Screening Assessment for the Challenge

7-Oxa-3,20-diazadispiro[5.1.11.2]heneicosan-21-one, 2,2,4,4-tetramethyl-

Chemical Abstracts Service Registry Number
64338-16-5

Environment Canada
Health Canada

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Synopsis

Pursuant to section 74 of the *Canadian Environmental Protection Act, 1999* (CEPA 1999), the Ministers of the Environment and of Health have conducted a screening assessment on 7-Oxa-3,20-diazadispiro[5.1.11.2]heneicosan-21-one, 2,2,4,4-tetramethyl- (ODHO), Chemical Abstracts Service Registry Number 64338-16-5. This substance was identified as a high priority for screening assessment and included in the Challenge because it was found to meet the ecological categorization criteria for persistence, bioaccumulation potential and inherent toxicity to non-human organisms and is believed to be in commerce in Canada.

The substance, ODHO, was not considered to be a high priority for assessment of potential risks to human health, based upon application of the simple exposure and hazard tools developed by Health Canada for categorization of substances on the Domestic Substances List. Therefore, this assessment focuses principally on information relevant to the evaluation of ecological risks.

ODHO is an organic substance that is used to protect plastic polymers and industrial materials from photochemical degradation. The substance does not occur naturally in the environment. Surveys conducted under section 71 of CEPA 1999 determined that, in 2005 and 2006, ODHO was not manufactured in Canada in quantities equal to or greater than 100 kg; however, in both years, imports of the substance into Canada were in the range of 100–1000 kg/year.

A predicted acid dissociation constant (pK_a) value of greater than 9 for the amine suggests that ODHO will exist almost entirely as a charged molecule in the environmentally-relevant pH range of 6–9, with the substance existing primarily as a protonated cation and acting as a weak base. Therefore, when released to the environment ODHO is expected to partition predominantly into water, although partitioning to soil and, to a lesser extent sediment, may also occur depending upon the compartment of release.

With a predicted atmospheric oxidation half-life of 0.11 day, ODHO is expected to be rapidly oxidized in air. Biodegradation modelling predicts that ODHO in water, soil and sediment will undergo primary biodegradation in less than 182 days, but the identities of the degradation products are not known. However, ultimate biodegradation modelling indicates that complete mineralization will occur only slowly, and the substance and/or its degradation products may therefore persist in water, soil and sediment. Based on the available data, ODHO meets the persistence criteria in water, soil and sediment (half-lives in soil and water $\geq$ 182 days and half-life in sediment $\geq$ 365 days), but does not meet the criterion for air (half-life criterion of $\geq$ 2 days) as set out in the *Persistence and Bioaccumulation Regulations.*

ODHO was initially categorized as potentially bioaccumulative based on model predictions for the neutral compound. However, given the evidence for molecular charge at ambient pHs (6–9), as well as a new measured bioconcentration factor of about 4.0 and new predicted bioaccumulation and bioconcentration factors (BAF/BCF) ranging from 12.8 to 1580 that take into account the fact that the charged form is expected to predominate, it is considered unlikely that ODHO will accumulate in large amounts in organisms. Therefore, it is considered not to meet the bioaccumulation criteria as set out in the *Persistence and Bioaccumulation Regulations*.

Empirical data suggest that ODHO has a moderate to low potential for acute toxicity in aquatic organisms. However, no empirical data are available on possible effects following long-term exposure, an issue of importance given the evidence for stability of the substance in the environment. For this reason, predicted data were also considered in evaluating the potential for toxicity. Model estimates which take into consideration the presence of the charged form of the substance suggest that ODHO will generally have moderate toxicity to aquatic organisms. However, a chronic toxicity estimate of 0.3 mg/L is considered to indicate that ODHO may have the potential to cause adverse effects following long-term exposure of aquatic organisms to relatively low concentrations in the environment.

ODHO is considered to have low exposure potential based on relatively low import volumes and information indicating that when added to plastics and coatings during processing operations, it becomes chemically reacted into the matrix material thereby reducing the potential for release into the environment from finished products.

A risk quotient analysis, integrating a conservative predicted environmental concentration (PEC) with a conservative predicted no-effect concentration (PNEC) resulted in a risk quotient (PEC/PNEC) value of 0.4, indicating that current estimated exposure concentrations of ODHO in water are unlikely to cause ecological harm at the current and foreseeable level of use in Canada.

With regard to human health, no measured concentrations of ODHO in environmental media were identified in Canada and elsewhere. However, the potential for exposure of the general population to ODHO from environmental media is expected to be negligible according to estimates based on the quantity of ODHO in Canadian commerce in 2006. No information with regard to the presence of ODHO in foods was identified. Exposure from food, if any, would be negligible. No consumer products were identified in Canada that contain ODHO.

There are very limited toxicological data available for ODHO, and quantitative structure activity relationship (QSAR) programs for carcinogenicity, genotoxicity, and reproductive and developmental toxicity did not generate predictions in most cases.

Since exposure of the general population to ODHO in Canada is expected to be negligible, and since ODHO was not identified as posing a high hazard to human health based on the limited information available, it is concluded that ODHO is not entering the environment in a quantity or concentration or under conditions that constitute or may constitute a danger in Canada to human life or health.

It is further concluded that ODHO is not entering 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 or that constitute or may constitute a danger to the environment on which life depends. ODHO meets the criteria for persistence but does not meet criteria for bioaccumulation potential as set out in the *Persistence and Bioaccumulation Regulations*.

Based on the information available, it is concluded that ODHO does not meet any of the criteria set out in section 64 of the *Canadian Environmental Protection Act, 1999*.

This substance will be considered for inclusion in the *Domestic Substances List* inventory update initiative. In addition and where relevant, research and monitoring will support verification of assumptions used during the screening assessment.

Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) (Canada 1999) requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that have met the categorization criteria set out in the Act to determine whether these substances present or may present a risk to the environment or human health.

Based on the information obtained through the categorization process, the Ministers identified a number of substances as high priorities for action. These include substances that

- met all of the ecological categorization criteria, including persistence (P), bioaccumulation potential (B) and inherent toxicity to aquatic organisms (iT), and were believed to be in commerce in Canada; and/or
- met the categorization criteria for greatest potential for exposure (GPE) or presented an intermediate potential for exposure (IPE), and had been identified as posing a high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity.

The Ministers therefore published a notice of intent in the *Canada Gazette*, Part I, on December 9, 2006 (Canada 2006), that challenged industry and other interested stakeholders to submit, within specified timelines, specific information that may be used to inform risk assessment, and to develop and benchmark best practices for the risk management and product stewardship of those substances identified as high priorities.

The substance 7-Oxa-3,20-diazadispiro[5.1.11.2]heneicosan-21-one, 2,2,4,4-tetramethyl- was identified as a high priority for assessment of ecological risk as it was found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and is believed to be in commerce in Canada. The Challenge for this substance was published in the *Canada Gazette* on March 14, 2009 (Canada 2009). A substance profile was released at the same time. The substance profile presented the technical information available prior to December 2005 that formed the basis for categorization of this substance. As a result of the Challenge, submissions of information pertaining to the physical and chemical properties, bioaccumulation potential, aquatic toxicity, uses and environmental exposure of the substance were received.

Although 7-Oxa-3,20-diazadispiro[5.1.11.2]heneicosan-21-one, 2,2,4,4-tetramethyl- was determined to be a high priority for assessment with respect to the environment, it did not meet the criteria for GPE or IPE and high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity. Therefore, this assessment focuses principally on information relevant to the evaluation of ecological risks.

Screening assessments focus on information critical to determining whether a substance meets the criteria as set out in section 64 of CEPA 1999. Screening assessments examine scientific information and develop conclusions by incorporating a weight-of-evidence approach and precaution[1].

This final screening assessment includes consideration of information on chemical properties, hazards, uses and exposure, including the additional information submitted under the Challenge. Data relevant to the screening assessment of this substance were identified in original literature, review and assessment documents, stakeholder research reports and from recent literature searches, up to June 2010 for ecological sections of the document and January 2010 for human health-related sections. Key studies were critically evaluated; modelling results may have been used to reach conclusions.

When available and relevant, information presented in hazard assessments from other jurisdictions was considered. The final screening assessment does not represent an exhaustive or critical review of all available data. Rather, it presents the most critical studies and lines of evidence pertinent to the conclusion.

This final screening assessment was prepared by staff in the Existing Substances Programs at Health Canada and Environment Canada and incorporates input from other programs within these departments. The ecological portion of this assessment has undergone external written peer review/consultation.

Additionally, the draft of this screening assessment was subject to a 60-day public comment period. While external comments were taken into consideration, the final content and outcome of the screening assessment remain the responsibility of Health Canada and Environment Canada. Approaches used in the screening assessments under the Challenge have been reviewed by an independent Challenge Advisory Panel.

The critical information and considerations upon which the final assessment is based are summarized below.

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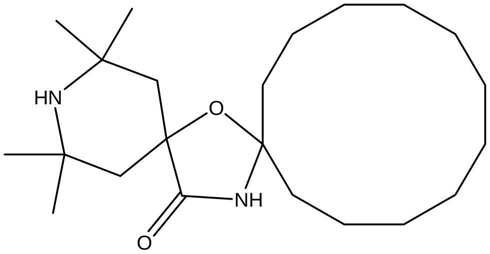
[1] A determination of whether one or more of the criteria of section 64 are met is based upon an assessment of potential risks to the environment and/or to human health associated with exposures in the general environment. For humans, this includes, but is not limited to, exposures from ambient and indoor air, drinking water, foodstuffs, and the use of consumer products. A conclusion under CEPA 1999 on the substances in the Chemicals Management Plan (CMP) Challenge Batches 1-12 is not relevant to, nor does it preclude, an assessment against the hazard criteria specified in the *Controlled Products Regulations*, which is part of regulatory framework for the Workplace Hazardous Materials Information System [WHMIS] for products intended for workplace use.

Substance Identity

Substance Name

For the purposes of this document, 7-Oxa-3,20-diazadispiro[5.1.11.2]heneicosan-21-one, 2,2,4,4-tetramethyl- will be referred to as ODHO, derived from the Domestic Substances List (DSL) inventory name.

Table 1. Substance identity for ODHO

Chemical Abstracts Service Registry Number (CAS RN)	**64338-16-5**
DSL name	**7-Oxa-3,20-diazadispiro[5.1.11.2]heneicosan-21-one, 2,2,4,4-tetramethyl-**
National Chemical Inventories (NCI) names[1]	*7-Oxa-3,20-diazadispiro[5.1.11.2]heneicosan-21-one, 2,2,4,4-tetramethyl-* (AICS, ASIA-PAC, NZIoC, PICCS) *2,2,4,4-tetramethyl-7-oxa-3,20-diazadispiro[5.1.11.2]-henicosan-21-one* (ECL, EINECS, ENCS, PICCS) *DISPIRO[5,1,11,2]-HENEICOSANE-21-ONE, 2,2,4,4-TETRAMETHYL-7-OXA-3,20-DIAZA-* (PICCS)
Other names	*2,2,4,4-Tetramethyl-21-oxo-7-oxa-3,20-diazadispiro [5.1.11.2] heneicosane; Hostavin N 20; Hostavin TMN 20; N 20; Sanduvor 3051PDR*
Chemical group (DSL Stream)	Discrete organics
Major chemical class or use	Heterocyclic organic compounds
Major chemical sub-class	Hindered Amine Light Stabilizers (HALS)
Chemical formula	$C_{22}H_{40}N_2O_2$
Chemical structure	
SMILES[2]	O=C1C2(OC3(N1)CCCCCCCCCCC3)CC(C)(C)NC(C2)(C)C
Molecular mass	364.58 g/mol

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[1] National Chemical Inventories (NCI). 2009: AICS (Australian Inventory of Chemical Substances); ASIA-PAC (Asia-Pacific Substances Lists); ECL (Korean Existing Chemicals List); EINECS (European Inventory of Existing Commercial Chemical Substances); ENCS (Japanese Existing and New Chemical Substances); NZloC (New Zealand Inventory of Chemicals); and PICCS (Philippine Inventory of Chemicals and Chemical Substances).

[2] Simplified Molecular Input Line Entry System.

Physical and Chemical Properties

Table 2 contains experimental and modelled physical and chemical properties of ODHO that are relevant to its environmental fate.

Water solubility values of 0.2 and approximately 3 mg/L have been reported for ODHO at 20°C or room temperature (Study Submission 2006, 2009a). The variability between the empirical values may be attributable to differences in procedural and analytical techniques, as well as to the chemical characteristics of the water used to derive the solubility value (e.g., pH and water hardness).

A predicted pK_a of 9.89 (ACD/pK_aDB 1994–2009) for the amine group suggests that ODHO will exist almost entirely as a charged molecule in the environmentally relevant pH range of 6 to 9, existing primarily as a protonated cation that acts as a weak base. The molecular charge influences both the water solubility and partitioning behaviour of a substance. Charged substances have enhanced water solubility relative to the neutral form, while partitioning to organic phases, such as the organic fraction of particulate matter in sediment and soil and the lipid fraction of biota, is reduced. The reported empirical water solubility values of 0.2 and 3 mg/L are higher than that of 0.02 mg/L predicted for the neutral form of ODHO (WSKOWWIN 2008), which is consistent with what would be expected given the presence of the charged form at environmental pH. In addition, WSKOWWIN (2008) estimates a higher water solubility of 12.08 mg/L for charged ODHO (Table 2).

Both the neutral and charged forms of ODHO are expected to have low water solubility. In addition, the neutral form has high predicted partition coefficients (log K_{ow} and log K_{oc}), while comparable expressions of partitioning behaviour that take into account the presence of the charged form are substantially lower. ACD/pK_aDB (1994–2009) estimates distribution coefficient (log D) values of 2.72 to 4.81 at pH 6 to 9, substantially lower than the log K_{ow} of 6.39 and 5.75 predicted for the neutral form (KOWWIN 2008; ACD/pK_aDB 1994–2009; Table 2).

Table 2. Physical and chemical properties for ODHO

Property	Type	Value[1]	Temperature (°C)	Reference
Melting point (ºC)	Experimental	229–230 (minimum)		Clariant 2007, 2009
		231.5		Bayer and Zäh 2001

Property	Type	Value[1]	Temperature (°C)	Reference
	Modelled	212		MPBPWIN 2008
Boiling point (ºC)	Modelled	498		MPBPWIN 2008
Density (kg/m^3)	Experimental	1060	20	Clariant 2005
Vapour pressure (Pa)	Modelled (neutral form)	4.36 × 10^{-8} (3.27 × 10^{-10} mm Hg)	25	MPBPWIN 2008
Henry's Law constant (Pa·m^3/mol)	Modelled (neutral form)	9.84 × 10^{-6} (9.71 × 10^{-11} atm·m^3/mol; Bond estimate)	25	HENRYWIN 2008
		7.95 × 10^{-5} (7.84 × 10^{-10} atm·m^3/mol; VP/Wsol estimate[2])		
		5.30 × 10^{-6} (5.23 × 10^{-11} atm·m^3/mol; VP/Wsol estimate[3])		
Log K_{ow} (Octanol-water partition coefficient) (dimensionless)	Modelled (neutral form)	6.39	25	KOWWIN 2008
		5.75*		ACD/pK$_a$DB 1994–2009
Log D (Distribution coefficient)[4] (dimensionless)	Modelled (taking into account charged form)	2.72–4.81 (pH 6–9) 3.07* (pH 7)	25	ACD/pK$_a$DB 1994–2009
Log K_{oc} (Organic carbon-water partition coefficient)	Modelled (neutral form)	4.30–4.40	25	KOCWIN 2008

Property	**Type**	**Value**[1]	**Temperature** (°C)	**Reference**
(dimensionless)				
Log K_{oa} (Organic carbon-air partition coefficient) (dimensionless)	Modelled (neutral form) (taking into account charged form)	15.0 11.5	25	KOAWIN 2008
Water solubility (mg/L)	Experimental	0.2* 3* (approximately)	20	Study Submission 2006, 2009a
	Modelled	0.02[5] (neutral form) 12.08[6] (taking into account charged form)	25	WSKOWWIN 2008
pK_a (Acid dissociation constant) (dimensionless)	Modelled	9.89[7]	25	ACD/pK_aDB 1994–2009

[1] Values in parentheses represent the original ones as reported by the authors or as estimated by the models.

[2] Input values used for VP/WSol estimate were 4.36×10^{-8} Pa for vapour pressure (MPBPWIN 2008) and reported water solubility value of 0.2 mg/L (Study Submission 2006).

[3] Input values used for VP/WSol estimate were 4.36×10^{-8} Pa for vapour pressure (MPBPWIN 2008) and reported water solubility value of 3 mg/L (Study Submission 2009a).

[4] Distribution coefficient taking into account the presence of the ionic species; represents the net amount of the neutral and ionic forms expected to partition into the lipid or organic carbon phases at a given pH.

[5] Estimate based on log K_{ow} of 6.39 (neutral form of substance).

[6] Estimate based on log D of 3.07 (taking into account presence of charged form of substance).

[7] Substance is protonated, acting as a weak base at environmental pH 6–9.

*indicates selected value for modelling

Sources

There is no reference in the published literature to the natural occurrence of ODHO.

Surveys conducted under section 71 of CEPA 1999 determined that for the calendar years 2005 and 2006, ODHO was not manufactured in Canada at or above the reporting threshold of 100 kg. However, in both years, imports of the substance into Canada were in the range of 100–1000 kg/year (Environment Canada 2006, 2009a).

ODHO is a low production volume chemical (10–1000 tonnes produced per year) in the European Union (ESIS c1995–2009). ODHO was used in Sweden from 1999 to 2001 and from 2004 to 2007, Denmark from 2000 to 2007, and Norway and Finland from 2005 to 2007 (SPIN 2007). In Finland, 9.1 tonnes of ODHO were used in 2007; use quantities in other countries and years are confidential.

Uses

Information provided in the section 71 surveys indicated that, for the 2005 and 2006 calendar years, business activities associated with the use of ODHO in Canada were in the wholesale trade and distribution of chemicals (except agricultural) and allied products (Environment Canada 2006, 2009a). This Canadian industry comprises establishments primarily engaged in wholesaling industrial and household chemicals, cleaning compounds and preparations, plastics resins, plastic basic forms and shapes, and industrial gases. The 1984–1986 DSL nomination information classified ODHO as a paint/coating additive and photosensitive agent with applications in the plastics industry (Environment Canada 1988).

Clariant (2006a, 2009) identifies ODHO as a low molecular weight hindered amine light stabilizer (HALS) that is used to protect plastic polymers from photochemical degradation. The commercial ODHO product Hostavin N 20 is primarily used in thick-walled plastic products, although it is also suitable for films. Common applications include high-density polyethylene (HDPE), polypropylene (PP), polystyrene and its copolymers, polyamides, ethylene vinyl acetate, polyoxymethylene and acrylonitrile butadiene styrene (Clariant 2006a). Products that may contain Hostavin N 20 include HDPE injection moulding, such as that used in crates and dustbins, extrusion blow moulding, HDPE long-gap stretching tapes, PP containers and vehicle bumpers, and some transparent and colourless plastic articles.

ODHO is also a component of several formulations with applications in coatings and binder systems, including the commercial products Hostavin 3225-2 disp XP, Hostavin 3051 P and Hostavin 3051-2 disp XP (Clariant 2009). These products are used as protective coatings in industrial coatings, automotives, plastics and wood. ODHO is also used in the formulation of tubing for transferring food during manufacturing; however, this application would lead to negligible exposures.

Releases to the Environment

As an additive in plastics and coatings, releases of ODHO to the Canadian environment could occur during processing activities, including the transportation and storage of materials, preparation of masterbatches[2] containing the substance, addition to plastic or coating material, as well as during service life and disposal of finished products. Based

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[2] OECD (2004) defines masterbatches as compounds which are made up to contain high concentrations of specific additives. Masterbatches are dispersed into plastic polymer matrices by simple mixing.

on this, both non-dispersive and dispersive releases of ODHO to the environment are possible. While releases are expected to be primarily to wastewater, there is potential for emission to air with subsequent deposition to surface water or soil. Results from the section 71 notices conducted for the years 2005 and 2006 (Environment Canada 2006, 2009a) indicated that ODHO was not manufactured in Canada during this period and, for this reason, potential releases associated with manufacturing of the substance will not receive further consideration in the assessment.

The available information indicates that when added to plastics or coatings during processing operations, ODHO becomes chemically reacted into the matrix of the material (Environment Canada 2009a), thereby reducing the potential for release into the environment.

A method has been developed by Environment Canada to estimate a substance's losses during different stages of its life cycle, including its fate within a finished product or article (Environment Canada 2008). This method, referred to as Mass Flow, consists of a life cycle analysis and a spreadsheet tool (Mass Flow Tool or MFT) that integrates information on the manufacturing, importation and use data available for the substance. Starting with an identified mass of the substance, each life cycle stage is subsequently evaluated until all of the mass has been accounted for. Relevant factors are considered, uncertainties recognized and assumptions may be made during each stage, depending on information available. The estimated losses represent the complete mass balance over the life cycle of the substance and include releases to wastewater and other receiving compartments (land, air), chemical transformation, transfer to recycling activities and transfer to waste disposal sites (landfill, incineration). However, unless specific information on the rate or potential for release of the substance from landfills and incinerators is available, the method does not quantitatively account for releases to the environment from disposal. Ultimately, the estimated losses provide a first tier in the exposure analysis of a substance and help to estimate environmental releases and focus exposure characterization later in the assessment.

In general, releases of a substance to the environment depend upon various losses from its manufacture, industrial use, and/or consumer/commercial use. These losses can be grouped into seven types: (1) discharge to wastewater; (2) emission to air; (3) loss to land; (4) chemical transformation; (5) disposal to landfill; (6) loss to incineration; and (7) disposal through recycling (i.e., recycling is deemed a loss and not considered further). They are estimated using regulatory survey data, industry data and data published by different organizations. The discharge to wastewater refers to raw wastewater prior to any treatment, whether it be on-site industrial wastewater treatment or off-site municipal sewage treatment. In a similar manner, the loss via chemical transformation refers to changes in a substance's identity that may occur within the manufacture, industrial use, and consumer/commercial use stages, but excludes those during waste management operations such as incineration and wastewater treatment. The loss to land includes unintentional transfer or leakage to soil or paved/unpaved surfaces during the substance's use and service life (e.g., from the use of agricultural machinery or automobiles). The loss to land, however, does not include transfers subsequent to a substance's use and service life (e.g., land application of biosolids and atmospheric deposition).

The losses estimated for ODHO over its life cycle (based on conservative assumptions) are presented in Table 3 (Environment Canada 2009b). The results indicate that most ODHO (92.3%) is expected to be disposed of to landfill, while a further 2.9% will undergo incineration during industrial use or at product end-of-life. It should be noted that most ODHO directed to landfill and/or incineration has been chemically incorporated into end products and is therefore less available for direct release into the environment. The substance is also expected to be released to wastewater at 4.3% of the total quantity used in Canadian commerce (Environment Canada 2009b). This value incorporates consideration of potential losses from consumer use as well as industrial handling during the preparation of masterbatches and the addition of masterbatch or the substance itself into plastic and coating materials during processing operations.

Table 3. Estimated losses of ODHO during its life cycle (Environment Canada 2009b)

Type of loss	Proportion (%)	Pertinent life cycle stages
Wastewater	4.3	Industrial use, and consumer/commercial use
Air emission	0.5	Industrial use
Land	0.0	-
Chemical transformation	0.0	-
Landfill	92.3	Industrial use, and consumer/commercial use
Incineration	2.9	Consumer/commercial use
Recycling	0.0	-

ODHO may also be released to the environment via routes other than wastewater. The MFT predicts that a small proportion (0.5%) of the total quantity of ODHO used in industrial processes will be emitted to air. Air emission can lead to atmospheric exposure if the substance remains in air, or soil and aquatic exposure if the substance is subject to atmospheric deposition. In addition, landfills have the potential to leach substances into groundwater.

Environmental Fate

Based on its physical and chemical properties (Table 2), ODHO is expected to predominantly reside in water or soil, depending upon the compartment of release.

Results from the MFT indicate that the majority of ODHO will be disposed of to landfill after industrial use and consumer/commercial use. However, a small proportion is expected to be released into wastewater (4.3%) and air (0.5%; see Table 3 above).

If released into water, ODHO is expected to remain primarily within this compartment. The dissociation constant (pK_a) of 9.89 (Table 2) indicates that ODHO will occur primarily as the charged (protonated) form when present in aquatic systems, giving the substance higher water solubility than the neutral form and less tendency than the neutral form to partition to suspended solids and sediments. For this reason, while some portion of the substance may adsorb to suspended particulates in the water column with subsequent settling to bed sediment or form complexes with dissolved organic acids, a significant proportion of ODHO is also expected to be found in the dissolved form in the water column. It should be noted that as the pH of the test systems used to derive the reported empirical water solubility values of 0.2 and 3 mg/L is not known, it is possible that these values may underestimate the solubility of ODHO under some environmental conditions, given the charged nature of the substance. This, in turn, would influence the mass fraction of the substance present in the water column.

The low volatility of ODHO suggests that if released to air, the substance will be removed from this compartment to soil or surface water through wet or dry deposition processes. Based on properties estimated for the neutral compound (Table 2), EPI Suite (2008) predicts that nearly all ODHO present in air will occur in the particulate form.

ODHO entering soil through direct release or through settling from air will likely remain in the soil, although a portion may move into surface waters, for example in runoff during a rainfall event. The dominance of the charged form at environmentally relevant pH and low volatility of the neutral form suggests that volatilization from the soil surface is unlikely to occur.

Persistence and Bioaccumulation Potential

Environmental Persistence

The above analysis of environmental fate indicates that this substance will partition mainly into water or soil, depending upon the compartment of release. Some partitioning into sediment may also occur.

No experimental degradation data for ODHO have been identified, although Clariant (2005) describes the commercial product Hostavin N 20 Pwd as “sparingly degradable.” Given the ecological importance of the water compartment, the fact that most of the available models include a water compartment and the fact that ODHO is expected to be released to this compartment, persistence in water was primarily examined using predictive quantitative structure-activity relationship (QSAR) models for biodegradation.

Table 4 summarizes the results of available QSAR models for degradation in various environmental media.

Table 4. Modelled data for degradation of ODHO

Fate process	Model and model basis	Model result and prediction	Extrapolated half-life (days)
AIR			
Atmospheric oxidation	AOPWIN 2008[1]	$t_{1/2} = 0.11$ day	< 2
Ozone reaction	AOPWIN 2008[1]	n/a[2]	n/a
WATER			
Hydrolysis	HYDROWIN 2008[1]	Very slow	> 182
Primary biodegradation			
Biodegradation (aerobic)	BIOWIN 2008[1] Sub-model 4: Expert Survey (qualitative results)	2.9[3] “may biodegrade quickly”	< 182
Ultimate biodegradation			
Biodegradation (aerobic)	BIOWIN 2008[1] Sub-model 3: Expert Survey (qualitative results)	1.5[3] “biodegrades slowly”	> 182
Biodegradation (aerobic)	BIOWIN 2008[1] Sub-model 5: MITI linear probability	0.3[4] “biodegrades slowly”	> 182
Biodegradation (aerobic)	BIOWIN 2008[1] Sub-model 6: MITI non-linear probability	0.06[4] “biodegrades very slowly”	> 182
Biodegradation (aerobic)	TOPKAT 2004 Probability	0.0[4] “biodegrades very slowly	> 182
Biodegradation (aerobic)	CATABOL c2004–2008 % BOD (biological oxygen demand)	% BOD = 1.1 “biodegrades very slowly”	> 182

[1] EPI Suite (2008).
[2] Model does not provide an estimate for this type of structure.
[3] Output is a numerical score from 0 to 5.
[4] Output is a probability score.

In air, a predicted atmospheric oxidation half-life value of 0.11 day (see Table 4) demonstrates that this substance is likely to be rapidly oxidized. There is no estimate for the reaction half-life of this substance with other photo-oxidative species in the atmosphere, such as ozone. However, it is expected that reactions with hydroxyl radicals will be the most important degradation process in the atmosphere for gas-phase ODHO. With a half-life of 0.11 day via reactions with hydroxyl radicals in the gas phase, ODHO is considered not persistent in air.

The presence of an amide group in the ODHO molecule indicates that the substance may undergo hydrolysis. However, the rate is likely to be extremely slow (half-life measured in centuries) at pH 7 and 25°C (HYDROWIN 2008), and therefore hydrolysis is expected to be a relatively unimportant fate process for this substance.

The biodegradation models predict that ODHO will undergo primary biodegradation in much less than 182 days, but the identities of the degradation products are not known. However, ultimate biodegradation models indicate that complete mineralization will occur only slowly and the substance and/or its degradation products may therefore persist in the environment. There is consistency in results of ultimate biodegradation modelling indicating that the half-life for ultimate biodegradation of ODHO in water is > 182 days. In addition, the ODHO molecule contains structural features commonly associated with persistency, including a high degree of branching and the presence of multiple rings, which further supports the ultimate degradation modelling results.

Using an extrapolation ratio of 1:1:4 for a water: soil: sediment biodegradation half-life (Boethling et al. 1995), the ultimate degradation half-life in soil is also > 182 days and the half-life in sediments is > 365 days. This indicates that ODHO is expected to be persistent in soil and sediment.

Based on the modelled data presented in Table 4 above, ODHO meets the persistence criteria in water, soil and sediment (half-lives in soil and water ≥ 182 days and half-life in sediment ≥ 365 days), but does not meet the criteria for air (half-life in air ≥ 2 days) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential for Bioaccumulation

Modelled log K_{ow} values of 6.39 (KOWWIN 2008) and 5.75 (ACD/pK_aDB 1994–2009) for the neutral form of ODHO (Table 2) suggest that this chemical has the potential to bioaccumulate. However, the predicted acid dissociation constant (pK_a) of 9.89 indicates that ODHO will occur primarily as the charged form in the environment and the bioaccumulation potential of this form, as described by the log D value (2.72–4.81 in the pH range 6–9), is likely to be much less than for the neutral form.

Only one bioaccumulation factor (BAF) and/or bioconcentration factor (BCF) study was available for ODHO, as listed in Table 5a.

Table 5a. Empirical data for bioaccumulation of ODHO

Test organism	Endpoint	Value wet weight (L/kg)	Reference
Carp, *Cyprinus carpio*	BCF	3.2–4.2	Study Submission 2009b

Study Submission (2009b) reported a BCF range of 3.2 to 4.2 in carp, *Cyprinus carpio*, exposed for 8 weeks to a concentration of 0.05 mg/L ODHO. The study followed methods described in Organisation for Economic Co-operation and Development (OECD) Test Guideline 305C (OECD 1981) and used hydrogenated castor oil (HCO-40) as a dispersant for the test substance.

Since only one experimental BAF and/or BCF study was available for ODHO, a predictive approach was also applied using available BAF and BCF models as shown in Table 5b below. According to the *Persistence and Bioaccumulation Regulations* (Canada 2000), a substance is bioaccumulative if its BCF or BAF is ≥ 5000. Measures of BAF are generally the preferred metric for assessing bioaccumulation potential as the BCF may not adequately account for dietary uptake, which predominates for substances with a log

K_{ow} of greater than around 4.0 (Arnot and Gobas 2003). ODHO is predicted to be almost completely ionized at environmental pH 6–9 and the log D value of 3.07 (pH 7; ACD/pK_aDB 1994–2009), which takes into account the presence of the charged form, was therefore used to derive estimates of bioaccumulation potential. As this value is less than 4.0, direct uptake from the surrounding aqueous medium, such as that occurring across gill surfaces, is expected to predominate over dietary uptake and for this reason, dietary uptake with subsequent metabolic transformation potential are not considered in the following analysis of bioaccumulation potential.

Table 5b: Modelled data for bioaccumulation for ODHO

Test organism	Endpoint	Value wet weight (L/kg)	Reference
Fish	BCF BAF	81 85	BCFBAF 2008
Fish	BCF	12.8–1580 (pH 6–9) 28.8 (pH 7)	ACD/pK_aDB 1994–2009

With a predicted BAF of 85 (Arnot and Gobas 2003) and predicted BCF values of 81 (Arnot and Gobas 2003) and 12.8–1580 (ACD/pK_aDB 1994–2009), as well as empirical BCF values of 3.2–4.2, it is considered that ODHO in the environment has relatively low bioaccumulation potential and does not meet the bioaccumulation criteria (BAF or BCF ≥ 5000) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential to Cause Ecological Harm

Only limited empirical toxicity data are available for ODHO and, for this reason, estimates derived from modelling are included in the analysis of potential for adverse effects.

Ecological Effects Assessment

A – In the Aquatic Compartment

Empirical aquatic toxicity data for ODHO are summarized in Table 6a below. Endpoint values include median lethal (LC_{50}) concentrations ranging from > 3.62 to 62.2 mg/L for fish (Study Submission 2009a,b,c) and a no-effect (EC_0) range of 100 to 1000 mg/L for bacterial toxicity (Clariant 2005). In addition, a 48-hour median effect (EC_{50}) concentration of >100 mg/L has been determined for the water flea, *Daphnia magna* (Study Submission 2006). All empirical data provide endpoint values at or above the reported water solubility limit of 0.2 to 3 mg/L (see Table 2), suggesting the studies may have been conducted at saturation of the test substance or under conditions of fluctuating pH and therefore variable water solubility.

Table 6a. Empirical data for aquatic toxicity

Test organism	Type of test	Endpoint	Value (mg/L)	Reference
Fish Orange-red Killifish, *Oryzias latipes*	Acute (48 hours)	LC_{50}[1]	8.35	Study Submission 2009a,b,c
Zebrafish, *Brachydanio rerio*	(96 hours)		> 3.62 62.2	
Water Flea, *Daphnia magna*	Acute (48 hours)	EC_{50}[2]	> 100	Study Submission 2006
Bacteria	Duration of exposure not specified	EC_0[3]	100–1000	Clariant 2005

[1] LC_{50} – The concentration of a substance that is estimated to be lethal to 50% of the test organisms.

[2] EC_{50} – The concentration of a substance that is estimated to cause some effect on 50% of the test organisms.

[3] EC_0 – The highest concentration of a substance at which no effects are observed in the test organisms.

Based on the results obtained for the species tested, ODHO has only a moderate to low potential to cause acute adverse effects to aquatic organisms. However, there are no laboratory studies of possible effects following long-term exposure to ODHO, such as impacts to growth and/or reproduction, and this issue is of importance given the evidence for stability of this substance in the environment. For this reason, ecotoxicity models were also considered in the evaluation of potential for aquatic toxicity.

Table 6b provides predicted ecotoxicity values that were considered reliable and used in the QSAR weight-of-evidence approach for assessing aquatic toxicity (Environment Canada 2007). Only estimates which take into account the presence of the charged form in the environment (i.e., those derived using the log D value of 3.07) are presented in the table.

Table 6b. Modelled data for aquatic toxicity

Test organism	Type of test	Endpoint	Value (mg/L)	Reference
Fish	Acute (96 hours)	LC_{50}[1]	6.7[4], 14.5[5]	ECOSAR 2008
			0.2	OASIS Forecast 2005
Daphnia	Acute (48 hours)	LC_{50}	1.8[5], 5.5[4]	ECOSAR 2008
Algae	Acute (96 hours)	EC_{50}[2]	0.4[4], 1.1[5]	ECOSAR 2008
	Chronic	MATC[3]	0.3[5]	ECOSAR 2008

[1] LC_{50} – The concentration of a substance that is estimated to be lethal to 50% of the test organisms.

[2] EC_{50} – The concentration of a substance that is estimated to cause some effect on 50% of the test organisms.

[3] MATC – The maximum allowable toxicant concentration, generally presented as the range between the NOEC (no-observed-effect concentration) and LOEC (lowest-observed-effect concentration) or as the geometric mean of the two measures. The NOEC and LOEC are, respectively, the highest concentration in a toxicity test not causing a statistically significant effect compared to the controls, and the lowest concentration causing a statistically significant effect compared to the controls.

[4] Prediction based on Amide chemical class.

[5] Prediction based on Aliphatic Amine chemical class.

The modelling results suggest that ODHO will generally have moderate toxicity to aquatic organisms, with acute effects at concentrations of 0.2 mg/L to 14.5 mg/L. In addition, ECOSAR (2008) predicts a chronic toxicity value of 0.3 mg/L for algae and, in the absence of empirical chronic data, this will be considered to indicate that ODHO may have the potential to cause adverse effects to aquatic plants following long-term exposure to low concentrations in water.

It should be noted that some predicted effect concentrations presented in Table 6b are above the reported water solubility limits of 0.2 or 3 mg/L and, in these cases, ECOSAR (2008) warns that the substance may not be sufficiently soluble to measure the predicted effect. Given the lack of information regarding derivation of the empirical solubility data, it is also possible that they may underestimate the solubility of ODHO under some environmental conditions, particularly as WSKOWWIN (2008) predicts a higher solubility of 12.08 mg/L when the presence of the charged form is taken into account.

Overall, based on the available information, it is considered that ODHO may have the potential to cause adverse effects in sensitive aquatic organisms exposed for long periods of time to relatively low concentrations.

B – In Other Environmental Compartments

No ecological effects studies were found for this compound in media other than water.

ODHO has exhibited low oral toxicity in laboratory studies conducted using terrestrial mammalian species, with an acute oral median lethal dose (LD_{50}) of 2800 mg/kg-bw reported for the rat (Clariant 2005).

Ecological Exposure Assessment

No data concerning concentrations of this substance in water in Canada have been identified. Therefore, environmental concentrations are estimated from available information, including estimated substance quantities, release rates, and size of receiving water bodies.

A – Industrial Release

Aquatic exposure to ODHO would be expected if the substance is released from industrial use to a wastewater treatment plant (WWTP) and the treatment plant discharges its effluent to a receiving water body. The concentration of the substance in the receiving water near the discharge point of the wastewater treatment plant is used as the predicted environmental concentration (PEC) in evaluating the aquatic risk of the substance. It can be calculated using the equation:

$$C_{water-ind} = \frac{1000 \times Q \times L \times (1-R)}{N \times F \times D}$$

where

$C_{water\text{-}ind}$:	aquatic concentration resulting from industrial releases, mg/L
Q:	total substance quantity used annually at an industrial site, kg/yr
L:	loss to wastewater, fraction
R:	wastewater treatment plant removal rate, fraction
N:	number of annual release days, d/yr
F:	wastewater treatment plant effluent flow, m^3/d
D:	receiving water dilution factor, dimensionless

As ODHO is used industrially and is expected to be released to water, a worst-case industrial release scenario was used to estimate the aquatic concentration of the substance with the help of Environment Canada's (2009c) Industrial Generic Exposure Tool – Aquatic (IGETA). The scenario was made conservative by estimating the largest total quantity of the substance that may be used by a single Canadian industrial facility and assuming loss to wastewater from this site of 1.15% based on reasonable worst-case release factors described in OECD (2004). The scenario also assumed that the release occurs 250 days per year, typical for small and medium-sized facilities, and is sent to a local WWTP with a zero-removal rate for the substance. Upon combining with the WWTP effluent, the receiving water in a small watercourse normally has an actual or equivalent flow of 34 560 m^3 per day. Based on the above assumptions, the substance at a total quantity of 1000 kg/yr for industrial use (equal to the upper value of the reported 100–1000 kg import range; see Sources section) yields a predicted environmental concentration (PEC) of 0.0012 mg/L (Environment Canada 2009d).

B – Consumer Release

While no consumer products containing ODHO were identified in Canada, conservative assumptions were applied to estimate down-the drain release of ODHO from potential consumer uses. Mega Flush, Environment Canada's spreadsheet model was employed to derive these estimates for the potential substance concentration in multiple water bodies receiving STP effluents to which consumer products containing the substance may have been released (Environment Canada 2009e).

By default, the model assumes primary and secondary WWTP removal rates to be 0%, consumer use of the substance to be more than 365 days/year, and the flow rate at all discharge sites to be at the low end (tenth percentile) of the typical range. These estimates are made for approximately 1000 release sites across Canada, which account for most of the major WWTPs in the country. The equation and inputs used to calculate the maximum PEC of ODHO in receiving water bodies are described in Environment Canada (2009f). A scenario was run assuming a total consumer use quantity of 1000 kg/year based on information provided in the section 71 notices for the calendar years 2005 and 2006 (see Sources section above), and 0.2% losses from consumer use based on information available in OECD (2004). Using this scenario, Mega Flush estimates a maximum PEC in receiving water bodies of 2.4×10^{-6} mg/L.

Characterization of Ecological Risk

The approach taken in this ecological screening assessment was to examine various supporting information, and develop conclusions based on a weight-of-evidence approach and using precaution as required under CEPA 1999. Lines of evidence considered include results from a conservative risk quotient calculation, as well as information on persistence, bioaccumulation, toxicity, sources, and fate of the substance.

ODHO is expected to be persistent in water, soil and sediment. The substance is not expected to persist in air. The charged form of the substance is predicted to predominate in the environmental pH range of 6 to 9 and, as a consequence, ODHO is expected to have low bioaccumulation potential. While only limited toxicity data are available, it is considered that ODHO may have the potential to cause toxicity to sensitive aquatic species exposed for long periods of time to relatively low concentrations. Based on its use as an additive in plastics and coatings, industrial releases of ODHO into the Canadian environment are expected to occur mainly during processing operations and to be primarily to wastewater, although emission to air could also occur with subsequent removal to surface water or soil. However, the available information indicates that when added to plastics or coatings during processing operations, most ODHO will be chemically incorporated into the matrix of the product, thereby substantially reducing the potential for release into the environment from finished products.

A risk quotient analysis, integrating conservative estimates of exposure with toxicity information, was performed for the aquatic medium to determine whether there is potential for ecological harm in Canada. The exposure estimation modelling described in the previous section (Ecological Exposure Assessment) determined that highest potential releases of ODHO into the aquatic environment will likely result from industrial processing activities. For this reason, the conservative PEC of 0.0012 mg/L calculated using the IGETA exposure tool (Environment Canada 2009d) was used in the quantitative analysis of risk. A conservative predicted no-effect concentration (PNEC) was derived from the chronic toxicity value of 0.3 mg/L, predicted taking into account exposure of algae to the charged form of ODHO at ambient pH (ECOSAR 2008). This toxicity value was then divided by an assessment factor of 100 (10 to account for interspecies and intraspecies variability in sensitivity, and 10 to estimate a long-term no-effects concentration in the field from a laboratory-based estimated chronic-effect concentration) to give a PNEC value of 0.003 mg/L. The resulting conservative risk quotient (PEC/PNEC) is 0.4. Based on this, it is concluded that current estimated exposure concentrations of ODHO in Canada are unlikely to exceed those predicted to elicit adverse effects in aquatic organisms.

Considered together, the available information suggests that ODHO has low potential to cause ecological harm at the current and foreseeable level of use in Canada.

Uncertainties in Evaluation of Ecological Risk

There is uncertainty regarding the physical and chemical properties of ODHO, and this influences the estimation of environmental behaviour, fate, and potential toxicity. Gaps in the experimental database were filled through the use of QSARs. However, the extent to which the modelled data reflect the actual properties of ODHO is unclear, given indications that the substance is charged at environmental pH. In the absence of adequate measured data, estimations based on modelled data and professional judgement have been used to provide a conservative assessment of potential risk to the environment.

In addition, there is uncertainty associated with the empirical water solubility values for ODHO, given the absence of information detailing their derivation. However, it is considered that this uncertainty did not significantly impact the outcome of the assessment.

Regarding ecotoxicity, the lack of empirical data on chronic effects introduces uncertainty into the analysis of potential for risk. As well, the predicted partitioning behaviour of this chemical suggests that it may have some presence in soil and sediment, and this is not well addressed by the available effects data. Indeed, the only effects data identified apply primarily to pelagic aquatic exposures, although the water column may not be the only medium of concern. In addition, while there is some limited empirical evidence of low toxicity in rodents, the extent to which this applies to other mammalian and non-mammalian terrestrial species is unknown.

Potential to Cause Harm to Human Health

Exposure Assessment

Environmental Media and Food

Empirical data on concentrations of ODHO in environmental media in Canada or elsewhere were not identified. ChemCAN, a Canada-specific environmental exposure model, was used to estimate concentrations of ODHO in various environmental media (ChemCAN 2003). This model is a level III fugacity model that is used to estimate average concentrations in various media to estimate general population exposures from the environment. ChemCAN differs from the point source models used in the ecological assessment section of the document.

Based on the information submitted in response to a notice published under section 71 of CEPA 1999, the total quantity in commerce was reported to range from 100 kg to 1 000 kg in 2006 (Environment Canada 2009a). The loss percentages predicted by the Mass Flow tool (see Table 3) were applied to the upper value of the range (1 000 kg) of ODHO in Canadian commerce in 2006. The annual release quantities are estimated to be 43 kg to water from loss to wastewater, 5 kg to air from loss to air emissions and 923 kg to soil from loss to landfill. These release quantities to the environmental media are considered to be overestimates (as explained in the Releases to the Environment section), especially related to landfilling since only a small fraction of the substance would likely escape from landfills (e.g. in leachate).

Conservative upper-bounding daily intakes of ODHO for the general population in Canada were derived based on the estimated environmental concentrations. The upper-bounding total daily intake estimate of ODHO from environmental media was on the order of magnitude of nanograms (10^{-6} mg)/kg-bw per day.

Uncertainty in this exposure estimation is high because no empirical data on environmental concentrations of ODHO were used to estimate exposure. In addition, there is uncertainty due to assumptions used in the model.

No studies were identified reporting the presence of ODHO in food. The copolymer synthesized from ODHO and epichlorohydrin, identified by the CAS RN 202483-55-4, is approved for use as an antioxidant and/or stabilizer additive for polyolefins intended for contact with food (US FDA 2009). This CAS RN corresponds to Hostavin N 30, a copolymer manufactured by Clariant (Clariant 2006b).

In Canada, it was reported that a copolymer comprised of ODHO as one of the monomers is used in the formulation of tubing for transferring food during manufacturing. This application leads to negligible exposures (2009 email from Food Directorate, Health Canada, to Risk Management Bureau, Health Canada; unreferenced).

Consumer Products

Based on available information, no consumer products in Canada were identified that contain ODHO.

Health Effects Assessment

Very limited toxicological data are available for ODHO. Information from the submission of Clariant Corporation to the United States Environmental Protection Agency (US EPA) (US EPA 2005) indicates that ODHO has an oral LD_{50} of 2800 mg/kg-bw (rat) and an inhalation LC_{50} of 1.6 mg/L (species not specified). ODHO also induced severe and possibly irreversible irritation to the eyes of rabbits, but it was found to be a non-irritant when tested on rabbit skin (US EPA 2005). In addition, a publication of the European Commission (2005) indicated the availability of three *in vitro* mutagenicity studies for Hostavin N 20 (trade name for ODHO, Bayer and Zäh 2001), however, no results or study details were provided, and additional information could not be obtained by contacting the European Food Safety Authority (2010, email from Food Contact Materials, Enzymes, Flavourings and Processing Aids Unit, European Food Safety Authority, to Risk Assessment Bureau, Health Canada; unreferenced). The

(Q)SAR programs DEREK (2008), TOPKAT (2004), CASETOX (2008), Toxtree (2009) and Leadscope Model Applier (2009) did not generate predictions in most cases.

Potential analogues for ODHO were identified based on chemical similarity; however, none of the identified substances provided additional health effects information and so are not further discussed here.

In the absence of data on analogues, the safety evaluation of Hostavin N 30 (a formulation containing ODHO) by the National Industrial Chemicals Notification and Assessment Scheme (NICNAS 1995) was also considered in this assessment. Hostavin N 30 is a copolymer of ODHO and epichlorohydrin, and may contain up to 0.2% unreacted monomer. Since exposure of ODHO to the general population would likely be through residual ODHO in a formulation such as Hostavin N 30, toxicity data for Hostavin N 30 is considered to contribute to the overall safety profile of ODHO. In the NICNAS evaluation, Hostavin N 30 was reported to have low oral toxicity in the rat (LD50 > 2000 mg/kg-bw) and no skin irritation, and slight eye irritation in the rabbit. Hostavin N 30 was also not mutagenic in both *Salmonella typhimurium* and *Escherichia coli*, either with or without metabolic activation. NICNAS (1995) concluded that neither the polymeric Hostavin N 30 nor the low molecular weight species are expected to contribute to acute oral toxicity, skin or eye irritancy or mutagenicity, and the residual monomer would not be expected to pose a health hazard to the public. The existence of additional toxicity data on Hostavin N 30, including a subchronic oral study, were indicated in a European Commission publication (European Commission 2005), however, no details were provided and the data could not be obtained (2010, email from Food Contact Materials, Enzymes, Flavourings and Processing Aids Unit, European Food Safety Authority, to Risk Assessment Bureau, Health Canada; unreferenced).

As there was very limited health effects information available for ODHO and no health effects information on suitable analogues was identified, the confidence in the toxicity database is considered to be very low.

Characterization of Risk to Human Health

The very limited empirical hazard data identified for ODHO indicate a low potential for acute hazard by the oral and inhalation routes. Although severe eye irritation was observed for ODHO in rabbits, direct occular exposure of ODHO to the general population is unlikely. Although mutagenicity studies for ODHO have been cited, the results for these studies could not be obtained. Computer (Q)SAR models did not generate predictions for ODHO except in few instances. While no suitable analogue substances could be identified, limited data for a polymer formulation containing ODHO as a residual indicated a low hazard potential. Based on the limited information available, ODHO was not identified as posing a high hazard to human health although the confidence in hazard characterization is considered to be very low.

The maximum potential for exposure to the general population to ODHO from environmental media is estimated to be on the order of magnitude of nanograms (10^{-6} mg/kg-bw per day). General population exposure to ODHO from use of consumer products is not expected. Although the limited human health effects data preclude the selection of a critical health effect level for the purposes of risk characterization, based on the limited information available, ODHO was not identified as posing a high hazard to human health. As exposure of the general population in Canada is expected to be negligible, potential risk to human health is also considered to be low.

Uncertainties in Evaluation of Risk to Human Health

Confidence in the toxicity database is considered to be very low, due to the limited information available. Literature data were not identified for ODHO concentrations in environmental media. Nonetheless, confidence is high that exposure to ODHO from environmental sources is negligible. Upper-bound release estimates were rendered by the conservative use of loss percentages predicted by the MFT applied to the total quantity of ODHO in Canadian commerce in 2006. Hence it is likely that the resulting exposure estimates are very conservative. Although ODHO was not identified in consumer products in Canada, this was based on limited information, and is an area of uncertainty.

Conclusion

Based on the information presented in this screening assessment, and in particular the low to negligible exposure potential for human and non-human organisms in Canada, it is concluded that ODHO is not entering 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 or that constitute or may constitute a danger to the environment on which life depends. Additionally, ODHO meets the criteria for persistence but does not meet criteria for bioaccumulation potential as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Based on the information presented in this screening assessment, it is concluded that ODHO is not entering the environment in a quantity or concentration or under conditions that constitute or may constitute a danger in Canada to human life or health.

It is therefore concluded that ODHO does not meet any of the criteria set out in section 64 of CEPA 1999.

This substance will be considered for inclusion in the Domestic Substances List inventory update initiative. In addition and where relevant, research and monitoring will support verification of assumptions used during the screening assessment.

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Appendix I – Robust Study Summary

Robust Study Summary: Aquatic B				
No.	**Item**	**Weight**	**Yes/No**	**Specify**
1	Reference: 13365Submission023, Bioconcentration study of N20 in carp (Study Submission 2009b)			
2	Substance identity: CAS RN	n/a	N	64338-16-5
3	Substance identity: chemical name(s)	n/a	Y	Chemical formula and structure, as well as trade name, provided but in Japanese
4	Chemical composition of the substance	2	Y	
5	Chemical purity	1	Y	100%
6	Persistence/stability of test substance in aquatic solution reported?	1	Y	
7	If test material is radio-labelled, were precise position(s) of the labelled atom(s) and the percentage of radioactivity associated with impurities reported?	2		n/a
Method				
8	Reference	1	Y	OECD TG 305C
9	OECD, EU, national, or other standard method?	3	Y	
10	Justification of the method/protocol if a non-standard method was used	2		n/a
11	GLP (good laboratory practice)	3	Y	
Test organism				
12	Organism identity: name	n/a	Y	Carp *(Cyprinus carpio)*
13	Latin or both Latin and common names reported?	1	Y	
14	Life cycle age / stage of test organism	1		See comments below
15	Length and/or weight	1		See comments below
16	Sex	1		n/a
17	Number of organisms per replicate	1		See comments below
18	Organism loading rate	1		See comments below
19	Food type and feeding periods during the acclimation period	1		See comments below
Test design / conditions				
20	Experiment type (laboratory or field)	n/a	Y	Laboratory
21	Exposure pathways (food, water, both)	n/a		See comments below
22	Exposure duration	n/a	Y	8 weeks
23	Number of replicates (including controls)	1		See comments below
24	Concentrations	1	Y	0.005 and 0.05 mg/L
25	Food type/composition and feeding periods during the test	1		See comments below

26	If BCF/BAF was derived as a ratio of chemical concentration in the organism and in water, was experiment duration equal to or longer than the time required for the chemical concentrations to reach steady state?	3	Y	Report shows graphic to establish steady state
27	If BCF/BAF was derived as a ratio of chemical concentration in the organism and in water, were measured concentrations in both water and organism reported?	3	Y	
28	Were concentrations in the test water measured periodically?	1	Y	
29	Were the exposure media conditions relevant to the particular chemical reported? (e.g., for the metal toxicity – pH, DOC/TOC, water hardness, temperature.)	3		See comments below
30	Photoperiod and light intensity	1		See comments below
31	Stock and test solution preparation	1		See comments below
32	Analytical monitoring intervals	1		See comments below
33	Statistical methods used	1		See comments below
34	Was solubilizer/emulsifier used if the chemical was unstable or poorly soluble?	n/a	Y	HCO-40
Information relevant to the data quality				
35	Was the test organism relevant to the Canadian environment?	3	Y	
36	Were the test conditions (pH, temperature, DO, etc.) typical for the test organism?	1	Y	
37	Do system type and design (static, semi-static, flow-through; sealed or open; etc.) correspond to the substance's properties and organism's nature/habits?	2	Y	
38	Was pH of the test water within the range typical for the Canadian environment (6–9)?	1	Y	
39	Was temperature of the test water within the range typical for the Canadian environment (5–27°C)?	1	Y	
40	Was lipid content (or lipid-normalized BAF/BCF) reported?	2	Y	See comments below
41	Were measured concentrations of a chemical in the test water below the chemical's water solubility?	3	Y	
42	If radio-labelled test substance was used, was BCF determination based on the parent compound (i.e., not on total radio-labelled residues)?	3		
Results				
43	Endpoints (BAF, BCF) and values	n/a	n/a	BCF 3.2–4.2 after 8 weeks at 0.05 mg/L, < 23 at 0.005 mg/L
44	Was BAF/BCF determined as: 1) the ratio of chemical concentration in the organism and in water, or 2) the ratio of the chemical uptake and elimination rate constants?	n/a	Y	1)

45	Was BAF/BCF derived from a 1) tissue sample or 2) whole organism?	n/a	n/a	See comments below
46	Was 1) average or 2) maximum BAF/BCF used?	n/a	n/a	See comments below
47	***Score: ... %***	***100.0***		
48	***Environment Canada reliability code:***	***1***		
49	***Reliability category (high, satisfactory, low):***	***High confidence***		
50	***Comments***	***Study was conducted by MITI(Japanese Institute of Technology and Evaluation) and is considered to be reliable in terms of procedures used. However, the majority of the report is written in Japanese, with only a 3-page English summary of results provided, and for this reason it is not possible to answer some of the points on the RSS form. Given that this agency developed this bioconcentration method, which is widely accepted and used by agencies such as the OECD, the inability to determine details relating to standard procedures used in the method has not been applied as a negative result in evaluating the acceptability of the endpoint data.***		

Appendix II – Model Inputs Summary Table for Environmental Modelling

	Phys-Chem/Fate	**Fate**	**Fate**	**Persistence, Bioaccumulation and Toxicity (PBT) Profiling**	**Ecotoxicity**
Model input parameters	EPIWIN Suite (all models, including: AOPWIN, KOCWIN, BCFWIN BIOWIN and ECOSAR)	EQC (required inputs are different if Type I vs. Type II chemical)	Arnot-Gobas BCF/BAF Model	Canadian-POPs (including: Catabol, BCF Mitigating Factors Model, OASIS Toxicity Model)	Artificial Intelligence Expert System (AIES)/ TOPKAT/ ASTER
SMILES code	O=C1C2(OC3(N1)CCCCCCCCCCC3)CC(C)(C)NC(C2)(C)C			O=C1C2(OC3(N1)CCCCCCCCCCC3)CC(C)(C)NC(C2)(C)C	O=C1C2(OC3(N1)CCCCCCCCCCC3)CC(C)(C)NC(C2)(C)C
Molecular weight (g/mol)		364.58			
Data temperature (°C)		25			
Log K_{aw} (Air-water partition coefficient) (dimensionless)		-8.40 ($K_{aw} = 3.97 \times 10^{-9}$)			
Log K_{ow} (Octanol-water partition coefficient) (dimensionless)	5.75		5.75		
Log D (Octanol-water partition coefficient including both neutral and ionized forms of substance) (dimensionless)	3.07		3.07		
Log K_{oc} (Organic carbon-water partition coefficient – L/kg)		1.82 ($K_{oc} = 66.5$)			
Water solubility (mg/L)	0.2, 3				
Soil-water		1.33			

partition coefficient (L/kg)[1]					
Sediment-water partition coefficient (L/kg)[1]		2.66			
Suspended particles-water partition coefficient (L/kg)[1]		13.3			
Fish-water partition coefficient (L/kg)[2]		28.8			
Aerosol-water partition coefficient (dimensionless)[3]		100			
Half-life in air (days) [4]		0.05			
Half-life in water (days)		180			
Half-life in sediment (days)		720			
Half-life in soil (days)		180			
Metabolic rate constant (1/days)			0.12		

[1] Derived from K_{oc} value of 66.5 at pH 7 (ACD/pK_aDB 1994–2009).

[2] Derived from BCF at pH 7 (ACD/pK_aDB 1994–2009).

[3] Default value.

[4] Based on 12-hour day (i.e., 1.298 hours).