Screening Assessment for the Challenge

4-[[5-[[[4-(Aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyphenyl]azo]-*N*-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxynaphthalene-2-carboxamide
(Pigment Red 187)

Chemical Abstracts Service Registry Number
59487-23-9

Environment Canada
Health Canada

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Synopsis

Pursuant to section 74 of the *Canadian Environmental Protection Act, 1999* (CEPA 1999), the Ministers of the Environment and of Health have conducted a screening assessment on 2-Naphthalenecarboxamide, 4-[[5-[[[4-(aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyphenyl]azo]-*N*-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxy- (Pigment Red 187), Chemical Abstracts Service Registry Number 59487-23-9. This substance was identified as a high priority for screening assessment, and included in the Ministerial Challenge because it had been found to meet the ecological categorization criteria for persistence, bioaccumulation potential and inherent toxicity to non-human organisms and is believed to be in commerce in Canada.

The substance Pigment Red 187 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 (i.e., it did not meet the criteria of both being considered to present greatest or intermediate potential for exposure and having been classified by another national or international regulatory agency on the basis of carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity). Therefore, this assessment focuses on information relevant to the evaluation of ecological risks.

Pigment Red 187 is an organic substance that is used in Canada and elsewhere primarily as a colour pigment in plastics, inks, paints and textiles, and is also used in the food and beverage sector. Its secondary use is as an inert ingredient in pesticides. The substance is not naturally produced in the environment. It is not reported to be manufactured in Canada; however, between 1001 and 100 000 kg of the pigment were imported into the country in 2006.

Based on certain assumptions and reported use patterns in Canada, most of the substance ends up in waste disposal sites. Assumptions and input parameters used in making these estimates are based on information obtained from a variety of sources including responses to regulatory surveys, Statistics Canada, manufacturers' websites and technical databases. Estimates predict that as much as 4.1% and 2.5% of Pigment Red 187 may be released to water and soil, respectively. No releases are predicted to air. Pigment Red 187 presents very low experimental solubilities in water and octanol (< 50 µg/L). It is present in the environment primarily as micro-particulate matter that is not volatile and rather chemically stable, and it has a tendency to partition by gravity to sediments if released to surface waters, and to soils if released to air in terrestrial environments.

Based on its physical and chemical properties, Pigment Red 187 is expected to be persistent in the environment. However, new experimental data relating to its solubility in octanol and water suggest that this pigment has a low potential to accumulate in the lipid tissues of organisms. The substance therefore meets the persistence criterion but does not meet the bioaccumulation criterion 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 saturated solutions of the substance do not cause acute harm to aquatic organisms.

For this screening assessment, a very conservative exposure scenario was selected in which whereby an industrial operation (user of the pigment) discharges Pigment Red 187 into the aquatic environment. The predicted environmental concentration in water was many orders of magnitude below predicted no-Effect concentrations calculated for fish, daphnids and algae.

This substance will be included in the Domestic Substances List inventory update initiative, to be launched in 2009. In addition and where relevant, research and monitoring will support verification of assumptions used during the screening assessment.

Based on the information available, Pigment Red 187 does not meet any of the criteria set out in Section 64 of the *Canadian Environmental Protection Act, 1999*.

Introduction

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

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

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

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

The substance Pigment Red 187 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 Pigment Red 187 was published in the *Canada Gazette* on February 3, 2007 (Canada 2007a). 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 were received.

Although Pigment Red 187 was determined to be a high priority for assessment with respect to the environment, it did not meet the criteria for GPE or IPE and high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity. Therefore, this assessment focuses principally on information relevant to the evaluation of ecological risks.

Screening assessments under CEPA 1999 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 develops conclusions by incorporating a weight of evidence approach and precaution.

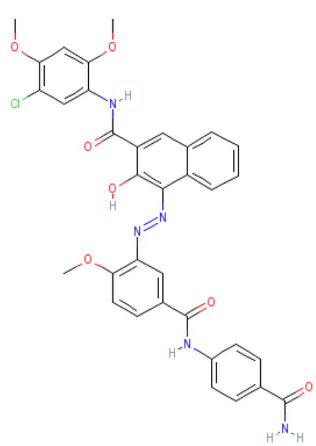
This screening assessment includes consideration of information on chemical properties, hazards, uses and exposure, including the additional information submitted under the Challenge. Data relevant to the screening assessment of this substance were identified in original literature, review and assessment 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, the draft of this screening assessment was subject to a 60-day public comment period. The critical information and considerations upon which the assessment is based are summarized below.

Substance Identity

For the purpose of this document, this substance will be referred to as Pigment Red 187. This pigment belongs to the group of Naphthol AS III organic pigments, for which the basic entity is the anilide of 2-hydroxy-3-naphthoic acid (Table 1; Herbst and Hunger 2004).

Table 1. Substance identity

CAS Registry Number	59487-23-9
DSL name	4-[[5-[[[4-(Aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyphenyl]azo]-*N*-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxynaphthalene-2-carboxamide
Inventory names	2-Naphthalenecarboxamide, 4-[[5-[[[4-(aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyphenyl]azo]-*N*-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxy- (TSCA, AICS, PICCS, ASIA_PAC) ; 4-[[5-[[[4-(aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyphenyl]azo]-*N*-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxynaphthalene-2-carboxamide (EINECS); Pigment Red 187 (ENCS); C.I. Pigment Red 187 (ECL, PICCS).
Other names	2-Naphthanilide, 4-[[5-[(p-carbamoylphenyl)carbamoyl]-2-methoxyphenyl]azo]-5'-chloro-3-hydroxy-2',4'-dimethoxy-; C.I. 12486; Novoperm Red HF 4B
Chemical group	Discrete organics
Chemical sub-group	Monoazo Organic Color Pigments (Naphthol AS pigments III)
Chemical formula	$C_{34}H_{28}ClN_5O_7$
Chemical structure	
SMILES	O=C(Nc(c(OC)cc(OC)c1Cl)c1)c(c(O)c(N=Nc(c(OC)ccc2C(=O)Nc(ccc(C(=O)N)c3)c3)c2)c(c4ccc5)c5)c4
Molecular mass	654.08 g/mol

Source: National Chemical Inventories (NCI), 2007: AICS (Australian Inventory of Chemical Substances); ASIA-PAC (Combined Inventories from the Asia-Pacific Region); 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

The pigment industry synthesizes organic pigments that have low to very low solubilities in nearly all solvents (i.e., < 1 mg L^{-1} to < 0.01 mg L^{-1}). This arises from the desire of the industry to produce chemicals that will retain their colour for a long time and in any type of material. Low solubility is enhanced by designing chemicals that have strong interactive forces between molecules. For Naphthol AS compounds, this is achieved by the introduction of substituents like $–CONH_2$, $–SO_2NH–$, or –Cl in the molecule (Herbst and Hunger 2004; Lincke 2003). The resulting intermolecular bonds, in turn, generate a crystal structure that is at the origin of the stability of organic pigments (Lincke 2003).

As is the case with the majority of organic pigments, Naphthol AS III pigments generally do not exist as individual molecules but are principally particles in the submicron range. The pigment powder is typically composed of primary particles (i.e., the crystal lattice of a pigment), aggregates and agglomerates. Manufacturers usually provide the physical specifications of their pigments, which include the average particle size of the pigment powder. In doing so, users can determine which pigment is the most appropriate to colour their product(s), since performance is chiefly controlled by the particle size distribution (Herbst and Hunger 2004).

Table 2 contains modelled and experimental physical and chemical properties of Pigment Red 187 that are relevant to its environmental fate. Modelled estimates for these properties, as well as for rate constants and environmental partitioning are typically generated using quantitative structure-activity relationship (QSAR) models. These models, in turn, base their predictions on the individual characteristics of the molecules. The modelled log K_{OW} of 7.07 (KOWWIN 2000) implies that the solubility of Pigment Red 187 is much higher in octanol than in water. Experimental solubility data, however, reveals that the substance is approximately equally soluble in the two solvents, indicating that the modelled partition coefficient is likely overestimated. The modelled estimate of log K_{OW} has therefore been disregarded for this assessment.

The experimental solubilities in Table 2 have been determined using an aggressive approach with long contact times between pigment particles and the solvent, and a filtration step removing as much of the particulate matter in the suspension as possible. These studies have been critically reviewed, and although none reported using reference chemicals of known solubilities, they were determined to have a satisfactory degree of reliability for the present assessment.

Table 2. Physical and chemical properties for Pigment Red 187

Property	Type	Value	Temperature (°C)	Reference
Physical state	Experimental	Bluish red and very transparent powder	--	Herbst and Hunger 2004
Average size of the crystal particle (nm)	Experimental	110	--	Clariant 2007
Melting point (ºC)	Experimental	NA	NA	--
	Modelled	350	--	MPBPWIN v1.41
Boiling point (ºC)	Experimental	NA	NA	--
	Modelled	992	--	MPBPWIN v1.41
Density (g/cm^3)	Experimental	1.45	NA	Clariant 2007
	Modelled	NA	NA	--
Vapour pressure (Pa)	Experimental	NA	NA	--
	Modelled	3.84×10^{-25}	25	MPBPWIN v1.41
Henry's Law constant ($Pa{\cdot}m^3/mol$)	Experimental	NA[1]	NA[1]	--
	Modelled	9.66×10^{-28}	25	HENRYWIN v3.10
Log K_{OW} (Octanol-water partition coefficient) (dimensionless)	Experimental	0.40	23–24	See text
	Modelled	NA[1]	NA[1]	See text
Log K_{OC} (Organic carbon-water partition coefficient) (L/kg)	Experimental	NA	NA	--
	Modelled	NA	NA	--
Water solubility (µg/L)	Experimental	8.9	23–24	Study Submission 2007b
	Modelled	0.092	25	WSKOWWIN v1.41
Other solubilities (µg/L)	Experimental (octanol)	22.1	23–24	Study Submission 2007b

NA: Not available; NA[1]: not applicable

Sources

Pigment Red 187 is not known to be formed in nature. In Canada, no manufacture of this substance was reported in response to a CEPA section 71 survey notice for the 2006 calendar year in a quantity meeting the 100 kg reporting threshold. Two companies reported importing this substance for use in the manufacturing of various coloured products, with one company in the 0–100 kg/year range and one company in the 1001–100 000 kg/year range (Environment Canada 2007a).

Products containing Pigment Red 187 may enter the country even if they are not identified as such in the Section 71 survey. These quantities are currently not known. According to information from the United States Environmental Protection Agency (US EPA 2002), the import and production of Pigment Red 187 in that country was in the order of 4.5–225 tonnes per year from 1986 to 2002. The Substances in Preparations in Nordic Countries (SPIN) database indicated that Pigment Red 187 was used in Denmark, Norway, and Sweden from 1999 to 2004. Denmark reported a use volume in the order of 35.8–59.7 tonnes from 2000 to 2004. The consumption in Norway was less than 2 tonnes. Quantity in Sweden was not specified (SPIN 2006).

Uses

According to the submissions made under Section 71 of CEPA 1999, the only known current use pattern code for Pigment Red 187 in Canada is as a colourant/pigment/ stain/dye/ink (Environment Canada 2007a). In Canada, Pigment Red 187 is used as a colourant in some polyethylene and polyvinyl chloride plastics under the Food and Drug Act (Health Canada 2007a). Pigment Red 187 is a formulant (<3.0%) in three commercial class pest control products registered for use in Canada under the *Pest Control Products Act* (Health Canada 2007b; 2007c).

Internationally, uses of Pigment Red 187 include:

- in plastics such as polyolefins, acrylic, polystyrene, HIPS and ABS resins (CII 2007; Herbst and Hunger 2004);
- as a colourant in printing inks and gravures (CII 2007; Clariant 2007; Herbst and Hunger 2004);
- as a colourant for home textiles such as upholstery and carpeting, and for artificial leathers in the automobile sector (Clariant 2007; Herbst and Hunger 2004);
- as a colourant in industrial paints such as in films or bicycle paints, metallic finishes and automotive refinishes (Clariant 2007; Herbst and Hunger 2004);

Uses in Canada as a colourant/pigment/stain/dye/ink are considered to be similar to those identified above.

Releases to the Environment

The two companies that reported importing this substance in 2006 did not indicate any releases of this chemical to the environment.

Mass Flow Tool

To estimate potential release of the substance to the environment at different stages of its life cycle, a mass flow tool was used. Empirical data concerning releases of specific substances to the environment are seldom available. Therefore, for each identified type of use of the substance, the proportion and quantity of release to the different environmental media are estimated, as is the proportion of the substance chemically transformed or sent for waste disposal. Assumptions and input parameters used in making these estimates are based on information obtained from a variety of sources including responses to regulatory surveys, Statistics Canada, manufacturers' websites and technical databases. Of particular relevance are emission factors, which are generally expressed as the fraction of a substance released to the environment, particularly during its manufacture, processing and use associated with industrial processes. Sources of such information include emission scenario documents, often developed under the auspices of the Organisation for Economic Co-operation and Development (OECD) and default assumptions used by different international chemical regulatory agencies. It is noted that the level of uncertainty in the mass of substance and quantity released to the environment generally increase further down the life cycle.

Results indicate that Pigment Red 187 can be expected to be found largely in waste management sites (82.6%), due to the eventual disposal of manufactured items containing it. The calculations assume that there is no release of the substance from these sites, although long-term releases may be possible. A small fraction of solid waste is incinerated, which is expected to result in the transformation of the substance. It has also been assumed that 8.8% of the pigment may be treated as hazardous waste. Based largely on information contained in OECD emission scenario documents for processing and uses associated with this substance, it is estimated that 4.1 percent and 2.5 percent of Pigment Red 187 may be released to water and soil, respectively (Table 3).

Although no information is available on the volume of consumer products containing Pigment Red 187 that are imported into Canada, it is anticipated that the quantities of Pigment Red 187 that are released to the various environmental media would not be significantly different from those estimated here. However, the quantities sent for waste management would be higher if importation of these products were taken into consideration.

Table 3. Estimated releases and losses of Pigment Red 187 to environmental media, chemical transformation and distribution to management processes, based on the Mass Flow Tool.

Fate	Proportion of the mass (%)[1]	Major life cycle stage involved[2]
Releases to receiving media:		
To soil	2.5	Consumer use
To air	0.0	Manufacture
To sewer[3]	4.1	Manufacture, formulation, consumer use
Chemically transformed	1.9	Waste disposal
Transferred to waste disposal **sites (e.g., landfill, incineration, hazardous waste)**	91.4	Waste disposal

[1] For Pigment Red 187, information from the following OECD emission scenario documents was used to estimate releases to the environment and distribution of the substance as summarized in this table: (OECD 2006; 2004). Values presented for release to environmental media do not account for possible mitigation measures that may be in place in some locations (e.g., partial removal by sewage treatment plants). Specific assumptions used in derivation of these estimates are summarized in Environment Canada (2007b).

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

[3] Wastewater before any form of treatment

Environmental Fate

The very low modelled vapour pressure and a negligible Henry's Law constant of $\sim10^{-28}$ Pa·m^3/mol for Pigment Red 187 are consistent with the fact that it is a large and complex molecule (Baughman and Perenich 1988; Danish EPA 1998). This pigment is not expected to volatilize at environmentally realistic temperatures.

Because of its very low solubility in water, this pigment may be considered not available for aerobic biodegradation. In addition, direct contact with biota probably does not occur when the pigment is sealed in the matrix of coloured materials.

The particulate character of Pigment Red 187 should have a key influence on its fate in the environment. Its particle size and density, which is 45 percent greater than that of water (cf. Wetzel 2001; Reynolds *et al*. 1987), together with its chemical stability and low aqueous solubility, indicates that it will partition by gravity to sediments if released to surface waters and will tend to remain in soils if released to terrestrial environments.

Persistence and Bioaccumulation Potential

Persistence

Jaffe (1996) has stated that once a pigment is incorporated into a matrix (e.g., plastic), it is expected to be durable and withstand the combined chemical and physical stresses of weather, solar radiation, heat, water, and industrial pollutants.

Industries that manufacture pigments recognize that their substances are persistent. For example, the Color Pigments Manufacturers Association, Inc. (CPMA 2003) has indicated that pigments are designed to be durable or persistent in the environment in order to provide color to finished coatings, inks and paints.

The environmental persistence of Naphthol AS III pigments, such as Pigment Red 187, in anoxic environments is an important area of uncertainty. Azo dyes are reported to be degraded in anoxic waters via anaerobic reduction of the azo bond (-N=N-: Van der Zee 2002). Naphthol AS III pigments have azo chromophores in their structure as well. However, no documentation has been found regarding a possible degradation potential of these pigments in aqueous media in the absence of oxygen. In principle, the crystal would have to dissolve first, releasing its constituent molecules. Then, the azo bonds in these molecules would be available for biotic reduction.

Based on the weight of evidence provided by the above-described literature, Pigment Red 187 is considered to meet the persistence criteria defined in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Bioaccumulation

There is a predictable relationship between K_{OW} and the bioconcentration factor in lipids (Mackay 1982). The ratio log (C_O/C_W) has been estimated from the experimental solubilities of Pigment Red 187 in octanol (C_O) and water (C_W) (Table 2), and this experimentally derived ratio has been preferred over the model-derived log K_{OW} for this pigment. This approach is supported by the observation that partitioning into octanol is a good indicator of a substance's potential to partition into the lipid phase of aquatic biota (Bertelsen et al. 1998) and, for pigments, the observation that a reduced solubility in octanol translates into a similarly reduced bioconcentation factor (BCF) and bioaccumulation factor (BAF) in an aquatic organism (Banerjee and Baughman 1991).

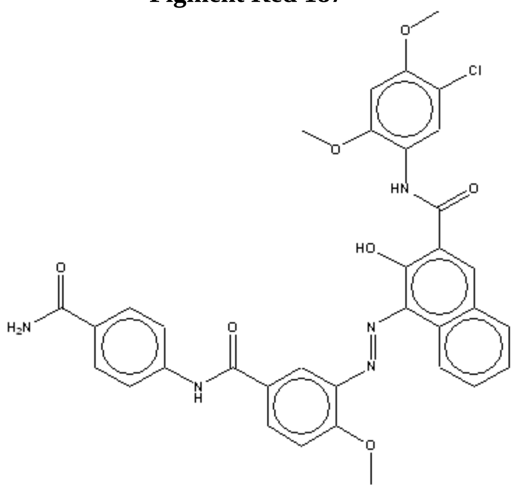
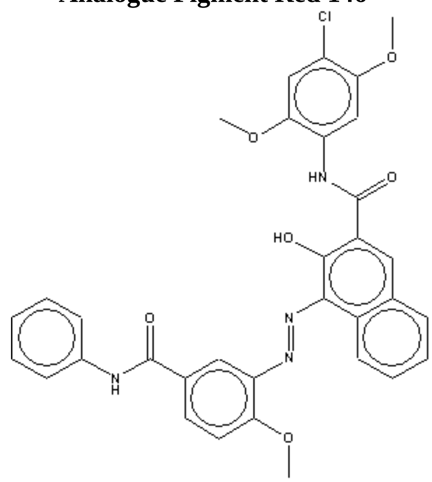
A new set of BCF and BAF estimates for Pigment Red 187 has been obtained from quantitative structure-activity relationship (QSAR)-based bioaccumulation models, using the experimentally based value log (C_O/C_W) in place of the overestimated log K_{OW} by KOWWIN (2000). In addition, modelled BCF and BAF estimates have been obtained for a reasonably close analogue of Pigment Red 187, namely Pigment Red 146 (CAS RN 5280-68-2), using a log (C_O/C_W) derived from experimental solubilities as well (Study Submission 2007b). Table 4 shows that the new modelled BCF and BAF estimates are well below 1000 (log BCF/BAF of 3) for both Pigment Red 187 under evaluation and its analogue, Pigment Red 146.

To identify chemical analogues, the guidance provided by the OECD (2007) has been generally followed. In the present case, the crystalline nature of the pigments (Re: OECD 2007), and therefore their solubilities in water and octanol, is a key factor when determining an analogue for use in read-across. Pigment Red 187 and Pigment Red 146 have reasonably similar solubilities in water and octanol. For example, water and octanol solubilities of Pigment Red 146 are 8.7 and 100 µg/L, respectively (Study Submission 2007b; solubilities of Pigment Red 187 are given in Table 2).

Thus, Pigment Red 187 is expected to present a low bioaccumulation potential because of its very limited affinity for the lipid phase of living organisms. Further support is provided by experimental determinations for six representative organic pigments, all with BCF values of less than 100 wet wt (MITI 1992).

The above weight of evidence indicates that Pigment Red 187 does not meet the bioaccumulation criterion (BCF, BAF > 5000) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Table 4. Modelled bioaccumulation data for Pigment Red 187 and its analogue, Pigment Red 146

Chemical structure			
Pigment Red 187 [a]			**Analogue Pigment Red 146** [a]
			
Test organism	**Endpoint**	**Value wet wt**	**Reference**
Pigment Red 187 [log (C_O/C_W) = 0.40]			
Fish	BAF	0.0415 L/kg	Gobas BAF T2MTL (Arnot & Gobas 2003)
Fish	BCF	0.0278 L/Kg	Gobas BCF T2LTL (Arnot & Gobas 2003)
Fish	BCF	1.12 L/kg	OASIS, 2005
Fish	BCF	10 L/kg [b]	BCFWIN v2.15
Pigment Red 146 [log (C_O/C_W) = 1.1]			
Fish	BAF	1.69 L/kg	Gobas BAF T2MTL (Arnot & Gobas 2003)
Fish	BCF	1.46 L/kg	Gobas BCF T2LTL (Arnot & Gobas 2003)
Fish	BCF	19.2 L/kg	OASIS, 2005
Fish	BCF	10 L/kg [b]	BCFWIN v2.15

[a] Pigment Red 187 differs from Pigment Red 146 in two chemical features: an additional residue H_2NOC on one terminal benzene ring, and O and Cl differently substituted on the other terminal benzene ring.
[b] Default value for non-ionizable azo pigments.

Potential to Cause Ecological Harm

A quantitative evaluation based on exposure and ecological effects was conducted for this pigment as part of the weight of evidence evaluation of its potential to cause harm.

First, a predicted environmental concentration (PEC) was determined based on an analysis of exposure pathways. Then, pertinent endpoint organisms were selected. For each endpoint organism, a conservative (reasonable worst-case) predicted no-effect concentration (PNEC) was derived. The PNEC is obtained by selecting the lowest critical toxicity value (CTV) for the organism of interest and dividing it by an application factor appropriate for the endpoint.

Ecological Exposure Assessment

No data have been found regarding concentrations of Pigment Red 187 in the Canadian environment. The mass flow tool estimated that ~93 percent of the mass of this pigment ends up in waste disposal facilities. Off-site chemical migration from these facilities is unlikely, or can be predicted to be minor, because of the negligible geochemical mobility of the pigment indicated by its very low solubility in water and in organic solvents. Consequently, it is anticipated that there are negligible releases associated with the waste management stage of this substance.

The mass flow tool estimated that up to nearly 5 percent of the total mass of Pigment Red 187 in use could be released to water. In addition, available industrial information suggested that these releases would be generated by industrial users who employed the pigment to manufacture other coloured products (Environment Canada 2007a). The Industrial Generic Exposure Tool – Aquatic (IGETA) was selected to model the reasonable worst-case discharge of an industrial operation (user of the pigment) to the aquatic environment. IGETA is a modelling tool developed by Environment Canada to estimate surface water concentrations. 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 PEC. The maximum mass, per year, purchased by an industrial facility (1000 kg: Environment Canada 2007a) was used to calculate the loading rate for the PEC estimation. Based on the IGETA results, the average annual PEC is 0.0056 mg/L in the receiving watercourse.

Ecological Effects Assessment

A – In the Aquatic Compartment

Although no experimental toxicity data were found for Pigment Red 187, there are experimental toxicity data available for Pigment Red 146, which is a close analogue of Pigment Red 187 (Table 4, CAS RN 5280-68-2). Furthermore, predicted ecotoxicity values were obtained using the experimental log (C_O/C_W) of Pigment Red 187 (0.40). These experimental and predicted toxicity data (Table 5a and 5b) are considered reliable and have been used in the weight of evidence approach to determine the aquatic toxicity potential of this pigment.

Juveniles of *Daphnia magna* were exposed to a saturated solution of Pigment Red 146 for 48 hours under static conditions (Study Submission 2007c; Table 5a). The pH was maintained between 7.6 and 7.7, the temperature oscillated between 18 and 22°C and dissolved oxygen ranged between 8.0 and 8.5 mg/L. The test water had a hardness of 249 mg $CaCO_3$/L. An experimental treatment consisted of five specimens placed in a 50-mL glass beaker. One test concentration of 100 mg/L was established, using four replicates per test. In order to make a saturated solution, a stock solution of 100 mg Pigment Red 146 in one litre of test water was made. The stock solution was shaken at room temperature at 20 rpm for 24 hours (rotating shaker). Undissolved particles were removed by filtration on 0.45-µm membrane. This approach followed the guidance provided by the OECD for sparingly soluble substances (OECD 2000). The chemical was not measured during the test. No biologically significant effects (immobilization) were observed at saturation.

The degree of reliability of this study was deemed satisfactory for the present assessment. Notably, a reference toxicant was used and good laboratory practices were followed.

Aquatic toxicity predictions, recalculated using log (C_O/C_W), were obtained using the ECOSAR model (ECOSAR 2004). It is assumed that Pigment Red 187 has a narcotic mode of action similar to that of phenols. Table 5b presents these modelled ecotoxicity results.

The model data are all well above the estimated water solubility of the substance, and therefore are consistent with results of the experimental acute toxicity test, which indicate no effects at saturation.

B - In Other Media

No empirical or predicted effects data for non-aquatic organisms were identified for this compound. However, given the current release scenarios and quantities used in Canada, exposures through soils, suspended solids and sediment are not likely to be significant at this time.

Table 5a. Experimental aquatic toxicity value for Pigment Red 187

Organism	Test type	Endpoint	Duration	Value	Reference
Daphnid	Acute	EC_{50} [1]	48 hours	No effect at saturation (100 mg/L)	Study Submission 2007c

[1] Immobilization

Table 5b. Modelled aquatic toxicity values for Pigment Red 187

Organism	Endpoint	Duration	Value (mg/L)	Chemical class/mode of action	Reference
Fish	LC_{50}	14 days	21 958	Neutral Organic SAR (baseline toxicity)	ECOSAR 2004
Fish	LC_{50}	96 hours	936	Phenols	
Daphnid	LC_{50}	48 hours	160	Phenols	
Green Algae	EC_{50}	96 hours	8551	Phenols	

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 section 76.1 of CEPA 1999. Particular consideration has been given to risk quotient analysis, persistence, bioaccumulation, toxicity, sources and fate in the environment.

Pigment Red 187 is determined to be persistent, based on published evidence. However, it has been determined not to be bioaccumulative in accordance with the *Persistence and Bioaccumulation Regulations* of CEPA 1999 (Canada 2000), based on observations of its very low solubility in octanol, low modelled BCFs, and low experimental BCFs determined for a number of analogous organic pigments (CITI 1992).

Newly acquired empirical data for a chemical analogue, as well as modelled aquatic toxicity results, also suggest that this pigment is not very harmful, indicating no acute effects at saturation. There is uncertainty that effect concentrations are greater than the solubility of the compound; the OECD (2000) protocol is currently the best available approach for the evaluation of sparingly soluble substances.

Since Pigment Red 187 is considered a persistent but not bioaccumulative substance, a quantitative evaluation of exposure and of ecological effects was conducted as part of the weight of evidence evaluation of this pigment’s potential to cause harm.

In view of the limited amount of empirical Canadian exposure data, the IGETA model was used, along with industrial information, to estimate worst-case PECs. Three categories of organisms were considered for derivation of PNECs: fish, daphnids and algae. An application factor of 100 was used to extrapolate from acute to chronic effects, and from laboratory species to different species in the field. CTVs and PNECs are based on the most conservative effect values and are presented in Table 6. The resulting risk quotients are in all cases much less than 1, suggesting that the substance is unlikely to be present at concentrations that could cause harm to aquatic organisms.

Given the high persistence of the substance in the environment, chronic exposure is likely to occur. However, in view of the absence of any acute effects at saturation, and taking into account the relatively low solubility of the substance (9 µg/L) and its low bioaccumulation potential, long-term environmental exposure to the substance is not expected to cause adverse effects to aquatic organisms.

Considering these findings and given that this chemical is imported in relatively low quantities, it is concluded that Pigment Red 187 is unlikely to be causing ecological harm in Canada.

Table 6. Summary of values used for the risk characterization of Pigment Red 187

Endpoint organism	CTV	PNEC	PEC	Scenario	Risk quotient (PEC/PNEC)
	(mg/L)				
Fish	936	9.36	0.0056	IGETA model: discharge to a watercourse from an industrial plant.	0.0006
Daphnid	160	1.6			0.0035
Algae	8551	85.5			6.5×10^{-5}

Uncertainties in Evaluation of Ecological Risk

This section summarizes the key uncertainties associated with the risk assessment of Pigment Red 187.

Environmental fate processes could increase the bioavailability of the individual pigment molecule in biotic compartments. For example, long-term stability of Pigment Red 187 in anoxic sediments, as well as in anoxic layers in the soil column of waste disposal sites, is largely unknown.

Nanoscale materials are informally defined as substances having at least one dimension less than 100 nm. There is increasing evidence to the effect that nanoparticles can be absorbed by non-specific biouptake pathways such as pinocytosis (Leroueil et al. 2007). Organic pigments, such as Pigment Red 187, typically have a certain proportion of their particle size spectra in the nanoparticle range (e.g., Table 2). Presently, the bioaccumulation mechanisms and potential of these particles is poorly understood, as is the nature of the relationship between their bioaccumulation and their toxicity. Furthermore, certain less commonly considered environmental fate processes may have an important influence on the propensity of the pigment nanoparticles to be taken up by biota (e.g., importance of aggregation in nature: Wiesner et al. (2006)).

Conclusion

Based on the information presented in this draft screening assessment, it is concluded that Pigment Red 187 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. Similarly, it is concluded that Pigment Red 187 is persistent but does not meet the criterion for bioaccumulation as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Therefore it is concluded that Pigment Red 187 does not meet the definition of toxic as set out in paragraph 64(a) of the Canadian Environmental Protection Act, 1999.

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Appendix I - Robust Study Summaries

Evaluation of experimental data using Kollig's approach*

Item	Weight	Response	Mark
Reference: 13365Challenge003. Determination of the solubility in water and in octanol at ambient temperature – Sample: pure Pigment Red 187.			
Test substance: CAS RN: **59487-23-9;** Pigment Red 187			
Could you repeat the experiment with available information?	5	Fairly well	3.5
Is a clear objective stated?	1	Yes	1
Is water quality characterized or identified (distilled or deionized)?	2	Yes (water and octanol)	2
Are the results presented in detail, clearly and understandably?	3	Fair	1.5
Are the data from a primary source and not from a referenced article?	3	Primary	3
Was the chemical tested at concentrations below its water solubility?	5	N/A	N/A
Were particulates absent?	2	Not indicated	0
Was a reference chemical of known constant tested?	3	Not indicated	0
Were other fate processes considered?	5	N/A	N/A
Was a control (blank) run?	3	Not indicated	0
Was temperature kept constant?	5	Assumed	4
Was the experiment done near room temperature (15-30^{o} C)?	3	Yes	3
Is the purity of the test chemical reported (> 98%)?	3	Yes	3
Was the chemical's identity proven?	3	Partly	1.5
Is the source of the chemical reported?	1	Yes	1
Results: (X±SE)			
Solubility (water): 8.9±1.2 µg/L	Solubility (octanol): 22.1±2.6 µg/L		
Score:	23.5/37 or 63.5%		
Degree of reliability**	Satisfactory		

* Kollig, H.P. 1988. Criteria for evaluating the reliability of literature data on environmental process constants. Toxicol. Environ. Chem. 17: 287-311.

** The reliability code for ecotoxicological studies of DSL categorization is used.

Evaluation of experimental data using Kollig's approach*

Item	Weight	Response	Mark
Reference: 13365Challenge005. Determination of the solubility in water and in octanol at ambient temperature – Sample: pure Pigment Red 146.			
Test substance: CAS RN: **5280-68-2;** Pigment Red 146			
Could you repeat the experiment with available information?	5	Fairly well	3
Is a clear objective stated?	1	Yes	1
Is water quality characterized or identified (distilled or deionized)?	2	Yes (water and octanol)	2
Are the results presented in detail, clearly and understandably?	3	OK	2.5
Are the data from a primary source and not from a referenced article?	3	Primary	3
Was the chemical tested at concentrations below its water solubility?	5	N/A	N/A
Were particulates absent?	2	Assumed	2
Was a reference chemical of known constant tested?	3	Not indicated	0
Were other fate processes considered?	5	N/A	N/A
Was a control (blank) run?	3	Not indicated	0
Was temperature kept constant?	5	Assumed	4
Was the experiment done near room temperature (15-30^{o} C)?	3	Yes	3
Is the purity of the test chemical reported (> 98%)?	3	Qualitatively	1.5
Was the chemical's identity proven?	3	Assumed	3
Is the source of the chemical reported?	1	Yes	1
Results: ($\overline{X}$±SE)			
Solubility (water): 8.7±2.4 µg/L	Solubility (octanol): 100±3 µg/L		
Score:	26/37 or 70%		
Degree of reliability**	Satisfactory		

* Kollig, H.P. 1988. Criteria for evaluating the reliability of literature data on environmental process constants. Toxicol. Environ. Chem. 17: 287-311.

** The reliability code for ecotoxicological studies of DSL categorization is used.

Robust Study Summaries Form and Instructions: Aquatic iT				
No	**Item**	**Weight**	**Yes/No**	**Specify**
1	13365Challenge007. Acute Immobilisation Test (Static, 48h) to Daphnia magna STRAUS, Limit-Test, 2006			
2	Substance identity: CAS RN	n/a		5280-68-2
3	Substance identity: chemical name(s)	n/a		Pigment Red 146
4	Chemical composition of the substance	2		N/A
5	Chemical purity	1	Y	95.33%
6	Persistence/stability of test substance in aquatic solution reported?	1	Y	More than 72-h stable
Method				
7	Reference	1	Y	
8	OECD, EU, national, or other standard method?	3	Y	OECD 202
9	Justification of the method/protocol if not a standard method was used	2		N/A
10	GLP (Good Laboratory Practice)	3	Y	
Test organism				
11	Organism identity: name	n/a	Y	*Daphnia magna*
12	Latin or both Latin & common names reported?	1	Y	
13	Life cycle age / stage of test organis	1	Y	2-24 h old
14	Length and/or weight	1		N/A
15	Sex	1		N/A
16	Number of organisms per replicate	1	Y	5
17	Organism loading rate	1	N	
18	Food type and feeding periods during the acclimation period	1	Y	Fed ad libidum with algae
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	48 hours
23	Negative or positive controls (specify)	1	Y	positive & negative; positive = potassium dichromate
24	Number of replicates (including controls)	1	Y	4
25	Nominal concentrations reported?	1	Y	1
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	pH, dissolved oxygen concentration
30	Photoperiod and light intensity	1	Y	16/8 light:dark; 20 µE/cm2/s
31	Stock and test solution preparation	1	Y	100 mg of test item in 1 liter of water
32	Was solubilizer/emulsifier used, if the chemical was poorly soluble or unstable?	1	N	
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	Analytical monitoring intervals	1	N	For daphnid immobilization only.
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	Assumed there were no shading effect
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	Y	Around 7.6
42	Was temperature of the test water within the range typical for the Canadian environment (5 to 27°C)?	1	Y	Around 20

43	Was toxicity value below the chemical's water solubility?	3		N/A
Results				
44	Toxicity values (specify endpoint and value)	n/a	n/a	0% immobilization at saturation. EC50 > 100 mg/L (WAF)
45	Other endpoints reported - e.g. BCF/BAF, LOEC/NOEC (specify)?	n/a	N	
46	Other adverse effects (e.g. carcinogenicity, mutagenicity) reported?	n/a	N	
47	***Score*: ... %**	***81.1***		
48	***EC Reliability code*:**	***1***		
49	***Reliability category (high, satisfactory, low)*:**	***High Confidence***		
50	***Comments***	***The toxicity test was performed at saturation i.e., the maximum dissolved concentration of the test item that can be achieved under the test conditions. In order to make a saturated solution (i) a stock solution of 100 mg test item in one liter of water was made. (ii) The stock solution was shaken at room temperature with 20 rpm for 24 hours (rotating shaker). Undissolved particles were removed by filtration on 0.45 µm membrane. The submission states that this approach followed the guidance provided by OECD Test Series on Testing and Assessment, No. 23. The test concentration should be a saturated solution at the maximum solubility limit (15 µg/L, experimentally determined)***		