TSCA Section 5(a)(3) Determination for Premanufacture Notice (PMN) P-18-0068

Number: P-18-0068
TSCA Section 5(a)(3) Determination: The chemical substance is not likely to present an unreasonable risk (5(a)(3)(C))

Chemical Name:
Generic: Metal, oxo alkylcarboxylate complexes

Conditions of Use (intended, known, or reasonably foreseen)[1]:
Intended conditions of use (generic): Manufacture for use as, and use as a polymer composite additive, 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 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 hydrolysis products of the new chemical substance may be persistent or very persistent, the hydrolysis products have low potential for bioaccumulation, such that repeated exposures are not expected to be cumulative. Based on EPA's TSCA New Chemicals Program Chemical Categories for [claimed CBI] and Respirable, Poorly Soluble Particulates[2] and test data on analogous chemical substances, EPA estimates that the chemical substance has low environmental hazard and potential for the following human health hazards:

[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.

skin, eye, and lung irritation and pulmonary 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 this new chemical substance and its hydrolysis products using data for analogous chemicals and EPI (Estimation Programs Interface) Suite™, a suite of physical/chemical property and environmental fate estimation programs (http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface). The new chemical substance is estimated to be removed during wastewater treatment with an efficiency of 90% via sorption and slow hydrolysis. The one hydrolysis product, [claimed CBI], is estimated to be removed during wastewater treatment with an efficiency of 90% via sorption and biodegradation, and the other hydrolysis product, [claimed CBI], is estimated to be removed with an efficiency of 90% via sorption. For the new chemical substance, removal by biodegradation is expected to be negligible based on data for high molecular volume substances. Removal by biodegradation is expected to be high for one hydrolysis product, [claimed CBI], based on the structure and negligible for the other hydrolysis product, [claimed CBI], based on structure and data on analogous chemicals.

For the new chemical substance, sorption to sludge is estimated to be strong based on data for high molecular volume substances and sorption to soil and sediment is also estimated to be strong. For one hydrolysis product, [claimed CBI], sorption to sludge is estimated to be strong based on estimated physical/chemical properties and sorption to soil and sediment is also expected to be strong. For the other hydrolysis product, [claimed CBI], sorption to sludge is estimated to be strong based on the structure and data on analogous chemicals and sorption to soil and sediment is also estimated to be strong. The estimates of strong sorption result in slow migration to groundwater for the new chemical substance and its hydrolysis products. Volatilization to air is estimated to be negligible for the new chemical substance because of the high molecular volume, negligible for the one hydrolysis product, [claimed CBI], based on estimated physical/chemical properties, and negligible for the other hydrolysis product, [claimed CBI], based on structure and data for analogous chemicals. Overall, these estimates are indicative of low potential for this chemical substance and its hydrolysis products to volatilize into the air and a low potential to migrate into groundwater.

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

[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)

data for analogous chemicals, EPA estimated the hydrolysis half-life of the new chemical substance to be days to weeks. Based on data for analogous chemicals, one hydrolysis product's, [claimed CBI], anaerobic biodegradation half-life is estimated to be months based on the aerobic biodegradation half-life; the aerobic biodegradation half-life is estimated to be weeks. Based on data for analogous chemicals, the other hydrolysis product's, [claimed CBI], anaerobic and aerobic biodegradation half-lives are estimated to be greater than six months. These estimates for biodegradation indicate that the new chemical substance will not be persistent in aerobic environments (e.g., surface water) or anaerobic environments (e.g., sediment). The estimates indicate that the one hydrolysis product, [claimed CBI], may be persistent in anaerobic environments, and the other hydrolysis product, [claimed CBI], may be very persistent in both aerobic and anaerobic environments.

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 food chains. The new chemical substance has low bioaccumulation potential based on hydrolysis. One hydrolysis product, [claimed CBI], has low bioaccumulation potential based on physical/chemical properties and metabolism of [claimed CBI] (bioconcentration/bioaccumulation factor = 100). The other hydrolysis product [claimed CBI], has low bioaccumulation potential based on data on analogous chemicals. Although EPA estimated that the hydrolysis products could be persistent or very persistent, the chemical substance and its hydrolysis products have 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

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[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)

[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.

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 new chemical substance based on its estimated physical/chemical properties and analogous chemical substances for which there is information on human health hazard. Absorption of the new chemical substance is expected to be poor by all routes of exposure based on physical/chemical properties. For the new chemical substance, EPA identified lung overload as a potential hazard based on the TSCA New Chemicals Program Chemical Category of Respirable, Poorly Soluble Particulates, and for skin, eye, and lung irritation based on information in the Safety Data Sheet provided by the submitter. EPA identified skin sensitization as a potential hazard to the extent a component, [claimed CBI], of the substance is bioavailable; in an occupational setting it is not expected to be bioavailable. EPA identified a NOAEC of 4 mg/m^3 for lung overload from a 90-day inhalation toxicity study with an analogue described in the TSCA New Chemical Category for Respirable, Poorly Soluble Particulates. This NOAEC was used to derive exposure route- and population-specific points of departure for quantitative risk assessment, described below.

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. The new chemical substance falls within the TSCA New Chemicals Program Chemical Category of [claimed CBI]. EPA estimated environmental hazard of this new chemical substance based on the negligible water solubility of the new chemical substance. Hazards from acute and chronic exposures are not expected at concentrations up to the water solubility limit of the new chemical substance (i.e., no effects at saturation). These toxicity values indicate that the new chemical substance is expected to have a low environmental hazard. Because no effects are expected at any concentration soluble in water, no concentrations of concern were identified.

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

[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).

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 new chemical assessment, EPA assessed exposure to workers via the inhalation route based on potential generation of respirable poorly soluble particles during processing and use scenarios. EPA also assessed exposure to workers via the dermal route. Releases to water and air were estimated. Exposure to the general population was assessed via drinking water. Exposure to the general population via inhalation was not assessed because releases to air are expected to be negligible (below modeling thresholds). Exposures to consumers were not assessed because consumer uses were not identified as conditions of use. Exposure to aquatic organisms was not quantitatively assessed because environmental hazards are not expected for the new chemical substance up to the water solubility limit.

Risk Characterization: EPA applies a margin of exposure approach to calculate potential human health risks of new chemicals. A benchmark (acceptable) margin of exposure is derived by applying uncertainty factors for the following types of extrapolations: intra-species extrapolation (UF_H = 10 to account for variation in sensitivity among the human population), inter-species extrapolation (UF_A = 10 to account for extrapolating from experimental animals to humans) and LOAEL-to-NOAEL extrapolation (UF_L = 10 to account for using a LOAEL when a NOAEL is not available). Hence, in the New Chemicals Program, a benchmark MOE is typically 100 and 1000 when NOAELs and LOAELs, respectively, are used to identify hazard. When allometric scaling or pharmacokinetic modeling is used to derive an effect level, the UF_H may be reduced to 3, for a benchmark MOE of 30. The benchmark MOE is used to compare to the MOE calculated by comparing the toxicity NOAEL or LOAEL to the estimated exposure concentrations. When the calculated MOE is equal to or exceeds the benchmark MOE, the new chemical substance is not likely to present an unreasonable risk. 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 to human health for the new chemical substance were evaluated using the route-specific effect level (i.e., NOAEC) described above. Risks were identified for workers for lung effects from lung overload via inhalation (MOE = 70; benchmark MOE = 100). Risks can be mitigated if exposures can be controlled by the use of appropriate, effective PPE, including a respirator with an APF of 10. Irritation hazard to workers was identified, but cannot be quantified due to lack of dose-response information for this hazard. However, exposures can be controlled by the appropriate use of PPE, such as gloves, eye protection, and respiratory protection. EPA expects

that workers will use appropriate PPE consistent with the Safety Data Sheet prepared by the submitter, in a manner adequate to protect them. Sensitization hazard to workers was not identified because the sensitizing component of the new chemical substance, [claimed CBI], is not expected to be bioavailable in an occupational setting.

Sensitization hazard to the general population via ingestion of drinking water is not expected because sensitization is unlikely via this exposure route. Irritation hazard to the general population via drinking water is not expected due to the low concentrations estimated to be in water. Risks were not evaluated for the general population for lung overload via inhalation because releases to air are expected to be negligible (below modeling thresholds). Risks to consumers were not evaluated because consumer uses were not identified as conditions of use.

Due to low environmental hazard, EPA believes that this chemical substance is not likely to present an unreasonable risk to the environment even if potential exposures were high.

Because worker exposures can be controlled by PPE, no unreasonable risks to the general population or environment were identified, and there are no expected consumer exposures, 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.

12/12/18
Date:

/s/
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