APPENDIX B

GENERIC NAMES FOR CONFIDENTIAL

CHEMICAL SUBSTANCE IDENTITIES

The following list contains generic chemical names for the substances included in the category "Chemical Substances with Confidential Identities," which appears in the TSCA Inventory. The identities of these substances have been claimed as confidential business information by submitters to the Inventory. The fact that these substance identities are listed as confidential does not mean that EPA has made a determination that all of these claims of confidentiality are valid.

Some of the substances that appeared as confidential in Volume I of the Initial Inventory or Cumulative Supplement II may have been transferred to the non-confidential portion of the **TSCA Chemical Substance Inventory: 1985 Edition.** This is because either EPA determined that the chemical identity fails to meet the standard for confidential treatment in section 14 of TSCA, or submitters decided to withdraw their claims of confidentiality. Also, the Agency may have denied the confidentiality claim based on the fact that another person submitted the same substance without claiming confidentiality for the chemical identity. These substances are published on the non-confidential portion of the TSCA Inventory. Their generic names and accession numbers have been removed from this list of confidential substances. The Agency encourages submitters to withdraw their claims of confidentiality for chemical identity when confidential treatment is no longer needed.

This appendix includes generic names for substances that were submitted under the TSCA Inventory Reporting Regulations and claimed as confidential by their submitters as well as generic names for substances that were not claimed as confidential for purposes of the Inventory by their submitters, but which include as reactants confidential trademark products manufactured by other companies. For these substances, the EPA has developed generic names that mask only the portion of the Inventory substance that represents the confidential trademark reactant.

This appendix also includes generic names for substances that have been placed on the Inventory following premanufacture review and receipt by EPA of a notice of commencement of manufacture or import. Companies must reassert and substantiate confidential chemical identity claims at the time of submitting a notice of commencement. EPA reviews the submitter's substantiation to determine whether a claim of confidentiality is justified. EPA also determines whether the generic name submitted in the premanufacture notice is appropriate for Inventory listing purposes. In most cases, the EPA finds that the submitter's generic name is too generic, and develops a mutually agreeable generic name following the procedures in the Premanufacture Notice Requirements and Review Procedures (4) CFR 720.85). This generic name is then listed in the Inventory.

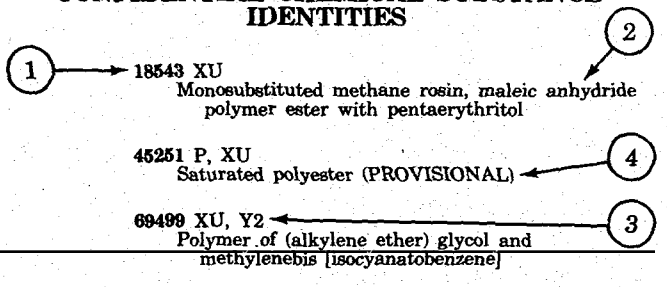
At the time of this printing, a number of commenced PMN substances for which notices of commencement have been received were undergoing substantiation review or generic name development. To represent these substances on the printed Inventory, EPA has published some generic names as submitted in the premanufacture notices, accompanied by the word PROVISIONAL in parentheses after the name. If the claims of confidentiality are neither dropped by the submitter nor held invalid by EPA, EPA will publish the final generic names for these substances in future updates or supplements to the Inventory.

With the exception of the provisional generic names, the generic names in this appendix were created according to the guidelines presented in the following pages. These guidelines were published in the introduction to Appendix B of the TSCA Initial Inventory and made available by EPA to assist persons who wished to claim the precise identity of a chemical substance as confidential for purposes of the Inventory. Such persons were required to submit a proposed generic name for the reported substance that was "only as generic as necessary to protect the confidential identity of the particular chemical substance."

Persons who intend to manufacture or import for a commercial purpose a chemical substance that is not included on the Inventory by a specific chemical name but falls within one of the generic names included in this list may ask EPA whether the specific chemical identity is included on the Inventory. EPA may disclose such information provided the person establishes a *bona fide intent* to manufacture or import the substance for commercial purposes, in accordance with the procedures outlined in section 720.25 of the Premanufacture Notice Requirements and Review Procedures (48 FR 21722).

EPA assigns a unique five-digit accession number to each confidential chemical identity on the TSCA Inventory. Each substance in this appendix is listed in order of its accession number; any applicable flags follow the accession number. The flags used are: P, S, XU, Y1, and Y2.

ILLUSTRATIVE KEY TO ENTRIES AS THEY APPEAR IN APPENDIX B: GENERIC NAMES FOR CONFIDENTIAL CHEMICAL SUBSTANCE IDENTITIES



1. The **Accession Number** appears in *boldface* type.

2. The **Generic Name** appears in lightface type under the Accession Number.

3. The **flags** for SNUR substances, PMN substances, *et al.* appear in lightface type following the Accession Number. The following flags are used:

   — **P** indicates a commenced PMN substance.

   — **S** indicates a substance identified in a proposed or final Significant New Use Rule. See the *SNUR Index.*

   —**XU** indicates a substance exempt from reporting under the proposed rule for Partial Updating of the TSCA Inventory Data Base Production and Site Reports.

   —**Y1** indicates an exempt polymer that has a number-average molecular weight of 1,000 or greater.

   —**Y2** indicates an exempt polymer that is a polyester and is made only from the specified list of low concern reactants.

4. The label **PROVISIONAL** follows the generic name and indicates that the generic name is not considered final by EPA and that it is subject to change.

GUIDELINES FOR CREATING PROPOSED GENERIC NAMES FOR CONFIDENTIAL CHEMICAL SUBSTANCE IDENTITIES FOR THE TSCA INVENTORY

The procedures presented below were designed by EPA to provide guidance in developing proposed generic names for chemical substances whose specific identities were claimed as confidential for purposes of the Inventory. They are included in this Appendix to assist a company in deciding if a particular chemical substance is possibly included in the class defined by a generic name and, hence, on the Inventory. The company would then file a *bona fide* inquiry to make a more precise determination of the Inventory status of the substance.

These guidelines are based on the masking of selected parts of a specific substance name to disguise the full identity of the substance. Although the guidelines illustrate the masking of a single structural feature, multiple masking is permitted if the company reporting the substance justifies in writing the need for such additional masking.

Because of inherent differences in naming Class 1 and Class 2 chemical substances, the guidelines address each separately. However, in certain instances the procedure for creating proposed generic names for Class 1 substances is applicable to the creation of generic names for Class 2 substances as well.

Class 1 Chemical Substances

The composition of a Class 1 chemical substance, except for impurities, can be represented by a definite chemical structure diagram.

The names of Class 1 chemical substances normally disclose the following chemical structure information:

1. Identity of parent structure (i.e., a chain of carbon atoms, a ring system, or a coordinated metal).
2. Identity, number, and position of chemical group(s) which are attached to the parent structure(s) or to other chemical groups.
3. Identity and number of counter ions (for salts).
4. Stereochemical relationships.

Generic chemical names are created for Class 1 chemical substances by masking structurally descriptive parts of their specific chemical names. Masking can be accomplished by substituting non-descriptive terms (e.g., "substituted") for descriptive parts of the name.

The structurally descriptive parts of a Class 1 chemical name that could be masked when creating a proposed generic name, are listed below:

1. A locant which specifies the placement of a single chemical group.
2. Locant and multiplicative prefixes (e.g., di-, tri-, tetra-) which together specify the number and placement of a given chemical group.
3. Identity (but **not** placement and number) of a given chemical group.
4. Identity of a given parent structure, and locants of substituent chemical groups.
5. Identity and multiplicative prefixes (specifying the number) of a given simple cation or anion of a salt.

Chemical Group Masking

Table 1 of these guidelines lists by name and molecular formula the type of chemical groups which can be masked to create a proposed generic name for a Class 1 chemical substance.

The groups of atoms found in Table 1 are common chemical structural units; a given group may be listed under more than one name. Each group includes at least one atom other than carbon or hydrogen.

A chemical group which includes a carbon atom having more than one single free valence (e.g., carbonyl —CO—) can not be masked if the carbon atom is directly attached to an acyclic carbon atom or is included within a ring system; in this circumstance, only the atom or group of atoms attached to the carbon atom can be masked. (See Example 2, below, where the oxo group is masked.)

Table 1 lists most of the **common** chemical functional groups which contain oxygen, e.g., H_2NCO-. While not always listed, the Group VIa element (sulfur, selenium and tellurium) analogs of these functional groups, e.g., H_2NCSe-, are considered included within Table 1 and, accordingly, can be used in masking.

Parent Masking

A parent structure which is a chain of carbon atoms or a ring system can be masked in the chemical name only by the following generic terms:

alkyl *or* alkane

alkenyl *or* alkene
alkynyl *or* alkyne
carbomonocyclic *or* carbomonocycle (e.g., benzene, cyclopentane)
carbopolycyclic *or* carbopolycycle (e.g., naphthalene, spiroundecane)
heteromonocyclic *or* heteromonocycle (e.g., pyrrole, *p*–dioxane)
heteropolycyclic *or* heteropolycycle (e.g., indole, benzothiazole)

In the case of a coordinated metal compound, the identity of the metal atom can be masked by the term "metal" in the chemical name.

Only one such parent group or multiple occurrences of the **same** parent group can be masked.

The following examples show how several hypothetical compounds can be named by masking only **one** structural detail (other than stereochemistry). (As pointed out earlier, multiple masking is allowed if the reporting company can establish to the satisfaction of the Agency the need for the additional masking.)

Example 1 $CF_3CF_2CF_2CF_2CF_2CN(CH_2CH_2OH)_2$
$$\begin{matrix} & & & & & & || & & \\ & & & & & & O & & \end{matrix}$$

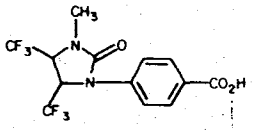
FULLY DEFINED NAME:

2,2,3,3,4,4,5,5,6,6,6–Undecafluoro–*N,N*–bis(2–hydroxyethyl)hexanamide

ACCEPTABLE GENERIC NAMES:

fluorine atoms masked:
N,N–Bis(2–hydroxyethyl), 2,2,3,3,4,4,5,5,6,6,6–undecasubstituted hexanamide
number of fluorine atoms masked:
Polyfluoro–*N,N*–bis(2–hydroxyethyl)hexanamide
hydroxyl groups masked:
2,2,3,3,4,4,5,5,6,6,6–Undecafluoro–*N,N*–bis(2–substituted ethyl)hexanamide
hexane parent (plus locants) masked:
Undecafluoro–*N,N* –bis(2–hydroxyethyl)alkanamide
amide group (plus nitrogen locants) masked:
2,2,3,3,4,4,5,5,6,6,6–Undecafluorobis(2–hydroxyethyl)hexane derivative

Example 2



FULLY DEFINED NAME:

4–[3–Methyl–2–oxo–4,5–bis(trifluoromethyl)–1–imidazolidinyl] benzoic acid

ACCEPTABLE GENERIC NAMES:

oxo group masked:
4–[3–Methyl–2–substituted–4,5–bis(trifluoromethyl)–1–imidazolidinyl] benzoic acid
(NOTE: Only the oxo and not the carbonyl group has been masked.)
fluorine atoms masked:
4–[3–Methyl–2–oxo–4,5–bis(trisubstituted methyl)–1–imidazolidinyl] benzoic acid
benzene ring (plus locant) masked:
[3–Methyl–2–oxo–4,5–bis(trifluoromethyl)–1–imidazolidinyl] carbomonocyclic carboxylic acid
imidazolidine ring (plus locants) masked:
4–[Methyloxobis(trifluoromethyl)heteromonocycle] benzoic acid

Class 2 Chemical Substances

The composition of a Class 2 chemical substance cannot be represented by a definite chemical structure diagram. The specific name used to describe such a substance on the Inventory was based, in whole or in part, on the supplemental information provided for each substance, i.e., the information which further established the identity of the substance.

The composition of some Class 2 substances can be represented by a partial or incomplete chemical structure diagram. In other instances, the composition can only be described in terms of a complex combination of several different known or unknown components.

The method by which a Class 2 substance is manufactured can also serve to identify the substance. For a substance manufactured by chemical reaction, identification can be stated in terms of the immediate precursor substances and other reactants which participate in the final reaction sequence used to manufacture the substance, and the nature of the reaction, e.g., ethoxylation, or bromination. For a substance derived from a source without chemical reaction, processing information identifies the source and method of derivation, e.g., distillation, or extraction with methylene chloride.

Because Class 2 chemical substance names may be based on such variable types of information, these guideline procedures for creating proposed Class 2 generic names are necessarily stated in only the most general terms. Nonetheless, in instances such as those described below, the guideline procedure presented earlier for creating generic names for Class 1 substances may be applicable.

The composition of a Class 2 chemical substance which can be represented by a partial or incomplete chemical structure diagram can generally be described by a common chemical name which encompasses the variability or incompleteness in the structure. EPA generally will accept a proposed generic name for such a substance if created by following the guidelines specified for masking Class 1 chemical substances.

In other instances, the preferred name for a Class 2 chemical substance may identify a predominant component or components of its composition, an immediate precursor or precursors, and other reactants by specific chemical name. EPA generally will accept a proposed generic name for such a substance if it is constructed by masking the chemical name of **one** such component, precursor, or reactant according to the guideline procedure specified for Class 1 substances.

The following example shows how one hypothetical substance could be identified by names which mask only **one** structural detail.

Example

Ethoxylated mixed esters derived from hydrogenated palm oil fatty acids and D–mannitol

FULLY DEFINED NAME:

Hydrogenated palm-oil fatty acids, esters with D-mannitol, ethoxylated

ACCEPTABLE GENERIC NAMES:

oil source masked:

Hydrogenated fatty acids, esters with D-mannitol, ethoxylated

hydrogenation masked:

Modified palm-oil fatty acids, esters with D-mannitol, ethoxylated

carbohydrate masked:

Hydrogenated palm-oil fatty acids, esters with hexahydroxyalkane, ethoxylated

ethoxylation masked:

Hydrogenated palm-oil fatty acids, esters, with D-mannitol, alkoxylated