Screening Assessment for the Challenge

Phosphonium, triphenyl(phenylmethyl)-, salt with 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (1:1)

Chemical Abstracts Service Registry Number
75768-65-9

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 Phosphonium, triphenyl(phenylmethyl)-, salt with 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (1:1) (PTPTT), Chemical Abstracts Service Registry Number 75768-65-9. This substance was identified as a high priority for screening assessment and included in the Ministerial Challenge because it had been found to meet the ecological categorization criteria for persistence, bioaccumulation potential and inherent toxicity to non-human organisms and was believed to be in commerce in Canada.

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

PTPTT is an organic salt that is used in Canada primarily as a cross linking agent and vulcanization accelerator in the manufacture of fluoroelastomers, a class of synthetic rubbers used in industrial applications requiring high resistance to chemicals and heat. The substance is not naturally produced in the environment. It is not reported to be manufactured in Canada; however, between 100 and 1000 kg of the salt were imported into the country in 2006 for use in the manufacturing of fluoroelastomer containing products.

Based on reported use patterns and certain assumptions, in Canada most of the substance is chemically transformed during the curing process of the fluoroelastomer rubbers. About 0.1% is estimated to be released to wastewater, 0.1 % is expected to be sent to landfills and no releases are predicted to air. PTPTT is an ionic compound which (based on new information) is expected to dissociate into a benzyltriphenyl phosphonium (BTP) cation and bisphenol AF (BPAF) if released in the aquatic environment. The BPAF component will be in a neutral form in the aquatic environment at circum-neutral to acidic pH but will dissociate into its anionic form at alkaline pH. Because of this dissociation behaviour, the assessment of PTPTT focuses to a large extent on the dissociation products BTP and BPAF.

PTPTT and its dissociation products present low experimental and predicted solubility in water and, in the case of BTP, moderate measured solubility in 1-octanol (920 mg/L). Upon dissociation if released into the aquatic environment, BTP and BPAF are expected to largely remain in the water column with a smaller amount likely binding to suspended solids and settling to sediments. Neither PTPTT nor its dissociation products are volatile, and the substances are expected to be largely immobile if released to soil.

Based on their physical and chemical properties, PTPTT's dissociation products are expected to be persistent in all media with the exception of the atmosphere. In addition,

experimental data relating to the solubility of BTP in octanol and water, as well as bioaccumulation model predictions for BTP and BPAF, suggest that these substances have a low potential to accumulate in the lipid tissue of organisms. The dissociation products of PTPTT therefore meet the persistence criteria but do not meet the bioaccumulation criteria as set out in the *Persistence and Bioaccumulation Regulations*. Aquatic toxicity data for PTPTT's dissociation products suggest that BTP has a low potential to harm aquatic organisms, but that BPAF may be harmful depending on exposure concentrations.

Based on a very conservative exposure scenario in which an industrial operation (user of PTPTT) discharges the substance into the aquatic environment, and assuming complete PTPTT dissociation in solution, predicted environmental concentration in water (PEC) for BTP and BPAF were below predicted no-effect concentrations (PNECs) calculated for sensitive aquatic species. Therefore, based on the information presented in this screening assessment, it is concluded that PTPTT 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.

Exposure of the general population in Canada to PTPTT from environmental media is expected to be negligible based on the limited amount imported into Canada on an annual basis, the form that it is imported in, and its use. PTPTT is imported as a component of solid-state fluoroelastomer precompounds, which are subsequently cured at fluoroelastomer processing facilities. It is believed that PTPTT is almost fully consumed (transformed) during this process and that potential residual levels in manufactured products would be only at trace levels, leading to negligible exposure of the general population. Since very small amounts (< 1 kg) of PTPTT could be potentially released into water each year, exposure to any dissociation products would be negligible and therefore these dissociation products were not considered in the human health screening assessment.

There is a limited health effects database available for PTPTT however, the available empirical data and information from predictive models is not suggestive of high hazard.

As exposure of the general population in Canada is expected to be negligible, the risk to human health is considered to be low. On the basis of the carcinogenicity of PTPTT, for which there may be a probability of harm at any level of exposure, and applying a precautionary approach, it is concluded that PTPTT 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 PTPTT does not meet any of the criteria set out in section 64 of the *Canadian Environmental Protection Act, 1999*.

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

Introduction

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

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

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

The Ministers therefore published a notice of intent in the *Canada Gazette*, Part I, on December 9, 2006 (Canada 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 phosphonium, triphenyl(phenylmethyl)-, salt with 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (1:1) was identified as a high priority for assessment of ecological risk as it had been found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and is believed to be in commerce in Canada.

The Challenge for this substance was published in the *Canada Gazette* on January 31st 2009 (Canada 2009). A substance profile was released at the same time. The substance profile presented the technical information available prior to December 2005 that formed the basis for categorization of this substance. As a result of the Challenge, submissions of information pertaining to the use and physical and chemical properties of the substance were received.

Although phosphonium, triphenyl(phenylmethyl)-, salt with 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (1:1) 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 September 2009. 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 also undergone external written peer review/consultation. Additionally, the draft of this screening assessment was subject to a 60-day public comment period. While external comments were taken into consideration, the final content and outcome of the screening assessment remain the responsibility of Health Canada and Environment Canada. Approaches used in the screening assessments under the Challenge have been reviewed by an independent Challenge Advisory Panel. The critical information and considerations upon which the assessment is based are summarized below.

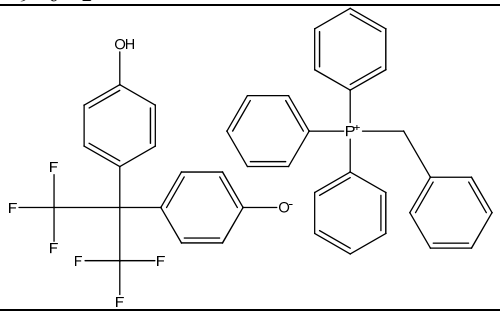
[1] A determination of whether one or more of the criteria of section 64 are met is based upon an assessment of potential risks to the environment and/or to human health associated with exposures in the general environment. For humans, this includes, but is not limited to, exposures from ambient and 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 PTPTT, derived from the DSL inventory name Phosphonium, triphenyl(phenylmethyl)-, salt with 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (1:1). Information on the identity of PTPTT is presented in Table 1a. Since the substance is an organic salt, it is expected to dissociate upon its release in the environment and to dissolve in water into equal proportions of the positively charged cation benzyltriphenyl phosphonium (BTP) (CAS RN 15853-35-7) and the negatively charged anion phenol, 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis- whose neutral form corresponds to the substance bisphenol AF (BPAF) (CAS RN 1478-61-1). Because of the particular behavior of PTPTT as a salt, information on the identities of its dissociation products is also presented in Table 1b and 1c. It is noted that the Simplified Molecular Input Line Entry System (SMILES) notations presented in Tables 1a and 1b do not reflect the ionic nature of each compound since quantitative structure-activity relationship (QSAR) models only accept the neutral form of a chemical as input.

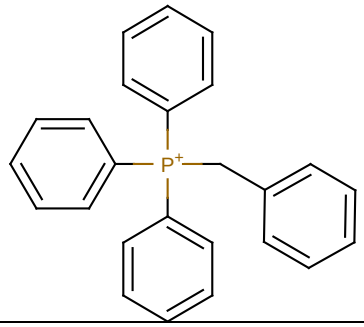
Table 1a. Substance identity for PTPTT

Chemical Abstracts Service Registry Number (CAS RN)	**75768-65-9**
DSL name	**Phosphonium, triphenyl(phenylmethyl)-, salt with 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (1:1)**
National Chemical Inventories (NCI) names[1]	*Phosphonium, triphenyl(phenylmethyl)-, salt with 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (1:1)* (PICCS, ASIA-PAC, NZIoC) *benzyltriphenylphosphonium, salt with 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (1:1)* (EINECS) *Phosphonium, triphenyl(phenylmethyl)-, salt with 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (1:1)* (AICS) *Benzyltriphenylphosphonium, salt with 4, 4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (1:1)* (ECL) *Phosphonium,triphenyl(phenylmethyl)-,salt with 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethyl idene)bis[phenol](1:1)* (PICCS)
Other names	*4,4'-(Hexafluoroisopropylidene)diphenol benzyltriphenylphosphonium salt (1:1)*
Chemical group (DSL Stream)	Discrete organics
Major chemical class or use	Phenols
Major chemical sub-class	Fluorinated
Chemical formula	$C_{25}H_{22}P$. $C_{15}H_9F_6O_2$
Chemical structure	
SMILES used in QSAR models[2]	c1cccc(c1)P(c1ccccc1)(c1ccccc1)(Cc1ccccc1)Oc1ccc(C(C(F)(F)F)(C(F)(F)F)c2ccc(O)cc2)cc1
Molecular mass	688.645 g/mol

[1] National Chemical Inventories (NCI). 2009: AICS (Australian Inventory of Chemical Substances); ASIA-PAC (Asia-Pacific Substances Lists); ECL (Korean Existing Chemicals List); EINECS (European Inventory of Existing Commercial Chemical Substances); 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 Line Input Entry System used in quantitative structure-activity relationship modelling taken from EPIWEB (2009)

Table 1b. Substance identity for benzyltriphenylphosphonium (BTP)

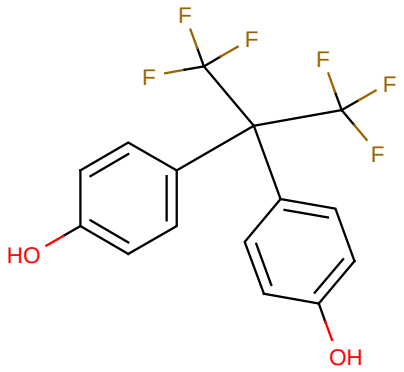
Chemical Abstracts Service Registry Number (CAS RN)	**15853-35-7**
DSL name	**n/a**
National Chemical Inventories (NCI) names[1]	*benzyltriphenylphosphonium* (EINECS, ENCS) *Phosphonium, triphenyl(phenylmethyl)-* (ASIA-PAC)
Other names	*NSC 167253* *Phosphonium, benzyltriphenyl-* *Triphenylbenzylphosphonium ion*
Chemical group (DSL Stream)	Discrete organics
Major chemical class or use	Phosphonium compounds; phenyl compounds
Major chemical sub-class	Phenylphosphonium compounds
Chemical formula	$C_{25}H_{22}P$
Chemical structure	
SMILES used in QSAR models[2]	c1(ccccc1)CP(c1ccccc1)(c1ccccc1)c1ccccc1
Molecular mass	353.423 g/mol

[1] National Chemical Inventories (NCI). 2009: ASIA-PAC (Asia-Pacific Substances Lists); EINECS (European Inventory of Existing Commercial Chemical Substances) and ENCS (Japanese Existing and New Chemical Substances);.

[2] Simplified Molecular Line Input Entry System used in quantitative structure-activity releationship modelling taken from EPIWEB (2009)

Table 1c. Substance identity for bisphenol AF (BPAF)

Chemical Abstracts Service Registry Number (CAS RN)	**1478-61-1**
DSL name	**Phenol, 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis-**
National Chemical Inventories (NCI) names[1]	*4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]diphenol* (EINECS) *4,4'-[2,2,2-Trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol]* (ENCS) *Phenol, 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis-* (AICS) *4,4'-[2,2,2-Trifluoro-1-(trifluoromethyl)ethylidene]bisphenol* (ECL) *BISPHENOL AF* (PICCS) *BISPHENOL, 4,4'-[2,2,2-TRIFLUORO-1-(TRIFLUOROMETHYL)ETHYLIDENE]-* (PICCS))
Other names	*1,1,1,3,3,3-Hexafluoro-2,2-bis(4-hydroxyphenyl)propane* *2,2-Bis(4'-hydroxyphenyl)hexafluoropropane* *2,2-Bis(4-hydroxyphenyl)-1,1,1,3,3,3-hexafluoropropane* *2,2-Bis(4-hydroxyphenyl)hexafluoropropane* *2,2-Bis(4-hydroxyphenyl)perfluoropropane* *2,2-Bis(p-hydroxyphenyl)hexafluoropropane* *4,4'-(Hexafluoroisopropylidene)diphenol* *4,4'-[2,2,2-Trifluoro-1-(trifluoromethyl)ethylidene]bisphenol* *Biphenol AF, BIS-AF, Bisphenol AE, Cheminox BAF* *Curative 30, GP 21, Hexafluorobisphenol A* *Hexafluorodiphenylolpropane* *Hexafluoroisopropylidenebis(4-hydroxybenzene)* *NSC 152522* *Phenol, 4,4'-(bis(trifluoromethyl)methylene)di-* *Phenol, 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]di-* *Phenol, 4,4'-[trifluoro-1-(trifluoromethyl)ethylidene]di*
Chemical group (DSL Stream)	Discrete organics
Major chemical class or use	Phenols
Major chemical sub-class	Bisphenols
Chemical formula	$C_{15}H_{10}F_6O_2$

Chemical structure	
SMILES used in QSAR models[2]	FC(F)(F)C(c1ccc(O)cc1)(c1ccc(O)cc1)C(F)(F)F
Molecular mass	336.23 g/mol

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

[2] Simplified Molecular Line Input Entry System used in quantitative structure-activity relationship modelling taken from EPIWEB (2009)

Physical and Chemical Properties

Table 2 contains experimental, analogue and modelled physical and chemical properties of PTPTT and its dissociation products BTP and BPAF that are relevant to their environmental fate. The key study from which experimental data were reported for some of these properties was critically reviewed for validity. This review (Robust Study Summary) is found in Appendix I.

Models based on quantitative structure-activity relationships (QSARs) were used to generate data for some of the physical and chemical properties of PTPTT and its dissociation products BTP and BPAF. These models (except WSKOWWIN 2000) are mainly based on fragment addition methods, i.e., they rely on the structure of a chemical. Since these models only accept the neutral form of a chemical as input (in SMILES form), the modelled values shown in Table 2 apply to the neutral forms of PTPTT, BTP and BPAF.

The experimental log K_{ow} value of 2.6 and water solubility value of 4.5 mg/L generated for PTPTT (Environment Canada 2009a) were used as empirical inputs in all models when possible, to generate more accurate predictions by decreasing the dependency on modelled data. It is noted that although PTPTT's log K_{ow} value and solubility were measured indirectly by monitoring the solubility of the BTP cation in both aqueous and octanol solutions, this information is weighted more heavily than modelled information. In addition, the experimental log K_{ow} value of 2.6 and water solubility value of 2.31 mg/L were used as empirical inputs for BTP in all models when possible (Environment Canada 2009a).

Although melting point and water solubility data from Material Safety Data Sheets (MSDS) are available for many halogen arylphosphonium salts (Acros Organic N.V. 1999; Alfa Aesar Lancaster Synthesis 2003; Fisher Scientific 2005; Chemconserve 2008a, 2008b, 2008c, 2008d, 2008e), these substances are not considered suitable analogues to PTPTT due to vast differences in water solubility values. Indeed, halogen arylphosphonium salts' read-across water solubility values range between from 19 000 to 297 000 mg/L (Chemconserve 2008a, 2008b, 2008c, 2008d, 2008e), compared to an experimental water solubility value of 4.5 mg/L submitted by industry (Environment Canada 2009a). In addition, there are inconsistencies between the literature and the MSDS data. For example, while the MSDS for the potential analogue substance tetraphenylphosphonium bromide (CAS RN 2751-90-8) indicates that it has a water solubility of 19 000 mg/L, a study conducted by Bergeron et al. (2009) on the interaction of arylphosphonium salts with DNA to modulate cytotoxicity observed that tetraphenylphosphonium bromide was insoluble in water.

A corrected log K_{ow} value of 4.15 was generated for BPAF using the "Experimental value adjustment method" of KOWWIN, based on an experimental log K_{ow} value of 3.32 for Bisphenol A (BPA) (CAS RN 80-05-7) (Howard 1989; Hansch et al. 1995). However,

the uncorrected modelled log K_{ow} value of 4.47 was used in subsequent modelling such as EPIWEB in order to generate conservative predictions for the risk characterization.

Table 2. Physical and chemical properties for PTPTT, BTP, BPAF and analogue substances

Substance	Type	Value	Temperature (°C)	Reference
Physical form				
PTPTT salt	na	Fine white powder, odourless		MSDSonline 2006[1]
PTPTT salt	na	Pink to purple pellets		DuPont 2006a[2]
Melting point (ºC)				
PTPTT (neutral form)[3]	Modelled	310.51		MPBPWIN 2000
Notified new substance (PTPTT salt analogue)[4]	Experimental	207–208		Environment Canada 1999a
		230–234		Environment Canada 1999b
BPAF (neutral form)[5]	Experimental	160–163		Sigma-Aldrich 2008[6]
		159–164		Halocarbon 2007[7]
	Modelled	125.78		MPBPWIN 2000
BTP (neutral form)[3]	Modelled	174.03		MPBPWIN 2000
Boiling point (ºC)				
PTPTT (neutral form)[3]	Modelled	690.34		MPBPWIN 2000
Notified new substance (PTPTT analogue)[4]	Experimental	> 300		Environment Canada 1999a

Substance	Type	Value	Temperature (°C)	Reference
BPAF (neutral form)[5]	Experimental	400		Halocarbon 2007[7]
	Modelled	347.16		MPBPWIN 2000
BTP (neutral form)[3]	Modelled	469.38		MPBPWIN 2000
Density (kg/m^3)				
PTPTT salt	Experimental	1380		DuPont 2006a[2]
PTPTT salt	Experimental	1400		MSDSonline 2006[1]
Vapour pressure (Pa)				
PTPTT (neutral form)[3]	Modelled	1.63×10^{-15} (1.22×10^{-17} mmHg)	25	MPBPWIN 2000
Notified new substance (PTPTT salt analogue)[4]	Experimental	0.01 (7.5×10^{-5} mmHg)		Environment Canada 1999a
BPAF (neutral form)[5]	Experimental	< 13.33 (< 0.1 mmHg)		Halocarbon 2007[7]
	Modelled	6.98×10^{-5} (5.23×10^{-7} mmHg)		MPBPWIN 2000
BTP (neutral form)[3]	Modelled	6.16×10^{-7} (4.62×10^{-9} mmHg)		MPBPWIN 2000
Henry's Law constant (Pa·m^3/mol)				
BPAF (neutral form)[5]	Modelled	1.07×10^{-2} (1.06×10^{-7} atm-m3/mole)[8]		HENRYWIN 2000

Substance	Type	Value	Temperature (°C)	Reference
BTP (ionic form)[3]	Modelled	9.45 x 10^{-5} (9.33 x 10^{-10} atm-m3/mole)[8]		HENRYWIN 2000
Log K_{ow} (Octanol-water partition coefficient) (dimensionless)				
Notified new substance (PTPTT salt analogue)[4]	Calculated	0.2[9]		Environment Canada 1999a
BPAF (neutral form)[5]	Modelled	4.47		KOWWIN 2000
		4.15[10]		KOWWIN 2000
BPAF (ionic form)	Modelled	1.87		Cahill 2008[11]
BTP (neutral form)	Modelled	5.78[12]		KOWWIN 2000
BTP (ionic form)	Experimental	2.6		Environment Canada 2009a[13]
Notified new substance (Cation of PTPTT salt analogue)[4]	Modelled	-0.04[14]		Environment Canada 1999a
Log K_{oc} (Organic carbon-water partition coefficient) (dimensionless)				
Notified new substance (PTPTT analogue)[4]	Experimental	3.80[15]	20	Environment Canada 1999a
		4.35[16]	20	
		5.09[17]	20	
BPAF (neutral form)[5]	Modelled	3.73		PCKOCWIN 2000

Substance	Type	Value	Temperature (°C)	Reference
BTP (neutral form)[3]	Modelled	5.02[12]		PCKOCWIN 2000
BTP (ionic form)[3]	Modelled	2.26		PCKOCWIN 2000
Water solubility (mg/L)				
PTPTT salt	Experimental	Insoluble		DuPont 2006a[2]
	Experimental	Negligible		MSDSonline 2006[1]
	Experimental	4.5		Environment Canada 2009a[13]
Notified new substance (PTPTT salt analogue)[4]	Experimental	120 000		Environment Canada 1999a
	Experimental	175 000		Environment Canada 1997
BPAF (neutral form)[5]	Modelled	4.3		WSKOWWIN 2000
		0.84		WATERNT 2000-2008
		1.73[18]		WATERNT 2000-2008
BTP (ionic form)	Experimental	2.31		Environment Canada 2009a[13]
BTP (ionic form)[3]	Modelled	35.06	25	WSKOWWIN 2000
		2.43×10^{-4}		WATERNT 2000-2008
1-octanol solubility (mg/L)				

Substance	Type	Value	Temperature (°C)	Reference
BTP (ionic form)	Experimental	919		Environment Canada 2009a[13]
pKa (Acid dissociation constant) (dimensionless)				
BPAF (neutral form)[5]	Modelled	pKa1 = 8.11 pKa2 = 8.86		ACD/pK_aDB (2005)
BTP (ionic form)	Modelled	n/a[19]		ACD/pK_aDB (2005)

[1] This information refers to PTPTT salt with a purity < 99% CAS RN 75768-65-9 (MSDSonline 2006).
[2] This information refers to the commercial products "VITON" Curative No 50, VC-50, "VITON" RCR-7325, "VITON" RCX 7325, RCX-7325 which contain 0–-90% Bisphenol AF (CAS RN 1478-61-1) and 10–-100% PTPTT salt (CAS RN 75768-65-9) (Dupont 2006a).
[3] Since salt compounds are out of EPIWEB's domain, modelling was conducted assuming a covalent structure for the ion pair. Correction factors, namely experimental water solubility data for PTPTT (4.5 mg/L) and BTP (2.31 mg/L) as well as an experimental log K_{ow} value (2.6) for both substances were added in EPIWEB as input for the neutral form of PTPTT and BTP unless otherwise specified.
[4] Data for this structurally similar substance were received through the *New Substances Notification Regulations*. The substance identity is considered confidential business information.
[5] The substantial fraction of the anion BPAF will be converted to its neutral form in the natural environment. Therefore, the neutral form was used in the modelling activities.
[6] Purity of BPAF (CAS RN 1478-61-1) is 97 % (Sigma-Aldrich 2008).
[7] Purity of BPAF (CAS RN 1478-61-1) is not specified (Halocarbon 2007).
[8] These Henry's Law constants were estimated using EPIWEB's VP/WSol method.
[9] Log K_{ow} was determined using the water solubility (120 000 mg/L) and the solubility in n-octanol of the substance (Environment Canada 1999a).
[10] This value was modelled using the "Experimental value adjustment method" of KOWWIN 2000,; which estimated the log K_{ow} of the substances based on the experimental log K_{ow} value of 3.32 for the analogue bisphenol A CAS RN 80-05-7 (Howard 1989; Hansch et al. 1995).
[11] Changes in log K_{ow} value from 4.47 for the neutral substance are based on fragment values and changes of example chemicals during ionization (Cahill 2008).
[12] This value was estimated without any correction factors.
[13] Octanol and water solubility of the PTPTT salt were determined by employing a stirred flask method at 20°C over a period of 25 hours on a PTPTT containing commercial substance with an excess of BPAF anion. The K_{ow} of the substance was subsequently estimated by dividing the substances' respective octanol and water solubility (Environment Canada 2009a).
[14] Log K_{ow} was determined with EPIWEB by substituting a nitrogen group for the phosphorous group in the neutral triphenyl counterion (Environment Canada 1999a).
[15] Log K_{oc} for clay loam at a temperature of 20°C according to OECD Test Guideline 106 (Environment Canada 1999a).
[16] Log K_{oc} for silt loam at a temperature of 20°C according to OECD Test Guideline 106 (Environment Canada 1999a).
[17] Log K_{oc} for loamy sand at a temperature of 20°C according to OECD Test Guideline 106 (Environment Canada 1999a).
[18] This value was modelled using the "Experimental value adjustment method" of WATERNT 2000; which estimated the water solubility of the substances based on the water solubility value of 301 mg/L for the analogue bisphenol A CAS 80-05-7 (Bayer AG 1988).

[19] Modelling results indicate that BTP as a cation does not ionize further in water; therefore the cation is expected to exist in water as is (ACD/pK_aDB 2005).

Sources

PTPTT and its dissociation products are not naturally produced in the environment.

Recent information was collected through industry surveys conducted for the years 2005 and 2006 under *Canada Gazette* notices issued pursuant to section 71 of CEPA 1999 (Canada 2006b, 2009). These notices requested data on the Canadian manufacture and import quantities of the substances. In the notice for 2006, data were also requested on use quantity of PTPTT.

No manufacture of PTPTT in Canada above the threshold of 100 kg/year was reported in response to the CEPA 1999 section 71 survey notice for the 2006 calendar year. Fewer than four companies imported between 100 and 1000 kg of PTPTT in Canada in 2006 (Environment Canada 2009b). PTPTT is imported as a component of fluoroelastomer precompound which is subsequently cured at fluoroelastomer processing facilities (Environment Canada 2009a). Four other companies also expressed interest as stakeholders in this substance.

Information received in response to the CEPA 1999 section 71 survey notice for the 2005 calendar year indicate that PTPTT was not manufactured in Canada in 2005 in a quantity greater than the 100 kg reporting threshold. However, information from this survey notice indicated that one company imported between 1001 and 100 000 kg of PTPTT in Canada (Environment Canada 2006).

The quantity reported under the Domestic Substances List (DSL) to be manufactured, imported or in commerce in Canada during the 1986 calendar year for PTPTT was 1000-10 000 kg. There were fewer than four notifiers for the calendar years 1984–1986.

It appears that the import volume and the number of users of PTPTT have been relatively stable in Canada in recent decades, or seem to be decreasing. Indeed, one company which declared importing PTPTT in 2006 reported importing less PTPTT in 2008.

Elsewhere, PTPTT was in use in Sweden during the period 1999 to 2007 (the most recent year for which data were available) (SPIN 2009). However, the usage volumes were considered to be confidential information (SPIN 2009). PTPTT is an existing substance in the European Union, but is not on the high production volume (HPV) or low production volume (LPV) chemical lists (ESIS 2009). The U.S. does not collect manufacture/import information for PTPTT through the *Toxic Substances Control Act* (TSCA) Inventory Updates (US EPA 2009).

Uses

Information on uses for the 2005 and 2006 calendar years was gathered in response to the CEPA 1999 section 71 notices (Canada 2006b, 2009).

In 2006, one company importing PTPTT described its business activity as "Other Chemical and Allied Products Merchant Wholesalers". This company reported commercializing the substance as a compounded polymer (Environment Canada 2009b). Another company importing PTPTT listed the following business activities (Environment Canada 2009b):

- "All Other Automotive Repair and Maintenance CAN";
- "Automotive Oil Change and Lubrication Shops";
- "Other Automotive Repair and Maintenance";
- "Automotive Repair and Maintenance";
- "All Other Support Activities for Transportation";
- "Pipeline Transportation of Refined Petroleum Products";
- "Pipeline Transportation of Natural Gas";
- "Pipeline Transportation of Crude Oil";
- "Automotive Parts and Accessories Stores U.S.";
- "Automotive Parts, Accessories and Tire Stores U.S.";
- "Chemical (except Agricultural) and Allied Product Wholesaler-Distributors CAN";
- "Mining and Oil and Gas Well Machinery, Equipment and Supplies Wholesaler-Distributors CAN";
- "Oil and Gas Field Machinery and Equipment Manufacturing";
- "All Other Miscellaneous Chemical Product Manufacturing CAN"; and
- "All Other Chemical Product Manufacturing".

The company that reported importing PTPTT in 2005 was primarily engaged in manufacturing basic organic chemicals (Environment Canada 2006).

The DSL use codes identified for PTPTT during the 1986 calendar year were:

40 - Processing aid; and
56 - Automotive, Aircraft and Watercraft.

A review of the available scientific and technical information indicates that PTPTT is a catalyst present in low concentrations (≤ 5%) in uncured fluoroelastomers precompounds (3M 2007a, 2007b, 2008; Changshu Xinhua Chemical Co. Ltd. 2006; DuPont 2006b, 2006c; and Rhodia 2008). PTPTT is an incorporated cure system comprising an organic phosphonium cation cure accelerator (BTP) and a cross-linking agent (BPAF) which improves fluoroelastomer compounds performance and resistance following cross-linking curing (Dupont 2006d, KOECT 2000). Cross-linking curing is a chemical reaction used in rubber processing to alter polymer properties of a compound by forming covalent, hydrogen or other bonds between polymer molecules (Datta 2001). The curing of PTPTT

containing fluoroelastomer is a two- step process involving the application of heat and pressure in a mold to shape an article, followed by a high temperature oven cycle at atmospheric pressure to obtain the final cure properties (KOECT 2000). The chemistry of this curing process indicates that PTPTT reacts chemically with the polymer chain (KOECT 2000), and it has been reported that PTPTT is, essentially, fully consumed following curing since only trace amounts of PTPTT (in the order of ppb) would remain free in the polymer (November 2009 email from Food Directorate, to Risk Management Bureau, Health Canada; unreferenced).

The fluoroelastomers class of synthetic rubber provides a high level of resistance to chemicals, oil and heat, while providing useful service life above 200°C (IISRP 2009). These materials are used in products in a wide variety of high-performance applications such as O-ring seals in fuel, lubricant and hydraulic systems, valve seals and valve liners, firewall, shaft and tire valve stem seals, fuel hoses and fuel injector O-rings, fuel tanks, diaphragms and gaskets in multiple industries, but notably in the aerospace and automotive industries (IISRP 2009). PTPTT is found in O-rings and plugs of stainless steel valves used for sanitary sampling in biopharmaceutical process systems (Millipore Corporation 2008).

The United States Food and Drugs Administration (FDA) has also authorized the use of PTPTT at a concentration of 1.9% by weight as vulcanization agents in the manufacture of vinyl fluoride-hexafluoropropylene and vinyl fluoride-hexafluoropropylene-tetrafluoroethylene copolymers regulated in 2 1 CFR 177.2600 destined for use in the manufacture of repeat-use rubber articles that may contact all types of food at temperatures of up to 250^{o}F (US FDA 2000).

Releases to the Environment

According to information received in response to a CEPA 1999 section 71 survey notice for the year 2006, releases of PTPTT associated with its import in fluoroelastomer precompounds are likely to be very small (Environment Canada 2009a, 2009b). Indeed, fluoroelastomer precompounds are imported in solid forms such as block, slabs, pellets or sheets (3M 2007a 2007b, 2008; Dupont 2006b, 2006c). These solid forms usually contain low levels (≤ 5%) of PTPTT (3M 2007a, 2007b, 2008, Changshu Xinhua Chemical Co. Ltd. 2006 and DuPont 2006b, 2006c) incorporated within a hydrophobic fluoropolymer matrix which likely limits the potential for release to the environment. PTPTT is then believed to be almost fully consumed (transformed) during the curing of the fluoroelastomer precompounds (KOETC 2000, November 2009 email from Food Directorate, to Risk Management Bureau, Health Canada; unreferenced).

A method has been developed to estimate a substance's losses during different stages of its life cycle, including its fate within a finished product or article (Environment Canada 2009c). This method, referred to as Mass Flow, consists of a life cycle analysis and a spreadsheet tool (Mass Flow Tool or MFT) that integrates information on the manufacturing, importation and use available for the substance. Starting with an identified mass of the substance, in commerce, loss of the substance at each life cycle stage is subsequently evaluated until all of the mass is accounted for. Relevant factors are considered, uncertainties recognized and assumptions may be made during each stage, depending on information available. The estimated losses represent the complete mass balance of the substance over the life cycle of the substance and include releases to wastewater and other receiving compartments (land, air), chemical transformation, transfer to recycling facilities and transfer to waste disposal sites (landfill, incineration). However, unless specific information on the rate or potential for release of the substance from landfills and incinerators is available, the method does not quantitatively account for releases to the environment from such disposal. Ultimately, the estimated losses provide a first tier in the exposure analysis of a substance and help to estimate environmental releases and focus exposure characterization later in the assessment.

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

The losses estimated for PTPTT over its lifecycle are presented in Table 3 (Environment Canada 2009c).

Table 3. Estimated Losses of PTPTT during Its Lifecycle

Type of Loss	Proportion (%)	Pertinent Lifecycle Stages
Wastewater	0.1	Industrial use
Air emission	0.0	n/a
Land	0.0	n/a
Chemical transformation	99.8	Industrial use
Landfill	0.1	Consumer/commercial use
Incineration	0.0	n/a
Recycling	0.0	n/a

The major losses of PTPTT are expected to occur during the industrial use stage through chemical transformation (99.8%). A very small proportion is expected to be lost to wastewater (0.1%), associated with container handling and curing operations. A small proportion of PTPTT is also estimated to be lost through waste disposal (landfill 0.1%)

The above loss estimates indicate that PTPTT has a low potential for release to the environment. In general, wastewater is a common source for releases of a substance to water through wastewater treatment facilities and to soil through application of biosolids from treated wastewater to land surfaces . Finally, landfills have the potential to leach substances into groundwater, if no liners and leachate collection systems are present, or there may be releases of substances to the atmosphere through landfill gas, if not collected and combusted.

Environmental Fate

The very low modelled vapour pressure value of 1.6×10^{-15} Pa of PTPTT, consistent with the fact that this is a large and complex molecule, indicate that PTPTT is not volatile. Therefore this substance will not be found in the atmosphere. Upon its release into the aquatic environment, PTPTT is expected to completely and rapidly dissociate into its BTP cation and BPAF anion (Environment Canada 2009a). Since it is not appropriate to use QSAR predictions to describe the environmental fate of PTPTT itself, because as a salt it is expected to completely dissociate in solution, the following discussion focuses on the environmental fate of its dissociation products.

If released to air, no amount of BTP is expected to reside in that compartment. The negligible modelled vapour pressure of 6.16×10^{-7} Pa and Henry's Law constant of 9.451×10^{-5} Pa·m^3/mol indicate that BTP is non-volatile. Therefore, if released solely to air, it will leave this compartment to enter water and soil.

Substances like BTP found in the water column will actively bind to suspended organic matter and will eventually be deposited to sediment because of their charge (Perdue 1985). If released to water, BTP is expected to strongly adsorb to suspended solids and sediment because of its electrostatic interaction with negatively charged dissolved and suspended particulate matter. Volatilization from water surfaces is expected to be an unimportant fate process based upon this compound's estimated Henry's Law constant. Thus, if water is a receiving medium, BTP is expected to reside both in the water column and sediments.

If released to soil, BTP is expected to have a high adsorptivity to soil because of its cationic character. Indeed, adsorption/desorption testing conducted on the analogue notified substance according to OECD Test guideline 106 in clay loam, silt loam and loamy sand at 20° C determined that more than 95% of the substance was adsorbed to all three soils with less than 5% desorbed after two soil washings (Environment Canada 1999a). Volatilization from moist soil surfaces seems to be an unimportant fate process, based upon the substance's estimated Henry's Law constant. This chemical will not volatilize from dry soil surfaces based upon its vapour pressure. Therefore, if released to soil, BTP will mainly reside in this environmental compartment.

For the BPAF anion, the moderately high acid dissociation constant (pK_{a1}) of 8.11 indicates that the anion will be substantially protonated to its neutral form under slightly acidic or circum-neutral conditions. Therefore, in water bodies at pH 6 to 7, more than 90% of the BPAF will be undissociated, which indicates that the biotic exposure to BPAF will mainly be from the neutral chemical. Based on its physical and chemical properties (Table 2), the predictions from the Cahill multispecies model which is capable of handling ionizing substances (Cahill 2008; pH of 7 assumed)), indicate that upon continuous releases to the environment the substance will primarily reside in soil, water or sediment, depending upon the mode of entry.

Table 4. Results of the Cahill multispecies model for BPAF at pH 7 (Cahill 2008)

	Percentage of substance partitioning into each compartment			
Substance released to:	**Air**	**Water**	**Soil**	**Sediment**
Air (100%) – neutral	0.7	3.0	88	1.3
Air (100%) – anion	0.0	0.2	6.8	0.1
Water (100%) – neutral	0.0	64	0.0	29
Water (100%) – anion	0.0	5.0	0.0	2.2
Soil (100%) – neutral	0.0	1.4	91	0.6
Soil (100%) – anion	0.0	0.1	7.1	0.1

If released to air, a negligible amount of the substance in its neutral form is expected to reside in air (see Table 4 above). Based on the negligible modelled vapour pressure of 6.98×10^{-5} Pa and Henry's Law constant of 1.071×10^{-2} Pa·m^3/mol, BPAF is non-volatile. Therefore, if released solely to air, it will leave this compartment and partition mainly to the soil compartment (88% neutral and 6.8% anionic; see Table 4b above).

If released to water, BPAF is expected to adsorb relatively strongly to suspended solids and sediment based upon a moderately high estimated log K_{oc} value of ~3.73. Volatilization from water surfaces is expected to be an unimportant fate process based upon this compound's estimated Henry's Law constant. Thus, if water is a receiving medium, BPAF is expected to mainly reside in water and partition to sediment (see Table 4 above).

If released to soil, BPAF is expected to have high adsorptivity to soil (i.e. expected to be immobile) based upon its estimated log $K_{oc.}$ Volatilization from moist soil surfaces seems to be an unimportant fate process, based upon this substance's estimated Henry's Law constant. This chemical will not volatilize from dry soil surfaces based upon its vapour pressure. Therefore, if released to soil, BPAF will mainly reside in this environmental compartment (see Table 4 above).

Based on their physical and chemical properties (Table 2) and potential uses, if released into the environment, BTP and BPAF would be expected to be found in water, sediments and soil, depending on the compartment of release.

Persistence and Bioaccumulation Potential

Environmental Persistence

No experimental degradation data for PTPTT or its dissociation products have been identified. Given the ecological importance of the water compartment, the fact that most of the available models apply to water and the fact that PTPTT is expected to be released to this compartment (Environment Canada 2009b) and dissociate into BTP and BPAF, the persistence of BTP and BPAF in water was primarily examined using predictive quantitative structure-activity relationship (QSAR) models for biodegradation. Neither BTP nor BPAF contain functional groups expected to undergo hydrolysis.

Tables 5a and 5b summarize the results of available QSAR models for degradation in air and water for BTP and BPAF.

Table 5a. Modelled data for degradation of BTP (neutral form)

Fate process	Model and model basis	Model result and prediction	Extrapolated half-life (days)
AIR			
Atmospheric oxidation	AOPWIN 2000	$t_{1/2}$ = 0.92 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)	2.5040[2] "biodegrades fast"	< 182
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 4: Expert Survey (primary biodegradation)	3.3559[2] "biodegrades fast"	< 182
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 5: MITI linear probability	-0.2336.[3] "biodegrades very slowly"	> 182
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 6: MITI non-linear probability	0.0044[3] "biodegrades very slowly"	> 182
Biodegradation (aerobic)	TOPKAT 2004 Probability	n/a[1,3]	n/a
Biodegradation (aerobic)	CPOPs 2008 % BOD (biological oxygen demand)	% BOD = 25.6 "biodegrades slowly"	<182

[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

Table 5b. Modelled data for degradation of BPAF (neutral form)

Fate Process	Model and model basis	Model Result and Prediction	Extrapolated Half-life (days)
Atmospheric oxidation	AOPWIN 2000	$t_{1/2}$ = 0.133 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)	1.3[2] "biodegrades slowly"	> 182
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 4: Expert Survey (primary biodegradation)	2.74[2] "biodegrades relatively slowly"	>182 (for complete mineralization)
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 5: MITI linear probability	0.08.[3] "biodegrades very slowly"	> 182
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 6: MITI non-linear probability	0.00[3] "biodegrades very slowly"	> 182
Biodegradation (aerobic)	TOPKAT 2004 Probability	0.00[3] "biodegrades very slowly"	> 182
Biodegradation (aerobic)	CPOPs 2008 % BOD (biological oxygen demand)	% BOD = 0.10 "biodegrades very slowly"	>182

[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

The CPOPs aerobic biodegradation model considers the structure of BTP (neutral form) and BPAF to be 80.77% and 95.65% within the model domain, respectively. Therefore, despite some uncertainty, the CPOPs biodegradation results are considered reliable for both substances. An estimate of aerobic biodegradation could not be generated for BTP by TOPKAT since the structure was found to be outside of the model's domain. The BPAF TOPKAT prediction indicates that, while the chemical is not in the model's database, all structure fragments are covered.

In air, a predicted atmospheric oxidation half-life value of 0.92 days (see Table 5a above) demonstrates that BTP is likely to be rapidly oxidized. The substance is not expected to react 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 BTP. Similar results are observed for BPAF (see Table 5b below), which is expected to be rapidly oxidized as illustrated by a half-life value of 0.133 days. Although BPAF is not expected to react with O_3 or to degrade via photolysis, reaction with nitrates may be an important fate process (AOPWIN 2000). With half-lives of 0.92 and 0.133 days respectively via reactions with hydroxyl radicals, BTP (neutral form) and BPAF (neutral form) are considered not persistent in air.

There are conflicting model results for the biodegradation of BTP (neutral form). Two of the four ultimate biodegradation models (BIOWIN Sub-models 5 and 6) suggest that biodegradation is very slow and that the half-life in water is > 182 days, whereas the other two (CPOPs and BIOWIN Sub-model 3) suggest a half-life of ≤ 182 days (Environment Canada 2009d). Results for the primary biodegradation model (BIOWIN Sub-model 4) indicate potential for rapid primary degradation, but since the identity of the degradation products is not known, this result is given less weight. The result of the BIOWIN Sub-model 3 (ultimate biodegradation), would suggest the substance has a primary half-life of ≤ 182 days, but that degradation could take as long as "months". On the other hand, results from BIOWIN Sub-models 5 and 6 are both well below the suggested threshold for persistence (< 0.3), suggesting clearly that the substance is persistent. The CPOPs prediction suggests that the rate of ultimate biodegradation is slow (half-life of about two months assuming first-order degradation kinetics) but that there is likely significant primary biodegradation based on the predicted BOD of > 20% (persistence threshold for CPOPs - Environment Canada (2009c)). Therefore, considering the comparative strength of the BIOWIN 5 and 6 results indicating slow degradation, and the fact that both BIOWIN 3 and CPOPs suggest that the ultimate degradation half-life of BTP could be as long as "months" there is greater evidence to suggest that the rate of ultimate biodegradation is slow and that BTP is likely persistent (half-life > 182 days) in water.

BPAF biodegradation results from Table 5b show that the three BIOWIN ultimate biodegradation models (3, 5 and 6) suggest that it does not biodegrade quickly and that its half-life in water is > 182 days. In fact, both BIOWIN probability results are much less than 0.3, the cut-off suggested by Aronson et al. (2006) for identifying substances as having a half-life > 60 days (based on the MITI probability models). The ultimate survey model (BIOWIN 3) result of 1.33 may be equated to a half-life value of 180–240 days (Aronson et al 2006). The overall conclusion from BIOWIN (2000) is that BPAF is not readily biodegradable. Other ultimate degradation models (CPOPs and TOPKAT) predict that BPAF does not undergo mineralization in a 28-day timeframe with probability or extent of biodegradation in the range of very persistent chemicals. TOPKAT, which simulates the Japanese MITI 28-day biodegradation test, predicted a probability of 0, which is much below the suggested cut-off for persistent substances in this model (< 0.3) (note: 0.7 is suggested for non-persistence chemicals) (TOPKAT 2004). CPOPs predicted only a 0.1 % extent of biodegradation based on the OECD 301 ready biodegradation test (%BOD) which has been suggested as meaning the compound is likely to be persistent (Aronson and Howard 1999) and have a half-life in water of >182 days.

Using a 1:1:4 ratio for a water:soil:sediment half-life extrapolation (Boethling et al. 1995), the ultimate biodegradation half-lives in soil are also > 182 days and the half-lives in sediments are > 365 days for both BTP and BPAF.

Therefore, considering all model results and structural features (e.g. presence of trifluoromethyl groups in BPAF and un-substituted aromatic rings sterically hindering attack of the phosphorous in BTP), there is more reliable evidence to suggest that the biodegradation half-lives of PTPTT's dissociation products are > 182 days in water.

Based on the modelled data (see Tables 4a and 4b above) PTPTT's dissociation products BTP and BPAF meet the persistence criteria in water, soil and sediment (half-lives in soil and water ≥ 182 days and half-life in sediment ≥ 365 days), but do 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

Experimental log K_{ow} values for BTP suggest that this chemical has a relatively low potential to bioaccumulate in biota (see Table 2). However, the elevated modelled log K_{ow} value for the other dissociation product, BPAF, suggests that it has a higher potential to bioaccumulate in biota.

Since no experimental bioaccumulation factor (BAF) and/or bioconcentration factor (BCF) data for PTPTT's dissociation products were available, a predictive approach was applied using available BAF and BCF models as shown in Tables 6a and Table 6b below. According to the *Persistence and Bioaccumulation Regulations* (Canada 2000), a substance is bioaccumulative if its BCF or BAF is $\geq$ 5000. Measures of BAF are the preferred metric for assessing bioaccumulation potential of substances 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 metabolism correction as long as the log K_{ow} of the substance is within the log K_{ow} domain of the model.

It is noted that the bioaccumulative potential of BTP may not be accurately evaluated by solely assessing its bioconcentration and bioaccumulation factors estimated based on log K_{ow}. Indeed, arylphosphonium salts have both lipophilic and cationic character, allowing them transport through plasma membranes or cell walls to accumulate in the cytoplasm or mitochondria of cells and to bind to DNA (Bergeron et al. 2009). For instance, lipophilic cations such as the cation of the analogue methyltriphenyl phosphonium bromide (CAS RN 1779-49-3), are known to accumulate in mitochondria and cells (Ross et al. 2006). Their cationicity makes them attracted to cell walls or lipid bilayers with negative energy potentials, while their lipophilic nature (≥ 3 aromatic rings) allows easy transport through the membrane to accumulate in the interior of cells or cellular compartments (Bergeron et al 2009). The structure of the tetra-substituted cation is relatively stable to further chemical modification once in the organism (Bergeron et al. 2009).

The sterically crowded chemical structure of BTP, however, could negatively affect its cationicity. Indeed, in the case of the analogue tetraphenylphosphonium bromide (TPP-Br, CAS RN 2751-90-8), it has been shown that electrostatic association with negatively

charged DNA may be decreased by the presence of the four large phenyl rings which may partially obscure its cationic character (Bergeron et al. 2009). The lack of water solubility of TPP-Br seems to further support this hypothesis (Bergeron et al. 2009).

The BCFBAF v 3.00 model from EPIWEB (2009) was used to estimate whole-body primary biotransformation rate estimate (k_M), bioconcentration factors (BCFs) and bioaccumulation factors (BAFs) for fish, for BTP and BPAF. Metabolic rates of 4.172/day and 0.3584/day were estimated for BTP (neutral form) and BPAF (neutral form), respectively, for a generic 10 g fish at a temperature of 15°C, which was then corrected for the body weight of the middle trophic level fish in the Arnot-Gobas model (184 g). The middle trophic level fish was used to represent overall model output as it is most representative of fish weight likely to be consumed by an avian or terrestrial piscivore.

Table 6a. Fish BAF and BCF predictions for BTP and BPAF (neutral forms) using the Arnot-Gobas kinetic model (2003) corrected for metabolic rate.

Substance	Metabolic rate constant k_M (1/days)[1]	LogK_{ow} Used	BCF (L/kg)	BAF (L/kg)	Biological half-life[2] (days)	Reference
BTP (ionic form) (CAS RN 15853-35-7)	4.172	2.6	21.13	21.13	0.34	Gobas BCF/BAF Middle Trophic Level (Arnot and Gobas 2003)
	0	2.6	28.2	28.8	0.12	
BPAF (neutral form) (CAS RN 1478-61-1)	0.3584	4.47	715.6	742.7	4.00	Gobas BCF/BAF Middle Trophic Level (Arnot and Gobas 2003)
	0	4.47	1995	3981	7.4	

[1] Metabolic rate constant km (1/days) for 10 gram fish

[2] Half-life ($t_{1/2}$) calculated using the following equation: $t_{1/2} = \ln 2/k_M$. In the case of $k_M = 0$, the half-life is calculated based on the sum of other rate constants used for loss of compound by fish (fecal egestion, loss via the gills, growth dilution).

Metabolism-corrected BCF values for BTP (ionic form) and BPAF (neutral form) were 21.13 L/kg and 715.6 L/kg respectively. Metabolism-corrected BAF values for the same substances were 21.13 L/kg and 742.7 L/kg. Their respective biological half-lives normalized for a 10 g fish at 15°C were approximately 4 hrs and 46.4 hrs.

Table 6b: Additional Modelled data for bioaccumulation for BTP and BPAF (neutral forms)

Substance	Log K_{ow} used	Test organism	Endpoint	Value wet weight (L/kg)	Reference
BTP (ionic form)	2.6	Fish	BCF	35.65 ± 2.7	OASIS Forecast 2005
		Fish	BCF	96.2	Baseline BCF Model (BCF Max) Dimitrov et al. 2005
		Fish	BCF	24	BCFWIN 2000
BPAF (neutral form)	4.47	Fish	BCF	11.59 ± 189.23	OASIS Forecast 2005
		Fish	BCF	2188	Baseline BCF Model (BCF Max) Dimitrov et al. 2005
		Fish	BCF	416	BCFWIN 2000

Some of the modelled values for BTP (ionic form) and BPAF (neutral form) in Table 6b (Oasis Forecast 2005 and Baseline BCF Model) are out of the total domain of the models, and thus are not considered as reliable as other predictions.

The available evidence indicates that the dissociation products of PTPTT are expected to have low bioaccumulation potentials. Therefore, considering the available evidence, PTPTT's dissociation products —BTP and BPAF— do 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 evidence that the neutral form of BPAF causes harm to aquatic organisms at relatively low concentrations (acute $LC/EC_{50} \leq 1.0$ mg/L; see Tables 7a below).

Table 7a. Empirical data for aquatic toxicity

Substance	Test organism	Type of test	Endpoint	Value (mg/L)	Reference
BPAF	Fish	Acute (96 hours)	LC_{50}[1]	< 1	Study Submission 2007
	Daphnia	Acute (48 hours)	EC_{50}[2]	3.2	Study Submission 2007
	Algae	Acute (72 hours)	EC_{50}[2]	0.156[3]	Study Submission 2007
				> 0.808[4]	

[1] LC_{50} – The concentration of a substance that is estimated to be lethal to 50% of the test organisms.
[2] EC_{50} – The concentration of a substance that is estimated to cause some effect on 50% of the test organisms.
[3] The effect measured is inhibition of yield.
[4] The effect measured is inhibition of growth rate.

Since there are no acceptable experimental data available for aquatic toxicity, BTP modelled data were used to estimate its potential for aquatic toxicity. Additional modelled data were also used to support BPAF experimental aquatic toxicity data. Table 7b contains predicted ecotoxicity values that were considered reliable and were used in the QSAR weight-of-evidence approach for aquatic toxicity (Environment Canada 2007). Input parameters used for ecotoxicity modelling are shown in Appendix II.

Table 7b. Modelled data for aquatic toxicity

Substances	Test organism	Type of test	Endpoint	Value (mg/L)	Reference
BTP (ionic form)	Fish	Acute (96 hours)	LC_{50}[1]	81[3]	ECOSAR 2004[4]
				20.84	AIEPS 2003–2007
		Acute (14 day)	LC_{50}[1]	82.7[3]	ECOSAR 2004[4]
		Chronic (30 day)	ChV[5]	8.785	
	Daphnia	Acute (48 hours)	LC_{50}[1]	49.9[3]	ECOSAR 2004[4]
		Chronic	ChV[5]	6.364	
	Algae	Acute (96 hours)	EC_{50}[2]	30.7[3]	ECOSAR 2004[4]
		Chronic	ChV[5]	12.984	
BPAF (neutral form)	Fish	Acute (96 hours)	LC_{50}[1]	1.129	ECOSAR 2004
				0.245	OASIS Forecast 2005
				7.94	AIEPS 2003–2007
		Chronic (30 day)	ChV[5]	0.228	ECOSAR 2004
	Daphnia	Acute (96 hours)	EC_{50}[2]	1.624	ECOSAR 2004
				0.810	TOPKAT 2004
		Chronic	ChV[5]	0.571	ECOSAR 2004
	Algae	Acute (96 hours)	EC_{50}[2]	1.726	ECOSAR 2004
		Chronic	ChV[5]	0.198	

[1] LC_{50} – The concentration of a substance that is estimated to be lethal to 50% of the test organisms.
[2] EC_{50} – The concentration of a substance that is estimated to cause some effect on 50% of the test organisms.
[3] No effects at saturation are predicted for this organism since the toxicity value exceeds the water solubility of 2.3 mg/L of BTP (Environment Canada 2009b) by 10-fold (ECOSAR 2004).
[4] Experimental water solubility value of 2.31 mg/L and experimental log K_{ow} of 2.6 (Environment Canada 2009b) were added to ECOSAR.
[5] ChV – Chronic toxicity value (ECOSAR 2004)

A range of aquatic toxicity predictions were obtained from the various QSAR models considered. These results indicate that the ionic form of BTP is moderately toxic to aquatic organisms and that the neutral form of BPAF is potentially highly hazardous to aquatic organisms (acute $LC/EC_{50} \leq 1.0$ mg/L**).**

B - In Other Environmental Compartments

While no acceptable experimental ecological effects studies were found for PTPTT, BTP or BPAF in whole organisms, some work is available on the effect of BTP and BPAF in mammalian cell lines.

The ability of BTP to accumulate in the cytoplasm or mitochondria of mammalian cells where it will likely be persistent and has the potential bind to DNA has been noted previously (Bergeron et al 2009).

Evidence of disruption to reproductive and developmental processes following exposure to bisphenol A (BPA), a BPAF analogue (NTP 2008), at concentrations below those causing acute effects has been reported in fish, aquatic invertebrates, amphibians and reptiles (Canada 2008). Although there is widespread variation in the reported levels resulting in hormonally related effects from BPA in aquatic organisms, many values fall in the range of 0.001 to 1 mg/L. Although studies on such effects in fauna are not available for BPAF, the endocrine-disrupting activities of BPAF along with BPA and 17 related compounds were examined by means of different *in vitro* and *in vivo* reporter assays (Kitamura et al. 2005). The endocrine-disrupting activities of the substances were examined using hormone-responsive reporter assays: the human breast cancer cell-line MCF-7 for estrogenic activity, the mouse fibroblast cell line NIH3T3 for androgenic activity, and the pituitary cell line GH3 for thyroid hormonal activity (Kitamura et al. 2005). Results indicate that BPAF showed greater estrogenic activity (EC_{50} of 0.05 μM or 1.68×10^{-2} mg/L), than BPA (EC_{50} of 0.63 μM). In addition, BPAF showed significant inhibition of the androgen activity of dihydrotestosterone in the NIH3T3 luciferase reporter assay as illustrated by an IC_{50} of 1.3 μm (0.437 mg/L), compared with the IC_{50} of 4.3 μm for BPA (Kitamura et al. 2005). Like BPA however, BPAF did not affect thyroid activity.

A chemical information profile of BPAF released by the National Toxicology Program (NTP) in 2008 indicates that BPAF was an agonist of estrogen (bonds to estrogen receptors) in all of the 10 studies evaluated, an antagonist (or had no effect) on androgen in one study, and is an antagonist (or had no effect) on thyroid in another study (NTP 2008).

There is evidence that BPAF causes endocrine disruption. More studies are required to determine these effects in fauna in the environment.

Ecological Exposure Assessment

Industrial Release

Aquatic exposure to PTPTT's dissociation products is expected when the substance is released from industrial use to a wastewater treatment plant and the treatment plant discharges its effluent to a receiving water body. The concentration of the substance, or in this case its dissociation products, in the receiving water near the discharge point of the wastewater treatment plant is used as the predicted environmental concentration (PEC) in evaluating the aquatic risk of each dissociation product. It can be calculated using the equation

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

where

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

As PTPTT is used industrially with the potential to be released to water, a worst-case industrial release scenario is used to estimate the aquatic concentration of the substance's dissociation products. The scenario is made conservative by assuming that the upper limit of the 2006 Confidential Business Information (CBI) quantity interval, 1000 kg PTPTT/yr, is used by a single industrial facility at a small, hypothetical site and the loss to sewer is at 0.1% of the total quantity resulting from the cleaning of container residue and process equipment residue, both in a solid form. 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 sewage treatment plant (STP) with a zero removal rate for the substance. In Canada, the receiving water at such a small site normally has a 10-fold dilution capacity for the STP effluent which was conservatively assumed to be 3456 m^3 per day (Environment Canada 2009d). Since PTPTT may dissociate completely and rapidly upon its release into the aquatic environment, the conservative scenario assumes complete dissociation of PTPTT into 51.3 mass% BTP and 48.7 mass% BPAF. Based on the above assumptions, the 0.1% release of 1000 kg/yr of PTPTT yields aquatic concentrations of 5.94×10^{-5} mg/L for BTP and 5.64×10^{-5} mg/L for BPAF..

Characterization of Ecological Risk

The approach taken in this ecological screening assessment was to examine various relevant pieces of 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 conservative risk quotient calculations, as well as information on persistence, bioaccumulation, toxicity, sources, behaviour and fate of the substance.

In contact with the water phase, PTPTT will dissolve and dissociate into equal molar proportions of BTP and BPAF. Both of the dissociation products are expected to be persistent in water, soil and sediment, but they are anticipated to have a low to moderate bioaccumulation potential. The low importation volume of the parent compound PTPTT into Canada, along with information on its use as a vulcanization accelerator, indicate a low potential for point-source releases into the Canadian environment (0.2 % of mass) (Environment Canada 2009c). Once released into surface waters, it will be found mainly in the water column and sediment. The dissociation products have been demonstrated to have a moderate to high 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 generic industrial scenario presented above yielded predicted environmental concentrations (PEC) of 5.94×10^{-5} mg/L for BTP and 5.64×10^{-5} mg/L for BPAF (Environment Canada 2009e and 2009f, respectively). A predicted no-effect concentration (PNEC) for BTP was derived from the chronic toxicity value of 6.36 mg/L for daphnid (ECOSAR 2004) by dividing it by an assessment factor of 10 (to account for interspecies and intraspecies variability in sensitivity and model to field extrapolation) to give a value of 0.63 mg/L. The resulting risk quotient (PEC/PNEC) = 9.4×10^{-5}.

A second PNEC was derived for BPAF (neutral form) from the experimental 72-hrs acute EC_{50} value of 0.156 for algae (Study Submission 2007) by dividing this value by an assessment factor of 100 (to account for interspecies and intraspecies variability in sensitivity, acute to chronic and, laboratory to field) to give a value of 1.56×10^{-3} mg/L. The resulting risk quotient (PEC/PNEC) = 0.03613.

Therefore harm to aquatic organisms from the dissociation products of PTPTT is unlikely in the reasonable worst-case scenario considered. This suggests that PTPTT does not have the potential to cause ecological harm in Canada.

Uncertainties in Evaluation of Ecological Risk

Uncertainties in this risk assessment exist due to a lack of physical and chemical property data specific to PTPTT, notably the extent of its dissociation in water. However, based on experimental evidence, an assumption of total dissociation of the substance at

environmentally relevant pH was used, and the assessment focussed on the risk associated with PTPTT's dissociation products BTP and BPAF.

The general lack of experimental physical and chemical property data specific to the dissociation products, notably the water solubility of BPAF and the absence of octanol-water partition coefficients and carbon-water partition coefficient for both substances, is a source of uncertainty for this assessment. However, read-across approaches, analogue data and modelled data (including the modelled values using the experimental value adjustment method of EPIWEB (2009) were used to identify conservative physical and chemical property values which were then used for further modelling.

Since QSAR models are unable to account for ionic compounds or charged compounds such as PTPTT salt or the BTP cation, neutral structures were often used to obtain model predictions. Although uncertainties exist regarding these predictions, they are considered representative since the sterically crowded chemical structure of BTP seem to be negatively affecting its cationic character, as illustrated by its physical and chemical properties.

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 well addressed by the effects data available. Indeed, most of effects data identified for BPAF and all of the effects data for BTP were estimated from models and apply primarily to pelagic aquatic exposures, although the water column may not be the only medium of concern based on partitioning estimates.

There are uncertainties in the risk characterization associated with the endocrine disruption potential of BPAF. While there is evidence that BPAF causes endocrine disruption, more empirical data is required to properly evaluate the risks associated with this potential. As BPAF was found to meet the ecological categorization criteria for persistence and inherent toxicity to non-human organisms and was believed to be in commerce in Canada during Categorization, it will be the object of a more in-depth risk assessment.

Potential to Cause Harm to Human Health

Exposure Assessment

There were no data identified in the literature for PTPTT in air, water, soil or sediment, in Canada or elsewhere. Given the limited amount imported into Canada on an annual basis, the form that it is imported in, and its use, concentrations of this substance released to environmental media, specifically water, are expected to be very small (i.e., < 1 kg per year).

PTPTT is used as a curing agent in some specific fluoroelastomers, including repeated use parts such as gaskets, O-rings, and valves for food processing equipment (November 2009 email from Food Directorate to Risk Management Bureau, Health Canada; unreferenced). During the curing of the fluoroelastomer precompounds, PTPTT reacts chemically with the polymer chain and is almost fully consumed (transformed). Any residuals remaining in the final manufactured product are expected to be found only at traces levels; therefore exposures from use of these products would be expected to be negligible.

Overall confidence in the exposure characterization for environmental, dietary and consumer product exposures is considered to be low due to the lack of experimental data. There is uncertainty in the exposure to PTPTT through these sources, however, given that the amount imported into Canada is very small, and residuals in products are expected to be very low, exposures through all sources are expected to be negligible. Since the amount of PTPTT potentially released into water each year is very small (< 1 kg), exposure to any dissociation products would be negligible and therefore these dissociation products were not considered in the human health screening assessment.

Health Effects Assessment

Only limited empirical toxicological data are available for PTPTT. No evidence of mutagenicity was observed in *Salmonella typhimurium* strains TA98, TA100, TA1537 and TA1538 exposed to PTPTT with or without metabolic activation (Environment Canada 2009a). The acute toxicity is low, with an LD_{50} of 4385 mg/kg in rats (Environment Canada 2009a). The outputs of predictive models, summarized in Appendix 2, were also considered using four different models, DEREK, TOPKAT, CASETOX and Leadscope Model Applier. The resulting predictions for carcinogenicity, genotoxicity, developmental toxicity and reproductive toxicity were predominately negative (DEREK 2008; TOPKAT 2004; CASETOX 2008; Leadscope 2009). The confidence in the toxicity database is considered to be low due to the limited available data for PTPTT.

Characterization of Risk to Human Health

There is potential for exposure of the general population to PTPTT through food (i.e. from its use in food processing equipment) and other consumer products; however, given the limited amount of PTPTT imported into Canada and very low residual levels in these products, these exposures are expected to be negligible.

There are limited toxicological data available for PTPTT; however, the available empirical data and information from predictive models are not suggestive of high hazard.

As exposure of the general population in Canada is expected to be negligible, the risk to human health is considered to be low.

Uncertainties in Evaluation of Risk to Human Health

Due to the limited data available for PTPTT 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.

Overall confidence in the exposure characterization for environmental, dietary and consumer product exposures is considered to be low due to the lack of experimental data. There is uncertainty in the exposure to PTPTT through these sources. However, given that the amount imported into Canada is very small, and residuals in products are expected to be very low, exposures through all sources are expected to be negligible.

Conclusion

Based on the information presented in this screening assessment, it is concluded that PTPTT 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, based on the results from PTPTT's dissociation products (BPT and BPAF), PTPTT meets the criteria for persistence but does not meet the criteria of bioaccumulation potential as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).).

It is also concluded that PTPTT 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 PTPTT 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.

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Appendix 1 - Robust Study Summary

Evaluation of experimental data using Kollig's approach*

Item	Weight	Response	Mark
Reference: 11344Submission001, Determination of solubility, stability and octanol/water partition coefficient for triphenyl(phenylmethyl)phosphonium salt with 4,4-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol], Environment Canada 2009a			
Test substance: Two commercial substances containing CAS RN 75768-65-9 Substance 1 : PTPTT Substance 2 : PTPTT			
Could you repeat the experiment with available information?	5	Y Guidelines and SOPpresented: 1. Laboratory guidelines on solubility verification and determination of limit solubility of test substance in aquatic dilution water. 2. OECD (2005) Guidelines for the testing of chemicals: 105 Water Solubility 3. OECD (2006) Guidelines for the testing of chemicals: 123 Partition Coefficient (1-Octanol/water): Slow-stirring method 4. USEPA Product properties test guidelines: OPPTS 830.7550 Partition Coefficient (n-Octanol/water), Shake-Flask Method The experimental procedure is clear.	5
Is a clear objective stated?	1	Y To estimate a valid estimate of the K_{ow} for PTPTT by measuring the solubility of the substance independently in octanol and in water.	1
Is water quality characterized or identified (distilled or deionized)?	2	N The water solubility testing was conducted using well water which had a pH of 7.86. The water is not distilled or deionized; it was selected based on its availability, phys/chem. characterization and relevance as an environmental groundwater matrix. 1-octanol solubility was determined using > 98% pure octanol purchased from a commercial source.	0
Are the results presented in detail, clearly and understandably?	3	Y	3
Are the data from a primary source and not from a referenced article?	3	Y	3

Was the chemical tested at concentrations below its water solubility?	5	n/a The aim of the study was to determine the substance solubility in water and octanol, in order to calculate a log K_{ow}	n/a
Were particulates absent?	2	Y The complete dissociation of PTPTT in the acidified water/methanol solution used as the column mobile phase was confirmed by the peak shape for both the BTPP and BPAF fragments, the absence of normal baseline anomalies associated with on-column decomposition, and the absence of any detectable signal for the undissociated PTPTT (Environment Canada 2009a)	2
Was a reference chemical of known constant tested?	3	Y Primary stock solution containing benzyltriphenyl phosphonium chloride and BPAF reference standards were prepared to prepare calibration standard solutions for the high-performance liquid chromatography with mass spectrometric detection.	3
Were other fate processes considered?	5	N	0
Was a control (blank) run?	3	N	0
Was temperature kept constant?	5	Y The bottles containing saturated solutions of the test materials in 1-octanol and in well water were placed in temperature-controlled water bath at 20C	5
Was the experiment done near room temperature (15-30^{o} C)?	3	Y	3
Is the purity of the test chemical reported (> 98%)?	3	Y However the commercial substances tested had purity below 98%. To remediate to this situation, water and 1-octanol solubility were determined based on benzyltriphenyl phosphonium cation measurements. Solubility of PTPTT was then extrapolated by stoichiometric conversion	1.5
Was the chemical's identity proven?	3	Y	3
Is the source of the chemical reported?	1	Y	1.5
Results:			
BTP (benzyltriphenyl phosphonium) cation		Water solubility = 2.31 mg/L mg/L 1-Octanol solubility = 919 mg/L K_{ow} = 398 Log K_{ow} = 2.60	
PTPTT		Water solubility = 4.5 mg/L K_{ow} = 398 Log K_{ow} = 2.60	
Score: **Degree of reliability****		31/42 = 74 % 2	

* Kollig, H.P. 1988. Criteria for evaluating the reliability of literature data on environmental process constants. Toxicol. Environ. Chem. 17: 287-311.
** The reliability code for ecotoxicological studies of DSL categorization is used.

Appendix 2 – PBT Model Inputs Summary Table

	Phys-Chem/Fate	**Fate**	**Fate**	**PBT Profiling**	**Ecotoxicity**
Model input parameters	EPIWEB Suite (all models, including: AOPWIN, KOCWIN, BCFWIN; BIOWIN and ECOSAR)	Cahill Multispecies Model	Arnot-Gobas BCF/BAF Model	Canadian-POPs (including: Catabol, BCF Mitigating Factors Model, OASIS Toxicity Model)	Artificial Intelligence Expert System (AIES)/ TOPKAT
SMILES Code	**PTPTT (75768-65-9, non ionic form)** c2cccc(c2)P(c3ccccc3)(c4ccccc4)(Cc1ccccc1)Oc5ccc(C(C(F)(F)F)(C(F)(F)F)c6ccc(O)cc6)cc5 **BTP** c(cccc1)(c1)CP(c(cccc2)c2)(c(cccc3)c3)c(cccc4)c4 **BPAF** FC(F)(F)C(c(ccc(O)c1)c1)(c(ccc(O)c2)c2)C(F)(F)F		**Same as EPIWEB**	**Same as EPIWEB**	**Same as EPIWEB**
Molecular weight (g/mol)	**PTPTT =** 688.66 **BTP =**354.44 **BPAF =** 336.24	Neutral = 336.24 Anion = 335.24			
Melting point (ºC)	*				
Boiling point (ºC)	*				
Data temperature (ºC)					
Density (kg/m^3)					
Vapour pressure (Pa)	*				
Henry's Law constant (Pa·m^3/mol)	*	1.071x10^{-2} Pa-m^3/mol (HENRYWIN, 2000)			
Log K_{aw} (Air-water partition coefficient) (dimensionless)		Neutral = -5.4 (calculated from Henry's Law constant)			

		Anion = -15.4 (Cahill 2008)			
Log K_{ow} (Octanol-water partition coefficient) (dimensionless)	When not specified other wise (see footnotes Table 2), the following correction factor was used for the salt and its dissociation product: Log K_{ow} = 2.6 (Environment Canada 2009a)	Neutral = 4.47 (KOWWIN, 2000) Anion = 1.87 (Cahill 2008)			BTP in ECOSAR Log K_{ow} = 2.6 (Environment Canada 2009a)
K_{ow} (Octanol-water partition coefficient) (dimensionless)					
Log K_{oc} (Organic carbon-water partition coefficient – L/kg)					
Water solubility (mg/L)	When not specified other wise (see footnotes Table 2), the following correction factor was used for the salt and its dissociation product: **PTPTT** = 4.5 mg/L **BTP** = 2.31 mg/L **BPAF** = 2.19 mg/L	Neutral = $4.3x10^{-3}$ g/L (WSKOWWIN 2000)			BTP in ECOSAR Water solubility = 2.31 mg/L (Environment Canada 2009a)
Log K_{oa} (Octanol-air partition coefficient) (dimensionless)					
Soil-water partition coefficient (L/kg)[1]					
Sediment-water partition coefficient (L/kg)[1]					
Suspended particles-water partition					

coefficient (L/kg)[1]					
Fish-water partition coefficient (L/kg)[2]					
Aerosol-water partition coefficient (dimensionless)[3]					
Vegetation-water partition coefficient (dimensionless)[1]					
Enthalpy (K_{ow})					
Enthalpy (K_{aw})					
Half-life in air (days)		0.13 d (Cahill 2008)			
Half-life in water (days)		182 d (Cahill 2008)			
Half-life in sediment (days)		728 d (Cahill 2008)			
Half-life in soil (days)					
Half-life in vegetation (days)[4]					
Metabolic rate constant (1/days)					
Biodegradation rate constant (1/days) or (1/hr) -specify					
Biodegradation half-life in primary clarifier ($t_{1/2\text{-}p}$) (hr)					
Biodegradation half-life in aeration vessel ($t_{1/2\text{-}s}$) (hr)					
Biodegradation half-life in settling tank ($t_{1/2\text{-}s}$) (hr)					

[1] derived from $\log K_{oc}$
[2] derived from BCF data
[3] default value
[4] derived from half-life in water

Appendix 3: Summary of (Q)SAR Results for the Health Assessment

(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

N – Negative
P – Positive
BB – Benigni-Bossa rule
ND – not in domain
'-' no model available in QSAR suite
NR – no result

(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 cancer alert
Model Applier	ND	ND	ND	N	N	N	ND	N	N	N	N	N	ND	-	N	N	N	N	N	N	N	-
Multicase Casetox	NR	-	-	NR	-	NR	-	-	-	-	NR	-	-	NR	-	-	-	-	-	-	NR	-
Topkat	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	NR	-
ToxTree	-	-	-	-	N	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	N

N – Negative
P – Positive
BB – Benigni-Bossa rule
ND – not in domain
'-' no model available in QSAR suite
NR – no result

(Q)SAR PREDICTIONS ON DEVELOPMENTAL TOXICITY

Model Applier

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

Multicase Casetox

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

N – Negative
P – Positive
BB – Benigni-Bossa rule
ND – not in domain
'-' no model available in QSAR suite
NR – no result

(Q)SAR PREDICTIONS ON REPRODUCTIVE TOXICITY

Model Applier

Model/ endpoint	Female			Male		
Species	mice	rat	rodent	mice	rat	rodent
repro	ND	ND	N	ND	N	N
sperm	-	-	-	ND	N	N

Multicase Casetox

mice	rat	rabbit	human
NR	NR	NR	NR

N – Negative
P - Positive
BB – Benigni-Bossa rule;
ND – not in domain;
'-' no model available in QSAR suite
NR – no result