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Office of
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Toxic Substances Control Act Chemical Substance Inventory

Initial Inventory

Volume I

TOXIC SUBSTANCES CONTROL ACT (TSCA)
CHEMICAL SUBSTANCE INVENTORY

VOLUME I

INITIAL INVENTORY

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SDA SUBSTANCE IDENTIFICATION PROCEDURE

FOR CLASS 2 CHEMICAL SUBSTANCES DERIVED FROM NATURAL FATS AND OILS AND SYNTHETIC SUBSTITUTES

The substance identification system presented here is an alternate and relatively simple method which was used to identify for the Inventory certain multicomponent Class 2 chemical substances derived from natural fats and oils and synthetic long-chain alkyl substitutes. The system was developed by The Soap and Detergent Association in conjunction with the EPA and is intended to standardize the identification of substances manufactured and used extensively in the soap and detergent industry. Accordingly, the system was used to identify multicomponent soaps and surface active agents (and also their precursors and derivatives) manufactured, imported, or processed for such uses as wetting agents, emulsifiers, dispersants, and penetrants. Its applicability, however, extended beyond the soap and detergent industry.

This system was not to be used to identify any single component Class 1 chemical substance (i.e., a substance whose composition may be represented by a definite chemical structure diagram) or any combination of such substances prepared by mixing without chemical reaction. Furthermore, it was not to be used in those cases where the person reporting considered its applicability to be marginal or in question.

The Class 2 chemical substances which were reported using this system are complex, multicomponent materials whose individual components have a common structural feature: one or more long-chain alkyl groups to which is attached a chemically functional group or groups. These components differ from one another with respect to one or more of the following long-chain alkyl group characteristics: length (carbon number), saturation, structure (linear or branched), and/or the position of functional group attachment(s).

Under the SDA Substance Identification Procedure, certain of these Class 2 chemical substances are identified by SDA Substance Names and by corresponding SDA Numbers and Substance Definitions.

SDA SUBSTANCE NAMES

SDA Substance Names are systematically-derived, and, within the limitations of the system, are as precisely descriptive of the chemical composition of a substance as possible.

SDA Substance Names consist of two or, in some cases, three parts. The two parts common to all SDA Substance Names are: (1) the Alkyl Descriptor, **A**, which describes the long-chain alkyl groups of the substance, and (2) the Functionality Descriptor, **F**, which identifies the functional group(s) of the substance. A third part, the Salt Descriptor, **S**, identifies the cation(s) of any salt.

SDA Substance Names are systematically constructed according to the following formats:

(**A**) alkyl (**F**),
or in the case of salts,
(**A**) alkyl (**F**) (**S**),

where **A** denotes the Alkyl Descriptor; **F**, the Functionality Descriptor; and **S**, the Salt Descriptor.

For example, the SDA Substance Name for a fatty amine which contains predominantly C_{10}–C_{16} saturated alkyl chain-length is:

C_{10}–C_{16} alkyl amine

where the phrase "C_{10}–C_{16}" corresponds to the Alkyl Descriptor (**A**), and "amine", to the Functionality Descriptor (**F**).

Similarly, the SDA Substance Name for the sodium salt of a fatty carboxylic acid comprised predominantly of C_{18} saturated and C_{18} unsaturated alkyl chains is:

C_{18} and C_{18} unsaturated alkyl carboxylic acid sodium salt

where the phrase "C_{18} and C_{18} unsaturated" corresponds to the Alkyl Descriptor (**A**); "carboxylic acid" to the Functionality Descriptor (**F**); and "sodium salt", to the Salt Descriptor (**S**).

The Class 2 chemical substances covered by this system are limited to those whose composition may be described using the Alkyl, Functionality, and Salt Descriptors listed below in Tables 1, 2, and 3, respectively. These descriptors, discussed in detail below, can be combined in the SDA Substance Name format to describe more than 5,000 multicomponent Class 2 chemical substances.

Alkyl Description

Table I lists the Alkyl Descriptors covered by this system of substance identification; assigned to each is a two-digit Alkyl Descriptor Code used in generating the SDA Reporting Numbers, described later. Each Descriptor identifies a distribution of alkyl groups in terms of carbon chain length, saturation and/or unsaturation, and linear or branched structure. Alkyl group distributions are inclusive of both even and odd alkyl chain lengths.

The Descriptors of Table 1 were chosen to cover the predominant long-chain alkyl group distributions actually present as of 1978, in most commercial multicomponent Class 2 substances of this type, and to provide for each as precise a description as practical. *Use of this system is predicated on selecting the narrowest alkyl distribution (Alkyl Descriptor) which describes the predominant long-chain alkyl groups of the substance reported.* In this context, the term "predominant" means that about 80 to 100 percent of all long-chain alkyl groups are included within the description.

In the Alkyl Descriptor, a saturated, linear long-chain alkyl group is denoted by "C_x" where the subscript x indicates the number of carbon atoms in the alkyl chain. Unsaturated and multiple branched alkyl groups are denoted by "C_x unsaturated" and "C_x branched", respectively.

By convention, the number of carbon atoms in a long-chain alkyl group includes all long-chain alkyl and functional group carbon atoms, other than those contained in an aromatic ring, which are connected to each other in a unbroken chain of carbon–carbon–bonds. For example, the alkyl chainlength, designated by "R" in the representative structural diagrams

found in Table 2, includes the acyl carbon of carboxylic acids and their derivatives, and the total number of carbon atoms in such structures as R–CH_2–OH or R–CH:CH_2. The alkyl group does not include, however, functional group carbon atoms which are part of a phenyl ring, or are separated from the alkyl chain by a phenyl group or an atom other than carbon, e.g., R–Ph, R–$N(CH_3)_2$, or R–$O(CH_2)_3NH_2$.

Unless specified otherwise, the alkyl groups identified by each Alkyl Descriptor are linear, or essentially linear, hydrocarbon chains. The natural fats and oils listed below provide such alkyl groups:

Vegetable	*Animal*
Avocado	Grease
Babassu	Lard
Castor	Neatsfoot
Coconut	Poultry
Corn	Tallow
Cottonseed	
Crambe	*Marine*
Linseed	
Olive	Herring
Oiticica	Menhaden
Palm	Salmon
Palm-kernel	Sardine
Peanut	Sperm Body
Rapeseed	(whale)
Rice Bran	Sperm Head
Safflower	(whale)
Safflower	Whale
(high oleic)	
Sesame	
Sorghum	
Soybean	
Sunflower	
Tung	
Wheat Germ	

These sources provide both saturated and unsaturated alkyl groups; castor oil provides a C_{18} hydroxy substituted alkyl group. Alkyl groups derived from other natural sources are not covered by this system.

Synthetic sources can provide linear or essentially linear alkyl groups, i.e., chain branching, if any, is limited to no more than one secondary methyl (CH_3–) or ethyl (C_2H_5–) group per alkyl chain. For purposes of this system, the latter type of alkyl chain is included within the designation "linear". Multiple branched alkyl groups, derived exclusively from synthetic sources, have separate Alkyl Descriptors.

Some Class 2 chemical substances covered by this procedure are comprised of components which have two or more long-chain alkyl groups, e.g., (dialkyl) amine, or (dialkyl) dimethyl ammonium chloride. This system could be used to identify such substances *provided* that each long-chain alkyl group is describable, in its predominant composition, by an Alkyl Descriptor found in Table 1 and that none of these long-chain alkyl groups is a single component structure describable by a definite chemical structural diagram.

Functionality Description

Table 2 lists the Functionality Descriptors which could be used in this system of substance identification; assigned to each is a three-digit Functionality Descriptor Code used in generating SDA Reporting Numbers. The partial chemical substance nomenclature (Functionality Descriptors) for each identifies a specific functional group or groups. Different Descriptors are provided for salts, and for their corresponding acids.

Associated with each Functionality Descriptor in Table 2 is a representative structure diagram or diagrams. In many cases, these diagrams depict only one of several possible isomers of a substance identified by a given Functionality Descriptor. For example, a C_{14}–C_{18} alkyl amine identified by this system may contain components which have the amine functional group (–NH_2) attached to a terminal alkyl carbon, as shown in Table 2 for Functionality Descriptor Code 029, or to any other carbon atom in the alkyl chain. *The applicability and limitations of each representative structural diagram are defined by a Substance Definition.* (See Substance Definition, below.)

Salt Description

Table 3 lists the Salt Descriptors covered by this system of substance identification; assigned to each is a two-digit Salt Descriptor Code used in generating the SDA Reporting Number. SDA Substance Names for Class 2 chemical substance which are not salts contain no Salt Descriptor part; the Salt Descriptor Code for such substances is *00*.

Mixed salts of monovalent anions are considered mixtures of the individual salts, each of which were to be identified separately. Mixed salts of divalent anions, however could be identified as a single substance.

SDA REPORTING NUMBER

The SDA Reporting Number is derived using the two- or three-digit codes associated with each Alkyl, Functionality, or Salt Descriptor contained in Tables 1, 2, and 3. The SDA Reporting Number is generated by systematically combining these codes for a given substance in a manner similar to that used to derive the SDA Substance Name. SDA Reporting Numbers have the following formats:

SDA **aa–fff–ss**
or for mixed salts of divalent anions,
SDA **aa–fff–ss,s′s′**

where "**aa**" denotes the appropriate Alkyl Descriptor Code; "**fff**", the appropriate Functionality Descriptor Code; and "**ss**" (and "**s′s′**") the appropriate Salt Descriptor Code(s).

For example, the SDA Reporting Number for C_{10}–C_{16} alkyl amine is:

SDA 15–029–00

This number was generated using the Descriptor Codes found in Tables 1 to 3. Table 1 identifies the Alkyl Descriptor Code for "C_{10}–C_{16}": *15*. Table 2 identifies the Functionality Descriptor Code for "(alkyl) amine": *029*. Table 3 identifies the Salt Descriptor Code to be used when the substance is not a salt: *00*. Inserting these numbers in the standard format yields the correct SDA Reporting Number.

SUBSTANCE DEFINITION

Each Functionality Descriptor listed in Table 2 is assigned a Substance Definition Format number ranging from 1 to 6. Through this number, the SDA Substance Name is linked to one of six generalized Substance Definitions appearing in Table 4. For each substance reported by this procedure, a unique definition can be generated by inserting the Alkyl, Functionality, and Salt Descriptor parts of its SDA Substance Name, and the corresponding representative structural diagram found in Table 2 into the appropriate generalized Substance Definition. Examples contained in Table 4 illustrate how such definitions are generated. *The Substance Definitions provide a chemical description of each substance identified by an SDA Substance Name and specify the applicability and limitation of the corresponding representative structure diagram.*

[Note: In Table 4, the term "positional isomers", appearing

in some Substance Definitions refers to substances which are otherwise similar except for the position of funcitonal group attachment(s) on the long-chain alkyl group(s).]

A seven step method, described in Addendum III of the Toxic Substances Control Act Candidate List of Chemical Substances (March 1978), was useful in applying the nomenclature of this system to the identification and reporting of particular chemical substances. Additional examples which further illustrate the applicability and limitations of the system are also presented there.

TABLE 1

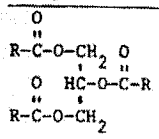
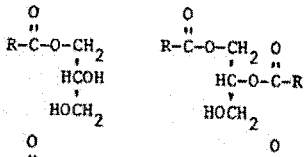
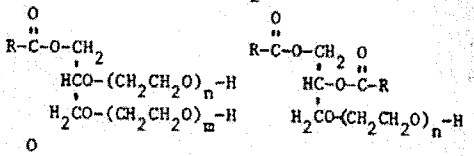
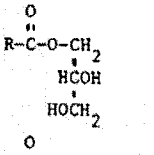
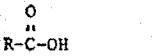
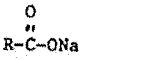
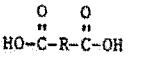
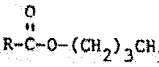
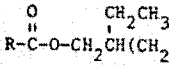
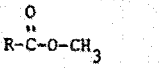
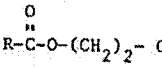
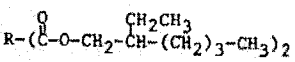
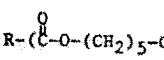
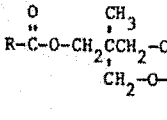
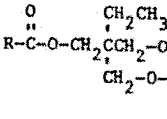
Alkyl Descriptors

Alkyl Descriptor Code	Predominant Carbon Chainlength Distribution Saturated	Unsaturated	Branched	Alkyl Descriptor (A) Nomenclature
01	8-18	18	No	C_8-C_{18} and C_{18} unsaturated
02	10-16	12-20	No	C_{10}-C_{16} and C_{12}-C_{20} unsaturated
03	14-18	12-20	No	C_{14}-C_{18} and C_{12}-C_{20} unsaturated
04	14-18	16-18	No	C_{14}-C_{18} and C_{16}-C_{18} unsaturated
05	14-18	16-22	No	C_{14}-C_{18} and C_{16}-C_{22} unsaturated
06	14-18	16-26	No	C_{14}-C_{18} and C_{16}-C_{26} unsaturated
07	14-22	16-22	No	C_{14}-C_{22} and C_{16}-C_{22} unsaturated
08	16-22	18	No	C_{16}-C_{22} and C_{18} unsaturated
09	16	18	No	C_{16} and C_{18} unsaturated
10	16	18,18*	No	C_{16} plus C_{18} unsaturated and C_{18} hydroxy unsaturated
11	16-18	18	No	C_{16}-C_{18} and C_{18} unsaturated
12	18	18	No	C_{18} and C_{18} unsaturated
13	6-12		No	C_6-C_{12}
14	8-26		No	C_8-C_{26}
15	10-16		No	C_{10}-C_{16}
16	12-18		No	C_{12}-C_{18}
17	14-18		No	C_{14}-C_{18}
18	14-26		No	C_{14}-C_{26}
19	16-18		No	C_{16}-C_{18}
20	16-18,18*		No	C_{16}-C_{18} and C_{18} hydroxy
21	16-22		No	C_{16}-C_{22}
22	8		Yes	C_8 branched
23	9		Yes	C_9 branched
24	12		Yes	C_{12} branched
25	11-13		Yes	C_{11}-C_{13} branched
26		10-16	No	C_{10}-C_{16} unsaturated
27		14-18	No	C_{14}-C_{18} unsaturated

*Hydroxy substituted alkyl group derived from Castor Oil

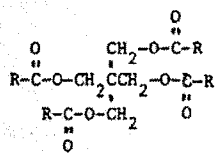
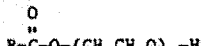
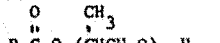
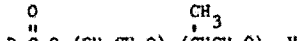
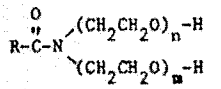
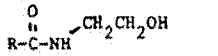
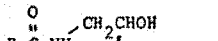
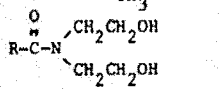
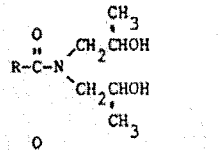
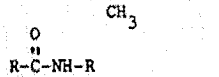
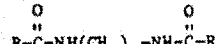
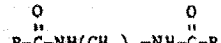
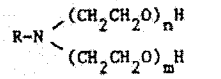
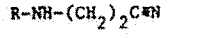
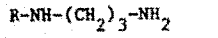
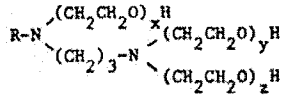
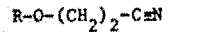
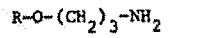
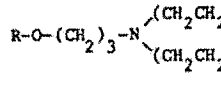
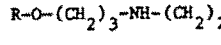
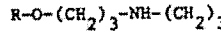
TABLE 2

Functionality Descriptors

Func. Desc. Code	Functionality Descriptor (F) Nomenclature	Common Name	Representative Structural Diagram[a]	Substance Definition Format[b]
001	(trialkyl) glyceride	refined fat or oil		1
002	(alkyl) and (dialkyl) glyceride			1
003	(alkyl) and (dialkyl) glyceride ethoxylate			2
004	(alkyl) glyceride			1
005	(alkyl) carboxylic acid	fatty acid		1
006	(alkyl) carboxylic acid (salt)	soap		1
007	(alkyl) dicarboxylic acid	fatty dibasic acid		1
008	(alkyl) carboxylic acid n-butyl ester	fatty butyl ester		1
009	(alkyl) carboxylic acid 2-ethylhexyl ester	fatty 2- ethylhexyl ester		1
010	(alkyl) carboxylic acid methyl ester	fatty methyl ester		1
011	(dialkyl) carboxylic acid ethylene glycol diester	fatty ethylene glycol diester		1
012	(alkyl) dicarboxylic acid 2-ethylhexyl diester	fatty 2-ethylhexyl diester		1
013	(alkyl) dicarboxylic acid hexyl diester	fatty hexyl diester		1
014	(trialkyl) carboxylic acid trimethylolethane triester			1
015	(trialkyl) carboxylic acid trimethylolpropane triester			1

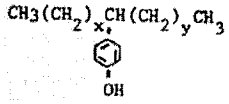
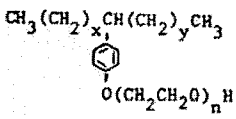
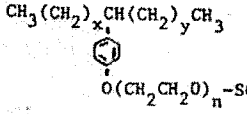
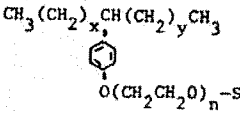
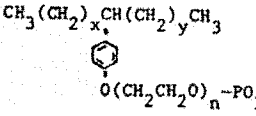
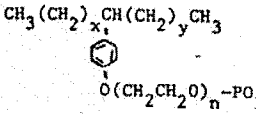
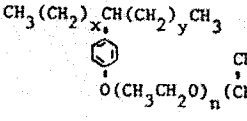
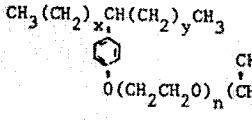
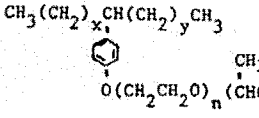
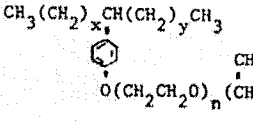
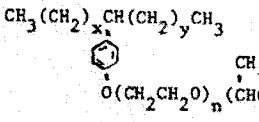
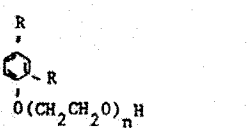
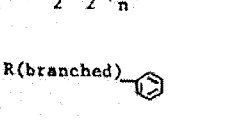
[a] Salts are depicted in terms of sodium cation(s).

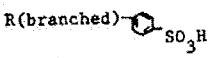
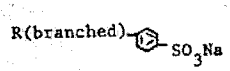
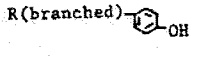
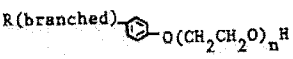
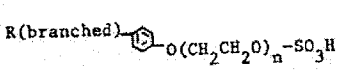
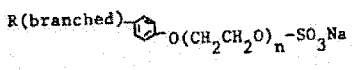
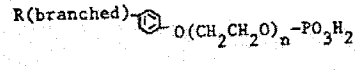
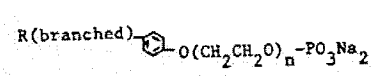
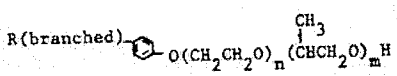
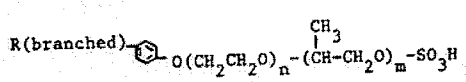
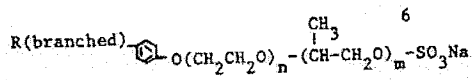
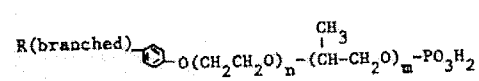
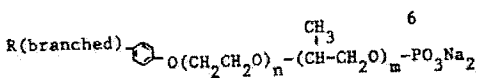
[b] Refer to corresponding Substance Definition Format number (1-6) in Table 4.

016	(tetradlkyl) carboxylic acid pentaerythritol tetraester			2
017	(alkyl) carboxylic acid ethoxylate	ethoxylated fatty acid		2
018	(alkyl) carboxylic acid propoxylate	propoxylated fatty acid		2
019	(alkyl) carboxylic acid ethoxylate propoxylate	ethoxylated propoxylated fatty acid		2
020	(alkyl) carboxylic acid amide	fatty amide		1
021	(alkyl) carboxylic acid amide ethoxylate	ethoxylated fatty amide		2
022	(alkyl) carboxylic acid amide monoethanol	monoethanol fatty amide		1
023	(alkyl) carboxylic acid amide monoisopropanol	monoisopropanol fatty amide		1
024	(alkyl) carboxylic acid amide diethanol	diethanol fatty amide		1
025	(alkyl) carboxylic acid amide diisopropanol	diisopropanol fatty amide		1
026	(alkyl) carboxylic acid amide (alkyl)			1
027	N,N'-(dialkyl) ethylene bis amide			1
028	N,N'-(dialkyl) propylene bis amide			1
029	(alkyl) amine	fatty amine		3
030	(alkyl) amine ethoxylate	ethoxylated fatty amine		4
031	(alkyl) amino ethylene nitrile	fatty amine nitrile		3
032	N-(alkyl) propylene diamine			3
033	N-(alkyl) propylene diamine ethoxylate			4
034	(alkyl) alkoxy ethylene nitrile	fatty ether nitrile		3
035	(alkyl) alkoxy propylene amine			3
036	(alkyl) alkoxy propylene amine ethoxylate			4
037	(alkyl) alkoxy ethylene amino nitrile	fatty ether amino nitrile		3
038	(alkyl) alkoxy propylene amine propylene amine	fatty ether diamine		3

039	(alkyl) nitrile	fatty nitrile	$R-C\equiv N$	3
040	(alkyl) dimethyl amine	fatty dimethyl amine	$R-N-(CH_3)_2$	3
041	(alkyl) dimethyl amine oxide	fatty dimethyl amine oxide	$R-\overset{CH_3}{\underset{CH_3}{N}}\rightarrow O$	3
042	(dialkyl) amine	dialkyl amine	$\overset{R}{\underset{R}{NH}}$	3
043	(dialkyl) methyl amine	dialkyl methyl amine	$\overset{R}{\underset{R}{N}}-CH_3$	3
044	(trialkyl) amine	trialkyl amine	$\overset{R}{\underset{R}{N}}-R$	3
045	(alkyl) trimethyl ammonium chloride	alkyl trimethyl ammonium chloride	$\left[\overset{R}{\underset{CH_3}{N}}\overset{CH_3}{\underset{CH_3}{}}\right]^+ Cl^-$	3
046	(alkyl) trimethyl ammonium bromide	alkyl trimethyl ammonium bromide	$\left[\overset{R}{\underset{CH_3}{N}}\overset{CH_3}{\underset{CH_3}{}}\right]^+ Br^-$	3
047	(dialkyl) dimethyl ammonium chloride	dialkyl dimethyl ammonium chloride	$\left[\overset{R}{\underset{R}{N}}\overset{CH_3}{\underset{CH_3}{}}\right]^+ Cl^-$	3
048	(dialkyl) dimethyl ammonium bromide	dialkyl dimethyl ammonium bromide	$\left[\overset{R}{\underset{R}{N}}\overset{CH_3}{\underset{CH_3}{}}\right]^+ Br^-$	3
049	(dialkyl) dimethyl ammonium methyl sulfate	dialkyl dimethyl ammonium methyl sulfate	$\left[\overset{R}{\underset{R}{N}}\overset{CH_3}{\underset{CH_3}{}}\right]^+ CH_3SO_4^-$	
050	(trialkyl) methyl ammonium chloride		$\left[\overset{R}{\underset{R}{N}}\overset{R}{\underset{CH_3}{}}\right]^+ Cl^-$	3
051	(trialkyl) methyl ammonium bromide		$\left[\overset{R}{\underset{R}{N}}\overset{R}{\underset{CH_3}{}}\right]^+ Br^-$	3
052	(alkyl) benzyl dimethyl ammonium chloride		$\left[\bigcirc\!\!-CH_2-\overset{CH_3}{\underset{CH_3}{N}}\overset{}{\underset{R}{}}\right]^+ Cl^-$	3
053	(dialkyl) benzyl methyl ammonium chloride		$\left[\bigcirc\!\!-CH_2-\overset{R}{\underset{CH_3}{N}}\overset{}{\underset{R}{}}\right]^+ Cl^-$	3
054	(trialkyl) benzyl ammonium chloride		$\left[\bigcirc\!\!-CH_2-\overset{R}{\underset{R}{N}}\overset{}{\underset{R}{}}\right]^+ Cl^-$	3
055	(alkyl) chloride	alkyl chloride	RCH_2-Cl	3
056	(alkyl) bromide	alkyl bromide	RCH_2-Br	3
057	(alkyl) alpha olefin	alpha olefin	$R-CH=CH_2$	3
058	(alkyl) alkene and (alkyl) hydroxy sulfonic acid		$R(CH_2)_xCH=CH(CH_2)_y-SO_3H$, $R(CH_2)_x\underset{OH}{CH}(CH_2)_y-SO_3H$	3
059	(alkyl) alkene and (alkyl) hydroxy sulfonic acid (salts)	olefin sulfonate	$R(CH_2)_xCH=CH(CH_2)_y-SO_3Na$ $R(CH_2)_x\underset{OH}{CH}(CH_2)_y-SO_3Na$	3

060	(alkyl) alcohol	fatty alcohol	$R-CH_2-OH$	3
061	(alkyl) alcohol sulfuric acid		$R-CH_2-OSO_3H$	3
062	(alkyl) alcohol sulfuric acid (salt)	alkyl sulfate	$R-CH_2-OSO_3Na$	3
063	(alkyl) alcohol phosphoric acid		$R-CH_2-OPO_3H_2$	3
064	(alkyl) alcohol phosphoric acid (salt)	alkyl phosphate ester	$R-CH_2-OPO_3Na_2$	3
065	(alkyl) alcohol ethoxylate	ethoxylated fatty alcohol	$R-CH_2-O-(CH_2CH_2O)_n-H$	4
066	(alkyl) alcohol ethoxylate sulfuric acid		$R-CH_2-O-(CH_2CH_2O)_n-SO_3H$	4
067	(alkyl) ethoxylate sulfuric acid (salt)	ethoxylated alkyl sulfate	$R-CH_2-O-(CH_2CH_2O)_n-SO_3Na$	4
068	(alkyl) alcohol ethoxylate phosphoric acid		$R-CH_2-O-(CH_2CH_2O)_n-PO_3H_2$	4
069	(alkyl) alcohol ethoxylate phosphoric acid (salt)	ethoxylated alkyl phosphate ester	$R-CH_2-O-(CH_2CH_2O)_n-PO_3Na_2$	4
070	(alkyl) alcohol ethoxylate propoxylate	ethoxylated propoxylated fatty alcohol	$R-CH_2-O-(CH_2CH_2O)_n(CHCH_2O)_m-H$ (CH$_3$)	4
071	(alkyl) alcohol ethoxylate propoxylate sulfuric acid		$R-CH_2-O-(CH_2CH_2O)_n(CHCH_2O)_m-SO_3H$ (CH$_3$)	4
072	(alkyl) alcohol ethoxylate propoxylate sulfuric acid (salt)	ethoxylated propoxylated alkyl sulfate	$R-CH_2-O-(CH_2CH_2O)_n(CHCH_2O)_m-SO_3Na$ (CH$_3$)	4
073	(alkyl) alcohol ethoxylate propoxylate phosphoric acid		$R-CH_2-O-(CH_2CH_2O)_n(CHCH_2O)_m-PO_3H_2$ (CH$_3$)	4
074	(alkyl) alcohol ethoxylate propoxylate phosphoric acid (salt)	ethoxylated propoxylated alkyl phosphate ester	$R-CH_2-O-(CH_2CH_2O)_n(CHCH_2O)_m-PO_3Na_2$ (CH$_3$)	4
075	(alkyl) glyceryl ether chloride		$R-O-CH_2CHCH_2-Cl$ (OH)	3
076	(alkyl) glycidyl ether		$R-O-CH_2CHCH_2$ (O)	3
077	(alkyl) glyceryl ether sulfonic acid (salt)	fatty glycerol sulfonate	$R-O-CH_2CHCH_2-SO_3Na$ (OH)	3
078	(alkyl) epoxide		$R-CHCH_2$ (O)	1
079	(alkyl) benzene	LAB	$CH_3(CH_2)_x\underset{\text{(C}_6\text{H}_4\text{)}}{CH}(CH_2)_yCH_3$	3
080	(alkyl) benzene sulfonic acid		$CH_3(CH_2)_x\underset{\text{(C}_6\text{H}_4\text{SO}_3\text{H)}}{CH}(CH_2)_yCH_3$	3
081	(alkyl) benzene sulfonic acid (salt)	LAS	$CH_3(CH_2)_x\underset{\text{(C}_6\text{H}_4\text{SO}_3\text{Na)}}{CH}(CH_2)_yCH_3$	3

082	(alkyl) phenol	linear alkyl phenol		3
083	(alkyl) phenol ethoxylate	ethoxylated linear alkyl phenol		4
084	(alkyl) phenol ethoxylate sulfuric acid			4
085	(alkyl) phenol ethoxylate sulfuric acid (salt)	ethoxylated linear alkyl sulfate ester		4
086	(alkyl) phenol ethoxylate phosphoric acid			4
087	(alkyl) phenol ethoxylate phosphoric acid (salt)	ethoxylated linear alkyl phosphate ester		4
088	(alkyl) phenol ethoxylate propoxylate	ethoxylated propoxylated linear alkyl phenol		4
089	(alkyl) phenol ethoxylate propoxylate sulfuric acid			4
090	(alkyl) phenol ethoxylate propoxylate sulfuric acid (salt)	ethoxylated propoxylated alkyl phenol sulfate		4
091	(alkyl) phenol ethoxylate propoxylate phosphoric acid			4
092	(alkyl) phenol ethoxylate propoxylate phosphoric acid (salt)	ethoxylated propoxylated linear alkyl phenol phosphate ester		4
093	(dialkyl) phenol	linear dialkyl phenol		3
094	(dialkyl) phenol ethoxylate	ethoxylated linear dialkyl phenol		4
095	(branched alkyl) benzene	AB		5

096	(branched alkyl) benzene sulfonic acid			5
097	(branched alkyl) benzene sulfonic acid (salt)	ABS		5
098	(branched alkyl) phenol	branched alkyl phenol		5
099	(branched alkyl) phenol ethoxylate	ethoxylated branched alkyl phenol		6
100	(branched alkyl) phenol ethoxylate sulfuric acid			6
101	(branched alkyl) phenol ethoxylate sulfuric acid (salt)	ethoxylated branched alkyl phenol sulfate		6
102	(branched alkyl) phenol ethoxylate phosphoric acid			6
103	(branched alkyl) phenol ethoxylated phosphoric acid (salt)	ethoxylated branched alkyl phenol phosphate ester		6
104	(branched alkyl) phenol ethoxylate propoxylate	ethoxylated propoxylated branched alkyl phenol		6
105	(branched alkyl) phenol ethoxylate propoxylate sulfuric acid			6
106	(branched alkyl) phenol ethoxylate propoxylate sulfuric acid (salt)	ethoxylated propoxylated branched alkyl phenol sulfate		6
107	(branched alkyl) phenol ethoxylate propoxylate phosphoric acid			6
108	(branched alkyl) phenol ethoxylate propoxylate phosphoric acid (salt)	ethoxylated propoxylated branched alkyl phenol phosphate ester		6

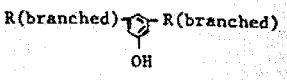
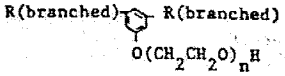
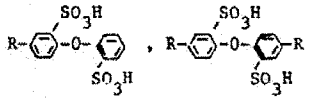
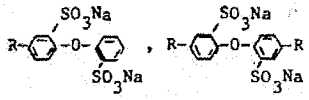
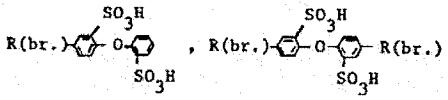
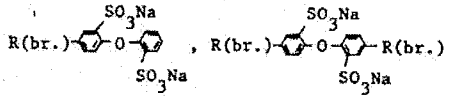
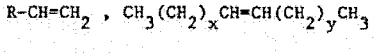
109	(branched dialkyl) phenol	branched dialkyl phenol		5
110	(branched dialkyl) phenol ethoxylate	ethoxylated branched dialkyl phenol		6
111	(alkyl) and (dialkyl) phenoxy benzene sulfonic acid			5
112	(alkyl) and (dialkyl) phenoxy benzene sulfonic acid (salt)			5
113	(branched alkyl) and (branched dialkyl) phenoxy benzene sulfonic acid			5
114	(branched alkyl) and (branched dialkyl) phenoxy benzene sulfonic acid (salt)			5
115	(alkyl) alpha and (alkyl) internal oletin			3

TABLE 3
Salt Descriptors

Salt Descriptor Code	Salt Descriptor (S) Nomenclature
00	(none)
01	ammonium salt
02	lithium salt
03	potassium salt
04	sodium salt
05	barium salt
06	calcium salt
07	magnesium salt
08	nickel salt
09	zinc salt
10	aluminum salt
11	titanium salt
12	monoethanol amine salt
13	diethanol amine salt
14	triethanol amine salt

TABLE 4 (continued)

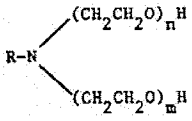
Substance Definition Format	SDA Reporting Number	SDA Substance Name	Substance Definition
3	SDA 00-000-00	(A) alkyl (F) (S) or (A) alkyl (F)	The combination of alkyl (F)(S) having predominantly (A) alkyl chainlengths that generally conform to, or are positional isomers of, the following structural diagram: [Insert the Representative Structural Diagram from Table 2 which corresponds to F; indicate proper salt form(s), if applicable.]
EXAMPLE:			
	SDA 13-060-00	C_6-C_{12} alkyl alcohol	The combination of alkyl alcohols having predominantly C_6-C_{12} alkyl chainlengths that generally conform to, or are positional isomers of, the following structural diagram: $R-CH_2-OH$
4	SDA 00-000-00	(A) alkyl (F) (S) or (A) alkyl (F)	The combination of alkyl (F)(S) having predominantly (A) alkyl chainlengths and ethoxylate and/or propoxylate homologues (as appropriate) that generally conform to, or are positional isomers of, the following structural diagram: [Insert the Representative Structural Diagram from Table 2 which corresponds to F; indicate proper salt form(s), if applicable.]
EXAMPLE:			
	SDA 13-030-00	C_6-C_{12} alkyl amine ethoxylate	The combination of alkyl amine ethoxylates having predominantly C_6-C_{12} alkyl chainlengths and ethoxylate homologues that generally conform to, or are positional isomers of, the following structural diagram: 

TABLE 4
Chemical Substance Identification
with Examples

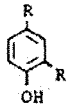
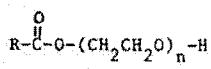
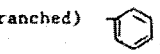
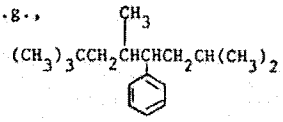
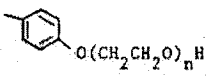
Substance Definition Format	SDA Reporting Number	SDA Substance Name	Substance Definition
1	SDA 00-000-00	(A) alkyl (F) (S) or (A) alkyl (F)	The combination of alkyl (F)(S) having predominantly (A) alkyl chainlengths that generally conform to the following structural diagram: [Insert the Representative Structural Diagram from Table 2 which corresponds to F; indicate proper salt form(s), if applicable.]
EXAMPLES:			
	SDA 13-006-04	C_6-C_{12} alkyl carboxylic acid sodium salt	The combination of alkyl carboxylic acid sodium salts having predominantly C_6-C_{12} alkyl chainlengths that generally conform to the following structural diagram: 
	SDA 13-093-00	C_6-C_{12} dialkyl phenol	The combination of dialkyl phenols having predominantly C_6-C_{12} alkyl chainlengths that generally conform to the following structural diagram: 
2	SDA 00-000-00	(A) alkyl (F) (S) or (A) alkyl (F)	The combination of alkyl (F)(S) having predominantly (A) alkyl chainlengths and ethoxylate and/or propoxylate homologues (as appropriate) that generally conform to the following structural diagram: [Insert the Representative Structural Diagram from Table 2 which corresponds to F; indicate proper salt form(s), if applicable.]
EXAMPLE:			
	SDA 13-017-00	C_6-C_{12} alkyl carboxylic acid ethoxylate	The combination of alkyl carboxylic acid ethoxylates having predominantly C_6-C_{12} alkyl chainlengths and ethoxylate homologues that generally conform to the following structural diagram: 

TABLE 4 (continued)

Substance Definition Format	SDA Reporting Number	SDA Substance Name	Substance Definition
5	SDA 00-000-00	(A) alkyl (F) (S) or (A) alkyl (F)	The combination of alkyl (F)(S) positional isomers having predominantly (A) alkyl chainlengths that generally conform to the following structural diagram: [Insert the Representative Structural Diagram from Table 2 which corresponds to F; indicate proper salt form(s), if applicable.]
EXAMPLE:			
	SDA 24-095-00	C_{12} branched alkyl benzene	The combination of alkyl benzene positional isomers having predominantly C_{12} branched alkyl chainlengths that generally conform to the following structural diagram: R(branched)  e.g., 
6	SDA 00-000-00	(A) alkyl (F) (S) or (A) alkyl (F)	The combination of alkyl (F)(S) having predominantly (A) alkyl chainlengths and ethoxylate and/or propoxylate homologues (as appropriate) that generally conform to, or are positional isomers of, the following structural diagram: [Insert the Representative Structural Diagram from Table 2 which corresponds to F; indicate proper salt form(s), if applicable.]
EXAMPLE:			
	SDA 24-099-00	C_{12} branched alkyl phenol ethoxylate	The combination of alkyl phenol ethoxylates having predominantly C_{12} branched alkyl chainlengths and ethoxylate homologues that generally conform to, or are positional isomers of, the following structural diagram: R(branched  e.g.,