# Substance Profile for The Challenge Phenol, 4,4' -(1-methylethylidene)bis-(Bisphenol A) CAS No. 80-05-7

# Introduction

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

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

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

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

Based on a consideration of the ecological and/or human health concerns associated with these substances, and the requirement under section 76.1 of CEPA 1999 for the Ministers to apply a weight of evidence approach and the precautionary principle when conducting

and interpreting the results of an assessment, sufficient data are currently available to conclude whether these substances meet the criteria under section 64 of CEPA 1999.

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

The substance Phenol, 4,4' -(1-methylethylidene)bis- (Bisphenol A) was identified as a high priority for action as it was determined to have a high potential for exposure to individuals in Canada (GPE), and is considered to present a high hazard to human health. The technical human health and ecological information that formed the basis for concern associated with this substance is contained in Appendices I and II, respectively.

CAS Registry Number	80-05-7			
Inventory names	Phenol, 4,4' -(1-methylethylidene)bis-			
Other names	Bisphenol A, 4,4'-Isopropylidenediphenol, Diphenylolpropane, BPA			
Chemical group	Organics			
Chemical sub-group	Phenols			
Chemical formula	$C_{15}H_{16}O_2$			
Chemical structure				
SMILES	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1			
Molecular mass	228.29 g/mol			

# Substance Identity

Based on information submitted by the 19 companies that notified this substance to the Domestic Substances List, approximately 12,100,000 kilograms of bisphenol A were in commerce in 1986 for a variety of uses including (but not limited to) the categories of paint/coating additives, antioxidant/corrosion inhibitors, monomers, polymers and formulation components. Other potential uses of the substance in Canada include: adhesive/ binder/sealant, catalyst/accelerator/initiator/, colourant in pigments and dyes, and plastics and synthetic resins.

# THE CHALLENGE

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

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

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

## Section 71 Notice

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

The information mandated through the notices may relate to, among other things; quantity of the substance imported, manufactured, used, or released, concentrations, suppliers, customers, as well as types of uses of the substance. Copies of the section 71 notice and guidance on how to comply with it are available from the Government of Canada Chemicals Portal (www.chemicalsubstanceschimiques.gc.ca), or from the contact provided below.

# **Opportunity to Submit Additional Information to Inform Screening** Assessment

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

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

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

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

<sup>&</sup>lt;sup>1</sup> "Guidelines for the Notification and Testing of New Substances: Chemicals & Polymers (version 2005)", Government of Canada, Available from <u>http://www.ec.gc.ca/substances/nsb/eng/cp\_guidance\_e.shtml</u>

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

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

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

Additional information is being invited in the following areas:

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

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

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

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

#### **Request for Documents and Submission of Information**

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

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

# Appendix I Human Health Information to Support The Challenge for Phenol, 4,4'-(1-methylethylidene)bis-(Bisphenol A) CAS No. 80-05-7

# Introduction

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

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

Bisphenol A (CAS No. 80-05-7) is considered to meet the criteria for GPE under SimET and for high hazard under SimHaz. This document summarizes the currently available information used to support the inclusion of this substance in the Challenge.

# **Exposure Information from Health Related Components of DSL Categorization**

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

#### **Results of the Application of SimET**

Bisphenol A has been determined to be GPE based on a consideration of the DSL nomination information listed below.

## **Nomination Information for DSL**

#### **Quantity in Commerce**

The quantity reported to be manufactured, imported or in commerce in Canada during the calendar year 1986 was 12,100,000 kg.

#### Number of Notifiers

The number of notifiers for the calendar years 1984-86 was 19.

#### **Use Codes and Description**

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

- 4 Adhesive/binder/sealant/filler Antioxidant/corrosion inhibitor/tarnish
- 7 inhibitor/scavenger/antiscaling agent
- 8 Catalyst/accelerator/initiator/activator
- 13 Colourant pigment/stain/dye/ink
- 21 Formulation component
- 28 Monomer
- 34 Polymer additive
- 36 Polymer, component of a formulation
- 51 Function other than that listed in codes 02-50
- 52 Adhesive and Sealant Production
- 76 Organic Chemicals, Industrial
- 77 Organic Chemicals, Specialty
- 80 Paint and Coating
- 86 Plastics
- 87 Plastics and Synthetic Resins
- 98 Used in industry other than those specified in codes 51-97

#### Potential Uses in Canada

Bisphenol-A is used primarily as an industrial raw precursor to the manufacturing of polycarbonates and, epoxy resins.

Use of bisphenol-A in polycarbonate manufacturing can impart the following desired properties including clarity, impact resistance and ductility to many polycarbonate end-products. Examples of polycarbonate products include compact discs and their jewel cases, medical devices, food and beverage contact containers such as milk and water bottles (EU RAR, 2003). Tablewares such as plates and mugs are some consumer products manufactured. Copolycarbonates have a variety of uses in both the automotive and electronic industries as functional components in injection moulding manufacturing techniques.

Bisphenol-A is also used in the manufacturing of epoxy resins for applications as protective coatings, structural composites, electrical laminates and as adhesives and sealants including dental sealants. Use of bisphenol-A in epoxy resin manufacturing can impart the following desired properties including chemical resistance, heat resistance and adhesion. Cured epoxy resins are inert and have been used as liners in metal cans for foods and beverages.

Bisphenol A can also be used as a precursor for the manufacturing of other resins such as phenolplast resins, phenolic resins and unsaturated polyester resins.

# Hazard Information from Health Related Components of DSL Categorization

#### Simple Hazard Tool (SimHaz)

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

#### **Results of the Application of SimHaz**

Bisphenol A is considered to be a potentially high hazard substance based on its classification for reproductive toxicity by the European Commission (EC).

The European Commission has classified Bisphenol A as Category 3 for reproductive toxicity (Substance which causes concern for human fertility) (ECB, 2003).

## Uncertainties

SimET and SimHaz have been developed as robust tools for effectively identifying substances from the DSL that are considered to be human health priorities for further consideration. It is recognized that they do not include a number of elements normally considered in a human health risk assessment such as a comprehensive characterization of exposure and hazard, a comparison of exposure metrics to hazard metrics and a detailed analysis of uncertainties; however, as a result of the combination of the severe hazard properties of these substances and their high potential for exposure to humans, evaluation of the need for preventative and protective actions is required.

## References

ECB (European Chemicals Bureau. Summary Record). 2003. Meeting of the Commission Working Group on the Classification and Labelling of Dangerous Substances. ECBI/50/03.

http://ecb.jrc.it/classlab/SummaryRecord/6302r5 sr CMR0902.doc

EU RAR. 2003. European Union Risk Assessment Report on Bisphenol A. http://ecb.jrc.it/DOCUMENTS/Existing-Chemicals/RISK\_ASSESSMENT/REPORT/bisphenolareport325.pdf

Health Canada. 2003. Proposal for Priority Setting for Existing Substances on the Domestic Substances List under the Canadian Environmental Protection Act, 1999: Greatest Potential for Human Exposure.

http://www.hc-sc.gc.ca/ewh-semt/alt formats/hecs-

sesc/pdf/pubs/contaminants/existsub/exposure/greatest\_potential\_human\_exposurerisque\_exposition\_humaine\_e.pdf

Health Canada 2005. Proposed Integrated Framework for the Health-Related Components of Categorization of the Domestic Substances List under CEPA 1999. http://www.hc-sc.gc.ca/ewh-semt/alt\_formats/hecssesc/pdf/contaminants/existsub/framework-int-cadre\_e.pdf

# Appendix II Ecological Information to Support The Challenge for Phenol, 4,4 -(1-methylethylidene)bis-(Bisphenol A) CAS No. 80-05-7

# Introduction

The information in this document will form the basis of a screening assessment under section 74 of CEPA 1999. Data relevant to an ecological screening assessment were identified in original literature, review documents, commercial and government databases prior to December 2005. Properties and characteristics may also have been estimated using Quantitative Structure Activity Relationship (QSAR) models. Additional information relating to the potential persistence, bioaccumulation and inherent toxicity of bisphenol A in the environment was submitted in April 2005 by the BPA (Bisphenol A) Global Industry Group of the American Plastics Council/PlasticsEurope/Japan Chemical Industry Association, and this information was considered in the determination of these characteristics for the purposes of categorization.

# **Physical and Chemical Properties**

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

<b>D</b> uce outer	T-m o	Value	Tommonotrano	Defener ee
Property	туре	value	remperature	Reference
			( <b>C</b> °)	
Melting point	Experimental	153		Syracuse Research
(°C)				Corporation 2003
	Modelled	131.76		MPBPWIN v1.41
Boiling point	Modelled	363.54		MPBPWIN v1.41
(°C)				
Density (kg/m <sup>3</sup> )	Experimental	1.195	25	Dorn et al. 1987
Vapour pressure	Experimental	5.3E-6	25	Bayer AG 1988
(Pa)	Modelled	3.026E-5	25	MPBPWIN v1.41
		(2.27E-7 mm		
		Hg)		
Henry's Law	Experimental	1.0E-6		Hine and Mookerjee
constant		(1.0E-11		1975
(Pa·m <sup>3</sup> /mol)		atm·m <sup>3</sup> /mol)		
	Modelled	9.28E-7	25	HENRYWIN v3.10
		(9.159E-12		
		atm·m <sup>3</sup> /mol)		
Log Kow	Experimental	3.32		Howard 1989;
(Octanol-water				Hansch et al. 1995
partition coefficient)	Modelled	3.64		KOWWIN v1.67

 Table 1. Physical and chemical properties for bisphenol A

(dimensionless)				
Water solubility	Experimental	120	25	Dorn et al. 1987
(mg/L)	Modelled	172.7	25	WSKOWWIN v1.41
pKa (Acid dissociation constant) (dimensionless)	Experimental	9.59 - 11.30		Staples et al. 1998
Log Koc (Organic carbon-water partition coefficient) (dimensionless)	Modelled	4.876		PCKOCWIN v1.66

# Manufacture, Importation, and Uses

Available information is presented in Appendix I.

# **Releases, Fate and Presence in the Environment**

#### Releases

There are no references in the published literature to the natural occurrence of bisphenol A in the environment.

Based on moderate water solubility, wastewaters and washing residue generated during manufacturing and processing activities are the most likely sources of bisphenol A into the environment (Cousins et al. 2002). Unintentional release of fugitive dust from closed systems during processing, handling and transportation of the substance may also occur. Bisphenol A has low vapour pressure at typical environmental temperatures; however, elevated temperatures occurring during some processing operations may increase the vapour pressure, resulting in formation and possible emission of gaseous bisphenol A from manufacturing facilities. The potential for fugitive gaseous emission from products in use is considered negligible, as the majority of the substance is reacted to completion during product manufacturing and any residual unreacted amount would have low vapour pressure and be nonvolatile (Cousins et al. 2002).

The National Pollutant Release Inventory (NPRI) has tracked the release of bisphenol A from industrial facilities in Canada since the 1990's. Table 2 provides a summary of NPRI on-site release and total disposal data over the period 2001 to 2005. Where information was provided, on-site releases were exclusively to the air compartment. Most recent reporting (2005) indicates total on-site releases of 120 kilograms, a decrease from that seen in previous years (Environment Canada 2007).

In addition, it should also be acknowledged that only facilities that meet established reporting criteria are required to report to the NPRI.

Year	Releases to air	Releases to	Releases to	Total releases	Total disposed
		water	land		
2001	2904	-	-	2904	4919
2002	-	-	-	44	5543
2003	5	-	-	8770	13953
2004	5523	-	-	5525	8452
2005	120	-	-	120	1154

Table 2: NPRI release and disposal data (kg) for bisphenol A from 2001 to 2005

#### Fate

Bisphenol A is characterized by having low vapour pressure, moderate water solubility and moderately high partition coefficients. The high pKa range of 9.59 to 11.30 (see Table 1) indicates that bisphenol A is a very weak acid. While ionization of the substance may occur at high pH, there is unlikely to be appreciable ionization at environmental pH levels of 7 and lower (Cousins et al. 2002). Cousins et al. (2002) consider that chemicals such as bisphenol A which have measurable vapour pressures, aqueous solubilities and octanol-water partition coefficients (Kow), will likely partition to some extent in all available environmental phases. As a moderately hydrophobic substance with some water solubility, bisphenol A can be expected to partition to organic phases such as sediments and soils; however, an appreciable fraction will also likely be present in the dissolved phase (Cousins et al. 2002). This suggests that the medium of release may be particularly important in predicting the partitioning behaviour and fate of bisphenol A in the environment.

Level III fugacity modelling (Table 3) predicts that when bisphenol A is released exclusively into water, the majority (95.5%) will remain within the water column with only a small fraction (4.53%) moving into sediment. When released to air or soil, or when equal proportions are released to all three media, most bisphenol A (87.5% to 99.3%) will partition to the soil compartment, with smaller amounts expected to be present in water and sediment. Bisphenol A is not predicted to remain within air, even when released exclusively into that compartment.

	Fraction of Substance Partitioning to Each Medium (%)					
Substance Released to:	Air	Water	Soil	Sediment		
- Air (100%)	0.00	3.06	96.8	0.15		
- Water (100%)	0.00	95.5	0.0	4.53		
- Soil (100%)	0.00	0.68	99.3	0.03		
- Air, water, soil (33% each)	0.00	11.9	87.5	0.57		

 Table 3: Results of the Level III fugacity modelling (EPIWIN v3.12)

Eisenreich et al. (1981) predicted that bisphenol A released into the atmosphere would exist almost entirely in the particulate phase and would be subject to removal through dry deposition or photolysis. The small fraction present as vapour would react with photochemically generated hydroxyl radicals (half-life approximately 0.13 days; AOPWIN v1.91) or undergo photolysis. Photodegradation products formed include

phenol, 4-isopropylphenol, and a semiquinone derivative of bisphenol A (Syracuse Research Corporation 2003).

Biodegradation is expected to be the dominant fate process for bisphenol A released into water. Biodegradation half-lives of less than four days were measured in natural waters following an adaptation period (acclimation) of from one to four days (Dorn et al. 1987). A slower rate of biodegradation is expected to occur in non-acclimated waters; other processes such as sorption to suspended solids and sediments and photolysis may also take place. Bisphenol A is not expected to undergo hydrolysis due to the lack of hydrolyzable functional groups (Lyman et al. 1982). The low Henry's Law constant suggests that volatilization is unlikely to be a significant removal process.

The moderate water solubility of bisphenol A implies the substance will exhibit low to moderate mobility when released to soil (Dorn et al. 1987). Results from biodegradation testing in aqueous systems (Dorn et al. 1987; Matsui et al. 1975) suggest bisphenol A may biodegrade in aerobic soils following acclimation; however, it is not expected to undergo chemical hydrolysis or to volatilize significantly from soil surfaces (Syracuse Research Corporation 2003).

#### Presence in the Environment

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

# **Evaluation of P, B and iT Properties**

#### **Environmental Persistence**

Based on empirical and modelled data, bisphenol A is not expected to be persistent in the environment.

Bisphenol A demonstrated rapid biodegradation in standard 28-day ready biodegradability testing (West et al. 2001; Table 4a) and can therefore be considered not persistent in water and soil. The modelled data support this conclusion, with BIOWIN v4.02 predicting an ultimate biodegradation half-life of 37.5 days (Table 4b).

The predicted half-life for atmospheric degradation due to reaction with the hydroxyl radical is 0.133 day (Table 4b), indicating that bisphenol A will likely be rapidly oxidized in air. As well, the substance may be subject to reaction with atmospheric nitrate radicals (AOPWIN v1.91).

1 abic 4a. 1	able 4a. Emphical data for persistence								
Medium	Fate Process	Degradation Value	<b>Endpoint/Units</b>	Reference					
Water	Biodegradation	89	Biodegradation, %	West et al. 2001					

#### Table 4a. Empirical data for persistence

Medium	Fate Process	Degradation Value	<b>Endpoint/Units</b>	Reference
Air	Atm. oxidation	0.133	Half-life, days	AOPWIN v1.91
Air	Ozone reaction	No estimate. Reaction with nitrate radicals may be important.	Half-life, days	AOPWIN v1.91
Water/Soil	Biodegradation	37.5	Half-life, days	BIOWIN v4.02, Ultimate survey
Water/Soil	Biodegradation	0.6866	Probability	BIOWIN v4.02, Linear
Water/Soil	Biodegradation	0.4653	Probability	BIOWIN v4.02, Non-linear
Water/Soil	Biodegradation	0.2956	Probability	BIOWIN v4.02, MITI linear
Water/Soil	Biodegradation	0.1559	Probability	BIOWIN v4.02, MITI non-linear

Table 4b. Modelled data for persistence

A biodegradation half-life for sediment was estimated using Boethling's extrapolation factors (Boethling et al. 1995); that is,  $t_{1/2 \text{ soil}} : t_{1/2 \text{ water}} : t_{1/2 \text{ sediment}} = 1$ : 1: 4. BIOWIN v4.02 estimates a soil half-life of 37.5 days (Table 4a), therefore the predicted half-life in water is also 37.5 days and that in sediment is 150 days.

The empirical and modelled data (Tables 4a and 4b) demonstrate that bisphenol A does not meet the persistence criteria (half-life in air  $\ge 2$  days, in soil and water  $\ge 182$  days, in sediment  $\ge 365$  days) as set out in the Persistence and Bioaccumulation Regulations (Government of Canada 2000).

#### Potential for Bioaccumulation

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The empirical and modelled log Kow values of 3.32 and 3.64, respectively, suggest that bisphenol A may have some potential to accumulate in organisms. However, laboratory-derived bioconcentration factor (BCF) values of 9.16 and 43.7 L/kg (Table 5a) obtained in testing with fish indicate the substance has low bioaccumulation potential. The observed difference may be attributable to metabolic capability, a factor not incorporated into estimations of bioaccumulation based on the log Kow.

A range of QSAR modelled bioaccumulation and bioconcentration values are available, with bioaccumulation factor (BAF) or BCF values of 5.20 (GOBAS BCF 5%T2LTL) to 956 (OASIS; Table 5b). Nearly all values support the conclusion of low bioaccumulation potential derived from the experimental data.

Table 5a. Empirical data for bioaccumulation					
Test Organism Endpoint Value wet wt Reference					
Fish	BCF	9.16 – 43.7 L/kg	CITI 1992		

Table 5b. Modelled data for bioaccumulation						
Test Organism	Endpoint	Value wet wt	Reference			
Fish	BAF	5.23 L/kg	GOBAS BAF T2MTL			
		-	(Arnot and Gobas 2003)			
Fish	BCF	5.20 L/Kg	GOBAS BCF 5%T2LTL			
		_	(Arnot and Gobas 2003)			

Fish	BCF	956 L/kg	OASIS v1.20
Fish	BCF	71.8 L/kg	BCFWIN v2.15

The weight of evidence indicates that bisphenol A does not meets the bioaccumulation criteria (BCF,  $BAF \ge 5000$ ) as set out in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000).

#### **Ecological Effects**

#### A - In the Aquatic Compartment

Empirical and modelled data indicate that bisphenol A has the potential to cause acute adverse effects in aquatic organisms at low concentrations (i.e.,  $L(E)C_{50}$  values at or approaching 1 mg/L; see Tables 6a and b).

- word own minipulate						
Test Organism	Type of Test	Endpoint	Value	Reference		
			(mg/L)			
Algae (Diatom)	Acute	$EC_{50}^{1}$	1	Alexander et al. 1988		
Crustacean (Mysid)	Acute	$LC_{50}^{2}$	1.1	Alexander et al. 1988		
Frog	Acute	$LT_{50}^{3}$	1	Koponen and Kukkonen		
				2002		

#### Table 6a. Empirical data for aquatic toxicity

Notes:

<sup>1</sup> median effective concentration

<sup>2</sup> median lethal concentration

<sup>3</sup> median lethal time

Alexander et al. (1988) examined the acute toxicity of bisphenol A to the diatom, *Skeletonema costatum*, and mysid shrimp, *Mysidopsis bahia*. The 96-h EC<sub>50</sub> for *S. costatum* was 1.0 mg/L, based on significantly reduced cell counts, while the mean 96-h  $LC_{50}$  for *M. bahia* was 1.1 mg/L (range 0.92 to 1.2 mg/L).

Bisphenol A was shown to adversely affect embryo development in the frog, *Rana temporaria* (Koponen and Kukkonen 2002). An LT50 (time to 50% lethality) of 72 hours was reported at a test concentration of 1 mg/L, indicating significant toxicity occurred at this concentration.

Test Organism	Type of Test	Endpoint	Value	Reference
			(mg/L)	
Fish	Acute	LC <sub>50</sub>	3.275	ECOSAR v.0.99h
Fish	Acute	LC <sub>50</sub>	4.3	TOPKAT v6.2
Fish	Acute	LC <sub>50</sub>	4.797763	ASTER
Fish	Acute	LC <sub>50</sub>	7.2217	OASIS
Fish	Acute	LC <sub>50</sub>	8.47996	PNN (Kaiser et al. 2002)
Daphnid	Acute	LC <sub>50</sub>	2.623	ECOSAR v.0.99h
Daphnid	Acute	EC <sub>50</sub>	5.2	TOPKAT v6.2
Green Algae	Acute	EC <sub>50</sub>	4.01	ECOSAR v.0.99h

#### Table 6b. Modelled data for aquatic toxicity

Acute aquatic toxicity estimates derived from QSAR models are in the range of 2 to 9 mg/L (Table 6b), slightly above results obtained experimentally. However, the predicted values are sufficiently close to those of laboratory studies to support a decision of potential acute aquatic toxicity at low concentrations. The weight of experimental and modelled evidence indicate that bisphenol A can be considered highly hazardous to the aquatic environment.

#### **B** - In Other Media

No effects studies for non-aquatic non-human organisms were found for this substance.

# Potential to Cause Ecological Harm

Based on the available information, bisphenol A does not persist in the environment and is not bioaccumulative based on criteria defined in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000). Information on concentrations of bisphenol A in the environment has not been identified at this time. However, the experimental and modelled ecotoxicological data indicate that bisphenol A could cause harm to aquatic organisms at relatively low concentrations. Information on potential impacts in other environmental compartments has not been identified.

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