TOXIC SUBSTANCES CONTROL ACT
INVENTORY REPRESENTATION FOR

PRODUCTS CONTAINING TWO OR MORE SUBSTANCES: FORMULATED AND STATUTORY MIXTURES

I. Introduction

This paper explains the conventions that are applied to listings of certain mixtures for the Chemical Substance Inventory that is maintained by the U.S. Environmental Protection Agency (EPA) under the Toxic Substances Control Act (TSCA). This paper discusses the Inventory representation of mixtures of substances that do not react together (i.e., formulated mixtures) as well as those combinations that are formed during certain manufacturing activities and are designated as mixtures by the Agency (i.e., statutory mixtures). Complex reaction products are covered in a separate paper. The Agency's goal in developing this paper is to make it easier for the users of the Inventory to interpret Inventory listings and to understand how new mixtures would be identified for Inventory inclusion.

Fundamental to the Inventory as a whole is the principle that entries on the Inventory are identified as precisely as possible for the commercial chemical substance, as reported by the submitter. Substances that are chemically indistinguishable, or even identical, may be listed differently on the Inventory, depending on the degree of knowledge that the submitters possess and report about such substances, as well as how submitters intend to represent the chemical identities to the Agency and to customers. Although these chemically indistinguishable substances are named differently on the Inventory, this is not a "nomenclature" issue, but an issue of substance representation. Submitters should be aware that their choice for substance representation plays an important role in the Agency's determination of how the substance will be listed on the Inventory.

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II. Definition of Terms

TSCA identifies two types of materials: (1) chemical substances and (2) mixtures of chemical substances. The Inventory lists only chemical substances. It does not list mixtures; however, the individual components of mixtures are listed separately.

"Chemical substance" is defined in section 3 of TSCA (and in section 710 of the Agency's implementing regulations) by chemical composition, by source or origin and by identification of certain categories of materials that are not considered "chemical substances":

"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, ...

"Chemical substance" does not include:

(i) any mixture [710.2(q)], ...

"Mixture" is defined in section 710.2(q) as:

any combination of two or more chemical substances if the combination does not occur in nature and is not, in whole or in part, the result of a chemical reaction; except that "mixture" does include:
(1) Any combination which occurs, in whole or in part, as a result of a chemical reaction if the combination could have been manufactured for commercial purposes without a chemical reaction at the time the chemical substances comprising the combination were combined and if, after the effective date of premanufacture notification requirements, none of the chemical substances comprising the combination is a new chemical substance, and
(2) Hydrates of a chemical substance or hydrated ions formed by association of a chemical substance with water.

III. Inventory Representations with Illustrative Examples

A. Mixtures resulting from blending substances that do not react.

A blend of two or more substances that has been physically combined without a chemical reaction is considered to be a mixture. Such a blend, as a whole entity, is excluded from the Inventory and premanufacture notification (PMN) requirements for new chemical substances. Individual components of such a mixture are separately reportable for the Inventory, however, and are considered to be "new substances" if they are not currently listed on the Inventory.

Note, however, that salt formation, the creation of ionic bonds, is considered to be a chemical reaction.

1. Combinations of materials that are physically blended or mixed together and do not themselves result in a chemical reaction are always considered to be mixtures.

The exclusion of these mixtures from the Inventory applies only to the mixture itself and not to the individual chemical substances of which the mixture is comprised. Each chemical substance in a mixture requires a separate Inventory listing. This approach affords considerable flexibility to processors, who are allowed to make many different mixtures of Inventory-listed substances without submitting PMNs.

Example 1. Consider two petroleum streams, each of which is a complex chemical substance. The two streams are mixed, but no reaction occurs. The Agency considers

that the combination of the two petroleum streams themselves is a mixture; each would be listed separately on the Inventory. A similar example from the petroleum industry is a blended gasoline to which a non-reactive corrosion inhibitor has been added.

Example 2. Solid solutions are treated as mixtures; they are found in certain alloys. For example, gold and copper form solid solutions in which some of the copper atoms in the lattice are replaced by gold atoms. In general, the gold atoms are distributed at random, and a range of gold-copper compositions is possible, according to this mixture representation for gold and copper.

Example 3. Consider a substance that is encapsulated in a second substance. If the two substances do not react together, they are considered to be a mixture under TSCA if they do not constitute an article.

Example 4. A commercial product described as "coating material of linseed oil and titanium dioxide," formed by the intentional mixing of two or more substances, which produces no new substance(s) and results only in a combination of the mixed substances, is not itself a substance under TSCA. The component substances of such mixtures (e.g., linseed oil and titanium dioxide), however, are individually reportable as substances.

Example 5. Consider a multi-nutrient "mixed fertilizer" that could have been prepared by physically blending dry products such as urea, superphosphate and potash or by chemical reaction when liquid ammonium phosphate was granulated with potash. The Agency considers this "mixed fertilizer" a mixture of urea, superphosphate and potash regardless of the method used to make it.

Example 6. If commercially-available pine oil, a non-ionic surfactant, and sodium soap of coconut oil acids are mixed, without chemical reaction, a combination is produced that is a mixture. Alternatively, if that same combination is prepared by mixing pine oil, the non-ionic surfactant, coconut oil acids and sodium hydroxide, and carrying out the saponification reaction to form the sodium soap of coconut oil acids, the combination would be identical to that manufactured by mixing the first set of substances without chemical reaction. The three substances in the final combination (i.e., pine oil, the surfactant and the sodium salt of coconut oil) constitute a mixture and each one is subject to Inventory reporting, regardless of the method used to manufacture the mixture.

In some cases two substances may be physically intertwined such that they cannot be separated without breaking bonds of one or the other. As long as they have not reacted with each other (i.e., there are no covalent bonds between the two types of molecules), they are considered to be a mixture. As an extreme example, two or more intertwined rings (i.e., concatenated molecules) that had different chemical compositions would be considered a mixture under TSCA if, in fact, they had no covalent bonds connecting them.

B. Combinations that are considered to be statutory mixtures under TSCA

1. Certain alloys, inorganic glasses, ceramics, frits and cements, including Portland cement are considered to be statutory mixtures by the Agency.

Inorganic glasses, ceramics, frits and cements, including Portland cements, are considered to be statutory mixtures under TSCA. Manufacturers of these products are not required to report them. When the initial Inventory was being developed, both EPA and industry recognized that the individual substances comprising these mixtures are complex solids and would be very difficult to identify. Therefore, instead of requiring industry to identify and report every such substance for the Inventory, several special categories were created to include the various substances formed when cement, glass, frit or ceramic are produced. These categories were reported during the initial Inventory reporting period and are currently listed on the TSCA Inventory. Each category contains a definition that describes the various components of that category in terms of the elements and the various types of chemical substances that may be formed with these elements. These categories of substances are:

Cement, Portland, Chemicals	[65997-15-1*]
Cement, Alumina, Chemicals	[65997-16-2*]
Glass, Oxide, Chemicals	[65997-17-3*]
Frits, Chemicals	[65997-18-4*]
Steel Manufacture, Chemicals	[65997-19-5*]
Ceramic Materials and Wares, Chemicals	[66402-68-4*]

For example, a category such as Ceramic Material and Wares, Chemicals includes any combination of the elements listed in the Inventory definition, as oxides, borides, carbides, etc., in multiple oxidation states, or in more complex compounds. The listed elements included in the definition of each of these categories are not intended to be inclusive. EPA recognizes that the list of elements may need to be updated from time to time as the state of the technology changes.

Example 7. Glass, oxide, chemicals (CASRN 65997-17-3*)

The definition of this substance is as follows:

Synonym: Chemical substances manufactured in the production of inorganic glass

This category encompasses the various chemical substances manufactured in the production of inorganic glasses. For purposes of this category, "glass" is defined as an amorphous, inorganic, transparent, translucent or opaque material traditionally formed by fusion of sources of silica with a flux, such as an alkali-metal carbonate, boron oxide, etc. and a stabilizer, into a mass which is cooled to a rigid condition without crystallization in the case of transparent or liquid-phase separated glass or with controlled crystallization in the case of glass-ceramics. The category consists of the various chemical substances, other than by-products or impurities, which are formed during the production of various glasses and concurrently incorporated into a glass mixture. All glasses contain one or more of

these substances, but few, if any, contain all of them. The elements listed below are principally present as components of oxide systems but some may also be present as halides or chalcogenides, in multiple oxidation states, or in more complex compounds. Trace amounts of other oxides or chemical compounds may be present. Oxides of the first seven elements listed* comprise more than 95 percent, by weight, of the glass produced.

Aluminum*	Lanthanum
Boron*	Lead
Calcium*	Lithium
Magnesium*	Manganese
Potassium*	Molybdenum
Silicon*	Neodymium
Sodium*	Nickel
Antimony	Niobium
Arsenic	Nitrogen
Barium	Phosphorus
Bismuth	Praseodymium
Cadmium	Rudibium
Carbon	Selenium
Cerium	Silver
Cesium	Strontium
Chromium	Sulfur
Cobalt	Tellurium
Copper	Tin
Germanium	Titanium
Gold	Tungsten
Holmium	Uranium
Iron	Vanadium
	Zinc

Definitions such as this may be subject to revision to reflect changes in the underlying technology.

Alloys that are solid or liquid mixtures of two or more metals or of one or more metals with certain nonmetallic elements (e.g., certain carbon steels), are considered mixtures and are not reportable. However, intermetallic compounds of well-defined stoichiometry are not considered alloys and should be reported.

2. Certain combinations of metals, inorganic metal compounds and inert supports, which are frequently used for commercial purposes, including for use as solid phase heterogeneous catalysts, are also considered to be mixtures for the purposes of the TSCA Inventory.

Example 8. Consider the following supported catalysts:
Pt supported on SiO_2, Al_2O_3 or C
Pd supported on SiO_2, Al_2O_3 or C
Rh supported on SiO_2, Al_2O_3 or C
Ni supported on SiO_2, Al_2O_3 or C

In supported catalysts, the catalytic ingredient is dispersed in the internal porosity of such supports as silica gel, alumina or charcoals. Tiny crystallites of such metals as platinum, palladium, rhodium and nickel can be formed in the pore structure. Supported catalysts have much larger surface area of the catalytic ingredient and are much more resistant to coalescence of the catalytic ingredient than are

powders. For example, the supported catalyst Pt/C was prepared by the reduction of $PtCl_2$ adsorbed on charcoal. Although a reaction was involved in the preparation, the resultant catalyst is represented in terms of the products formed and is viewed under TSCA as a mixture of the two substances, platinum and carbon.

Example 9. Zeolites are considered for TSCA purposes to be mixtures of the substances used to manufacture them. The individual reactant materials used to produce zeolites are required to be listed separately on the Inventory. The application of EPA's guidance is not affected by the chemical composition of the zeolite under consideration.

EPA recognizes zeolites as a family of aluminosilicates manufactured from a number of commercial processes and techniques that utilize different proportions of alumina, silica and a variety of sources of different inorganic and organic cations. The final zeolites are characterized by covalently linked AlO_4 and SiO_4 tetrahedra. Zeolites as a class of substances are considered mixtures under TSCA regardless of the commercial manufacturing processes and reactants utilized to achieve the desired chemical composition of the final zeolite structure.

Example 10. Consider a cobalt oxide-aluminum oxide catalyst. A mixed hydroxide precipitate formed by the reaction of sodium hydroxide and an aqueous solution of cobalt (II) nitrate and aluminum nitrate is heated in air to produce a mixed oxide catalyst. Some of the cobalt is known to be oxidized to Co(III) in the process. In this case, cobalt (II) oxide, cobalt (III) oxide and aluminum oxide would each be reported for the Inventory. More complex compounds of cobalt and/or aluminum which may be formed incidentally in the manufacture of the catalyst mixture are not reported.

C. Hydrates of a chemical substance or hydrated ions formed by association of a chemical substance with water are considered to be mixtures of the anhydrous form of the chemical substance and water.

Hydrated forms of chemical substances are exempt from the Inventory as mixtures; the anhydrous chemical substances, however, are reportable for the Inventory. Thus the manufacturer of hydrated copper sulfate, $CuSO_4.(H_2O)x$, would use the anhydrous form, $CuSO_4$, for Inventory purposes.

Example 11. $Na_2CO_3.10H_2O$ is a mixture of Na_2CO_3 and H_2O; $CuSO_4.5H_2O$ is a mixture of $CuSO_4$ and H_2O. The anhydrous forms, Na_2CO_3 and $CuSO_4$, are subject to reporting under TSCA.

This provision does not apply to the product of discrete chemical reactions in which either water or a solvent is a reactant. For example, hydrates are not formed when water reacts with an ester to form an acid and an alcohol; likewise, substances with Chemical Abstracts (CA) names containing the term "hydrolyzed" are not hydrates. Similarly, metal hydroxides formed by the reactions of metal oxides with water are not considered to be hydrates for TSCA Inventory purposes.

Example 12. A stable, hydrated complex of two substances and water is considered to be a mixture of the three chemicals. In this case, the only chemical interaction between the three entities is hydrogen bonding, which EPA does not recognize as bonding for purposes of chemical identification under TSCA.

Hydrogen bonding does not result in the formation of a new chemical substance for the purposes of TSCA, even though it has significant effects on physical properties. For example, the hydrogen of the chloroform molecule, Cl3CH, forms hydrogen bonds with an electron pair of the oxygen of the acetone molecule, Cl3CH O=C(CH3)2, and chloroform-acetone mixtures have higher boiling points than either pure component. This type of interaction between two molecules is caused by the electronegative atoms (such as fluorine, nitrogen or oxygen) in one molecule and hydrogen atoms bound to electronegative atoms in another molecule. The hydrogen-bonded materials are considered to be mixtures for the purposes of TSCA.

Example 13. Consider the reaction of calcium oxide (CaO) (CASRN 1305-78-8) with water (CASRN 7732-18-5) to form calcium hydroxide (Ca(OH)2) (CASRN 1305-62-0). The calcium hydroxide is not a hydrate with water and thus would require its own Inventory listing.

CaO + H2O Ca(OH)2

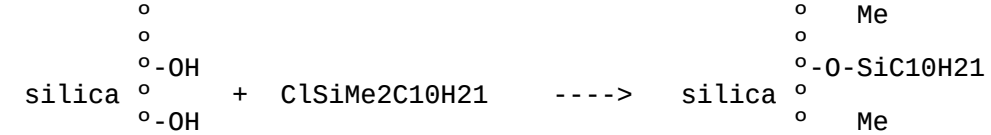
Example 14. Consider the reaction of acetyl chloride (CASRN 75-36-5) with water (CASRN 7732-18-5) to form acetic acid (CASRN 64-19-7) and hydrochloric acid (CASRN 7647-01-0). Both products of this reaction would require Inventory listing.

CH3-COCl + H2O CH3-COOH + HCl

D. Surface Treatment

With this term the Agency generally means the process of chemically treating the surface of a substance, the substrate, with another substance so as to enhance some physical property of the surface of the substrate or to impart chemical reactivity to the surface (i.e., to functionalize the surface chemically). The surface-treating substance adheres to the surface by van der Waal's forces, ionic bonds or covalent bonds. If the substance only alters a physical characteristic, the combination of the surface treatment substance and the substrate is considered to be a mixture of two substances, each requiring its own Inventory listing. If, however, the surface treatment is intended to impart chemical reactivity, the reaction product is required to be on the Inventory.

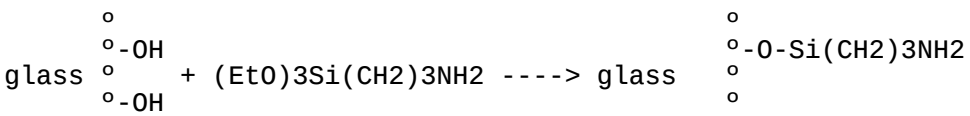
Example 15. Consider the following reaction:



silica surface hydrophobic silica

In this example, the silica surface was modified by a chemical reaction to introduce a material onto the outermost layer of the silica, contributing the property of hydrophobicity to the silica without changing the bulk properties of the silica. This type of reaction is usually not stoichiometric and would not be reportable under TSCA.

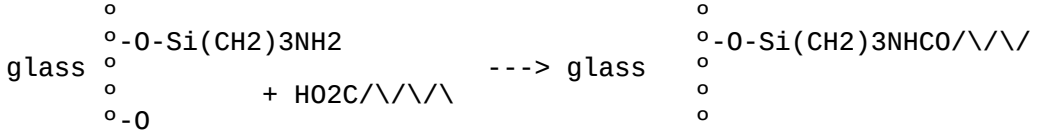
Example 16. On the other hand, if the surface of the substrate is functionalized, the reaction product formed upon reaction of the substrate and surface treating substance is considered to be a reportable substance, as illustrated below:



glass surface silane coupling agent chemically bonded to surface, providing amine functionality

The glass filler (particles, spheres, flakes and fibers) is coated with an organofunctional silane. Chemical modification of the filler through treatment with the silane is necessary to promote interfacial adhesion between the filler and a polymer in making polymer blends, which allows for uniform dispersion of the filler in the polymer blend. Such functionalized glasses, which are formed by chemical reactions, are reportable substances and not considered mixtures under TSCA. Generally, when the surface of glass or silica is modified to incorporate certain functional group(s) intended to react with other chemical substance(s), the Agency considers the surface modified glass or silica to be a chemical substance.

Example 17. If a functionalized glass sphere is coated with a polymer having reactive sites capable of reaction with the functionalized glass, the functionalized glass-polymer reaction product is not reportable. This type of substance is generally a combination of two or more materials present as separate phases and combined to form desired structures that take advantage of certain desirable mechanical/physical properties of each component. Chemical reactions merely take place over the interface region of the polymeric matrix and the dispersed particulate (filler) phases. The Agency considers such combinations comprising separate phases in the polymer blend to be, for purposes of TSCA, the same as a physical suspension of the functionalized filler in the polymer. Consequently, this type of material is considered to be a mixture of the suspending filler(s) and polymer(s), even though a reaction was involved.



Functionalized Glass	Polyester molecule with its acid end group	The linking moiety at the interface between polyester and glass