Screening Assessment for the Challenge

Amines, C18-22-tert-alkyl, (chloromethyl)phosphonates (2:1)

Chemical Abstracts Service Registry Number
79357-73-6

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 of Amines, C_{18-22}-*tert*-alkyl, (chloromethyl)phosphonates (2:1) (ATACP), Chemical Abstracts Service Registry Number 79357-73-6. This substance was identified as a high priority for screening assessment and included in the Challenge because it had originally been found to meet the ecological categorization criteria for persistence, bioaccumulation potential and inherent toxicity to non-human organisms and is believed to be in commerce in Canada.

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

ATACP is a complex organic substance, not naturally produced in the environment. While no companies have reported the manufacture (whether alone, in a product or in a mixture) of ATACP in Canada, between 100 and 1000 kg of ATACP were imported into Canada in 2006. All uses of ATACP in Canada have been claimed as confidential business information. However, these uses have been taken into consideration in conducting this assessment. In other countries, ATACP is reported to be used as a lubricant and an additive. The potentially dispersive uses of this substance, indicate that there may be releases into the Canadian environment.

Based on reported use patterns and certain assumptions, the majority of the substance is expected to end up in waste disposal facilities (96.8%). The rest is expected to be chemically transformed during incineration (3.0%), or released to air (0.1%), or released to sewers (0.1%).

ATACP is a salt which dissociates in water and for this reason, an assessment was made of its two components , a positively charged alkyl amine and a negatively charged phosponic acid counterion. Based on modelled physical and chemical properties, the alkyl amine is expected to degrade relatively quickly in air, but is likely persistent in water, soil and sediment. The phosphonic acid counterion is persistent in air on the other hand, but is not likely to persist in water, soil and sediment. Both counterions are also not expected to accumulate to a significant extent in organisms or biomagnify in food chains. While the components of ATACP do not meet the bioaccumulation criteria, they do meet some of the persistence criteria (in air for phosphonic acid and in water soil and sediment for the alkyl amine) as set out in the *Persistence and Bioaccumulation Regulations*. Modelled acute aquatic toxicity values suggest that the alkyl amine has a moderate to high potential for toxicity to aquatic organisms, whereas the phosphonic acid counterion exhibits little or no potential for aquatic toxicity.

As minimal releases into the aquatic environment from industrial operations or other sources are expected, this substance is not believed to cause ecological harm in the aquatic environment.

Based on the information available, it is concluded that ATACP 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.

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

Based on the information available, it is concluded that ATACP does not meet any of the criteria set out in section 64 of CEPA 1999.

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 results of a screening assessment, the Ministers can propose to take no further action with respect to the substance, to add the substance to the Priority Substances List (PSL) for further assessment, or to recommend that the substance be added to the List of Toxic Substances in Schedule 1 of the Act and, where applicable, the implementation of virtual elimination.

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

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

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

The substance Amines, C18-22-tert-alkyl, (chloromethyl)phosphonates (2:1), 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 November 17, 2007 (Canada 2007). 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 uses of the substance were received.

Although Amines, C18-22-tert-alkyl, (chloromethyl)phosphonates (2:1) 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 was not 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. Therefore, this assessment focuses principally on information relevant to the evaluation of ecological risks.

Under CEPA 1999, screening assessments focus on information critical to determining whether a substance meets the criteria for defining a chemical as toxic as set out in section 64 of the Act, where

> "64. [...] a substance is toxic if it is entering or may enter the environment in a quantity or concentration or under conditions that
>
> (*a*) have or may have an immediate or long-term harmful effect on the environment or its biological diversity;
> (*b*) constitute or may constitute a danger to the environment on which life depends; or
> (*c*) constitute or may constitute a danger in Canada to human life or health."

Screening assessments examine scientific information and develop conclusions by applying a weight-of-evidence approach and precaution.

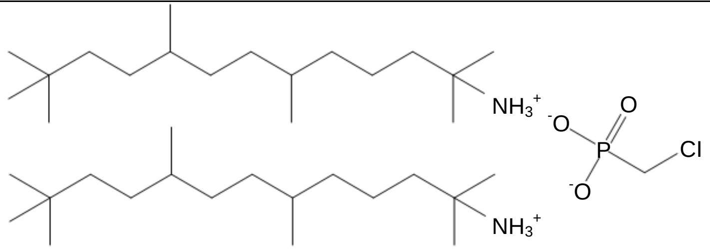
This screening assessment includes consideration of information on chemical properties, hazards, uses and exposure identified after December 2005, including the additional information submitted under the Challenge. Data relevant to the screening assessment of this substance were identified in original literature, review and assessment documents, stakeholder research reports and from recent literature searches up to March 2008. Key studies were critically evaluated and generally only results from studies of good quality were used to reach conclusions, although other studies and modelling results may have been considered as part of the weight of evidence. When available and relevant, information presented in hazard assessment 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.

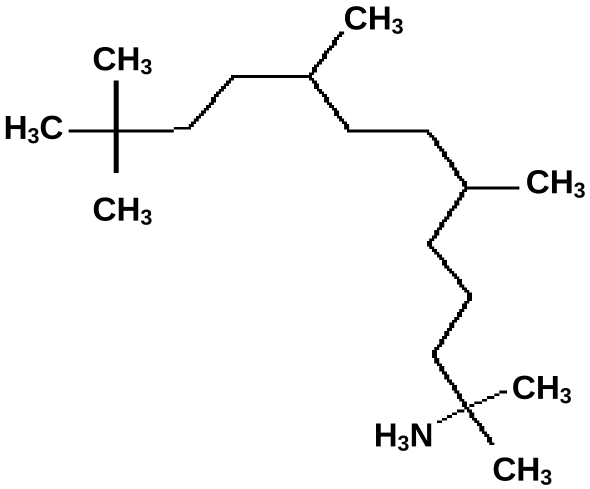
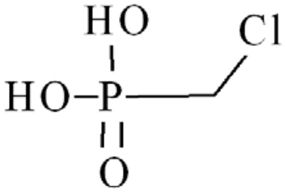
This screening assessment was prepared by staff in the Existing Substances Programs at Health Canada and Environment Canada and incorporates input from other programs within these departments. This assessment has undergone external written peer review/consultation. Additionally, a draft of this screening assessment was subject to a 60-day public comment period. While external comments were taken into consideration, the final content and outcome of the screening risk assessment remain the responsibility of Environment Canada and Health Canada. The critical information and considerations upon which the assessment is based are summarized below.

Substance Identity

For the purposes of this document, this substance will be referred to as ATACP, derived from the DSL inventory name. This substance is a UVCB (**U**nknown or **V**ariable Composition, **C**omplex Reaction Products, or **B**iological Materials). That is, it is not a discrete chemical and thus was characterized by a representative structure and corresponding SMILES notation which were subsequently used in modelling and throughout the assessment.

Table 1. Substance identity for ATACP

Chemical Abstracts Service Registry Number (CAS RN)	**79357-73-6**
Domestic Substances List (DSL) name	**Amines, C18-22-tert-alkyl, (chloromethyl)phosphonates (2:1)**
National Chemical Inventories (NCI) name[1]	*Amines, C18-22-tert-alkyl, (chloromethyl)phosphonates (2:1)* (TSCA, DSL, EINECS, ASIA-PAC, NZIoC*)*
Other names	*Monochloromethyl phosphonic acid, tert C18-C22 alkyl amine salt*
Chemical group (DSL Stream)	UVCB[2]
Major chemical class or use	Amines
Representative chemical formula for the alkyl amine component, the chemical moiety of most ecological concern for this UVCB	$C_{18}H_{39}N$
Representative chemical formula for the phosphonic acid component.	CH_4ClO_3
Chemical structure for the 2:1 salts for $C_{18}H_{39}N$	

Chemical structure representative of the alkyl amine component used to run the estimation models [2]	
Chemical structure representative of the phosphonic acid component used to run the estimation models	
Simplified Molecular Input Line Entry (SMILES) for the alkyl amine and phosphonic acid components used to run the estimation models [2]	CC(C)(C)CCC(C)CCC(C)CCCC(C)(C)N and [O-]P(O)(CCl)=O
Molecular mass for the alkyl amine and phosphonic acid components	269.52 g/mol (alkyl amine) and 130.47 g/mol (phosphonic acid)

[1] National Chemical Inventories (NCI). 2006: ASIA-PAC (Asia-Pacific Substances Lists); EINECS (European Inventory of Existing Commercial Chemical Substances); NZIoC (New Zealand Inventory of Chemicals); and TSCA (Toxic Substances Control Act Chemical Substance Inventory).

[2] This substance is a UVCB (**U**nknown or **V**ariable Composition, **C**omplex Reaction Products, or **B**iological Materials); i.e., it is not a discrete chemical and thus may be characterized by a variety of structures. To assist with modelling and throughout the assessment, the structure and corresponding SMILES presented here were chosen to represent the substance.

Physical and Chemical Properties

Table 2 contains the physical and chemical properties of ATACP that are relevant to its environmental fate. As no experimental data have been identified for ATACP, properties have been estimated using models mostly based on quantitative structure-activity relationship (QSAR) models, where applicable.

Two counterions were chosen to represent ATACP, an alkyl amine and a phosphonic acid component. A **counterion** is an ion that accompanies another ionic species in order to maintain the electric neutrality of a substance. ATACP is a salt that dissociates in water into a positively charged alkyl amine and a negatively charged phosphonic acid component. Ionization of the components significantly affects their physical and chemical properties such as water solubility, log K_{ow} and log K_{oc} (Table 2).

Table 2. Modelled physical and chemical properties of ATACP (alkyl amine ionic form and phosphonic acid)

Property	Type	Value[1] For alkyl amine	Value for phosphonic acid component	Temperature (°C)	Reference
Melting point (ºC)	Modelled	69.34	24.04		MPBPWIN 2000
Boiling point (ºC)	Modelled	299.34	292.26		MPBPWIN 2000
Density (kg/m^3)	N/A	N/A	N/A	N/A	N/A
Vapour pressure (Pa)	Modelled	0.103. (7.73 × 10^{-4} mm Hg)	0.0164		MPBPWIN 2000
Henry's Law constant) (Pa m^3/mol)	Modelled	9.48×10^{1}	4.35×10^{-7}	25	HENRYWIN 2000
Log K_{ow} [2] (Octanol-water	Modelled	3.5	-4.9		ADME/Tox Web

Property	Type	Value[1] For alkyl amine	Value for phosphonic acid component	Temperature (°C)	Reference
partition coefficient) (dimensionless)					
Log K_{oc} (Organic carbon-water partition coefficient) (dimensionless)	Modelled	4.81	0.44		PCKOCWIN 2000
Water solubility (mg/L)	Modelled	192.1	$1.0x10^6$	25	WSKOWWIN 2000
pK_a (Acid dissociation constant) (dimensionless)	Modelled	10.6 (base form)	1.2 (acid form)		ADME/Tox Web

[1] Values and units in parentheses represent those originally reported by the authors or estimated by the models.
[2] Log Kow values have been adjusted for ionization using using LogD estimate at pH 7 from ADME Boxes
N/A: not available.

Sources

The two counterions are not reported to be naturally produced in the environment.

As a result of a survey conducted under section 71 of CEPA 1999 for the year 2006 (Environment Canada 2008b), fewer than five companies reported having imported a combined total of between 100 and 1000 kg of this substance into Canada, either in a product, in a mixture or in a manufactured item. No companies reported manufacturing this substance in any quantity (below or above the prescribed threshold) in Canada during 2006. Fewer than five companies indicated stakeholder interest in this substance (Environment Canada 2008b).

As a result of an earlier survey conducted under section 71 of CEPA 1999 for the year 2005 (Environment Canada 2007), it appears that ATACP was not manufactured or imported into Canada in the year 2005 in a quantity meeting the 100 kg reporting threshold. However, fewer than five companies had indicated a stakeholder interest in this substance.

The quantity reported to be manufactured, imported or in commerce in Canada during the 1986 calendar year was between 0 and 1000 kg. The number of notifiers for the 1984–1986 calendar years was fewer than five (Environment Canada 1988).

Elsewhere, ATACP has been listed on the European Inventory of Existing Commercial Chemical Substances (EINECS) (ESIS 2007). It is not classified by the European Union (EU) industry as a High Production Volume (HPV) or Low Production Volume (LPV) chemical. ATACP was also reported to be used in Denmark and Norway between 2001 and 2005; however, the use and quantities were not identified (SPIN 2008).

Uses

Use information submitted in response to the section 71 notice for the 2006 calendar year (Environment Canada 2008b) has been claimed as confidential business information (CBI). However, these uses have been taken into consideration in conducting this assessment.

Fewer than five companies reported use of the substance during the calendar year 1986 (Environment Canada 1988) for the following uses: lubricating agent/lubricant additive/mould release agent.

According to the Substances in Preparations in Nordic Countries database (SPIN 2008), this chemical was used in Finland in lubricants and additives and in air transport, in 2004.

Releases to the Environment

Mass Flow Tool

To estimate potential releases of substances to the environment at different stages of their life cycle, a Mass Flow Tool was developed (Environment Canada 2008c). Empirical data concerning releases of specific substances to the environment are seldom available. Therefore, for each identified type of use of the substance, the proportion and quantity of release to the different environmental media are estimated, as is the proportion of the substance chemically transformed or sent for waste disposal. Unless specific information on the rate or potential for release of the substance from landfills and incinerators is available, the Mass Flow Tool does not quantitatively account for releases to the environment from disposal.

Assumptions and input parameters used in making the release estimates are based on information obtained from a variety of sources including responses to regulatory surveys, Statistics Canada, manufacturers' websites, technical databases and documents. Of particular relevance are emission factors, which are generally expressed as the fraction of a substance released to the environment, particularly during its manufacture, processing, and use associated with industrial processes. Sources of such information include emission scenario documents, often developed under the auspices of the Organisation for Economic Co-operation and Development (OECD), and default assumptions used by different international chemical regulatory agencies. It is noted that the level of uncertainty in the mass of substance and quantity released to the environment generally increases toward the end of the life cycle.

Results from the Mass Flow Tool (Table 3) indicate that most of the ATACP can be expected to be sent to waste disposal (96.8%), due to the eventual disposal of imported items containing it. A small fraction of solid waste is incinerated, which is expected to result in chemical transformation of the substance (3.0%). Based largely on information contained in OECD emission scenario documents for processing and uses associated with this type of substance, it is estimated that 0.1% of ATACP may be released to each of air and water (the latter via sewer).

Table 3. Estimated releases and losses of ATACP to environmental media, chemical transformation and transfer to waste disposal sites, based on the Mass Flow Tool.

Fate	Proportion of the mass (%)[1]	Major life cycle stage involved[2]
Releases to receiving media:		
Soil	0.0	Consumer use
Air	0.1	Service life
Sewer[3]	0.1	Service life
Chemically transformed	3.0	
Transferred to waste disposal sites (e.g., landfill, incineration)	96.8	Waste disposal

[1] For ATACP. values presented for release to environmental media do not account for possible mitigation measures that may be in place in some locations (e.g., partial removal by sewage treatment plants). Specific assumptions used in derivation of these estimates are summarized in Environment Canada 2008b.

[2] Applicable stage(s): consumer use-service life of article/product-waste disposal.

[3] Wastewater before any form of treatment.

Environmental Fate

Since ATACP is a salt, in water it dissociates into a positively charged (basic) alkyl amine and a negatively charged (acidic) phosphonic acid component. . Ionization has an impact on log K_{ow}, log K_{oc} and water solubility of the substance (Table 2). For example, the log K_{ow} of the ionized alkyl amine - estimated to be about 3.5 at a pH of 7 (Table 2) – is less than that of the neutral form.

Based on the physical and chemical properties of the counterions of ATACP (Table 2), the results of Level III fugacity modelling (Table 4) suggest that phosphonic acid will predominantly reside in water and soil, depending on the compartment of release . The alkyl amine will predominantly reside in water ,sediment or soil, depending on the compartment of release.

Table 4. Results of the Level III fugacity for the Alkyl Amine and Phosphonic acid Counterions of ATACP (Environment Canada 2008d)

	Percentage of ATACP components partitioning into each compartment				
Substance released to	**Form**	**Air**	**Water**	**Soil**	**Sediment**
Air (100%)	Alkyl amine	77.1	2.2	10.1	10.6
Water (100%)	Alkyl amine	0.3	17.4	0.004	82.3
Soil (100%)	Alkyl amine	0	0	100	0.03
Air (100%)	Phosponic acid	0	31.1	68.8	0.1
Water (100%)	Phosponic acid	0	99.8	0	02
Soil (100%)	Phosponic acid	0	27.8	72.1	0.1

The alkyl amine exhibits moderate volatility and will remain largely in air (77.1%) if released to air. If the phosphonic acid counterion is released to air, the substance will mostly partition to water and soil (see Table 4).

If released into water, the alkyl amine is expected to remain in water or to a larger extent partition to sediment (17.4 and 82.3%, respectively). Volatilization from water surfaces is expected to be an unimportant fate process based upon this compound’s estimated Henry’s Law constant. If water is a receiving medium, the phosphonic acid counterion is expected to mainly remain in water (see Table 4 above).

If released to soil, the alkyl amine is expected to have high adsorptivity to soil (i.e., expected to have somewhat limited mobility) based upon its estimated log $K_{oc,}$ whereas the phosphonic acid component is expected to be very mobile. Volatilization from moist soil surfaces seems to be an unimportant fate process based upon the estimated Henry’s Law constants. Moderate volatilization from dry soil surfaces is possible, based on the vapour pressure of the phosphonic acid component. Therefore, if released to soil, both counterions will mainly remain in this environmental compartment and, in the case of the phosphonic acid component partition to water, which is illustrated by the results of the multispecies modelling (see Table 4).

Persistence and Bioaccumulation Potential

Environmental Persistence

No experimental degradation data for both counterions have been identified. Table 5 summarizes the results of available QSAR models for degradation in various environmental media.

Table 5. Modelled data for degradation of the Alkyl Amine

Fate Process	Model and model basis	Model Result and Prediction	Extrapolated Half-life (days)
AIR			
Atmospheric oxidation	AOPWIN 2000	$t_{1/2}$ = 0.282 day	< 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)	2.2[2] “months”	< 182[4]
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 4: Expert Survey (primary biodegradation)	3.19[2] “weeks”	< 182[4]
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 5: MITI linear probability	0.32[3] “does not biodegrade fast”	< 182[4]
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 6: MITI non-linear probability	0.14[3] “does not biodegrade fast”	> 182[4]
Biodegradation (aerobic)	CATABOL 2004-2008 % BOD (biological oxygen demand)	% BOD = 24.86.4 “biodegrades slowly”	> 182[4]

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

Table 5. Modelled data for degradation of the Phosphonic Acid Counterion

Fate Process	Model and model basis	Model Result and Prediction	Extrapolated Half-life (days)
AIR			
Atmospheric oxidation	AOPWIN 2000	$t_{1/2}$ = 16.8 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)	2.73[2] “weeks to months”	< 182[4]
Biodegradation	BIOWIN 2000	3.55[2]	< 182[4]

(aerobic)	Sub-model 4: Expert Survey (primary biodegradation)	“days to weeks”	
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 5: MITI linear probability	0.37[3] “does not biodegrade fast”	< 182[4]
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 6: MITI non-linear probability	0.19[3] “does not biodegrade fast”	> 182[4]
Biodegradation (aerobic)	CATABOL 2004-2008 % BOD (biological oxygen demand)	% BOD = 0.6 “biodegrades slowly”	> 182[4]

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

In air, these chemicals are likely to react mainly with hydroxyl radicals. The compounds are not expected to react with other photo-oxidative species in the atmosphere, such as O_3. With a half-life of 0.28 days via reactions with hydroxyl radicals, the alkyl amine component of ATACP is considered not persistent in air. However, the phosphonic acid component is quite persistent in air, with an estimated half-life of 16.8 days.

Results for the alkyl amine generally suggest a low rate of ultimate biodegradation. Both BIOWIN sub-model 6 and Catabol indicate that ultimate biodegradation half lives would be greater than 182 days. The BIOWIN 5 result of 0.32 indicates that this substances “does not biodegrade fast”. The BIOWIN 3 result of “months” has been suggested to equate to a primary half-life of 120 days, suggesting that the ultimate degradation half-life could be longer than 182 days. Although primary degradation could occur relatively rapidly, the identities of the degradation products are not known.

For the phosphonic acid component, the results from BIOWIN sub-models 3 ,4,and 5 indicate that the biodegradation half life is less than 182 days. BIOWIN 6 and Catabol results on the other hand suggest that the half-life in water would be >182 days. However, in light of the BIOWIN 3 ,4 and 5 predictions and the fact that empirical data indicate that a related chemical ethephon degrades quickly in soil (Etoxnet, 2009), it is concluded that the ultimate degradation half life of the phosphonic acid component is significantly less than 182 days.

Using an extrapolation ratio of 1:1:4 for a water:soil:sediment biodegradation half-life (Boethling et al. 1995), the ultimate degradation half-life in soil is predicted to be >182 days and the half-life in sediments is predicted to be >365 days for the alkyl amine. This indicates that the alkyl amine is persistent in soil and sediment. The half-life for the phosphonic acid is expected to be significantly less than 182 days in soil (based mainly on degradation information for a related chemical - ethephon - noted above), and therefore the half-life in sediment is expected to be less than 365 days.

Based on the modelled data available (see Table 5), the alkyl amine meets the criteria for persistence in water, soil (i.e., half-lives in soil and water ≥ 182 days), and sediment (half-life in sediment ≥ 365 days), but does not meet the criteria for air (half-life in air ≥ 2 days) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000). For the phosphonic acid counterion, modelled data suggest that the substance does not meet the criteria for persistence in water, soil and sediment, but does meet the criteria in air as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential for Bioaccumulation

The modelled log K_{ow} estimated for the ionized form of phosphonic acid (-4.9) suggests that this chemical has a relatively low potential to bioaccumulate in the environment (see Table 2). The log K_{ow} estimated for the ionized form of the alkyl amine component (3.5) suggests moderate potential for bioaccumulation.

Since no experimental bioaccumulation factor (BAF) and bioconcentration factor (BCF) data were available for the counterions, a predictive approach was applied using available BAF and BCF models as shown in Table 6. Log K_{ow}s (adjusted for ionization) of 3.5 and -4.9 for the alkyl amine and phosphonic acid components respectively, were used for these estimations.

Table 6. Predicted BAF and BCF in fish for the alkyl amine and phosphonic acid using the Arnot and Gobas (2003) kinetic model with default of no metabolism.

Test organism	Endpoint	Value wet weight (L/kg) (alkyl amine)	Value wet weight (L/kg) (phosphonic acid)	Reference
Fish	BCF in middle trophic level fish	171.8	0.95	(Arnot and Gobas 2003)
Fish	BAF in middle trophic level fish	172.3	0.95	(Arnot and Gobas 2003)
Fish	BCF	94.69	3.162	BCFWIN (2000)

The results of BAF and BCF model calculations provide evidence of the low potential of both of these substances to bioaccumulate or bioconcentrate in the environment.

Metabolism information for these substances was not available, nor was it considered in the models. It is expected that metabolism information, if it were available, would lower the predicted BAF and BCFs.

Based on the available modelled values, neither of the components of ATACP meet the bioaccumulation criteria (BCF or 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

No experimental ecotoxicity data were identified for the two counterions. Therefore, QSAR modelling and a weight-of-evidence approach were used to estimate the potential for aquatic toxicity for ATACP.

Under the environmentally relevant pHs of 6 to 9, the components of ATACP will almost exclusively be found in their ionized forms in aquatic ecosystems. The ECOSAR model was run for the alkyl amine using log Kow of 3.5 and water solubility of 192 mg/L(Table 7). This substance is a narcotic toxicant (narcotic amine) and the model results suggest that this alkyl amine in this form has a high to moderate potential to cause toxicity to aquatic organisms However, due to its low bioaccumulation factor, it is not expect to accumulate to a significant extent in the tissues of exposed organisms.

When the ECOSAR model was run for the phosphonic acid component of ATACP - using the estimated log Kow of the ionized form of the substance (i.e., -4.9) - the toxicity values were generally above saturation (1.0×10^6 mg/L), indicating that this substance has little if any potential to cause aquatic toxicity.

Table 7. Modelled data for aquatic toxicity of alkyl amine counterions

Test organism	Type of test	Endpoint	Value (mg/L) Alkyl amine	Reference
Fish	96 hr	LC_{50}[1]	5.9	ECOSAR 2004
Fish	96 hr	LC_{50}		AIES 2003-2005
Daphnid	48 hr	LC_{50}[1]	0.82	ECOSAR 2004
Daphnid	48 hr	LC_{50}		AIES 2003-2005
Green algae	96 hr	EC_{50}[2]	0.57	ECOSAR 2004
Green algae	96 hr	ChV[3]	0.15	ECOSAR 2004

[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 toxic sublethal effect on 50% of the test organisms.
[3] ChV – Chronic toxicity.

B - In Other Environmental Compartments

No ecological effects studies were found for this compound in media other than water (e.g., soil or sediment). No QSAR models were available that generate toxicity data for ATACP or its components in the other media.

Ecological Exposure Assessment

No monitoring data on the presence of ATACP or the two counterions in environmental media (air, water, soil, sediment) have been found.

Based on the use pattern information submitted confidentially under section 71 of CEPA 1999 for ATACP, 96.8 % of the substance is expected to end up in waste disposal facilities and 3% is expected to undergo chemical transformation. Releases from the substance during the service life are expected to be low (0.1% to each of air and water) and disperse.

As this substance is not manufactured in Canada, and very little is used by industry in Canada, it is concluded that little or no industrial release of ATACP is expected.

Characterization of Ecological Risk

The characterization of ecological risk is based on the evaluation of scientific and other information using a weight-of-evidence approach and precaution. Attention is given in particular to potential for release, persistence and bioaccumulation in the environment, and potential to cause aquatic toxicity.

A risk quotient analysis was not performed as it is expected, based on the use patterns, that there is little release and exposure. The quantities of ATACP imported into Canada (range 100 – 1000 kg in 2006) are low, and the proportion of the imported ATACP that is released (0.2 %) is very low.

Once released in the environment, the alkyl amine is persistent in water, soils and sediment, while the phosphonic acid component is expected to be persistent in air. Neither of the components of ATACP is expected to bioaccumulate or biomagnify in food chains. Although the alkyl amine moiety has moderate to high potential for toxicity to aquatic organisms, the phosphonic acid component has a negligible toxicity potential.

Therefore, based mostly on the anticipated very low and disperse nature of releases it is not believed that ATACP is causing harm to organisms in Canada.

Uncertainties in Evaluation of Ecological Risk

The modelling of a substance’s physical and chemical properties and P, B and iT characteristics is based on chemical structures. This substance is a UVCB (**U**nknown or

Variable composition, **C**omplex reaction product or **B**iological material), specifically its composition is unknown or variable. It could not be represented by a single, discrete chemical structure. Therefore, for the purposes of modelling, a “representative structure” that would provide conservative estimates was identified. Within the representative structure, two counterions were identified, an akyl amine and a phosphonic acid moiety. Where possible, both counterions were considered in the assessment and the alkyl amine was determined to have the higher potential to cause adverse effects in the environment. Given that more than one representative structure may be derived for the same UVCB, it is recognized that structure-related uncertainties exist for this substance

As no empirical data were available for the components of ATACP, modeling was performed to determine the physical and chemical properties, persistence, bioaccumulation and ecological effects. The predicted values may add an additional source of uncertainty associated with the evaluation of the fate and toxicity of the components of ATACP.

There are uncertainties associated with releases predicted by the Mass Flow Tool, however, there is confidence that the releases to the environment will be small.

Conclusion

Based on the information presented in this screening assessment, it is concluded that ATACP 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.

It is therefore concluded that ATACP does not meet the definition of toxic as set out in section 64 of CEPA 1999. Additionally, while the alkyl amine does meet the criteria for persistence. The phosphonic acid counterion does not, and neither counterions meets the criteria for bioaccumulation potential as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

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Appendix II – PBT Model Inputs Summary Table

	Phys-Chem/Fate	**Fate**	**Fate**	**Fate**	**Fate**	**PBT Profiling**	**Ecotoxicity**
Model Input Parameters	EPIWIN Suite (all models, including: AOPWIN, KOCWIN, BCFWIN BIOWIN and ECOSAR)	STP (1) ASTreat (2) SimpleTreat (3) (required inputs are different depending on model)	EQC (required inputs are different if Type I vs. Type II chemical)	TaPL3 (required inputs are different if Type 1 vs. Type 2 chemical)	Arnot-Gobas BCF/BAF Model	Canadian-POPs (including: Catabol, BCF Mitigating Factors Model, OASIS Toxicity Model)	Artificial Intelligence Expert System (AIES)/ TOPKAT/ ASTER
SMILES Code	Alkyl amine:CC(CCCC(C)CCCC(C)CCCC([NH3+])(C)C)(C)C Phosphonic acid: [O-]P(O)(CCl)=O				Alkyl amine:CC(CCCC(C)CCCC(C)CCCC([NH3+])(C)C)(C)C Phosphonic acid: [O-]P(O)(CCl)=O	Alkyl amine:CC(CCCC(C)CCCC(C)CCCC([NH3+])(C)C)(C)C Phosphonic acid: [O-]P(O)(CCl)=O	Alkyl amine:CC(CCCC(C)CCCC(C)CCCC([NH3+])(C)C)(C)C Phosphonic acid: [O-]P(O)(CCl)=O
Molecular weight (g/mol)		269.52 g/mol (alkyl amine) and 130.47 g/mol (phosphonic acid)	269.52 g/mol (alkyl amine) and 130.47 g/mol (phosphonic acid)	269.52 g/mol (alkyl amine) and 130.47 g/mol (phosphonic acid)			
Melting point (ºC)	Alkyl amine: 69.34 Phosphonic acid: 24.04*		x Alkyl amine: 69.34 Phosphonic acid: 24.04*	Alkyl amine: 69.34 Phosphonic acid: 24.04*			
Boiling point (ºC)	Alkyl amine: 299.34 Phosphonic acid:						

	292.26*						
Data temperature (ºC)	20		20	20			
Density (kg/m^3)	Not available						
Vapour pressure (Pa)	Alkyl amine: 0.101 Phosphonic acid: 0.0164*	Alkyl amine: 0.101 Phosphonic acid: 0.0164*	Alkyl amine: 0.101 Phosphonic acid: 0.0164 (I)	Alkyl amine: 0.101 Phosphonic acid: 0.0164 (I)			
Henry's Law constant (Pa·m^3/mol)	* Alkyl amine: 9.48x10^{01} Phosphonic acid: 4.35x10^{-7}						
Log K_{aw} (Air-water partition coefficient; dimensionless)							
Log K_{ow} (Octanol-water partition coefficient; dimensionless)	Alkyl amine: 3.5 Phosphonic acid: -4.9*	Alkyl amine: 3.5 Phosphonic acid: -4.9*	Alkyl amine: 3.5 Phosphonic acid: -4.9*	Alkyl amine: 3.5 Phosphonic acid: -4.9*	Alkyl amine: 3.5 Phosphonic acid: -4.9*		
K_{ow} (Octanol-water partition coefficient; dimensionless)							
Log K_{oc}	Alkyl amine: 4.81						

(Organic carbon-water partition coefficient – L/kg)	Phosphonic acid: 0.44*						
Water solubility (mg/L)	Alkyl amine: 192.1 Phosphonic acid: $1.0x10^6$*	Alkyl amine: 192.1 Phosphonic acid: $1.0x10^6$*	Alkyl amine: 192.1 Phosphonic acid: $1.0x10^6$* (I)	Alkyl amine: 192.1 Phosphonic acid: $1.0x10^6$*			
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)							
Half-life in water (days)							
Half-life in sediment (days)							
Half-life in soil (days)							
Half-life in vegetation (days)[4]							
Metabolic rate constant (1/days)					Alkyl amine: 0.4796 Phosphonic acid:29.1		
Biodegradation rate constant (1/days) or							

(1/hr) -specify							
Biodegradation half-life in primary clarifier ($t_{1/2-p}$) (hr)		Alky; amine: 5587.93 Phosphonic acid: 17.42					
Biodegradation half-life in aeration vessel ($t_{1/2-s}$) (hr)		Alkyl amine: 5587.93 Phosphonic amine: 17.42					
Biodegradation half-life in settling tank ($t_{1/2-s}$) (hr)		Alkyl amine: 5587.93 Phosphonic acid: 17.42					

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