



## GUIDANCE

### Developing a Generic Chemical Name

(December 1, 2015)

#### 1.0 Purpose

The intent of this document is to provide suppliers with guidance on developing a generic chemical name (GCN) for the purpose of ingredient disclosure on safety data sheets (SDSs), for use under the *Hazardous Products Regulations* (HPR) and *Hazardous Materials Information Review Act* (HMIRA). A GCN may also be used for a non-hazardous ingredient (not required for disclosure on an SDS) so long as the SDS makes clear that the ingredient is not hazardous under the *Hazardous Products Act* (HPA).

#### 2.0 Background

A supplier or employer may seek an exemption from the requirement to disclose the name of a confidential ingredient on an SDS under the HPR by filing a claim for exemption with Health Canada under the HMIRA. In such cases, the claimant must disclose a GCN on the SDS in lieu of the chemical name (HPR 5.7 (5)). The GCN also must be submitted to Health Canada as part of the claim for exemption filed under the HMIRA.

The subject of developing a GCN has produced many questions by claimants seeking to apply for an exemption.

#### 3.0 Guidance for the derivation of a GCN

A GCN is a chemical name which is less specific than the true chemical name but no more general than is necessary to protect the Confidential Business Information (CBI). A GCN should be unique and unambiguous, and a claimant should be able to explain or justify to Health Canada, upon request, the extent of the name modification that is necessary to protect the CBI. The GCN, like all other information in the SDS, is subject to the prohibition in section 14.2 of the HPA, and as such, must not convey false or misleading information about the nature of the chemical.

#### 3.1 Strategy for developing a GCN

Several sources for a chemical name can be used as the starting point to develop a GCN. Most chemical names are derived using systematic nomenclature such as the one developed by the International Union of Pure and Applied Chemistry (IUPAC) or from the Chemical Abstract Services (CAS). Several sources are available to obtain systematic chemical names, such as ChemID through the National Library of Health (1), the CRC Handbook of Chemistry and Physics (2) and the Merck Index (3).

One method of developing a GCN is to use the approach set out by the *Masked Name Regulations* under the *Canadian Environmental Protection Act, 1999*. This method is useful in that it is very systematic and its application to develop a GCN as required under the HPR and HMIRA is considered acceptable by Health Canada.

A less systematic method is to mask the identity, position or number of functional groups on the chemical molecule. For example:

- The position and/or number and/or type of constituents can be masked;
- The parent structure and its primary functional group can be masked;
- The presence and number of other functional groups can be masked.
- Any combination of the above mentioned options

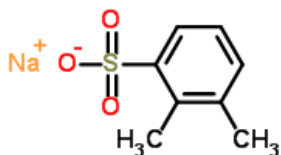
IUPAC has published documents on class names (4) which can be used to replace the parent structure and functional groups on the molecule.



The GCN should retain some aspect of the chemical structure, as well as one or more functional groups or radicals. For example, a salt should be identified and not masked if there are hazards very specific to its metal cation which are required to be disclosed on the SDS or label.

### 3.2 Examples of GCNs based on the outlined strategies

#### 1. CAS Name: Sodium dimethylbenzene sulphonate (CAS no: 1300-72-7)

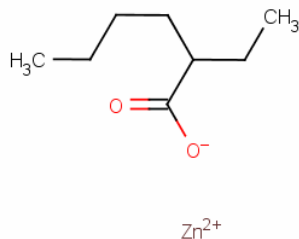


The GCN could be developed by starting with the CAS name and masking the following:

- $\text{Na}^+$ : the presence of the cation, or salt
- The two  $\text{CH}_3$  groups (alkyl groups): the specific constituents, the number of constituent groups, position of the constituent groups (positions "5" and "6" on the benzene ring), or even the presence of the constituent groups
- Benzene ring (aryl group): the parent compound

Possible GCNs include:

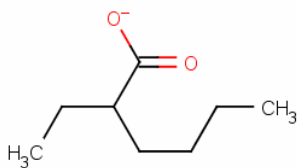
- dimethylbenzene sulphonate (salt)
- dialkylbenzenesulphonate sodium salt
- dialkylarylsulphonate sodium salt
- dialkylarylsulphonate (salt)
- alkylarylsulphonate (salt)
- substituted arylsulphonate (salt)
- dimethylbenzene inorganic acid, sodium salt



#### 2. CAS Name: Hexanoic acid, 2-ethyl-, zinc salt (CAS no: 136-53-8): $2(2-(\text{C}_2\text{H}_5)\text{C}_6\text{H}_{10}\text{O}_2)\text{Zn}$

The name Hexanoic acid, 2-ethyl-, zinc salt could be used to start, or zinc bis(2-ethylhexanoate), where the bis indicates two ethylhexanoate components could be used, and the following could be masked:

- $\text{Zn}^{2+}$ : the presence of the cation, or salt.
- The ethyl ( $\text{C}_2\text{H}_5$ ) group (alkyl group): the specific constituent, position of the constituent group (the "2" position), or even the presence of the constituent groups
- Hexanoic acid (carboxylic acid group): the parent compound



Possible GCNs include:

- salt of an alkyl substituted carboxylic acid
- alkylcarboxylic acid, zinc salt.

Keeping the identity of zinc salt would allow the linking of hazards to the organic functional group and structural features of the compound.



### 3.3 Common errors in developing a GCN

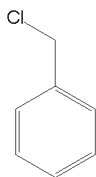
#### (a) Terms for product/chemical use

Terms such as dye, surfactant (even if qualified with the type such as anionic, cationic, or nonionic), catalyst, binder, colorant, emulsifier, inhibitor, or organic solvent are descriptors of product use and do not provide sufficient information on the chemical itself.

#### (b) Pseudo chemical names or misleading names

Syllables or masked syllables from the conventional chemical nomenclature may misrepresent a chemical structure. This includes using prefix and suffix syllables in the GCN, when these radicals or functional groups are not present in the molecule.

Juxtaposing a series of simple chemical terms such as “oxo-alcohol ether sulfate” or using creative phrases such as “oxygenated ketone” could cause confusion when considering the chemical functionality.



The order of the components of the name should usually relate to the actual chemical name. For example:

“alkylaryl halide” for chloromethylbenzene would be confusing as it indicates the halide is on the aryl (benzene) group (in this case, the GCN would be more correctly arylalkylhalide or haloalkylarene).

Where the precise structure of the reaction product is known, developing a GCN based on precursor or starting ingredient(s) of a reaction would be too ambiguous.

#### (c) Long descriptive phrases or a list of atoms.

Long descriptive phrases may be too general. For example, referral to a specific chemical ingredient as a “long chain hydrocarbon containing sulphur and nitrogen” gives no indication of whether the hydrocarbon is saturated, unsaturated, branched or linear; does not indicate whether the sulphur and nitrogen only have hydrogen attached to them or something more complex; and does not indicate whether sulphur or nitrogen is the main functional group, such as an amide or imide, or sulfonate or sulfoxide.

### 4.0 References

1. ChemID, National Library of Medicine, National Institute of Health. Available at: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
2. CRC Handbook of Chemistry and Physics, 96th Edition, Published by CRC Press, Editor(s):William M. Haynes, 2015
3. The Merck Index, 15<sup>th</sup> Edition, Royal Society of Chemistry, 2013
4. International Union of Pure and Applied Chemistry, (1995) Glossary of Class Names of Organic Compounds and Reactive Intermediates Based on Structure. Pure &App/. Chem., Vol. 67, Nos 819, pp. 1307-1375.