

TSCA Section 5(a)(3) Determination for Premanufacture Notice (PMN) P-18-0382

Number: P-18-0382

TSCA Section 5(a)(3) Determination: The chemical substance is not likely to present an unreasonable risk (5(a)(3)(C)).

Chemical Name:

Generic: Xanthylium, bis[dicarboxycyclic]sulfonylamino-alkylcyclicamino-disulfo-sulfocyclic-, inner salt, monocationic salt

Conditions of Use (intended, known, or reasonably foreseen)¹:

Intended conditions of use (generic): Import and process for use as and use as dye for printing ink, consistent with the manufacturing, processing, use, distribution, and disposal information described in the PMN.

Known conditions of use: Applying such factors as described in footnote 1, EPA evaluated whether there are known conditions of use and found the same use as the intended use.

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. The new chemical substance is a salt that is comprised of both an anion and cation ([claimed CBI]). Although EPA estimated that the anion could be very persistent, the substance has a low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms. Estimations of physical/chemical and fate properties are not applicable for the cation ([claimed CBI]); the cation ([claimed CBI]) is [claimed CBI] and is unlikely to impact the overall persistence and bioaccumulation of the new chemical substance. Based on available data on the new chemical substance and by comparing it

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.

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to structurally analogous chemical substances for which there is information on human health hazard, EPA estimates that the chemical substance has moderate environmental hazard and potential for the following human health hazards: systemic effects. 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 the anion using data for analogue(s) (soluble, non-azo dyes) and data submitted for the new chemical substance. The cation ([claimed CBI]) is not expected to drive the human health and eco hazard assessments. The cation ([claimed CBI]) is also not expected to be a concern for food chain effects and was not evaluated for persistence and bioaccumulation. In wastewater treatment, the anion is expected to be removed with an efficiency of 0% due to low biodegradability, low sorption, and low stripping. Removal of the anion by biodegradation is negligible. Sorption of the anion to sludge, soil, and sediment is expected to be low. Migration of the anion to groundwater is expected to be rapid due to low sorption to soil and sediment. Due to low estimated vapor pressure and Henry's law constant, the anion is expected to undergo negligible volatilization to air. Overall, these estimates indicate that the anion has low potential to volatilize to air and has high potential to migrate to groundwater.

Persistence²: 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. EPA estimated degradation half-lives of the new chemical substance using data for analogue(s) (soluble, non-azo dyes) and data submitted for the new chemical substance. EPA estimated that the new chemical substance's aerobic and anaerobic biodegradation half-lives are > 6 months. These estimates indicate that the new chemical substance may be very persistent in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediment).

Bioaccumulation³: 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 food chains. EPA estimated the potential for the new chemical substance to bioaccumulate using data for

² 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)

³ 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)

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analogues (soluble, non-azo dyes). EPA estimated that the new chemical substance has low bioaccumulation potential based on data for soluble, non-azo dyes in addition to high water solubility, which increases elimination. Although EPA estimated that the new chemical substance could be very persistent, the substance has a low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms.

Human Health Hazard⁴: 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 (and 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 its estimated physical/chemical properties, available data on the new chemical substance, and by comparing it to structurally analogous chemical substances for which there is information on human health hazard. Absorption is expected to be nil via all routes when neat and poor via the lungs and gastrointestinal (GI) tract when in solution based on physical/chemical properties. For the new chemical substance, EPA identified hazards for systemic effects based on analogue data. EPA identified a NOAEL of 500 mg/kg-bw/day based on systemic effects (decreased food intake, growth retardation, and increased kidney/testes weights) in a 90-day oral toxicity study (Test Guideline Not Specified). EPA considered this value protective for all health concerns identified and was used to derive exposure route- and population-specific points of departure for quantitative risk assessment.

Environmental Hazard⁵: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risk because the significance of the risk is dependent

⁴ 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](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.

⁵ 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

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upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA determined the environmental hazard for this new chemical substance based on acute toxicity data submitted for the new chemical substance. This substance falls within the TSCA New Chemicals Category of Acid Dyes and Amphoteric Dyes.⁶ Acute toxicity values measured for fish, aquatic invertebrates, and algae are >98.8 mg/L, >100 mg/L, and 100 mg/L, respectively. Chronic toxicity values measured for fish, aquatic invertebrates, and algae are >9.88 mg/L (Acute-to-Chronic Ratio (ACR) of 10), >10 mg/L (ACR of 10), and 1.78 mg/L, respectively. These toxicity values indicate that the new chemical substance is expected to have moderate environmental hazard. Application of assessment factors of 5 and 10 to acute and chronic toxicity values, respectively, results in acute and chronic concentrations of concern of 19.76 mg/L (or 19,760 ppb) and 0.178 mg/L (or 178 ppb).

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.

For this assessment, EPA assessed worker exposures via the dermal route; inhalation exposures are not expected. Releases to water, landfill, and air were estimated. Exposure to the general population was assessed via drinking water. Exposures to the general population via inhalation and groundwater ingestion impacted by landfill leaching were not assessed because releases to air and to landfills are expected to be negligible (below modeling thresholds) or via fish ingestion because bioaccumulation potential was evaluated to be low. EPA assessed consumer exposures via the dermal route.

ChVs is less than 0.1 mg/L (Sustainable Futures <https://www.epa.gov/sustainable-futures/sustainable-futures-p2-framework-manual>).

⁶ 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>.

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Risk Characterization: EPA assesses risks to workers considering engineering controls described in the PMN but in the absence of personal protective equipment (PPE) such as gloves and respirators. If risks are preliminarily identified, EPA then considers whether the risks would be mitigated by the use of PPE (e.g., impervious gloves, respirator).

Risks were not identified for workers for systemic effects via dermal exposure based on quantitative hazard data for an analogue (MOE = 2,545; Benchmark MOE = 100). Risks were not evaluated for workers via inhalation because exposures are expected to be negligible.

Risks were not identified for the general population for systemic effects via drinking water based on quantitative hazard data for an analogue (MOE_{Drinking Water (DW) adults} > 100,000; MOE_{DW infants} > 100,000; Benchmark MOE = 100). Risks were not evaluated for the general population via fish ingestion because bioaccumulation potential was evaluated to be low. Risks were not evaluated for the general population via groundwater ingestion impacted by landfill leaching or stack/fugitive air inhalation because exposures are expected to be negligible. Risks were not identified for consumers for systemic effects via dermal exposure based on quantitative hazard data for an analogue (MOE > 10,000,000; Benchmark MOE = 100).

Risks to the environment were evaluated by comparing estimated surface water concentrations with the estimated acute and chronic COCs. Risks from acute and chronic exposures to the environment were not identified due to releases to water that did not exceed the acute or chronic COC.

Because no unreasonable risks to workers, the general population, consumers, or environment were identified, 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.

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Date:

/s/

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