

Supporting Documents for Initial Risk-Based Prioritization of High Production Volume Chemicals

Sponsored Chemical

C.I. Disperse Blue 79:1 (CAS No. 3618-72-2)
(9th CI Name: Acetamide, N-[5-[bis]2-(acetyloxy)ethyl]amino]-
2-[(2-bromo-4,6-dinitrophenyl)azo]-4-methoxyphenyl]-)

Supporting Chemical

C.I. Disperse Blue 79 (CAS No. 12239-34-8)
(9th CI Name: Acetamide, N-[5-[bis]2-(acetyloxy)ethyl]amino]-
2-[(2-bromo-4,6-dinitrophenyl)azo]-4-ethoxyphenyl]-)

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BACKGROUND

Screening-level hazard, exposure and risk characterizations for high production volume chemicals (HPV) are important contributions to the chemicals cooperation work being done in North America¹ through the EPA Chemical Assessment and Management Program (ChAMP)². These screening-level characterizations are developed by EPA for individual chemicals or chemical categories to support initial Risk-Based Prioritizations (RBPs) for HPV chemicals. These screening-level characterizations are technical documents intended primarily to inform the Agency's internal decision-making process. Accordingly, they are written for assessment professionals and assume a degree of technical understanding. Each of the support documents is described below.

The Risk-Based Prioritizations are found in an accompanying document and are written for a general audience. They present EPA's initial thinking regarding the potential risks presented by these chemicals and future possible actions that may be needed.

Hazard Characterizations for HPV Chemicals

EPA's screening-level hazard characterizations are based primarily on the review of the summaries of studies and other information submitted by the chemical sponsor(s) under the HPV Challenge Program³. These studies included in the scope of the HPV Challenge comprise the Screening Information Data Set (SIDS) of the Organization for Economic Cooperation and Development (OECD)⁴, an internationally recognized battery of tests that provides the basic data necessary to make an initial evaluation of a chemical's hazards and fate. In preparing the initial hazard characterizations, EPA also consulted a variety of reliable sources⁵ for additional relevant information and considered its own comments and public comments on the original submission as well as the sponsor's responses to comments and revisions made to the submission. In order to determine whether any new hazard information was developed since the time of an HPV submission, EPA also searched publicly available databases⁶ for information entered from one year prior to the HPV submission through May 2008. The screening-level hazard characterization is performed according to established EPA guidance⁷. A more detailed description of the hazard characterization process is available on the EPA website⁸.

With respect to chemicals for which internationally-accepted OECD SIDS Initial Assessment Profiles (SIAP) and Initial Assessment Reports (SIAR) were available, EPA did not generate its own screening-level hazard characterization, but did check for and incorporate updated information in the risk characterization.

Exposure Characterizations for HPV Chemicals

EPA recently received exposure-related data on chemicals submitted in accordance with the requirements of Inventory Update Reporting (IUR)⁹. The 2006 IUR submissions pertain to chemicals manufactured in

¹ U.S. EPA – U.S. Commitments to North American Chemicals Cooperation: <http://www.epa.gov/hpv/pubs/general/sppframework.htm>.

² U.S. EPA – ChAMP information: <http://www.epa.gov/champ/>.

³ U.S. EPA – HPV Challenge Program information: <http://www.epa.gov/hpv>.

⁴ U.S. EPA – Technical Guidance Document, OECD SIDS Manual Sections 3.4 and 3.5: <http://www.epa.gov/chemrtk/pubs/general/sidsappb.htm>.

⁵ U.S. EPA – Public Database Hazard Information: <http://www.epa.gov/hpvis/hazardinfo.htm>.

⁶ U.S. EPA – Public Database Update Information: <http://www.epa.gov/chemrtk/hpvis/updateinfo.htm>.

⁷ U.S. EPA – Risk Assessment Guidelines: <http://cfpub.epa.gov/ncea/raf/rafguid.cfm>.

⁸ U.S. EPA – About HPV Chemical Hazard Characterizations: <http://www.epa.gov/hpvis/abouthc.htm>.

⁹ U.S. EPA – Basic IUR Information: <http://www.epa.gov/opptintr/iur/pubs/guidance/basic-information.htm>.

(including imported into) the U.S. during calendar year 2005 in quantities of 25,000 pounds or more at a single site. The reports include the identity, the quantity, and the physical form of the chemical manufactured or imported, and the number of workers reasonably likely to be exposed during manufacture of the chemical. For chemicals manufactured or imported in quantities of 300,000 pounds or more at a single site, additional reported information includes: the industrial processing and uses of the chemical; the number of industrial processing sites and workers reasonably likely to be exposed to the chemical at those sites; the consumer and commercial uses of the chemical; and an indication whether the chemical was used in products intended for use by children under 14 years of age.

EPA's screening-level exposure characterizations are based largely on the information submitted under the IUR reporting, although other exposure information submitted to the Agency (for example, in HPV submissions) or readily available through a limited set of publicly accessible databases¹⁰ was also considered. The screening-level Exposure Characterizations identify a potential (high, medium, or low) that each of five populations – the environment, the general population, workers, consumers, and children – might be exposed to the chemical. In most cases, this potential doesn't address the quantity, frequency, or duration of exposure, but refers only to the likelihood that an exposure could occur.

In many instances EPA is not able to fully disclose to the public all the IUR exposure-related data reviewed or relied upon in the development of the screening-level documents because some of the material was claimed as confidential business information (CBI) when it was submitted to the Agency. These CBI claims do limit the Agency's ability to be completely transparent in presenting some underlying exposure and use data for chemicals in public documents. EPA does consider all data, including data considered to be CBI, in the screening-level exposure and risk characterization process, and endeavors whenever possible to broadly characterize supporting materials claimed as confidential in ways that do not disclose actual CBI.

Risk Characterizations for HPV Chemicals

EPA combines the information from the screening-level exposure characterization with the screening-level hazard characterization to develop a qualitative screening-level risk characterization, as described in the Agency's guidance on drafting risk characterizations¹¹. These screening-level risk characterizations are technical documents intended to support subsequent priority-setting decisions and actions by OPPT. The purpose of the qualitative screening-level risk characterization is two-fold: to support initial risk-based decisions to prioritize chemicals, identify potential concerns, and inform risk management options; and to identify data needs for individual chemicals or chemical categories.

These initial characterization and prioritization documents do not constitute a final Agency determination as to risk, nor do they determine whether sufficient data are available to characterize risk. Recommended actions reflect EPA's relative judgment regarding this chemical or chemical category in comparison with others evaluated under this program, as well as the uncertainties presented by gaps that may exist in the available data.

¹⁰ U.S. EPA – Summary of Public Databases Routinely Searched: <http://www.epa.gov/chemrtk/hpvis/pubdtsum.htm>.

¹¹ U.S. EPA – Risk Characterization Program: <http://www.epa.gov/osa/spc/2riskchr.htm>.

**QUALITATIVE SCREENING-LEVEL RISK CHARACTERIZATION
OF HIGH PRODUCTION VOLUME CHEMICALS**

SPONSORED CHEMICAL

C.I. Disperse Blue 79:1 (CAS No. 3618-72-2)

[9th CI Name: Acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-methoxyphenyl]-]

SUPPORTING CHEMICAL

C.I. Disperse Blue 79 (CAS No. 12239-34-8)

[9th CI Name: Acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-ethoxyphenyl]-]

July 2008

Prepared by

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Economics, Exposure and Technology Division
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QUALITATIVE SCREENING-LEVEL RISK CHARACTERIZATION FOR C.I. Disperse Blue 79:1 (CAS No. 3618-72-2)

1. Physical-Chemical Properties and Environmental Fate

C.I. Disperse Blue 79:1 is a solid at room temperature. It has low water solubility, negligible vapor pressure, and is minimally volatile. It is moderately mobile in soil. It is slow to biodegrade under aerobic conditions and hydrolysis is negligible under environmental conditions. Bioconcentration is expected to be low. C.I. Disperse Blue 79:1 is expected to have moderate persistence (P2) and low bioaccumulation potential (B1).

2. Hazard Characterization

Aquatic Organism Toxicity. Acute aquatic toxicity is not expected at the chemical's solubility limit (0.0052 mg/L). Evaluation of data from an early life stage (chronic) toxicity test for rainbow trout indicates that the potential hazard of C.I. Disperse Blue 79:1 to aquatic organisms is low.

Human Health Toxicity. The acute oral toxicity of C.I. Disperse Blue 79:1 to rats is low. No treatment-related adverse effects were found in a 90-day repeated-dose gavage study in rats. Although a reproductive toxicity study was not available, examination of tissues/organs from the repeated-dose toxicity study showed that reproductive organs were not affected by exposure to the test chemical. No developmental effects were observed in prenatal developmental toxicity studies in rats and rabbits. C.I. Disperse Blue 79:1 is mutagenic in multiple strains of *Salmonella* (*in vitro*), but negative in the *Drosophila* sex-linked recessive lethal mutagenicity test (*in vivo*). Because of its physical-chemical properties (a solid with low water solubility and high molecular weight), C.I. Disperse Blue 79:1 is not expected to have significant absorption and azo-reduction *in vivo*, which may explain its negative mutagenic response *in vivo*. The supporting chemical, C.I. Disperse Blue 79, yielded negative results in both *in vitro* and *in vivo* genetic toxicity tests.

The potential health hazard C.I. Disperse Blue 79:1 is low.

3. Exposure Characterization

Disperse Blue 79:1 (CAS # 3618-79-2) has an aggregated production and/or import volume in the United States of 10,000 to 500,000 pounds. Disperse Blue 79:1 and related products are used almost exclusively for dyeing or printing polyester fibers.

Exposure to the General Population and the Environment. Based on the information considered such as potential water releases, slow biodegradation, and a moderate persistence, known uses, EPA identifies, for purposes of risk-based prioritization, a medium relative ranking for potential exposure to the general population and the environment.

Exposure to Workers. Based on the totality of the information considered (primarily IUR data) in combination with Agency's professional judgment, EPA identifies, for the purposes of risk-based prioritization, a high relative ranking for potential worker exposure. This relative ranking is based mainly on potential inhalation and dermal exposures to particulates.

Exposure to Consumers. No uses in products intended to be used by consumers were reported in the IUR, nor were any found in other data sources. Although this chemical is used in fabric dyes, EPA's experience indicates that the dye process "fixes" the dye in the fiber, such that the chemical is not available for exposure simply through physical contact with the fabric. Accordingly, EPA identifies, for the purposes of risk-based prioritization, a low potential for consumer exposures.

Exposure to Children. No uses in products intended to be used by children were reported in the IUR, nor were any found in other data sources. Based on the same rationale as the consumer exposure scenario, EPA identifies, for the purposes of risk-based prioritization, a low potential for children's exposures.

4. Risk Characterization

The statements and rationale provided below are intended solely for the purpose of this screening-level and qualitative risk characterization and will be used for prioritizing substances for future work in the Chemical Assessment and Management Program (ChAMP).

Risk Statement and Rationale

Potential Risk to Aquatic Organisms from Environmental Releases (LOW CONCERN).

EPA identifies a medium potential for exposure to aquatic organisms from environmental releases. C.I. Disperse Blue 79:1 has moderate persistence and low bioaccumulation. These characteristics, in combination with the low potential hazard to aquatic organisms, suggest a low concern for potential risk to aquatic organisms from environmental releases.

Potential Risk to the General Population from Environmental Releases (LOW CONCERN).

EPA identifies a medium potential for exposure to the general population from environmental releases. Based on toxicity studies in animals by oral exposure, the potential human health hazard is low. Given the low human health hazard and environmental fate characteristics (moderate persistence and low bioaccumulation), the available information suggests a low concern for potential risks to the general population.

Potential Risk to Workers (LOW CONCERN). EPA identifies a high potential for worker exposure. This relative ranking is based mainly on potential inhalation and dermal exposures to particulates. Based on toxicity studies in animals by oral exposure, the potential human health hazard is low. The available information suggests a low concern for potential risks to workers.

Potential Risk to Consumers from Known Uses (LOW CONCERN). EPA identifies a low potential that consumers may be exposed. Although this chemical is used in fabric dyes,

EPA's experience indicates that the dye process "fixes" the dye in the fiber, such that the chemical is not available for exposure simply through physical contact with the fabric. The available toxicity data indicated that the potential human health hazard is low. Therefore, taken together, the available information suggests a low concern for potential risks to consumers.

Potential Risk to Children (LOW CONCERN). Based on the same rationale as the consumer exposure scenario, EPA identifies a low potential for children's exposures. The potential human health hazard is low. Therefore, taken together, the available information suggests a low concern for potential risks to children.

**SCREENING-LEVEL HAZARD CHARACTERIZATION
FOR HIGH PRODUCTION VOLUME CHEMICALS**

SPONSORED CHEMICAL

C.I. Disperse Blue 79:1 (CAS No. 3618-72-2)
[9th CI Name: Acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-methoxyphenyl]-]

SUPPORTING CHEMICAL

C.I. Disperse Blue 79 (CAS No. 12239-34-8)
[9th CI Name: Acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-ethoxyphenyl]-]

July 2008

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**SCREENING-LEVEL HAZARD CHARACTERIZATION
OF HIGH PRODUCTION VOLUME CHEMICALS
SCREENING-LEVEL HAZARD CHARACTERIZATION
C.I. Disperse Blue 79:1 (CAS No. 3618-72-2)**

Introduction

The sponsor, ETAD North America, submitted a Test Plan and Robust Summaries to EPA for C.I. Disperse Blue 79:1 (CAS No. 3618-72-2; 9th CI name: acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-methoxyphenyl]-) on January 7, 2002. EPA posted the submission on the ChemRTK HPV Challenge website on February 20, 2002 (<http://www.epa.gov/oppt/chemrtk/pubs/summaries/acetamid/c13461tc.htm>). EPA comments on the original submission were posted to the website on October 3, 2002. The sponsor submitted updated/revised documents on June 6, 2003, which were posted to the ChemRTK website on June 30, 2003.

This screening level hazard characterization is based primarily on the review of the test plan and robust summaries of studies submitted by the sponsor(s) under the HPV Challenge Program. In preparing the hazard characterization, EPA considered its own comments and public comments on the original submission as well as the sponsor's responses to comments and revisions made to the submission. In order to determine whether any new hazard information was developed since the time of the HPV submission, a search of the following databases was made from 2004 to April 2008: the NLM databases (ChemID to locate available data sources including Medline/PubMed, Toxline, HSDB, ATSDR, EPA SRS, etc.), STN/CAS online databases (Registry file for locators, ChemAbs for toxicology data, RTECS, Merck, etc.) and Science Direct. A summary table of SIDS endpoint data with the structure(s) of the sponsored chemical(s) is included in the appendix. The screening-level hazard characterization for environmental and human health effects is based largely on SIDS endpoints and is described according to established EPA or OECD effect level definitions and hazard assessment practices.

Justification for Supporting Chemical

In some instances, test data do not exist for C.I. Disperse Blue 79:1. The sponsor provided data for the supporting chemical, C.I. Disperse Blue 79 (CAS No. 12239-34-8) for these endpoints. Nearly identical structure and physical-chemical properties, such as log K_{ow} , water solubility and modeled fate parameters, provide rationale for the use of C.I. Disperse Blue 79 as a supporting chemical.

Hazard Characterization

C.I. Disperse Blue 79:1 is a solid at room temperature. It has low water solubility, negligible vapor pressure, and is minimally volatile. It is moderately mobile in soil. It is slow to biodegrade under aerobic conditions and hydrolysis is negligible under environmental conditions. Bioconcentration is expected to be low. C.I. Disperse Blue 79:1 is expected to have moderate persistence (P2) and low bioaccumulation potential (B1).

Acute aquatic toxicity is not expected at the chemical's solubility limit (0.0052 mg/L). Evaluation of data from an early life stage (chronic) toxicity test for rainbow trout indicates that the potential hazard of C.I. Disperse Blue 79:1 to aquatic organisms is low.

The acute oral toxicity of C.I. Disperse Blue 79:1 to rats is low. No treatment-related adverse effects were found in a 90-day repeated-dose gavage study in rats. Although a reproductive toxicity study was not available, examination of tissues/organs from the repeated-dose toxicity study showed that reproductive organs were not affected by exposure to the test chemical. No developmental effects were observed in prenatal developmental toxicity studies in rats and rabbits. C.I. Disperse Blue 79:1 is mutagenic in multiple strains of *Salmonella* (*in vitro*), but negative in the *in vivo* *Drosophila* sex-linked recessive lethal mutagenicity test. Because of its physical-chemical properties (a solid with low water solubility and high molecular weight), C.I. Disperse Blue 79:1 is not expected to have significant absorption and azo-reduction *in vivo*, which may explain for its negative mutagenic response *in vivo*. The supporting chemical, C.I. Disperse Blue 79, yielded negative results in both *in vitro* and *in vivo* genetic toxicity tests.

The potential health hazard C.I. Disperse Blue 79:1 is low.

No data gaps were identified under the HPV Challenge Program.

1. Physical-Chemical Properties and Environmental Fate

The physical-chemical properties of C.I. Disperse Blue 79:1 are summarized in Table 1a, while its environmental fate properties are provided in Table 1b. The structure of the compound is provided in the Appendix.

Physical-Chemical Properties Characterization

C.I. Disperse Blue 79:1 is a solid at room temperature, with a low water solubility and negligible vapor pressure.

Property	Value	Value
Chemical Name	C.I. Disperse Blue 79:1	C.I. Disperse Blue 79
CAS No.	3618-72-2	12239-34-8
Molecular Weight	625.39	639.42
Physical State	Solid	Solid
Melting Point	≥138°C	No data
Boiling Point	No data	476°C
Vapor Pressure	No data	3.40 × 10 ⁻⁹ mm Hg at 25°C
Water Solubility	0.0052 mg/L at 25°C (measured)	0.0054 mg/L at 25°C (measured)
Henry's Law constant	9.8 × 10 ⁻²⁵ atm-m ³ /mole (estimated)	No data
Dissociation constant(s) (pKa)	Not applicable	
Log K _{ow}	4.44 (measured)	4.1 (measured)

¹ ETAD North America. 2003. Robust Summaries for Acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-methoxyphenyl] Disperse Blue 79:1.

<http://www.epa.gov/chemrtk/pubs/summaries/acetamid/c13461tc.htm>.

² US EPA. 2008. Estimation Programs Interface Suite™ for Microsoft® Windows, v 3.20. United States Environmental Protection Agency, Washington, DC, USA. <http://www.epa.gov/opptintr/exposure/pubs/episuite.htm>.

Environmental Fate Characterization

If released to the atmosphere, C.I. Disperse Blue 79:1 will exist primarily in the particulate phase. Particulate-phase C.I. Disperse Blue 79:1 will be removed from the atmosphere by wet and dry deposition. Any vapor-phase C.I. Disperse Blue 79:1 will be degraded rapidly in the atmosphere by reaction with photochemically-produced hydroxyl radicals. C.I. Disperse Blue 79:1 will be moderately mobile in soil and will adsorb to sediments or suspended solids in water bodies. C.I. Disperse Blue 79:1 is minimally volatile. Hydrolysis is expected to be negligible based on an estimated hydrolysis half-life of 250 days at pH 7. Adequate biodegradation data were not provided; however, based on ready biodegradation data for chemical analogs, C.I. Disperse Blue 79:1 is considered not readily biodegradable under aerobic conditions, but undergoes reductive degradation under anaerobic conditions, producing 2-bromo-4,6-dinitroaniline as a degradation byproduct. The log K_{ow} for C.I. Disperse Blue 79:1 indicates that its potential to bioaccumulate is expected to be high; however, based on the BCF, (estimated), bioconcentration is expected to be low. C.I. Disperse Blue 79:1 is expected to have moderate persistence (P2) and low bioaccumulation potential (B1).

Chemical name	Disperse Blue 79:1	Disperse Blue 79
Photodegradation Half-life	0.57 hours	0.55 hours ²
Direct Photolysis	Stable	Stable
Hydrolysis Half-life	25 days at pH 8 (estimated) ² 250 days at pH 7 (estimated) ²	25 days at pH 8 (estimated) ² 250 days at pH 7 (estimated) ²
Biodegradation	Not readily biodegradable (estimated) ²	Not readily biodegradable (estimated) ²
Bioconcentration	10 (estimated) ²	10 (estimated) ²
Log K _{oc}	3.2 (estimated) ²	3.5 (estimated) ²
Fugacity (Level III Model) ²	Air <1% Water 6.69% Soil 79.4% Sediment 13.9%	Air <1% Water 3.68% Soil 60.9% Sediment 35.4%
Persistence	P2 (moderate) ³	P2 (moderate) ³
Bioaccumulation	B1 (low) ³	B1 (low) ³

¹ ETAD North America. 2003. Robust Summaries for Acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-methoxyphenyl] Disperse Blue 79:1.

<http://www.epa.gov/chemrtk/pubs/summaries/acetamid/c13461tc.htm>

² US EPA. 2008. Estimation Programs Interface Suite™ for Microsoft® Windows, v 3.20. United States Environmental Protection Agency, Washington, DC, USA. <http://www.epa.gov/opptintr/exposure/pubs/episuite.htm>

³ FR 1999, Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances. *Federal Register* 64, Number 213 (November 4, 1999) Page 60194-60204.

Conclusion: Adequate biodegradation data were not provided; however, based on ready biodegradation data for chemical analogs, C.I. Disperse Blue 79:1 is considered not readily biodegradable, indicating that it is expected to persist in the environment. It is slow to biodegrade under aerobic conditions and hydrolysis is negligible under environmental conditions. The log K_{ow} for C.I. Disperse Blue 79:1 indicates that its potential to bioaccumulate is expected to be high; however, based on the BCF (estimated), bioconcentration is expected to be low. C.I. Disperse Blue 79:1 is expected to have moderate persistence (P2) and low bioaccumulation potential (B1).

2. Environmental Effects – Aquatic Toxicity

The submitted acute data for aquatic invertebrates and aquatic plants were judged inadequate because endpoints were tested above the chemical's aqueous water solubility, test durations were inadequate and chemical purity was not characterized. However, chronic test data are preferable in this case because acute effects are not expected at the chemical's solubility limit. The available chronic fish data for C.I. Disperse Blue 79:1 are adequate for assessing aquatic toxicity endpoints for the purpose of the HPV Challenge Program.

Acute Toxicity to Aquatic Invertebrates

C.I. Disperse Blue 79 (CAS No. 12239-34-8, supporting chemical)

The aquatic toxicity test submitted was conducted above the aqueous solubility limit of C.I. Disperse Blue 79:1. Given the low water solubility of C.I. Disperse Blue 79:1, chronic toxicity data are preferable; the available chronic fish data for C.I. Disperse Blue 79:1 are adequate for assessing aquatic toxicity endpoints for the purpose of the HPV Challenge Program.

Toxicity to Aquatic Plants

C.I. Disperse Blue 79 (CAS No. 12239-34-8, supporting chemical)

The aquatic toxicity test submitted was conducted above the aqueous solubility limit of C.I. Disperse Blue 79:1. Given the low water solubility of C.I. Disperse Blue 79:1, chronic toxicity data are preferable; the available chronic fish data for C.I. Disperse Blue 79:1 are adequate for assessing aquatic toxicity endpoints for the purpose of the HPV Challenge Program.

Chronic Toxicity to Fish

C.I. Disperse Blue 79:1 (CAS No. 3618-72-2)

In an early life stage test, newly fertilized eggs (fertilized < 4 hours before study initiation) from rainbow trout (*Oncorhynchus mykiss*) were exposed to C.I. Disperse Blue 79:1 at nominal test concentrations of 0.31, 0.63, 1.3, 2.5 and 5.0 µg/L under flow-through conditions for 122 days post-hatch. The mean measured concentrations of test substance were 0.36, 0.58, 1.2, 2.5 and 4.8 µg/L. The highest test concentration was considered the limit of solubility for the test substance. Hatchability, survival and fry growth (length and weight) were not affected by any concentration tested, and the reported 122-d NOEC = 0.0048 mg/L (measured). No effects at saturation.

Conclusion: Acute effects are not expected at the chemical's solubility limit. Evaluation of data from an early life stage (chronic) toxicity test for rainbow trout indicates that the potential hazard of C.I. Disperse Blue 79:1 to aquatic organisms is low.

3. Human Health Effects

Acute Oral Toxicity

Acute oral toxicity study was not provided. Instead the sponsor provided data for a two-week range-finding study.

Sprague-Dawley rats (5/sex/dose) were administered C.I. Disperse Blue (in corn oil) via gavage at 100, 500, 1000 or 2500 mg/kg-bw for 5 days/week for two weeks for a total of 11 doses. No treatment-related effects on daily clinical signs, body weights, body weight gains, food consumption and necropsy were observed at any dose level.

LD₅₀ > 2500 mg/kg-bw

Repeated-Dose Toxicity

C.I. Disperse Blue 79:1 (CAS No. 3618-72-2)

(1) Male and female Sprague-Dawley rats (number per group not specified) were administered C.I. Disperse Blue 79:1 via gavage at doses of 0, 250, 1250 or 2500 mg/kg-bw/day, 5 days/week for 13 weeks. Blue coloration of the body and/or tail was observed in some animals; however, this coloration is not considered biologically significant since the test substance is a dye with an intense blue color. No reported treatment-related effects on food consumption, mortality, clinical pathology, ophthalmic examinations, body weight or body weight gain, organ weights, necropsy or histopathology were observed at any dose.

NOAEL = 2500 mg/kg-bw/day (based no effects at highest dose tested)

(2) Male and female rats (5/group) were administered C.I. Disperse Blue 79:1 via gavage at doses of 0, 100, 500, 1000 or 2500 mg/kg-bw/day, 5 days/week for 2 weeks plus an additional dose on the following Monday (11 doses). No treatment-related effects on daily clinical signs, body weights, body weight gains, food consumption or necropsy were observed at any dose level.

NOAEL = 2500 mg/kg-bw/day (based on no effects at highest dose tested)

Reproductive Toxicity

C.I. Disperse Blue 79:1 (CAS No. 3618-72-2)

A reproductive toxicity study was not provided; however, the histopathological evaluation of reproductive organs in the 13-week repeated-dose toxicity study described above and available developmental toxicity data address the endpoint for the purpose of the HPV Challenge Program.

Histopathological evaluation was performed on all tissues including reproductive organs from each dose group and the control group. There were no gross or microscopic lesions attributed to treatment for either sex animal at any dose level.

Developmental Toxicity

C.I. Disperse Blue 79:1 (CAS No. 3618-72-2)

(1) Pregnant Sprague-Dawley rats (number per group not specified) were administered C.I. Disperse Blue 79:1 via gavage (in corn oil) at doses of 0, 500, 1000 or 2000 mg/kg-bw/day on days 6 – 15 of gestation and were sacrificed on gestation day 20. No treatment-related effects were reported for maternal weight or weight gain, food consumption, gestational parameters (pre- and post-implantation loss and fetal body weights/litter) or incidences of gross, visceral or skeletal malformations or variations.

NOAEL (maternal/developmental toxicity) = 2000 mg/kg-bw/day (based on no effects at highest dose tested)

(2) Pregnant New Zealand White rabbits (16/group) were administered C.I. Disperse Blue 79:1 via gavage (in corn oil) at doses of 0, 100, 300 or 600 mg/kg-bw/day on days 6 – 18 of gestation and were sacrificed on gestation day 30. There was a significant reduction in maternal weight gains at the mid- and high-dose groups. No treatment-related effects were seen for food consumption, gravid uterine or liver weights in dams, or pre- and post-implantation loss. No treatment-related increase in the incidence of gross, visceral or skeletal malformations or variations was observed.

LOAEL (maternal toxicity) = 300 mg/kg-bw/day (based on decreased maternal weight gain)

NOAEL (maternal toxicity) = 100 mg/kg-bw/day

NOAEL (developmental toxicity) = 600 mg/kg-bw/day (based on no effects at the highest dose tested)

Genetic Toxicity – Gene Mutation

In vitro

C.I. Disperse Blue 79:1 (CAS No. 3618-72-2)

Salmonella typhimurium TA98, TA100, TA1537 and TA1538 strains were exposed to Foron Navy SE-2GRL (purity not known) at concentrations ranging from 1 to 1000 µg/plate in the presence and absence of metabolic activation. Information on the use of controls and cytotoxic concentration is not provided.

Foron Navy SE-2GRL was mutagenic in this assay.

C.I. Disperse Blue 79 (CAS No. 12239-34-8, supporting chemical)

C.I. Mammalian cells V79 were exposed to Disperse Blue 79 at concentrations ranging from 0.05 – 1.0 µg/mL without metabolic activation and 2.5 – 750 µg/mL with metabolic activation. Information of the use of controls and cytotoxic concentration is not provided. **C.I. Disperse Blue 79 was not mutagenic in this assay.**

Genetic Toxicity – Chromosomal Aberrations

In vivo

C.I. Disperse Blue 79 (CAS No. 12239-34-8, supporting chemical)

NMRI mice (male and female) were administered C.I. Disperse Blue 79 via gavage at 5000 mg/kg-bw. C.I. Disperse Blue did not induce chromosomal mutations. The details on this study were limited.

C.I. Disperse Blue 79 did not cause chromosomal aberrations in this assay.

C.I. Disperse Blue 79:1 (CAS No. 3618-72-2)

In a *Drosophila* (fruit fly) sex-linked recessive lethal mutagenicity test, males were injected with 50 ppm of C.I. Disperse Blue 79:1 and were mated with untreated females (Basc females crossed with Canton-S wild type males) to assess lethal mutations in post-meiotic germ cells.

C.I. Disperse Blue 79:1 was not mutagenic in this assay.

Conclusion: The acute oral toxicity of C.I. Disperse Blue 79:1 to rats is low. No treatment-related adverse effects were found in a 90-day repeated-dose gavage study in rats. Although a reproductive toxicity study was not available, examination of tissues/organs from the repeated-dose toxicity study showed that reproductive organs were not affected by exposure to the test chemical. No developmental effects were observed in prenatal developmental toxicity studies in rats and rabbits. C.I. Disperse Blue 79:1 is mutagenic in multiple strains of *Salmonella* (*in vitro*), but negative in the *in vivo* *Drosophila* sex-linked recessive lethal mutagenicity test. Because of its physical-chemical properties (a solid with low water solubility and high molecular weight), C.I. Disperse Blue 79:1 is not expected to have significant absorption and azo-reduction *in vivo*, which may explain its negative mutagenic response *in vivo*.

The supporting chemical, C.I. Disperse Blue 79, yielded negative results in both *in vitro* and *in vivo* genetic toxicity tests.

The potential health hazard C.I. Disperse Blue 79:1 is low.

APPENDIX

Summary Table of the Screening Information Data Set as Submitted under the U.S. HPV Challenge Program		
Endpoints	SPONSORED CHEMICAL C.I. Disperse Blue 79:1 (3618-72-2)	SUPPORTING CHEMICAL C.I. Disperse Blue 79 (12239-34-8)
Structure		
Summary of Environmental Effects – Aquatic Toxicity Data		
Fish 96-h LC ₅₀ (mg/L)	—*	—*
Aquatic Invertebrates 48-h EC ₅₀ (mg/L)	—*	—*
Aquatic Plants 72-h EC ₅₀ (mg/L) (growth) (biomass)	—*	—*
Chronic Toxicity to Fish 122-d NOEC (mg/L)	0.0048	—*
Summary of Human Health Data		
Acute Oral Toxicity LD ₅₀ (mg/kg-bw)	>2500	—*
Repeated-Dose Toxicity NOAEL/LOAEL Oral (mg/kg-bw/day)	NOAEL = 2500 (14-d) NOAEL = 2500	—*
Reproductive Toxicity NOAEL/LOAEL Oral (mg/kg-bw/day)	Evaluation of reproductive organs from the 90-day study indicated no effects.	—*
Developmental Toxicity NOAEL/LOAEL Oral (mg/L/day) Maternal Toxicity	(rat) NOAEL = 2000 (rabbit) NOAEL = 100 LOAEL = 300	—*
Developmental Toxicity	(rat) NOAEL = 2000 (rabbit) NOAEL = 600	

Summary Table of the Screening Information Data Set as Submitted under the U.S. HPV Challenge Program		
Endpoints	SPONSORED CHEMICAL C.I. Disperse Blue 79:1 (3618-72-2)	SUPPORTING CHEMICAL C.I. Disperse Blue 79 (12239-34-8)
Genetic Toxicity – Gene Mutation <i>In vitro</i>	Positive	Negative
Genetic Toxicity – Gene Mutation <i>In vivo</i>	Negative	—*
Genetic Toxicity – Chromosomal Aberrations <i>In vivo</i>	No Data Negative (RA)	Negative

– indicates endpoint was not addressed for this chemical; * indicates endpoint not necessary for supporting chemical; (RA) = Read Across

Screening Level Exposure Characterization for HPV Challenge Chemical

**Acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-
dinitrophenyl)azo]-4-methoxyphenyl]-
(Disperse Blue 79:1)**

CAS # 3618-72-2

July 2008

Prepared by

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Screening Level Exposure Characterization
Acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-methoxyphenyl]-

(Disperse Blue 79:1) (CAS # 3618-72-2)

Non-CBI Executive Summary

This exposure characterization was completed using both public, non-confidential sources, and one or more IUR submissions. Disperse Blue 79:1 (CAS # 3618-79-2) has an aggregated production and/or import volume in the United States of 10,000 to 500,000 pounds.¹² Disperse Blue 79:1 and related products are used almost exclusively for dyeing or printing polyester fibers¹³.

Exposure to the General Population and the Environment. Based on the information considered such as potential water releases, slow biodegradation, and a moderate persistence, known uses, EPA identifies, for purposes of risk-based prioritization, a medium relative ranking for potential exposure to the general population and the environment.

Exposure to Workers. Based on the totality of the information considered (primarily IUR data) in combination with Agency's professional judgment, EPA identifies, for the purposes of risk-based prioritization, a high relative ranking for potential worker exposure. This relative ranking is based mainly on potential inhalation and dermal exposures to particulates.

Exposure to Consumers. No uses in products intended to be used by consumers were reported in the IUR, nor were any found in other data sources. Although this chemical is used in fabric dyes, EPA's experience indicates that the dye process "fixes" the dye in the fiber, such that the chemical is not available for exposure simply through physical contact with the fabric. Accordingly, EPA identifies, for the purposes of risk-based prioritization, a low potential for consumer exposures.

Exposure to Children. No uses in products intended to be used by children were reported in the IUR, nor were any found in other data sources. Based on the same rationale as the consumer exposure scenario, EPA identifies, for the purposes of risk-based prioritization, a low potential for children's exposures.

Volume and Use Information

Disperse Blue 79:1 (CAS # 3618-79-2) has an aggregated production and/or import volume in the United States of 10,000 to 500,000 pounds.¹⁴ Non-confidential information in the Inventory

¹² USEPA, 2006 Partial Updating of TSCA Chemical Inventory.

¹³ USEPA, 1989. CI Disperse Blue 79:1; Testing Consent Order. Federal Register, Volume 54, Number 223, Tuesday, November 21, 1989. p. 48102. Accessed 4/16/08 at <http://www.epa.gov/oppt/chemtest/pubs/sun93.pdf>.

¹⁴ USEPA, 2006 Partial Updating of TSCA Chemical Inventory.

Update Rule (IUR) indicates that this chemical was produced and/ or imported at the following companies and sites: Ciba Specialty Chemicals Corporation, High Point, NC and DyStar L.P., Charlotte, NC. There may be other companies and sites that are claimed confidential. Persons submitting IUR information for 2005 asserted that some or all of the information was confidential. Only non-confidential reported IUR data are included in this summary.

No industrial processing and uses (IPUs) or commercial/ consumer uses of this chemical were reported in IUR submissions.

The High Production Volume submission for this chemical did not include information on use¹⁵.

Disperse Blue 79:1 and related products are used almost exclusively for dyeing or printing polyester fibers¹⁶. Other publicly-available data sources, including the Hazardous Substances Data Bank¹⁷ (HSDB), that were checked for this report did not indicate any uses of disperse blue 79:1.

Exposures to Workers

Based on the totality of the information considered (primarily IUR data) in combination with Agency's professional judgment, EPA identifies, for the purposes of risk-based prioritization, a high relative ranking for potential worker exposure. This relative ranking is based mainly on potential inhalation and dermal exposures to particulates. The following is a summary of relevant information affecting occupational exposure.

Summary of Parameters affecting Worker Exposure

Parameter	
Volume*	10,000-500,000 lbs
Physical Form(s)*	Dry powder, liquid
Vapor Pressure	Negligible
Concentration*	up to 60% by weight
Number of Industrial Workers*	less than 100 (see details below)
Uses	Dyeing or printing polyester fibers
Key MSDS Info	None available
Other hazard characteristics	None found

* Only non-confidential versions of reported IUR data are included in this summary.

Based on IUR data, the maximum total number of workers reasonably likely to be exposed to this chemical during manufacturing and industrial processing and use may be less than 100. There may be additional potentially exposed industrial workers that are not included since not all submitters were required to report on industrial processing and use. This does not include

¹⁵ USEPA, 2007a. <http://www.epa.gov/chemrtk/pubs/summaries/dbe/c13453tc.htm>.

¹⁶ USEPA, 1989. CI Disperse Blue 79:1; Testing Consent Order. Federal Register, Volume 54, Number 223, Tuesday, November 21, 1989. p. 48102. Accessed 4/16/08 at <http://www.epa.gov/oppt/chemtest/pubs/sun93.pdf>.

¹⁷ HSDB, 2008. Hazardous Substances Data Bank. Accessed, 4/4/08, Disperse blue 79:1. <http://toxnet.nlm.nih.gov/>.

potentially exposed commercial workers. The National Occupational Exposure Survey (NOES), conducted from 1981 to 1983, estimated a total of 46,074 workers potentially exposed to this chemical¹⁸. Differences between numbers of workers estimated by IUR submitters and by the NOES are attributable to many factors, including time, scope, and method of the estimates. For example, NOES estimates are for all workplaces while IUR are for industrial workplaces only, and NOES used a survey and extrapolation method while IUR submitters simply provide their best estimates based on available information for the specific reporting year.

Worker exposures by inhalation and dermal routes are possible for this chemical. This chemical is manufactured/ imported in powder and liquid forms. Past EPA assessment experience has shown that use and handling of powders, including many dyes, in workplaces often results in significant worker inhalation exposures to particulates. Dermal exposures are also possible to both the liquid and powder forms. Also, the non-confidential maximum concentration is 60% by weight. There may be other physical forms and concentrations that are claimed as confidential business information (CBI). This chemical has a negligible vapor pressure¹⁹. EPA experience has shown that worker exposures to vapors have not been an issue for chemicals with vapor pressures below 0.001 torr. This chemical's vapor pressure is at a level at which worker exposures to vapors may generally be considered insignificant for most common handling of liquids at ambient conditions. No additional information on worker exposure was found from public data search.

This chemical does not have OSHA Permissible Exposure Limits (PELs)²⁰.

Environmental Releases

Environmental releases may impact general population and environmental exposures. Factors affecting releases include volumes produced, processed and used; numbers of sites; and, processes of manufacture, processing, and use.

There are two non-confidential manufacturing sites and may be other confidential manufacturing and/ or import sites. The number of industrial processing and use sites is not reported.

The chemical is not on the Toxics Release Inventory²¹. No emission data was found from other sources.

Many chemicals used in dyeing and printing of fibers are used in aqueous processes and have releases to aqueous media. Disperse dyes are known to have exhaustion rates between 75% and

¹⁸ NIOSH, 1983. National Occupational Exposure Survey (NOES, 1981-1983). Accessed, 4/4/08. <http://www.cdc.gov/noes/srch-noes.html>.

¹⁹ USEPA, 2008. Screening-Level Hazard Characterization for High Production Chemical, Disperse Blue 79:1, 3618-72-2.

²⁰ NIOSH, 1988. OSHA PEL Project Documentation. <http://www.cdc.gov/niosh/pel88/npelcas.html>. Accessed, 4/7/08.

²¹ USEPA, 2006. Toxic Release Inventory. Accessed, 4/11/08. <http://www.epa.gov/tri/>.

95%²², which means that 5% to 25% of the amount used can be released in a water effluent before treatment. The actual percentage and quantity of release of the reported chemical associated with this use category are not known.

This chemical has a negligible vapor pressure²³. Experience has shown that air releases due to volatilization have not been an issue for chemicals with vapor pressures below 0.01 torr. This chemical's vapor pressure is at a level at which air releases may generally be considered insignificant from volatilization.

Exposures to the General Population and the Environment

Based on the information under the release section above, it is likely that there would be releases to water and during use in dyeing and printing of fibers. No uses were reported to the IUR. A search of additional relevant databases did not provide any further information on releases of this chemical. EPA assumes, for the purposes of risk-based prioritization, that the potential for environmental release and subsequent exposure to the general population and the environment are likely. The IUR ranking for general population and the environment is high due to the likelihood that there will be exposure to this chemical from releases during its use in the dyeing and printing of fibers.

C.I. disperse blue 79:1 is a solid at room temperature. It has low water solubility, negligible vapor pressure, and is minimally volatile. It is moderately mobile in soil. It is slow to biodegrade under aerobic conditions and hydrolysis is negligible under environmental conditions. Bioconcentration is expected to be low. The persistence and bioaccumulation ranking for C.I. disperse blue 79:1 is P2 (moderate) B1 (low). These ratings suggest that this chemical is persistent in the environment; and is not very bioaccumulative

Based on the information considered such as for potential water releases slow biodegradation, and a moderate persistence, known uses, and the Agency's expert judgment, EPA identifies, for purposes of risk-based prioritization, a medium relative ranking for potential exposure to the general population and the environment.

Exposures to Consumers

No uses in products intended to be used by consumers were reported in the IUR, nor were any found in other data sources. Although this chemical is used in fabric dyes, EPA's experience indicates that the dye process "fixes" the dye in the fiber, such that the chemical is not available for exposure simply through physical contact with the fabric. Accordingly, EPA identifies a low potential for consumer exposures.

²² USEPA 1992. Textile Dyes. From 1997 Chemical Engineering Branch Compilation of Generic Scenarios [for industry-specific workplace release and exposure estimation]. Accessed at <http://www.epa.gov/oppt/exposure/pubs/1997cebcollectionofindustriescenarios.zip>.

²³ USEPA, 2008. Screening-Level Hazard Characterization for High Production Chemical, Disperse Blue 79:1, 3618-72-2.

Exposures to Children

No uses in products intended to be used by children were reported in the IUR, nor were any found in other data sources. Based on the same rationale as the consumer exposure scenario, EPA identifies a low potential for children’s exposures.

Non Confidential IUR Data Summary

Manufacturing/ Import Information

Production and import volume: 10,000-500,000 lbs
 List of non-CBI companies/ sites*: Ciba Specialty Chemicals Corp. / NC
 DyStar L.P. / NC
 Highest non-CBI maximum concentration*: 60%
 Non-CBI physical forms*: Dry powder, liquid

* Note: There may be other companies/ sites, concentrations, and physical forms that are claimed CBI.

Table 1 Industrial Processing and Use Information Reported in 2006 IUR		
Processing Activity	Industrial Sector	Function in Ind. Sector
None reported		

Table 2 Commercial/ Consumer Uses Information Reported in 2006 IUR		
Commercial/ Consumer Product Category Description	Highest maximum concentration range	Use in Children’s Products
None reported		