Screening Assessment for the Challenge

2-Anthracenesulfonic acid, 4,4'-[(1-methylethylidene)bis(4,1-phenyleneimino)]bis[1-amino-9,10-dihydro-9,10-dioxo-, disodium salt (Acid Blue 127)

Chemical Abstracts Service Registry Number
6471-01-8

Environment Canada
Health Canada

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Synopsis

Pursuant to section 74 of the *Canadian Environmental Protection Act, 1999* (CEPA 1999), the Ministers of the Environment and of Health have conducted a screening assessment on 2-Anthracenesulfonic acid, 4,4'-[(1-methylethylidene)bis(4,1-phenyleneimino)]bis[1-amino-9,10-dihydro-9,10-dioxo-, disodium salt (Acid Blue 127), Chemical Abstracts Service Registry Number 6471-01-8. This substance was identified as a high priority for screening assessment and included in the Challenge because it was 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 Acid Blue 127 was not considered to be a high priority for assessment of potential risks to human health, based upon application of the simple exposure and hazard tools developed by Health Canada for categorization of substances on the *Domestic Substances List*. Therefore, this assessment focuses on information relevant to the evaluation of ecological risks.

Since there were no reports of import or manufacture at or above the reporting threshold of 100 kg in 2005 or 2006, releases of this substance into the Canadian environment are expected to be low.

Based on its physical and chemical properties, Acid Blue 127 does not have the potential to accumulate to a significant extent in aquatic organisms, and empirical acute aquatic toxicity values of analogues of Acid Blue 127 suggest that the substance is not highly hazardous to aquatic organisms. However, Acid Blue 127 does not degrade quickly in the environment and therefore it is expected to be persistent in water, soil and sediments. This substance meets the persistence criteria but does not meet the bioaccumulation criteria as set out in the *Persistence and Bioaccumulation Regulations*.

For this screening assessment, a very conservative exposure scenario was designed in which it is assumed that 100 kg (the reporting threshold) of Acid Blue 127 is used at a single industrial operation (user of the dye) and that a large proportion of the amount used is discharged into the aquatic environment. The predicted environmental concentration in water was well below the predicted no-effect concentration for sensitive aquatic organisms.

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

Based on the information available, it is concluded that Acid Blue 127 does not meet any of the criteria set out in section 64 of CEPA 1999.

Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) (Canada 1999) requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that have met the categorization criteria set out in the Act to determine whether these substances present or may present a risk to the environment or human health. Based on the results of a screening assessment, the Ministers can propose to take no further action with respect to the substance, to add the substance to the Priority Substances List (PSL) for further assessment, or to recommend that the substance be added to the List of Toxic Substances in Schedule 1 of the Act and, where applicable, the implementation of virtual elimination.

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

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

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

The substance 2-Anthracenesulfonic acid, 4,4`-[(1-methylethylidene)bis(4,1-phenyleneimino)]bis[1-amino-9,10-dihydro-9,10-dioxo-, disodium salt (Acid Blue 127) was identified as a high priority for assessment of ecological risk as it had been found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and is believed to be in commerce in Canada. The Challenge for Acid Blue 127 was published in the *Canada Gazette* on August 18, 2007 (Canada 2007a). A substance profile was released at the same time (Canada 2007b). 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 were not received.

Although Acid Blue 127 was determined to be a high priority for assessment with respect to the environment, it did not meet the criteria for GPE or IPE and high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity. Therefore,

this assessment focuses principally on information relevant to the evaluation of ecological risks.

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

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

Screening assessments examine scientific information and develop conclusions by incorporating a weight-of-evidence approach and precaution as required under CEPA 1999.

This screening assessment includes consideration of information on chemical properties, hazards, uses and exposure, including the additional information submitted under the Challenge. Data relevant to the screening assessment of this substance were identified in original literature, review and assessment documents, stakeholder research reports and from recent literature searches, up to July 2007. Key studies were critically evaluated; modelling results may have been used to reach conclusions. When available and relevant, information presented in hazard assessment from other jurisdictions was considered. The screening assessment does not represent an exhaustive or critical review of all available data. Rather, it presents the most critical studies and lines of evidence pertinent to the conclusion.

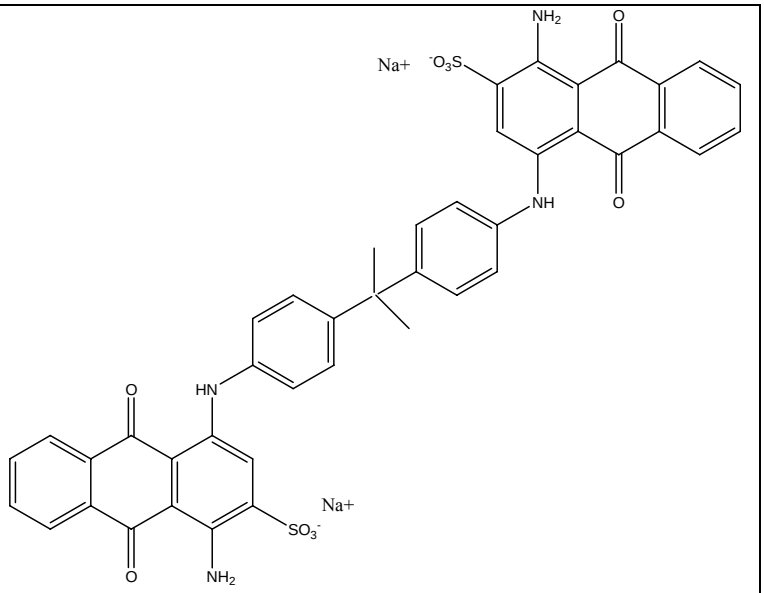
This screening assessment was prepared by staff in the Existing Substances Programs at Health Canada and Environment Canada and incorporates input from other programs within these departments. Additionally, a draft of this screening assessment was subject to a 60-day public comment period. While external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

Substance Identity

For the purposes of this report, this substance will be referred to as Acid Blue 127.

Table 1. Substance identity for Acid Blue 127

Chemical Abstracts Service Registry Number (CAS RN)	**6471-01-8**
DSL name[1]	2-Anthracenesulfonic acid, 4,4'-[(1-methylethylidene)bis(4,1-phenyleneimino)]bis[1-amino-9,10-dihydro-9,10-dioxo-, disodium salt
National Chemical Inventories (NCI) names[2]	2-anthracenesulfonic acid, 4,4'-[(1-methylethylidene)bis(4,1-phenyleneimino)]bis[1-amino-9,10-dihydro-9,10-dioxo-, disodium salt (AICS, PICCS, ASIA-PAC) 2-anthracenesulfonic acid, 4,4'-[(1-methylethylidene)bis(4,1-phenyleneimino)]bis[1-amino-9,10-dihydro-9,10-dioxo-, disodium salt (1:2) (TSCA) Disodium 4,4'-[(1-methylethylidene)bis(4,1-phenyleneimino)]bis[1-amino-9,10-dihydro-9,10-dioxoanthracene-2-sulphonate (EINECS) Acid Blue 127 (ENCS) C.I. acid blue 127(ECL, PICCS)
Other names	2-anthracenesulfonic acid, 4,4'-[isopropylidenebis(p-phenyleneimino)]bis[1-amino-9,10-dihydro-9,10-dioxo-, disodium salt; 2-anthraquinonesulfonic acid, 4,4'-[isopropylidenebis(p-phenyleneimino)]bis[1-amino-, disodium salt; Brilliant Alizarine Milling Blue G-MCI; C.I. 61135; Kayakalan Brilliant Blue G; Lanyl Brilliant Blue G; Lanyl Brilliant Blue G Extra Conc.; Nylosan Blue F-GBL; Optanol Fast Blue 2G; Shimazaki Alizarine Brilliant Milling Blue GS; Suminol Milling Brilliant Blue G; Supranol Fast Blue GG; Telon Fast Blue GGN; Vondamol Fast Blue 2G
Chemical group (DSL stream)	Discrete organics
Chemical sub-group	Anthraquinones
Chemical formula	$C_{43}H_{30}N_4O_{10}S_2.2Na$

Chemical structure	
SMILES	c1c(S(=O)(=O)O[Na])c(N)c2C(=O)c3ccccc3C(=O)c2c1Nc4ccc(cc4)C(C)(C)c5ccc(cc5)Nc6c7C(=O)c8ccccc8C(=O)c7c(N)c(S(=O)(=O)O[Na])c6
Molecular mass	872.83 g/mol

[1] DSL (Domestic Substances List).

[2] **Source:** National Chemical Inventories (NCI). 2006: AICS (Australian Inventory of Chemical Substances); ASIA-PAC (Asia-Pacific Substances Lists); ECL (Korean Existing Chemicals List); EINECS (European Inventory of Existing Chemical Substances); ENCS (Japanese Existing and New Chemical Substances); PICCS (Philippine Inventory of Chemicals and Chemical Substances); TSCA (Toxic Substances Control Act Chemical Substance Inventory).

Physical and Chemical Properties

At the Environment Canada-sponsored Quantitative Structure-Activity Relationship (QSAR) Workshop in 1999 (Environment Canada 2000), Environment Canada and other invited modelling experts identified many structural classes of pigment and dyes as difficult to model using QSARs. The inherent properties of many of the structural classes of dyes and pigments (including acid and disperse dyes) are not amenable to model prediction because they are considered "out of the model domain of applicability" (e.g., structural and/or property parameter domains). Therefore, to determine the domain of applicability, Environment Canada reviews the applicability of QSAR models to dyes and pigments on a case-by-case basis. It has been considered inappropriate to use QSAR models to predict the physical and chemical properties of Acid Blue 127 and consequently a "read-across" approach was used to determine the approximate physical and chemical properties in Table 2. These properties were subsequently used for further modelling in this assessment. Table 2 shows some calculated and extrapolated physical and chemical properties of Acid Blue 127.

Table 2. Physical and chemical properties for Acid Blue 127

Property	Type	Value	Temperature (°C)	Reference
Physical state	Information not available			
Boiling point (°C)	Read-across[1]	> 150	n/a	ETAD 1995
Decomposition point (°C)	Read-across[1]	> 300	n/a	ETAD 1995
Vapour pressure (Pa)	Read-across[1]	10^{-8} to 10^{-10}	25	ETAD 1995 Baughman and Perenich 1988
Henry's Law constant ($Pa \cdot m^3/mol$)	Calculated[2]	8.4×10^{-15}	25	HENRYWIN 2000
Log K_{ow} (Octanol-water partition coefficient) (dimensionless)	Read-across[1]	< 3	25	Anliker et al 1981 Anliker and Moser 1987
Log K_{oc} (Organic carbon-water partition coefficient) (L/kg)[3]	Information not available			
Water solubility (mg/L)	Read-across[1]	10 000	25	MSDS 2006
	Read-across[1]	Readily soluble		ETAD 1995
pK_a (Acid dissociation constant) (dimensionless)	Calculated	-1.45[4]		ACD/pK_aDB 2005

[1] The extrapolated values used for substances in the disulfonic acid dyes group are based on evidence for disulfonic acid dyes submitted to Environment Canada under the *New Substances Notification Regulations* and/or available evidence from other di-sulfonic acid dye analogues (e.g., ETAD 1995).

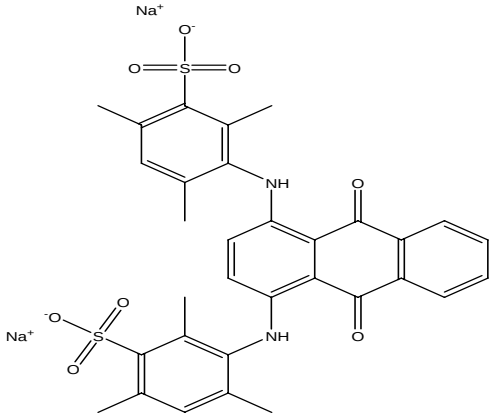
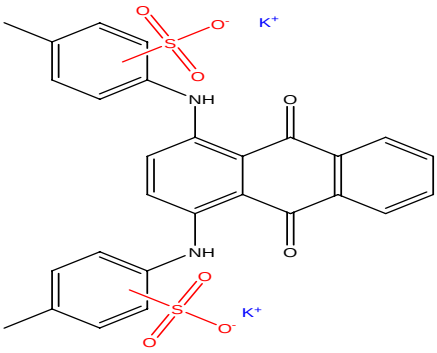
[2] Calculated using the following read-across physical and chemical properties from Table 2: water solubility (WS), vapour pressure (VP) and molecular weight (MW). Water solubility at 10 000 mg/L and upper range limit of 10^{-8} Pa for vapour pressure were used in the calculation.

[3] Highly soluble ionic substances such as acid dyes are not expected to undergo adsoption to solids as a function of the octanol-carbon partition coefficient (little or no solubility in n-octanol). However, acids dyes have been observed to have a high degree of adsorption to positively charged substrates (as they are designed to do, for example, cellulosic fibres) and have been observed to be removed to sludges in sewage treatment plants (STPs) via sludge adsorption and/or precipitation and settling out (e.g., ETAD 1995, acid dyes submitted to Environment Canada under the *New Substances Notification Regulations*).

[4] pKa of the acid (protonated) form.

In addition, empirical toxicity data from two analogues: Benzenesulfonic acid, 3,3'-[(9,10-dihydro-9,10-dioxo-1,4 anthracenediyl)diimino]bis[2,4,6-trimethyl-, disodium salt (CAS RN 4474-24-2) and 9,10-Anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts (CAS RN 125351-99-7), listed in Table 3, were used in support of the weight of evidence.

Table 3. Structural analogues for Acid Blue 127

i. Benzenesulfonic acid, 3,3'-[(9,10-dihydro-9,10-dioxo-1,4 anthracenediyl)diimino]bis[2,4,6-trimethyl-, disodium salt (CAS RN 4474-24-2)	**ii. 9,10-Anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts (CAS RN 125351-99-7)**
	
Comparison with Acid Blue 127 CAS RNs 4474-24-2 and 125351-99-7 are reasonable ecotoxicological analogues of Acid Blue 127 due to the similarities in the number and position of SO_3^- groups and the lack of extra substituent of ecotoxicological concern. Acid Blue 127 contains two anthraquinone structures with the sulfonic acid moiety and a primary amine attached on each anthraquinone. However, for CAS RNs 4474-24-2 and 125351-99-7, the sulfonic acid moieties are attached to the anthraquinone structure by a phenylamine.	

Sources

Acid Blue 127 is not naturally produced in the environment.

Recent information was collected through industry surveys conducted for the years 2005 and 2006 under *Canada Gazette* notices issued pursuant to section 71 of CEPA 1999 (Canada 2006b and Environment Canada 82008a). These notices requested data on the Canadian manufacture, import and use of the substance.

No companies reported manufacturing or importing Acid Blue 127 above the prescribed threshold of 100 kg/year in Canada in 2005 or 2006. In addition, no companies reported using a total quantity greater than 1000 kg of the substance, whether alone, in a mixture, in a product or in a manufactured item at any concentration in 2006. In the Declaration of Stakeholder Interest form associated with the section 71 survey for 2006, two companies reported a stakeholder interest in this substance despite not meeting mandatory reporting requirements. One company reported a stakeholder interest in 2005.

It should be noted that products containing Acid Blue 127 may enter the country even though they are not identified as such in the section 71 survey because they are imported unknowingly in manufactured items, or in quantities below the 100-kg reporting threshold for the survey.

According to the Domestic Substances List (DSL) nomination, the quantity reported to be manufactured, imported or in commerce in Canada during the calendar year 1986 was 1000 kg. Acid Blue 127 is an existing chemical in Europe, but is not on the low or high production volume chemicals lists (ESIS 82008).

Uses

The following use codes were specified for the substance during the DSL nomination: "Soap and Cleaning Products" and "Function Other than Listed."

In the United States, employees in the leather and leather products industry were potentially exposed to Acid Blue 127 from 1981 to 1983 (NIOSH 1983), which suggests it may be used in this sector. Acid Blue 127 may also be used as a colorant for textiles such as wool, paper and leather (Chemische Fabriek Triade 2008).

The above information suggests that Acid Blue 127 has dispersive uses.

Releases to the Environment

Since there were no reports of import or manufacture at or above the reporting threshold of 100 kg in 2005 or 2006 in response to section 71 notices (Canada 2006b; Environment Canada 82008a), releases of this substance to the Canadian environment are estimated to be low.

However releases of Acid Blue 127 from imported down-the-drain products such as soap and cleaning products cannot be quantified, because no information on the amount of the substance imported into Canada in such products has been specifically identified (Environment Canada 8a2008a).

Environmental Fate

Most of the above uses would result in releases to aqueous waste streams. Since it is a salt, and the pK_a of the acid form is very low (-1.45), Acid Blue 127 is expected to be present mainly as a dissociated anion in water. Because of its ionic character, it is expected to have a high water solubility value (10 000 mg/L) and to a large extent reside the aqueous phase.

Acid dyes, however, have high fixation rates, being attracted to positively charged substrates (e.g., nitrogen-containing particles, cationic metals) and consequently they can settle out to bed sediments or wastewater treatment plant (WWTP) sludges (ETAD 1995). Acid Blue 127 may thus be released to soil with WWTP sludges used for soil enrichment. Sludges may also be deposited in landfills. Volatilization from dry or moist soil surfaces seems to be an unimportant fate process based upon the low estimated

vapour pressure and Henry's law constant. If released to soil, because of its high water solubility Acid Blue 127 may be leached from solids and migrate to the water phase of the soil (e.g., groundwater) or undergo surface runoff attached to particulate matter.

Given the use in aqueous-based dye treatments and products, Acid Blue 127 will not be released directly to air and is not expected to partition to this compartment based on a very low calculated Henry's Law constant of 8.4×10^{-15} Pa·m^3/mol. Moreover, air is not considered to be a transport medium for dyes (including acid dyes), as these substances exhibit low or negligible volatility (ETAD 1995).

Persistence and Bioaccumulation Potential

Environmental Persistence

No environmental monitoring data relating to the presence of Acid Blue 127 in the Canadian environment (air, water, soil, sediment) have been identified. Furthermore, no experimental biological degradation data for Acid Blue 127 have been identified.

According to the Ecological and Toxicological Association of Dyes and Organic Pigments Manufacturers, with some exceptions, dyes are considered essentially non-biodegradable under aerobic conditions (ETAD 1995). Repeated evaluation of ready and inherent biodegradability using accepted screening tests (see the *OECD Guidelines for the Testing of Chemicals* website) have confirmed this assumption (Pagga and Brown 1986; ETAD 1992). Based on the chemical structure of Acid Blue 127, there is no reason to suspect that biodegradation will be other than that described for dyes generally (ETAD 1995). As described below, modelled data in Table 4 support this assumption of non-degradability.

Given that the majority of Acid Blue 127 is expected to be released into wastewater, persistence was primarily examined using predictive QSAR models for biodegradation in water. Because these degradation models are structure-based, their results are considered reliable since chemicals of structural comparability to Acid Blue 127 are contained in their training sets. Acid Blue 127 does not contain functional groups expected to undergo hydrolysis (dyes are designed to be stable in aqueous conditions).

Table 4. Modelled data for biodegradation of Acid Blue 127

Model	Model basis	Medium	Value	Interpretation	Extrapolated half-life (days)	Extrapolation reference and/or source
BIOWIN1* v4.1 (2000)	Linear probability	water (aerobic)	-1.19	Does not biodegrade fast	n/a: not applicable	
BIOWIN2* v4.1 (2000)	Non-linear probability	water (aerobic)	0	Does not biodegrade fast	n/a	
BIOWIN3* v4.1 (2000)	Expert Survey (ultimate biodegradation)	water (aerobic)	0.81	Recalcitrant	182	US EPA 2002
BIOWIN4*	Expert Survey	water	2.02			US EPA 2002

Model	Model basis	Medium	Value	Interpretation	Extrapolated half-life (days)	Extrapolation reference and/or source
v4.1 (2000)	(primary biodegradation)	(aerobic)		Recalcitrant (m)Months	60	
BIOWIN5* v4.1 (2000)	MITI linear probability	water (aerobic)	-1.65	Does not biodegrade fast	n/a	
BIOWIN6* v4.1 (2000)	MITI non-linear probability	water (aerobic)	0	Does not biodegrade fast	n/a	
BIOWIN7* v4.1 (2000)	Linear probability	anaerobic	-4.81	Does not biodegrade fast		
BIOWIN Overall Conclusion[1]	BIOWIN 3 + BIOWIN 5	water (aerobic)	no	Not ready biodegradable	n/a	
CATABOL v.5.100 (c2004−2008)	% BOD (OECD 301C)	water (aerobic)	0	Persistent (< 20%)	> 182	First-order-rate kinetics

*BIOWIN 1−7 are outputs obtained from the predictive model BIOWIN (2000). BIOWIN estimates aerobic and anaerobic biodegradability of organic chemicals using seven different models.
[1] Based on outcome of BIOWIN 3 and BIOWIN 5.

The results from Table 4 show that all the probability models (BIOWIN 1, 2, 5, 6 and 7) suggest this substance does not biodegrade rapidly. In fact, all probability results are less than 0.3, the cut-off suggested by Aronson et al. (2006) identifying substances as having a half-life > 60 days (based on the MITI probability models) and less than 0.5, the cut-off suggested by the model developers below which biodegradation is considered not to be fast. The half-life from the primary survey model (BIOWIN 4) result of months is suggested to mean approximately 60 days (US EPA 2002; Aronson et al. 2006), however the nature of the degradation products is unknown. The ultimate survey model (BIOWIN 3) result of recalcitrant is suggested to mean approximately 182 days or more (US EPA 2002; Aronson et al. 2006). The substance is also not expected to degrade rapidly under anaerobic conditions. The overall conclusion from BIOWIN (2000) is that this substance is not ready biodegradable.

Another ultimate degradation model, CATABOL predicted a 0% biodegradation based on the OECD 301 28-day ready biodegradation test (% BOD), which has been suggested mean likely persistent (Aronson and Howard 1999) and having a half-life in water of > 182 days (assuming first-order-rate kinetics).

When the results of the BIOWIN models and CATABOL are considered, there is a high likelihood that the ultimate degradation half-life in water is > 182 days, which is consistent with what would be expected for this chemical structure (i.e., few degradable functional groups). Although there is some potential for primary degradation, the estimated half-life is relatively long (months) and the nature of the degradation products is not known.

Using a 1:1:4 for a water:soil:sediment half-life extrapolation (Boethling et al. 1995), the ultimate degradation half-life in soil is also > 182 days and the half-life in sediments is > 365 days.

Based on the results of predictive modelling, Acid Blue 127 meets the persistence criteria for water and soil (half-life in soil and water ≥ 182 days) as well as sediments (half-life in sediments ≥ 365 days) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential for Bioaccumulation

There are no empirical bioaccumulation data available for this substance.

As indicated in Table 2, anionic dyes in general will have relatively low log K_{ow} values (< 3.0) and high water solubility values (10 000 mg/L). This pattern has been observed based on data from previous bioconcentration and partition studies with dyes (ETAD 1995).

The low estimated log K_{ow} value for Acid Blue 127 suggests that it does not have the potential to bioaccumulate in the environment. The high estimated water solubility of Acid Blue 127 also provides an indication that Acid Blue 127 is likely to have a low potential to bioaccumulate/bioconcentrate in aquatic biota.

High solubility and low bioaccumulation potential for Acid Blue 127 would be expected given is its low pK_a and consequent high degree of dissociation under typical environmental conditions. The high degree of ionization is expected to limit the lipid partitioning tendency of this acid dye as is its large molecular size.

It has been stated by ETAD (1995) that the molecular characteristics indicating the absence of bioaccumulation are a molecular weight of > 450 g/mol and a cross-sectional diameter of > 1.05 nm. Recent investigation by Dimitrov et al. (2002), Dimitrov et al. (2005) and the BBM (2008) suggests that the probability of a molecule crossing cell membranes as a result of passive diffusion declines significantly with increasing maximum cross-sectional diameter (D_{max}). The probability of passive diffusion lowers appreciably when cross-sectional diameter is > ~1.5 nm and more significantly for molecules having a cross-sectional diameter of >1.7 nm. Sakuratani et al. (2008) have also investigated the effect of cross-sectional diameter on passive diffusion from a test set of about 1200 new and existing chemicals. They also observed that substances not having a very highly bioconcentration potential often have a D_{max} (>2.0 nm) and an effective diameter (D_{eff}) >1.1 nm.

Acid Blue 127 has a molecular weight of 872.83 g/mol (see Table 1); this characteristic does not indicate a bioaccumulation capability of this substance if molecular weight is used as the only parameter. An Environment Canada (2007) report points out that there

are no clear relationships for establishing strict molecular size cut-offs for assessing bioaccumulation potential. However, the report does not dispute the notion that a reduction in uptake rate can be associated with increasing cross-sectional diameter as demonstrated by Dimitrov et al. (2002, 2005). The maximum diameter of Acid Blue 127 and its conformers ranges from 0.54 to 2.8 nm (BBM 2008) suggesting that a potential for a reduced uptake rate and in vivo bioavailability exists with this dye.

The weight of evidence indicates that Acid Blue 127 does not meet the bioaccumulation criterion (BCF, BAF ≥ 5000) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential to Cause Ecological Harm

Ecological Effects Assessment

A - In the Aquatic Compartment

There are no empirical ecotoxicity data available for this substance.

Aquatic toxicity predictions for Acid Violet 48 obtained using predictive QSAR models were considered unreliable and are not included. These models lack the ability to accurately estimate log K_{ow} for this substance.

Experience with new dyes at Environment Canada as well as at the United States EPA Office of Pollution Prevention and Toxics (OPPT) has shown that, in general, the number of sulphonic acid groups determines potential for toxicity. Dyes with one or two sulphonic acid groups have shown moderate to high acute toxicity (< 1–10 mg/L) to some aquatic biota, while dyes with more than two sulphonic acid groups have shown very low acute (> 100 mg/L) and chronic (> 10 mg/L) toxicity to most aquatic biota. Furthermore, Environment Canada has evaluated numerous acid dyes under the *New Substances Notification Regulations* and has generally found anionic dyes to be of low toxicity regardless of the number of acid groups, but some exceptions have been found (e.g., when a reactive functional group is not hindered). Therefore Acid Blue 127, as an anionic dye with two sulphonic acid groups and no reactive functional groups, is more likely to have only a moderate toxicity to aquatic organisms.

A search for suitable analogues resulted in two structural anthraquinone analogues being identified: CAS RNs 125351-99-7 and 4474-24-2 (Table 3). Because these molecules are smaller, they are expected to more readily taken up and hence more toxic than Acid Blue 127. An empirical acute toxicity study on *Salmo gairdneri*, *oncorhynchus mykiss* (Table 5) found a 48-hr LC_{50} of 75 mg/L for a structural analogue (CAS RN 4474-24-2). The result of this study was deemed to be of medium reliability, as detailed test methods were not provided. It is however generally consistent with the result from another empirical

acute toxicity study for a structural analogue (CAS RN 125351-99-7) on *Poecilia reticulata* (Table 5) which reported a 96-hr LC_{50} of 14.3 mg/L based on nominal concentrations.

Based on experience with new dyes, available experimental evidence for the above analogues (Table 5) and an analysis of functional groups, Acid Blue 127 is therefore not expected to cause harm to aquatic organisms at low concentrations (acute LC_{50}s are expected to be in the 10–100 mg/L range or higher).

Table 5. Empirical data for aquatic toxicity of analogues of Acid Blue 127

CAS RNs[1]	Test organism	Type of test	Duration (hours)	Endpoint	Value (mg/L)	Reference
4474-24-2	*Salmo gairdneri*, *oncorhynchus mykiss* (rainbow trout)	Acute	48	LC_{50}[2]	75	Sandoz 1977
	Bacteria (activated sludge)	Respiration Inhibition	3	IC_{50}[3]	> 1.000	Clariant 1989
125351-99-7	*Poecilia reticulata* (guppy)	Acute	96	LC_{50}[2]	14.3	Häner 1996

[1] Chemical Abstracts Service Registry Numbers.
[2] LC_{50} – The median or nominal lethal concentration (LC_{50}) is the concentration of a substance that is estimated to be lethal to 50% of the test organisms.
[3] IC_{50} – The concentration of a substance that is estimated to cause inhibition of 50% of the test organisms.

B - In Other Environmental Compartments

Acid Blue 127 could be released to soil from the disposal of products that degrade and release Acid Blue 127 as well as from the intentional application of biosludges. Accumulations are also possible in sediment after release to water. It would thus be desirable to obtain toxicity data for soil and sediment-dwelling organisms. However, no suitable ecological effects studies were found for this compound for media other than water.

Ecological Exposure Assessment

No data concerning concentrations of this substance in water in Canada have been identified. Environmental concentrations are, therefore, estimated from available information using models. As Acid Blue 127 is used in industrial facilities and can be released to water, Environment Canada's Industrial Generic Exposure Tool – Aquatic (IGETA) was employed to estimate a conservative substance concentration in a generic water course receiving industrial effluents (Environment Canada 2008b).

The generic scenario is designed to provide these estimates based on conservative assumptions regarding the amount of chemical processed and released, the number of

processing days, the sewage treatment plant removal rate and the size of the receiving watercourse. The tool models an industrial-release scenario based on loading data from sources such as industrial surveys and knowledge of the distribution of industrial discharges in the country and calculates a predicted environmental concentration (PEC).

The PEC for Acid Blue 127 was calculated assuming that the maximum mass of chemical used at a single facility is the threshold reporting value of 100 kg for the 2006 section 71 notice, a level that was not reached by any company. As a conservative estimate, handling and processing losses were assumed to be 100%, with no removal (0%) by sewage treatment plant. The receiving body information is highly conservative, assuming the chemical is released to a very small river without treatment. The equation and inputs used to calculate the PEC in the receiving watercourse are described in Environment Canada (2008b).

The conservative PEC for water, resulting from industrial releases, was calculated to be 0.011 mg/L (Environment Canada 2008c).

Characterization of Ecological Risk

The approach taken in this ecological screening assessment was to examine the available scientific information and develop conclusions based on a weight-of-evidence approach and using the precautionary principle as required under CEPA 1999. Particular consideration has been given to potential for environmental exposure, persistence, bioaccumulation, and potential to cause toxicity.

A predicted no-effect concentration (PNEC) was estimated based on the nominal lethal concentration (LC_{50}) to fish (*Poecilia reticulata*). The 96-hr LC_{50} for 9,10-Anthracenedione, 1,4-bis[(4-methylphenyl)amino]-, sulfonated, potassium salts (CAS RN 125351-99-7), an analogue which may be somewhat more toxic than Acid Blue 127, was 14.3 mg/L (Table 5). A factor of 100 was then applied to account for uncertainty in extrapolating acute to chronic (long-term) toxicity and from laboratory results to the field. The resulting PNEC is 0.143 mg/L. When compared to the conservative PEC calculated above, the resulting risk quotient (PEC/PNEC) is 0.011/0.143 = 0.078. Therefore, concentrations of Acid Blue 127 in surface waters in Canada pose little risk to populations of aquatic organisms. The calculated risk coefficient is less than 1 with a more than a ten-fold margin of safety afforded by the conservative risk quotient to account for uncertainty.

Based on the available information, although Acid Blue 127 is expected to be persistent in water, soil and sediment; it is also expected to have a low bioaccumulation potential. The low importation volumes of Acid Blue 127 into Canada indicate a low potential for releases into the Canadian environment. Once released into the environment, it will be found mainly in water and possibly sediment. It has also been demonstrated to have only a moderate potential for toxicity to aquatic organisms. Risk quotients for aquatic exposures indicate that Acid Blue 127 concentrations likely do not exceed concentrations

associated with adverse effects, even when using conservative scenarios and assumptions. Therefore Acid Blue 127 is unlikely to be causing harm to populations of aquatic organisms in Canada.

Uncertainties in Evaluation of Ecological Risk

The persistence assessment is limited by the lack of experimental biodegradation data, which necessitated generation of model predictions.

The lack of evidence from empirical studies with Acid Blue 127 is a source of uncertainty in the bioaccumulation assessment. Data for chemical analogues were used to fill this gap.

The uncertainties also exist because of the lack of information on environmental concentrations (e.g., monitoring data) in Canada for Acid Blue 127. Consequently some conservative assumptions were made when using models to estimate concentrations near point sources.

Although it is possible that the total mass of the substance in commerce has been underestimated - because of its unreported presence in down-the-drain consumer products imported into Canada – any releases associated with such uses would be spread over wide areas and the resulting exposure concentrations should thus be lower than those resulting from industrial releases and thus are also expected to pose little risk.

Regarding toxicity, based on the anticipated release pattern for the substance, the significance of soil and sediment as possible media of exposure is not well addressed by the effects data available. Indeed, the only effects data identified apply primarily to pelagic aquatic exposures. Similarly for the exposure assessment, the predicted environmental concentration (PEC) accounts for concentrations in water only, so exposure through soils, suspended solids and sediments is not considered. However, given the current release pathways and quantities used in Canada, overall exposure is not likely to be significant at this time.

Conclusion

Based on the information presented in this screening assessment, it is concluded that Acid Blue 127 is not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity, or that constitute or may constitute a danger to the environment on which life depends.

It is, therefore, concluded that Acid Blue 127 does not meet the definition of “toxic” as set out in section 64 of CEPA 1999. Additionally, Acid Blue 127 does not meet criteria

for bioaccumulation potential but meets criteria for persistence as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

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