

# **Screening Assessment**

## **Aromatic Azo and Benzidine-based Substance Grouping**

## **Certain Azo Metal Complexes and Other Azo Substances**

**Environment Canada  
Health Canada**

**April 2015**

Cat. No.: En14-215/2015E-PDF  
ISBN 978-1-100-25667-2

Information contained in this publication or product may be reproduced, in part or in whole, and by any means, for personal or public non-commercial purposes, without charge or further permission, unless otherwise specified.

You are asked to:

- Exercise due diligence in ensuring the accuracy of the materials reproduced;
- Indicate both the complete title of the materials reproduced, as well as the author organization; and
- Indicate that the reproduction is a copy of an official work that is published by the Government of Canada and that the reproduction has not been produced in affiliation with or with the endorsement of the Government of Canada.

Commercial reproduction and distribution is prohibited except with written permission from the author. For more information, please contact Environment Canada's Inquiry Centre at 1-800-668-6767 (in Canada only) or 819-997-2800 or email to [enviroinfo@ec.gc.ca](mailto:enviroinfo@ec.gc.ca).

© Her Majesty the Queen in Right of Canada, represented by the Minister of the Environment, 2015.

Aussi disponible en français

## 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 four azo metal complexes and two other azo substances. These six substances constitute two subgroups of the Aromatic Azo and Benzidine-based Substance Grouping being assessed as part of the Substance Groupings Initiative of the Government of Canada's Chemicals Management Plan based on structural similarity and applications. Substances in this Grouping were identified as priorities for assessment as they met the categorization criteria under subsection 73(1) of CEPA 1999 and/or were considered as a priority based on other human health concerns.

These substances are considered together in this assessment, as they constitute the azo metal complexes subgroup and other individual azo substances that do not belong in any of the aromatic azo and benzidine-based substance subgroups. The Chemical Abstracts Service Registry Number (CAS RN)<sup>1</sup> and *Domestic Substances List* (DSL) name of the four azo metal complexes and two other azo substances are presented in the following table.

### Identity of four Azo Metal Complexes and two Other Azo Substances in the Aromatic Azo and Benzidine-based Substance Grouping

CAS RN	DSL name
6708-61-8 <sup>a</sup>	1-Triazene, 1-(4-nitro-1-naphthalenyl)-3-[4-(phenylazo)phenyl]-
63224-47-5 <sup>b</sup>	Benzenediazonium, 4-[(2,6-dichloro-4-nitrophenyl)azo]-2,5-dimethoxy-, (T-4)-tetrachlorozincate(2-) (2:1)
72391-06-1 <sup>b</sup>	Spiro[isobenzofuran-1(3H),9'(8'aH)-xanthylum], 3',6'-bis(diethylamino)-3-oxo-, chloride, compd. with [4-[(4,5-dihydro-3-methyl-5-oxo-1-phenyl-1H-pyrazol-4-yl)azo]-3-hydroxy-1-naphthalenesulfonato(3-)]chromium (1:1)
83221-38-9 <sup>a</sup>	Benzenesulfonamide, 4-[[4-[[4-(2-hydroxybutoxy)-3-methylphenyl]azo]phenyl]amino]-3-nitro- <i>N</i> -(phenylsulfonyl)-, monolithium salt
85029-57-8 <sup>b,c</sup>	Amines, C10–14-branched and linear alkyl, bis[2,4-dihydro-4-[(2-hydroxy-4-nitrophenyl)azo]-5-methyl-2-phenyl-3H-pyrazol-3-onato(2-)]chromate(1-)

---

<sup>1</sup> The Chemicals Abstract Service Registry Number (CAS RN) is the property of the American Chemical Society, and any use or redistribution, except as required in supporting regulatory requirements and/or for reports to the Government of Canada when the information and the reports are required by law or administrative policy, is not permitted without the prior, written permission of the American Chemical Society.

CAS RN	DSL name
94276-35-4 <sup>b</sup>	Xanthylum, 9-[2-(ethoxycarbonyl)phenyl]-3,6-bis(ethylamino)-2,7-dimethyl-, hydroxy[2-hydroxy-5-nitro-3-[[2-oxo-1-[(phenylamino)carbonyl]propyl]azo] benzenesulfonato(3-)]chromate(1-)

<sup>a</sup> Other Azo Substances.

<sup>b</sup> Azo Metal Complexes.

<sup>c</sup> Substance of unknown or variable composition, complex reaction product or biological material (UVCB).

All six substances in this Screening Assessment do not occur naturally in the environment. No manufacture of any substance above the 100 kg/year reporting threshold has been reported in response to any recent surveys under section 71 of CEPA 1999. One substance, CAS RN 85029-57-8, has been reported as having an import quantity above the 100 kg/year survey reporting threshold. No import or use in Canada has been identified for any of the remaining five substances (CAS RN 6708-61-8, CAS RN 63224-47-5, CAS RN 72391-06-1, CAS RN 83221-38-9 and CAS RN 94276-35-4).

All six substances in this screening assessment do not occur naturally in the environment. No manufacture of any substance above the 100 kg/year reporting threshold has been reported in response to any recent surveys under section 71 of CEPA 1999. One substance, CAS RN 85029-57-8, has been reported as having an import quantity above the 100 kg/year survey reporting threshold. No import or use in Canada has been identified for any of the remaining five substances (CAS RN 6708-61-8, CAS RN 63224-47-5, CAS RN 72391-06-1, CAS RN 83221-38-9 and CAS RN 94276-35-4).

An assessment approach based on rapid screening principles was applied to the five substances with no reported import or use in Canada to confirm that there are no sources of exposure in the environment or to the general population of Canada from these substances. The remainder of this screening assessment focuses on the one substance in commerce in Canada, CAS RN 85029-57-8.

## Environment

As part of the rapid screening assessment approach for the five substances with no identified commercial activity in Canada, generic aquatic exposure values were calculated to be below the predicted concentrations of concern for aquatic organisms. Furthermore, no information was identified by domestic or international initiatives to indicate these substances as possibly being of greater concern due to their ecological hazard properties or elevated potential for environmental release.

CAS RN 85029-57-8 has relatively low water solubility (0.002–0.5 mg/L) and is not expected to dissociate at environmentally relevant pH levels. Considering its physical and chemical properties, when released to water, CAS RN 85029-57-8 is expected to remain in the water column for a period of time before ultimately partitioning via

electrostatic interactions and sorption to suspended solids and ultimately sediments. When released to soil, it is expected to remain in that compartment.

Available experimental and modelled data regarding the abiotic and biotic degradation of CAS RN 85029-57-8 indicate that this substance is expected to persist in water, sediment and soil. In anaerobic environments (i.e., anoxic layers of sediments), there is the potential for this substance to degrade to aromatic amines as a result of cleavage of the azo bond under anaerobic or reducing conditions.

Based on limited data, CAS RN 85029-57-8 is expected to have a low bioaccumulation potential due to its low octanol–water partition coefficient and relatively high molecular weight. Read-across aquatic toxicity data suggest that CAS RN 85029-57-8 is not highly hazardous to aquatic organisms (median lethal concentrations predominantly between 3 and 10 mg/L). No data were available on toxicity to soil- and sediment-dwelling organisms.

The risk quotient analysis for CAS RN 85029-57-8 focused on exposure scenarios representing major potential environmental releases of the substance due to industrial activities. Predicted environmental concentrations (PECs) associated with releases of the substance during its use in industrial formulation activities were calculated for the aquatic environment. The PECs were not found to exceed the predicted no-effect concentrations (PNECs) for water. Due to a lack of data, no risk quotients were calculated for the soil or sediment compartments.

Considering all available lines of evidence presented in this screening assessment, there is low risk of harm to organisms and the broader integrity of the environment from the four azo metal complexes and two other azo substances evaluated in this assessment. It is concluded that these six substances do not meet the criteria under paragraphs 64(a) or 64(b) of CEPA 1999, as they are 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.

## **Human Health**

Exposure of the general population to four azo metal complexes and two other azo substances from environmental media is not expected due to limited commercial quantities in Canada; therefore risk to human health from this source is not expected.

As part of the rapid screening assessment approach for the five substances with no identified commercial activity in Canada (CAS RN 6708-61-8, CAS RN 63224-47-5, CAS RN 72391-06-1, CAS RN 83221-38-9 and CAS RN 94276-35-4), no other sources of exposure of the general population of Canada were identified. Therefore, based on current information for exposure, risk to human health is not expected for these substances. Additionally, none of these substances has been classified by any national

or international agency for hazard potential, and available information does not indicate that these substances have effects of concern based on potential carcinogenicity.

CAS RN 85029-57-8 was identified to be used in wood coatings and stains at concentrations of 2.5–10%. While dermal exposure to this substance is possible for the general population during wood coating and staining, exposure to this substance is expected to be limited for the general population of Canada. Therefore, risk to human health is considered to be low for this substance.

Based on the information presented in this screening assessment, it is concluded that the four azo metal complexes and two other azo substances evaluated in this assessment do not meet the criteria under paragraph 64(c) of CEPA 1999 as they are not entering the environment in a quantity or concentration or under conditions that constitute or may constitute a danger in Canada to human life or health.

## **Overall Conclusion**

It is concluded that the four azo metal complexes and two other azo substances evaluated in this assessment do not meet any of the criteria set out in section 64 of CEPA 1999.

# Table of Contents

<b>Synopsis</b> .....	<b>i</b>
<b>1. Introduction</b> .....	<b>1</b>
<b>2. Identity of Substances</b> .....	<b>4</b>
2.1 Selection of Analogues and Use of (Q)SAR Models .....	6
<b>3. Physical and Chemical Properties</b> .....	<b>8</b>
3.1 Melting Point and Decomposition .....	8
3.2 Solubility in Water .....	8
3.3 Octanol–Water Partition Coefficient ( $K_{ow}$ ) .....	8
3.4 Cross-sectional Diameter .....	9
3.5 Acid Dissociation Constant ( $pK_a$ ) .....	9
3.6 Vapour Pressure and Henry’s Law Constant .....	9
<b>4. Sources and Uses</b> .....	<b>11</b>
4.1 Sources .....	11
4.2 Uses .....	11
<b>5. Environmental Fate and Behaviour</b> .....	<b>13</b>
5.1 Releases to Water and Sediment .....	13
5.2 Releases to Soil .....	13
5.3 Releases to Air .....	13
5.4 Environmental Persistence .....	14
5.5 Potential for Bioaccumulation .....	15
<b>6. Assessment of the Five Substances with No Commercial Activity in Canada Based on Rapid Screening Principles</b> .....	<b>17</b>
6.1 Potential to Cause Ecological Harm .....	17
6.2 Potential to Cause Harm to Human Health .....	18
6.3 Characterization of Risk .....	18
<b>7. Screening Assessment of CAS RN 85029-57-8</b> .....	<b>18</b>
7.1 Potential to Cause Ecological Harm .....	18
7.2 Potential to Cause Harm to Human Health .....	26
<b>8. Conclusion</b> .....	<b>30</b>
<b>References</b> .....	<b>31</b>
<b>Appendices</b> .....	<b>38</b>
Appendix A: Supplementary Data Tables .....	38
Appendix B: Ecological Aquatic Exposure Calculations for the Azo Metal Complex CAS RN 85029-57-8 .....	45

## List of Tables

Table 2-1. Identity of four Azo Metal Complexes.....	4
Table 2-2. Identity of two Other Azo Substances .....	6
Table 2-3. Identities of analogues used to inform the physical and chemical properties, environmental fate and potential to cause ecological harm of substances in this assessment.....	7
Table 3-1. Summary of physical and chemical properties of CAS RN 85029-57-8 a and analogues.....	9
Table 6-1. Critical toxicity values and risk quotients for three Azo Metal Complexes and two Other Azo Substances .....	17
Table 7-1. Empirical aquatic toxicity data for analogues of CAS RN 85029-57-8.....	19



# 1. Introduction

Pursuant to sections 68 or 74 of the *Canadian Environmental Protection Act, 1999* (CEPA 1999) (Canada 1999), the Minister of the Environment and the Minister of Health conduct screening assessments of substances to determine whether these substances present or may present a risk to the environment or to human health.

The Substance Groupings Initiative is a key element of the Government of Canada's Chemicals Management Plan (CMP). The Aromatic Azo and Benzidine-based Substance Grouping consists of 358 substances that were identified as priorities for assessment, as they met the categorization criteria under section 73 of CEPA 1999 and/or were considered as a priority based on human health concerns (Environment Canada and Health Canada 2007). Some substances within this Substance Grouping have been identified by other jurisdictions as a concern due to the potential cleavage of the azo bonds, which can lead to the release of aromatic amines that are known or likely to be carcinogenic.

While many of these substances have common structural features and similar functional uses as dyes or pigments in multiple sectors, diversity within the substance group has been taken into account through the establishment of subgroups. Subgrouping based on structural similarities, physical and chemical properties, and common functional uses and applications accounts for variability within this Substance Grouping and allows for subgroup-specific approaches in the conduct of screening assessments. This Screening Assessment considers substances that belong to both the Azo Metal Complexes and Other Azo Substances subgroups. Consideration of potential azo bond cleavage products (aromatic amines) is a key element of human health assessment in each subgroup. Some aromatic amines, commonly referred to as EU22 aromatic amines<sup>2</sup>, as well as associated azo dyes, are restricted in other countries (EU 2006). Information on the subgrouping approach for the Aromatic Azo and Benzidine-based Substance Grouping under Canada's CMP, as well as additional background information and regulatory context, is provided in a separate document prepared by the Government of Canada (Environment Canada and Health Canada 2013a).

Four Azo Metal Complexes and two Other Azo Substances are considered together in this Screening Assessment, as they constitute the Azo Metal Complexes subgroup and other individual azo substances that do not belong in any of the Aromatic Azo and Benzidine-based Substance subgroups.

---

<sup>2</sup> Twenty-two aromatic amines listed in Appendix 8 of Regulation (EC) No. 1907/2006.

Another substance included in this assessment, CAS RN 63281-10-7, was previously included as part of a screening assessment, in April 2008, of 145 persistent, bioaccumulative, and inherently toxic (PBiT) substances that were considered not to be in commerce. This assessment was not updated for CAS RN 63281-10-7 as no significant new information was identified.

Screening assessments focus on information critical to determining whether substances meet the criteria as set out in section 64 of CEPA 1999, by examining scientific information to develop conclusions based on a weight of evidence approach and using precaution<sup>3</sup>.

This Screening Assessment includes consideration of information on chemical properties, environmental fate, hazards, uses and exposure, including additional information submitted by stakeholders. Relevant data were identified up to June 2013. Empirical data from key studies as well as some results from models were used to reach conclusions. When available and relevant, information presented in assessments 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.

The 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 and human health portions of this assessment have undergone external written peer review and/or consultation. Comments on the technical portions relevant to the environment were received from Dr. Harold Freeman (North Carolina State University, USA) and Dr. Gisela Umbuzeiro (University of Campinas, Brazil). Comments on the technical portions relevant to human health were received from Dr. Harold Freeman (North Carolina State University, USA), Dr. David Josephy (University of Guelph, Canada), Dr. Michael Bird (University of Ottawa, Canada) and Dr. Kannan Krishnan (University of Montreal, Canada). 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

---

<sup>3</sup> 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 is not relevant to, nor does it preclude, an assessment against the hazard criteria specified in the *Controlled Products Regulations*, which are part of the regulatory framework for the Workplace Hazardous Materials Information System for products intended for workplace use. Similarly, a conclusion based on the criteria contained in section 64 of CEPA 1999 does not preclude actions being taken under other sections of CEPA 1999 or other Acts.

of the Screening Assessment remain the responsibility of Health Canada and Environment Canada.

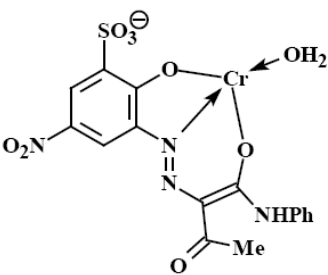
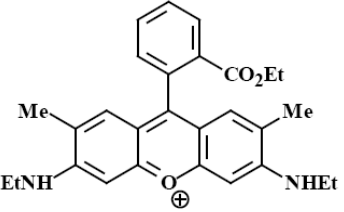
The critical information and considerations upon which the Screening Assessment is based are given below.

## 2. Identity of Substances

This Screening Assessment focuses on the four Azo Metal Complexes and two Other Azo Substances subgroups that are part of the Aromatic Azo and Benzidine-based Substance Grouping. The identities of the individual substances in this Screening Assessment are presented in Tables 2-1 and 2-2. The CAS RNs, *Domestic Substances List* (DSL) names are presented in Table 2-1 and Table 2-2, with their chemical structures or, for substances with mixed composition, up to two of the most representative structures (a and b). A list of additional chemical names (e.g., trade names) is available from the National Chemical Inventories (NCI 2012).

**Table 2-1. Identity of four Azo Metal Complexes**

CAS RN	DSL name	Chemical structure
63224-47-5	Benzenediazonium, 4-[(2,6-dichloro-4-nitrophenyl)azo]-2,5-dimethoxy-, (T-4)-tetrachlorozincate(2-) (2:1)	
72391-06-1 <sup>a</sup>	Spiro[isobenzofuran-1(3H),9'(8'aH)-xanthylium], 3',6'-bis(diethylamino)-3-oxo-, chloride, compd. with [4-[(4,5-dihydro-3-methyl-5-oxo-1-phenyl-1H-pyrazol-4-yl)azo]-3-hydroxy-1-naphthalenesulfonato(3-)]chromium (1:1)	
85029-57-8 <sup>b</sup>	Amines, C10–14-branched and linear alkyl, bis[2,4-dihydro-4-[(2-hydroxy-4-nitrophenyl)azo]-5-methyl-2-phenyl-3H-pyrazol-3-onato(2-)]chromate(1-)	<p>a.</p> <p>b. variable structure (not shown)</p>

CAS RN	DSL name	Chemical structure
94276-35-4	Xanthylium, 9-[2-(ethoxycarbonyl)phenyl]-3,6-bis(ethylamino)-2,7-dimethyl-, hydroxy[2-hydroxy-5-nitro-3-[[2-oxo-1-[(phenylamino)carbonyl]propyl]azo] benzenesulfonato(3-)]chromate(1-)	<p>a.</p>  <p>b.</p> 

<sup>a</sup> "a" is the metal ion component of the substance; "b" is the counter ion component of substance.

<sup>b</sup> Note that this is a substance of unknown or variable composition, complex reaction product or biological material (UVCB), and the structure presented is the one selected as most representative among possible structures.

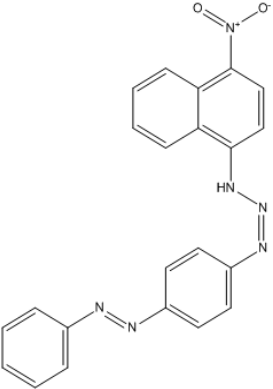
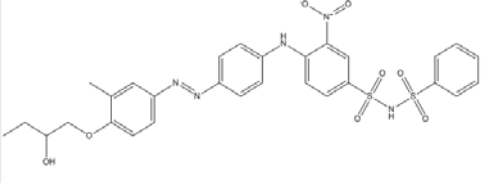
Three of the four Azo Metal Complexes contain trivalent chromium. Trivalent chromium has been assessed by the Government of Canada as part of a Priority Substances List assessment of chromium and its compounds (Canada 1994).

CAS RN 85029-57-8 is considered to be a substance of unknown or variable composition, complex reaction product or biological material (UVCB) and cannot be represented by a single chemical structure. The structure of this substance presented in Table 2-1 is considered to be the most representative among various possible structures that are not shown. The poorly defined chemical identity of this substance is due, in part, to the use of various additives and different manufacturing methods during synthesis of the material, making characterization with regard to physical-chemical properties difficult. CAS RN 85029-57-8 is a symmetrical 1:2 metal:dye complex, where the metal is chromium and the ligands are tridentate, having a non-planar structure when the ligand and metal are bound (Hunger 2003). The C10–14 branched and linear alkyl amine is considered to be present as a counterion. When considered as a metal:dye complex, CAS RN 85029-57-8 has a high molecular weight and carries an ionic charge. Dissociation of the metal:dye complex under environmental conditions would occur only under highly acidic conditions (Zollinger 2003).

The structure of CAS RN 63224-47-5 is consistent with that of a "stabilized diazonium salt," in the form of a zinc chloride double salt (Zollinger 2003). This compound is a suitable precursor for disazo dye formation via coupling with 2-naphthol and its derivatives. The structure of CAS RN 6708-61-8 is consistent with that of a "masked diazonium salt," also known as a "diazo amine" or "triazine" (Zollinger 2003). This

compound is a suitable precursor for diazo coupling with, for instance, arylamines, to give monoazo dyes.

**Table 2-2. Identity of two Other Azo Substances**

CAS RN	DSL name	Chemical structure
6708-61-8	1-Triazene, 1-(4-nitro-1-naphthalenyl)-3-[4-(phenylazo)phenyl]-	
83221-38-9	Benzenesulfonamide, 4-[[4-[[4-(2-hydroxybutoxy)-3-methylphenyl]azo]phenyl]amino]-3-nitro- <i>N</i> -(phenylsulfonyl)-, monolithium salt	

## 2.1 Selection of Analogues and Use of (Q)SAR Models

Guidance on the use of read-across approaches has been prepared by various organizations, such as the Organisation for Economic Co-operation and Development (OECD 2014). It has been applied in various regulatory programs, including the European Union's (EU) Existing Substances Programme. The general method for analogue selection and the use of (quantitative) structure–activity relationship ((Q)SAR) models is provided in Environment Canada and Health Canada (2013). For characterization of human health effects, the basis for the use of analogues and/or (Q)SAR modelling data is documented in the Health Effects Assessment section of this report.

Analogues used to inform the ecological assessment were selected based on structural similarity and the availability of relevant empirical data pertaining to physical-chemical properties, persistence, bioaccumulation and ecotoxicity. Such data were used as read-across data for those Azo Metal Complexes and Other Azo Substances that lacked empirical data, where appropriate, or to support the weight of evidence of existing empirical information. Although analogue data are used preferentially to fill data gaps for the substances in this assessment, the applicability of (Q)SAR models to dyes is determined on a case-by-case basis.

Data submitted to the New Substance Notification System (regulated under CEPA 1999) were also considered for read-across. These analogues are referred to as Substances A, B and C throughout this report, due to confidentiality of the information.

The selected analogues used in this Screening Assessment are listed in Table 2-3, with an indication of the potential read-across data available for different parameters (refer to Tables A-1-1 and A1-2 in Appendix A for more details).

**Table 2-3. Identities of analogues used to inform the physical and chemical properties, environmental fate and potential to cause ecological harm of substances in this assessment**

CAS RN	C.I. name or common name	Chemical name	Read-across to CAS RN (structure a or b, as indicated)	Experimental data to be considered in the report
1787-61-7	Mordant Black 11	3-Hydroxy-4-((1-hydroxy-2-naphthalenyl)azo)-7-nitro-1-naphthalenesulfonic acid, monosodium salt	85029-57-8 a, 94276-35-4 a and 72391-06-1 a	Ecotoxicity
5610-64-0	Acid Black 52	Chromium, 3-hydroxy-4-[(2-hydroxy-1-naphthalenyl)azo]-7-nitro-1-naphthalenesulfonic acid complex	85029-57-8 a, 94276-35-4 a and 72391-06-1 a	Ecotoxicity
NA	Substance A	NA	85029-57-8 a, 94276-35-4 a and 72391-06-1 a	MP, K <sub>ow</sub> , ecotoxicity
NA	Substance B	NA	85029-57-8 a, 94276-35-4 a and 72391-06-1 a	MP, K <sub>ow</sub> , WS, ecotoxicity
NA	Substance C	NA	85029-57-8 a, 94276-35-4 a and 72391-06-1 a	MP, K <sub>ow</sub> , WS, ecotoxicity
6300-37-4	Disperse Yellow 7	Phenol, 2-methyl-4-[[4-(phenylazo)phenyl]azo]-	6708-61-8 and 63224-47-5	Ecotoxicity

Abbreviations: K<sub>ow</sub>, octanol–water partition coefficient; MP, melting point; NA, not available; WS, water solubility

### 3. Physical and Chemical Properties

Limited experimental and modelled data are available on those physical and chemical properties of the Azo Metal Complexes and Other Azo Substances and their analogues that are relevant to their environmental fate and ecotoxicity. The primary focus is placed on CAS RN 85029-57-8, as presented on Table 3-1, although available information on the other substances is given in Tables A-2-2–A-26 of Appendix A. The relevant component of the substance (a or b) is indicated in the respective tables. Pivotal values, including either single mean data points (e.g., melting point and decomposition) or a range of values, have been chosen to represent the properties of each substance.

#### 3.1 Melting Point and Decomposition

Results indicate that four of the six substances, CAS RN 85029-57-8 (component a), CAS RN 94276-35-4 (component b), CAS RN 72391-06-1 (component a), and CAS RN 6708-61-8 have melting points in the range from 126 to < 300°C.

Component b of substance CAS RN 85029-57-8 is variable, and thus its melting point depends on what form it takes. Modelled results show that melting points for this substance are less than 134°C and that they increase with the number of carbons and amines in the structure.

#### 3.2 Solubility in Water

Based on analogue data, the water solubility of CAS RN 85029-57-8 (component a) ranges from 0.002 to 0.5 mg/L. The actual solubility of CAS RN 85029-57-8 is expected to be slightly lower than that of its analogues due to the lack of sulfonyl groups in CAS RN 85029-57-8. The only specific (non-analogue) water solubility datum available for a substance in this assessment was a qualitative description noting that CAS RN 85029-57-8 is insoluble (BASF Canada 2003).

The solubility of metal complexes can differ greatly due to differences in structure. For example, CAS RN 94276-35-4 is a 1:1 chromium complex dye and is much more water soluble than CAS RN 85029-57-8, which is a 1:2 chromium complex dye. Chromium complex dyes that occur in a 1:1 ratio are stable only at pH < 4 and tend to be more water soluble when they contain sulfonic acid groups (Hunger 2003). Chromium complex dyes that occur in a 1:2 ratio, however, are more stable and less soluble at high pH (Hunger 2003).

#### 3.3 Octanol–Water Partition Coefficient ( $K_{ow}$ )

CAS RN 85029-57-8 has a very low log  $K_{ow}$ . Log  $K_{ow}$  values for analogues of the substance range from –2.8 to –1.4. No experimental data on log  $K_{ow}$  are available for



the other substances. Furthermore, no suitable analogues were identified that had log  $K_{ow}$  data.

### 3.4 Cross-sectional Diameter

The effective cross-sectional diameter of molecules of the Azo Metal Complexes ranges from approximately 0.84 to 1.13 nm. Average effective cross-sectional diameters of molecules of the Other Azo Substances are > 1.0 nm, while average maximum diameters vary significantly. Since this parameter is important in determining the permeation of substances through biological membranes, detailed discussion on cross-sectional diameters of these substances is presented in the “Potential for Bioaccumulation” section.

### 3.5 Acid Dissociation Constant ( $pK_a$ )

No experimental  $pK_a$  data were available for these substances. Furthermore, no suitable analogues were identified that had  $pK_a$  data.

### 3.6 Vapour Pressure and Henry’s Law Constant

While experimental data are limited, Azo Metal Complexes such as CAS RN 85029-57-8 are expected to have very low vapour pressures and very low Henry’s Law constant values (Øllgaard et al. 1998).

**Table 3-1. Summary of physical and chemical properties of CAS RN 85029-57-8 a and analogues**

Property	Type of data (all conducted at 25°C)	Value(s) or range (for more than three data points)	Pivotal value(s) for this assessment (basis for selection)
Melting point and decomposition (°C)	Experimental	< 300	< 300 (sole estimated value)
Melting point and decomposition (°C)	Modelled	134 (melting point increases in the number of carbons and amines in the structure is correlated with)	134
Water solubility (mg/L)	Experimental	0.002–0.5	0.251 (mean value)
Water solubility (mg/L)	Modelled	1.946	1.946 (mean value)
Log $K_{ow}$ (dimensionless)	Experimental	-2.8 to -1.4	-2.1 (mean value)

<b>Property</b>	<b>Type of data (all conducted at 25°C)</b>	<b>Value(s) or range (for more than three data points)</b>	<b>Pivotal value(s) for this assessment (basis for selection)</b>
D <sub>min</sub> (nm)	Modelled	0.84	0.84 (sole estimated value)
D <sub>max</sub> (nm)	Modelled	1.09	1.09 (sole estimated value)
pK <sub>a</sub> (dimensionless)	Experimental	NA	NA

Abbreviations: D<sub>max</sub>, effective maximum cross-sectional diameter; D<sub>min</sub>, effective minimum cross-sectional diameter; NA, not available; pK<sub>a</sub>, acid dissociation constant

## 4. Sources and Uses

### 4.1 Sources

All Azo Metal Complexes and Other Azo Substances are anthropogenically produced and are not expected to occur naturally in the environment.

Based on the information submitted in the recent surveys (2005–2011) issued pursuant to section 71 of CEPA 1999, only CAS RN 85029-57-8 was identified to be imported commercially and used in Canada, in the Paints and Coatings Sector. Fewer than four companies reported a combined import total of 100–1000 kg/year for this substance. The other five substances in this screening assessment are not known to be in commerce in Canada above the section 71 survey reporting thresholds (Environment Canada 2012).

CAS RN 85029-57-8 and CAS RN 63224-47-5 are identified as low production volume (LPV) substances in other countries, according to Substances in Preparations in Nordic Countries (SPIN), the *Toxic Substances Control Act* (TSCA) of the United States and the European Chemical Substances Information System (ESIS). The other four substances were below the LPV trigger quantity (less than one metric ton per year).

### 4.2 Uses

CAS RN 85029-57-8 was identified as being in commerce in Canada for use in wood coatings based on recent section 71 surveys (Environment Canada 2012). It has also been identified as being in use in Canada in automotive coatings (PPG Industries Inc. 2012) and in printing inks (BASF Canada 2012). No uses have been identified for the remaining five substances.

CAS RN 85029-57-8 is present in several wood coatings in the United States (Sherwin-Williams 2013), Germany (Akzo Nobel Deco GmbH 2010) and Finland (Tikkurila Oyj 2010). It is also present in some paints in Germany (MIPA AG 2012) and in automotive paints in the United States (PPG Industries Inc. 2012). It is used in some printing inks in the United States (BASF 2012), as well as for correction pens in the Czech Republic (AGFA 2007).

In Canada, food colouring agents are regulated as food additives under the *Food and Drug Regulations*. Colours that are permitted for use in food are listed in the *List of Permitted Colouring Agents* incorporated by reference in the *Marketing Authorization for Food Additives That May Be Used as Colouring Agents*, issued under the authority of the *Food and Drugs Act*. None of the six substances in this screening assessment are listed on the *List of Permitted Colouring Agents* as permitted food colouring agents or identified as being used in food packaging applications (July and September 2011 emails from the Food Directorate, Health Canada to the Risk Management Bureau, Health Canada, unreferenced).

Colouring agents permitted to be used in drugs in Canada are regulated under Part C, Division 1 of the *Food and Drug Regulations* (Canada [1978]). None of the substances in this subgroup is listed as a permitted colouring agent in drugs nor have any been identified to be present in pharmaceuticals, veterinary drugs or biologics (August 2011 email from the Therapeutic Products Directorate, Health Canada to the Risk Management Bureau, Health Canada; unreferenced; June 2011 email from the Veterinary Drugs Directorate, Health Canada to the Risk Management Bureau, Health Canada; unreferenced; June 2011 email from the Biologics and Genetic Therapies Directorate, Health Canada to the Risk Management Bureau, Health Canada; unreferenced) in Canada.

None of the substances in this assessment are listed in the Natural Health Products Ingredients Database (NHPID) as an ingredient for use in natural health products and are not listed in the Licensed Natural Health Products Database (LNHPD) to be present in currently licensed natural health products (NHPID 2011; LNHPD 2011).

Based on notifications submitted under the *Cosmetic Regulations* to Health Canada, none of the substances in this Screening Assessment are used in certain cosmetic products in Canada (2011 and 2013 emails from the Consumer Product Safety Directorate, Health Canada, to the Existing Substances Risk Assessment Bureau, Health Canada; unreferenced). These substances are not included on the List of Prohibited and Restricted Cosmetic Ingredients (more commonly referred to as the Cosmetic Ingredient Hotlist or simply the Hotlist), an administrative tool that Health Canada uses to communicate to manufacturers and others that certain substances, when present in a cosmetic, may contravene the general prohibition found in section 16 of the *Food and Drugs Act* or a provision of the *Cosmetic Regulations* (Health Canada 2011).

None of these six substances was identified as being present in pest control products registered in Canada (June 2011 email from the Pest Management Regulatory Agency, Health Canada to the Risk Management Bureau, Health Canada; unreferenced). In addition, no uses of the Azo Metal Complexes or Other Azo Substances were identified for military applications in Canada (July 2011 email from the Department of National Defence to the Risk Management Bureau, Health Canada; unreferenced).

According to use quantities of these substances in other countries (SPIN, TSCA and ESIS), CAS RN 85029-57-8 and CAS RN 63224-47-5 were LPV substances. The other four substances were below LPV trigger quantities.

## 5. Environmental Fate and Behaviour

The environmental fate of chemicals describes the processes by which they move and are transformed in the environment. As explained in Environment Canada and Health Canada (2013), the Equilibrium Criterion model or EQC (EQC 2011) is not applicable for many Aromatic Azo and Benzidine-based Substances, as they do not fall under the model domain. In this section, some general characteristics of Azo Metal Complexes and Other Azo Substances are described in an effort to understand their environmental fate, distribution, persistence and bioaccumulation in organisms.

### 5.1 Releases to Water and Sediment

When released to water, Azo Metal Complexes and Other Azo Substances are not expected to hydrolyse, nor are they likely to evaporate from the surface, due to their low vapour pressures and Henry's Law constants. The substances are expected to remain in the water column for a period of time before partitioning, via electrostatic interactions and sorption, to suspended solids and ultimately sediments, where they may bind reversibly and become resuspended over time or where they may bind irreversibly and remain buried. If released into wastewater, these substances are expected to be adsorbed during the wastewater treatment process (ETAD 1995).

Other factors, such as increasing molecular size, water hardness and salinity and decreasing pH, are thought to favour some sorption of azo dyes to suspended solids (HSDB 1983– ; Øllgaard et al. 1998). It has been stated generally that, due to the recalcitrant nature of azo dyes in aerobic environments, they eventually end up in anaerobic sediments, shallow aquifers and groundwater (Razo-Flores et al. 1997).

### 5.2 Releases to Soil

Azo Metal Complexes and Other Azo Substances may be released indirectly to soil via the application of wastewater biosolids to agricultural land or deposition in landfills. These types of substance tend to be strongly adsorbed to sludges and are not easily released to become biologically available (other than direct ingestion of the biosolids by organisms) (ETAD 1995).

### 5.3 Releases to Air

Azo Metal Complexes and Other Azo Substances are not expected to be released to air or to partition to this compartment due to their very low vapour pressures and Henry's Law constants (Øllgaard et al. 1998).

Given their low levels of volatility and physicochemical preference for partitioning to other media, it is also not expected that these substances will be subject to long-range atmospheric transport.

## 5.4 Environmental Persistence

In order to characterize the environmental persistence of Azo Metal Complexes and Other Azo Substances, empirical and modelled data for these substances were considered under both aerobic and anaerobic conditions.

No empirical biodegradation data related to the persistence of Azo Metal Complexes and Other Azo Substances were found. Substances with read-across data available for persistence were not deemed to have enough structural similarity to be used for read-across.

A (Q)SAR-based weight of evidence approach (Environment Canada 2007) was applied using biodegradation models. These models are considered acceptable for use, as they are based on chemical structure, and the azo structure is represented in the training sets of all the BIOWIN models used, thereby increasing the reliability of the predictions.

All of the model outputs for Azo Metal Complexes and Other Azo Substances (BIOWIN Submodels 3–6 and CATALOGIC) consistently predicted that these substances would biodegrade slowly in water, soil and sediment under aerobic conditions (Appendix A, Table A-3). These results are consistent with information included in Environment Canada and Health Canada (2013), which outlines the general persistence of azo dyes in aerobic environments.

All model results from AOPWIN (2010) indicate that Azo Metal Complexes and Other Azo Substances are not expected to persist in air. Half-lives for these substances ranged from 0.01 to 0.73 day.

Modelled persistence data for these substances in aerobic environments show little to no biodegradation in the time scale of the studies. This is consistent with the understanding that these dyes must be chemically stable in order to be effective in their applications (Øllgaard et al. 1998). Azo Metal Complexes and Other Azo Substances are expected to biodegrade slowly under aerobic conditions.

Under anaerobic conditions, azo substances are likely to undergo biodegradation by microbial agents, resulting in the cleavage of the azo bond and the formation of aromatic amines (Brown and Hamburger 1987; Øllgaard et al. 1998). In a study by Brown and Hamburger (1987), the biodegradation of azo dyes under anaerobic conditions was examined. Mordant Black 11 achieved 99% degradation in 7 days in an anaerobic environment. However, the presence of a metal complex in azo substances has been proven to prevent the reduction of the azo bond in this manner (Deb et al. 2011).

The majority of the Azo Metal Complexes and Other Azo Substances do not contain functional groups expected to undergo hydrolysis. This is consistent with published studies that note hydrolysis as being an insignificant factor in the cleavage of azo

compounds (Baughman and Perenich 1988). However, one substance (CAS RN 94276-35-4) contained an amide functional group that was flagged by EPI Suite (2012) as having the potential to undergo some degree of hydrolysis.

Due to the persistence of Azo Metal Complexes and Other Azo Substances in aerobic environments in combination with their moderate water solubility, it is expected that these substances will have relatively long residence times in water. As these substances are predicted to stay in the water for long periods of time, they may disperse widely from point sources of release. Eventually, due to electrostatic interactions with negatively charged particulate matter, they will be deposited to sediment, where they will persist under aerobic conditions and remain a source of exposure to organisms until buried due to sedimentation. Deeper layers of sediment are likely under anaerobic conditions, which will transform (reduce) the dyes via azo hydrolysis. Exposure of the benthos under anaerobic conditions is not expected to be significant. Short residence times in air are expected to result in low potential for long-range atmospheric transport.

## 5.5 Potential for Bioaccumulation

In this assessment, various lines of evidence have been investigated to determine the bioaccumulation potential of the Azo Metal Complexes and Other Azo Substances. Due to the general lack of information on the bioaccumulation potential of these substances, this section will focus on CAS RN 85029-57-8. The use of (Q)SAR bioaccumulation modelling was not pursued, since these substances were outside the model domains of applicability.

As indicated in Table 3-1, CAS RN 85029-57-8 has relatively low water solubility (0.002–0.5 mg/L). Experimental log  $K_{ow}$  data were limited to read-across data for CAS RN 85029-57-8, with values ranging from  $-2.8$  to  $-1.4$ . The above suggests that CAS RN 85029-57-8 may have a low bioaccumulation potential according to equilibrium partitioning theory.

No bioconcentration factor (BCF) values were found for CAS RN 85029-57-8. Furthermore, no suitable analogues were identified that had BCF data for read-across.

In terms of bioaccumulation, it is also useful to consider molecular size and cross-sectional diameter, which are parameters commonly used by international jurisdictions in weight of evidence conclusions on bioaccumulation potential. For example, ECHA (2012) showed that some additional indicators for low bioaccumulation potential might be applicable for substances with low solubility in *n*-octanol and water. In particular, a maximum cross-sectional diameter ( $D_{max}$  average) of  $> 1.7$  nm may be considered as one of these additional indicators.

Investigations relating fish BCF data to 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  $D_{\max}$  is above ~1.5 nm, and much more so for molecules having a  $D_{\max}$  of > 1.7 nm. Sakuratani et al. (2008) 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 (i.e., BCF < 5000) often have a  $D_{\max}$  of > 2.0 nm and an effective diameter ( $D_{\text{eff}}$ ) of > 1.1 nm. Anliker et al. (1981) also proposed that a second largest cross-section of > 1.05 nm with a molecular weight of > 450 would suggest a lack of bioconcentration for organic colourants. Therefore,  $D_{\text{eff}}$  values of > 1.05–1.1 nm and  $D_{\max}$  values of > 1.5–1.7 nm can be considered indicators of a reduced rate of uptake from water. A reduced rate of uptake allows other internal elimination processes, such as metabolism and fecal egestion, to reduce the overall burden of chemical in the tissues of organisms, reducing bioaccumulation on a whole-body basis.

Due to the lack of empirical bioaccumulation data available for CAS RN 85029-57-8, available data on water solubility, molecular weight and cross-sectional diameter are considered in order to determine the bioaccumulation potential of this substance.

CAS RN 85029-57-8 was found to have effective cross-sectional diameters that ranged from 0.84 nm ( $D_{\min}$ ) to 1.09 nm ( $D_{\max}$ ) (Table 3-1). The molecular weight of this substance is not known due to its UVCB nature; however, the molecular weight of this substance is relatively high (> 400 g/mol), which may slow the uptake of the substance into biological organisms. The small cross-sectional diameters for this substance would likely not be a factor in restricting its rate of uptake when crossing cell membranes.

It should, however, be noted that according to Arnot et al. (2010), there are some uncertainties associated with the thresholds proposed by Dimitrov et al. (2002, 2005) and Sakuratani et al. (2008), as the bioaccumulation studies used to derive them were not always critically evaluated. Arnot et al. (2010) pointed out that 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 uptake = slow elimination). 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. However, if the rate of gill uptake is sufficiently mitigated by steric hindrance to the point where the rate of elimination exceeds the rate of uptake, bioconcentration will be decreased.

CAS RN 85029-57-8, based on limited data, is expected to have a low bioaccumulation potential due to its low log  $K_{\text{ow}}$  and relatively high molecular weight.



## 6. Assessment of the Five Substances with No Commercial Activity in Canada Based on Rapid Screening Principles

As a result of a survey conducted under section 71 of CEPA 1999 (Canada 2011), none of these five Azo Metal Complexes and Other Azo Substances (CAS RN 6708-61-8, CAS RN 63224-47-5, CAS RN 72391-06-1, CAS RN 83221-38-9 and CAS RN 94276-35-4) is manufactured, imported or used in Canada. These substances are also not expected to occur naturally. A rapid screening-type assessment approach was therefore applied to evaluate these five substances. This modified approach adheres to the rapid screening approach previously applied by Health Canada and Environment Canada to confirm low risk to the environment or to human health (Environment Canada, Health Canada 2013b, 2014). This section summarizes the critical information and considerations that served as the basis for this evaluation.

### 6.1 Potential to Cause Ecological Harm

The ecological component of the rapid screening approach consists of multiple steps that address different factors relating to the potential for a substance to cause ecological harm. The first step in the ecological approach involves applying different generic scenarios or fate models to estimate environmental exposure. Two generic aquatic exposure scenarios, industrial and residential, were applied to identify potential concerns near the point of discharge of a substance to the environment. A risk quotient (RQ) analysis followed, which involved comparing conservative (i.e., ecologically protective) estimates of exposure in receiving waters (predicted environmental concentration [PEC]) with an effects threshold (predicted no-effects concentration [PNEC]) to evaluate whether a chemical is expected to cause harm to the local aquatic environment. The effects thresholds were a combination of ecotoxicity data for analogues and categorization data. Results of the RQ analysis (PEC divided by the PNEC) are presented in Table 6-1. RQs exceeding 1 would be indicative of ecological concern; however, RQs were significantly below 1 for all five substances when using the industrial release scenario (scenario A) and the residential release scenario (scenario B).

**Table 6-1. Critical toxicity values and risk quotients for three Azo Metal Complexes and two Other Azo Substances**

CAS RN	CTV (mg/L)	RQ (industrial release scenario)	RQ (residential release scenario)
6708-61-8	0.025 <sup>a</sup>	0.25	0.11
63224-47-5	0.025 <sup>a</sup>	0.25	0.11
72391-06-1	0.4 <sup>a</sup>	0.02	0.01
83221-38-9	0.65 <sup>b</sup>	0.01	< 0.00
94276-35-4	0.4 <sup>a</sup>	0.02	0.01

Abbreviation: CTV, critical toxicity value; RQ, risk quotient

<sup>a</sup> CTV derived from analogue data.

<sup>b</sup> CTV derived from categorization data.

A substance-specific evaluation was then conducted to determine whether any of the substances have elevated ecological hazard profile or a high potential for environmental release that may not have been adequately addressed using the generic exposure scenarios. No information from national or international initiatives was found that identified these substances as possibly being of greater concern due to their ecological hazard properties or elevated potential for environmental release.

## **6.2 Potential to Cause Harm to Human Health**

None of these five substances has been classified by any national or international agencies as having effects of concern based on potential carcinogenicity. No health effects studies were identified for these substances except for one on “Fast Dark Blue Salt,” which corresponds to the diazo compound identified by CAS RN 63224-47-5 (Kundu 1977). No empirical data on concentrations of the five substances in environmental media in Canada or elsewhere were identified. Due to the relatively low volatility and water solubility of Azo Metal Complexes in general, this type of substance is expected to be absorbed onto soil and sediments when released to the environment and not to partition into water. In addition, due to the very low expected vapour pressures of these substances, inhalation of the volatile fraction via air is not expected to be a significant route of exposure. However, no information was submitted in the recent surveys (2005–2011) issued pursuant to section 71 of CEPA 1999 to indicate activity of these substances in Canada above the reporting threshold of 100 kg/year (Environment Canada 2012). Therefore, overall exposure to any of the five substances for the general population of Canada via environmental media is not expected. In addition, direct exposure to any of the five substances is not expected, considering no uses of these substances in Canada were identified. Therefore, risk to human health is not expected.

## **6.3 Characterization of Risk**

Based on the information presented above, these five substances, CAS RN 6708-61-8, CAS RN 63224-47-5, CAS RN 72391-06-1, CAS RN 83221-38-9 and CAS RN 94276-35-4, are not posing a risk to organisms or the broader integrity of the environment or the general population of Canada.

# **7. Screening Assessment of CAS RN 85029-57-8**

## **7.1 Potential to Cause Ecological Harm**

### **7.1.1 Ecological Effects Assessment**

Empirical data for CAS RN 85029-57-8 and its analogues were considered for the assessment of the ecological effects of CAS RN 85029-57-8, given the high level of

uncertainty associated with modelling the ecotoxicity of this substance as well as the physical and chemical properties used as inputs for the models (e.g., log  $K_{ow}$ ).

### Aquatic Compartment

The majority of empirical acute aquatic toxicity values for CAS RN 85029-57-8 were below 10 mg/L (Table 7-1). Confidential data received through New Substance Notifications for close analogues to CAS RN 85029-57-8 spanned the range of available toxicity data. Among the more sensitive studies were a 72-hour median effective concentration ( $EC_{50}$ ) immobilization study on *Daphnia magna* and a 96-hour median lethal concentration ( $LC_{50}$ ) study on rainbow trout. Both toxicity tests were conducted on Substance C.

Among the lowest and most reliable of these values are those from studies by Little and Lamb (1973) and Little et al. (1974) on fathead minnows, *Pimephales promelas*. These bioassays were carried out according to published standard methods and evaluated lethal concentrations of various dyes over 24-, 48- and 96-hour periods. The studies yielded  $LC_{50}$  values of 6–7 mg/L for two key analogues of the chromium-containing substances, Mordant Black 11 and Acid Black 52.

Material Safety Data Sheets for chromium-based azo dyes indicate that these substances are very toxic to aquatic organisms. BASF Canada (2012) reported an  $EC_{50}$  of 0.1–1 mg/L for a 48-hour bioassay of Orasol (formerly Neozapon) Red 395, a substance that consists of CAS RN 85029-57-8 and another similar compound. An  $EC_{50}$  value of 0.21 mg/L was reported for the same compound (BASF Canada 2003). However, given that the full study for either toxicity test was not available, the reliability of these data could not be verified.

Whether chromium has an effect on the observed ecotoxicity of these substances remains unknown. It has been shown for some substances that the addition and identity of the metal have no effect on the ecotoxicity of the substance; for other substances, however, the metal complex enhances the toxicity of the substance (Freeman et al. 1999).

**Table 7-1. Empirical aquatic toxicity data for analogues of CAS RN 85029-57-8**

CAS RN C.I. name	Test organism	Test duration (h)	Endpoint	Value (mg/L)	Reference
1787-61-7 Mordant Black 11	Fathead minnow <i>Pimephales promelas</i>	24	$LC_{50}$	10	Little et al. 1974
1787-61-7 Mordant	Fathead minnow <i>Pimephales</i>	48	$LC_{50}$	6 <sup>a</sup>	Little et al. 1974

CAS RN C.I. name	Test organism	Test duration (h)	Endpoint	Value (mg/L)	Reference
Black 11	<i>promelas</i>				
1787-61-7 Mordant Black 11	Fathead minnow <i>Pimephales promelas</i>	96	LC <sub>50</sub>	6 <sup>a</sup>	Little et al. 1974
1787-61-7 Mordant Black 11	Fathead minnow <i>Pimephales promelas</i>	96	LC <sub>50</sub>	6 <sup>a</sup>	Little and Lamb 1973
5610-64-0 Acid Black 52	Fathead minnow <i>Pimephales promelas</i>	24	LC <sub>50</sub>	7	Little et al. 1974
5610-64-0 Acid Black 52	Fathead minnow <i>Pimephales promelas</i>	48	LC <sub>50</sub>	6.2	Little et al. 1974
5610-64-0 Acid Black 52	Fathead minnow <i>Pimephales promelas</i>	96	LC <sub>50</sub>	6.2	Little et al. 1974
5610-64-0 Acid Black 52	Fathead minnow <i>Pimephales promelas</i>	96	LC <sub>50</sub>	7	Little and Lamb 1973
Substance A	<i>Daphnia magna</i>	24	EC <sub>50</sub> (immobilization)	480.7	Confidential information
Substance A	Carp ( <i>Cyprinus carpio</i> )	96	LC <sub>50</sub>	> 1200	Confidential information
Substance B	<i>Daphnia magna</i>	48	EC <sub>50</sub> (immobilization)	> 100	Confidential information
Substance B	Rainbow trout <i>Oncorhynchus mykiss</i>	48	LC <sub>50</sub>	100	Confidential information
Substance C	<i>Daphnia magna</i>	72	EC <sub>50</sub> (immobilization)	1.7	Confidential information
Substance C	Rainbow trout <i>Oncorhynchus mykiss</i>	96	LC <sub>50</sub>	0.4	Confidential information
Substance C	Fathead minnow <i>Pimephales promelas</i>	96	LC <sub>50</sub>	37.0	Confidential information

Abbreviations: C.I. Colour Index; EC<sub>50</sub>, the concentration of a substance that is estimated to cause some effect on 50% of the test organisms; LC<sub>50</sub>, the concentration of a substance that is estimated to be lethal to 50% of the test organisms

<sup>a</sup> Value used as CTV. Robust study summaries were conducted to determine the quality of the studies and are available upon request.

## **Derivation of Aquatic Predicted No-Effect Concentration (PNEC)**

Analogue substances A, B and C were the closest in structural similarity to CAS RN 85029-57-8 (with Substances A and B being more structurally similar to CAS RN 85029-57-8 than Substance C). However, for this assessment, the PNEC was not calculated from the lowest 96-hour LC<sub>50</sub> value of 0.4 mg/L for rainbow trout, because the study contains confidential information that was received through a New Substance Notification and therefore is not readily available to readers.

Instead, ecotoxicity data for Acid Black 52 and Mordant Black 11 were chosen as read-across data for CAS RN 85029-57-8, since both share chemical structural similarity with CAS RN 85029-57-8 and have reliable ecotoxicity information available. The 96-hour LC<sub>50</sub> of 6 mg/L for fathead minnows (Little et al. 1974) was selected as the CTV because it was the most sensitive valid experimental value available for review.

A PNEC was derived by dividing the CTV by an assessment factor of 100 (to account for interspecies and intraspecies variability in sensitivity and to estimate a long-term no-effects concentration from a short-term LC<sub>50</sub>), to give a value of 0.06 mg/L.

## **Other Environmental Compartments**

No empirical studies were found on the toxicity of CAS RN 85029-57-8 to soil or sediment-dwelling organisms. Therefore, no soil or sediment PNEC was calculated for this assessment.

## **Summary of Ecological Effects**

Based on lines of evidence involving empirical and read-across aquatic toxicity data, it is concluded that CAS RN 85029-57-8 may be hazardous to aquatic organisms at low concentrations.

### **7.1.2 Ecological Exposure Assessment**

#### **Releases to the Environment**

CAS RN 85029-57-8 was not manufactured in Canada for the 2010 calendar year according to a survey issued pursuant to section 71 of CEPA 1999 (Environment Canada 2012). The substance was identified as being imported and formulated into paints and coatings used for automotive parts and wood. As no data on measured environmental concentrations (in water, soil or sediment) for this substance in Canada (or elsewhere) have been identified, environmental concentrations were estimated from available information.

Anthropogenic releases of a substance to the environment depend upon various losses that occur during the manufacture, industrial use, consumer or commercial<sup>4</sup> use and disposal of a substance. Factors relevant to key life cycle stages of these substances have been considered, uncertainties have been recognized and assumptions have been made, subject to the availability of information. Exposure scenarios for the uses or media of concern have been developed, including the determination of applicable PECs.

### **Identification of Important Exposure Scenarios**

Exposure characterization is focused on important exposure scenarios. These scenarios represent major environmental releases and relatively high concentrations. In general, the magnitude of releases is a direct function of the quantity of a substance manufactured or used and its applicable emission factors. In cases where industrial releases are similar in quantity to consumer and/or commercial releases, the former normally results in higher environmental concentrations than the latter. This is in part because industrial releases are concentrated at a limited number of sites, while consumer and/or commercial releases are dispersed across the country.

CAS RN 85029-57-8 was imported into Canada and formulated into paints and coatings for use on automotive parts and wood. The use of the formulated paints/coatings on automotive parts and wood was expected to be more dispersive than the formulation and to yield lower environmental concentrations. The formulation was therefore considered as the principal exposure scenario and selected for a quantitative analysis.

### **Estimates for Predicted Environmental Concentrations (PECs)**

The PECs for CAS RN 85029-57-8 were estimated for the formulation of paints and coatings. These concentrations are based on available information on the quantities of the substance, sector-specific emission factors for emissions to wastewater, characteristics of the wastewater treatment systems involved and characteristics of the receiving environments. A detailed explanation of the exposure calculations as well as assumptions used is given in Appendix B.

While it is expected that CAS RN 85029-57-8 will eventually partition to biosolids during publically-owned wastewater treatment or to sediment after it is released to receiving water, the water column is expected to be the major compartment of environmental concern. Thus, PECs were not calculated for sediment or biosolids-amended soil.

---

<sup>4</sup> Commercial use is the use of a chemical substance, or the use of a mixture, product or manufactured item containing a chemical substance, in a commercial enterprise providing saleable goods or services.

The aquatic PECs of the substance were estimated according to its quantities used in the formulation of paints and coatings, found from a survey issued pursuant to section 71 of CEPA 1999 (Canada 2011). The total import quantity of the substance was between 100 and 1000 kg for the 2010 calendar year. This quantity was distributed and used in the formulation of paints and coatings across various facilities.

Ten facilities that formulated the substance into paints and coatings were identified from the survey. The 10 facilities were located in 10 different municipalities in British Columbia, Ontario and Quebec. These municipalities are referred to as sites in this assessment, as they each represent a common point of entry to the environment via a wastewater treatment system.

The survey data were not sufficient for determining which facilities were involved with the substance when a survey respondent was found to operate multiple facilities. These multiple facilities were identified based on Environment Canada's National Pollutant Release Inventory database (NPRI 2006). When a respondent cited use at multiple facilities, each of these facilities was conservatively assumed to use the substance at an annual quantity equal to the total annual quantity reported by the respondent.

The aquatic PEC from each of the 10 facilities was estimated based on the use quantity at each facility, an emission factor for emissions to wastewater, on-site and off-site wastewater treatment removal efficiencies and dilution provided by both wastewater and receiving water. The use quantity at each facility was between 10 and 1000 kg/year, according to the survey data.

The emission factor used was 0.3%, which was found from an analysis of industry data as a loss from the cleaning of paint/coating formulation equipment (Environment Canada 2012). This value is in line with the range of 0.25–0.5% loss to wastewater from equipment residue estimated in an emission scenario document on coatings produced by the OECD (2009).

The on-site wastewater treatment removal efficiency was approximated as 90% from literature data (OECD 2009), considering the substance is sparsely soluble in water (water solubility below 1 mg/L) and solids settling tanks are common at paint/coating formulation facilities.

The off-site wastewater treatment removal efficiency was conservatively assumed to be 0%, considering the substance is not likely to partition to sludge, is not volatile and lacks biodegradation data.

The wastewater flow of the local wastewater treatment system identified at each formulation site was used to determine the concentrations of the substance in influent and effluent. Dilution was considered in the determination of the concentration in effluent in the case of lagoons because of their long hydraulic retention times.

An appropriate dilution factor of the receiving water was then used to derive the aquatic PEC from the concentration in effluent near the discharge point.

The calculated PECs were considered to be realistic estimates for aquatic exposure because they were based on actual use quantities and realistic emission factors. They ranged from 0.0001 to 1.1 µg/L.

### **7.1.3 Ecological Risk Characterization**

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 RQ analysis, as well as information on persistence, bioaccumulation, ecological effects, sources, fate of the substance and presence and distribution in the environment. Various lines of evidence are summarized below, along with relevant uncertainties leading to overall conclusions.

The presence of trivalent chromium in this substance is not expected to be an ecological concern. Chromium and its compounds have been previously assessed under the *Canadian Environmental Protection Act* (Canada 1994). Furthermore, it is unlikely that this substances (and above chromium containing substances) —all of which are believed to have very little or no commercial presence at this time—will become significant contributors to the total chromium concentration in the environment relative to other sources of release of chromium.

#### **Risk Quotient Analysis**

An RQ analysis was conducted by comparing the aquatic PEC value (obtained from the relevant exposure scenario) with the aquatic PNEC (extrapolated from the ecotoxicity data).

The aquatic PEC resulting from each of 10 mills was estimated from a number of parameters, as mentioned above, including quantities used in the formulation of paints and coatings found from a survey issued pursuant to section 71 of CEPA 1999 (Canada 2011), the emission factor for emissions to wastewater, the wastewater treatment flow and removal, and the receiving water dilution factor. Given that some key factors remain unknown, the overall predictions were based on conservative assumptions.

The PECs from the mills ranged from 0.0001 to 1.1 µg/L and were well below the PNEC value of 60 µg/L. Furthermore, if the more conservative toxicity value of 0.4 mg/L for rainbow trout (resulting PNEC would have been 4 µg/L) had been used, the PEC would still be well below the PNEC at all sites. The RQ analysis outcome suggests that there is limited potential for the environmental releases of CAS RN 85029-57-8 to cause adverse effects on aquatic organisms in the environment.



## Characterization of Ecological Risk

Release of CAS RN 85029-57-8 from use in the formulation of paints and coatings to the aquatic environment via wastewater treatment plants and to soil via biosolids application is expected. No releases are expected to air, where, due to its very low expected vapour pressure and Henry's Law constant, the substance is not expected to remain, and long-range atmospheric transport is not a concern.

CAS RN 85029-57-8 has relatively low water solubility (< 1 mg/L) and is not expected to dissociate at environmentally relevant pH levels. When released to water, CAS RN 85029-57-8 is expected to remain in the water column for a period of time before partitioning, via electrostatic interactions and sorption, to suspended solids and ultimately sediments. When released to soil, it is expected to remain in that compartment.

No BCF and limited log  $K_{ow}$  data for CAS RN 85029-57-8 were found. While the small cross-sectional diameter for this substance would likely not be a factor in restricting its rate of uptake when crossing cell membranes, its higher molecular weight may slow its uptake into biological organisms. Bioaccumulation resulting from exposures of organisms to this substance in soil and sediment is not well understood due to minimal and limited data. Due to the low log  $K_{ow}$  for CAS RN 85029-57-8, this substance is not believed to readily bioaccumulate.

According to modelled data, CAS RN 85029-57-8 is expected to biodegrade very slowly in aerobic environments and is therefore considered to be persistent in water, sediment and soil, according to the *Persistence and Bioaccumulation Regulations*.

Based on the available empirical and analogue aquatic toxicity data, CAS RN 85029-57-8 is expected to be hazardous to aquatic organisms at low concentrations (most acute toxicity values below 10 mg/L). No toxicity data were available for other substances in this assessment, nor were any ecotoxicity data for soil- and sediment-dwelling organisms found.

An RQ analysis was performed for the release of CAS RN 85029-57-8 from its use in the formulation of paints and coatings. This sector was anticipated to present the highest potential ecological risk related to industrial releases to the environment for this substances. RQ analysis showed that conservative PECs for CAS RN 85029-57-8 released from 10 facilities across Canada were well below the PNEC calculated for aquatic organisms. Due to the paucity of soil and sediment toxicity data and the fact that water is believed to be the primary medium of concern, an RQ was not calculated for these compartments.

Based on all lines of evidence presented, CAS RN 85029-57-8 is unlikely to cause ecological harm in Canada.

## **Uncertainties in Evaluation of Ecological Risk**

The substances addressed in this report are data poor. As a result, a read-across approach using data from selected analogues was the best alternative to estimating physical and chemical properties. The availability of structural analogues was lacking, which led to the use of some analogues for read-across purposes that were not ideal in terms of structural similarity, which further increases the uncertainty.

Long-term (chronic) toxicity data would be beneficial in evaluating these substances due to the fact that the substances are predicted to be persistent in the environment, but the availability of such data is minimal. The use of an assessment factor of 100 in determining an aquatic PNEC is intended to address this uncertainty. While the soil and sediment exposure media are most likely the ultimate destination for these substances, no data were available on toxicity to soil- or sediment-dwelling organisms, and no RQs for soil or sediment were calculated.

The lack of measured environmental concentrations of these substances (e.g., monitoring data) in Canada resulted in the need to evaluate risk based on predicted concentrations in water near industrial point sources. Conservative assumptions were made when using models to estimate concentrations in receiving water bodies.

## **7.2 Potential to Cause Harm to Human Health**

### **7.2.1 Exposure Assessment**

No empirical data on concentrations of CAS RN 85029-57-8 in environmental media in Canada or elsewhere were identified. Due to its relatively low volatility and water solubility, this substance is expected to be absorbed onto soil and sediments when released to the environment and not to partition into water. In addition, due to the very low expected vapour pressure of this substance, inhalation of the volatile fraction via air is not expected to be a significant route of exposure (refer to Environmental Fate and Behaviour chapter). Therefore, general population exposure to CAS RN 85029-57-8 from environmental media is not expected.

CAS RN 85029-57-8 was identified to be used in wood coatings and stains in Canada, where concentrations ranging from 2.5% to 10% are expected, based on German product information (Akzo Nobel Deco GmbH 2010). While dermal exposure to CAS RN 85029-57-8 is possible for the general population during the application of the product containing this substance to a wooden deck or to wooden furniture, potential exposure to this substance via the dermal route for the general population of Canada is expected to be limited. In determining the exposure to be limited, a number of parameters were considered, including 1) the physical and chemical properties of the substance, such as its large molecular size and charge, which indicate limited potential for dermal absorption, 2) its limited dissociation potential in the application media (formulations for wood coatings and stains) as well as its stability under ambient conditions, which

indicate limited bioavailability, and 3) limited direct contact with the hands during application of the product.

Based on the information available, exposure to CAS RN 85029-57-8 for the general population of Canada is not expected via environmental media and exposure is expected to be limited via use in wood coatings and stains.

## 7.2.2 Health Effects Assessment

Limited empirical toxicity data were identified for evaluation of the potential health effects associated with CAS RN 85029-57-8. CAS RN 85029-57-8 has not been classified for human health effects by any national or international agencies.

Carcinogenicity and genotoxicity are generally considered to be the critical health effects of potential concern for substances in the Aromatic Azo and Benzidine-based Substance Grouping. The primary mechanism by which these substances exert their toxicity involves the reductive cleavage of the azo bonds and the subsequent release of the free aromatic amines. These aromatic amines are, in turn, converted to reactive electrophilic intermediates through metabolic oxidation (Environment Canada and Health Canada 2013a). However, a recent study by Deb et al. (2011) showed that azo substances that are bound by metal ions, such as chromium, are much less reactive than their metal complex-free counterparts. In human lung carcinoma (A549) cells *in vitro* study, 2-hydroxyphenyl-azo-2'-naphthol (HPAN) caused significant cytotoxicity through changes in the cell viability and morphology in addition to deoxyribonucleic acid (DNA) fragmentation, while no significant change was observed with its cobalt(II) complex, even at high concentrations. In addition, the cobalt(II) complex was noted to have weaker interaction with calf thymus DNA *in vitro* compared to HPAN alone. Deb et al. (2011) note that the preferential reduction of the metal ion protects the azo bond, which results in lack of aromatic amine formation. Therefore, while biologically azo bond cleavage is generally considered to be an important metabolic reaction resulting in toxicity, the generation of an azo reductive cleavage product is not considered likely to occur for CAS RN 85029-57-8.

Positive results were observed for a standard reverse mutation assay for *Salmonella typhimurium* TA1537 and TA98 in the presence and absence of induced rat liver S9 at concentrations of CAS RN 85029-57-8 ranging from 100 to 5000 µg/plate (Study Submission 2012). Negative results were obtained for a Prival modified Ames assay conducted under standard (uninduced hamster liver S9) and reductive conditions (flavin mononucleotide) in *S. typhimurium* TA98 and TA100 in the presence of reductive S9 at concentrations up to 5000 µg/plate (BioReliance 2012). Negative results were also obtained for *S. typhimurium* TA100 and TA1535 and *Escherichia coli* WP2 uvrA in a standard reverse mutation assay. No bacterial toxicity was noted at all dose levels tested (20–5000 µg/plate); however, the substance was observed to precipitate from dose levels of 500 µg/plate and upward (Study Submission 2012), thus data at these higher dose levels were not useful.

Experimental studies in which animals were administered CAS RN 85029-57-8 via the oral and inhalation routes have been identified for the determination of acute toxicity. Acute oral toxicity was reported to be low in rats (median lethal dose [LD<sub>50</sub>] greater than 10 000 mg/kg body weight), while the inhalation of a highly enriched/saturated vapour–air mixture by rats did not represent a likely acute hazard, and an inhalation median lethal concentration (LC<sub>50</sub>) could not be determined. This substance was considered to be not irritating to either the skin or eyes of rabbits (BASF 2012).

No appropriate analogues were identified to inform the health effects assessment of CAS RN 85029-57-8 due to limited data on the associated effects, although several metal:dye complexes were identified to be structurally similar to this substance. Chromium complexes (2:1) are stable at ambient conditions. In highly acidic environments, chromium forms a 1:1 metal:dye complex and an unbound dye molecule (Hunger 2003). A conservative assumption of complete dissociation of this complex would result in release of trivalent chromium and the ligand organic dye component; however, there is no indication that these substances have effects of concern based on potential carcinogenicity (Canada 1994; Environment Canada and Health Canada 2013c).

Overall, available information does not indicate CAS RN 85029-57-8 to be a substance with effects of concern based on potential carcinogenicity.

### **7.2.3 Characterization of Risk to Human Health**

Exposure of the general population to Azo Metal Complexes and Other Azo Substances from environmental media is not expected due to limited commercial quantities in Canada; therefore risk to human health from this source is not expected.

For CAS RN 85029-57-8, based on limited potential for general population exposure and the absence of indications of health effects of concern, risk to human health is considered to be low for this substance.

#### **Uncertainties in Evaluation of Risk to Human Health**

There is uncertainty regarding the exposure characterization from environmental media due to the lack of data. No Canadian specific data was obtained on the concentration of CAS RN 85029-57-8 used in wood coatings and stains; however, the concentration is likely within the same range obtained from the German product information.

Uncertainties are recognized in the human health characterization of CAS RN 85029-57-8 due to the limited nature of the health effects database.

There is also uncertainty with respect to potential health effects of trace level of impurities or minor components of unknown or variable compositions that may be

present in the dye because of the purity of the chemical and methods used in its manufacture are not standardized.

## 8. Conclusion

Considering all available lines of evidence presented in this Screening Assessment, there is low risk of harm to organisms and the broader integrity of the environment from the four Azo Metal Complexes and two Other Azo Substances evaluated in this assessment. It is concluded that the four Azo Metal Complexes and two Other Azo Substances do not meet the criteria set out in paragraphs 64(a) and 64(b) of CEPA 1999, as they are 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. .

Based on the information presented in this Screening Assessment, it is concluded that the four Azo Metal Complexes and two Other Azo Substances evaluated in this assessment do not meet criteria set out in paragraph 64(c) of CEPA 1999, as they are not entering the environment in a quantity or concentration or under conditions that constitute or may constitute a danger in Canada to human life or health.

It is concluded that the four Azo Metal Complexes and two Other Azo Substances do not meet any of the criteria set out in section 64 of CEPA 1999.

## References

- AGFA. 2007. [Material Safety Data Sheet: KC091 ADDITION PEN] [Internet]. Prague (CZ): AGFA. [cited 2013 Apr 10]. Available from: [www.elektronika-navratil.cz/download.php?FNAME=1191592269.upl&ANAME=Agfa%20KN091.pdf](http://www.elektronika-navratil.cz/download.php?FNAME=1191592269.upl&ANAME=Agfa%20KN091.pdf). [in Czech].
- Akzo Nobel Deco GmbH. 2010. Material Safety Data Sheet: Colorkonzentrat bordeaux [Internet]. Hilden (DE): Akzo Nobel Deco GmbH, Geschäftsbereich Zweihorn. [cited 2013 Apr 10]. Available from: [www.zweihorn.com/assets/templates/zweihorn/files/en/Sicherheitsdatenblaetter/Beizen/CK%2004\(1\).pdf](http://www.zweihorn.com/assets/templates/zweihorn/files/en/Sicherheitsdatenblaetter/Beizen/CK%2004(1).pdf)
- Anliker R, Clarke EA, Moser P. 1981. Use of the partition coefficient as an indicator of bioaccumulation tendency of dyestuffs in fish. *Chemosphere* 10(3):263–274.
- [AOPWIN] Atmospheric Oxidation Program for Windows [Estimation Model]. 2010. Version 1.92a. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: [www.epa.gov/oppt/exposure/pubs/episuite.htm](http://www.epa.gov/oppt/exposure/pubs/episuite.htm)
- Arnot JA, Arnot MI, Mackay D, Couillard Y, MacDonald D, Bonnell M, Doyle P. 2010. Molecular size cutoff criteria for screening bioaccumulation potential: fact or fiction? *Integr Environ Assess Manag* 6(2):210–224.
- Bartlett A. 2013. Toxicity summary: effects of Disperse Yellow 7, Sudan Red G, Disperse Orange 13, Acid Red 97, and Bismarck Brown Y on the survival and growth of the freshwater amphipod *Hyalella azteca* in chronic, water-only exposures. Unpublished Environment Canada study.
- [BASF] BASF Corporation. 2012. Material Safety Data Sheet: Orasol® Red 335 (old Neozapon® Red 335) [Internet]. Florham Park (NJ): BASF. [cited 2013 Apr 10]. Available from: [worldaccount.basf.com/wa/NAFTA~fr\\_FR/Catalog/FunctionalPolymers/doc4/BASF/PRD/30047779/.pdf?title=&asset\\_type=msds/pdf&language=EN&validArea=US&urn=urn:documentum:ProductBase\\_EU:09007af88009c034.pdf](http://worldaccount.basf.com/wa/NAFTA~fr_FR/Catalog/FunctionalPolymers/doc4/BASF/PRD/30047779/.pdf?title=&asset_type=msds/pdf&language=EN&validArea=US&urn=urn:documentum:ProductBase_EU:09007af88009c034.pdf)
- BASF Canada. 2003. Material Safety Data Sheet: Neozapon Red 395. Toronto (ON): BASF Canada Inc.
- BASF Canada. 2012. Material Safety Data Sheet: Orasol® Red 395 (old Neozapon® Red 395) [Internet]. Mississauga (ON): BASF Canada Inc. [cited 2013 Jun 10]. Available from: [worldaccount.basf.com/wa/NAFTA/Catalog/FunctionalPolymers/doc4/BASF/PRD/30047](http://worldaccount.basf.com/wa/NAFTA/Catalog/FunctionalPolymers/doc4/BASF/PRD/30047)

175/.pdf?title=&asset\_type=msds/pdf&language=EN&validArea=CA&urn=urn:documentum:ProductBase\_EU:09007af8802c037d.pdf

Baughman GL, Perenich TA. 1988. Fate, solubility and partitioning of hydrophobic dyes. *Environ Toxicol Chem* 7:183–199.

BioReliance. 2012. Bacterial reverse mutation assay of selected azo dyes. Unpublished report prepared for Health Canada. Rockville (MD): BioReliance. Study Report No.: AD46RB-RL.502.BTL.

[BIOWIN] Biodegradation Probability Program for Windows [Estimation Model]. 2010. Version 4.10. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: [www.epa.gov/oppt/exposure/pubs/episuite.htm](http://www.epa.gov/oppt/exposure/pubs/episuite.htm)

Brown D, Hamburger B. 1987. The degradation of dyestuffs: Part III—Investigations of their ultimate degradability. *Chemosphere* 16(7):1539–1555.

Canada. [1978]. *Food and Drug Regulations*, C.R.C., c. 870. Available from: [www.canlii.org/en/ca/laws/regu/crc-c-870/latest/crc-c-870.html](http://www.canlii.org/en/ca/laws/regu/crc-c-870/latest/crc-c-870.html)

Canada. 1994. Chromium and its compounds [Internet]. Ottawa (ON): Environment Canada; Health Canada. (Priority substances list assessment report). Available from: [www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/chromium\\_chrome/index-eng.php](http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/chromium_chrome/index-eng.php)

Canada. 1999. *Canadian Environmental Protection Act, 1999*. S.C., 1999, c. 33. Part III, vol. 22, no. 3. Available from: <http://laws-lois.justice.gc.ca/eng/acts/c-15.31>

Canada, Dept. of the Environment. 2011. *Canadian Environmental Protection Act, 1999: Notice with respect to certain aromatic amines and aromatic azo- and benzidine-based substances*. Canada Gazette, Part I, vol. 145, no. 51, Supplement to the Canada Gazette. Available from: [www.gazette.gc.ca/rp-pr/p1/2011/index-eng.html](http://www.gazette.gc.ca/rp-pr/p1/2011/index-eng.html)

CATALOGIC [Computer Model]. 2012. Version 5.11.6. Bourgas (BG): Bourgas Prof. Assen Zlatarov University, Laboratory of Mathematical Chemistry. Available from: [www.oasis-lmc.org/?section=software&swid=1](http://www.oasis-lmc.org/?section=software&swid=1)

[Crechem] Crechem Technologies Inc. 2003. Release scenarios for Canadian coating facilities. Prepared for Environment Canada (Gatineau, QC) by Crechem Technologies Inc. (Ottawa, ON), March 31, 2003.

Deb T, Choudhury D, Guin PS, Saha MB, Chakrabarti G, Das S. 2011. A complex of Co(II) with 2-hydroxyphenyl-azo-2'-naphthol (HPAN) is far less cytotoxic than the parent



compound on A549-lung carcinoma and peripheral blood mononuclear cells: reasons for reduction in cytotoxicity. *Chem Biol Interact* 189:206–214.

Dimitrov S, Dimitrova N, Walker J, Veith G, Mekenyan O. 2002. Predicting bioconcentration potential of highly hydrophobic chemicals. Effect of molecular size. *Pure Appl Chem* 74(10):1823–1830.

Dimitrov S, Dimitrova N, Parkerton T, Comber M, Bonnell M, Mekenyan O. 2005. Base-line model for identifying the bioaccumulation potential of chemicals. *SAR QSAR Environ Res* 16(6):531–554.

[DS TOPKAT] Discovery Studio TOxicity Prediction by Komputer Assisted Technology [Prediction Module]. ©2005–2009. Version 2.5.0.9164. San Diego (CA): Accelrys Software Inc. Available from: [www.accelrys.com/products/](http://www.accelrys.com/products/)

[ECHA] European Chemicals Agency. 2012. Guidance on information requirements and chemical safety assessment. Chapter R.11: PBT assessment. [Guidance for the implementation of REACH. Version 1.1]. Helsinki (FI): European Chemicals Agency; 97 p. Available from: [echa.europa.eu/documents/10162/13632/information\\_requirements\\_r11\\_en.pdf](http://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf)

Environment Canada. 2007. Guidance for conducting ecological assessments under CEPA, 1999: Science resource technical series, technical guidance module: QSARs. Reviewed draft working document. Gatineau (QC): Environment Canada, Ecological Assessment Division.

Environment Canada. 2012. Data for certain aromatic amines and aromatic azo- and benzidine-based substances collected under the *Canadian Environmental Protection Act, 1999*, section 71: *Notice with respect to certain aromatic amines and aromatic azo- and benzidine-based substances*. Data prepared by: Environment Canada, Program Development and Engagement Division.

Environment Canada, Health Canada. 2007. Chemical substances: Categorization [Internet]. Ottawa (ON): Government of Canada. [updated 2007 April 20; cited 2014 June 10]. Available from: <http://www.chemicalsubstanceschimiques.gc.ca/approach-approche/categor-eng.php>

Environment Canada, Health Canada. 2013a. The Chemicals Management Plan Substance Grouping Initiative. Subgrouping Approach and Background Information for the Screening Assessment of Aromatic Azo and Benzidine-based Substances. May 2013. Environment Canada, Health Canada. Available upon request.

Environment Canada, Health Canada. 2013b. Rapid screening of substances of lower concern. Results of the screening assessment. Ottawa (ON): Environment Canada;

Health Canada. Available from: [www.ec.gc.ca/ese-ees/default.asp?lang=En&n=2A7095CD-1](http://www.ec.gc.ca/ese-ees/default.asp?lang=En&n=2A7095CD-1)

Environment Canada, Health Canada. 2013c. Screening Assessment: Aromatic Azo and Benzidine-based Substance Grouping. Certain Solvent Dyes. Ottawa (ON): Environment Canada, Health Canada. (Final screening assessment to be published at a later date).

Environment Canada, Health Canada. 2014. Rapid screening of substances from Phase One of the Domestic Substances List Inventory Update. Ottawa (ON): Environment Canada; Health Canada. Available from: <http://www.ec.gc.ca/ese-ees/default.asp?lang=En&n=7340E1B7-1>

[EPI Suite] Estimation Programs Interface Suite for Microsoft Windows [Estimation Model]. 2012. Version 4.1. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: [www.epa.gov/oppt/exposure/pubs/episuite.htm](http://www.epa.gov/oppt/exposure/pubs/episuite.htm)

[EQC] Equilibrium Criterion Model. 2011. Version 1.00 (Beta). Peterborough (ON): Trent University, Canadian Centre for Environmental Modelling and Chemistry. Available from: [www.trentu.ca/academic/aminss/envmodel/models/NewEQCv100.html](http://www.trentu.ca/academic/aminss/envmodel/models/NewEQCv100.html)

[ETAD] The Ecological and Toxicological Association of Dyes and Organic Pigments Manufacturers. 1995. Health and environmental information on dyes used in Canada. An overview to assist in the implementation of the *New Substances Notification Regulations* under the *Canadian Environmental Protection Act*. Prepared by the ETAD Canadian Affiliates. Report No.: 7/21/95.

[EU] European Union. 2006. Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC [Internet]. Off J Eur Union L 396:1–849. Available from: [eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=oj:l:2006:396:0001:0849:en:pdf](http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=oj:l:2006:396:0001:0849:en:pdf)

Freeman HS, Lye J, Sokolowska-Gajda J. 1999. Iron complex dyes in pollution prevention. In: Proceedings of the Colour Science Conference, p. 61–71. Harrogate, England

Health Canada. 2011. The Cosmetic Ingredient Hotlist March 2011 [Internet]. Ottawa (ON): Health Canada, Consumer Product Safety. [cited 2013 Apr 26]. Available from: [www.hc-sc.gc.ca/cps-spc/cosmet-person/indust/hot-list-critique/hotlist-liste-eng.php](http://www.hc-sc.gc.ca/cps-spc/cosmet-person/indust/hot-list-critique/hotlist-liste-eng.php)

[HSDB] Hazardous Substances Data Bank [database on the Internet]. 1983– . Bethesda (MD): National Library of Medicine (US). [cited year mon day]. Available from: [www.toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB](http://www.toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB)

Hunger K, editor. 2003. Industrial dyes: chemistry, properties, applications. WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim. 685 p. ISBN 3-527-30426-6.

[HYDROWIN] Hydrolysis Rates Program for Microsoft Windows [Estimation Model]. 2010. Version 2.00. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: [www.epa.gov/oppt/exposure/pubs/episuite.htm](http://www.epa.gov/oppt/exposure/pubs/episuite.htm)

Kundu D. 1977. Effects of diazo compounds on chromosomes and spindle. *Biologia (Bratisl)* 32(6):423–430.

Little LW, Lamb JC III. 1973. Acute toxicity of 46 selected dyes to the fathead minnow, *Pimephales promelas*. In: Dyes and the environment—Reports on selected dyes and their effects. Vol. 1. American Dye Manufacturers Institute, Inc.; 130 p.

Little LW, Lamb JC III, Chillingworth MA, Durkin WB. 1974. Acute toxicity of selected commercial dyes to the fathead minnow and evaluation of biological treatment for reduction of toxicity. In: Proceedings of the 29th Industrial Waste Conference, Purdue University, West Lafayette (IN); p. 524–534.

[LNHPD] Licensed Natural Health Products Database [database on the Internet]. 2008. Version 1.0. Ottawa (ON): Health Canada. [cited 2013 Apr 16]. Available from: [webprod3.hc-sc.gc.ca/lnhpd-bdpsnh/index-eng.jsp](http://webprod3.hc-sc.gc.ca/lnhpd-bdpsnh/index-eng.jsp)

MIPA AG. 2012. Material Safety Data Sheet: Brilliant Design [Internet]. Essenbach (DE): MIPA AG. [cited 2013 Apr 10]. Available from: [www.mipa-paints.com/gb/sdb/auto/Brillant\\_Design\\_GB.pdf](http://www.mipa-paints.com/gb/sdb/auto/Brillant_Design_GB.pdf)

[NCI] National Chemical Inventories [database on a CD-ROM]. 2012. Issue 2. Columbus (OH): American Chemical Society, Chemical Abstracts Service. [cited 2011 May 1]. Available from: [www.cas.org/products/other-cas-products/nci-on-cd](http://www.cas.org/products/other-cas-products/nci-on-cd)

[NHPIID] Natural Health Products Ingredients Database [database on the Internet]. 2011. Version 2.1. Ottawa (ON): Health Canada. [cited 2013 Apr 16]. Available from: [webprod.hc-sc.gc.ca/nhpid-bdipsn/search-rechercheReq.do](http://webprod.hc-sc.gc.ca/nhpid-bdipsn/search-rechercheReq.do)

[NPRI] National Pollutant Release Inventory [database on the Internet]. 2006. Gatineau (QC): Environment Canada. [cited 2013 May 16]. Available from: [www.ec.gc.ca/pdb/querysite/query\\_e.cfm](http://www.ec.gc.ca/pdb/querysite/query_e.cfm)

[OECD] Organisation for Economic Co-operation and Development. 2009. Emission scenario document on coating industry (paints, lacquers and varnishes). Paris (FR): OECD, Environment Directorate. (Series on Emission Scenario Documents No. 22). Report No.: ENV/JM/MONO(2009)24. Available from: [www.oecd.org/officialdocuments/displaydocument/?cote=env/jm/mono\(2009\)24&doclanguage=en](http://www.oecd.org/officialdocuments/displaydocument/?cote=env/jm/mono(2009)24&doclanguage=en)

OECD QSAR Toolbox [Read-across tool]. 2012. Version 3.0. Paris (FR): Organisation for Economic Co-operation and Development, Environment Directorate. [June 2013]. Available from: [www.oecd.org/document/23/0,3343,en\\_2649\\_34379\\_33957015\\_1\\_1\\_1\\_1,00.html](http://www.oecd.org/document/23/0,3343,en_2649_34379_33957015_1_1_1_1,00.html)

“[OECD] Organisation for Economic Co-operation and Development. 2014. [Guidance on Grouping of Chemicals. Second Edition. Series on Testing & Assessment No. 194. Available at: \[http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono\\(2014\\)4&doclanguage=en\]\(http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono\(2014\)4&doclanguage=en\)](#)

Øllgaard H, Frost L, Galster J, Hansen OC. 1998. Survey of azo-colorants in Denmark: consumption, use, health and environmental aspects. Copenhagen (DK): Danish Ministry of Environment and Energy, Environmental Protection Agency. Available from: [www2.mst.dk/udgiv/publications/1999/87-7909-548-8/pdf/87-7909-546-1.pdf](http://www2.mst.dk/udgiv/publications/1999/87-7909-548-8/pdf/87-7909-546-1.pdf)

PPG Industries Inc. 2012. Material Safety Data Sheet: YELLOW SHADE DYE RED [Internet]. Pittsburgh (PA): PPG Industries Inc. [cited 2013 Apr 10]. Available from: [buyat.ppg.com/EHSDocumentManagerPublic/documentSearch.aspx?CodeValue=DMX212&CodeCondition=BeginsWith&Language=en-US](http://buyat.ppg.com/EHSDocumentManagerPublic/documentSearch.aspx?CodeValue=DMX212&CodeCondition=BeginsWith&Language=en-US)

Razo-Flores E, Luijten M, Donlon B, Lettinga G, Field J. 1997. Biodegradation of selected azo dyes under methanogenic conditions. *Water Sci Technol* 36(6–7):65–72.

Sakuratani Y, Noguchi Y, Kobayashi K, Yamada J, Nishihara T. 2008. Molecular size as a limiting characteristic for bioconcentration in fish. *J Environ Biol* 29(1):89–92.

[Sherwin-Williams] The Sherwin-Williams Company. 2013. Material Safety Data Sheet: SHER-WOOD® Simplicity Stain Concentrate, Red [Internet]. Cleveland (OH): The Sherwin-Williams Company. [cited 2013 Apr 10]. Available from: [www.paintdocs.com/webmsds/webPDF.jsp?SITEID=STORECAT&lang=E&doctype=MSDS&prodno=S81R2](http://www.paintdocs.com/webmsds/webPDF.jsp?SITEID=STORECAT&lang=E&doctype=MSDS&prodno=S81R2)

Smyth SA. 2012. Wastewater 101: for CMP monitoring. Presentation to Science Risk Assessment Division, Gatineau (QC), October 16.

Study Submission. 2012. Unpublished confidential studies submitted to Environment Canada under the Chemicals Management Plan initiative. Gatineau (QC): Environment Canada, Health Canada; Existing Substances Program.

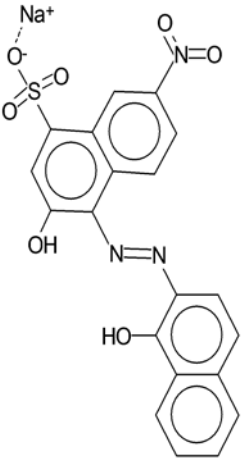
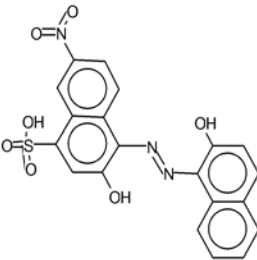
Tikkurila Oyj. 2010. Material Safety Data Sheet: DICCO COLOR [Internet]. Vantaa (FI): Tikkurila Oyj. [cited 2013 Apr 10]. Available from:  
[www.tikkurila.com/files/3482/DICCO\\_COLOR\\_GB-ENG\\_.PDF](http://www.tikkurila.com/files/3482/DICCO_COLOR_GB-ENG_.PDF)

Zollinger H, editor. 2003. Azo dyes and pigments. In: Color chemistry: syntheses, properties, and applications of organic dyes and pigments. 3rd rev. ed. Zurich (CH): Verlag Helvetica Chimica Acta; p. 165–253.

## Appendices

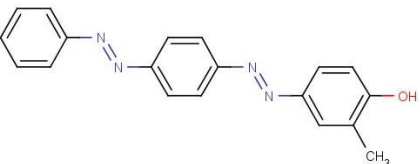
### Appendix A: Supplementary Data Tables

**Table A1-1: Substance identities for analogues of CAS RN 85029-57-8, CAS RN 94276-35-4 and CAS RN 72391-06-1**

CAS RN C.I. name	Chemical structure and formula	% similarity <sup>a</sup>	Read-across to
1787-61-7 Mordant Black 11		60–70; 70–80; 80–90	85029-57-8 a; 94276-35-4 a; 72391-06-1 a
5610-64-0 Acid Black 52		60–70; 70–80; 80–90	85029-57-8 a; 94276-35-4 a; 72391-06-1 a

<sup>a</sup> Percent similarity based on OECD QSAR Toolbox (2012) structural comparisons.

**Table A1-2: Substance identity for analogue of CAS RN 6708-61-8 and CAS RN 63281-10-7**

CAS RN C.I. name	Chemical structure and formula	% similarity <sup>a</sup>	Read-across to
Disperse Yellow 7 6300-37-4		NA	6708-61-8 and 63224-47-5

Abbreviations: NA, not available

<sup>a</sup> Percent similarity based on OECD QSAR Toolbox (2012) structural comparisons.

**Table A2-1: Physical and chemical properties for analogues of CAS RN 85029-57-8**

Substance identity	Property	Value	Reference
Substance A	Melting point (°C)	> 269	Confidential data
Substance A	Water solubility (g/L)	20	Confidential data
Substance A	Log K <sub>ow</sub> (dimensionless)	-2.8	Confidential data
Substance A	Molecular weight (g/mol)	NA	Confidential data
Substance B	Melting point (°C)	< 300	Confidential data
Substance B	Water solubility (mg/L)	0.5	Confidential data
Substance B	Log K <sub>ow</sub> (dimensionless)	-1.4	Confidential data
Substance B	Molecular weight (g/mol)	NA	Confidential data
Substance C	Melting point (°C)	< 300	Confidential data
Substance C	Water solubility (mg/L)	0.002	Confidential data
Substance C	Log K <sub>ow</sub> (dimensionless)	NA	Confidential data
Substance C	Molecular weight (g/mol)	NA	Confidential data

Abbreviations: NA, not available

**Table A2-2: Summary of physical and chemical properties of CAS RN 6708-61-8 and analogues (experimental data at 25°C)**

Property	Value(s) or range (for more than three data points)	Pivotal value(s) for this assessment (basis for selection)
Melting point and decomposition (°C)	211	211 (sole experimental value)
Water solubility (mg/L)	0.0096–0.35	0.18 (mean value)
Log K <sub>ow</sub> (dimensionless)	NA	NA
D <sub>min</sub> (nm)	0.92	0.92 (sole estimated value)
D <sub>max</sub> (nm)	1.10	1.10 (sole estimated value)
pK <sub>a</sub> (dimensionless)	NA	NA

Abbreviations: D<sub>max</sub>, effective maximum cross-sectional diameter; D<sub>min</sub>, effective minimum cross-sectional diameter; NA, not available; pK<sub>a</sub>, acid dissociation constant

**Table A2-3: Summary of physical and chemical properties of CAS RN 63224-47-5 and analogues (experimental data at 25°C)**

Property	Value(s) or range (for more than three data points)	Pivotal value(s) for this assessment (basis for selection)
Melting point and decomposition (°C)	NA	NA
Water solubility (mg/L)	NA	NA
Log K <sub>ow</sub> (dimensionless)	NA	NA
D <sub>min</sub> (nm)	1.54	1.54 (sole estimated value)
D <sub>max</sub> (nm)	1.54	1.54 (sole estimated value)
pK <sub>a</sub> (dimensionless)	NA	NA

Abbreviations: D<sub>max</sub>, effective maximum cross-sectional diameter; D<sub>min</sub>, effective minimum cross-sectional diameter; NA, not available; pK<sub>a</sub>, acid dissociation constant

**Table A2-4: Summary of physical and chemical properties of CAS RN 72391-06-1 and analogues (experimental and modelled data at 25°C)**

Property	Substance	Type of data	Value(s) or range (for more than three data points)	Pivotal value(s) for this assessment (basis for selection)
Melting point and decomposition (°C)	72391-06-1 a and analogues	Experimental	NA	NA
Melting point and decomposition (°C)	72391-06-1 b	Modelled	248.14	248.14 (sole estimated value)
Water solubility (mg/L)	72391-06-1 a and analogues	Experimental	NA	NA
Water solubility (mg/L)	72391-06-1 b	Modelled	2.80 × 10 <sup>-4</sup>	2.80 × 10 <sup>-4</sup> (sole estimated value)
Log K <sub>ow</sub> (dimensionless)	72391-06-1 a and analogues	Experimental	NA	NA
Log K <sub>ow</sub> (dimensionless)	72391-06-1 b	Modelled	6.63	6.63 (sole estimated value)
D <sub>min</sub> (nm)	72391-06-1 a and analogues	Experimental	1.25	1.25 (sole estimated value)
D <sub>max</sub> (nm)	72391-06-1 a and analogues	Experimental	1.25	1.25 (sole estimated value)
pK <sub>a</sub> (dimensionless)	72391-06-1 a and analogues	Experimental	NA	NA

Abbreviations: D<sub>max</sub>, effective maximum cross-sectional diameter; D<sub>min</sub>, effective minimum cross-sectional diameter; NA, not available; pK<sub>a</sub>, acid dissociation constant



**Table A2-5: Summary of physical and chemical properties of CAS RN 83221-38-9 and analogues (experimental data at 25°C)**

Property	Value(s) or range (for more than three data points)	Pivotal value(s) for this assessment (basis for selection)
Melting point and decomposition (°C)	NA	NA
Water solubility (mg/L)	NA	NA
Log K <sub>ow</sub> (dimensionless)	NA	NA
D <sub>min</sub> (nm)	0.96	0.96 (sole estimated value)
D <sub>max</sub> (nm)	1.30	1.30 (sole estimated value)
pK <sub>a</sub> (dimensionless)	NA	NA

Abbreviations: D<sub>max</sub>, effective maximum cross-sectional diameter; D<sub>min</sub>, effective minimum cross-sectional diameter; NA, not available; pK<sub>a</sub>, acid dissociation constant

**Table A2-6: Summary of physical and chemical properties of CAS RN 94276-35-4 and analogues (experimental and modelled data at 25°C)**

Property	Substance	Type of data	Value(s) or range (for more than three data points)	Pivotal value(s) for this assessment (basis for selection)
Melting point and decomposition (°C)	94276-35-4 a and analogues	Experimental	165	165 (sole value)
Water solubility (mg/L)	94276-35-4 a and analogues	Experimental	1.2 × 10 <sup>4</sup>	1.2 × 10 <sup>4</sup> (sole value)
Log K <sub>ow</sub> (dimensionless)	94276-35-4 a and analogues	Experimental	1.95	1.95 (sole value)
D <sub>min</sub> (nm)	94276-35-4 a and analogues	Experimental	0.89	0.89 (sole estimated value)
D <sub>max</sub> (nm)	94276-35-4 a and analogues	Experimental	1.14	1.14 (sole estimated value)
pK <sub>a</sub> (dimensionless)	94276-35-4 a and analogues	Experimental	NA	NA
Melting point and decomposition (°C)	94276-35-4 b and analogues	Experimental	217.85	217.85 (sole experimental value)
Melting point and decomposition (°C)	94276-35-4 b	Modelled	217.85	217.85 (sole estimated value)

Property	Substance	Type of data	Value(s) or range (for more than three data points)	Pivotal value(s) for this assessment (basis for selection)
Water solubility (mg/L)	94276-35-4 b and analogues	Experimental	1.946	1.946 (sole experimental value)
Water solubility (mg/L)	94276-35-4 b	Modelled	1.946	1.946 (sole estimated value)
Log K <sub>ow</sub> (dimensionless)	94276-35-4 b and analogues	Experimental	4.81	4.81 (sole experimental value)
Log K <sub>ow</sub> (dimensionless)	94276-35-4 b (989-38-8)	Modelled	4.81	4.81 (sole estimated value)
D <sub>min</sub> (nm)	94276-35-4 b and analogues	Experimental	NA	NA
D <sub>max</sub> (nm)	94276-35-4 b and analogues	Experimental	NA	NA
pK <sub>a</sub> (dimensionless)	94276-35-4 b and analogues	Experimental	NA	NA

Abbreviations: D<sub>max</sub>, effective maximum cross-sectional diameter; D<sub>min</sub>, effective minimum cross-sectional diameter; NA, not available; pK<sub>a</sub>, acid dissociation constant

**Table A3: Summary of modelled data for degradation of chromium-containing Azo Metal Complexes<sup>a</sup>**

Fate process	Model and model basis	Model result and prediction	Extrapolated half-life (days)
Atmospheric oxidation (air)	AOPWIN 2010 <sup>b</sup>	t <sub>1/2</sub> = 0.01–0.73 day	≤ 2
Ozone reaction (air)	AOPWIN 2010 <sup>b</sup>	N/A <sup>c</sup>	N/A
Primary biodegradation (aerobic) (water)	BIOWIN 2010 <sup>b</sup> Submodel 4: Expert Survey (qualitative results)	2.7859–3.5638 <sup>d</sup> (borderline)	≥ 182
Ultimate biodegradation (aerobic) (water)	BIOWIN 2010 <sup>b</sup> Submodel 3: Expert Survey (qualitative results)	1.5815–2.47 <sup>d</sup> (borderline)	≥ 182
Biodegradation (aerobic) (water)	BIOWIN 2010 <sup>b</sup> Submodel 5:	–0.7244 to 0.1139 <sup>e</sup> (biodegrades slowly)	≥ 182

Fate process	Model and model basis	Model result and prediction	Extrapolated half-life (days)
	MITI linear probability		
Biodegradation (aerobic) (water)	BIOWIN 2010 <sup>b</sup> Submodel 6: MITI non-linear probability	0–0.0038 <sup>e</sup> (biodegrades slowly)	≥ 182
Biodegradation (aerobic) (water)	DS TOPKAT ©2005–2009 Probability	N/A	N/A
Biodegradation (aerobic) (water)	CATALOGIC 2012 % BOD	N/A	N/A

Abbreviations: BOD, biological oxygen demand; MITI, Ministry of International Trade and Industry (Japan); N/A, not applicable;  $t_{1/2}$ , half-life

<sup>a</sup> Substances used in this summary include the following: CAS RN 85029-57-8, CAS RN 94276-35-4 and CAS RN 72391-06-1.

<sup>b</sup> EPI Suite (2012).

<sup>c</sup> Model does not provide an estimate for this type of structure.

<sup>d</sup> Output is a numerical score from 0 to 5.

<sup>e</sup> Output is a probability score.

**Table A4-1: Toxicity data for analogues of CAS RN 85029-57-8, CAS RN 94276-35-4 and CAS RN 72391-06-1**

CAS RN C.I. name	Test organism	Duration of test (h)	Endpoint	Value (mg/L)	Reference
1787-61-7 Mordant Black 11	Fathead minnow <i>Pimephales promelas</i>	24	LC <sub>50</sub>	10	Little et al. 1974
1787-61-7 Mordant Black 11	Fathead minnow <i>Pimephales promelas</i>	48	LC <sub>50</sub>	6	Little et al. 1974
1787-61-7 Mordant Black 11	Fathead minnow <i>Pimephales promelas</i>	96	LC <sub>50</sub>	6	Little et al. 1974
1787-61-7 Mordant Black 11	Fathead minnow <i>Pimephales promelas</i>	96	LC <sub>50</sub>	6	Little and Lamb 1973
5610-64-0 Acid Black 52	Fathead minnow <i>Pimephales promelas</i>	24	LC <sub>50</sub>	7	Little et al. 1974
5610-64-0 Acid Black 52	Fathead minnow <i>Pimephales promelas</i>	48	LC <sub>50</sub>	6.2	Little et al. 1974
5610-64-0	Fathead minnow	96	LC <sub>50</sub>	6.2	Little et al.

CAS RN C.I. name	Test organism	Duration of test (h)	Endpoint	Value (mg/L)	Reference
Acid Black 52	<i>Pimephales promelas</i>				1974
5610-64-0 Acid Black 52	Fathead minnow <i>Pimephales promelas</i>	96	LC <sub>50</sub>	7	Little and Lamb 1973
Substance A	<i>Daphnia magna</i>	24	EC <sub>50</sub> (immobilization)	480.7	Confidential information
Substance A	Carp ( <i>Cyprinus carpio</i> )	96	LC <sub>50</sub>	> 1200	Confidential information
Substance B	<i>Daphnia magna</i>	48	EC <sub>50</sub> (immobilization)	> 100	Confidential information
Substance B	Rainbow trout <i>Oncorhynchus mykiss</i>	48	LC <sub>50</sub>	100	Confidential information
Substance C	<i>Daphnia magna</i>	72	EC <sub>50</sub> (immobilization)	1.7	Confidential information
Substance C	Rainbow trout <i>Oncorhynchus mykiss</i>	96	LC <sub>50</sub>	0.4	Confidential information
Substance C	Fathead minnow <i>Pimephales promelas</i>	96	LC <sub>50</sub>	37.0	Confidential information

Abbreviations: EC<sub>50</sub>, the concentration of a substance that is estimated to cause some effect on 50% of the test organisms; LC<sub>50</sub>, the concentration of a substance that is estimated to be lethal to 50% of the test organisms

**Table A4-2: Toxicity data for analogue of CAS RN 6708-61-8 and CAS RN 63224-47-5**

CAS RN C.I. name	Test organism	Endpoint	Reference
Disperse Yellow 7 6300-37-4	<i>Hyalella</i>	7 d LC <sub>50</sub> = 0.18 mg/L 14 d LC <sub>50</sub> = 0.16 mg/L 20 d LC <sub>50</sub> = 0.025 mg/L 21 d LC <sub>50</sub> = 0.12 mg/L 28 d LC <sub>50</sub> = 0.12 mg/L 28 d EC <sub>50</sub> > 0.2 mg/L	Bartlett 2013

Abbreviations: EC<sub>50</sub>, the concentration of a substance that is estimated to cause some effect on 50% of the test organisms; LC<sub>50</sub>, the concentration of a substance that is estimated to be lethal to 50% of the test organisms

## Appendix B: Ecological Aquatic Exposure Calculations for the Azo Metal Complex CAS RN 85029-57-8

The predicted environmental concentrations (PECs) of the only in-commerce substance (CAS RN 85029-57-8) were estimated in water for the 10 paint/coating formulation sites identified. The estimates were based on several parameters: annual use quantity, emission factor for emissions to wastewater, removal by on-site wastewater treatment and dilution by wastewater and receiving water.

The annual use quantity of the substance at each facility was obtained from a survey issued pursuant to section 71 of CEPA 1999 (Canada 2011). This quantity was between 10 and 1000 kg for the 2010 calendar year:

Annual use quantity of substance CAS RN 85029-57-8 at a facility  
= Actual annual quantity found from CEPA section 71 survey (Canada 2011)  
= 10 to 1000 kg/year

The use of the actual quantities found from the survey in these exposure calculations is intended to provide more accurate release and exposure estimates whenever possible with the data available. This would improve the certainty in risk characterization and avoid false risk conclusions. However, conservative assumptions are still needed as a precautionary measure in the case of data gaps and data uncertainties.

The number of annual operation days involved with the substance at each facility was unknown. This parameter was conservatively assumed to be 1 day/year:

Number of annual operation days = 1 day/year

The daily use quantity of the substance at each facility was then calculated by dividing the annual use quantity by the number of annual operation days. As an example, for an annual use quantity of 100 kg/year, the daily use quantity was calculated as

Daily use quantity of substance CAS RN 85029-57-8 at a facility  
= Annual use quantity of substance CAS RN 85029-57-8 at a facility / Number of annual operation days  
= 100 kg/year / 1 day/year  
= 100 kg/day

The emission factor for emissions to wastewater from the cleaning of paint/coating formulation facilities was obtained from an analysis of industry data (Environment Canada 2012). This parameter was found to be 0.3%:

Emission factor to wastewater = 0.3%

The daily release quantity of the substance to wastewater from a facility was estimated by multiplying a facility's daily use quantity of the substance by the emission factor to wastewater. As an example, for a daily use quantity of 100 kg/day, the daily quantity of the substance released to wastewater from a facility was estimated as follows:

$$\begin{aligned} & \text{Daily release quantity of substance CAS RN 85029-57-8 to wastewater at a} \\ & \text{facility} \\ & = \text{Daily use quantity of substance CAS RN 85029-57-8 at a facility} \times \text{Emission} \\ & \text{factor to wastewater} \\ & = 100 \text{ kg/day} \times 0.3\% \\ & = 0.3 \text{ kg/day} \end{aligned}$$

Several site visits to paint/coating formulation facilities indicated that settling tanks were used as on-site wastewater treatment for solids removal (Crechem 2003). These site visits also indicated that the treated wastewater was treated further by off-site local wastewater treatment systems before being discharged to the aquatic environment. Both on-site and off-site wastewater treatment were therefore assumed to occur, and both are reflected in the exposure calculations.

Dyes with water solubility under 1 mg/L are expected to be removed by 90% via settling tanks (OECD 2009). The removal mechanism is precipitation when a substance is present in water at concentrations above its water solubility. Since the substance CAS RN 85029-57-8 has a water solubility below 1 mg/L (0.002–0.5 mg/L) and on-site wastewater treatment systems are expected to have settling tanks, the removal efficiency is expected to be 90% for the on-site treatment:

$$\text{On-site wastewater treatment removal} = 90\%$$

The quantity of the substance released from a facility to sewer was then determined from the daily release quantity to wastewater and the on-site wastewater treatment removal. As an example, for a daily release quantity of 0.3 kg/day to wastewater, the daily release quantity to sewer was estimated as:

$$\begin{aligned} & \text{Daily release quantity of substance CAS RN 85029-57-8 to sewer at a facility} \\ & = \text{Daily release quantity of substance CAS RN 85029-57-8 to wastewater at a} \\ & \text{facility} \times (1 - \text{On-site wastewater treatment removal}) \\ & = 0.3 \text{ kg/day} \times (1 - 0.9) \\ & = 0.03 \text{ kg/day} \end{aligned}$$

The concentration of the substance in influent to a local publically-owned wastewater treatment system depends upon the influent flow. The concentration of the substance in influent was estimated by dividing the daily release quantity to sewer at a facility by the influent flow. The example below is used to illustrate the calculations for a daily release quantity of 0.03 kg/day to sewer and an influent flow of 200 000 L/day:

Concentration of substance CAS RN 85029-57-8 in influent  
= Daily release quantity of substance CAS RN 85029-57-8 to sewer at a facility /  
Influent flow  
= 0.03 kg/day / 200 000 L/day  
=  $1.5 \times 10^{-7}$  kg/L  
= 150 µg/L

It should be noted that the influent and effluent flows of a local wastewater treatment system were assumed to be equal in all concentration calculations. For the sake of convenience, they were also referred to as the flow of a wastewater treatment system.

The removal efficiencies of the off-site local wastewater treatment systems for the 10 paint/coating formulation sites are assumed to be negligible. This is because the substance has low affinity for solids due to its low octanol–water partition coefficient ( $\log K_{ow} = -2.8$  to  $-1.4$ ). Thus, the removal by sludge sorption is expected to be insignificant. In addition, the substance is not volatile, so the removal by volatilization is negligible. The substance is assumed to be non-biodegradable under wastewater treatment conditions due to a lack of biodegradation data. The overall removal is therefore assumed to be 0%.

Two of the off-site local wastewater treatment systems were identified as lagoons. Lagoons contain large volumes of water and have long hydraulic retention times. The retention time of a lagoon was in weeks to months, according to field data collected through the Chemicals Management Plan's Monitoring and Surveillance Program at Environment Canada (Smyth 2012). The implication of a long retention time is that the substance entering a lagoon within a relatively short duration is subject to dilution, although the removal is negligible. As a result, the concentration of the substance in lagoon effluent is reduced by such dilution. The duration of the aquatic release of the substance within a year was 1 day, as assumed in this analysis:

Duration of aquatic release of substance CAS RN 85029-57-8 at a facility = 1 day

This duration was relatively short compared with a lagoon's residence time. Dilution was therefore justified. Such dilution was, however, not expected in primary or secondary treatment systems, because their hydraulic retention times were short, typically in hours.

No quantitative method was available to determine the degree of lagoon dilution. Nevertheless, the ratio of a lagoon's retention time to a substance's release duration could be used as an approximation to the lagoon dilution, because the ratio represented the full dilution or the volume ratio of the entire lagoon water to the wastewater containing a specific substance. As an estimate, the lagoon retention time in weeks to months was interpreted as 42 days (6 weeks) to 84 days (12 weeks), with an average of 63 days. The full dilution was then determined by dividing this average by the release duration (1 day):

$$\begin{aligned} & \text{Lagoon dilution} \\ &= \text{Average lagoon hydraulic retention time} / \text{Release duration} \\ &= 63 \text{ day} / 1 \text{ day} \\ &= 63 \end{aligned}$$

The concentration of the substance in lagoon effluent was estimated by considering lagoon dilution. As an example, for a concentration of 150 µg/L in influent, the concentration of the substance in effluent was estimated as:

$$\begin{aligned} & \text{Concentration of substance CAS RN 85029-57-8 in lagoon effluent} \\ &= \text{Concentration of substance CAS RN 85029-57-8 in lagoon influent} / \text{Lagoon dilution} \\ &= 150 \text{ µg/L} / 63 \\ &= 2.4 \text{ µg/L} \end{aligned}$$

For primary or secondary systems, the concentration of the substance in effluent equals the concentration in influent.

The aquatic PEC was determined by applying the receiving water dilution to the concentration in effluent. Since the aquatic PEC was assessed near the discharge point, the receiving water dilution selected should also be applicable to this condition. The full dilution potential of a river was considered appropriate if it was between 1 and 10, based on its 10th percentile flow. Otherwise, the dilution was kept at 10 for both large rivers and still waters.

As an example, for a concentration of 2.4 µg/L in effluent discharging at 200 000 L/day to a river with a 10th percentile flow of 34 000 000 L/day, the full dilution of the receiving water was calculated as 170 (34 000 000 L/day / 200 000 L/day). The dilution factor of 10 was therefore selected in determining the concentration near the discharge point:

$$\begin{aligned} & \text{Aquatic PEC} \\ &= \text{Concentration of substance CAS RN 85029-57-8 in effluent} / \text{Receiving water dilution factor} \\ &= 2.4 \text{ µg/L} / 10 \\ &= 0.24 \text{ µg/L} \end{aligned}$$