TSCA Section 5(a)(3) Determination for Premanufacture Notice (PMN) P-18-0197

Number: P-18-0197
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, alkylcarboxylate oxo complexes

Conditions of Use (intended, known, or reasonably foreseen)[1]:
Intended conditions of use (generic): Manufacture and process for 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 new chemical substance and the hydrolysis product ([claimed CBI]) could be persistent, the substances have a low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms. Although EPA estimated that the hydrolysis product ([claimed CBI] oxides) could be very persistent, the substance does not bioaccumulate by lipophilic partitioning and there is low concern that it will accumulate in organisms by other mechanisms; thus, repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms. Based on physical/chemical properties and data for analogous chemical substances, EPA estimates that the

[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.

chemical substance has low environmental hazard and potential for the following human health hazards: lung overload and irritation. 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 new chemical substance using data for analogue(s) (reactive polymers); of the hydrolysis product ([claimed CBI]) using data for analogue(s) ([claimed CBI]); and of the hydrolysis product ([claimed CBI] oxides) using data for analogues (metal oxides). In wastewater treatment, the new chemical substance is expected to be removed with an efficiency of 90% due to sorption and hydrolysis; the hydrolysis product ([claimed CBI]) is expected to be removed with an efficiency of 90% due to sorption and biodegradation; and the hydrolysis product ([claimed CBI] oxides) is expected to be removed with an efficiency of 90% due to sorption. Removal of the new chemical substance by biodegradation is negligible; removal of the hydrolysis product ([claimed CBI]) by biodegradation is high; and removal of the hydrolysis product ([claimed CBI] oxides) by biodegradation is negligible. Sorption of the new chemical substance and the hydrolysis product ([claimed CBI]) to sludge, soil, and sediment is expected to be strong; and sorption of the hydrolysis product ([claimed CBI] oxides) to sludge is expected to be strong and to soil and sediment is expected to be very strong. Migration of the new chemical substance and the hydrolysis product ([claimed CBI]) to groundwater is expected to be slow due to strong sorption to soil and sediment; and migration of the hydrolysis product ([claimed CBI] oxides) to groundwater is expected to be negligible due to very strong sorption to soil and sediment. Due to low estimated vapor pressure and Henry's law constant, the new chemical substance; the hydrolysis product ([claimed CBI]); and the hydrolysis product ([claimed CBI] oxides) are expected to undergo negligible volatilization to air. Overall, these estimates indicate that the new chemical substance, the hydrolysis product ([claimed CBI]), and the hydrolysis product ([claimed CBI] oxides) have low potential to volatilize to air and low potential to migrate to groundwater.

Persistence[2]: 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) (reactive polymers); of the hydrolysis product ([claimed CBI]) using data for analogue(s) ([claimed CBI]); and of the hydrolysis product ([claimed CBI] oxides) using data for analogues (metal oxides). EPA estimated that the new chemical substance's aerobic and anaerobic

[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)

biodegradation half-lives range from < 2 months to 6 months and its hydrolysis half-life is weeks; the hydrolysis product ([claimed CBI]) has an aerobic biodegradation half-life of < 2 months and anaerobic biodegradation half-life of 2 to 6 months; and the hydrolysis product ([claimed CBI] oxides) have aerobic and anaerobic biodegradation half-lives of > 6 months. These estimates indicate that the new chemical substance may be persistent in aerobic environments (e.g., surface water) and in anaerobic environments (e.g., sediments). Further, these estimates indicate that the hydrolysis product ([claimed CBI]) may have limited persistence in aerobic environments (e.g., surface water) and may be persistent anaerobic environments (e.g., sediment). These estimates also indicate that the hydrolysis product ([claimed CBI] oxides) may be very persistent in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediment).

Bioaccumulation[3]: 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 analogue(s) (reactive polymers), of the hydrolysis product ([claimed CBI]) to bioaccumulate using data for analogue(s) ([claimed CBI]) and of the hydrolysis product ([claimed CBI] oxides) to bioaccumulate using data for analogues (metal oxides). EPA estimated that the new chemical substance has low bioaccumulation potential based on hydrolysis and that the hydrolysis product ([claimed CBI]) has low bioaccumulation potential based on bioconcentration or bioaccumulation data reported for [claimed CBI]. EPA also estimated that the hydrolysis product ([claimed CBI] oxides) does not bioaccumulate by lipophilic partitioning, and there is low concern that it may accumulate in organisms by other mechanisms. Although EPA estimated that the new chemical substance and the hydrolysis product ([claimed CBI]) could be persistent, the substances have a low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms. In addition, although EPA estimated that the hydrolysis product ([claimed CBI] oxides) could be very persistent, the substance does not bioaccumulate by lipophilic partitioning and there is low concern that it will accumulate in organisms by other mechanisms; thus, repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms.

Human Health Hazard[4]: 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

[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)

[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

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 its estimated physical/chemical properties and by comparing it to structurally analogous chemical substance for which there is information on human health hazard. Absorption of the new chemical is expected to be nil via all routes based on physical/chemical properties. For the new chemical substance, EPA identified lung overload as a hazard based on the substance being a respirable, poorly soluble particulate and respiratory irritation as a hazard is based on its reactivity in water. EPA identified a NOAEC of 10 mg/m^3 based on lung effect, which was used to derive exposure route- and population-specific points of departure for quantitative risk assessment, described below. Respiratory irritation was assessed qualitatively.

Environmental Hazard[5]: 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 predictions based on the negligible water solubility of the new chemical substance. Acute and chronic toxicity values estimated for fish, aquatic invertebrates, and algae are all no effects at saturation. These toxicity values indicate that the new chemical substance is expected to have low environmental hazard. Because hazards are not expected up to the water solubility limit, acute and chronic concentrations of concern are not 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

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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.

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

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 new chemical assessment, EPA assessed worker exposure via inhalation exposure. Dermal exposure to workers was not assessed since no hazards were identified for this route of exposure. Releases to air were estimated. Releases to water and landfill were not estimated. EPA assessed general population exposure via inhalation exposure to fugitive emissions, but not to water or landfill since no hazards were identified for this route. EPA did not assess consumer exposure since consumer uses were not identified as conditions of use.

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 1,000 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 levels (i.e., NOAEC) described above. Risks were not identified for workers for lung effects via inhalation based on quantitative hazard data for an analogue (MOE = 690; benchmark MOE = 100). Irritation hazards to workers via inhalation were identified based on the reactivity of the new chemical substance. Risks for these endpoints were not quantified due to a lack of dose-response for this hazard. However, exposures can be mitigated by the use of appropriate personal protective equipment (PPE), including respiratory protection. EPA expects that employers will require and that workers will use appropriate PPE consistent with the Safety Data

Sheet prepared by the new chemical submitter, in a manner adequate to protect them. Risks were not evaluated for workers via dermal exposure since no hazards were identified for this route of exposure.

Risks were not identified for the general population for lung effects via fugitive air inhalation based on quantitative hazard data for an analogue (MOE >> 10,000; benchmark MOE = 100). Risks to the general population via oral and dermal routes were not evaluated since no exposures are expected via these routes. Risks to consumers were not assessed because consumer use was not identified as a condition of use.

Risks to the environment from acute and chronic exposure are not expected at any concentration of the new chemical substance soluble in the water (i.e., no effects at saturation).

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.

8/9/2019 /s/

Date: Tala R. Henry, Ph.D.
Deputy Director for Programs
Office of Pollution Prevention and Toxics