Screening Assessment for the Challenge

Spiro[isobenzofuran-1(3*H*),9'-[9*H*]xanthen]-3-one, 3',6'-bis(diethylamino)-
(Solvent Red 49)

Chemical Abstracts Service Registry Number
509-34-2

Environment Canada
Health Canada

September 2010

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 Spiro[isobenzofuran-1(3*H*),9'-[9*H*]xanthen]-3-one, 3',6'-bis(diethylamino)- (Solvent Red 49), Chemical Abstracts Service Registry Number 509-34-2. 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 is believed to be in commerce in Canada.

The substance Solvent Red 49 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.

In 2006, no companies reported importing or manufacturing the substance above the reporting threshold of 100 kg/year. No company reported using the substance above the reporting threshold of 1000 kg/year in 2006; however five companies reported a stakeholder interest in Solvent Red 49.

Since there were no reports of use, import or manufacture of Solvent Red 49 in Canada in 2006 at or above the reporting thresholds specified in the CEPA section 71 notice, releases of this substance to the Canadian environment are expected to be very low. As a conservative measure, it was assumed that 100 kg/yr were used in both industrial and consumer use scenarios.

Solvent Red 49 has a high modelled water solubility and a low octanol-water partitioning coefficient. It is present in the environment primarily as a zwitterion (i.e., both positive and negative charges present) that is not volatile, is rather chemically stable, and is expected to have a tendency to partition to sediments if released to surface waters, and adsorb to soils if released to land. This behaviour is mainly governed by electrostatic interactions.

Based on its physical and chemical properties, Solvent Red 49 is expected to be persistent in water, soil and sediment. However, new experimental data relating to its solubility in octanol and water and empirical bioaccumulation data for a chemical analogue suggest that this dye has a low potential to accumulate in the lipid tissues of organisms. The substance therefore meets the persistence criteria but does not meet the bioaccumulation criteria as set out in the *Persistence and Bioaccumulation Regulations*. In addition, new experimental toxicity data for a chemical analogue, as well as new toxicity predictions that take into account revised estimates of bioaccumulation potential, suggest that the substance is likely to have only a moderate potential for toxicity to aquatic organisms.

For this screening assessment, two very conservative exposure scenarios were considered involving both industrial use and consumer use, which would result in discharges of Solvent Red 49 into the aquatic environment. The highest predicted environmental concentration in water, which was for the industrial use scenario, was more than two orders of magnitude below the predicted no-effect concentration calculated for sensitive aquatic biota.

Although the potential hazard to human health is recognized for Solvent Red 49, there were no reports of use, import or manufacture of Solvent Red 49 in Canada in 2006 at or above the reporting thresholds specified in the CEPA section 71 notice. The likelihood of exposure to the general population is therefore low, and hence the risk to human health is likewise considered to be low. Therefore, it is concluded that Solvent Red 49 is a substance that is not entering the environment in a quantity or concentration or under conditions that constitute a danger in Canada to human life or health.

Based on the information available, it is concluded that Solvent Red 49 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. Solvent Red 49 meets the persistence criteria but does not meet the bioaccumulation criteria as set out in the *Persistence and Bioaccumulation Regulations*.

Based on available information, it is concluded that Solvent Red 49 does not meet any of the criteria set out in section 64 of CEPA 1999.

Because this substance is listed on the *Domestic Substances List*, its import and manufacture in Canada are not subject to notification under subsection 81(1). Given the hazardous properties of this substance, there is concern that new activities that have not been identified or assessed could lead to the substance meeting the criteria set out in section 64 of the Act. Therefore, it is recommended to amend the *Domestic Substances List*, under subsection 87(3) of the Act, to indicate that subsection 81(3) of the Act applies with respect to this substance so that new manufacture, import or use of the substance is notified and undergoes ecological and human health risk assessments.

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 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 Spiro[isobenzofuran-1(3*H*),9'-[9*H*]xanthen]-3-one, 3',6'-bis(diethylamino)- was identified as a high priority for assessment of ecological risk as it was 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 March 14, 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 of the substance were received.

Although Spiro[isobenzofuran-1(3*H*),9'-[9*H*]xanthen]-3-one, 3',6'-bis(diethylamino)- was determined to be a high priority for assessment with respect to the environment, it did not meet the criteria for GPE or IPE. 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 final 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 December 2009 for human health and ecological sections of the document. Key studies were critically evaluated; modelling results may have been used to reach conclusions.

When available and relevant, information presented in hazard assessments from other jurisdictions was considered. The final 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 final 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 portion of this assessment has 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 final assessment is based are summarized below.

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[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

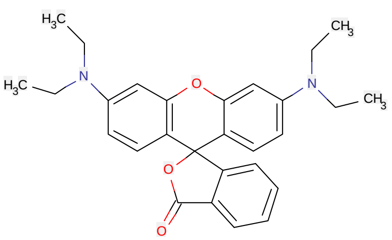
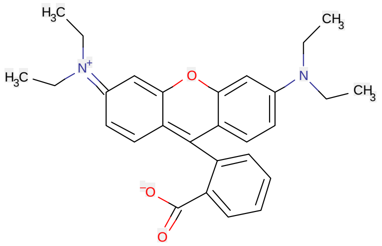
For the purposes of this document, this substance will be referred to as Solvent Red 49, derived from the ENCS (Japanese Existing and New Chemical Substances) and PICCS (Philippine Inventory of Chemicals and Chemical Substances) inventories.

Solvent Red 49 is defined by Colour Index International (CII 2002–2009) as a combination of multiple CAS numbers, including CAS RN 509-34-2. However, for the purposes of the present report and the assessment of this substance, the common name "Solvent Red 49" refers exclusively to the CAS RN 509-34-2.

The substance Solvent Red 49 is a free base compound that is expected to exist in solution in two tautomeric forms, the lactonic and quinonoid forms, with the latter form expected to prevail at environmental pHs.

Table 1. Substance identity for Solvent Red 49

Chemical Abstracts Service Registry Number (CAS RN)	**509-34-2**
DSL name	**Spiro[isobenzofuran-1(3*H*),9'-[9*H*]xanthen]-3-one, 3',6'-bis(diethylamino)-**
National Chemical Inventories (NCI) names[1]	*Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-bis(diethylamino)-* (TSCA, PICCS, ASIA-PAC, AICS, NZIoC) *3',6'-bis(diethylamino)spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3-one* (EINECS) *Solvent Red 49* (ENCS, PICCS) *C.I. solvent red 049* (ECL) *SPIRO[ISOBENZOFURAN-1(3H),9'-[9H]XANTHEN]-3-ONE 3'-6'-BIS(DIETHYLAMINO)-* (PICCS) *RHODAMINE B BASE* (PICCS) *C.I. SOLVENT RED 49, (SPIRO[ISOBENZOFURANYL(3H), 9'-[9H]XANTHEN]-3-ONE, 3',6'-BIS(DIETHYLAMINO)-)* (PICCS) *SPIRO[ISOBENZOFURANYL(3H),9'-[9H]XANTHEN]-3-ONE, 3',6'-BIS(DIETHYLAMINO)-* (PICCS)
Other names	*3',6'-Bis(diethylamino)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]; Aizen Rhodamine B Base, Aizen SOT Pink 1 Baso Red 546; Baso Red NB 546, Certiqual Rhodamine; Eljon Magenta Toner; Fast Oil Pink B, Fluoran, 3',6'-bis(diethylamino)-* *Lacquer Pink S; Neptune Red Base 543; Neptune Red Base NB 543LD, NSC 43944; Oil Pink 312; Oil Pink 330; Orient Oil Pink*

	312; Orient Pink 312; Rhodamine B Base Extra; Rhodamine B Extra Base; Rhodamine B lactone; Rhodamine Base B; Rhodamine Base B Extra; Rhodamine Base FB; Rhodamine S (Russian); lactone; Rhodamine S lactone, Waxoline Rhodamine B; Waxoline Rhodamine BS
Chemical group (DSL Stream)	Discrete organics
Major chemical class or use	Dyes
Major chemical sub-class	Xanthene Dyes
Chemical formula	$C_{28}H_{30}N_2O_3$
Chemical structure	 Lactonic tautomer  Quinonoid tautomer
SMILES[2]	C12(c3c(Oc4c1ccc(c4)N(CC)CC)cc(N(CC)CC)cc3)c1c(cccc1)C(O2)=O (lactonic tautomer)[3]
SMILES[2]	c12O\C\3=C\C(=N(CC)CC)\C=C/C3=C(\c3c(C(=O)O)cccc3)/c1ccc(N(CC)CC)c2 (protinated quinonoid tautomer)[4]
Molecular mass	442.56 g/mol

[1] National Chemical Inventories (NCI). 2007: AICS (Australian Inventory of Chemical Substances); ASIA-PAC (Asia-Pacific Substances Lists); ECL (Korean Existing Chemicals List); EINECS (European Inventory of Existing Commercial Chemical Substances); ENCS (Japanese Existing and New Chemical Substances); NZIoC (New Zealand Inventory of Chemicals); PICCS (Philippine Inventory of Chemicals and Chemical Substances); and TSCA (Toxic Substances Control Act Chemical Substance Inventory).

[2] Simplified Molecular Input Line Entry System.

[3] The lactonic form of the substance was used for water solubility modelling only, as this would be the most representative form of Solvent Red 49 in solid state prior to being solubilized in contact with water.

[4] Most models used in this assessment do not accept the ionized form of this substance, and thus this SMILES which was used for all modelling except water solubility, refers to the protonated form of the quinonoid tautomer (zwitterion) with a molecular weight of 443.56 g/mol.

Physical and Chemical Properties

Tautomers are isomeric forms of a substance generally formed through the delocalization of electrons and the mobility of a group or atom that normally only occur in a liquid state or in solution, but not in the solid state. In Solvent Red 49, this occurs reversibly through the opening of the lactone or cyclic ester group adjacent to the phenyl group and the delocalization of π-electrons in the xanthene group, resulting in positive and negative charges (i.e., zwitterion) forming ammonium and carboxylic groups, respectively (Arbeloa and Ojeda 1981). It is expected that, at pHs 6–9, the soluble quinonoid would be the predominant form.

As a result of the ionizable nature of Solvent Red 49 and due to the structural similarities with Rhodamine B (CAS RN 81-88-9) (i.e., the hydrochloride salt of Solvent Red 49), this salt will serve as a suitable analogue for this substance (further justification for the suitability of this analogue can be found in the environmental fate section). Table 2 contains the experimental and modelled physical and chemical properties of Solvent Red 49 and its hydrochloride salt analogue that are relevant to its environmental fate. Chemical structures for Solvent Red 49 and Rhodamine B are shown in Table 3. Key studies from which experimental data are reported for some of these properties have been critically reviewed for validity and are available in the peer-reviewed open literature.

Models based on quantitative structure-activity relationships (QSARs) were used to generate data for some of the physical and chemical properties of Solvent Red 49. These models are mainly based on fragment addition methods, i.e., they rely on the structure of a chemical. Since these models only accept the protonated form of a chemical as input (in SMILES form), most of the modelled values shown in Table 2 are for the protonated form of quinonoid tautomer Solvent Red 49 as detailed in Table 1.

The modelled log K_{ow} value for Solvent Red 49 of 1.93 was determined by KOWWIN (2000), using the experimental value adjustment (EVA) method with an empirical log K_{ow} of 2.28 for Rhodamine B salt (Benoit-Guyod et al. 1979). In addition, the modelled water solubility for Solvent Red 49 was estimated using a similar EVA approach; however, in this case, the lactonic structure was considered more relevant to this fate process as noted in Table 1. The EVA approach estimates a parameter (i.e., log K_{ow} or water solubility) for a queried chemical by comparing its structure to that of an analogue chemical that has an empirical parameter value. The empirical parameter for the analogue is adjusted based on the influence that structural differences have on the parameter when the two chemicals are compared. Finally, the log K_{oc} value was modelled based on the log K_{ow} using PCKOCWIN (2000). These adjustments largely correct the models for the ionization characteristics of Solvent Red 49 that may not have been adequately addressed.

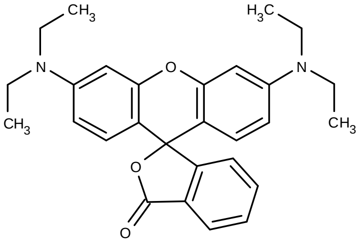
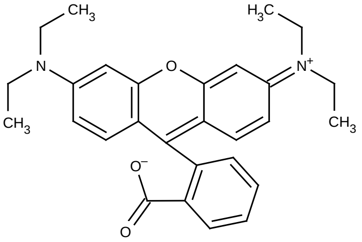
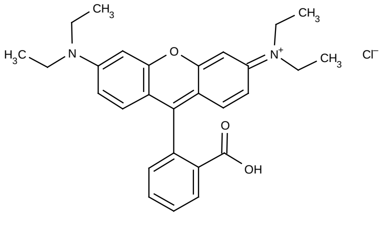
Table 2. Physical and chemical properties for Solvent Red 49 and its hydrochloride salt, Rhodamine B

Property	Type	Value	Temperature (°C)	Reference
Melting point (ºC)				
Solvent Red 49	Experimental	160		Standarcom 2009
Rhodamine B	Experimental	165		Rankin 2009
Boiling point (ºC)				
Solvent Red 49	Modelled	729.11[1]		MPBPWIN 2000
Rhodamine B	Experimental	Decomposes		MSDS 2008
Density (kg/m^3)				
Rhodamine B	Experimental	0.79		MSDS 2009
Maximum Cross-sectional diameter (nm)				
Solvent Red 49	Modelled	1.6-1.8		CPOPs 2008
Rhodamine B	Modelled	1.5-1.8		CPOPs 2008
Vapour pressure (Pa)				
Solvent Red 49	Modelled	1.52×10^{-13} (1.14×10^{-15} mm Hg)	25	MPBPWIN 2000
Henry's Law constant (Pa·m^3/mol)				
Solvent Red 49	Modelled	1.90×10^{-14} (1.88×10^{-19} atm-m^3/mol)	25	HENRYWIN 2000
Log K_{ow} (Octanol-water partition coefficient) (dimensionless)				

Property	**Type**	**Value**	**Temperature (°C)**	**Reference**
Solvent Red 49	Modelled	1.93[2]		KOWWIN 2000
Rhodamine B	Experimental	2.28		Benoit-Guyod et al. 1979
Log K_{oc} (Organic carbon-water partition coefficient) (dimensionless)				
Solvent Red 49	Modelled	1.21[3]		PCKOCWIN 2000
Water solubility (mg/L)				
Solvent Red 49	Modelled	11 000[4, 5]	25	WATERNT 2002
Rhodamine B	Experimental	20 000		Kasnavia et al. 1999
pK_a (Acid dissociation constant) (dimensionless)				
Rhodamine B	Experimental	3.1[6]	20	Arbeloa and Ojeda 1981
	Experimental	3.22[6]	20–25	Mchedlov-Petrossyan and Kukhtik 1994

[1] Substance will decompose before this temperature is reached.
[2] Used the experimental value adjustment (EVA) method with Rhodamine B and log K_{ow} of 2.28.
[3] Based on the estimated log K_{ow} of 1.93.
[4] Water solubility value modelled using the lactone structure (SMILES), as this will be the form of the solid state prior to going into solution.
[5] Used experimental value adjustment (EVA) method with Rhodamine B and water solubility of 20 000 mg/L.
[6] Protonation of the carboxylate group of the zwitterion.

Table 3. Solvent Red 49 tautomers and salt analogue

CAS RN	Common name (Molecular weight in g/mol)	DSL name	Chemical structure
509-34-2	Solvent Red 49 (442.56)	Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-bis(diethylamino)-	 (Lactone)
3375-25-5	Solvent Red 49 (442.56)	n/a	 (Quinonoid)
81-88-9	Rhodamine B (479.02)	Xanthylium, 9-(2-carboxyphenyl)-3,6-bis(diethylamino)-, chloride	 (HCl Salt)

Sources

Solvent Red 49 is not known to be naturally produced.

Recent information was requested through an industry survey conducted pursuant to section 71 of CEPA 1999 (Environment Canada 2009). This survey required the submission of data on the Canadian manufacture, import and use of Solvent Red 49 for the 2006 calendar year. In association with the section 71 survey notice for 2006, companies that did not meet the mandatory reporting requirements but had a business interest in the substance were invited to identify themselves as stakeholders.

In 2006, no companies reported importing or manufacturing the substance above the reporting threshold of 100 kg/year. No company reported using the substance above the reporting threshold of 1000 kg/year in 2006; however, five companies reported a stakeholder interest in Solvent Red 49.

During the development of the Domestic Substances List, 1000–10 000 kg of Solvent Red 49 were reported as being manufactured, imported or in commerce in 1986. The number of notifiers for the calendar years 1984–1986 was 7.

Solvent Red 49 has been identified as a European Union low production volume chemical, indicating that production within the EU has been estimated to be 10 tons per year or less (ESIS 2007). The annual production volume of Solvent Red 49 in the United States in 1986, 1990, 1994 and 1998 was between 4.5 and 225 tonnes (US EPA 1986-2002). Solvent Red 49 was in use in Sweden from 1999 to 2005, Norway and Denmark from 2000 to 2005, and Finland from 2001 to 2003 (SPIN 2006).

Uses

No manufacturing, importation or use was reported in Canada for 2006 above the reporting thresholds of the mandatory survey notice issued pursuant to section 71 of CEPA 1999 (Environment Canada 2009). However, one stakeholder reported that Solvent Red 49 is used in heat transfer fluids at very low concentrations.

Solvent Red 49 is used in Canada as a colorant in some pet collars at concentrations ranging from 0.018 to 0.03%. These products are registered for the control of fleas and ticks on dogs and cats and do not have any food uses (PMRA 2007; 2010 Personal communication from Pesticide Management Regulatory Agency, Health Canada, to Risk Management Bureau, Health Canada; unreferenced).

The following DSL use codes have been identified for Solvent Red 49:

13 - Colourant - pigment/stain/dye/ink
21 - Formulation component
44 - Solvent/carrier
61 - Electrical or Electronic Products
76 - Organic Chemicals, Industrial
77 - Organic Chemicals, Specialty
84 - Photographic/Photocopier
85 - Pigment, Dye and Printing Ink
89 - Printing and Publishing

Solvent Red 49 was used in the manufacture of transport equipment in Norway and in chemicals and chemical products for the paint industry in Sweden (SPIN 2006).

Additional evidence suggests that Solvent Red 49 may be used globally in various applications, including ballpoint ink, computer cartridge ink, gravure printing inks, and as a dye for oils, fats and waxes (CII 2002–2009).

In Canada, Solvent Red 49 is not listed in the *Food and Drug Regulations* under section C.01.040.2 (3)(*a*) as a colouring agent permitted in drugs for internal and external use (Canada 1978). Solvent Red 49 is not approved for any food additive use nor has the Food Directorate received submissions for its use in food packaging materials or formulations of incidental additives (2010 Personal communication from Food Directorate, Health Canada to Existing Substances Risk Assessment Bureau, Health Canada).

Solvent Red 49 (CAS RN 509-34-2) is not currently listed on Cosmetic Ingredient Hotlist (Health Canada 2009) and no products containing Solvent Red 49 were notified to Cosmetics Notification System (CNS) database under its common names “Solvent Red 49” or “Solvent Red 49:1” (CNS 2009). Rhodamine B (CAS RN 81-88-9), on the other hand, is currently on Health Canada’s Cosmetic Ingredient Hotlist as Solvent Red 49:1 (CI 45170:1) and Basic Violet 10 (CI 45170) (Health Canada 2009).

In Europe, "Colouring agent CI 45170" and "Colouring agent CI 45170:1" along with associated CAS RNs 509-34-2 (Solvent Red 49), 81-88-9 (Rhodamine B base), and 6373-07-5 (Rhodamine B-stearate) are listed on Annex II of the Cosmetics Directive and therefore are currently prohibited from use in cosmetic products (SCC 1990, European Commission 2009). In the United States, Rhodamine B (as D&C Red No.19) and Rhodamine B stearate (as D&C Red No.37) were delisted from approved use in 1988 and are no longer permitted for use as colourants in drugs and cosmetics (US FDA 1988; Lipman 1995).

Releases to the Environment

In principle, the releases of Solvent Red 49 to the environment could result from various losses of the substance during 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 paved/unpaved surfaces; (4) chemical transformation; (5) disposal to landfill; (6) disposal by recycling; and (7) disposal by incineration.

However, since there were no reports of any use, import or manufacture of Solvent Red 49 in Canada in 2006 at or above the reporting thresholds specified in the CEPA section 71 notice (Environment Canada 2009), releases of this substance to the Canadian environment are expected to be very low.

The threshold of 100 kg was used throughout this screening assessment to capture the potential mass of this substance in use in Canada that would be below the threshold reporting value.

Environmental Fate

The lactonic form of Solvent Red 49 (see Table 1) only predominates at pH < 1. Thus, at an environmentally relevant pH (6–9), the major form will be the quinonoid one (Arbeloa and Ojeda 1981). Furthermore, at an environmentally relevant pH, the zwitterionic (i.e., both positively and negatively charged) quinonoid form will be the most prevalent form of this substance, considering that the pK_a of the carboxylic group is 3.1–3.2 (see Table 2) and that the positive charge on the ammonium group is π-stabilized in the quinonoid (Wight 2000). As a result, the chemical speciation of Solvent Red 49 in aqueous media at an environmentally relevant pH is expected to be similar that of the analogue Rhodamine B (see Table 3). In fact, at an environmentally relevant pH and concentrations, the two are expected to be essentially the same zwitterionic substance, although Rhodamine B will have a chlorine counter ion while Solvent Red 49 would likely pick up another negatively charged counter ion from the environment.

The authors of a study on certain xanthene dyes in a municipal wastewater treatment plant (Borgerding and Hites 1994) stated that partitioning between the solid and liquid phases may be dependent on ionic interactions between the dyes and solids and/or on simple hydrophobic equilibrium processes. Evaluations of the use of Rhodamine B as a conservative hydraulic tracer dye have shown that Rhodamine dyes, including Rhodamine B and related substances, adsorb to organic and inorganic sediments based on the availability and charge of the particulates (Kasnavia et al. 1999). Considering that Rhodamine B exists as a zwitterion, adsorption to both positively (e.g., alumina) and negatively (e.g., clays, silica) charged mineral surfaces may occur. In fact, Smart and Laidlaw (1977) found that, of eight different fluorescent dyes used in surface water tracing, Rhodamine B most strongly sorbed to organic and inorganic sediments. Rhodamine B sorption to inorganic mineral surfaces was so strong that it was considered a poor choice as a hydraulic tracer dye in the environment (Kasnavia et al. 1999). Considering these trends for Rhodamine B, along with the lower predicted water solubility value for Solvent Red 49 (11 g/L) versus that measured for Rhodamine B (20 g/L), it is expected that, if released to water, Solvent Red 49 would partition to sediments with a lesser amount remaining in the water column.

Due to the high modelled water solubility of Solvent Red 49 (11 g/L) and its tendency to form a zwitterion in solution identical to Rhodamine B at an environmentally relevant pH, if released to soil, Solvent Red 49 would be expected to remain largely in soil with some partitioning into soil pore water. It is not expected to partition to air to any great extent.

Persistence and Bioaccumulation Potential

Environmental Persistence

No environmental monitoring data relating to the presence of Solvent Red 49 in the Canadian environment (air, water, soil or sediment) have been identified. According to the Ecological and Toxicological Association of Dyes and Organic Pigments Manufacturers, dyes are, with some exceptions, considered essentially non-biodegradable under aerobic conditions (ETAD 1995). Repeated evaluation of ready and inherent biodegradability using accepted screening tests (i.e., OECD Guidelines for Testing of Chemicals) have confirmed this assumption (Pagga and Brown 1986; ETAD 1992). Based on the chemical structure of Solvent Red 49 (e.g., tertiary amine-substituted and heterocyclic), there is no reason to suspect that biodegradation will be other than that described for dyes in general (ETAD 1995).

The only available empirical data on the biodegradation of Solvent Red 49 showed a negligible loss after a 4-week incubation with activated sludge (see Table 4a), suggesting that this substance biodegrades slowly.

Table 4a. Empirical data for degradation of Solvent Red 49 and Rhodamine B

Medium	Fate process	Degradation value	Degradation endpoint / units	Reference
Solvent Red 49				
Water	Biodegradation[1]	1%	Degradation in 4 weeks	NITE 2002
Rhodamine B				
Water	Photodegradation	61.6	Half-life / hours	Yager and Yue 1988
Water	Photo-oxidation	30	Half-life / days	Buxton et al. 1988

[1] OECD 301 C, Modified MITI Test (I).

Rhodamine B absorbs light in the UV spectrum above 290 nm (Arbeloa and Ojeda 1981); therefore, it has the potential to directly photolyze in sunlight. In a photolysis study that exposed distilled water solutions of Rhodamine B in test tubes to outdoor sunlight, Rhodamine B had a mean photodegradation half-life of 61.6 hours (Yager and Yue 1988). Since the dissolved forms of Rhodamine B and Solvent Red 49 are considered to be the same, Solvent Red 49 is expected to photolyze at a similar rate in sunlight.

In addition to direct photolysis, Rhodamine B and Solvent Red 49 may undergo photo-oxidation in natural water exposed to sunlight. Their structures contain functional groups (olefinic bonds, aromatic amine) that are susceptible to photo-oxidants (hydroxyl and peroxy radicals) in natural water (Mill and Mabey 1985). One reported experimental hydroxyl radical constant in water for Rhodamine B (Buxton et al. 1988) corresponds to a half-life of about 30 days of sunlight.

Since few experimental data on the degradation of Solvent Red 49 or its analogue Rhodamine B are available beyond the degradation values presented in Table 4a, a

QSAR-based weight-of-evidence approach (Environment Canada 2007) was also applied using the degradation models shown in Table 4b below. Given the ecological importance of the water compartment, the fact that most of the available models apply to water and the fact that Solvent Red 49 is expected to be released to this compartment, biodegradation in water was primarily examined.

In air, a predicted atmospheric oxidation half-life value of < 2 days for the gas phase of Solvent Red (see Table 4b) demonstrates that this substance may be rapidly oxidized, although the atmosphere is not a primary medium of concern for this substance and the effectiveness of this loss process will be limited by the fact that very little Solvent Red 49 is likely to exist in the gas phase.

Table 4b summarizes the results of available QSAR models for degradation in water and air .

Table 4b. Modelled data for degradation of Solvent Red 49

Fate process	**Model and model basis**	**Model result and prediction**	**Extrapolated half-life (days)**
AIR			
Atmospheric oxidation	AOPWIN 2000[1]	$T_{1/2} = 0.022$ days	< 2
Ozone reaction	AOPWIN 2000[1]	$t_{1/2} = 0.002$ days	< 2
Primary biodegradation			
Biodegradation (aerobic)	BIOWIN 2000[1] Sub-model 4: Expert Survey (qualitative results)	3.00[2] “biodegrades relatively quickly”	< 182
Ultimate biodegradation			
Biodegradation (aerobic)	BIOWIN 2000[1] Sub-model 3: Expert Survey (qualitative results)	2.00[2] “biodegrades slowly”	≥ 182
Biodegradation (aerobic)	BIOWIN 2000[1] Sub-model 5: MITI linear probability	0.15[3] “biodegrades very slowly”	≥ 182
Biodegradation (aerobic)	BIOWIN 2000[1] Sub-model 6: MITI non-linear probability	0.012[3] “biodegrades very slowly”	≥ 182
Biodegradation (aerobic)	CPOPs 2008 % BOD (biological oxygen demand)	100% “biodegrades fast”	< 182

[1] EPI Suite (2007).
[2] Output is a numerical score from 0 to 5.
[3] Output is a probability score.

In contrast to the BIOWIN model results in Table 4b, which predict a slow ultimate biodegradation, the CPOPs model predicts a fast biodegradation for Solvent Red 49. This latter result is not considered reliable since this substance is considered out of the domain of the model. The BIOWIN modelled values in Table 4b, however, are considered to be reliable, as several chemicals of structural comparability are contained in their training sets and thus Solvent Red 49 is considered to be within the domain of applicability of these models. Only the primary biodegradation BIOWIN (sub-model 4) suggests that the substance biodegrades quickly; however, this value is on the border of suggesting a quick (≥ 3.0) versus a slow (< 3.0) biodegradation when this result is viewed in terms of complete mineralization and thus carries less weight than the 3 previously mentioned ultimate biodegradation results.

All 3 reliable ultimate biodegradation model results suggest that biodegradation is very slow or slow and that the half-life in water would be ≥ 182 days. This result is consistent with the results from the experimental biodegradation study and with information on the chemical's structure, indicating the presence of structural features associated with chemicals that are not easily biodegraded (e.g., tertiary amine-substituted and heterocyclic). Although empirical data show that photolytic or photo-oxidative degradation of Rhodamine B, the hydrochloride salt of Solvent Red 49, proceeds relatively quickly (half-life ~ 30 days or less), the identities of the degradation products are not known. Therefore, considering all of the empirical and model results and structural features, there is more reliable evidence to suggest the biodegradation half-life of Solvent Red 49 is ≥ 182 days in water.

Using an extrapolation ratio of 1:1:4 for a water: soil: sediment biodegradation half-life (Boethling et al. 1995), and the ultimate degradation half-life of ≥ 182 days in water, the half-life in soil is also ≥ 182 days and the half-life in sediments is ≥ 365 days. This indicates that Solvent Red 49 is expected to be persistent in soil and sediment. Note that photolytic degradation processes that can be relatively rapid in water are not expected to be effective in sediments or subsurface soils due to limitations on light penetration.

Based on the empirical and modelled data (see tables 4a and 4b), Solvent Red 49 meets the persistence criteria in water, soil and sediment (half-lives in soil and water ≥ 182 days and half-life in sediment ≥ 365 days) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential for Bioaccumulation

The modelled log K_{ow} value for Solvent Red 49 (1.93) and empirical log K_{ow} value for the Rhodamine B analogue (2.28) (see Table 2) suggest that this chemical has a low potential to bioaccumulate in biota. This is further supported by the low experimental BCF for fish and mussels for Rhodamine B (see Table 5a).

Table 5a. Empirical data for bioaccumulation of Rhodamine B

Test organism	Endpoint	Value wet weight (L/kg)	Reference
Mussel (*Mytilus sp.*)	BCF	22	Galassi and Canzonier 1976
Fish (Carp)	BCF	< 1.7	Chem. Inspect. Test Inst. 1992

To provide further evidence of bioaccumulation potential for Solvent Red 49, a predictive approach was applied using available BAF and BCF models as shown in Table 5b below. According to the *Persistence and Bioaccumulation Regulations* (Canada 2000), a substance is bioaccumulative if its BCF or BAF is $\geq$ 5000. However, measures of BAF are the preferred metric for assessing bioaccumulation potential of substances. This is because BCF may not adequately account for the bioaccumulation potential of substances via the diet, which predominates for substances with log $K_{ow} > \sim 4.0$ (Arnot and Gobas 2003). BCF and BAF estimates were generated using the Arnot-Gobas mass balance model for BCF and BAF (Arnot and Gobas 2003). Mitigation of bioaccumulation via gut biotransformation was not relevant to consider because, given the low log K_{ow} of the substance, uptake and loss will be mainly a function of gill transfer and not the diet.

Table 5b: Modelled data for bioaccumulation for Solvent Red 49

BCF (L/kg)	BAF (L/kg)	Reference
6.62	6.62	Arnot and Gobas 2003 (Gobas BCF/BAF Middle Trophic Level)
3.16	n/a	BCFWIN 2000
6.92	n/a	CPOPs 2008

[1] Based on log K_{ow} of 1.93 modelled for Solvent Red 49.

The modelled BCF results (see Table 5b) using BCFWIN 2000 of 3.16 L/kg is considered the most reliable measure of the bioaccumulation potential of Solvent Red 49, as the CPOPs (2008) model does not contain many chemicals of structural comparability in its training set (only 30% of the structural domain of the model), and the Gobas BCF/BAF model does not contain ionizing compounds in its training set. The low estimated BCF and BAF values nevertheless indicate that Solvent Red 49 has a low potential to bioaccumulate, which is in general agreement with the empirical information presented in Table 5a for the Rhodamine B analogue.

Recent investigations relating fish BCF data and molecular size parameters (Dimitrov et al. 2002, 2005) suggest that the probability of a molecule crossing cell membranes as a result of passive diffusion declines significantly with increasing maximum diameter (D_{max}). The probability of passive diffusion decreases appreciably when the maximum diameter is greater than ~1.5 nm and much more so for molecules having a maximum diameter of greater than 1.7 nm. Sakuratani et al. (2008) have also investigated the effect of cross-sectional diameter on passive diffusion in a BCF test set of about 1200 new and existing chemicals. They observed that substances that do not have a very high bioconcentration potential (BCF < 5000) often have a D_{max} of > 2.0 nm and an effective diameter (D_{eff}) > 1.1 nm.

However, as Arnot et al. (2010) have noted there are uncertainties associated with the thresholds proposed by Dimitrov et al.(2002, 2005) and Sakuratani et al. (2008) since the BCF studies used to derive them were not critically evaluated. As Arnot et al. (2010) point out, molecular size influences solubility and diffusivity in water and organic phases (membranes), and larger molecules may have slower uptake rates. However, these same kinetic constraints apply to diffusive routes of chemical elimination (i.e., slow in = slow out). Thus, significant bioaccumulation potential may remain for substances that are subject to slow absorption processes, if they are slowly biotransformed or slowly eliminated by other processes. Consequently, when evaluating bioaccumulation potential molecular size information should be considered with care, and used together with other relevant lines of evidence in a weight of evidence approach.

The maximum cross-sectional diameter for Solvent Red 49 and its conformers (D_{max}) ranges from 1.6 to 1.8 nm (CPOPs 2008), which is comparable to some of the values cited above and suggests that the uptake rate of this substance may be slower compared to that of smaller more compact substances, thus, mitigating the overall bioconcentration potential.

The available evidence indicates that Solvent Red 49 likely has a low bioaccumulation potential due in part to its physical and chemical properties (i.e., low lipophilicity, ionic character, as well as, relatively high molecular weight and cross-sectional diameter). The predicted BCF and BAF values (e.g., maximum BCF = 3.16 L/kg) and empirical BCF values for Rhodamine B (22 L/kg and < 1.7 L/kg) are much less than the bioaccumulation criterion (BCF or BAF ≥ 5000) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000) and are consistent with what would be expected for an zwitterionic chemical with a high water solubility. It is also possible that this compound is metabolized *in vivo* should it be taken up via the gills and transported to the liver. Therefore, Solvent Red 49 is not considered to be bioaccumulative according to these criteria.

Potential to Cause Ecological Harm

Ecological Effects Assessment

A – In the Aquatic Compartment

There are empirical data on the aquatic toxicity of the analogue Rhodamine B (see Table 6a).

Table 6a. Empirical data for aquatic toxicity of Rhodamine B

Test organism	Type of test	Endpoint	Value (mg/L)	Reference
Daphnia magna	Acute (24 hours)	EC_{50}[1]	22	Rochat et al. 1978
Daphnia magna	Acute (24 hours)	NOEC	10	Rochat et al. 1978
Rainbow Trout (*Oncorhynchus mykiss*)	Acute (96 hours)	LC_{50}[2]	217	Marking 1969
Channel Catfish	Acute	LC_{50}[2]	526	Marking 1969

(*Ictalurus punctatus*)	(96 hours)			
Bluegill (*Lepomis macrochirus*)	Acute (96 hours)	$LC_{50}{}^{2}$	379	Marking 1969
Daphnia magna	Acute (24 hours)	$LC_{50}{}^{2}$	72	Benoit-Guyod et al. 1979
Daphnia magna	Acute (48 hours)	$LC_{50}{}^{2}$	42	Benoit-Guyod et al. 1979
Daphnia magna	Acute (72 hours)	$LC_{50}{}^{2}$	29	Benoit-Guyod et al. 1979
Guppy (*Lebistes reticulatus*)	Acute (24 hours)	$LC_{50}{}^{2}$	86	Benoit-Guyod et al. 1979

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

Using Rhodamine B as a source of surrogate data, Solvent Red 49 is expected to show similar moderate to low toxicity to various fish and daphnids (see Table 6a).

As empirical data were not available for Solvent Red 49, modelled ecotoxicity values were also generated and are shown in Table 6b. The SMILES for the quinonoid form of Solvent Red 49 and a log K_{ow} of 1.93 were used for this modelling (see tables 1 and 2).

Table 6b. Modelled data for aquatic toxicity

Test organism	Type of test	Endpoint	Value (mg/L)	Reference
Fish	Acute (96 hours)	$LC_{50}{}^{1}$	$912^{3,4}$	ECOSAR 2004
			1.31	AIEPS 2003–2007
Daphnia	Acute (48 hours)	$EC_{50}{}^{2}$	$495^{3,4}$	ECOSAR 2004
			16.9	AIEPS 2003–2007
Algae	Acute (96 hours)	$EC_{50}{}^{2}$	$174^{3,4}$	ECOSAR 2004
	Acute (72 hours)	$EC_{50}{}^{2}$	5.82	AIEPS 2003–2007

[1] EC_{50} – The concentration of a substance that is estimated to cause some effect on 50% of the test organisms.
[2] LC_{50} – The concentration of a substance that is estimated to be lethal to 50% of the test organisms.
[3] Estimate using a modelled log K_{ow} (1.93) for Solvent Red 49 in EPI Suite (2007)
[4] Neutral organic SAR (baseline toxicity)

The modelled data indicate that Solvent Red 49 is not expected to have a high acute aquatic toxicity and are in general agreement with the empirical analogue data in Table 6a .

The weight of evidence regarding experimental and modelled data for Solvent Red 49 indicates that this substance is likely to have a low to moderate potential for acute toxicity to aquatic organisms.

B – In Other Environmental Compartments

No suitable ecological effects studies were found for this compound in media other than water.

When Solvent Red 49 is released into a water body, it partitions into suspended particulate matter and to bottom sediments where sediment-dwelling organisms would be exposed to the substance. However, no suitable environmental monitoring data or toxicity data specific to sediment-dwelling organisms are available for this substance or its analogue.

Ecological Exposure Assessment

No data concerning concentrations of this substance in water in Canada have been identified; therefore, environmental concentrations are estimated from available information, including estimated substance quantities, release rates and size of receiving water bodies. Considering that there are no reports of use, import or manufacture of Solvent Red 49 in Canada in 2006 at or above the reporting thresholds specified in the CEPA section 71 notice (Environment Canada 2009), releases of this substance to the Canadian environment are expected to be very low. As a conservative measure, it was assumed that 100 kg/year were used in both industrial and consumer use scenarios.

A – Industrial Release

The aquatic exposure of Solvent Red 49 is expected if 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 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 the substance. 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

$C_{water\text{-}ind}$: 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 Solvent Red 49 may be used industrially and is expected to be released to water, a worst-case industrial release scenario has been developed to estimate the aquatic concentration of the substance using the Industrial Generic Exposure Tool – Aquatic (IGETA) (Environment Canada 2008a). The scenario is made conservative by assuming that the total quantity of the substance used by Canadian industry is used by one industrial facility at a small, hypothetical site and the loss to the sewers is 5% of the total quantity resulting from the cleaning of chemical containers and process equipment. 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. Upon combining with the STP effluent, the receiving water at such a site normally has an actual or equivalent flow of 34 560 m^3 per day. Based on the above assumptions, and assuming that the substance is used at a total quantity of 100 kg/year for industrial purposes, this results in a predicted environmental concentration (PEC) of 0.0006 mg/L (Environment Canada 2008b).

B – Consumer Release

Solvent Red 49 is found in some consumer products (i.e., pest control products for the control of fleas and ticks on dogs and cats) although none were identified in Canada at or above the reporting threshold in the CEPA section 71 notice (Environment Canada 2009). As consumer products may be released to water, Mega Flush, Environment Canada's spreadsheet tool for estimating down-the-drain releases from consumer uses, was employed to estimate the potential substance concentration in multiple water bodies receiving sewage treatment plant effluents to which consumer products containing the substance may have been released (Environment Canada 2008c). The spreadsheet tool is designed to provide these estimates based on conservative assumptions regarding the amount of the substance used and released by consumers.

By default, it was assumed that primary and secondary STP removal rates are 0%, losses from use are 100%, consumer use of the substance extends over 365 days/year and the flow rate at all sites is relatively low (i.e., the tenth percentile of annual flow values). These estimates were made for approximately 1000 release sites across Canada, which account for most of the major STPs in the country.

The equation and inputs used to calculate the PECs of Solvent Red 49 in the receiving water bodies are described in Environment Canada (2008d). A scenario was run, assuming a total consumer use quantity of 100 kg/year based on the reporting limit threshold.

Using this scenario, the model estimates that PECs in the receiving water bodies range from 2.7×10^{-6} to 1.5×10^{-4} mg/L.

Characterization of Ecological Risk

The approach taken in this ecological screening assessment was to examine various supporting information and develop conclusions based on a weight-of-evidence approach and using precaution as required under CEPA 1999. Lines of evidence considered include results from a conservative risk quotient calculation, as well as information on persistence, bioaccumulation, toxicity, sources and fate of the substance.

Solvent Red 49 is expected to be persistent in water, soil and sediment, and it is expected to have low bioaccumulation potential in aquatic organisms. The lack of any notified manufacture, import or use of Solvent Red 49 in Canada above 100 kg/year indicates a low potential for release into the Canadian environment. Once released into the environment, it will be found in water and associated with sediment and/or soil. It has also been demonstrated to have low to moderate potential for toxicity to aquatic organisms.

A risk quotient analysis, integrating conservative estimates of exposure with toxicity information, was performed for the aquatic medium to determine whether there is potential for ecological harm in Canada. The conservative generic industrial scenario presented above yielded the highest PEC of 0.0006 mg/L (Environment Canada 2008b).

The lowest empirical aquatic toxicity value for the analogue Rhodamine B (see Table 6a) is the 24-hour LC_{50} of 22 mg/L for *Daphnia sp.*, which is considered the critical toxicity value (CTV) for this substance. A predicted no-effect concentration (PNEC) was derived from this CTV by dividing it by an assessment factor of 100 (10 to account for interspecies and intraspecies variability in sensitivity and 10 to estimate a long-term no-effect concentration in the field from a short-term LC_{50}), to give a value of 0.22 mg/L. The resulting risk quotient (PEC/PNEC) is 0.0027. Therefore, harm to aquatic organisms is unlikely.

For this substance, a risk quotient based on exposure in sediment may be calculated based on the aquatic compartment PEC and PNEC values and used for sediment risk characterization. In the calculation, bottom sediment and its pore water are assumed to be in equilibrium with the overlying water, and benthic and pelagic organisms are assumed to have similar sensitivities to the substance. Therefore, the PEC and PNEC for pore water are considered to be the same as that of the aquatic compartment. This equilibrium approach would result in a risk quotient (PEC/PNEC) for the sediment compartment that is the same as that of the aquatic compartment.

This information suggests that Solvent Red 49 does not have the potential to cause ecological harm in Canada.

Uncertainties in Evaluation of Ecological Risk

Given the use of this substance in other countries, it is possible that the substance is entering the Canadian market as a component of manufactured items and consumer products. Available information is currently not sufficient to derive a quantitative estimate that would help determine the importance of this source. However, information obtained from the section 71 survey and other information sources indicated that it may be present in a limited number of these types of products in Canada. The threshold of 100 kg was used throughout this screening assessment to provide a conservative estimate of the potential mass of this substance in use in Canada that would be below the threshold reporting value.

Rhodamine B, a free acid salt of Solvent Red 49, was used as an analogue throughout this assessment. However, as it is a salt, it is expected to have slightly different physical and chemical properties, creating uncertainty in the predictions of fate, persistence, bioaccumulation potential and aquatic toxicity that are based on these properties. Nevertheless differences between the properties and environmental behaviour of Rhodamine B and Solvent Red 49 are expected to be small.

As for ecotoxicity, considering 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, the only effects data identified apply primarily to pelagic aquatic exposures, although the water column may not be the only medium of concern based on partitioning estimates.

The modelled values for vapour pressure (1.52×10^{-13} Pa) and Henry's Law constant (1.90×10^{-14} Pa·m3/mol) included in this assessment may be at the lower end of the range of accurate prediction and, thus, the values estimated for these properties need to be treated with caution. However, there was reasonably good confidence in concluding that the substance has a very low vapour pressure and Henry's Law constant in general, such that loss to due volatilization would be negligible.

Potential to Cause Harm to Human Health

As a limited toxicological information was identified for Solvent Red 49, toxicological dataset of its analogue, Rhodamine B ,was considered for human health effects assessment of Solvent Red 49. Based on experimental data for the acid dissociation constant of Rhodamine B (see Table 2), Rhodamine B is considered to be in the quinonoid form of Solvent Red 49 under physiologically relevant conditions (pH 6–8). Therefore, toxicity data for Rhodamine B are considered relevant to Solvent Red 49.

Based primarily on the health effects information on Rhodamine B, the potential hazard to human health is recognized for Solvent Red 49. The toxicological database for Rhodamine B is summarized in assessments conducted by EFSA (EFSA 2005), the U.S. FDA (Lipman 1995), IARC (IARC 1978) and the American Federal Color Additive Scientific Review Panel (Hart et al. 1986). The U.S. FDA concluded that Rhodamine B (as D&C Red No.19) was an animal carcinogen by the oral route based on dietary studies showing an increased incidence of liver tumours in mice and thyroid tumours in rats (Lipman 1995). The European Commission Scientific Committee on Cosmetology (SCC) also considered there to be a potential health concern for this substance based on the evidence of carcinogenicity in mice (SCC 1990). However, the U.S. FDA also concluded there was no evidence of carcinogenicity by the dermal route based on skin painting studies in mice (Lipman 1995). While genotoxicity of Rhodamine B was observed in some *in vitro* and *in vivo* assays, several of the positive results were confounded by the presence of impurities in the test samples (Hart et al. 1986, EFSA 2005). Non-cancer effects including body weight changes and increased weights of some organs (e.g. liver, kidney, etc.) have been reported in oral studies conducted with Rhodamine B. Solvent Red 49 may demonstrate the same hazard potential.

There were no reports of use, import or manufacture of Solvent Red 49 in Canada in 2006 at or above the reporting thresholds specified in the section 71 notice of CEPA 1999 (Environment Canada 2009). This substance has only limited use as a colourant in some pet collars registered as pest control products at concentrations ranging from 0.018 to 0.03%. Therefore, the likelihood of exposure to the general population is low, and hence the risk to human health is likewise considered to be low.

Conclusion

Based on the information presented in this screening assessment, it is concluded that Solvent Red 49 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.

Although the potential hazard to human health is recognized for Solvent Red 49, on the basis of information that indicates that it is not manufactured in or imported into Canada in amounts above the reporting threshold, the likelihood of exposure in Canada is considered to be low; hence the risk to human health is likewise considered to be low. Therefore, it is concluded that it is a substance that is not entering the environment in a quantity or concentration or under conditions that constitute a danger in Canada to human life or health.

Based on available information, it is concluded that Solvent Red 49 does not meet any of the criteria set out in section 64 of CEPA 1999. Additionally, Solvent Red 49 meets the criteria for persistence but does not meet the criteria for bioaccumulation potential as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Because this substance is listed on the Domestic Substances List, its import into, and manufacture in Canada are not subject to notification under subsection 81(1). Given the hazardous properties of this substance, there is concern that new activities that have not been identified or assessed could lead to this substance meeting the criteria set out in section 64 of the Act. Therefore, it is recommended to amend the Domestic Substances List, under subsection 87(3) of the Act, to indicate that subsection 81(3) of the Act applies with respect to the substance so that new manufacture, import or use of this substance is notified and undergoes ecological and human health risk assessments. In addition and where relevant, research and monitoring will support verification of assumptions used during this screening assessment.

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Appendix 2 – Robust Study Summary (RSS)

No	Item	Weight	Yes/No	Specify
1	Reference: Toxicologic study of a fluorescent tracer: rhodamine B (Original in French). Rochat et al. 1978. *Toxicol Europ Res* Vol. 1. pp. 23–26.			
2	Substance identity: CAS RN	n/a	N	
3	Substance identity: chemical name(s)	n/a	Y	Rhodamine B
4	Chemical composition of the substance	2	Y	Structure of components provided
5	Chemical purity	1	N	
6	Persistence/stability of test substance in aquatic solution reported?	1	N	
	Method			
7	Reference	1	Y	AFNOR Standard T 90.301 (april 1974)
8	OECD, EU, national, or other standard method?	3	Y	
9	Justification of the method/protocol if not a standard method was used	2		n/a
10	GLP (Good Laboratory Practice)	3	N	
	Test organism			
11	Organism identity: name	n/a	Y	*Daphnia magna (Strauss)*
12	Latin or both Latin & common names reported?	1	Y	
13	Life cycle age / stage of test organism	1	Y	<72 hrs
14	Length and/or weight	1	Y	0.8-0.56 mm grid
15	Sex	1		n/a
16	Number of organisms per replicate	1	Y	five
17	Organism loading rate	1	N	
18	Food type and feeding periods during the acclimation period	1	Y	
	Test design / conditions			
19	Test type (acute or chronic)	n/a	Y	Acute
20	Experiment type (laboratory or field)	n/a	Y	Laboratory
21	Exposure pathways (food, water, both)	n/a	Y	Water
22	Exposure duration	n/a	Y	24 hours
23	Negative or positive controls (specify)	1	Y	4 negative controls
24	Number of replicates (including controls)	1	Y	four
25	Nominal concentrations reported?	1	N	
26	Measured concentrations reported?	3	N	
27	Food type and feeding periods during the long-term tests	1		n/a
28	Were concentrations measured periodically (especially in the chronic test)?	1	N	
29	Were the exposure media conditions relevant to the particular chemical reported? (e.g., for the metal toxicity - pH, DOC/TOC, water hardness, temperature)	3	Y	
30	Photoperiod and light intensity	1	N	
31	Stock and test solution preparation	1	Y	
32	Was solubilizer/emulsifier used, if the chemical was poorly soluble or unstable?	1		n/a
33	If solubilizer/emulsifier was used, was its concentration reported?	1		n/a
34	If solubilizer/emulsifier was used, was its ecotoxicity reported?	1		n/a
35	Monitoring intervals (including observations and water quality parameters) reported?	1	N	
36	Statistical methods used	1	Y	
	Information relevant to the data quality			
37	Was the endpoint directly caused by the chemical's toxicity, not by organism's health (e.g. when mortality in the control >10%) or physical effects (e.g. 'shading effect')?	n/a	Y	
38	Was the test organism relevant to the Canadian environment?	3	Y	
39	Were the test conditions (pH, temperature, DO, etc.) typical for the test organism?	1	Y	
40	Does system type and design (static, semi-static, flow-through; sealed or open; etc.) correspond to the substance's properties and organism's nature/habits?	2	Y	
41	Was pH of the test water within the range typical for the Canadian environment (6 to 9)?	1		n/a
42	Was temperature of the test water within the range typical for the Canadian environment (5 to 27°C)?	1	Y	20°C
43	Was toxicity value below the chemical's water solubility?	3	Y	
	Results			
44	Toxicity values (specify endpoint and value)	n/a	n/a	24-h LC50=22 mg/L
45	Other endpoints reported - e.g. BCF/BAF, LOEC/NOEC (specify)?	n/a	Y	NOEC=10 mg/L
46	Other adverse effects (e.g. carcinogenicity, mutagenicity) reported?	n/a	N	
47	***Score : ... %***			***68.3***
48	***EC Reliability code :***			***2***
49	***Reliability category (high, satisfactory, low) :***			***Satisfactory Confidence***
50	***Comments:*** *Details of AFNOR Standard T 90.301 (april 1974) provided in Rambaud, A., Chan K.-S., Reboul B., Bontoux J. 1976. Toxicite d'effluents de raffineries petroliere evaluee par le test Daphnies. Trav. Soc. Pharm. Montpellier, 36, 65-72.*			

Appendix 2 – PBT Model Inputs Summary Table

	Phys-Chem/Fate	**Phys-Chem/Fate**	**Fate**	**PBT profiling**	**Ecotoxicity**
Model input parameters	EPIWIN Suite (all models except WATRNT, including: AOPWIN, KOCWIN, BCFWIN, BIOWIN and ECOSAR)	EPIWIN Suite (WATRNT only)	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	c12O\C\3=C\C(=N(CC)CC)\C=C/C3=C(\c3c(C(=O)O)cccc3)/c1ccc(N(CC)CC)c2	C12(c3c(Oc4c1ccc(c4)N(CC)CC)cc(N(CC)CC)cc3)c1c(cccc1)C(O2)=O	c12O\C\3=C\C(=N(CC)CC)\C=C/C3=C(\c3c(C(=O)O)cccc3)/c1ccc(N(CC)CC)c2	c12O\C\3=C\C(=N(CC)CC)\C=C/C3=C(\c3c(C(=O)O)cccc3)/c1ccc(N(CC)CC)c2	c12O\C\3=C\C(=N(CC)CC)\C=C/C3=C(\c3c(C(=O)O)cccc3)/c1ccc(N(CC)CC)c2
Molecular weight (g/mol)	443.57	442.56	443.57	443.57	443.57
Melting point (ºC)	160		160		
Boiling point (ºC)					
Data temperature (ºC)					
Density (kg/m^3)					
Vapour pressure (Pa)					
Henry's Law constant (Pa·m^3/mol)					
Log K_{aw} (Air-water partition coefficient; dimensionless)					
Log K_{ow} (Octanol-water partition coefficient; dimensionless)	1.93[1] for K_{oc}, LC_{50}		1.93[1]	1.93[1]	
Log K_{oc} (Organic carbon-water partition coefficient – L/kg)					
Water solubility					

(mg/L)					
Log K_{oa} (Octanol-air partition coefficient; dimensionless)					

[1] Derived from experimental value adjustment (EVA) using Rhodamine B structure and empirical log K_{ow} = 2.28.