TOXIC SUBSTANCES CONTROL ACT
INVENTORY REPRESENTATION FOR

CHEMICAL SUBSTANCES OF UNKNOWN OR VARIABLE COMPOSITION, COMPLEX REACTION PRODUCTS AND BIOLOGICAL MATERIALS: UVCB SUBSTANCES

I. Introduction

This paper is a compendium of information related to the broad class of chemical substances referred to as UVCBs: Unknown or Variable compositions, Complex reaction products and Biological materials. These chemical substances cannot be represented by unique structures and molecular formulas. This paper is a companion paper to other nomenclature papers including "Combinations of two or more substances: Complex reaction products" and "Products containing two or more substances: Formulated and statutory mixtures." The Agency's goal in developing this paper is to make it easier for the users of the Inventory to interpret listings for UVCB products and to understand some of the considerations that go into naming new UVCB substances for the Inventory.

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. Definitions

A. Class 1, Class 2 and UVCBs

Substances on the TSCA Inventory are divided into two classes for ease of identification. Class 1 substances are those single compounds composed of molecules with particular atoms arranged in a definite, known structure. Examples of Class 1 substances include: acetone, iron, benzene and dimethylmercury. These substances have discrete molecular formulas and fully-defined structural diagrams. They are included in the molecular formula index of the printed Inventory and are searchable in many computerized databases by molecular formula, name or structural fragments.

Many commercial substances that are subject to TSCA are not Class 1 substances, however. They may have unknown or variable compositions or be composed of a complex combination of different molecules. These are designated Class 2 substances.

Class 2 substances can be further divided into three subgroups. The first subgroup includes substances that can be represented by definite Hill ordered molecular formulas but have variable structural diagrams. An example of this first subgroup is xylene, in which the location of the substituent groups is variable. The second subgroup includes substances that can be represented by definite molecular formulas but have unknown structural diagrams, such as aluminum cerium nickel sulfide, AlCe3NiS7. The third subgroup includes substances that have no definite molecular formula representation and either partial structural diagrams or no structural diagrams. These are the UVCB substances. Each name for a UVCB substance includes more than one molecular entity: as such, each UVCB can be considered to be a category of molecules, often closely related. An example of this kind of substance is "Light oil (coal), coke-oven" (CASRN 65996-78-3*), which is defined on the Inventory as:

> "the volatile organic liquid extracted from the gas evolved in the high temperature (greater than 700oC (1292oF)) destructive distillation of coal. Composed primarily of benzene, toluene and xylenes. May contain other hydrocarbon constituents."

B. Natural Products: Product Combinations that are Generally Chemical Substances

A combination that occurs in nature is a chemical substance and not a mixture. If the natural product is processed for commercial purposes using only techniques from the restricted list below, the resulting substance is considered to be included implicitly on the Inventory and need not be listed explicitly. The definition from 40 CFR 710.4(b) follows:

> "Any chemical substance which is naturally occurring and
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> (1) Which is (i) unprocessed or (ii) processed only by

manual, mechanical, or gravitational means; by dissolution in water; by flotation; or by heating solely to remove water; or

(2) Which is extracted from air by any means,

shall automatically be included in the Inventory under the category 'Naturally Occurring Substances.'"

Many substances that are derived from natural products and are processed by methods other than those listed above are subject to Inventory reporting and fall within the UVCB category for Inventory listing purposes. For example, biologicals extracted with solvents other than water or extracted using steam also would not be considered to be naturally occurring and would thus be subject to Inventory reporting; many of these substances also fall into the UVCB category, as would a variety of crude petroleum products.

C. UVCBs vs Mixtures

A reaction product combination could, in theory, be named as either a group of individual Class 1 substances (if all of the individual molecules in the product are known and always present) or as a Class 2 UVCB complex reaction product. Complex reaction products are most often given UVCB names but not all UVCB substances are reaction products. Agency guidance to distinguish between complex reaction products and mixtures is found in the Inventory paper: "Combinations of two or more substances: Complex reaction products." Refer to that paper to determine the appropriate representation for this type of substance.

D. Definitions for UVCB Chemical Substances

Some UVCB substances are not adequately described by their CA Names. Their names are not specific or complete enough to permit unambiguous identification. The CA names for such substances may contain:

1. Process terms that are not chemically descriptive (e.g., distillation residues, distillation overheads, by-products, low-boiling, catalytic reformed);

2. Trade jargon (e.g., slack wax, spelter, winterized, deodorized distillates, steep liquor, foots oil);

3. Unqualified or very broadly qualified substance class terms (e.g., pyridine bases, petroleum resins, phenols (petroleum)); or

4. Physical rather than chemical terms (e.g., microcrystalline, pulp, agglomerates, sinter, viscous).

These substances have supplemental definitions that are considered integral parts of the names for TSCA purposes. In

general, the definitions serve to narrow the scope of the CA Names. Thus, any substance that matches a CA Name on the TSCA Inventory but is not covered by the corresponding substance definition is not considered to be covered by that Inventory name.

Example 1. Soybean, flour
CASRN 68513-95-1*

The definition of this substance is: "A fine-ground powder made by steaming soybeans, followed by removal of hulls and mechanical grinding." If another type of soybean flour were made without steaming the soybeans or without removal of the hulls, the resultant flour would not fit within this definition, and would require a different listing on the Inventory.

Example 2. Gelatins, hydrolyzates
CASRN 68410-45-7*

The definition of this substance is: "Enzymatic digest produced by hydrolysis of gelatin." If, on the other hand, the gelatin were hydrolyzed chemically rather than enzymatically, the resultant product would not fit the definition and would require a different Inventory listing.

Chemical substance definitions often include such information as the typical or allowed carbon number ranges or physical property ranges, the types of atoms or substances that may be included, and the raw material sources or processes of manufacture. Many definitions use a standard format. Typically, the first sentence states that the substance is a combination of substances of a certain class and indicates the nature or the process by which it was derived. The next sentence (or sentences) usually identifies the predominant components and perhaps an approximate boiling range or other characteristic physical data.

A dagger () is found next to the CASRN in the printed TSCA Inventory to indicate that a definition exists for that chemical substance. These definitions appear in Appendix A of Volume I of the 1985 Edition of the TSCA Chemical Substance Inventory. Persons using various on-line versions of the TSCA Inventory need to be certain that they obtain any definitions that may pertain to UVCB substances of interest before they make Inventory determinations. The definitions are usually found in fields separate from the main CA names, and so may be overlooked.

III. Examples of UVCB Nomenclature

A. Substances of Unknown Composition

1. General: Substances of Unknown Composition

A wide variety of substances of unknown composition are listed on the TSCA Inventory. Examples might include distillation residues, spent cooking or neutralizing liquors and residual oils. Each Inventory substance, however, has a commercial purpose under TSCA; if it were an impurity, a byproduct or a waste with no commercial use, it would not be eligible for TSCA Inventory listing.

Example 3. Dust, iron-ore, sinter
CASRN 69012-53-9*

The UVCB definition for this substance is: "Dust generated during the making, breaking and handling of sinter which is recovered through the use of pollution abatement equipment."

2. Substances named as "Reaction Products with"

"Reaction products with ..." names are used when it is difficult or impossible to assign a product-based name that accurately describes the chemical composition of the reaction product. Such names are only appropriate for those substances for which there is not enough information to identify the products completely or for which the products are comprised of a combination of different chemical classes. The Agency discourages the use of names including "reaction products with" unless there is no reasonable alternative. Substances reacting together to form only esters or only salts or only polymers, for example, would not be named as "reaction products with." Substances that meet the definition of polymer as given in the accompanying paper on polymers are named as polymers and not as "reaction products with."

The commercial intent behind this type of substance is important as well. For substances named as "reaction products with," all of the components that might be present in the reaction product would be present intentionally and have commercial value. If only some of the components within the product were present intentionally and of commercial value, the rest of the components would be considered as impurities and the name assigned would include only the commercially-valuable components. If only one chemical component were of commercial value, the reaction product would be named using that component.

A name that includes "reaction products with" is, of course, a reactant-based name. With this type of name, the reactants must always be the same; if different reactants were used to make an identical product, the name would be different and a different chemical substance would be created for TSCA purposes.

Example 4. Formaldehyde, reaction products with diethanolamine
CASRN 72624-00-1*

The reaction of formaldehyde and diethanolamine produces a complex set of products that may include adducts of formaldehyde and secondary amines, methylolated amines and cyclic amines, depending on reaction conditions and stoichiometry.

3. "Compounds with"

The terms "compd. with" or "compds. with" are generally used for acid/base salts, adducts, inclusion compounds, etc. It is to be distinguished from the term "reaction products with," which is used when a product-based name cannot be developed. "Reaction products with" usually refers to covalent bond formation.

Example 5. Fatty acids, linseed-oil, compds. with triethylamine
CASRN 68605-07-2*

This substance is the triethylamine salt of linseed oil fatty acids. It is a UVCB substance because linseed oil fatty acids are biological materials.

B. Substances of Variable Composition

Example 6. Alcohols, C8-18
CASRN 68551-07-5*

The relative amounts of the alcohol chain lengths that comprise this substance are variable. Because of the variable composition within the stated range, all substances containing ranges of alkyl chain lengths are UVCBs. See the Inventory representation paper titled: "Certain chemical substances containing varying carbon chain lengths (alkyl ranges using the CX-Y notation)" for more information.

Example 7. Alkenes, C14-18 à-
CASRN 68855-59-4*

The UVCB definition for this substance is: "This substance is identified by SDA Substance Name: C14-C18 alpha olefin and SDA reporting number: 17-057-00. Consult SDA Substance Identification Procedure." The relative amounts of the alkene chain lengths that comprise this substance are variable; see the Inventory representation paper on alkyl ranges. SDA nomenclature was developed in conjunction with the Soap and Detergent Manufacturers Association for use in describing this type of alkyl range substance for the TSCA Inventory. For further information see the end of Appendix A, Vol. 1 of the 1985 Edition of the TSCA

Inventory, SDA Substance Identification Procedure.

Example 8. Rutile, neodymium
CASRN 68516-14-3*

The UVCB definition for this substance is: "An inorganic pigment that is the reaction product of high temperature calcination in which neodymium (III) oxide and titanium (IV) oxide in varying amounts are homogeneously and ionically interdiffused to form a crystalline matrix of rutile."

Example 9. Natural gas (petroleum), raw liq. mix
CASRN 64741-48-6*

The UVCB definition for this substance is: "A complex combination of hydrocarbons separated as a liquid from natural gas in a gas recycling plant by processes such as refrigeration or absorption. It consists mainly of saturated aliphatic hydrocarbons having carbon numbers in the range of C2 through C8." This substance includes variable carbon chain lengths.

C. Substances that are Complex Reaction Products

Example 10. Pentene, hydroformylation products
CASRN 68527-03-7*

The definition of this substance is: "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 45oC to 290oC (113oF to 554oF)."

Example 11. Coal, carboxylated
CASRN 71949-31-0*

The UVCB definition of this substance is: "The oxidation product obtained from the reaction of coal with nitric acid. Composed primarily of complex organic acids, carbon and ash. The nature and proportion will vary with the characteristics of the coal used which may range from bituminous to lignite."

Example 12. 1,3-Propanediamine, N-octadecyl-, carboxymethyl derivs.
CASRN 68610-28-6*

In this case, the degree of carboxymethylation is unknown.

D. Substances that are Biological Materials or Made From

Biological Materials

Numerous relatively simple biological materials are listed as UVCB products on the TSCA Inventory, either by themselves or as components of further reaction products. The more complex biologicals, including enzymes, organisms and products of the biotechnology industry are also considered to be UVCB substances. Although some of these more complex biological substances were reported and included on the Inventory, EPA has not yet developed guidance for their Inventory representation.

Note that some biological materials are completely defined and, thus, are Class 1 substances, rather than UVCBs. An example of a Class 1 biological material is the polypeptide hormone, insulin.

1. Natural products vs explicit Inventory listings

The question is frequently raised whether a particular biological material is a natural product or not. (See the definition of natural product, section II.B. above.) An Inventory listing for a biological substance implies that the substance was prepared using other than purely mechanical means. If only mechanical means (or other techniques listed at 40 CFR 710.4(b)) are used to prepare a substance, an Inventory listing is not necessary as the substance is a natural product included implicitly on the Inventory.

Example 13. Beeswax
CASRN 8012-89-3*

The UVCB definition for this substance is: "The wax obtained from the honeycomb of the bee. It consists primarily of myricyl palmitate, cerotic acid and esters and some high-carbon paraffins." Although the method of isolation or purification is not stated in the definition, the listing assumes that other than mechanical means were used; this substance is not a natural product for purposes of TSCA.

Example 14. Gelatins
CASRN 9000-70-8*

The definition for this substance is: "A complex combination of proteins obtained by hydrolysis of collagen by boiling skin, tendons, ligaments, bones, etc." In this case no specific source is given, so the gelatin could be made from any species of animal.

2. Essential Oils

Essential oils are listed on the Inventory by names and definitions. TSCA definitions generally contain the phrase "Extractives and their physically modified derivatives" followed

by the genus and species of the biological source. The definition may also include a list of the primary components of the oil. Note that use of another source even if the same composition of oil were obtained would require a separate Inventory listing.

Example 15. Oils, eucalyptus
CASRN 8000-48-4*

The UVCB definition for this substance is: "Extractives and their physically modified derivatives. Eucalyptus, Myrtaceae."

3. Polymers that contain biologicals

Polymers containing biological materials are frequently named starting with the biological. If the first term in the name is singular, the polymer is named as "polymer with;" in contrast, if it is plural, the term "polymers with" is used.

Example 16. Rosin, polymer with formaldehyde, methanol and phenol
CASRN 68333-68-6*

This is a UVCB polymer because rosin is a biological material.

Example 17. Fatty acids, tall-oil, polymers with glycerol, isophthalic acid and rosin
CASRN 68956-34-3*

This second UVCB polymer has two biological reactants: tall oil fatty acids and rosin.