Substance Profile for The Challenge Thiourea (CAS No. 62-56-6)

Introduction

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

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

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

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

Based on a consideration of the ecological and/or human health concerns associated with these substances, and the requirement under section 76.1 of CEPA 1999 for the Ministers to apply a weight of evidence approach and the precautionary principle when conducting and interpreting the results of an assessment, sufficient data are currently available to conclude whether these substances meet the criteria under section 64 of CEPA 1999.

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

The substance thiourea (CAS No. 62-56-6) was identified as a high priority for action as it was determined to have a high potential for exposure to individuals in Canada (GPE), and is considered to present a high hazard to human health. The technical human health and ecological information, that formed the basis for concern associated with this substance, is contained in Appendices I and II, respectively.

CAS Registry Number	62-56-6		
Inventory names	Thiourea		
Other names	 β-thiopseudourea; 2-thiourea; isothiourea; NSC 5033; pseudothiourea; pseudourea (NH2·C(OH):NH), hio-; pseudourea, 2-thio-; thiocarbamide; THU; TsIZP 34; UN 2810; urea, 2-thio; urea, thio- 		
Chemical group	Discrete organics		
Chemical sub-group	Amines; thio compounds		
Chemical formula	CH ₄ N ₂ S		
Chemical structure	H ₂ N NH ₂ S		
SMILES	NC(=S)N		
Molecular mass	76.12 g/mol		

Substance Identity

Based on information submitted by the 16 companies that notified this substance to the Domestic Substances List, the quantity of thiourea reported to be manufactured, imported or in commerce in Canada during the calendar year 1986 was 1,240,000 kg. Reported uses include the categories of: Analytical reagent, Catalyst/accelerator/initiator/activator, Organic Chemical intermediate, Finishing agent, Formulation component, Fragrance/perfume/deodourizer/flavouring agent, Photosensitive agent - fluorescent agent/brightener/UV absorber, Stripper/etcher/discharge printing agent/de-inker, Electrical or Electronic Products, Explosive Materials, Metallurgical, Metal and Non-Metal Mining, Industrial and Specialty Organic Chemicals, Industrial, Pharmaceuticals, Photographic/Photocopier, Plating and Surface Finishing, Printing and Publishing, and Textile, Primary Manufacture.

In Canada, thiourea has been reported as being used in the non-ferrous metals smelting and refining sector (Refer to Appendix I), but other uses are likely. One of its main potential uses is as a chemical intermediate and/or reagent for a variety of industrial and chemical processes, such as ore leaching, metal cleaning and precipitation, electroplating, rubber vulcanization, production of flame retardant resins, pharmaceutical and pesticide synthesis, dry cleaning, photographic developing, and production of copy paper. It is also a corrosion inhibitor and may be used to inhibit nitrification in fertilizers. Thiourea has been used in hair preparations and as a mold inhibitor in cosmetics. Thiourea may also be produced naturally by certain shrubs and fungi.

THE CHALLENGE

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

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

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

Section 71 Notice

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

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

Opportunity to Submit Additional Information to Inform Screening Assessment

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

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

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

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

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

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

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

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

Submission of additional information is being invited in the following areas:

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

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

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

Responses to the questionnaire should be received at the address provided below by November 13, 2007.

Request for Documents and Submission of Information

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

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

Appendix I Human Health Information to Support The Challenge for Thiourea CAS No. 62-56-6

Introduction

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

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

Thiourea is considered to meet the criteria for GPE under SimET and for high hazard under SimHaz. This document summarizes the currently available information used to support the inclusion of this substance in the Challenge.

Exposure Information from Health Related Components of DSL Categorization

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

Results of the Application of SimET

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

Nomination Information for DSL

Quantity in Commerce

The quantity reported to be manufactured, imported or in commerce in Canada during the calendar year 1986 was 1,240,000 kg.

Number of Notifiers

The number of notifiers for the calendar years 1984-1986 was 16.

Use Codes and Description

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

- 05 Analytical reagent
- 08 Catalyst/accelerator/initiator/activator
- 10 Chemical intermediate organic
- 17 Finishing agent
- 21 Formulation component
- 22 Fragrance/perfume/deodourizer/flavouring agent
- 32 Photosensitive agent fluorescent agent/brightener/UV absorber
- 45 Stripper/etcher/discharge printing agent/de-inker
- 51 Function other than that listed in codes 02-50
- 61 Electrical or Electronic Products
- 62 Explosive Materials
- 71 Metallurgical
- 72 Mining, Metal and Non-Metal
- 76 Organic Chemicals, Industrial
- 77 Organic Chemicals, Specialty
- 83 Pharmaceuticals
- 84 Photographic/Photocopier
- 88 Plating and Surface Finishing
- 89 Printing and Publishing
- 94 Textile, Primary Manufacture

Potential Uses in Canada

The additional information below on potential uses of Thiourea was identified through searches of the available scientific and technical literature.

Thiourea is produced by fusing ammonium thiocyanate which is accomplished by heating dry ammonium thiocyanate followed by extraction with a concentrated solution of ammonium thiocyanate and subsequent crystallization (Lewis, 2001; O'Neil, 2001). It may also be prepared by reacting hydrogen sulphide (or ammonium sulphide or calcium hydrogen sulphide) with calcium cyanamide (WHO, 2003; Lewis, 2001).

Thiourea is found in nature in laburnum shrubs (*Laburnum anagyroides*) and is a natural metabolite of the fungi *Verticillium alboatrum* and *Bortrylius cinerea* (WHO, 2003).

Thiourea is a versatile chemical intermediate that is used in conversion of maleic to fumaric acid, in the production of thiourea dioxide, in the modification of resins, in the production and modification of textile and dyeing auxiliaries, and in the production of mercaptosilanes (WHO, 2003).

Thiourea may be used in ore leaching (e.g. gold and silver extraction), as a photographic fixing agent and to remove stains from negatives, as an auxiliary agent in diazo paper (light-sensitive photocopy paper) and many other types of copy paper, in metal cleaning (such as silver polishes), in the precipitation of heavy metals, as an additive in slurry explosives, used in electroplating and electroforming, and as a corrosion inhibitor (WHO, 2003; Lewis, 2001; O'Neil, 2001; Verschueren, 2001). In addition, it may be used as a dry cleaning agent, in the synthesis of pharmaceuticals and insecticides, in boiler water treatment, as a reagent for bismuth and selenite ions, and it may be used to inhibit nitrification in fertilizers (NTP, 2005; Lewis, 2001; O'Neil, 2001; WHO, 2003; Verchueren, 2001). Thiourea may also be used as a liquefying agent in animal hide glues, in the production of flame retardant resins and as a vulcanization accelerator (WHO, 2003).

Furthermore, Thiourea has been used in hair preparations and as a mold inhibitor in cosmetics, however, it is currently listed on Health Canada's Cosmetic Hotlist which prohibits its use in cosmetic products (Winter, 2005; Health Canada, 2005a). This substance is also prohibited in food products (US FDA, 2006; Winter, 2005).

Canadian specific uses were not identified however the company reporting to the National Pollutant Release Inventory (NPRI) on this substance in 2004 and 2005 is from the metal industry (non-ferrous metals – smelting, refining, etc.) (NPRI, 2006).

Hazard Information from Health Related Components of DSL Categorization

Simple Hazard Tool (SimHaz)

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

Results of the Application of SimHaz

Thiourea is considered to be a potentially high hazard substance based on its classification for carcinogenicity by the European Commission, United States National

Toxicology Program (NTP) and for developmental toxicity by the European Commission.

In the 11th Report on Carcinogens, NTP concluded that Thiourea is reasonably anticipated to be a human carcinogen based on sufficient evidence of carcinogenicity in experimental animals. (NTP, 2005)

The European Commission classified Thiourea as a Carcinogen Category 3 (Causes concern for humans owing to possible carcinogenic effects) and also as a Reproductive Category 3 based on a developmental endpoint (Possible risk of harm to the unborn child) (European Commission, 1998a; European Commission, 1998b; ESIS, 2006)

Uncertainties

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

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Appendix II Ecological Information to Support The Challenge for Thiourea CAS No. 62-56-6

Introduction

The information in this document will form the basis of a screening assessment under section 74 of CEPA, 1999. Data relevant to an ecological screening assessment were identified in original literature, review documents, commercial and government databases prior to December 2005. Properties and characteristics may also have been estimated using Quantitative Structure Activity Relationship (QSAR) models.

Physical and Chemical Properties

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

Property	Туре	Value	Temperature (°C)	Reference
Melting Point	Experimental	177.00 °C		Sax (1984)
		182.00 °C		SRC PHYSPROP Database (2003)
	Modelled	25.8 °C		MPBPWIN v1.41
Boiling Point	Modelled	157.8 °C		MPBPWIN v1.41
Vapour Pressure	Experimental	1.83 e-004 mm Hg (2.44E-02 Pa)	25	CHEMFATE (SRC, 2007)
	Modelled	7.8 Pa		MPBPWIN v1.41
Henry's Law Constant	Experimental	1.29e-10 atm- m3/mole (1.31e-05 Pa- m3/mole)		Hin and Mookerjee (1975)
	Modelled	1.58e-007 atm- m3/mole (1.61e-02 Pa- m3/mole)		HenryWin v3.10
log K _{ow} (Octanol-water partition coefficient)	Modelled	-1.31		Kowwin v.1.67

Table 1. Physical-chemical properties for thiourea

Property	Туре	Value	Temperature (°C)	Reference
	Experimental	-2.38 - 0.00		ISHOW; HSDB; ENVIROFATE; CHEMFATE (SRC, 2007); CESARS and CMR; Govers,H et al.(1986); Kent et al. (1991)
Water Solubility	Measured	91800 - 142000 mg/L		ISHOW; Kent et al. (1991); Milleman and Ehrenberg (1982)
	Modelled	554200 mg/L		WSKOW v.1.41
log K _{oc} (Organic carbon-water partition coefficient)	Modelled	0.44 unitless		PCKOCWIN v1.66

Manufacture, Importation, and Uses

Manufacture and Importation

Available information is presented in Appendix I.

Uses

Available information is presented in Appendix I.

Releases, Fate and Presence in the Environment

Releases

Appendix I provides information regarding the releases to the environment. Aside from anthropogenic sources, thiourea is also produced in the environment by natural sources including the fungi *Verticillium alboatrum* and *Bortrylius cinerea*, and, possibly, the shrub *Laburnum anagyroides* (WHO, 2003).

Fate

Thiourea is highly water soluble (WS > 91800 mg/L) and only slightly volatile (VP = 0.024 Pa) and, therefore, is expected to remain in soil or water, depending on the compartment of release. Level III fugacity modelling (Table 2) indicates that thiourea releases to air, or a combination of air/water/soil, will partition almost completely to the water and soil compartments. Releases to soil will result in almost 80% of the chemical remaining in the soil compartment with the remainder primarily entering the water compartment. Because of its high solubility, releases to water result in only slight partitioning to sediments and negligible partitioning to air or soil.

Receiving Media	% in Air	% in Water	% in Soil	% in Sediment
Air (100%)	0.12	26.0	73.8	0.05
Water (100%)	0.00	99.8	0.0	0.18
Soil (100%)	0.00	22.1	77.8	0.04
Air, Water, Soil (33.3% each)	0.04	39.4	60.5	0.07

 Table 2: Results of the Level III fugacity modelling (EPIWIN V3.04; CEMC, 2002)

Presence in the Environment

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

Evaluation of P, B and iT Properties

Environmental Persistence

Once released into the environment, thiourea appears to be relatively persistent in the environment, mainly in water, soil and sediments. No experimental persistence data in air are available for thiourea. A predicted atmospheric oxidation half-life value of 0.25 days (Table 3a) suggests that in air, this chemical is likely to be rapidly oxidized. This compound is not expected to react, or react appreciably, with other photo oxidative species in the atmosphere, such as O_3 and NO_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 thiourea. With a half life of 0.25 days via reactions with hydroxyl radical, thiourea does not meet the criterion for persistence in air (half-life ≥ 2 days) as set out in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000).

Medium	Fate Process	Degradation Value	Endpoint (units)	Model
Water/Soil	Biodegradation	15	half-life (days)	BIOWIN v4.02, Ultimate survey
Water/Soil	Biodegradation	0.77	Probability	BIOWIN v4.02 MITI Non-Linear Probability
Water/Soil	Biodegradation	1	Probability	ТОРКАТ
Air	Ozone reaction	Not reactive	half-life (days)	AOPWIN v1.91
Air	Atm. oxidation	0.25	half-life (days)	AOPWIN v1.91

Table 3a. Modeled data for persistence

Table 3b. Empirical data for persistence

Medium	Fate Process	Degradation Value	Endpoint (units)	Reference
Water	Biodegradation	2.6%	%BOD	MITI (1992)
Water	Hydrolysis	54750	half life (days)	Ellington et al. (1988)

Two studies with measured values were available for the degradation of thiourea in water (Table 3b). The studies were critically reviewed, and data were considered as reliable and the most appropriate for estimating persistence in water, although several QSAR predictions were also available (Table 3a). The empirical hydrolysis data (Ellington et al.; 1988) show negligible hydrolysis. The experimental biodegradation result (MITI 1992) shows very low biodegradation (2.6% over 28 days in a ready-biodegradation test, Table 3b), which indicates that the half-life in water is expected to be longer than 182 days (6 months). Therefore, thiourea can be considered persistent in water.

To extrapolate half-life in water to half-lives in soils and sediments, Boethling's extrapolation factors $t_{1/2 \text{ water}}$: $t_{1/2 \text{ soil}}$: $t_{1/2 \text{ soil}}$ = 1: 1: 4 (Boethling *et al.*, 1995) can be used. Therefore, it may be concluded that half-lives in soil and sediments are expected to be 182 days and 2 years, respectively.

Thus, the substance thiourea meets the persistence criteria (half-lives in soil and water \geq 182 days; half-life in sediment \geq 365 days) as set out in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000).

Potential for Bioaccumulation

Experimental and modelled log K_{ow} values (Table 1) for thiourea indicate that this chemical has very little potential to bioaccumulate in aquatic organisms.

The experimental bioconcentration factors (BCF) in fish are reported to be 0.2 and 2 L/kg (MITI 1992). The modelled bioaccumulation (BAF) and bioconcentration (BCF) values also agree quite well with the experimental value (Table 4b). The Modified GOBAS BAF middle trophic level model for fish produced a bioaccumulation factor (BAF) of 0.93 L/kg, indicating that thiourea has little potential to bioconcentrate and biomagnify in the environment. The three other BCF models for fish also provide a weight-of-evidence to support low bioconcentration potential of this substance (1-9 L/kg).

Table 4a. Empirical data for bioaccumulation

Test Organism	Endpoint	Value	Reference
Fish (carp)	BCF	2.0 (wet weight, L/kg)	MITI (1992)
Fish (carp)	BCF	0.2 (wet weight, L/kg)	MITI (1992)

Test Organism	Endpoint	Value	Reference
Fish	BAF	0.93 (wet weight, L/kg)	Modified GOBAS BAF Tier II 6.3% BAF (Arnot and Gobas, 2003)
Fish	BCF	9.12 (wet weight, L/kg)	OASIS BCF _{Max} (OASIS Forecast. 2005)
Fish	BCF	3.16 (wet weight, L/kg)	BCFWIN v2.15
Fish	BCF	0.95 (wet weight, L/kg)	Modified GOBAS BCFTier II 5.10% BCF (Arnot and Gobas, 2003)

Table 4b. Modelled data for bioaccumulation

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

Ecological Effects

A - In the Aquatic Compartment

The experimental toxicity data for thiourea (Table 5a) indicate that algae and daphnia are more sensitive species (acute LC50/EC50=5-18 mg/L) than fish (acute LC50=600 mg/L).

A range of aquatic toxicity predictions were obtained from the various QSAR models considered. Table 5b contains those predictions that were considered reliable and were used in the QSAR weight-of-evidence approach for aquatic toxicity (ESD 2006a). All models produced ecotoxicity values in the order of hundreds to thousands of mg/L.

Organism	Test type	Endpoint	Value (mg/L)	Reference
Algae	Acute	EC50	4.8* - 10.0	Geyer et al. (1985)
Daphnia	Acute	LC50	5.6 - 18	Maas (1990)
Fish	Acute	LC50	600	Curtis and Ward (1981)

Table 5a: Empirical data for aquatic toxicity.

*Pivotal iT value for categorization

Table 5b Modelled data for aquatic toxicity.

Organism	Type of Test	Endpoint	Value (mg/L)	Model
Fish	Acute	LC50	475	AI Expert
Fish	Acute	LC50	72925	ECOSAR v 099h
Daphnia	Acute	EC50	7500	TOPKAT v6.2
Algae	Acute	EC50	32123	ECOSAR v 099h
Daphnia	Chronic	EC50	749	ECOSAR v 099h,
Mysid Shrimp	Acute	LC50	223	ECOSAR v 099h,

Therefore, since experimental acute LC50/EC50 values vary from several mg/L to hundreds of mg/L, it is expected that thiourea will pose a moderate to low (acute or immediate) hazard to aquatic organisms.

B - In Other Media

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

Potential to Cause Ecological Harm

Based on the available information, thiourea is considered to be persistent in the environment (water, soil and sediment, but not bioaccumulative based on criteria defined in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000). Information on concentrations of thiourea in the environment has not been identified at this time. The relatively low observed and predicted toxicity of thiourea to aquatic organisms suggests that it poses a relatively low hazard to aquatic organisms in the Canadian environment. Information on potential impacts in other environmental compartments has not been identified.

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