TSCA Section 5(a)(3) Determination for Premanufacture Notice (PMN) P-18-0136

Number: P-18-0136
TSCA Section 5(a)(3) Determination: The chemical substance is not likely to present an unreasonable risk (5(a)(3)(C))

Chemical Name:
Generic: 1-Butanaminium, N,N,N-tributyl-, 2(or5)-[[benzoyldihydrodioxo[(sulfophenyl)amino]heteropolycycle]oxy]-5(or 2)-(1,1-dimethylpropyl)benzenesulfonate (2:1)

Conditions of Use (intended, known, or reasonably foreseen)[1]:
Intended conditions of use (generic): Import for use as a coloring agent, consistent with the manufacture, processing, use, and distribution described in the PMN.
Known conditions of use: Applying such factors as described in footnote 1, EPA evaluated whether there are known conditions and use and found none.
Reasonably foreseen conditions of use: Applying such factors as described in footnote 1, EPA evaluated whether there are reasonably foreseen conditions of use and found none.

Summary: The chemical substance is not likely to present an unreasonable risk of injury to health or the environment, without consideration of costs or other nonrisk factors, including an unreasonable risk to a potentially exposed or susceptible subpopulation identified as relevant by the Administrator under the conditions of use, based on the risk assessment presented below. Although EPA estimated that the new chemical substance could be very persistent, the new chemical substance has low potential for bioaccumulation, such that repeated exposures are not expected to be cumulative. Based on EPA's TSCA New Chemicals Program Chemical Category for Acid Dyes and Amphoteric Dyes[2] and test data on the chemical substance and analogous chemical substances, EPA estimates that the chemical substance has moderate environmental

[1] Under TSCA § 3(4), the term "conditions of use" means "the circumstances, as determined by the Administrator, under which a chemical substance is intended, known, or reasonably foreseen to be manufactured, processed, distributed in commerce, used, or disposed of." In general, EPA considers the intended conditions of use of a new chemical substance to be those identified in the section 5(a) notification. Known conditions of use include activities within the United States that result from manufacture that is exempt from PMN submission requirements. Reasonably foreseen conditions of use are future circumstances, distinct from known or intended conditions of use, under which the Administrator expects the chemical substance to be manufactured, processed, distributed, used, or disposed of. The identification of "reasonably foreseen" conditions of use will necessarily be a case-by-case determination and will be highly fact-specific. Reasonably foreseen conditions of use will not be based on hypotheticals or conjecture. EPA's identification of conditions of use includes the expectation of compliance with federal and state laws, such as worker protection standards or disposal restrictions, unless case-specific facts indicate otherwise. Accordingly, EPA will apply its professional judgment, experience, and discretion when considering such factors as evidence of current use of the new chemical substance outside the United States, evidence that the PMN substance is sufficiently likely to be used for the same purposes as existing chemical substances that are structurally analogous to the new chemical substance, and conditions of use identified in an initial PMN submission that the submitter omits in a revised PMN. The sources EPA uses to identify reasonably foreseen conditions of use include searches of internal confidential EPA PMN databases (containing use information on analogue chemicals), other U.S. government public sources, the National Library of Medicine's Hazardous Substances Data Bank (HSDB), the Chemical Abstract Service STN Platform, REACH Dossiers, technical encyclopedias (e.g., Kirk-Othmer and Ullmann), and Internet searches.

[2] TSCA New Chemicals Program (NCP) Chemical Categories. https://www.epa.gov/reviewing-new-chemicals-under-toxic-substances-control-act-tsca/chemical-categories-used-review-new.

hazard and potential for the following human health hazards: systemic toxicity from repeated exposures. EPA concludes that the new chemical substance is not likely to present an unreasonable risk under the conditions of use.

Fate: Environmental fate is the determination of which environmental compartment(s) a chemical moves to, the expected residence time in the environmental compartment(s) and removal and degradation processes. Environmental fate is an important factor in determining exposure and thus in determining whether a chemical may present an unreasonable risk. EPA estimated physical/chemical and fate properties of this new chemical substance using measured data submitted with the PMN and data on analogous chemicals. The chemical substance is estimated to be removed with an efficiency of 0-25 % during wastewater treatment due to low biodegradation, low sorption, and low stripping. Sorption to sludge is estimated to be low based on the measured octanol-water partition coefficient that was submitted with the PMN and data on analogous chemicals. Volatilization to air is estimated to be negligible based on high molecular volume and analogous chemicals. Sorption to soil and sediment is estimated to be low to moderate based on the measured octanol-water partition coefficient that was submitted for the PMN and data on analogous chemicals. Migration to groundwater is estimated to be moderate to rapid based on the measured octanol-water partition coefficient that was submitted with the PMN and data on analogous chemicals. Overall, these estimates are indicative of low potential for this chemical substance to volatilize into the air and a moderate to high potential for this chemical to migrate into ground water. Removal of the substance in wastewater treatment is unlikely due to low biodegradability, low sorption, and low stripping.

Persistence[3]: Persistence is relevant to whether a new chemical substance is likely to present an unreasonable risk because chemicals that are not degraded in the environment at rates that prevent substantial buildup in the environment, and thus increase potential for exposure, may present a risk if the substance presents a hazard to human health or the environment. Based on data for the new chemical substance and analogous chemicals, EPA estimated the aerobic and anaerobic biodegradation half-lives to be greater than six months. These estimates for biodegradation indicate that the chemical substance may be very persistent in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediment).

Bioaccumulation[4]: Bioaccumulation is relevant to whether a new chemical substance is likely to present an unreasonable risk because substances that bioaccumulate in aquatic and/or terrestrial species pose the potential for elevated exposures to humans and other organisms via

[3] Persistence: A chemical substance is considered to have limited persistence if it has a half-life in water, soil or sediment of less than 2 months or there are equivalent or analogous data. A chemical substance is considered to be persistent if it has a half-life in water, soil or sediments of greater than 2 months but less than or equal to 6 months or if there are equivalent or analogous data. A chemical substance is considered to be very persistent if it has a half-life in water, soil or sediments of greater than 6 months or there are equivalent or analogous data. (64 FR 60194; November 4, 1999)

[4] Bioaccumulation: A chemical substance is considered to have a low potential for bioaccumulation if there are bioconcentration factors (BCF) or bioaccumulation factors (BAF) of less than 1,000 or there are equivalent or analogous data. A chemical substance is considered to be bioaccumulative if there are BCFs or BAFs of 1,000 or greater and less than or equal to 5,000 or there are equivalent or analogous data. A chemical substance is considered to be very bioaccumulative if there are BCFs or BAFs of 5,000 or greater or there are equivalent or analogous data. (64 FR 60194; November 4 1999)

food chains. The new chemical substance has a low bioaccumulation potential based on high molecular volume, which limits bioavailability and bioaccumulation. Although EPA estimated that the new chemical substance could be very persistent, the chemical substance has low potential for bioaccumulation, such that repeated exposures are not expected to cause food chain effects via accumulation in exposed organisms.

Human Health Hazard[5]: Human health hazard is relevant to whether a new chemical substance is likely to present an unreasonable risk because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated the human health hazard of this chemical substance based on test data submitted for the new chemical and for analogous chemical substances. The submission included test data on both the new chemical substance and an analogue to the cation. EPA determined that the submitted analogue was not appropriate, and therefore EPA utilized the submitted data on the new chemical substance as well as data from alternative analogues to assess the anion and cation components of the new chemical substance. For this new chemical substance, EPA estimates absorption to be nil through the skin based on physical/chemical properties, and poor to nil through the GI tract and lungs based on physical/chemical properties and submitted data. During the initial assessment, EPA identified irritation as a hazard based on analogue data, which indicated that the anion and cation components may each cause irritation. Inconclusive results were reported in an *in vitro* skin irritation test (OECD 439) with the new chemical substance, but no irritation or corrosion to skin was observed in an acute dermal study (OECD 404) conducted with the new chemical substance. Therefore, EPA concludes that the new chemical substance is not an irritant. Genotoxicity bioassays (three types) conducted with both the anionic and cationic component analogues were all negative. Likewise, tests with both the anion analogues and the cation analogue showed negative results in sensitization bioassays (OECD 429 and 406). Tests of acute toxicity for analogues of both the anion and cation showed oral LD_{50}s greater than 300 and less than 2000 mg/kg. In a repeated-dose (28-day) study with an analogue of the anion, effects on stomach were noted at 150 mg/kg, but attributed to irritation of the stomach. In repeated-dose tests with an analogue of the cation, no (18-day) or equivocal (28-day) systemic effects were observed at high doses (e.g., 1000 mg/kg-day).

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[5] A chemical substance is considered to have low human health hazard if effects are observed in animal studies with a No Observed Adverse Effect Level (NOAEL) equal to or greater than 1,000 mg/kg/day or if there are equivalent data on analogous chemical substances; a chemical substance is considered to have moderate human health hazard if effects are observed in animal studies with a NOAEL less than 1,000 mg/kg/day or if there are equivalent data on analogous chemical substances; a chemical substance is considered to have high human health hazard if there is evidence of adverse effects in humans or conclusive evidence of severe effects in animal studies with a NOAEL of less than or equal to 10 mg/kg/day or if there are equivalent data on analogous chemical substances. EPA may also use Benchmark Dose Levels (BMDL) derived from benchmark dose (BMD) modeling as points of departure for toxic effects. See https://www.epa.gov/bmds/what-benchmark-dose-software-bmds. Using this approach, a BMDL is associated with a benchmark response, for example a 5 or 10 % incidence of effect. The aforementioned characterizations of hazard (low, medium, high) would also apply to BMDLs. In the absence of animal data on a chemical or analogous chemical substance, EPA may use other data or information such as from in vitro assays, chemical categories (e.g., Organization for Economic Co-operation and Development, 2014 Guidance on Grouping of Chemicals, Second Edition. ENV/JM/MONO(2014)4. Series on Testing & Assessment No. 194. Environment Directorate, Organization for Economic Co-operation and Development, Paris, France. (http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2014)4&doclanguage=en)), structure-activity relationships, and/or structural alerts to support characterizing human health hazards.

Environmental Hazard[6]: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risk because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using hazard data submitted for the new chemical substance and on analogous chemicals. The new chemical substance falls within the TSCA New Chemicals Program Chemical Category of Acid Dyes and Amphoteric Dyes. Acute toxicity values estimated for fish, aquatic invertebrates, and algae are >43 mg/L (data on an analogue), 1.93 mg/L (data on the new chemical substance), and 1.2 mg/L (data on an analogue), respectively. Chronic toxicity values estimated for fish, aquatic invertebrates, and algae are >10 mg/L (SARs for anionic dyes), 0.193 mg/L (data on the new chemical substance with an ACR of 10), and <0.21 mg/L (data on an analogue), respectively. These toxicity values indicate that the new chemical substance is expected to have moderate environmental hazard. Application of assessment factors of 4 and 10 to acute and chronic toxicity values, respectively, results in acute and chronic concentrations of concern (COCs) of 0.3 mg/L (300 ppb) and 0.0193 mg/L (19 ppb), respectively.

Exposure: The exposure to a new chemical substance is potentially relevant to whether a new chemical substance is likely to present unreasonable risks because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance.

EPA estimates occupational exposure and environmental release of the new chemical substance under the intended conditions of use described in the PMN using ChemSTEER (Chemical Screening Tool for Exposures and Environmental Releases https://www.epa.gov/tsca-screening-tools/chemsteer-chemical-screening-tool-exposures-and-environmental-releases). EPA uses EFAST (the Exposure and Fate Assessment Screening Tool; https://www.epa.gov/tsca-screening-tools/e-fast-exposure-and-fate-assessment-screening-tool-version-2014) to estimate general population, consumer, and environmental exposures.

EPA considers workers to be a potentially exposed or susceptible subpopulation (PESS) on the basis of greater exposure potential compared to the general population. EPA also considers PESS in conducting general population drinking water exposures by evaluating risks associated with water intake rates for multiple age groups, ranging from infants to adults. EPA considers consumers of specific products to be a potentially exposed or susceptible subpopulation on the basis of greater exposure potential compared to the general population who do not use specific products.

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[6] A chemical substance is considered to have low ecotoxicity hazard if the Fish, Daphnid and Algae LC50 values are greater than 100 mg/L, or if the Fish and Daphnid chronic values (ChVs) are greater than 10.0 mg/L, or there are not effects at saturation (occurs when water solubility of a chemical substance is lower than an effect concentration), or the log Kow value exceeds QSAR cut-offs. A chemical substance is considered to have moderate ecotoxicity hazard if the lowest of the Fish, Daphnid or Algae LC50s is greater than 1 mg/L and less than 100 mg/L, or where the Fish or Daphnid ChVs are greater than 0.1 mg/L and less than 10.0 mg/L. A chemical substance is considered to have high ecotoxicity hazard, or if either the Fish, Daphnid or Algae LC50s are less than 1 mg/L, or any Fish or Daphnid ChVs is less than 0.1 mg/L (Sustainable Futures https://www.epa.gov/sustainable-futures/sustainable-futures-p2-framework-manual).

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For this new chemical assessment, EPA did not assess exposures for workers, the general population, consumers or the environment because the form in which the new chemical substance is imported and handled prevents exposure.

Risk Characterization: Risks were not identified for human health from the new chemical substance. Risks posed by the substance were not quantified but are estimated to be negligible due to negligible human exposure under the conditions of use.

Risks to the environment were not identified because there are no expected releases to water.

Because the new chemical substance will be contained [claimed CBI] in a manner that prevents exposure, EPA has determined that the new chemical substance is not likely to present unreasonable risk to human health or the environment under the conditions of use.

11/20/2018 /s/

Date: Jeffery T. Morris, Director
Office of Pollution Prevention and Toxics