TSCA Section 5(a)(3) Determination for Premanufacture Notice (PMN) P-19-0029

Number: P-19-0029
TSCA Section 5(a)(3) Determination: The chemical substance is not likely to present an unreasonable risk (5(a)(3)(C))

Chemical Name:
Specific: Phosphonium, tributylethyl-, diethyl phosphate (1:1); CASRN 20445-94-7

Conditions of Use (intended, known, or reasonably foreseen)[1]:
Intended conditions of use (generic): Import for use as a catalyst, 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 that the new chemical substance is imported for use as catalyst, additive, extractant, solvent and polymer additive based on other TSCA submissions.

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, based on a patent search, the following reasonably foreseen uses: composite micro-capsule stopping agent for preventing spontaneous combustion of coal; biodegradable and biosourced polymers for use in manufacturing of plastic bags; Ionic liquid crosslinker for epoxy composites with thermoplastic polymer or rubber; carbon dioxide absorbent; ionic liquid release coat for use in metal flake manufacture; and component in cellulose-conducting polymer composites for solar cells.

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 and

[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.

the terms of the proposed Significant New Use Rule (SNUR) signed by EPA.[2] EPA estimated that the anion and the anion degradant (phosphate) could have limited persistence and 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 cation could be 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. Based on its estimated physical/chemical properties, available data on the new chemical substance, and by comparing it to structurally analogous chemical substances, EPA estimates that the chemical substance has moderate environmental hazard and potential for the following human health hazards: neurotoxicity, reproductive and developmental toxicity, liver toxicity, irritation and possible corrosion. The PMN describes conditions of use that mitigate the human health and environmental risks. Therefore, EPA concludes that the new chemical substance is not likely to present an unreasonable risk under the intended conditions of use.

As set forth below, the information available to EPA is sufficient to permit the Agency to conduct a reasoned evaluation of the health and environmental effects of the chemical substance under the conditions of use that are not subject to the proposed SNUR, in order to determine that the chemical substance is not likely to present an unreasonable risk under those conditions of use. As such, EPA does not need to impose testing requirements to conduct this evaluation. Whether testing is needed to evaluate the effects of the intended, known, or reasonably foreseen conditions of use of a chemical substance subject to a PMN is determined on a case-by-case basis. To the extent that testing may be necessary to conduct a reasoned evaluation of the health or environmental effects of the reasonably foreseen conditions of use that are subject to the proposed SNUR, EPA will make the appropriate determination if a SNUN is submitted following finalization of the SNUR.

EPA previously assessed the known conditions of use, assessed the intended conditions of use, and addressed reasonably foreseen conditions of use by proposing a SNUR. Therefore, EPA determines the new chemical substance is not likely to present unreasonable risk to human health or the environment.

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

[2] Reasonably foreseen conditions of use subject to a proposed SNUR are not likely to present an unreasonable risk of injury to health or the environment. Based on EPA's experience, it is the Agency's judgment that a new use would not commence during the pendency of a proposed SNUR because web posting of a proposed SNUR serves as the cut-off date for a significant new use. Therefore, manufacturers and processors would not commence a prohibited new use that would be legally required to cease upon the finalization of the SNUR. Once a SNUR is final and effective, no manufacturer or processor – including the PMN submitter – may undertake the conditions of use identified as a significant new use of the PMN substance in the SNUR. EPA must first evaluate the new use in accordance with the requirements of TSCA Section 5 and (a) either conclude that the new use is not likely to present an unreasonable risk under the conditions of use; or (b) take appropriate action under section 5(e) or 5(f). If EPA were not to finalize the proposed SNUR, then that decision would be based on information and data provided to the Agency during the comment period demonstrating that the reasonably foreseen conditions of use subject to the proposed SNUR are not likely to present an unreasonable risk. Under either scenario, the reasonably foreseen condition of use is not likely present an unreasonable risk.

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) (alkyl phosphate); of the cation using data for analogue(s) (alkyl phosphonium); and of the anion degradant (phosphate) using data for analogue(s) (phosphate). In wastewater treatment, the anion is expected to be removed with an efficiency of 90% due to biodegradation; the cation is expected to be removed with an efficiency of 50% to 90% due to sorption and possible biodegradation; and the anion degradant (phosphate) is expected to be removed with an efficiency of 35% due to possible biodegradation. Removal of the anion by biodegradation is moderate to high; removal of the cation by biodegradation is negligible to moderate; and removal of the anion degradant (phosphate) by biodegradation is negligible to moderate. Sorption of the anion to sludge is expected to be low and to soil and sediment is expected to be low to moderate; sorption of the cation to sludge, soil, and sediment is expected to be moderate; and sorption of the anion degradant (phosphate) to sludge is expected to be low and to soil and sediment is expected to be low to moderate. Migration of the anion to groundwater is expected to be negligible to slow due to low to moderate sorption to soil and sediment, mitigated by biodegradation; migration of the cation to groundwater is expected to be moderate due to moderate sorption to soil and sediment; and migration of the anion degradant (phosphate) to groundwater is expected to be moderate to rapid due to low to moderate sorption to soil and sediment. Due to low estimated vapor pressure and Henry's law constant, the anion, the cation and the anion degradant (phosphate) are expected to undergo negligible volatilization to air. Overall, these estimates indicate that the anion has low potential to volatilize to air or migrate to groundwater; that the cation has low potential to volatilize to air and has moderate potential to migrate to groundwater; and that the anion degradant (phosphate) has low potential to volatilize to air and has moderate to high potential to migrate to 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. EPA estimated degradation half-lives of the anion using data for analogue(s) (alkyl phosphate); of the cation using data for analogue(s) (alkyl phosphonium); and of the anion degradant (phosphate) using data for analogue(s) phosphate. EPA estimated that the anion's aerobic and anaerobic biodegradation half-lives are < 2 months; that the cation's aerobic and anaerobic biodegradation half-lives are 2 to 6 months; and that the anion degradant's aerobic and anaerobic biodegradation half-lives are < 2 months. These estimates indicate that the anion and anion degradant (phosphate) may have limited persistence in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediment). Further, these estimates indicate that the cation may be persistent in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediment).

[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)

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. EPA estimated the potential for the anion to bioaccumulate using data for analogue(s) (alkyl phosphate); of the cation to bioaccumulate using data for analogue(s) (alkyl phosphonium); and of the anion degradant (phosphate) to bioaccumulate using data for analogue(s) (phosphate). EPA estimated that the anion, the cation and the anion degradant (phosphate) have low bioaccumulation potential based on high water solubility, which increases elimination. EPA estimated that the anion and anion degradant (phosphate) could have limited persistence and 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 cation could be 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 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 (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 PMN data, and by comparing it to structurally analogous chemical substances for which there is information on human health hazard. Absorption of the new chemical substance is expected to be poor through the skin, lung and GI tract based on physical/chemical properties. For the new chemical substance, EPA identified neurotoxicity, reproductive and developmental toxicity, and liver toxicity as hazards based on analogue data; irritation and possible corrosion as hazards based analogue data and information provided in the SDS. Acute oral toxicity was identified based on submitted test data on the new

[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.

chemical substance (OECD 423). EPA quantitatively assessed the new chemical substance using test data (OECD 422 in rats) on tetrabutylphosphonium bromide which demonstrated systemic, reproductive, and developmental toxicities. EPA identified a NOAEL of 100 mg/kg-bw/day which 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. EPA determined environmental hazard for this new chemical substance based on submitted acute aquatic invertebrate and green algae test data on the new chemical substance and the standard toxicity profile for phosphate with molecular weight adjustment (24.7%). Acute toxicity values estimated for fish, aquatic invertebrates, and algae are >100 mg/L (standard toxicity profile for phosphate with molecular weight adjustment (24.7%)), 9.7 mg/L (acceptable submitted aquatic invertebrate test data), and 1.155 mg/L (acceptable submitted algal test data), respectively. Chronic toxicity values estimated for fish, aquatic invertebrates, and algae are >10 mg/L (standard toxicity profile for phosphate with molecular weight adjustment (24.7%)), 0.97 mg/L (ACR of acceptable submitted aquatic invertebrate test data), and 0.51 mg/L (ChV of acceptable submitted algal test data), 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 of 0.289 mg/L (289 ppb) and 0.051 mg/L (51 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 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 and environmental exposures.

[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).

EPA considers workers to be a potentially exposed or susceptible population (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 routes for multiple age groups, ranging from infants to adults. EPA considers consumers of specific products to be a potentially exposed or susceptible population on the basis of greater exposure potential compared to the general population who do not use specific products.

For this assessment, EPA assessed worker exposure via inhalation and dermal routes. Releases to water, air, and landfill were estimated. Exposure to the general population was assessed via drinking water, fish ingestion, landfill leachate, and stack air inhalation. Consumer exposures were not assessed because consumer uses were not identified as conditions of use.

Risk Characterization: EPA characterizes risks to human health and the environment by comparing the potential hazards and exposures for the chemical substance, estimated as described above. 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 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., NOAEL) described above. Risks were identified for workers for systemic, reproductive and developmental toxicities via dermal exposure based on quantitative hazard data for an analogue (MOE = 34; benchmark MOE = 100). Risks were not identified for workers for systemic, reproductive and developmental toxicities via inhalation based on quantitative hazard data for an analogue (MOE = 4,000; benchmark MOE = 100). Irritation and corrosion hazards to workers via dermal and inhalation exposure were identified based on information in the SDS and analogues. Risks for these endpoints were not quantified due to a lack of dose-response for these hazards. However, exposures can be mitigated by the use of appropriate personal protective equipment (PPE), including impervious gloves, eye protection, and a respirator. 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 identified for the general population for systemic, reproductive, and developmental effects via drinking water, fish ingestion, groundwater ingestion from landfill leaching or stack air inhalation based on quantitative hazard data for an analogue (all MOEs ≥ 27,000; benchmark MOE = 100). Irritation, corrosion, and acute oral toxicity hazards to the general population are not expected via drinking water, fish ingestion, or groundwater ingestion due to dilution of the chemical substance in the media. Risks to consumers were not evaluated because consumer uses were not identified as conditions of use.

Risks to the environment were evaluated by comparing estimated surface water concentrations with the acute and chronic concentrations of concern. Risks from acute exposure to the environment were not identified due to releases to water that did not exceed the acute COC. Risks from chronic exposure to the environment were not identified despite the 26 days of exceedence identified in the exposure report (26/250 days/year during use of the new chemical substance) because the predicted environmental concentration (surface water concentration) of 39.4 ppb does not exceed the chronic COC of 51 ppb.

It is reasonably foreseen, based on patent searches, that the new chemical substance could be manufactured, processed and used for uses other than the use described in the PMN, which may result in greater exposures for workers and greater environmental releases. The SNUR that has been proposed for this chemical substance defines certain conditions of use as significant new uses. The proposed significant new uses include any use other than the known or intended uses. Conditions of use that fall under the restrictions of the proposed SNUR are not likely to present unreasonable risk of injury to health or the environment because (1) those conditions of use are not likely to be commenced during the pendency of the proposed SNUR, and (2) upon finalization of the SNUR, those conditions of use would be prohibited unless and until EPA makes an affirmative determination that the significant new use is not likely to present an unreasonable risk or takes appropriate action under section 5(e) or 5(f).

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Date:

/s/
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