

TSCA Inventory Status of Nanoscale Substances – General Approach

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Purpose

The approach outlined in this document describes how EPA currently determines whether a nanoscale substance is a “new” chemical only for the purposes of the Toxic Substances Control Act (TSCA) Inventory. The Agency may use different approaches under its other authorities (e.g., the Federal Insecticide, Fungicide and Rodenticide Act (FIFRA)) in making regulatory status determinations. In adopting this approach under TSCA, EPA is not establishing a precedent on how nanotechnology issues arising under other EPA programs, other Federal Government agencies, or other federal statutes will be addressed.

Background

With the rapid advancement of nanotechnology and the introduction of nanoscale substances into U.S. commerce, it has become important for the U.S. Environmental Protection Agency (EPA) to consider the extent to which these substances may be “new chemical substances” under the Toxic Substances Control Act (TSCA), and thus subject to new chemical reporting under section 5(a) of TSCA. All substances, including nanoscale substances, that meet the TSCA definition of chemical substance are subject to TSCA.¹

The TSCA Chemical Substance Inventory, established under section 8(b) of the Act, is comprised of substances that are considered to be “existing” in U. S. commerce. A substance not already included on the Inventory is considered to be a “new” chemical substance pursuant to TSCA section 3(9). Under section 5(a) of TSCA, a person must submit a Premanufacture Notice (PMN) to EPA at least 90 days before commencing manufacture or import, for a commercial purpose, of a chemical substance not on the Inventory, unless the substance is exempt from reporting under section 5(h) of the Act. The notification must include the information described in subparagraphs (A), (B), (C), (D), (F), and (G) of section 8(a)(2). After PMN review and upon receipt of a Notice of

¹ Certain categories of chemical substances are not subject to TSCA. Examples include foods and food additives, pesticides, drugs, cosmetics, tobacco, nuclear material, or munitions.

Commencement of Manufacture or Import (NOC), a chemical substance is added to the Inventory and becomes an “existing” chemical substance. Certain nanoscale substances that will be manufactured or imported for commercial purposes are expected to be new chemical substances and therefore subject to TSCA new chemical reporting requirements, as are any other new chemical substances.

EPA does not expect, however, that all nanoscale substances will qualify as new chemicals under TSCA. EPA thus intends to determine whether nanoscale substances are new or existing chemical substances based on the case-by-case approach that the Agency has historically applied in determining the Inventory status of chemical substances.

Note that the principles in this paper are not rules or regulations, nor do they otherwise impose legally-binding requirements on EPA or the regulated community. Rather, this paper informs the public of the approach EPA has historically taken under TSCA in evaluating whether chemical substances are new, and further informs the public of EPA’s intention to follow this approach for nanomaterials that are chemical substances. Interested parties will be free to raise questions about the validity or applicability of these principles and EPA will consider whether the principles and their application are appropriate in that context at that time. Any decision regarding whether a chemical substance is a new chemical substance will be made based on the applicable statutory and regulatory requirements.

Determination of Whether A Chemical Substance is New or Existing

Section 3(2)(A) of TSCA defines the term “chemical substance” to mean “any organic or inorganic substance of a particular molecular identity....”² Thus, in determining whether a chemical substance is a new chemical for purposes of TSCA Section 5, or instead is an existing chemical, EPA determines whether the chemical substance has the same molecular identity as a substance already on the Inventory. A chemical substance with a molecular identity that is not identical to any chemical substance on the TSCA Inventory is considered to be a new chemical substance (i.e. not

² The text of section 3(2)(A) states that “the term ‘chemical substance’ means any organic or inorganic substance of a particular molecular identity, including - (i) any combination of such substances occurring in whole or in part as a result of a chemical reaction or occurring in nature, and (ii) any element or uncombined radical.”

on the Inventory); a chemical substance that has the same molecular identity as a substance listed on the Inventory is considered to be an existing chemical substance.

Molecular Identity of a Chemical Substance

In general, a molecule is the smallest unit of matter that retains all of its chemical properties. Molecules that are made up of two or more atoms of like or different elements are held together by chemical bonds, with the principal types of chemical bonds being the ionic, covalent, and metallic bonds.

EPA views molecular identity as being based on such structural and compositional features as the types and number of atoms in the molecule, the types and number of chemical bonds, the connectivity of the atoms in the molecule, and the spatial arrangement of the atoms within the molecule. EPA considers chemical substances that differ in any of these structural and compositional features to have different molecular identities. For example, EPA considers chemical substances to have different molecular identities for the purposes of TSCA when they:

- have different molecular formulas, i.e., they have the same types of atoms but a different number of atoms, e.g., ethane (C_2H_6) and propane (C_3H_8), or they have the same number of atoms but different types of atoms, e.g., bromomethane (CH_3Br) and chloromethane (CH_3Cl), or they differ in both the types and numbers of atoms.
- have the same molecular formulas but have different atom connectivities, i.e., they have the same types and number of atoms but are structural isomers (e.g., n-butane and isobutane) or positional isomers (e.g., 1-butanol and 2-butanol).
- have the same molecular formulas and atom connectivities but have different spatial arrangements of atoms, e.g., they have the same types, number, and connectivity of atoms but are isomeric (e.g., (*Z*)-2-butene and (*E*)-2-butene).
- have the same types of atoms but have different crystal lattices, i.e., they have different spatial arrangements of the atoms comprising the crystals, e.g., anatase (atoms arrayed tetragonally) and brookite (atoms arrayed orthorhombically) forms of titanium dioxide.
- are different allotropes of the same element, e.g., graphite (carbon atoms arranged in hexagonal sheets with each atom bonded to three other atoms in the plane of a given sheet) and diamond (carbon atoms arranged in a tetrahedral lattice with

each atom bonded to four other atoms).

- have different isotopes of the same elements.

Molecules can themselves be arranged or aggregated into particles or other physical forms of various types, shapes, and sizes with concomitant physical properties. EPA does not consider these particles or physical forms themselves to be different molecules with different molecular identities, but rather to be aggregates of molecules that have the same molecular identity, with no chemical bonding between the molecules. Consequently, EPA has not treated the mere aggregation of molecules into particles or varying physical forms to result in different chemical substances with different molecular identities for the purposes of TSCA.

Fundamental to TSCA is the identification of chemical substances as precisely as practicable for listing on the TSCA Inventory. Class 1 substances can be represented by a distinct chemical structure and specific molecular formula. Class 2 substances, including UVCB substances (substances of Unknown or Variable composition, Complex reaction products, and Biological materials), are an extremely broad category of chemical substances that cannot be represented by unique chemical structures or, in most cases, by unique molecular formulas. They can, however, be described using either partly indefinite names indicating variable structures (e.g., heptene), or names that are descriptive of complex or poorly defined compositions (e.g., tall-oil fatty acids), or that include sets of compositional characteristics (e.g., C15-18 .alpha.-alkenes). UVCB substance names may also include a supplemental definition (e.g., pentene, hydroformylation products, with the supplemental definition “A complex combination of products produced by the hydroformylation of pentene. It consists predominantly of C5 olefins and paraffins, C6 alcohols and aldehydes, and C18 acetals and boils in the range of approximately 45 degrees C to 290 degrees C...”). Class 2 substances that differ in such indefinite, variable, or complex structures, descriptive compositions, or sets of compositional characteristics, are considered different chemical substances with different molecular identities for the purposes of TSCA.

Since EPA generally has not considered units of matter beyond molecules, such as physical aggregates, to be reportable to the TSCA Inventory, EPA has not used particle size to distinguish for Inventory purposes two substances that are known to have the same molecular identity. Under principles of traditional chemistry these different forms of such substances would not be considered different chemicals. However, the form in

which a chemical is manufactured, processed, used, or disposed of may play a role in evaluating the risk of a substance and considering whether to address it in some fashion under TSCA.

TSCA Inventory Determination of Nanoscale Substances

As stated above, historically, EPA has not used particle size to distinguish substances that are known to have the same molecular identity for the purposes of the TSCA Inventory. In determining whether a nanoscale substance is a new or existing chemical, the Agency intends to continue to apply its current Inventory approaches based on molecular identity, rather than focus on physical attributes such as particle size.

New Chemicals

A chemical substance with a molecular identity that is not identical to any substance on the TSCA Inventory is considered to be a new chemical (i.e., not on the Inventory). A nanoscale substance might not have a non-nanoscale counterpart with the same molecular identity (e.g., nanotubes and carbon fullerenes), or a substance might be found in both nanoscale and non-nanoscale forms, but if the substance has not been reported previously to EPA and placed on the Inventory in either form, it is considered a new chemical.

A substance of this type would be subject to PMN reporting requirements regardless of whether it is manufactured or imported in the nanoscale form or the non-nanoscale form. When manufacture or importation commences and the substance is added to the Inventory, the listing is considered to encompass both nanoscale and non-nanoscale forms of the substance. Consequently, subsequent forms of the substance manufactured or imported, whether nanoscale or macroscale, which have the same molecular identity, would be considered existing chemical substances.

Systematic chemical nomenclature conventions may not exist for all nanoscale substances identified as new chemicals. In these cases, EPA will likely need to apply new nomenclature conventions to fully, uniquely, unambiguously, and consistently identify and name these new chemical substances for the purposes of the TSCA Inventory. As with existing nomenclature conventions, EPA expects that new nomenclature conventions developed for Inventory listing of these novel substances will

include data elements necessary to describe and distinguish their unique molecular identities but will not describe different physical forms (e.g., particle sizes) of these new substances. In the interim, EPA intends to describe new chemical substances (including new substances that exist in nanoscale forms) to the best of its ability for listing these substances on the Inventory, recognizing that names assigned to these substances and even their Inventory status may change once nomenclature conventions are developed. As necessary, EPA will provide interim guidance on molecular identity data elements that could be used by the notifier and the Agency to identify and name these new chemical substances for listing on the Inventory.

Existing Chemicals

Under the approach outlined in this paper, a nanoscale substance that has the same molecular identity as a substance listed on the Inventory (whether or not reported to the Agency as being manufactured or processed in nanoscale form) is considered an existing chemical, i.e., the nanoscale and non-nanoscale forms are considered the same chemical substance because they have the same molecular identity.

EPA's rationale for considering this group of nanoscale substances to be existing chemicals is based on the TSCA definition of "chemical substance." Although a nanoscale substance that has the same molecular identity as a non-nanoscale substance listed on the Inventory differs in particle size and may differ in certain physical and/or chemical properties resulting from the difference in particle size, EPA considers the two forms to be the same chemical substance because they have the same molecular identity. The Inventory listing in this case is considered to represent both the nanoscale and non-nanoscale forms of the substance and, as such, does not distinguish between two forms having the same molecular identity that differ only in particle size and/or physical/chemical properties resulting from the difference in particle size.

Assistance to Manufacturers and Importers

In order for manufacturers or importers of nanoscale substances to determine whether their substances are new or existing chemicals, and thus whether they are subject to PMN reporting requirements, EPA encourages companies to contact the New Chemicals Program to arrange a pre-notice consultation or to submit a request for an Inventory search under the *bona fide* intent to manufacture provision in 40 CFR §720.25.

As EPA cannot always judge *a priori* if a nanoscale substance has a molecular identity that is identical to a substance listed on the Inventory, EPA may require certain data on the nanoscale substance in order to determine whether it is an existing chemical covered by an existing Inventory listing, or whether it is a new chemical subject to PMN reporting requirements.