data is not available for air. It is expected to oxidize quickly by hydroxyl radical reactions (EPIWIN v3.12). As shown in Table 3a, it is not expected to react with O_3 or NO_3. In addition to the expected rapid loss by reaction with hydroxyl radicals, almost all organic peroxides are thermally and photolytically sensitive due to the weak oxygen-oxygen bonds. Di-tert butyl peroxide is structurally similar to DBTMC around the peroxide bond and absorbs light up to 340nm, and has been found to photolyze to form tert-butoxy radicals at low temperatures (HSDB, 2006). It is expected that photolytic decomposition will be the most important degradation process in the atmosphere for DBTMC resulting in rapid losses from air.

Table 3a Modelled data for persistence

Medium	Fate Process	Endpoint	Value	Reference
Air	Atm-oxidation	Half life (days)	1.232	AOPWIN v1.91
Air	Ozone reaction	Half life (days)	Not reactive	AOPWIN v1.91
Water/Soil	Biodegradation	Half life (days)	182	BIOWIN v4.02 (USM)
Water/Soil	Biodegradation	Probability	0.0207	BIOWIN v4.02 MITI Non-linear
Water/Soil	Biodegradation	Probability	0	TOPKAT

Table 3b Empirical data for persistence

Medium	Fate Process	Endpoint	Value	Reference
Water	Ready Biodegradation	% Biodeg	0-3%	ESD 2006a
Water	Ready Biodegradation	% Biodeg	12%	NITE Database

For estimating degradation in water, soil and sediment, a QSAR weight-of-evidence approach (ESD, 2006b) was applied using the models shown in Table 3a. Based on these results, the estimated measures for biodegradation indicate that DBTMC can be considered as persistent in water and soil.

Empirical data support the model predictions that DBTMC will persist in water and soil (Table 3b). Considering both the empirical and modelled data the data indicate that the half-life in water and soil is expected to be longer than 182 days.

To extrapolate to a half-life in sediments, an approach has been developed using Boethling's extrapolation factors (BIOWIN v4.02), which involves extrapolating the half life in sediment from that estimated for water ($t_{1/2\ water} : t_{1/2\ sediment} = 1:4$). Therefore, in sediments, the half-life is expected to exceed 728 days.

The long-range transport potential (LRTP) of DBTMC from its point of release to air is estimated to be low according to the model prediction presented in Table 3c. The TaPL3 model was used to estimate Characteristic Travel Distance (CTD), defined as the maximum distance traveled by 63% of the substance; or in other words, the distance that 37% of the substance may travel beyond. Beyer et al (2000) have selected CTD's of >2000 km as representing high LRTP, 700-2000 km as moderate, and <700 km as low. Based on the result shown in Table 3c, this substance is expected to remain primarily in the areas close to its emission sources.

Table 3c – Model Predicted Characteristic Travel Distance (CTD) for DBTMC

Characteristic Travel Distance	**Model (Reference)**
307 km	TaPL3 (CEMC, 2003)

The empirical and modelled data (Tables 3a and 3b) demonstrate that the substance meets the persistence criteria (half-lives 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

Modelled log Kow values and empirical data indicate that DBTMC has the potential to bioaccumulate in the environment (Table 4a and 4b).

QSAR modelled bioaccumulation and bioconcentration values (Table 4a) also agree quite well with the experimental values (Table 4b). The Modified GOBAS BAF middle trophic level model produced a BAF of 189,819 L/kg, indicating that DBTMC has the potential to bioconcentrate and biomagnify in the environment. Two other BCF models provide a weight of evidence to support the bioconcentration potential of this substance.

Table 4a. Predicted bioaccumulation values

Test Organism	Endpoint	Value wet wt	Reference
Fish	BAF	189,819 L/kg	GOBAS BAF T2MTL (Arnot and Gobas, 2003)
Fish	BCF	1,419 L/kg	Gobas BCF T2LTL (Arnot and Gobas, 2003)
Fish	BCF	25,119 L/kg	OASIS
Fish	BCF	10,965 L/kg	BCFWIN

Table 4b. Empirical bioaccumulation values

Test Organism	Concentration tested (mg/L)	Endpoint	Value wet wt	Reference
Cyprinus carpio (Common carp)	0.2	BCF	3500-9860 L/kg	NITE database
Cyprinus carpio (Common carp)	0.02	BCF	4960-13200 L/kg	NITE database

The results from the eight week BCF studies indicate that the models are conservative and that metabolism may reduce the bioaccumulation of DBTMC but typically not below the bioaccumulation criterion.

The weight of evidence indicates that the substance meets the bioaccumulation criterion (BCF, BAF ≥ 5000) as set out in the Persistence and Bioaccumulation Regulations (Government of Canada 2000).

Ecological Effects

A - In the Aquatic Compartment

There is modelled and experimental evidence that the substance causes harm to aquatic organisms at relatively low concentrations (e.g., acute LC50 < 1 mg/L) [Table 5a and b]. A range of aquatic toxicity predictions were obtained from the various QSAR models considered. Table 5a list those predictions that were considered reliable and were used in the QSAR weight of evidence approach for aquatic toxicity (ESD, 2006b). These results indicate a high potential for toxicity to aquatic organisms (i.e. acute LC/EC50≤1.0 mg/L).

Table 5a Modelled data for aquatic toxicity

Test Organism	Type of Test	Endpoint	Value (mg/L)	Reference
Fish	Acute	LC50	0.4395	OASIS
Fish	Acute	LC50	2.73	PNN (AI Expert)
Fish	Acute	LC50	0.006	ECOSAR
Fish	Acute	LC50	0.00006	ECOSAR Neutral Organic SAR

Table 5b Empirical data for aquatic toxicity

Test Organism	Type of Test	Endpoint	Value (mg/L)	Reference
Oryzias latipes (Medaka)	Acute	LC50	>500	NITE Database
Daphnia magna (Water flea)	Acute	EC50	0.13	ESD 2006c

Acute experimental data for DBTMC are presented in Table 5b. A MITI study found that the 48 hour LC50 for *Oryzias latipes* was greater than 500 mg/L, although this study has not been reviewed for robustness, the LC50 exceeds the water solubility by many orders of magnitude, calling into question the relevance of the test. A reviewed confidential study resulted in a 48 hour EC50 for *Daphnia magna* of 0.13 mg/L. A co-solvent was added to increase the substance's solubility. The co-solvent was also tested and revealed no toxicity (ESD, 2006c).

These results indicate that the substance is highly hazardous to aquatic organisms (i.e. acute LC/EC50≤1.0 mg/L).

B - In Other Media

The toxicity results listed in Table 6 have not been evaluated for robustness.

Table 6. Empirical data for Toxicity in Other Media

Test Organism	Test Type	Endpoint	Value (mg/kg)	Reference
Rat	Oral	LD50	12918-13000	ChemID Plus, 2006 and Kirk-Othmer, 2001

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, 2006d). Substances that are persistent remain in the environment for a long time after being released, 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 relatively large importation volumes of diperoxyketals into Canada indicate that DBTMC is likely entering the environment in Canada. Once released in the environment, because of its hydrophobicity, it will partition to sediments or soils where it will remain for long times due to its resistance to degradation. As it persists in the environment, and because of its lipophyllic character, it will likely bioaccumulate and may biomagnify in trophic food chains. It has also demonstrated relatively high toxicity to aquatic organisms. This information suggests that DBTMC has the potential to cause ecological harm in Canada.

Uncertainties

Information and data on concentrations in the Canadian environment are currently lacking. Yet, the relatively high volume of diperoxyketals imported in Canada in 2000 and the reported amount that was imported in 2005 indicate that there is a potential for release to the Canadian environment.

The evidence for high persistence and bioaccumulation potential is considered strong, since both modelled estimates and empirical data indicate that DBTMC meets the criteria set out in the Persistence and Bioaccumulation Regulations of CEPA 1999 (Government of Canada, 2000). Similarly convincing evidence that DBTMC can harm organisms at relatively low exposure concentrations, is provided by results from QSAR modelling and toxicity testing for pelagic organisms.

The effects data do not address toxicity in soil and sediments, which have been identified as the primary media of concern based on partitioning estimates. The only effects data identified apply to pelagic aquatic exposures, although the water column is not the medium of primary concern.

The experimental or predicted concentrations, associated with inherent toxicity for 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 (either experimental or predicted). Given that concentrations for both the 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 DBTMC 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 substances potential to cause environmental harm. However when risks for persistent and bioaccumulative substances such as DBTMC are estimated using such quantitative methods, they are highly uncertain and are likely to be underestimated (ESD, 2006d). Given that 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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