Considerations related to Listing Chemical Categories
Toxics Use Reduction Institute
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The following information may be useful when considering designation of a chemical category. This information is intended to be a helpful guide, and is not comprehensive.

General considerations

For listing a chemical category on the TURA list of Toxic and Hazardous Substances, a key consideration is to ensure the category is sufficiently well defined that companies know their reporting and planning responsibilities. In addition, it is important to have a clear rationale for listing the category.

Sometimes a category is listed because listing specific chemicals with CAS numbers is not feasible. In other cases, the principle reason is that a category better accomplishes the objectives of the listing. Sometimes both of these considerations are relevant.

Rationale for using categories

A category can be appropriate when:

- **Structure**: Substances with a similar structure or functional group pose or can be reasonably anticipated to pose similar hazards. (e.g., glycol ethers, C1-C4 NOL, lead compounds)
    - The toxic effect of concern may be identified for at least one member of the category; it may then be determined that the effect may reasonably be expected to be caused by all other members of the category.
        - e.g., "Because the individual members of this category can be reasonably anticipated to cause one or more of the following effects: …"
- **Precursors**: Substances break down into a similar set of toxic or hazardous degradation/transformation products. (e.g., nonylphenol ethoxylates)
- **Cumulative effects**: In aggregate, the substances can reasonably be anticipated to cause a cumulative health or environmental impact. (e.g., lead compounds)
- **Large groups**: It is not practical to review every chemical individually, either because of the number of possible substances or because EHS data are not available for all members of the group (e.g. C1-C4 NOL)
- **CAS # limitations**: When specific CAS #s do not adequately capture the chemical or category of concern or when use of CAS #s has caused confusion. Likewise, when proprietary ingredients are described generically, or the category is likely to be known by the user, but specific substances are not necessarily known by the user.
- **Mixtures**: When chemicals within the category are used in mixtures, and/or are present as contaminants.

Approaches to Defining a Category

A category can be defined based on:

- **Structure**: using chemical structure and text description, with or without a non-exhaustive list of CAS #s provided as guidance (e.g., glycol ethers)
- **Structure with exclusions**: using chemical structure and text, with specific substances excluded based on evidence that specific chemicals in the category are not sufficiently toxic or hazardous to warrant being on the list (e.g., glycol ethers)
- **Structure NOL**: using chemical structure and text, but only including chemicals not otherwise listed (NOL). Substances that fit the structure but are listed separately are reported individually. Typically this is done when there are chemicals already on the list before the category is added. (e.g., glycol ethers, C1-C4 NOL)
- **Delimited**: using a delimited series of chemical CAS #s. (e.g., nonylphenols and nonylphenol ethoxylates – note that EPA originally proposed that this be defined by structure, but changed to delimited list of CAS #s as a result of comments from industry; this could lead to the introduction of slightly different products with new CAS #s that are not included in the category)

Meeting the objectives of the listing

A chemical category may be preferable under certain circumstances, including:

- **Interchangeability & regrettable substitutes:** if a similar unregulated chemical within the category may be substituted for a regulated chemical for a particular functional use, a category may help prevent regrettable substitution and the "whack-a-mole" situation. (e.g., C1-C4 NOL)
- **New similar substances***:* when chemicals within the category are easily modified to create new similar substances (e.g., metal compounds)
- **Guidance**: when the objective is to communicate the hazard of a particular functional group or type of chemical, particularly when the structure is very complex (e.g., glycol ethers)

Examples – EPCRA TRI[1]

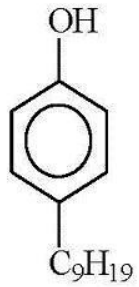
EPA **nonyl phenol** June 2013 listing criteria: (note that ultimately, EPA capitulated to industry's preference for a list of specific CAS numbers)

"Why is nonylphenol being added as a category instead of as an individual chemical?

Nonylphenol is being proposed for addition as a TRI chemical category because there is no single Chemical Abstracts Service Registry Number (CASRN) that adequately captures what is referred to by industry as nonylphenol.

How will the nonylphenol category be defined?

EPA is proposing to define the nonylphenol category using the chemical structure and text below:"



Where C9H19 = Branched or linear alkyl chain

From the Federal Register proposed rule:

"C. How is EPA proposing to list nonylphenol on the TRI?

> Because there is no one CASRN that adequately captures what is referred to as nonylphenol and because of the apparent confusion that has resulted from the use of multiple CASRNs, EPA is proposing to add nonylphenol as a category defined by a structure. EPA is proposing to define the nonylphenol category using the structure and text presented below.
>
> This category definition covers the chemicals that are included in CASRNs 84852–15–3 as well as those 4 position isomers covered by CASRN 25154–52–3. Any nonylphenol that meets the above category definition would be reportable regardless of its assigned CASRN."

From final rule:

> "All three commenters requested that EPA define the nonylphenol category by chemical name and CASRN rather than by a chemical structure. The commenters were concerned that reporting by chemical structure would be difficult for some reporters who lacked detailed knowledge of the chemicals they use. The commenters felt that using chemical names and CASRNs would simplify reporting and be less burdensome.
>
> There are several TRI chemical categories listed based on chemical structures or chemical formulas and reporting has not been a significant issue for those listings. EPA continues to believe that listing nonylphenol as a category defined by structure would be an appropriate way to list the category.

[1] US EPA https://www.epa.gov/toxics-release-inventory-tri-program/addition-nonylphenol-category#rule-history

However, since there are a limited number of CASRNs used to identify nonylphenol mixtures, EPA has decided to modify the category listing to address the commenter's concerns. EPA is listing nonylphenol as a delimited category defined by the existing names and CASRNs."

Nonylphenol Ethoxylate (NPE) Proposed category (Nov 2016)[2]

"On November 16, 2016, EPA proposed a rule that would add a nonylphenol ethoxylates (NPEs) category to the Toxics Release Inventory (TRI) list of reportable chemicals. NPEs are nonionic surfactants used in adhesives, wetting agents, emulsifiers, stabilizers, dispersants, defoamers, cleaners, paints, and coatings.

EPA proposed this rule because we believe that longer-chain NPEs can break down in the environment to short-chain NPEs and nonylphenol, both of which are highly toxic to aquatic organisms. For this reason, EPA believes NPEs meet the Emergency Planning and Community Right-to-Know Act (EPCRA) section 313(d)(2)(C) toxicity listing criteria.
Basis for Adding an NPEs Category

EPA believes that NPEs meet the ECPRA section 313(d)(2)(C) environmental effects listing criteria based on the available toxicity data, which indicate that short-chain NPEs are highly toxic to aquatic organisms. Long-chain NPEs, while not as toxic as short-chain NPEs, degrade in the environment to produce products that include highly toxic short-chain NPEs and nonylphenol. Nonylphenol is even more toxic to aquatic organisms than short-chain NPEs, and EPA added it to the TRI toxic chemical list in September 2014."

While this rule has not yet been finalized, it is interesting to note industry's objection to listing chemicals based on degradation products:
Where degradation intermediates themselves represent the hazard of interest that hazard is contingent on the conditions of disposal and treatment and ultimately the occurrence of those degradants in emissions and the receiving environment. Disposal of long-chain NPEs in one treatment scenario may generate degradation products of concern whereas disposal in another treatment scenario may not generate any degradants of concern.[3]

Polychlorinated Alkanes Category[4] Definition
The polychlorinated alkanes category is defined by the following formula and description:
$C_xH_{(2x-y+2)}Cl_y$
where:
x = 10-13;
y = 3-12; and

[2] US EPA https://www.epa.gov/toxics-release-inventory-tri-program/addition-npes-category-tri-list-proposed-rule

[3] Alkylphenols & Ethoxylates Research Council *Comments on US EPA Proposed Rule for Addition of Nonylphenol Ethoxylates Category to Community Right-to-Know Toxic Chemical Release Reporting under Section 313 of the Emergency Planning and Community Right-to-Know Act (November 16, 2016)*. Submitted to Docket ID No. EPA–HQ–TRI–2016–0222 via the Federal eRulemaking Portal www.regulations.gov. January 17, 2017. Accessed at https://www.regulations.gov/docket?D=EPA-HQ-TRI-2016-0222

[4]US EPA https://ofmpub.epa.gov/apex/guideme_ext/guideme_ext/guideme/file/polychlorinated%20alkanes.pdf

the average chlorine content ranges from 40 to 70 percent with the limiting molecular formulas set at $C_{10}H_{19}Cl_3$ and $C_{13}H_{16}Cl_{12}$.

Chemicals that meet this category definition are reportable.
EPA is providing two lists of CAS numbers and chemical names to aid the regulated community in determining whether they need to report for the polychlorinated alkanes category. The first list includes individual chemicals that meet the polychlorinated alkanes category definition. If a facility is manufacturing, processing, or otherwise using a chemical which is on this list, they must report this chemical. However, this list is not exhaustive. If a facility is manufacturing, processing, or otherwise using a polychlorinated alkane that meets the category definition, they must report this chemical, even if it does not appear on the list. The second list includes chemical mixtures which might contain polychlorinated alkanes that meet the category definition. If a facility is manufacturing, processing, or otherwise using a mixture which is on this list and contains a polychlorinated alkane that meets the category definition, they must report the polychlorinated alkane component. However, this list is not exhaustive. If a facility is manufacturing, processing, or otherwise using a mixture that contains a polychlorinated alkane that meets the category definition, they must report the polychlorinated alkane component, even if the mixture does not appear on the list.

Glycol Ethers
http://www.epa.gov/ttnatw01/glycol2000.pdf

On June 28, 1994, EPA promulgated a final rule (published in the Federal Register July 5, 1994) modifying the definition of the glycol ethers category on the list of toxic chemicals under Section 313 of the Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA), 42 U.S.C. 11001 *et.seq*. The effect of this modification, which is described at 59 FR 34386, is that many high molecular weight glycol ethers were excluded from the category…..
As part of this modification and as the result of public comment, EPA changed the category name at 40 CFR 372.65(c) from 'glycol ethers' to 'certain glycol ethers'.

Glycol Ethers Category Definition
The glycol ethers category is defined by the following formula:

$$R - (OCH_2CH_2)_n - OR'$$

where:
n = 1, 2, or 3;
R = Alkyl C7 or less, or phenyl or alkyl substituted phenyl;
R' = H or alkyl C7 or less, or
OR' consisting of a carboxylic acid ester, sulfate, phosphate, nitrate, or sulfonate.

EPA is providing three lists of CAS numbers and chemical names to aid the regulated community in determining whether they need to report for the glycol ethers category. Section 2 (pages 5 to 159) lists individual chemicals that meet the definition of the EPCRA section 313 'certain glycol ethers' category. This list consists only of chemicals that have been assigned CAS numbers and, thus, is not exhaustive. If a facility manufactures, processes, or otherwise uses, in greater than threshold quantities, a glycol ether that meets the category definition, whether or not that chemical is on this list, they must report the chemical.
….
Ethylene Glycol Ethers versus Propylene Glycol Ethers
The members of this category are glycol ethers derived from ethylene glycol, diethylene glycol, and triethylene glycol. This category does **not** contain glycol ethers based on propylene glycol,

dipropylene glycol, or tripropylene glycol.

Individually Listed Glycol Ethers

There are two chemicals, 2-methoxyethanol (CAS number 109-86-4) and 2-ethoxyethanol (CAS number 110-80-5) that are on the individual chemical list and CAS number list (40 CFR 372.65(a) and (b)). Threshold determinations should be made for each of these chemicals individually and separately from the glycol ethers category.

From Federal Register, July 5, 1994
http://www.gpo.gov/fdsys/pkg/FR-1994-07-05/html/94-16173.htm

SUMMARY: EPA is redefining the glycol ethers category list of toxic chemicals subject to reporting under section 313 of the Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA). EPA is changing the present definition of the glycol ethers category to exclude the high molecular weight glycol ethers that do not, in EPA's judgement, meet the criteria set out in EPCRA section 313(d). This redefinition of the glycol ethers category, which is based on EPA's review of available human health data on short-chain length glycol ethers, eliminates the EPCRA section 313 reporting requirements for those glycol ethers known as surfactant glycol ethers.

EPA has evaluated the current scope of the section 313 glycol ethers category and believes that it is overly broad. The existing category includes substances that traditionally have not been considered glycol ethers. Also, it is apparent that this category contains members that do not meet the EPCRA section 313(d)(2) criteria for listing. EPA has reviewed the current glycol ethers category and is redefining it to exclude the surfactant glycol ethers. Surfactant glycol ethers are those glycol ethers with pendant alkyl groups which typically consist of eight or more carbon atoms (i.e., high molecular weight glycol ethers). However, EPA does not believe that the category can be more narrowly defined at this time.

IV. Rationale for Redefinition

EPA's concerns for the included chemicals is based on a review of available human health data on short-chain length glycol ethers. Specifically, EPA believes that these chemicals meet the criterion of EPCRA section 313(d)(2)(B) because the individual members of this category can be reasonably anticipated to cause one or more of the following effects: Kidney toxicity, liver toxicity, adverse blood effects, adverse central nervous system effects, reproductive effects, and developmental effects. EPA believes that the category can be redefined to exclude those glycol ethers known as surfactant glycol ethers because these high molecular weight glycol ethers do not meet the listing criteria in section 313(d)(2)(A) or (B). None of the chemicals in the current glycol ethers category meet the toxicity criterion of section 313(d)(2)(C) based on their ecotoxicity. EPA's rationale for this redefinition is detailed in the proposed rule and is based on the Agency's review of various relevant materials.

Response to comments:
…However, several of the commenters expressed the opinion that the proposed rule does not narrow the definition sufficiently, and that EPA should consider a further narrowing of the definition in the future. As discussed below, EPA does not believe that it currently has sufficient

data to further narrow the category definition.
…. One commenter, General Electric, suggested that the definition should not identify reportable glycol ethers by molecular structure. Instead, the **commenter recommended listing the glycol ethers of concern individually**, and identifying those which must be reported on an individual basis. **All remaining glycol ethers would then be reported in an aggregate form**. EPA believes this approach to defining the category is inappropriate and unnecessary. EPA has identified by molecular formula a specific group of glycol ethers having a common structure that pose similar hazards. EPA currently believes that the most appropriate way to report on this group of glycol ethers is in aggregate by category. A listing of glycol ethers as proposed by the commenter may exclude from reporting certain glycol ethers within the scope of the definition in this rulemaking that meet the section 313(d)(2) criterion.

In the proposed rule, EPA requested comment on whether the definition of R' should include only straight chained alkyl groups of seven of fewer carbons or both straight and branched alkyl groups of seven or fewer carbons. No comments on this issue were received. Therefore, the definition of R' will include both straight and branched alkyl groups of seven or fewer carbons….

Henkel Corporation stated that ``[t]he C8, C9, and C12 alkyl phenol ethoxylates have also been used for many years as surfactants. There is no evidence that they present adverse human effects such as those which caused the listing of the glycol ether category or would otherwise meet the section 313 criteria.'' However, this commenter did not supply data to substantiate this Assertion……To evaluate the alkylphenol ethoxylates subcategory of the ethylene glycol ether category, EPA would require subchronic toxicity data for one or more specific members of the category (e.g., 2-nonylphenoxyethanol). In the absence of these data, the Agency believes that the glycol ethers category should continue to include these substances.

…General Electric contended that individual glycol ethers should be listed in lieu of a category because EPCRA section 313 ``clearly states that additions to the EPCRA section 313 list must be done on a chemical-by-chemical basis. Each statutory provision that deals with revising the section 313 list speaks only in terms of a chemical-by-chemical basis, and EPCRA is silent on the issue of regulating by chemical categories.'' The Agency believes that the statutory authority to add ``a chemical'' to the list may be reasonably interpreted to include the authority to add groups or categories of chemicals to the list, particularly in light of the fact that the original list adopted by Congress in section 313(c) of EPCRA included 20 chemical categories. These consist mostly of metal compounds categories, but also include categories of organic chemicals, such as glycol ethers (as noted in the proposed rule, Congress listed this category without a delimiting definition).

Re: whether listings should be consistent btwn TSCA and TRI,referred to EPCRA's goals: "EPCRA's goal is to provide the general public with a broad range of information on releases of certain chemicals."

Examples: TSCA New Chemicals Program[5] – *note different goals than EPCRA*

(p.ii)…chemicals for which sufficient assessment experience has been accumulated so that hazard concerns and testing recommendations vary little from chemical to chemical within the category.

In addition, EPA NCP is evaluating PFAS substances, including shorter chain-length telomer alternatives to PFOA and related chemicals.[6]

"For many PFAS chemicals, EPA's regulatory approach involves use of TSCA §5(e) Consent Orders to require testing while allowing production and use, with control measures where appropriate. For a subset of PFAS chemicals, EPA requires environmental degradation testing before the chemicals may be commercializsed. EPA is requiring the possible ultimate degradation products from telomers to be tested to demonstrate that they are less bioaccumulative and less toxic than PFOA and other longer-chain perfluorinated substances. These degradation products are being tested for the following endpoints: developmental and reproductive effects, subchronic toxicity (e.g. liver toxicity), pharmacokinetics and carcinogenicity and avian reproductive effects and chronic aquatic toxicity. In addition, EPA is requiring that the telomeric products be tested to determine their fate in the environment with a battery for each structural class of telomers, which includes biodegradability (water, soil, and sewage), photolysis, and hydrolysis testing."

On January 27, 2010, EPA published a final rule (75 FR 4295) that amends the Polymer Exemption Rule to exclude from eligibility polymers containing as an integral part of their composition, except as impurities, certain perfluoroalkyl moieties consisting of a CF3- or longer chain length. This exclusion includes polymers that contain any one or more of the following: perfluoroalkyl carboxylic acids (PFCAs); perfluoroalkane sulfonates (PFSAs); fluorotelomers; or perfluoroalkyl moieties that are covalently bound to either a carbon or sulfur atom where the carbon or sulfur atom is an integral part of the polymer molecule. This change to the regulation was necessary because, based on current information, EPA can no longer conclude that these polymers "will not present an unreasonable risk to human health or the environment" under the terms of the polymer exemption rule, which is the determination necessary to support an exemption under section 5(h)(4) of TSCA.

[5] US EPA. *TSCA NEW CHEMICALS PROGRAM (NCP) CHEMICAL CATEGORIES.* Aug 2010 https://www.epa.gov/reviewing-new-chemicals-under-toxic-substances-control-act-tsca/new-chemicals-program-under-tsca

[6] https://www.epa.gov/assessing-and-managing-chemicals-under-tsca/new-chemicals-program-review-alternatives-pfoa-and