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Office of Chemical Safety
and Pollution Prevention

Guidance for Creating Generic Names for Confidential Chemical Substance Identity Reporting under the Toxic Substances Control Act

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Preface

This guidance provides information to assist companies in creating structurally descriptive chemical names for chemical substances whose specific chemical identities are claimed confidential, for purposes of protecting the specific chemical identities from disclosure while describing the chemical substance as specifically as practicable, and for listing substances on the Toxic Substances Control Act (TSCA) Chemical Substance Inventory.

The Frank R. Lautenberg Chemical Safety for the 21st Century Act amends TSCA Section 14(c)(4) to require EPA to "develop guidance regarding – (A) the determination of structurally descriptive generic names, in the case of claims for protection from disclosure of specific chemical identity…" The Act also amends TSCA Section 14(c)(1)(C) to require submitters who assert a confidentiality claim for specific chemical identity to include a structurally descriptive generic name for the chemical substance that EPA may disclose to the public, which is consistent with EPA's guidance and which describes the chemical structure of the substance as specifically as practicable while protecting those features of the chemical structure that are claimed as confidential, and the disclosure of which would be likely to cause substantial harm to the competitive position of the claimant. Consistent with the TSCA Section 14(c)(4) and (c)(1)(C) requirements, this guidance updates and replaces the 1985 guidance published in the *TSCA Inventory, 1985 Edition (Appendix B: "Generic Names for Confidential Chemical Substance Identities").*

Also consistent with the TSCA Section 14(c)(4) and (c)(1)(C) requirements, EPA will be reviewing generic names upon receipt in TSCA filings where chemical identity is claimed as confidential for consistency with the guidance. Companies are encouraged to consult with the Agency prior to the submission of TSCA filings about creating generic names generally and in particular instances. Companies are particularly encouraged to consult the Agency (Office of Pollution Prevention and Toxics/Industrial Chemistry Branch; telephone (202) 564-8740) if they feel that it will be necessary to mask more than one structural element of a specific chemical name in order to mask a confidential chemical identity.

Disclaimer

This Guidance does not constitute rulemaking by the United States Environmental Protection Agency (EPA), and cannot be relied on to develop a substantive or procedural right enforceable by any party in litigation with the United States. Non-mandatory language such as "should" provides recommendations and does not impose any legally binding requirements.

The TSCA statutory provisions described in this document contain legally binding requirements relating to claims for protection from disclosure of a specific chemical identity. This document is not a regulation itself, nor does it change or substitute those provisions or other EPA regulations. While EPA has made every effort to ensure the accuracy of the discussion in this guidance, the obligations of EPA and the regulated community are determined by statutes, regulations, or other legally binding requirements, which supersede this guidance document.

Interested persons are free to raise questions and objections about the substance of this guidance and the appropriateness of the application of this guidance to a particular situation. EPA may make changes in this document at any time without public notice.

Background

A specific chemical name identifies every structural feature of a chemical substance possible, i.e., a specific chemical name is a structurally specific and descriptive chemical identifier. A generic name is the nonconfidential substitute for a specific chemical name that is treated as confidential. A generic name should also be structurally descriptive, i.e., a generic name should reveal the chemical identity of a substance to the maximum extent practicable while masking only those structural elements that are confidential. Generic names allow EPA to publicly identify confidential chemical substances. For example, generic names are routinely used to publicly identify the thousands of confidential substances on the TSCA Inventory.

This guidance and the 1985 guidance that it is replacing are based on the approach that an appropriate generic name generally starts with the specific Chemical Abstracts (CA) Index name and then masks only the structurally descriptive element(s) (or the compositionally descriptive element(s) or other element(s) for substances with variable or unknown structural features) of that name that are confidential; an appropriate generic name generally *does not* start with a very generic name to which some additional structural information is then reintroduced. Additionally, when masking a confidential element, it generally is not just removed from the name but is substituted with a more generic structural descriptor. Furthermore, because generic names, like CA Index names, are generally structure-based names, trade names generally are not acceptable as generic names, nor are names that mask confidential elements by substituting with non-structural descriptors, e.g., use or function information.

This guidance provides examples of the process for masking the structurally descriptive (or other) element(s) of the specific CA Index name for a chemical substance. Although examples primarily include masking one structural element, masking more than one structural element can be acceptable, provided that the submitter can justify their need for any additional masking.

Because of inherent differences in naming class 1 organic chemical substances, class 2 (including UVCB) organic substances, and inorganic substances, the guidance addresses each separately.

Class 1 Organic Chemical Substances

A class 1 organic chemical substance can be represented by a definite molecular formula and chemical structure diagram. A generic name is created for a class 1 organic chemical substance by masking the confidential elements of its specific chemical name. Masking is accomplished by substituting more generic structural descriptors for the confidential elements. The specific chemical name of a class 1 chemical substance generally discloses the following structure information:

1. Identity of the parent structure for a substance of a certain chemical class (e.g., alcohols, alkenes) which often also describes a chain of carbon atoms or a ring system.

2. Identity, number, and position of chemical group(s) that are attached to the parent structure or to other chemical groups.
3. Identity and number of counter ion(s) for salt(s).
4. Stereochemical relationship(s).

The structural elements of a class 1 organic chemical substance name that can be masked when creating a generic name therefore include the following:
1. Identity of a parent structure.
2. Identity of an attached chemical group.
3. Number or multiplicative prefix (e.g., di-, tri-, tetra-) of an attached chemical group.
4. Position or locant of an attached chemical group.
5. Identity or number (multiplicative prefix) of the cation(s) or anion(s) of a salt.
6. Stereochemical or isomeric identifiers (e.g., *D*- or *L*-, *R*- or *S*-, *E*- or *Z*-, *cis*- or *trans*-).

Parent Structure Masking

A parent structure describing a certain chemical class – often including a chain of carbon atoms or a ring system – can be masked in the specific chemical name by substituting the following examples of more generic descriptors:
- "*alkane*" for saturated carbon chains (e.g., butane, octane)
- "*alkene*" or "*alkyne*" for unsaturated carbon chains (e.g., 1-butene, 2-butyne)
- "*cycloalkane*" or "*carbomonocycle*" for non-aromatic, carbon-based, single ring systems (e.g., cyclohexane)
- "*carbomonocycle*" for aromatic, carbon-based, single ring systems (e.g., benzene)
- "*carbopolycycle*" for aromatic or non-aromatic, carbon-based fused, bridged, or spiro ring systems (e.g., 1H-indene, bicyclo[2.2.2]octane, spiro[5.5]undecane)
- "*heteromonocycle*" for aromatic or non-aromatic, carbon-based, single ring systems that contain at least one additional atom (heteroatom) in the ring (e.g., pyrrolidine; 1,4-dioxane)
- "*heteropolycycle*" for aromatic or non-aromatic, carbon-based, fused, bridged, or spiro ring systems that contain at least one additional atom (heteroatom) in the ring(s) (e.g., 1H-indole; 1,4-diazabicyclo[2.2.2]octane; 2,4,8,10-tetraoxaspiro[5.5]undecane)

Chemical Group Masking

An attached chemical group can be carbon-based (carbon chain or carbon-based ring system), heteroatom-based (e.g., hydroxyl, amino, nitro, chloro), or both (e.g., alkoxyl, acyl, amido, cyano). The attachment can be on the parent structure or on another chemical group. Similar to masking a parent structure, the identity of an attached chemical group can be masked in the specific chemical name by substituting the following examples of more generic descriptors:
- "*alkyl*," "*alkenyl*," or "*alkynyl*" for saturated or unsaturated carbon chains (e.g., butyl, 1-butenyl, 1-butynyl)
- "*carbomonocyclic*" or "*carbopolycyclic*" for carbon-based ring systems (e.g., cyclohexyl, phenyl, indenyl, bicyclooctyl, spiroundecyl); "*aryl*" also can be used for aromatic ring systems

- "*heteromonocyclic*" or "*heteropolycyclic*" for carbon-based ring systems that contain at least one additional atom (heteroatom) in the ring (e.g., pyrrolidinyl, indolyl, diazabicyclooctyl, tetraoxaspiroundecyl)
- "*halo*" for halogens (e.g., chloro, bromo)
- "*nitrogen-substituted*" for nitrogen containing chemical groups (e.g., nitro, azo); "*heteroatom-substituted*" also can be used for heteroatom-based chemical groups

Masking the number (multiplicative prefix) or position (locant) of an attached chemical group is illustrated in the examples below.

Examples

The generic names provided for the examples below illustrate only some of the possible ways that structural elements in class 1 organic chemical substances can be masked.

Example 1

Specific chemical name: "*2-Pentenoic acid, 2,4-dimethyl-, ethyl ester, (2E)-"*

Appropriate generic names:
- *"alkenoic acid, 2,4-dimethyl-, ethyl ester, (2E)-"* or *"unsaturated carboxylic acid, 2,4-dimethyl-, ethyl ester, (2E)-"* masks the identity of the 2-pentenoic acid parent group
- *"2-pentenoic acid, 2,4-dialkyl-, ethyl ester, (2E)-"* masks the identity of the methyl groups (but not the number and positions)
- *"2-pentenoic acid, methyl substituted, ethyl ester, (2E)-"* masks the locants and multiplicative prefix of the methyl groups (but not the identity)
- *"2-pentenoic acid, 2,4-dimethyl-, alkyl ester, (2E)-"* masks the identity of the ethyl ester group (but not the stereochemistry)
- *"2-pentenoic acid, 2,4-dimethyl-, ethyl ester, single isomer"* masks the stereochemistry

Example 2

Specific chemical name: *"Benzenesulfonic acid, 3-amino-5-chloro-4-ethyl-"*

Appropriate generic names:
- "*carbomonocycle hetero-acid, 3-amino-5-chloro-4-ethyl-"* or *"aryl hetero-acid, 3-amino-5-chloro-4-ethyl-"* masks the identity of the benzenesulfonic acid parent group
- *"benzenesulfonic acid, 3-nitrogen-substituted-5-chloro-4-ethyl-"* or *"Benzenesulfonic acid, 3-heteroatom-substituted-5-chloro-4-ethyl-"* masks the identity of the amino group (but not the number and position)
- *"benzenesulfonic acid, 3-amino-5-halo-4-ethyl-"* masks the identity of the chloro group (but not the number and position)
- *"benzenesulfonic acid, 3-amino-5-chloro-4-alkyl-"* masks the identity of the ethyl group (but not the number and position)

Example 3

Specific chemical name: "*1,1'-Biphenyl, 2,2',3,3',5,5',6,6'-octafluoro-"*

Appropriate generic names:

- *"carbopolycycle, 2,2',3,3',5,5',6,6'-octafluoro-"* masks the identity of the 1,1-biphenyl parent group
- *"1,1'-biphenyl, 2,2',3,3',5,5',6,6'-octahalo-"* masks the identity of the fluoro groups (but not the number and positions)
- *"1,1'-biphenyl, polyfluoro-"* masks the locants and multiplicative prefix of the fluoro groups (but not the identity)

Example 4

Specific chemical name: "*1H-Imidazole, 4,5-dihydro-2-(phenylmethyl)-, hydrochloride (1:1)"*

Appropriate generic names:

- *"heteromonocycle, 2-(phenylmethyl)-, hydrochloride (1:1)"* masks the identity of the 4,5-dihydro-1H-Imidazole parent group
- *"1H-imidazole, 4,5-dihydro-2-carbomonocyclic-, hydrochloride (1:1)"* masks the identity of the phenylmethyl group (but not the position)
- *"1H-imidazole, 4,5-dihydro-2-(phenylmethyl)-, 1:1 salt"* masks the identity of the hydrochloride salt

Class 2 Organic Chemical Substances

A class 2 organic chemical substance cannot be represented by a definite chemical structure diagram and may or may not be able to be represented by a definite molecular formula.

Class 2 organic chemical substances include less complex substances that have variable chemical structure diagrams in which the variability is known. Some have definite molecular formulas such as "*Benzene, dimethyl-*" (or xylene) in which the location of the attached methyl chemical group is variable resulting in three possible structural isomers: 1,2-dimethylbenzene, 1,3-dimethylbenzene, and 1,4-dimethylbenzene. The molecular formula for all three isomers is $C_6H_4(CH_3)_2$ or C_8H_{10}. Other class 2 organic chemical substances that have variable chemical structure diagrams in which the variability is known do not have definite molecular formulas. An example is "*Alkanes, C2-3*" which is comprised of ethane and propane.

Class 2 organic chemical substances also include more complex substances, such as those of Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCBs). These substances do not have definite molecular formulas or definite chemical structure diagrams. UVCBs often have variable structural elements that are not defined or have unknow structural elements. An example is "*Extracts (petroleum), light naphthenic distillate solvent*" which has the definition "*A complex combination of hydrocarbons obtained as the extract from a solvent extraction process. It consists predominantly of aromatic hydrocarbons*

having carbon numbers predominantly in the range of C15 through C30. This stream is likely to contain 5 wt. % or more of 4- to 6-membered condensed ring aromatic hydrocarbons."

A generic name is created for a class 2 organic chemical substance by masking the confidential elements of its specific chemical name which, for a class 2 organic substance, will often include variable or unknown structural elements. In instances where a variable structural element is known, the guidance presented above for creating generic names for class 1 substances may be applied in order to mask the variable structural element. For example, if a class 2 organic substance has a variable parent structure or a variable chemical group attached and the variability is known, such structural elements can be masked in a similar way as described for class 1 substances. To further illustrate, the substance "*Pyridine, C1-3-alkyl derivs.*" has the variable chemical group "*C1-3-alkyl derivs*." that could be masked by substituting with "*alkyl derivatives*," just as "*methyl*," "*ethyl*," and "*propyl*" can be masked by substituting with "*alkyl*."

If a class 2 organic chemical substance with more complex structural variability or with an unknown structural element can be represented by a partial or representative (e.g., predominant component) chemical structure diagram, the specific chemical name for the substance is generally a more common name that encompasses the variable or unknown element of the structure. In such instances, the variable or unknown structural element in the common name can be substituted with a more generic descriptor of the partial or representative structure by applying the guidance for class 1 substances. For example, the substance "*Resin acids and rosin acids*" is a common name representing a mixture of carboxylic acids generally comprised of the same fused ring parent structure that could be masked by substituting with "*polycyclic acids*." Similarly, "*Lignin*" is a common name representing a plant-based polymer generally comprised of crosslinked phenols that could be masked by substituting with "*polyphenols*" or "*polyarylalcohols*."

In other instances, the specific chemical name for a class 2 organic chemical substance with more complex structural variability or with an unknown structural element may include manufacturing, chemical processing, or related information as a means to identify the substance. Such information can include natural source material, synthetic precursors (e.g., monomers) or other reactants, or manufacturing or chemical processing methods. To mask precursors or other reactants in the specific chemical name, the guidance for creating generic names for class 1 substances may be directly applied. For example, the "*1-chloronaphthalene*" reactant in "*Formaldehyde, reaction products with 1-chloronaphthalene*" could be masked by substituting with "*halocarbopolycycle*." To mask source information, a more generic descriptor of the source should be substituted. For example, "*Oils, catnip*" could be masked by substituting with "*plant-based oils*," and "*Fatty acids, tallow, sodium salts*" could be masked by substituting with "*animal-based fatty acid salts.*" Finally, to mask manufacturing or chemical processing methods, either a more generic structure-based descriptor or a more generic descriptor of the method could be substituted. For example, "*methoxylated*" or "*ethoxylated*" could be masked by substituting with "*alkoxylated*," "*oxidized*" or "*hydrogenated*" could be substituted with "*modified*," and "*fumerated*" or "*maleated*" could be substituted with "*functionalized*."

Examples

The generic names provided for the examples below illustrate only some of the possible ways that structural elements in class 2 organic chemical substances can be masked.

Example 1

Specific chemical name: "*Nonanedioic acid, polymer with 1,2-ethanediamine, 1,6-hexanediamine and (9Z,12Z)-9,12-octadecadienoic acid dimer*"

Appropriate generic names:

- *"alkanedioic acid, polymer with 1,2-ethanediamine, 1,6-hexanediamine and (9Z,12Z)-9,12-octadecadienoic acid dimer"* or *"dicarboxylic acid, polymer with 1,2-ethanediamine, 1,6-hexanediamine and (9Z,12Z)-9,12-octadecadienoic acid dimer"* masks the identity of the nonanedioic acid starting material
- *"nonanedioic acid, polymer with mixed alkyldiamines and (9Z,12Z)-9,12-octadecadienoic acid dimer"* masks the identity of the two diamine monomers
- *"nonanedioic acid, polymer with 1,2-ethanediamine, 1,6-hexanediamine and a (Z,Z)-alkanedienoic acid dimer"* masks the identity of the 9,12-octadecadienoic acid dimer starting material (but not the stereochemistry)
- *"nonanedioic acid, polymer with 1,2-ethanediamine, 1,6-hexanediamine and a single isomer of octadecadienoic acid dimer"* masks the stereochemistry

Example 2

Specific chemical name: "*Hydrogenated palm-oil fatty acids, esters with D-mannitol, ethoxylated*"

Appropriate generic names:

- "*hydrogenated plant oil fatty acids, esters with D-mannitol, ethoxylated*" masks the natural source of the fatty acids parent group
- "*modified palm-oil fatty acids, esters with D-mannitol, ethoxylated*" masks that the fatty acid parent group is hydrogenated
- "*hydrogenated palm-oil fatty acids, esters with polyhydroxyalkane, ethoxylated*" masks the identity of the D-mannitol reactant
- "*hydrogenated palm-oil fatty acids, esters, with D-mannitol, alkoxylated*" masks that the chemical substance is ethoxylated

Example 3

Specific chemical name: "*Waste plastics, pyrolyzed, C5-12 fraction*"

Appropriate generic names:

- "*waste polymers, pyrolyzed, C5-12 fraction*" or "*waste solids, pyrolyzed, C5-12 fraction*" or "*wastes, pyrolyzed, C5-12 fraction*" masks the identity of the waste source of the starting material

- "*waste plastics, pyrolyzed, fractionated*" masks the specific carbon range of the fraction

Similarly, specific chemical name: "*Tires, wastes, pyrolyzed, C6-39 oil fraction*"

Appropriate generic names:
- "*waste polymers, pyrolyzed, C6-39 oil fraction*" or "*waste solids, pyrolyzed, C6-39 oil fraction*" or "*wastes, pyrolyzed, C6-39 oil fraction*" masks the identity of the waste source of the starting material
- "*tires, wastes, pyrolyzed, fractionated*" masks the specific carbon range of the fraction

Inorganic Chemical Substances

Inorganic chemical substances (which, for the purposes of this guidance, includes organometallic substances) may or may not include metals. In the case of metal-containing inorganic compounds or complexes, the identity of the metal atom can be masked by substituting with more generic terms such as "*metal*," "*transition metal*", "*alkali metal*," or "*alkaline earth metal*." Similarly, the identity of a metalloid atom can be masked by substituting with the more generic term "*metalloid*." Non-metal elements can be masked by applying the guidance for class 1 substances. For example, the metal in "*Potassium bromide*" can be masked by substituting "*alkali metal"* ("*alkali metal bromide*") and the bromide group can be masked by substituting "halide" ("*potassium halide*").

For mixed metal-containing inorganic compounds or complexes, the identity of one metal atom can be masked by substituting with more the generic term "*metal*," or the identities of two or more metal atoms can be masked by substituting with more the generic term "*mixed metal*." For example, one metal in "*Cadmium zinc sulfide*" can be masked by substituting "*transition metal*" ("*transition metal zinc sulfide*" or "*cadmium transition metal sulfide*") or both metals can be masked by substituting "*mixed metal"* or "*mixed transition metal*" ("*mixed transition metal sulfide*").

For inorganic substances with more complex structural elements (such as inorganic UVCB substances), such elements can be masked by applying the guidance for class 2 substances. For example, manufacturing, chemical processing, or related information used as a means to identify more complex structural variability or unknown structural elements of inorganic substances can be masked by substituting either a more generic structure-based descriptor or a more generic descriptor of the method. To mask source information, a more generic descriptor of the source should be substituted. To further illustrate, "*acid-leached*" or "*sintered*" could be substituted with "*modified*" or "*treated*," "*copper ore*" could be substituted with "*ore*," and "*copper refinery*" could be substituted with "*metal refinery*."

Examples

The generic names provided for the examples below illustrate only some of the possible ways that structural elements in inorganic chemical substances can be masked.

Example 1

Specific chemical name: "*Silicic acid, aluminum calcium salt*"

Appropriate generic names:

- "*metalloid acid, aluminum calcium salt*" or "*inorganic acid, aluminum calcium salt*" masks the identity of the silicic acid parent group
- "*silicic acid, mixed metal salt*" masks the identity of the aluminum calcium salt

Example 2

Specific chemical name: "*Copper(2+), tetraammine-, carbonate hydroxide (2:1:2)*"

Appropriate generic names:

- "*transition metal, tetraammine-, carbonate hydroxide"* masks the identity of the copper metal
- "*Copper(2+), nitrogen-substituted, carbonate hydroxide*" masks the identity of the tetramine group
- "*Copper(2+), tetraammine-, salt complex*" masks the identity of the carbonate hydroxide salt

Example 3

Specific chemical name: "*Zinc ores, concs., preleached*"

Appropriate generic names:

- "*ores, concs., preleached*" masks the identity of the zinc ores
- "*zinc ores, concs., modified*" masks that the zinc ores are preleached

Example 4

Specific chemical name: "*Copper, [2,9,16,23-tetrachloro-29H,31H-phthalocyaninato(2-)-.kappa.N29,.kappa.N30,.kappa.N31,.kappa.N32]-, (SP-4-1)-*"

Appropriate generic names:

- "*transition metal, [2,9,16,23-tetrachloro-29H,31H-phthalocyaninato(2-)-.kappa.N29,.kappa.N30,.kappa.N31,.kappa.N32]-, (SP-4-1)-*" masks the identity of the copper metal
- "*copper, [2,9,16,23-tetrahalo-29H,31H-phthalocyaninato(2-)-.kappa.N29,.kappa.N30,.kappa.N31,.kappa.N32]-, (SP-4-1)-*" masks identity of the chloro groups (but not the number and positions)
- "*copper, [polychloro-29H,31H-phthalocyaninato(2-)-.kappa.N29,.kappa.N30,.kappa.N31,.kappa.N32]-, (SP-4-1)-*" masks the locants and multiplicative prefix of the chloro groups (but not the identity)
- "*copper, [2,9,16,23-tetrachloro-heteropolycyclic]-*" masks identity of the phthalocyaninato group