Screening Assessment for the Challenge

Zinc, bis[*O*,*O*-bis(1,3-dimethylbutyl) phosphorodithioato-*S*,*S*']-, (*T*-4)-

Chemical Abstracts Service Registry Number
2215-35-2

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 Zinc, bis[*O,O*-bis(1,3-dimethylbutyl) phosphorodithioato-*S,S'*]-, (*T*-4)- (zinc BDBP), Chemical Abstracts Service Registry Number 2215-35-2. This substance was identified as a high priority for screening assessment and included in the Challenge because it had been 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 zinc BDBP 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 on information relevant to the evaluation of ecological risks.

Zinc BDBP is an organometallic dialkyldithiophosphate substance that is used in Canada and elsewhere as an anti-wear oil additive. It also acts as an antioxidant. The substance is not naturally produced in the environment. Between 10 000 and 100 000 kg of zinc BDBP were imported into Canada in 2005 and between 100 000 and 1 000 000 kg were imported in 2006 for use in the petroleum industry. The quantity of zinc BDBP imported into Canada indicates that it could be potentially released to the Canadian environment.

Based on reported use patterns and certain assumptions, most of the substance is transformed during use. Small proportions are estimated to be released to wastewater (1.9%) and to paved/unpaved land surfaces (0.9%). Zinc BDBP is somewhat soluble in water, is not volatile and has a tendency to partition to particles and lipids (fat) of organisms because of its hydrophobic nature. For these reasons, zinc BDBP will be likely found mostly in sediments and soil, and to a minor extent, in water. It is not expected to be significantly present in air. It is also not expected to be subject to long-range atmospheric transport.

Based on its physical and chemical properties, zinc BDBP is expected to be persistent in water, soil and sediments. New bioaccumulation predictions suggest that this substance has a low potential to accumulate in the lipid tissues of organisms. The substance therefore meets the persistence criteria but does not meet the bioaccumulation criteria as set out in the *Persistence and Bioaccumulation Regulations*.

For this screening assessment, a moderately conservative industrial exposure scenario was selected in which an operation discharges zinc BDBP into the aquatic environment. The predicted environmental concentration in water (PEC) was below the predicted aquatic no-effect concentration (PNEC) calculated from a Species Sensitivity

Distribution (SSD) using data from other substances within the dialkyldithiophosphate category. Additionally, results from a consumer release scenario, that estimates exposure (PECs) resulting from the down-the-drain release using conservative assumptions, indicate that the PNEC is unlikely to be exceeded. Consequently, exposure levels are not likely to exceed the aquatic PNEC in the conservative scenarios considered, whether based on consumer or industrial releases; that is, conservative risk quotients are almost always below 1.

Based on the information available, it is concluded that zinc BDBP 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.

The potential for exposure of the general population to zinc BDBP from environmental media is expected to be negligible. However, there is potential for dermal exposure from its use as a motor oil additive, which is typically used in an occupational setting, but may also be used directly by consumers.

The toxicological dataset for zinc BDBP is limited. However, health effects associated with zinc BDBP dermal exposure in experimental animals include dermal irritation, body weight loss, elevated white blood cell count and at higher exposure levels, effects on testes.

The margins between upper-bounding estimates of exposure from environmental media and consumer products (additive in motor oil) and levels associated with effects in experimental animals are considered to be adequately protective. It is thus concluded that zinc BDBP 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.

Based on the information available, it is concluded that zinc BDBP 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 to 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 2006a), 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 Zinc, bis[*O,O*-bis(1,3-dimethylbutyl) phosphorodithioato-*S,S'*]-, (*T*-4)- had been identified as a high priority for assessment of ecological risk because it had been found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and was believed to be in commerce in Canada.

The Challenge for this substance was published in the *Canada Gazette* on January 31, 2009 (Canada 2009a). 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, a submission of information pertaining to the bioaccumulation potential of the substance was received.

Although Zinc, bis[*O,O*-bis(1,3-dimethylbutyl) phosphorodithioato-*S,S'*]-, (*T*-4)- 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 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 2009 for the physical and chemical properties, and exposure and ecological effects sections of the document. 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 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 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 portions of the assessment have 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 risk 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 assessment is based are summarized below.

[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.

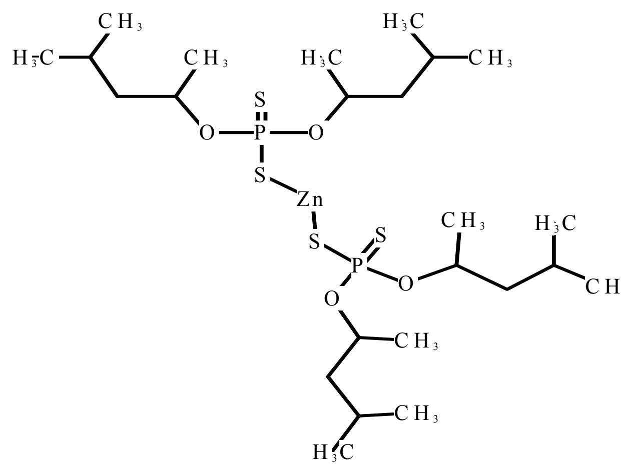
Substance Identity

Substance name

For the purposes of this document, this substance will be referred to as zinc BDBP, derived from the DSL inventory name: **Z**inc, **b**is[*O*,*O*-bis(1,3-**d**imethyl**b**utyl) **p**hosphorodithioato-*S*,*S'*], (*T*-4)-.

Table 1. Substance identity for zinc BDBP

Chemical Abstracts Service Registry Number (CAS RN)	**2215-35-2**
DSL name	**Zinc, bis[*O*,*O*-bis(1,3-dimethylbutyl) phosphorodithioato-*S*,*S'*], (*T*-4)-**
National Chemical Inventories (NCI) names[1]	*Zinc, bis[O,O-bis(1,3-dimethylbutyl) phosphorodithioato-kS,kS']-, (T-4)-* (TSCA, PICCS, ASIA-PAC, NZIoC) *Zinc, bis[O,O-bis(1,3-dimethylbutyl) phosphorodithioato-S,S']-, (T-4)-* (ENCS) *zinc O,O,O',O'-tetrakis(1,3-dimethylbutyl) bis(phosphorodithioate)* (EINECS) *2-Pentanol, 4-methyl-, hydrogen phosphorodithioate, zinc salt* (AICS) *4-Methyl-2-pentanol hydrogen phosphorodithioate zinc salt* (ECL) *Zinc O,O-DI(1,3-dimethylbutyl)phosphorodithioate* (PICCS) *Zinc,bis[O,O-bis(1,3-dimethylbutyl)phosphorodithioato-S,S']-,(T-4)-* (PICCS) *ZINC, BIS[O,O-BIS(1,3-DIMETHYLBUTYL)PHOSPHORODITHIOATO-S,S']-, (T-4)-* (PICCS)
Other names	*O,O-Bis(1,3-dimethylbutyl)dithiophosphate zinc salt;* *Phosphorodithioic acid, O,O-bis(1,3-dimethylbutyl) ester, zinc salt;* *Phosphorodithioic acid, O,O-bis(1,3-dimethylbutyl) ester, Zn salt;* *Zinc bis(1,3-dimethylbutyl) dithiophosphate;* *Zinc bis(1,3-dimethylbutyl)phosphorodithioate;* *Zinc O,O-bis(4-methyl-2-pentyl)phosphorodithioate*
Chemical group (DSL Stream)	Discrete organometallics
Major chemical class or use	Zinc-containing compounds
Major chemical sub-class	Dialkyldithiophosphates
Chemical formula	$C_{24}H_{54}O_4P_2S_4Zn$

Chemical structure	
SMILES[2]	CC(CC(C)OP(OC(CC(C)C)C)(S[Zn]SP(OC(C)CC(C)C)(OC(C)CC(C)C)=S)=S)C
Molecular mass	662.3 g/mol

[1] National Chemical Inventories (NCI). 2007 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); NZIoC (New Zealand Inventory of Chemicals); PICCS (Philippine Inventory of Chemicals and Chemical Substances); and TSCA (Toxic Substances Control Act Chemical Substance Inventory).

[2] Simplified Molecular Input Line Entry System

Physical and Chemical Properties

A number of models have been re-run for this SAR owing to (1) the availability of updated information on physical and chemical properties; and (2) identification of a different structure for zinc BDBP than the one that was used for the previously published substance profile. The structure used in the profile was incorrect as one half of the structure bonded to the zinc was missing.

Table 2 contains experimental and modelled physical and chemical properties of zinc BDBP that are relevant to its environmental fate. Note that this substance is expected to persist and not to transform nor dissociate in water (See fate and persistence sections). Therefore, physical and chemical properties of the substance apply to the parent molecule form of the substance.

Table 2. Physical and chemical properties for zinc BDBP

Property	Type	Value[1]	Temperature (C°)	Reference
Physical state	Experimental	Liquid	~20	US EPA 2008
Melting point (ºC)	Experimental	-16.00		European Commission 2000d
Boiling point (ºC)	Modelled	480	-	MPBPWIN 2008
Density (kg/m^3)	-	NA[2]	-	-
Vapour pressure (Pa)	Modelled	1.17×10^{-5} (8.76×10^{-8} mm Hg)	25	MPBPWIN 2008
Vapour pressure (Pa)	Experimental[3]	1.7×10^{-4} (1×10^{-6} mm Hg)	-	US EPA 2008
Henry's Law constant (Pa·m^3/mol)	Modelled	1.49×10^{-2} (1.47×10^{-7} atm·m^3/mol)	25	HENRYWIN 2008 (bond method)
Log K_{ow} (Octanol-water partition coefficient) (dimensionless)	Modelled	12.32	25	KOWWIN 2008

Log K_{oc} (Organic carbon partition coefficient) (dimensionless)	Modelled	6.55–7.56	25	PCKOCWIN 2008
Water solubility (mg/L)	Modelled (semi-experimental)	3.05 x 10^{-2}	25	WATERNT 2002
	Experimental, based on analogue I[4]	15.8	-	US EPA 2008
	Experimental, based on analogue II[5]	1.1	-	US EPA 2008

[1] Values and units in brackets represent those originally reported by the authors or estimated by the models.
[2] Not Available.
[3] Based on the vapour pressure of the lubricating oil in which the substance is used (US EPA 2008).
[4] Based on a discrete analogue organometallic substance, Phosphorodithioic acid, mixed *O,O*-bis(1,3-dimethylbutyl and iso-Pr) ester, zinc salt, CAS 84605-29-8
[5] Based on a discrete analogue organometallic substance, Phosphorodithioic acid, mixed *O,O*-bis(2-ethylhexyl) ester, zinc salt, CAS 4259-15-8

Sources

Zinc BDBP is not reported to occur naturally. According to the raw data submitted under the Challenge, for the year 2006 in Canada, no manufacture of zinc BDBP was reported (Environment Canada 2009a). However, fewer than four companies reported importing a total quantity between 100 000 and 1 000 000 kg (Environment Canada 2009a). For the year 2005 in Canada, no manufacture of zinc BDBP was reported (Canada 2006b). However, fewer than four companies reported importing, each, a total quantity between 1001 and 100 000 kg of zinc BDBP into Canada (Canada 2006b).

Products containing zinc BDBP may enter the country even if they are not identified as such in the section 71 survey because they may be imported unknowingly in manufactured items, or in quantities below the 100 kg reporting threshold for the survey.

Elsewhere, zinc BDBP has been identified as an International Council of Chemical Associations high production volume (HPV) chemical (ICCA 1999), an Organisation for Economic Co-operation and Development HPV chemical (OECD 2004), and as a United States HPV chemical (Zinc Dialkyldithiophosphate Category) (US EPA 2008). According to 1986-2002 information from the United States Environmental Protection Agency (US EPA 2009), the U.S. import/production was in the range of 454–4545 tonnes in 1986, 1990, 1994 and 2002. In 1998, the import/production was in the range of 4545–22 727 tonnes. In Sweden and Denmark, total use was 17–21 tonnes annually from 1999 through 2005, but dropped sharply to roughly 1 tonne annually in 2006 and 2007 (SPIN 2009).

Given the use of this substance in other countries, it is probable that the substance is entering the Canadian market as a component of industrial and/or consumer products. Available information is currently not sufficient to derive a quantitative estimate of the importance of this possible source.

Uses

Information on uses for the 2005 and 2006 calendar years was gathered in response to notices published under S.71 of CEPA 1999 (Canada 2006b; 2009b). Companies identified themselves as primarily engaged in refining crude petroleum; manufacturing petroleum products (including blending and compounding lubricating oils and greases from refined petroleum products and re-refining used products); and manufacturing miscellaneous chemical products.

The above industrial activities identified through the CEPA 1999 section 71 notice are based on the North American Industry Classification System (NAICS) codes. Over 3000 NAICS codes have been defined. NAICS codes describe a company’s sectors and business lines without, however, specifying the exact use of the substance or product within the company. NAICS codes differ from the functional use codes used for DSL nomination information in that functional use codes indicate specific applications or uses for the substance or products containing the substance.

Information on the use of this substance that was received through the notice indicates that zinc BDBP could be used in Canada in a dispersive manner.

Potential uses in Canada

The information below on potential uses of zinc BDBP was found through searches of the available scientific and technical literature.

In Canada, zinc BDBP is used in lubricity additive packages that may be added to form finished oils such as motor oil (ACC 2005; Environment Canada 2009a; Ford Motor Company 2002, 2005). According to the US EPA (2008), more generally, zinc dialkyldithiophosphates are used to formulate finished lubricating oils including all types of automotive and diesel engine crankcase oils, industrial oils and hydraulic fluids. They are used as anti-wear inhibitors to reduce wear in engines and hydraulic equipment parts, and also act as antioxidants. In Nordic countries, zinc BDBP is used industrially in the categories of lubricants/additives and base oils. More specifically, the substance is used in the manufacture, maintenance and repair of motor vehicles and motorcycles and in manufacture of automotive fuel (SPIN 2009). Zinc BDBP is believe added to motor oil as an extreme pressure additive, although it may serve as a corrosion inhibitor or anti-wear additive (Danish Environmental Protection Agency 2005).

Releases to the Environment

Responses to a notice issued under section 71 of CEPA 1999 indicated no reported releases of zinc BDBP to the environment in the 2006 calendar year (Environment Canada 2009a). Zinc BDBP is not a reportable substance to the National Pollutant Release Inventory (NPRI 2008) or to the U.S. Toxics Release Inventory (TRI 2007); therefore no release data were available from these sources.

The losses of zinc BDBP via various routes during its life cycle are estimated based on regulatory survey data, industry data and data published by different organizations. The losses are grouped into six types: (1) discharge to wastewater; (2) emission to air; (3) loss to paved/unpaved surfaces; (4) chemical transformation; (5) disposal to landfill; and (6) disposal by incineration. Losses may occur at one or more of the substance's life cycle stages that include manufacture, industrial use, consumer/commercial use, and disposal. To assist in estimating these losses, a spreadsheet (Mass Flow Tool) was used that incorporates all data and assumptions required for the estimation (Environment Canada 2009c). Unless specific information on the rate or potential for release of the substance from landfills and incinerators is available, the Mass Flow Tool does not quantitatively account for releases to the environment from waste disposal sites.

In the context of the estimation assisted by the Mass Flow Tool, the discharge to wastewater refers to raw wastewater prior to any treatment, either on-site industrial wastewater treatment or off-site municipal sewage treatment. In a similar manner, the loss via chemical transformation refers to changes in substance identity that occur within the manufacture, industrial use, or consumer/commercial use stages, but excludes those during waste management operations such as incineration and wastewater treatment.

The losses estimated for zinc BDBP over its life cycle are presented in Table 3 (Environment Canada 2009c). The substance is expected to be released to wastewater at 1.9% of the total quantity used in Canadian commerce. In general, loss to wastewater is a common source for releases to water through wastewater treatment facilities and to soil through application of biosolids. Most losses to wastewater are expected to result from consumer use.

Table 3. Estimated losses of zinc BDBP during its life cycle

Type of loss	Proportion (%)	Pertinent life cycle stages
Wastewater	1.9	Industrial use and consumer/commercial use
Air emission	0.0	-
Paved/unpaved surfaces	0.9	Consumer/commercial use
Chemical transformation	84.2	Consumer/commercial use
Landfill	1.1	Consumer/commercial use
Incineration	0.2	Consumer/commercial use
Recycling	11.7	Industrial use and Consumer/commercial use

Zinc BDBP is also expected to be released to the environment via routes other than wastewater. There are various mechanisms for the loss to paved/unpaved land surfaces such as leaks and spills. The substance lost to paved/unpaved surfaces can be blown to nearby soil or washed into sewers, resulting in releases to water and soil. The substance entering recycling facilities can find its way to water and/or soil, depending upon the operational characteristics of these facilities. The substance disposed of in landfill has a low potential to leach out into groundwater.

The above loss estimates indicate that zinc BDBP has a moderate potential for release to the environment.

This substance is also likely present in similar consumer products that are imported into Canada. Although available information is currently not sufficient to estimate the total volume released to the environment or sent for waste and wastewater management from the latter sources, it is anticipated that the proportions lost to each receiving medium would not be significantly different.

In summary, releases of zinc BDBP occur primarily during consumer use (leaks, spills during use, improper disposal) and, to a lesser extent during industrial handling, blending and repackaging.

Environmental Fate

The substance zinc BDBP is not expected to dissociate in water based on (1) its resistance to hydrolysis (see persistence section below); (2) the rather strong level of covalence (81%) of the bond between zinc and sulphur which likely confers high stability, indicating a negligible potential for dissociation of zinc from the molecule (the percentage covalence was calculated from the difference in electronegativity between the zinc and sulphur atoms); and (3) the level of aquatic toxicity that would be higher if there had been evidence of the liberation of significant amounts of dissolved zinc.[2] Therefore, in water bodies at environmentally relevant pH (6–9), zinc BDBP is expected to be undissociated, which indicates that the biotic exposure to zinc BDBP will be from the neutral chemical. This also indicates that partitioning behaviour predicted using the log K_{ow}, log K_{oa} and log K_{oc} is appropriate.

Based on its physical and chemical properties (Table 2), the results of Level III fugacity modelling (Table 4) suggest that zinc BDBP is expected to predominantly reside in soil and/or sediment, depending on the compartment of release.

Table 4. Results of the Level III fugacity modelling (EQC 2003)

	Percentage of substance partitioning into each compartment			
Substance released to:	**Air**	**Water**	**Soil**	**Sediment**
Air (100%)	0.9	0.3	78.7	20.1
Water (100%)	0.0	1.7	0.0	98.3
Soil (100%)	0.0	0.0	99.9	0.1
Water (68%); Soil (32%); Air (0%)[1]	0.0	1.4	18.8	79.8

1: It is estimated that, 1.9% of the total quantity of the substance is lost to wastewater and 0.9% is expected to be lost to paved/unpaved surfaces which is assumed to be released to soil. Therefore, 68% of the mass of the substance that is so lost is expected to reach wastewater and 32% goes to soil (the total loss is 2.8% (1.9% + 0.9%) and the total loss to water is 1.9%/2.8% = 68%; total loss to soil is 0.9%/2.8% = 32%).

If released to air, a very low amount of the substance is expected to reside in air (see Table 4 above). Based upon the low vapour pressure of 1.17 x 10^{-4} Pa and low Henry's Law constant of 1.49 x 10^{-2} Pa·m^3/mol, zinc BDBP is non-volatile. Therefore, if released solely to air, it will not tend to remain in this compartment; but rather the substance will partition mainly to soil (~ 79%) and to a lesser extent to sediment (~ 20%) (see Table 4 above).

If released to water, zinc BDBP is expected to strongly adsorb to suspended solids and sediment based upon a very high estimated log K_{oc} value of ~ 7. Volatilization from water surfaces is expected to be an unimportant fate process based upon this compound's

[2] For example, an analogue CAS RN 4259-15-8, Phosphorodithioic acid, *O,O*-bis(2-ethylhexyl) ester, zinc salt shows no effects at saturation to rainbow trout (*Oncorhynchus mykiss*) and at loading rates up to 100 mg/L (US EPA 2008).

estimated Henry's Law constant. Thus, if water is the receiving medium, zinc BDBP is expected to mainly partition into sediment (see Table 4).

If released to soil, zinc BDBP is expected to have high adsorptivity to soil (i.e., expected to be immobile in this environmental compartment) based upon its estimated log $K_{oc.}$ Volatilization from moist soil surfaces seems to be an unimportant fate process based upon its estimated Henry's Law constant. This chemical is not expected to volatilize from dry soil surfaces based upon its vapour pressure. Therefore, if released to soil, zinc BDBP will entirely reside in this environmental compartment, which is illustrated by the results of the Level III fugacity modelling (see Table 4).

As explained in footnote to Table 4 above, based on a more realistic scenario that takes into account the relative proportions likely to be lost to wastewater and soil most of the substance will partition to sediment (79.8%), followed by soil (18.8%) and water (1.4%).

Persistence and Bioaccumulation Potential

Environmental Persistence

Table 5a presents empirical persistence values that were found for two analogue substances in the zinc dialkydithiophosphate category. The closest analogue of zinc BDBP is CAS RN 84605-29-8, Phosphorodithioic acid, mixed *O,O*-bis(1,3dimethylbutyl and isopropyl) esters, zinc salts (US EPA 2008). This substance was considered closest based on the fewest differences in the number of carbons in the 4 chains and also because it has the nearest molecular weight. A substance in the same category but less related was also considered, CAS RN 54261-67-5, Phenol, dodecyl-, hydrogen phosphorodithioate, zinc salt. The ready-biodegradation studies (Modified Sturm Test, OECD 301B), for both substances, show relatively low (4.2- 5.9%) biodegradation of the substances over 28 days (Table 5a). The values are based on carbon dioxide evolution. These tests indicate that the half-life in water is likely to be longer than 182 days (6 months) and that the substances are therefore likely to persist in that environmental compartment.

Table 5a. Empirical analogue data for degradation of zinc BDBP

CAS RN	Medium	Fate process	Biodegradation value for analogues (%)	Reference
84605-29-8	Water	Biodegradation	5.9	US EPA 2008
54261-67-5	Water	Biodegradation	4.2-5.9	

Since few experimental data on the degradation of analogues of zinc BDBP are available, a quantitative structure-activity relationship (QSAR)-based weight-of-evidence approach

(Environment Canada 2007) was also applied using the degradation models shown in Table 5b below. The BIOWIN models and others were used to estimate the substances' persistence in water, and these predictions were extrapolated to soil and sediment, the compartments to which zinc BDBP is expected to primarily partition when released to the environment. Zinc BDBP contains functional groups (dithiophosphate esters) expected to undergo very slow hydrolysis.

Table 5b summarizes the results of available QSAR models for degradation in air and water.

Table 5b. Modelled data for degradation of zinc BDBP

Fate process	Model and model basis	Model result and prediction	Extrapolated half-life (days OR hours)
AIR			
Atmospheric oxidation	AOPWIN 2000	$t_{1/2}$ = 0.034 days	< 2
Ozone reaction	AOPWIN 2000	n/a[1]	n/a
WATER			
Hydrolysis	HYDROWIN 2000	n/a[1]	n/a
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 3: Expert Survey (ultimate biodegradation)	1.74[2] "does not biodegrade fast"	> 182[4]
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 4: Expert Survey (primary biodegradation)	2.90[2] "does not biodegrade fast"	> 182[4]
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 5: MITI linear probability	-1.45.[3] "does not biodegrade fast"	> 182[4]
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 6: MITI non-linear probability	0.00[3] "does not biodegrade fast"	> 182[4]
Biodegradation (aerobic)	TOPKAT 2004 Probability	n/a[1]	n/a
Biodegradation (aerobic)	Canadian POPs Model (CPOPs) % BOD (biological oxygen demand)	% BOD = 2.7 "biodegrades very slowly"	> 182[4]

[1] Model does not provide an estimate for this type of structure.
[2] Output is a numerical score from 0 to 5.
[3] Output is a probability score.
[4] Expected half-lives for BIOWIN and CPOPS models are determined based on Environment Canada 2009b.

In air, a predicted atmospheric oxidation half-life value of 0.034 days (see Table 5b above) demonstrates that this substance is likely to be rapidly oxidized in air. The compound is not expected to react (or react appreciably) with other photo-oxidative species in the atmosphere, such as O_3; nor is it likely to degrade via direct photolysis. Therefore, it is expected that reactions with hydroxyl radicals will be the most important fate process in the atmosphere for zinc BDBP. With a half-life of 0.034 days via reactions with hydroxyl radicals, zinc BDBP is considered not persistent in air.
The five biodegradation models suggest that biodegradation is not fast and that the half-life in water would be ≥ 182 days (Environment Canada 2009b). The models consider primary biodegradation and ultimate degradation. The prediction from CPOPs is

considered to be more reliable than the prediction from BIOWIN because of the slightly better and larger model training set coverage. The prediction from CPOPs suggests a very slow rate of biodegradation. The substance also contains two structural features associated with chemicals that are not easily biodegraded, as listed in Environment Canada (2009b): (1) terminal isopropyl groups attached to a non-cyclic chemical, and (2) a highly branched structure. Therefore, considering the model results, the empirical data for the closest analogue, and structural features, there is reliable evidence to suggest that the ultimate biodegradation half-life of zinc BDBP is > 182 days in water. In addition, the U.S. EPA considers all of the dialkyldithiophosphate group member substances, including zinc BDBP, as "P3" (i.e., high level of persistence) in their screening level hazard characterization (US EPA 2008; Federal Register 1999).

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 zinc BDBP is expected to be persistent in soil and sediment.

In addition, the long-range transport potential (LRTP) of zinc BDBP from its point of release to air is estimated to be negligible according to its very low partitioning to air and low persistence in this medium.

Based on the empirical and modelled data (see Tables 5a and 5b above) zinc BDBP 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

Since no experimental bioaccumulation factor (BAF) and/or bioconcentration factor (BCF) data for zinc BDBP were available, a predictive approach was applied using available BAF and BCF models as shown in Table 6 below. According to the *Persistence and Bioaccumulation Regulations* (Canada 2000) a substance is bioaccumulative if its BCF or BAF is ≥ 5000; however, measures of BAF are the preferred metric for assessing bioaccumulation potential of substances. This is because BCF may not adequately account for the bioaccumulation potential of substances via the diet, which predominates for substances with log K_{ow} > ~4.0 (Arnot and Gobas 2003). Kinetic mass-balance modelling is in principle considered to provide the most reliable prediction method for determining the bioaccumulation potential because it allows for correction based on ADME (absorption, distribution, metabolism and elimination) parameters as the log K_{ow} of the substance is within the log K_{ow} domain of the model. Unfortunately results from the Arnot and Gobas model could not be used in this assessment since few of the chemicals used in its training have log K_{ow}s above 9. The empirical log K_{ow} value for zinc BDBP is likely > 9 as the modelled log K_{ow} is 12.32 (see Table 2 above). This suggests that this chemical has low potential to bioaccumulate in the environment due to strong adsorption to organic materials and very low water solubility resulting from a high molecular weight, including many carbons. These factors favour a low bioavailability in water.

Table 6. Modelled data for bioaccumulation of zinc BDBP

Test organism	Endpoint	Value wet weight (L/kg)	Reference
Fish	BCF	14.5 L/kg	OASIS Forecast 2005
Fish	BCF	7.6 L/kg	
Fish	BCF	32.8 L/kg	BCFWIN 2000

The OASIS and BCFWIN modelled values in Table 6 are considered to be of acceptable reliability as some chemicals of structural comparability are contained in the training sets. The low values (7.6-32.8 L/Kg) from these models show that low bioavailability to water organisms and low dietary accumulation are likely.

The available evidence indicates that zinc BDBP is expected to have low bioaccumulation potential due to its physical and chemical properties. This conclusion is consistent with that of the U.S. EPA, which considers all of the dialkyldithiophosphate group member substances including zinc BDBP to be “B1” (i.e., low bioaccumulation potential) in their screening level hazard characterization (US EPA 2008; Federal Register 1999).

Therefore, considering the available evidence, zinc BDBP does not meet the bioaccumulation criteria (BCF, BAF ≥ 5000) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential to Cause Ecological Harm

Ecological Effects Assessment

A - In the Aquatic Compartment

There is experimental and modelled evidence that zinc BDBP causes harm to aquatic organisms at relatively low concentrations.

The U.S. EPA has requested that empirical data on the zinc dialkyldithiophospate category (that includes zinc BDBP) be generated in order to produce a screening-level risk assessment for this category of chemical to support its initial Risk-Based Prioritizations (RBPs) for High Production Volume (HPV) chemicals (US EPA 2008). The European Commission undertook a similar exercise where industry submitted data that were compiled in the form of IUCLID files following regulations on the Evaluation and Control of the Risks of European Existing Substances (European Commission 2000a;

2000b; 2000c; 2000d; 2000e). Seven substances of the dialkyldithiophospate category have IUCLID files, including zinc BDBP. The aquatic toxicity information, related to the dialkyditiohosphates, from these two sources was compiled and a Species Sensitivity Distribution (SSD) was then generated with the datasets (see Figure 1, below). The intent is to use the 5th percentile of the SSD as the critical toxicity value (CTV). The lowest acute aquatic toxicity value was identified for each of the 8 species included in the dataset (see Table 7, below). The group included two marine invertebrate species (*Crassostrea virginica* and *Mysidopsis bahia*). They were included in the SSD due to the limited number of species. The assumption made is that the SSD reflects the most toxic zinc dialkyldithiophosphate category member substances, which are shorter chain/lower molecular weight ones. The software SSD Master v2.0 (SSD Master 2008) was used to plot the SSD. Several cumulative distribution functions (CDFs) (normal, logistic, Gompertz, Weibull and Fisher-Tippett) were fit to the data using regression methods. Model fit was assessed using statistical and graphical techniques. The best model was selected based on consideration of goodness-of-fit and model feasibility. Model assumptions were verified graphically and with statistical tests. The Normal model provided the best fit of the models tested (Anderson-Darling Statistic (A^2) = 0.316) and the 5th percentile of the SSD plot is 0.017 mg/L with lower and upper confidence limits of 0.05 and 0.057 mg/L, respectively (Figure 1). This is selected as the short-term CTV. As no chronic data could be found in the dataset, a long-term SSD could not be drawn. Therefore, an application factor of 10 was used to convert the short-term CTV to a long-term (chronic) predicted no effect concentration (PNEC). As a result, the long-term (chronic) PNEC is calculated to be 0.017 mg/L.

Robust Study Summaries (RSS) could not be generated to assess the reliability of the studies, given the lack of information in the IUCLID sources. However, an RSS was created for the lowest value of the closest analogue of zinc BDBP (CAS RN 84605-29-8) (US EPA 2008). The LL_{50} (loading rate causing 50% mortality) for rainbow trout (*Oncorhynchus mykiss*) was 4.5 mg/L (see RSS in Appendix 1). The reliability of the study was satisfactory. An application factor (AF) of 100 was applied to the LL_{50} to account for interspecies and intraspecies variability in sensitivity and to estimate a long-term no-effects concentration from a short-term LL_{50}. Application of the AF to the LL_{50} results in a PNEC value of 0.045 mg/L.

The PNEC calculated from the SSD (0.017 mg/L) was used preferably over the single deterministic value from the analogue loading rate study because it is likely to more accurately reflect the natural variability of responses to the dialkyldithiophosphate category member substances. The SSD value of 0.017 mg/L is also below the predicted water solubility of zinc BDBP and the experimental water solubility of its analogues.

Table 7. Empirical data for aquatic toxicity of dialkyldithiophospate category member substances used in the SSD

Test organism	Substance	Type of test	Endpoint	Value (mg/L)	Reference
Crassostrea virginica (Eastern oyster-invertebrate)	zinc dialkyl (C8) dithiophosphate	Acute (96 hours)	EC_{50}[1] (growth)	0.25	European Commission (2000a)
Daphnia magna (water flea-invertebrate)	unknown	Acute (48 hours)	EC_{50} (immobilization)	1	IUCLID (2000b)
Pimephales promelas (Fathead minnow-fish)	unknown	Acute (96 hours)	LC_{50}[2]	1	IUCLID (2000c)
Selenastrum subcapitata (green algae)	zinc dialkyl (C8) dithiophosphate	Acute (96 hours)	EC_{50}	1	IUCLID (2000d)
Oncorhynchus mykiss (Rainbow trout- fish)	CAS RN 84605-29-8	Acute (96 hours)	LL_{50}[3]	4.5	US EPA (2008)
Cyprionodon variegatus (Sheepshead minnow- fish)	Phosphorodithioic acid, mixed O,O-diester with C4 and C5 alcohols, zinc salt; CAS not specified	Acute (96 hours)	LC_{50}	4.6	IUCLID (2000a)
Mysidopsis bahia (mysid shrimp-invertebrate)	CAS RN 4259-15-8	Acute (96 hours)	LC_{50}	6.9	IUCLID (2000e)
Scenedesmus subspicatus (algae)	CAS RN 84605-29-8	Acute (72 hours)	EC_{50} (growth)	21	US EPA (2008)

[1] EC_{50} – The concentration of a substance that is estimated to cause some effect on 50% of the test organisms.
[2] LC_{50} – The concentration of a substance that is estimated to be lethal to 50% of the test organisms.
[3] LL_{50} – The loading rate of a substance that is estimated to be lethal to 50% of the test organisms. It is not the concentration in the water. It is similar to the LC_{50} where only nominal concentrations would have been reported.

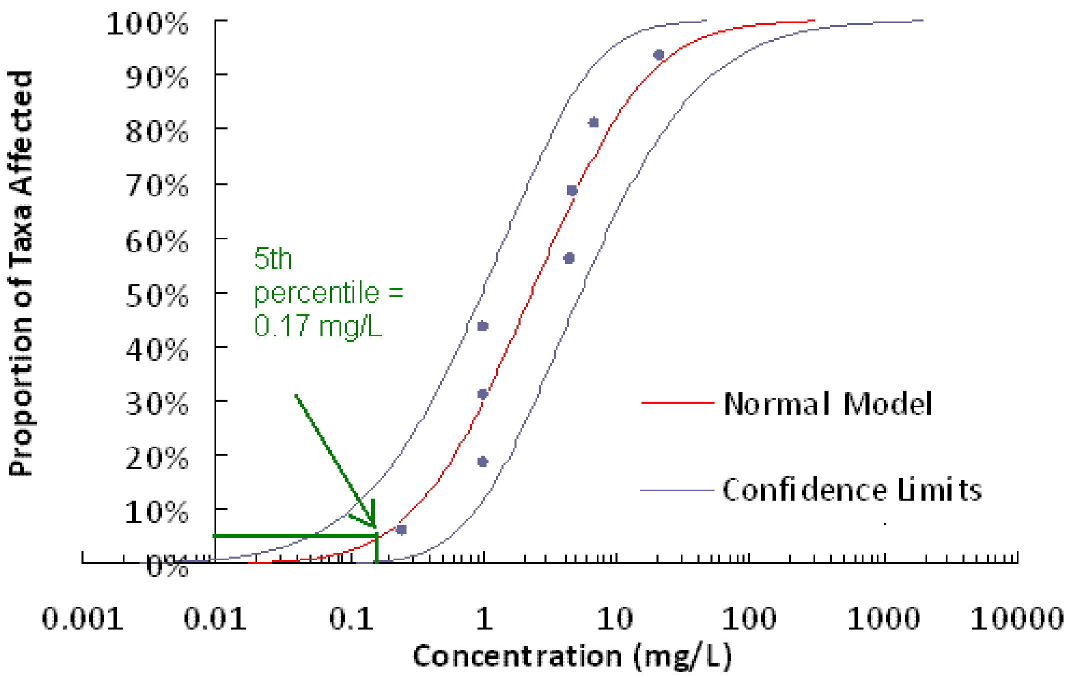


Figure 1. Species Sensitivity Distribution for the acute toxicity of the dialkydithiophosphate category

B - In Other Environmental Compartments

No ecological effects studies were found for this compound in media other than water. Effect levels have not been estimated for soil or sediment.

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 substance quantities, estimated release rates, and information on the potential size of receiving water bodies.

Industrial Release

As zinc BDBP is used industrially and is expected to be released to water, a conservative industrial release scenario is used to estimate the aquatic concentration of the substance (Environment Canada 2009d). The scenario is made conservative by assuming that the higher end of the range of the quantity of the substance subject to industrial releases (10 000 to 100 000 kg) is used by one single industrial facility at a small, hypothetical site. The loss to sewers is at 0.31% of the total quantity resulting from mainly container handling and blending. The scenario also assumes that the release occurs 250 days per year, typical for small and medium-sized facilities, and is sent to a local primary sewage treatment plant (STP) with a 57.3% removal rate for the substance based on AS treat 1.0 (Environment Canada 2009d). In Canada, the receiving water at such a small site normally has a 10-fold dilution capacity for the STP effluent, which equals 3456 m^3 per day for the size of the site. Based on the above assumptions, an aquatic concentration of 0.0153 mg/L is estimated for a small generic site (Environment Canada 2009e).

Consumer Release

As zinc BDBP is found in consumer products and is reported to be released to water, Mega Flush, Environment Canada's spreadsheet tool for estimating down-the-drain releases from consumer uses was employed to estimate the potential substance concentration in multiple water bodies receiving sewage treatment plant effluents to which consumer products containing the substance may have been released (Environment Canada 2009f). The spreadsheet tool is designed to provide these estimates based on conservative assumptions regarding the amount of substance used and released by consumers.

By default, primary and secondary STP removal rates are conservatively assumed to be 0%. Losses from use are assumed to be of 2.5%, consumer use of the substance to be over 365 days/year, and the flow rate at all sites to be low – i.e., equal to the tenth percentile of annual flows. These estimates are made for approximately 1000 release sites across Canada, which account for most of the major STPs in the country.

The equation and inputs used to calculate the predicted environmental concentration (PEC) of zinc BDBP in the receiving water bodies are described in Environment Canada (2009g). A scenario was run assuming a total consumer use quantity of 1 000 000 kg/year, which is a worst-case condition since it is the highest possible imported quantity in the reporting range (Environment Canada 2009g). In addition the proportion of the total mass that is lost to sewers was set at 2.5% based on the Mass Flow Tool which estimated potential releases to soil and sewers during the life cycle of the substance (leaks, spills during use, improper disposal). Default values were used for other parameters.

Using this scenario, the tool estimates that the PEC in the receiving water bodies ranges from 0.00098 to 0.038 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, inherent toxicity, sources and fate of the substance and its analogues.

Zinc BDBP is expected to be persistent in water, soil and sediment; it is also expected to have a low bioaccumulation potential. The high importation volumes of zinc BDBP into Canada, along with information on its uses, indicate moderate potential for releases to the Canadian environment. Once released to the environment, it will be found mainly in soil and sediments. It has also been demonstrated to have a low to moderate potential for toxicity to aquatic organisms.

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 conservative industrial scenario (the total quantity of the substance used by Canadian industry in the reporting range) presented above yielded a predicted environmental concentration (PEC) of 0.0153 mg/L (Environment Canada 2009e). A long-term (chronic) predicted no-effect concentration (PNEC) was derived using the 5th percentile short-term SSD value of 0.17 mg/L, and dividing this value by an assessment factor of 10 to give a value of 0.017 mg/L. The resulting risk quotient (PEC/PNEC) = 0.9. Given the conservatism in both the PEC and PNEC, this result indicates that harm to pelagic aquatic organisms is unlikely. Using a similar PEC/PNEC approach, the consumer release scenario tool predicted that conservative PECs for zinc BDBP do not exceed the PNEC in most (99.7%) of the water bodies receiving wastewater across Canada under low (10th percentile) flow conditions (Environment Canada 2009g) and assuming no STP removal. The highest PEC/PNEC ratio was 2.2.

As noted previously, when zinc BDBP is released to a water body, it partitions into suspended particulate matter and to bottom sediments, where sediment-dwelling organisms would be exposed to the substance. Because no environmental monitoring data or toxicity data specific to sediment-dwelling organisms are available, a risk quotient based on exposure in sediment pore water may be calculated based on the aquatic compartment PEC and PNEC values presented above and used for sediment risk characterization. In the calculation, bottom sediment and its pore water are assumed to be in equilibrium with the overlying water, and benthic and pelagic organisms are assumed to have similar sensitivities to the substance. Therefore the PEC and PNEC for sediment pore water is considered to be the same as for the aquatic compartment. This equilibrium approach would therefore result in risk quotients for the sediment compartment that are the same as for the aquatic compartment, i.e., almost all would be less than 1.

This information indicates that zinc BDBP does not have the potential to cause ecological harm in Canada.

Uncertainties in Evaluation of Ecological Risk

Although no information is available on the quantity of zinc BDBP that is imported in manufactured items or consumer products, it is expected that the quantities of zinc BDBP released to water would not be significantly greater than those estimated here. This is because a bounding high-end value of 1 000 000 kg was assumed to represent the mass in Canadian commerce for the consumer release scenario calculations. It is also recognized that potential releases from waste disposal sites could be possible and contribute to overall environmental concentration. However, available information is currently not sufficient to derive quantitative estimates for these releases.

Also, regarding ecotoxicity, based on the predicted partitioning behaviour of this chemical, the significance of soil and sediment as important media of exposure is not addressed by the effects data available. Indeed, the only effects data identified apply primarily to pelagic aquatic exposures, although the water column is likely not the medium of primary concern based on partitioning estimates.

The Species Sensitivity Distribution presented in this screening assessment does not meet the requirements of a type A guideline (CCME 2007) but was used since the PNEC derived from it is lower than the PNEC based on the lowest acceptable toxicity value and thus represents a more conservative scenario based on the whole dialkyldithiophosphate category.

Finally, there is uncertainty in concluding outside a moiety-based assessment on individual substances that can contribute to the total release of bioavailable zinc to the environment. The conclusion reached in this assessment, that zinc BDBP does not dissociate significantly (releasing zinc) in the environment and has a low potential to cause ecological harm in Canada, does not preclude the possible inclusion of this substance in a future moiety-based assessment of zinc-containing compounds.

Potential to Cause Harm to Human Health

Exposure Assessment

Environmental Media

There were no data identified for zinc BDBP in environmental media, regardless of location. In the absence of release data from publicly available inventories and since in responses to a notice issued under section 71 of CEPA 1999, no releases were reported, as a conservative approach, environmental concentrations were estimated using the loss percentages predicted by the Mass Flow Tool by Environment Canada (see Table 3) (Environment Canada 2009c). The percentages represent losses of a substance at different stages of the life cycle and were applied to the total quantity of zinc BDBP in Canadian commerce in 2006.

The total quantity in commerce was conservatively assumed to be the maximum of the import range for 2006, namely 1 000 000 kg (Environment Canada 2009a). The loss quantities are estimated as 19 000 kg to water through wastewater, 11 000 kg to soil through leaching from landfill and 9000 kg to paved/non-paved surfaces. These loss quantities to water and soil are considered as overestimates, as explained in the Releases to the Environment section.

The estimated losses were used in ChemCAN, a Canada-specific environmental exposure model, to estimate concentrations in various environmental media (ChemCAN 2003). The predicted concentrations are presented in Appendix II. This model differs from the point-source models used in the ecological assessment section of the document in that it is a regional far-field Level III fugacity model that is used to estimate average concentrations in various media to inform human exposure estimates. The estimated environmental concentrations were used as surrogates for measured data in deriving intake estimates. The estimated concentration in ambient air was used as a surrogate for indoor air data. In addition, the estimated concentration in surface water was used as a surrogate for drinking water. The intake estimates for each medium, in addition to total intake for each age group, are presented in Appendix III. The maximum total intake estimate was in the order of magnitude of 10^{-3} µg/kg-bw, which indicates that environmental exposure is considered negligible in comparison to potential exposure to zinc BDBP in consumer products.

Consumer Products

In order to estimate exposure to zinc BDBP for consumers, dermal exposure for a do-it-yourself (DIY) motor oil change was considered a worst-case source of exposure in finished oils due to the high likelihood of hand exposure during the change. Motor oils are agents that serve anti-wear and cooling functions for running equipment parts and must be periodically replaced, either at the dealer, repair garage or by the consumer.

A DIY motor oil change involves draining used oil, replacing the filter and pouring new oil into the engine crankcase using a funnel (eHow 2009). In an empirical study of zinc dithiophosphate levels in used motor oil, depletion of levels occurred at a roughly linear rate in two used oil samples tested at regular intervals of driving time (Yamaguchi et al. 2002). Assuming that some older cars require an oil change approximately every 4800 km, a vehicle traveling an average speed of 50 km/h would require an oil change every 96 hours (eHow 2009). At 96 hours of driving, approximately 40% of the total zinc BDBP would be depleted (Yamaguchi et al. 2002). Therefore, the dermal load of zinc BDBP after possible hand spillage during the draining phase of a motor oil change would be less than for exposure to new oil. However, the finger of the consumer is often used to lubricate the filter using new motor oil. In addition, the pouring of new motor oil into the engine crankcase presents another opportunity for potential hand spillage. A worst-case internal acute dose for dermal exposure to motor oil during an oil change of 0.858 mg/kg-bw per event was determined. The dermal scenario is presented in Appendix IV.

Health Effects Assessment

Only limited toxicological data are available for zinc BDBP. The acute toxicity is low, with an LD_{50} determined to be between 2000 and 5000 mg/kg-bw by gavage in rats (Anonymous 1986). New Zealand White rabbits dermally exposed to 0.8 mL/kg (converted to 884 mg/kg-bw/day[3]) or 1.6 ml/kg for three weeks showed irritation, body weight loss and elevated white blood cell count at both high and low doses. Effects in the high-dose groups included decreased mean testes weights, testes to body weights ratios and testes to brain weight ratios and decreased spermatogenic activity. A no-observed-effect level (NOEL) could not be established (Anonymous 1979).

The outputs of predictive models were also considered using four different models, Derek, TopKat, CaseTox and Leadscope Model Applier, of which the predictions for carcinogenicity, genotoxicity, developmental toxicity, and reproductive toxicity were predominately negative (DEREK 2008; TOPKAT 2004; CASETOX 2008; Leadscope 2009).

The U.S. EPA has conducted a screening level risk characterization of the zinc dialkyldithiophosphates which included zinc BDBP (US EPA 2008). The hazard characterization for zinc BDBP indicates that the acute oral toxicity is low based on measured data, and the acute dermal toxicity is low based on a read-across approach, which compared zinc BDBP to analogue substances. A no-observed-adverse-effect level (NOAEL) of 10 mg/kg-bw/day and a lowest-observed-adverse-effect level (LOAEL) of

[3] Conversion of 0.8 mL/kg to mg/kg
= (density of zinc BDBP)(volume conversion factor)(volume of substance/kg body weight)
= (1.105 g/cm^3)(1 cm^3/mL)(0.8 mL/kg-bw)
= 0.884 g/kg-bw
= 884 mg/kg-bw

50 mg/kg-bw/day was established for repeat-dose oral toxicity based on read-across data from one study of an analogue substance, which showed moderate systemic toxicity. The reproductive/developmental endpoint was filled, also using read-across data from a single oral study in which a NOAEL of 30 mg/kg-bw/day and a LOAEL of 100 mg/kg-bw/day were established for reproductive, developmental and systemic effects. Read-across data were negative for mutagenicity in bacterial cells, but showed a positive response in mammalian cells, and *in vivo* did not induce chromosome aberrations.

Characterization of Risk to Human Health

The potential for exposure of the general population to zinc BDBP from environmental media is expected to be negligible. However, there is potential for dermal exposure from the use of consumer products (additive in motor oil).

A comparison between the short-term dermal lowest-observed-effect level (LOEL) of 884 mg/kg-bw/day in New Zealand White rabbits and the estimated maximum total daily intake from all routes of environmental exposures in the order of magnitude of 10^{-3} µg/kg-bw/day results in a margin of exposure (MOE) in the order of magnitude of 10^{8}. This same short-term dermal LOEL of 884 mg/kg-bw/day and dermal exposure for consumer products (additive in motor oil) of 0.858 mg/kg-bw result in an MOE of 1030. Based on the information available, these margins are considered adequate to account for uncertainties in the database, in light of the conservative nature of the estimates of exposure and critical effect level.

Uncertainties in Evaluation of Risk to Human Health

Confidence in the environmental exposure estimates is moderate. Data in the literature were not identified for concentrations in environmental media. However, since no releases were reported in response to a notice issued under section 71 of CEPA 1999, in conjunction with the conservative use of loss quantities predicted by the Mass Flow Tool to represent worst-case release estimates, it is unlikely that the intake values are underestimates. Confidence in the consumer product exposure estimate is moderate. While end products in current use in Canada are considered to have been comprehensively captured in the responses to a notice issued under section 71 of CEPA 1999, the duration of dermal exposure and the skin surface area exposed were based on professional judgment in the do-it-yourself motor oil scenario.

The 3-week dermal study did not establish a NOEL. However, the effects observed at the LOEL were considered minor. Due to the limited data available for zinc BDBP, the confidence in the toxicological dataset is considered to be low. However, the available empirical data and information from predictive models are not suggestive of high hazard.

Conclusion

Based on the information presented in this screening assessment, it is concluded that zinc BDBP 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, Zinc BDBP meets the criteria for persistence but not for bioaccumulation potential as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

It is also concluded that zinc BDBP 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 zinc BDBP does not meet any of the criteria 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.

References

[ACC] American Chemistry Council. 2005. Final Submission for Zinc Dialkyldithiophosphate Category [Internet]. High Production Volume (HPV) Chemical Challenge Program. American Chemistry Council, Petroleum Additives Panel, Health Environmental and Regulatory Task Group. [cited 2009 Oct 6] 32p. Report No.: 201-15864A. Available from: http://www.regulations.gov/fdmspublic/ContentViewer?objectId=0900006480367cc3&disposition=attachment&contentType=pdf

Anonymous 1986. Unpublished study by an individual member company of the HERTG. [cited in HPVIS 2009]. Available from: http://iaspub.epa.gov/oppthpv/Public_Search.PublicTabs?SECTION=1&epcount=1&v_rs_list=24977145

Anonymous 1979. Unpublished study by an individual member company of the HERTG. [cited in HPVIS 2009]. Available from: http://iaspub.epa.gov/oppthpv/Public_Search.PublicTabs?SECTION=1&epcount=1&v_rs_list=24978911

[AOPWIN] Atmospheric Oxidation Program for Windows [Estimation Model]. 2000. Version 1.92a. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. [cited 2009 May]. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

Arnot JA, Gobas FAPC. 2003. A generic QSAR for assessing the bioaccumulation potential of organic chemicals in aquatic food webs. QSAR Comb Sci 22(3): 337-345.

[BCFWIN] BioConcentration Factor Program for Windows [Estimation Model]. 2000. Version 2.15. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. [cited 2009 May]. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

[BIOWIN] Biodegradation Probability Program for Windows [Estimation Model]. 2000. Version 4.10. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. [cited 2009 May]. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

Boethling RS, Howard PH, Beauman JA, Larosche ME. 1995. Factors for intermedia extrapolations in biodegradability assessment. Chemosphere 30(4):741−752.

Canada, Dept. of the Environment, Dept. of Health. 2009a. Canadian Environmental Protection Act, 1999: Notice with respect to Batch 8 Challenge substances. Canada Gazette, Part I, vol. 143, no. 5. Available from: http://www.gazette.gc.ca/rp-pr/p1/2009/2009-01-31/pdf/g1-14305.pdf

Canada, Dept. of the Environment, Dept. of Health. 2009b. Data for Batch 8 substances collected under the *Canadian Environmental Protection Act, 1999*, Section 71: *Notice with respect to certain Batch 8 Challenge substance,* Canada Gazette Part I, vol. 143, no. 5, p. 196–213. Data compiled by: Environment Canada, Program Development and Engagement Division.

Canada, Dept. of the Environment, Dept. of Health. 2006a. *Canadian Environmental Protection Act, 1999*: *Notice of intent to develop and implement measures to assess and manage the risks posed by certain substances to the health of Canadians and their environment*. Canada Gazette, Part I, vol. 140, no. 49, p. 4109–4117. Available from: http://canadagazette.gc.ca/partI/2006/20061209/pdf/g1-14049.pdf.

Canada, Dept. of the Environment, Dept. of Health. 2006b. *Canadian Environmental Protection Act, 1999*: *Notice with respect to selected substances identified as priority for action*. Canada Gazette, Part I, vol. 140, no. 9, p. 435–459. Available from: http://canadagazette.gc.ca/partI/2006/20060304/pdf/g1-14009.pdf

Canada. 2000. *Canadian Environmental Protection Act, 1999: Persistence and Bioaccumulation Regulations,* P.C. 2000-348, 29 March, 2000, SOR/2000-107. Available from: http://www.gazette.gc.ca/archives/p2/2000/2000-03-29/pdf/g2-13407.pdf

Canada. 1999. *Canadian Environmental Protection Act, 1999*. S.C., 1999, c. 33, Canada Gazette. Part III. Vol.22, no.3. Available from: http://www.gazette.gc.ca/archives/p3/1999/g3-02203.pdf

CASETOX [Prediction module]. 2008. Version 2.0. Beachwood (OH): MultiCASE. [cited 2009 September 30]. Available from: http://www.multicase.com/products/prod03.htm [restricted access].

[CCME] Canadian Council of Ministers of the Environment. 2007. A protocol for the derivation of water quality guidelines for the protection of aquatic life. In: Canadian environmental quality guidelines, 1999. Canadian Council of Ministers of the Environment, 1999.

ChemCAN [Level III fugacity model of 24 regions of Canada]. 2003. Version 6.00. Peterborough (ON): Trent University, Canadian Centre for Environmental Modelling and Chemistry. [cited 2009 Oct 6]. Available from: http://www.trentu.ca/academic/aminss/envmodel/models/CC600.html

[CPOPs] Canadian POPs Model. 2008. Gatineau (QC): Environment Canada, Ecological Assessment Division; Bourgas (BG): Bourgas Prof. Assen Zlatarov University, Laboratory of Mathematical Chemistry. [Model developed based on Mekenyan et al. 2005]. Available upon request.

Danish Environmental Protection Agency. 2005. Mapping and Development of Alternatives to Chlorinated Lubricants in the Metal Industry. Danish Ministry of the Environment. 142 p. Available from: http://www2.mst.dk/udgiv/publications/2005/87-7614-807-6/pdf/87-7614-808-4.pdf

[DEREK] Deducting Estimation from Existing Knowledge [Prediction module on CD ROM]. 2008. Version 10.0.2. Cambridge (MA): Harvard University, LHASA Group. [cited 2009 September 30]. Available from: http://lhasa.harvard.edu/?page=toxicology.htm [restricted access].

[ECOSAR] Ecological Structural Activity Relationships [Internet]. 2009. Version 1.00. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY):

eHow. 2009. How to change your motor oil [Internet]. [cited 2009 Oct 14]. Available from: http://www.ehow.com/video_11_change-motor-oil.html

Environment Canada. 2007. Guidance for Conducting Ecological Assessments under CEPA, 1999, Science Resource Technical Series, Technical Guidance Module: QSARs. Reviewed Draft Working Document. Gatineau (QC): Environment Canada, Ecological Assessment Division.

Environment Canada. 2009a. Data for Batch 8 substances collected under the Canadian Environmental Protection Act, 1999, Section 71: Notice with respect to Batch 8 Challenge substances. Data prepared by: Environment Canada, Existing Substances Program.

Environment Canada. 2009b. Guidance for Conducting Ecological Assessments under CEPA, 1999: Science Resource Technical Series, Technical Guidance Module: Suggested Approach to Determining the Persistence of a Chemical from Biodegradation Data. Reviewed Draft Working Document. Gatineau (QC): Environment Canada, Ecological Assessment Division. Ottawa, K1A 0H3

Environment Canada 2009c. Assumptions, limitations and uncertainties for zinc BDBP, CAS RN 2215-35-2 Unpublished report. Gatineau (QC): Environment Canada, Ecological Assessment Division.

Environment Canada. 2009d. Guidance for Conducting Ecological Assessments under CEPA, 1999, Science Resource Technical Series, Technical Guidance Module: The Industrial Generic Exposure Tool – Aquatic (IGETA). Working document. Gatineau (QC): Environment Canada, Ecological Assessment Division.

Environment Canada. 2009e. IGETA report: CAS RN 2215-35-2, 2009-09-15. Unpublished report. Gatineau (QC): Environment Canada, Ecological Assessment Division.

Environment Canada. 2009f. Guidance for Conducting Ecological Assessments under CEPA, 1999, Science Resource Technical Series, Technical Guidance Module: Mega Flush Consumer Release Scenario. Working Document. Gatineau (QC): Environment Canada, Ecological Assessment Division.

Environment Canada. 2009g. Mega Flush report: CAS RN 2215-35-2, 2009-09-15. Version xxx. Unpublished report. Gatineau (QC): Environment Canada, Ecological Assessment Division.

[EQC] Equilibrium Criterion Model. 2003. Version 2.02. Peterborough (ON): Trent University, Canadian Environmental Modelling Centre. Available from: http://www.trentu.ca/academic/aminss/envmodel/models/EQC2.html

European Commission. 2000a. IUCLID Dataset, phosphorodithioic acid mixed *O,O*-bis(iso-Bu and pentyl) esters, zinc salts CAS No. 68457-79-4 [Internet]. Year 2000 CD-ROM edition. [place unknown]:European Chemicals Bureau, European Commission. [created 2000 Feb 19; cited 2009 Sept 15]. Available from: http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/IUCLID/DATA_SHEETS/68457794.pdf

European Commission. 2000b. IUCLID Dataset, phosphorodithioic acid mixed *O,O*-C1-14-alkyl esters , zinc salts CAS No. 68649-42-3 [Internet]. Year 2000 CD-ROM edition. [place unknown]:European Chemicals Bureau, European Commission. [created 2000 Feb 19; cited 2009 Sept 15]. Available from: http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/IUCLID/DATA_SHEETS/68649423.pdf

European Commission. 2000c. IUCLID Dataset, zinc bis(*O-O*,diisooctyl) bis dithiophophate CAS No. 28629-66-5 [Internet]. Year 2000 CD-ROM edition. [place unknown]:European Chemicals Bureau, European Commission. [created 2000 Feb 19; cited 2009 Sept 15]. Available from: http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/IUCLID/DATA_SHEETS/28629665.pdf

European Commission. 2000d. IUCLID Dataset, zinc *O,O,O',O'*-tetrakis(1,3-dimethylbutyl) bis(phosphorodithioate CAS No. 2215-35-2 [Internet]. Year 2000 CD-ROM edition. [place unknown]:European Chemicals Bureau, European Commission. [created 2000 Feb 19; cited 2009 Sept 15]. Available from: http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/IUCLID/DATA_SHEETS/2215352.pdf

European Commission. 2000e. IUCLID Dataset, zinc bis[*O*-(1,3-dimethylbutyl)] bis[O-(isopropyl)] bis(dithiophosphate) CAS No. 14548-64-2 [Internet]. Year 2000 CD-ROM edition. [place unknown]:European Chemicals Bureau, European Commission. [created 2000 Feb 19; cited 2009 Sept 15]. Available from: http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/IUCLID/DATA_SHEETS/14548642.pdf

Federal Register 1999, Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances. *Federal Register* 64, Number 213 (November 4, 1999) Page 60194-60204.

Ford Motor Company. 2002. Material Safety Data Sheet: Motorcraft, Ford Internal Reference Number (Tox No.: 164586) [Internet]. 2002. Dearborn (MI): Ford Motor Company [cited 2009 Oct 6]. Available from: http://www.dcmsds.com/Demo/Car_Dealer/Service/MSDS%5CMotorcraft%5C164586_Super%20Duty%20Motor%20Oil%20-%20All%20Grades.pdf

Ford Motor Company. 2005. Material Safety Data Sheet: SAE (5W-20 and 5W-30 Premium Synthetic Blend, 10W-30 Super Premium, and 10W-40 Premium) Motor Oil [Internet]. 2005. Dearborn (MI): Ford Motor Company. [cited 2009 Oct 6]. Available from: http://www.canyonstateoil.com/msdssheets/Motorcraft/SAE_5W20_and_5W30_Premium_Synthetic_Blend_10W30_Super_Premium.pdf

Health Canada. 1998. Exposure factors for assessing total daily intake of priority substances by the general population of Canada. Unpublished report. Ottawa (ON): Health Canada, Environmental Health Directorate.

[HENRYWIN] Henry's Law Constant Program for Microsoft Windows [Estimation Model]. 2008. Version 3.20. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation [cited 2009 May]. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

[HYDROWIN] Hydrolysis Rates Program for Microsoft Windows [Estimation Model]. 2000. Version 2.00. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. [cited 2009 May]. Available from: http://www.epa.gov/oppt/exposure/pubs/episuite.htm

[ICCA] International Council of Chemical Associations. 1999 - . Website of the Global Initiative on High Production Volume (HPV) Chemicals. International Council of Chemical Associations. [revised 2005 October; cited 2006 January]. Available at: http://www.cefic.org/activities/hse/mgt/hpv/hpvinit.htm

[KOWWIN] Octanol-Water Partition Coefficient Program for Microsoft Windows [Estimation Model]. 2008. Version 1.67a. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. [cited 2009 May]. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

Leadscope [Prediction module]. 2009. Leadscope Model Applier Version 1.2.0-3. Columbus, OH: Leadscope, Inc. [cited 2009 September 30]. Available from: http://www.leadscope.com/all_products.php [restricted access].

[MPBPWIN] Melting Point Boiling Point Program for Microsoft Windows [Estimation Model]. 2008. Version 1.43. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. [cited 2009 May]. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

[NCI] National Chemical Inventories [database on CD-ROM]. 2007. Columbus (OH): American Chemical Society. [cited 2009 June]. Available from: http://www.cas.org/products/cd/nci/index.html

[NHW] Department of National Health and Welfare. 1990. Present patterns and trends in infant feeding in Canada. Catalogue No. H39-199/1999E; ISBN 0-662-18397-5. Ottawa (ON): Department of National Health and Welfare. 9 p. [cited in Health Canada 1998].

[NPRI] National Pollutant Release Inventory [database on the Internet]. 2008. Gatineau (QC): Environment Canada. [cited 2009 Oct 6]. Available from: http://www.ec.gc.ca/pdb/querysite/query_e.cfm

[OASIS Forecast] Optimized Approach based on Structural Indices Set [Internet]. 2005. Version 1.20. Bourgas (BG): Bourgas Prof. Assen Zlatarov University, Laboratory of Mathematical Chemistry. [cited May 2009]. Available from: http://oasis-lmc.org/?section=software

[OECD] Organisation for Economic Co-operation and Development. 2004. The 2004 OECD list of high production volume chemicals [Internet]. Paris (FR): OECD, Environment Directorate. [cited 2006 Jan 1]. Available from: http://www.oecd.org/dataoecd/55/38/33883530.pdf

[PCKOCWIN] Organic Carbon Partition Coefficient Program for Windows [Estimation Model]. 2008. Version 2.0. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. [cited 2009 May]. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

[RIVM] Rijksinstituut voor Volksgezondheid en Milieu. 2006. General Fact Sheet: Limiting conditions and reliability, ventilation, room size, body surface area. Updated version for ConsExpo 4 [Internet]. Report No.: 320104002/2006. Bilthoven (NL): RIVM (National Institute for Public Health and the Environment). [cited 2009 Oct 6]. Available from: http://www.rivm.nl/bibliotheek/rapporten/320104002.pdf

[SPIN] Substances in Products in Nordic Countries [database on the Internet]. 2009. Financed by the Nordic Council of Ministers, Chemical group. [cited 2009 Sept]. Available from: http://195.215.251.229/Dotnetnuke/Home/tabid/58/Default.aspx

[SSD master] Determination of Hazardous Concentrations with Species Sensitivity Distributions. [Computer Model]. 2008. Version 2. Ottawa (Canada). Intrinsikscience, Ottawa, Ontario.

[TOPKAT] Toxicity Prediction by Komputer Assisted Technology [Internet]. 2004. Version 6.2. San Diego (CA): Accelrys Software Inc. [cited May 2009]. Available from: http://www.accelrys.com/

[TRI] Toxics Release Inventory [database on the Internet]. 2007. TRI Explorer 4.8. Washington (DC): US Environmental Protection Agency. [cited 2009 Oct 6]. Available from: http://www.epa.gov/triexplorer/

[US EPA] United States Environmental Protection Agency. 2008. Supporting documents for initial risk-based prioritization of High Production Volume chemicals zinc dialkyldithiophosphates (ZDDP) Category. [cited 2009 November 6]. Available from http://www.epa.gov/champ/pubs/rbp/Cat_ZincDialkyldithiophosphates_Web_SuppDocs_Sept2008.pdf

[US EPA] US Environmental Protection Agency. 2009. High Production Volume Information System (HPVIS) [Internet]. Washington (DC): US EPA, Office of Pollution Prevention and Toxics. [cited 2009 July] Available from: http://www.epa.gov/hpvis/index.html

Versar. 1985. Methods of assessing exposure to chemical substances. Volume 7. Methods for assessing consumer exposure to chemical substances. Washington D.C.: U.S. Environmental Protection Agency. EPA 560/5-85-007.

[WATERNT] Water Solubility Program [Estimation Model]. 2002. Version 1.01. Washington (DC): U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. [cited 2009 June]. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm

Yamaguchi ES, Wilson DM, Kasrai M, Bancroft GM. 2002. XANES analysis of used engine oils and relationship to wear. Presented by: Society of Tribologists and Lubrication Engineers. Presented at: ASME/STLE Tribology Conference in Cancun, Mexico.

Appendix I. Robust Study Summary

Robust Study Summaries Form and Instructions: Aquatic iT				
No	**Item**	**Weight**	**Yes/No**	**Specify**
1	Reference: US EPA (2008)			
2	Substance identity: CAS RN	n/a		84605-29-8
3	Substance identity: chemical name(s)	n/a		Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and iso-propyl) esters, zinc salts
4	Chemical composition of the substance	2	N	
5	Chemical purity	1	N	
6	Persistence/stability of test substance in aquatic solution reported?	1	Y	
	Method			
7	Reference	1	Y	
8	OECD, EU, national, or other standard method?	3	Y	OECD Guideline for Testing of Chemicals #203 Fish Acute Toxicity Test
9	Justification of the method/protocol if a non-standard method was used	2		
10	GLP (good laboratory practice)	3	Y	
	Test organism			
11	Organism identity: name	n/a	Y	
12	Latin or both Latin and common names reported?	1	Y	*Oncorhynchus mykiss*
13	Life cycle age / stage of test organism	1	Y	Fingerlings
14	Length and/or weight	1	Y	Mean of 4.6 cm and 1.23 g
15	Sex	1		
16	Number of organisms per replicate	1	Y	
17	Organism loading rate	1	Y	0.62 g/L
18	Food type and feeding periods during the acclimation period	1	Y	Not fed during study
	Test design / conditions			
19	Test type (acute or chronic)	n/a		Acute
20	Experiment type (laboratory or field)	n/a		Lab
21	Exposure pathways (food, water, both)	n/a		Water
22	Exposure duration	n/a		96 hrs
23	Negative or positive controls (specify)	1	Y	Negative

24	Number of replicates (including controls)	1	N	
25	Nominal concentrations reported?	1	Y	
26	Measured concentrations reported?	3	N	
27	Food type and feeding periods during the long-term tests	1		
28	Were concentrations measured periodically (especially in the chronic test)?	1	N	
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	Y	
30	Photoperiod and light intensity	1	N	
31	Stock and test solution preparation	1	Y	
32	Was solubilizer/emulsifier used if the chemical was poorly soluble or unstable?	1		
33	If solubilizer/emulsifier was used, was its concentration reported?	1		
34	If solubilizer/emulsifier was used, was its ecotoxicity reported?	1		
35	Monitoring intervals (including observations and water quality parameters) reported?	1	Y	
36	Statistical methods used	1	Y	
Information relevant to the data quality				
37	Was the endpoint directly caused by the chemical's toxicity, not by organism’s health (e.g., when mortality in the control > 10%) or physical effects (e.g., shading effect)?	n/a	Y	
38	Was the test organism relevant to the Canadian environment?	3	Y	
39	Were the test conditions (pH, temperature, DO, etc.) typical for the test organism?	1	Y	
40	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	N	
41	Was pH of the test water within the range typical for the Canadian environment (6 to 9)?	1	Y	7.5–8.1
42	Was temperature of the test water within the range typical for the Canadian environment (5 to 27°C)?	1	Y	13.3–14.3

43	Was toxicity value below the chemical's water solubility?	3	Y	Empirical solubility is 15.8 mg/L
Results				
44	Toxicity values (specify endpoint and value)	n/a	n/a	LL_{50} (loading rate causing 50% mortality) = 4.5 mg/L
45	Other endpoints reported - e.g., BCF/BAF, LOEC/NOEC (specify)?	n/a	Y	No observed loading rate = 1.8 mg/L
46	Other adverse effects (e.g., carcinogenicity, mutagenicity) reported?	n/a	N	
47	***Score: ... %***	***73.8***		
48	***Environment Canada reliability code:***	***2***		
49	***Reliability category (high, satisfactory, low):***	***Satisfactory Confidence***		
50	***Comments***			

Appendix II: Estimated concentrations of zinc BDBP in environmental media using ChemCAN version 6.00 (ChemCAN 2003).[1]

Medium[2]	Estimated concentration
Ambient air[3]	0.0784 ng/m^3
Surface water[4]	14.5 ng/L
Soil[4]	415 ng/g solids
Sediment[4]	1149 ng/g solids

[1]The concentrations were estimated for the area of southern Ontario.
[2]Default inflow concentrations of 2 ng/m^3 in air and 3 ng/L in water were specified by ChemCAN.
[3]The degradation half-life in air was assumed to be 0.06709 day (AOPWIN 2000).
[4]Degradation processes in water, soil and sediment were assumed to be negligible. The HYDROWIN 2000 software is not capable of processing this structure to estimate an aqueous hydrolysis rate.

Appendix III. Estimates of total and media-specific daily intakes of zinc BDBP for various age groups

Route of exposure	Estimated intake (μg/kg-bw per day) of zinc BDBP by various age groups							
	0–0.5 years[1,2,3]			0.5–4 years[4]	5–11 years[5]	12–19 years[6]	20–59 years[7]	60+ years[8]
	Breast milk fed	Formula fed	Not formula fed					
Air[9]	$< 10^{-4}$	$< 10^{-4}$	$< 10^{-4}$	$< 10^{-4}$	$< 10^{-4}$	$< 10^{-4}$	$< 10^{-4}$	$< 10^{-4}$
Drinking water[10]	N/A	10^{-4}	10^{-3}	10^{-4}	10^{-4}	10^{-4}	10^{-4}	10^{-4}
Food and beverages[11]	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Soil[12]	10^{-3}	10^{-3}	10^{-3}	10^{-3}	10^{-4}	10^{-4}	10^{-4}	10^{-4}
Total intake	10^{-3}	10^{-3}	10^{-3}	10^{-3}	10^{-3}	10^{-4}	10^{-4}	10^{-4}
Maximum total intake from all routes of exposure: 10^{-3} μg/kg-bw per day								

1 No data were identified for concentrations of zinc BDBP in breast milk.

2 Assumed to weigh 7.5 kg, to breathe 2.1 m^3 of air per day, to drink 0.8 L of water per day (formula fed) or 0.3 L/day (not formula fed) and to ingest 30 mg of soil per day (Health Canada 1998).

3 For exclusively formula-fed infants, intake from water is synonymous with intake from food. The concentration of zinc BDBP in drinking water used to reconstitute formula was based on an estimated surface water concentration of 14.5 ng/L provided by ChemCAN version 6.00. For non-formula-fed infants, approximately 50% are introduced to solid foods by 4 months of age and 90% by 6 months of age (NHW 1990).

4 Assumed to weigh 15.5 kg, to breathe 9.3 m^3 of air per day, to drink 0.7 L of water per day and to ingest 100 mg of soil per day (Health Canada 1998).

5 Assumed to weigh 31.0 kg, to breathe 14.5 m^3 of air per day, to drink 1.1 L of water per day and to ingest 65 mg of soil per day (Health Canada 1998).

6 Assumed to weigh 59.4 kg, to breathe 15.8 m^3 of air per day, to drink 1.2 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

7 Assumed to weigh 70.9 kg, to breathe 16.2 m^3 of air per day, to drink 1.5 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

8 Assumed to weigh 72.0 kg, to breathe 14.3 m^3 of air per day, to drink 1.6 L of water per day and to ingest 30 mg of soil per day (Health Canada 1998).

9 The concentrations of zinc BDBP in ambient air and indoor air were based upon an estimated concentration in ambient air of 0.0784 ng/m^3 provided by ChemCAN version 6.00.

10 The concentration of zinc BDBP in drinking water was based upon an estimated concentration in surface water of 14.5 ng/L provided by ChemCAN version 6.00.

11 No data were identified upon which to estimate exposure from food.

12 The concentration of zinc BDBP in soil was based upon an estimated concentration in soil of 415 ng/g solids provided by ChemCAN version 6.00.

Appendix IV: Dermal exposure estimate for a do-it-yourself motor oil change

Assumptions	Calculations	Exposure estimates
DERMAL: Maximum weight fraction: 0.01 (Ford Motor Company 2002) Surface area of one hand: 0.043 m^2 (RIVM 2006) Density of motor oil: 0.89 g/mL (Ford Motor Company 2002) Film thickness retained on skin: 15.88×10^{-3} cm (Versar 1985) Adult body weight: 70.9 kg (Health Canada 1998) Uptake fraction: 1 (conservative)	Volume of product retained on one hand: $(0.043\ m^2)(15.88 \times 10^{-5}\ m)$ $= 6.828 \times 10^{-6}\ m^3$ = 6.828 mL Amount of product in contact with skin = (volume of product retained)(density) = (6.828 mL)(0.89 g/mL) = 6.08 g Amount zinc BDBP absorbed = (uptake fraction)(amount of product)(maximum weight fraction) / (adult body weight) = (1)(6.08 g)(0.01) / (70.9 kg) = 0.858 mg/kg-bw	Dermal acute (internal) dose: 0.858 mg/kg-bw

Appendix V: Summary of (Q)SAR Results for Zinc BDBP

(Q)SAR PREDICTIONS ON CARCINOGENICITY

Model/Species	Mice		Rat		Rat	Mice	Rodent	Mammal
	Male	Female	Male	Female				
Model Applier	N	N	N	N	N	N	N	-
Multicase CaseTox	NR	NR	NR	NR	-	-	NR	-
TopKat	NR	NR	NR	NR	-	-	-	-
Derek	-	-	-	-	-	-	-	NR

MA – Model Applier
CT – Multicase CaseTox
TK – TopKat
TT – Toxtree
BB – Benigni-Bossa rule
ND – not in domain
'-' No model available in QSAR suite
NR – No result
N- Negative

(Q)SAR PREDICTIONS ON GENOTOXICITY

Model/endpoints	chrom. ab.	chrom. ab. other rodent	chrom. ab. rat	micronucleus mice	micronucleus rodent	drosophila	drosophila HT	drosophila SLRL	mam. mutation	mam. mutation DL	UDS	UDS human lymphocytes	UDS rat hepatocytes	mouse lymphoma mut	*S. cerevisiae*	yeast	hgprt	*E. coli*	*E. coli* w	microbial	salmonella	BB
MA	N	N	ND	N	N	N	ND	N	ND	ND	N	N	ND	-	N	N	N	N	N	N	N	
CT	NR	-	-	NR	-	NR	-	-	-	-	NR	-	-	NR	-	-	-	-	-	-	NR	
TK	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	NR	
TT	-	-	-	-	N	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	N

MA – Model Applier
CT – Multicase CaseTox
TK – TopKat
TT – Toxtree
BB – Benigni-Bossa rule
ND – not in domain
'-' No model available in QSAR suite
NR – No result
N- Negative

(Q)SAR PREDICTIONS ON DEVELOPMENTAL TOXICITY

Model Applier

Endpoint/Species	Mice	Rabbit	Rat	Rodent
Retardation	ND	N	ND	N
Weight decrease	ND	N	N	N
Fetal death	ND	N	ND	N
Post impl. loss	ND	N	N	ND
Pre impl. loss	N	N	N	N
Structural	ND	N	ND	ND
Visceral	N	-	N	N

Multicase Casetox

Endpoint/Species	Hamster	Mammal	Miscellaneous
Teratogenicity	-	NR	NR
Developmental	NR	-	-

MA – Model Applier
CT – Multicase CaseTox
TK – TopKat
TT – Toxtree
BB – Benigni-Bossa rule
ND – not in domain
'-' No model available in QSAR suite
NR – No result
N- Negative

(Q)SAR PREDICTIONS ON REPRODUCTIVE TOXICITY

Model Applier

Model/ endpoint	Female			Male		
Species	Mice	Rat	Rodent	Mice	Rat	Rodent
Repro	ND	ND	ND	N	N	N
Sperm	-	-	-	N	N	N

Multicase CaseTox

Mice	Rat	Rabbit	Human
NR	NR	NR	NR

MA – Model Applier
CT – Multicase CaseTox
TK – TopKat
TT – Toxtree
BB – Benigni-Bossa rule
ND – not in domain
'-' No model available in QSAR suite
NR – No result
N- Negative

Appendix VI – PBT Model Inputs Summary Table

	Phys-Chem/Fate	Fate	Fate	Fate	PBT Profiling	Ecotoxicity
Model input parameters	EPI Suite (all models, including: AOPWIN, KOCWIN, BCFWIN, BIOWIN and ECOSAR)	STP (1) ASTreat (2) SimpleTreat (3) (required inputs are different depending on model)	EQC (required inputs are different if Type I vs. Type II chemical)	*Arnot-Gobas BCF/BAF Model (not used)*	*Canadian-POPs (including: Dimitrov Model, OASIS Toxicity Model) (not used)*	*Artificial Intelligence Expert System (AIEPS)/ TOPKAT/ (not used)*
SMILES	CC(CC(C)OP(OC(CC(C)C)C)(S[Zn]SP(OC(C)CC(C)C)(OC(C)CC(C)C)=S)=S)C					
Molecular weight (g/mol)	660.26	660.27	662.3			
Melting point (ºC)	-16		-16			
Boiling point (ºC)						
Data temperature (ºC)		20 (1)	20			
Density (kg/m^3)		0.96 (2)				
Vapour pressure (Pa)		1.17×10^{-4} (1, 3)	1.17×10^{-4}			
Henry's Law constant		1.49×10^{-2} (3)	1.49×10^{-2}			

(Pa·m³/mol)						
Log K_{aw} (Air-water partition coefficient) (dimensionless)						
Log K_{ow} (Octanol-water partition coefficient) (dimensionless)	12.32	12.32 (1)	12			
Log K_{oc} (Organic carbon-water partition coefficient – L/kg)						
Water solubility (mg/L)	3.05×10^{-2}	3.05×10^{-2} (1,3)	3.05×10^{-2}			
Log K_{oa} (Octanol-air partition coefficient) (dimensionless)						
Soil-water partition coefficient (L/kg)[1]		1.93×10^{8} (2,3)				
Half-life in air (hours)			0.816			
Half-life in water (days)			182			

Half-life in sediment (days)			728			
Half-life in soil (days)			182			
Metabolic rate constant (1/days)						
Biodegradation rate constant (1/days) or (1/hr) -specify		0.096 1/hr (3) 2.30 1/days (2)				
Biodegradation half-life in primary clarifier ($t_{1/2-p}$) (hr)		72 (1)				
Biodegradation half-life in aeration vessel ($t_{1/2-s}$) (hr)		7.2 (1)				
Biodegradation half-life in settling tank ($t_{1/2-s}$) (hr)		7.2 (1)				

[1] derived from log K_{oc}