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OECD GUIDANCE FOR CHARACTERISING OLEOCHEMICAL SUBSTANCES FOR ASSESSMENT PURPOSES

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OECD GUIDANCE FOR CHARACTERISING OLEOCHEMICAL SUBSTANCES FOR ASSESSMENT PURPOSES

IOMC
INTER-ORGANIZATION PROGRAMME FOR THE SOUND MANAGEMENT OF CHEMICALS
A cooperative agreement among FAO, ILO, UNDP, UNEP, UNIDO, UNITAR, WHO, World Bank and OECD

Environment Directorate
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or contact:

OECD Environment Directorate,
Environment, Health and Safety Division
2 rue André-Pascal
75775 Paris Cedex 16
France

Fax: (33-1) 44 30 61 80

E-mail: ehscont@oecd.org

FOREWORD

Substance identification is the cornerstone of the implementation of any chemical legislation. Unambiguous characterisation of a substance is a prerequisite to various regulatory processes and relies on information on composition and analytical information. While characterising well-defined substances (including mono-constituent and multi-constituent substances) can in general be regarded as straightforward, the characterisation of UVCB substances (Substances of Unknown or Variable composition, Complex reaction products or Biological materials) is often more challenging due to their complex origin and unknown and/or variable composition. A common understanding and approach to characterising UVCBs would enable regulatory authorities to increase cooperation in the field of hazard assessment and help industry deal with regulatory requirements from multiple jurisdictions.

The purpose of this document is to present a harmonised method for characterising, one specific subcategory of UVCBs: oleochemical substances for assessment purposes. Many oleochemicals are UVCBs, due to the variability in the composition of the starting materials. The method presented in this document gives guidance on how oleochemical substances can be characterised in a way that their composition is accurately and consistently reflected to ensure that substances with the same chemical composition, manufactured in different countries, can be characterised with the same description for hazard assessment purposes.

The concepts expressed herein are not, by default, expected to be applicable to other UVCB substance types which have their own specific substance characterisation issues.

This document has been prepared by the OECD correspondence group on characterisation of UVCB substances of the Task Force on Hazard Assessment. It is being published under the responsibility of the Joint Meeting of the Chemicals Committee and the Working Party on Chemicals, Pesticides and Biotechnology.

1. HISTORY

At its meeting on 13-14 June 2012, the OECD Task Force on Hazard Assessment agreed to launch a project on the characterisation, for hazard assessment purposes, of substances of Unknown or Variable composition, Complex reaction products or Biological materials (UVCBs). It was agreed that oleochemicals would act as a pilot substance group to investigate how to address the following priority areas:

1. Further guidance for UVCB substance characterisation

2. Compositional variability for UVCB substances

The content of this paper has been developed by the OECD correspondence group on characterisation of UVCB substances. It is a combination of ideas based on experience and current guidance, such as that produced by the US Environmental Protection Agency (EPA)[1] and the European Chemicals Agency (ECHA)[2].

2. INTRODUCTION

The purpose of this paper is to present a harmonised method for characterising oleochemical substances in a way that their composition is accurately and consistently described for hazard assessment purposes. This method ensures that substances with the same chemical composition can be characterised with the same description, whilst ensuring comparability of their toxicological and ecotoxicological properties. This facilitates a number of processes in terms of efficiency, consistency and accuracy, for example:

- Sharing of data
- Collaboration on hazard assessment between multiple producers or countries
- Chemical name searching
- Harmonisation of classification and labelling of substances

This guidance could be used for characterising substances assessed within several international collaborative frameworks e.g. the OECD Cooperative Chemicals Assessment Programme (CoCAP), the international program of chemical safety (IPCS) and the development of a global harmonised list of classification and labelling.

Countries/regions may also decide to utilise this guidance in their own hazard assessment activities.

It is also important to note that this guidance focuses solely on oleochemicals. The concepts expressed herein are not, by default, expected to be applicable to other UVCB substance types which have their own specific substance characterisation issues.

[1] EPA Toxic Substances Control Act Chemical Substance Inventory "TSCA Inventory: 1985 Edition Volume 1 – SDA Substance Identification Procedure for Class 2 chemical substances derived from natural fats and oils and synthetic substitutes"

[2] ECHA Guidance for identification and naming of substances under REACH version 1.2 March 2012

3. BACKGROUND ON OLEOCHEMICALS

UVCB oleochemicals are derivatives from animal and vegetable oils and fats and/or their alternatives based on synthetic (e.g. petrochemical) feedstocks. The major process for transforming animal and vegetable oils and fats into oleochemicals is hydrolysis, the splitting of natural triglycerides into crude glycerine and crude mixed fatty acids, under the influence of water, temperature and pressure. In the same way, methanolysis is used to produce crude glycerine and fatty acids methyl esters.

The difference between the types of fatty acids derived from different types of feedstock is mainly due to their degree of saturation and their carbon chain length distribution. The carbon chain length distribution depends on the initial fat or oil used as feedstock, although it might not be exclusive for a specific fat or oil. Due to the variability in the composition of the starting materials, many oleochemicals fall under the definition of a UVCB substance. The fatty acids carbon chain lengths obtained mainly appear between C6 and C24, with the vast majority between C12 and C18.

Source descriptor vs. Alkyl descriptor

The source descriptor describes the origin of the animal fat or plant oil used to manufacture a particular oleochemical substance e.g. tallow. In general every animal fat or plant oil source provides a typical carbon chain length distribution in the final oleochemical substance. For that reason often the source descriptor has been used instead of an alkyl descriptor e.g. *Hydrogenated tallow amines* as opposed to *C16-18 (even numbered) alkyl amines*. The source descriptor however, does not provide information on the variability in composition of the final products and is therefore less accurate than an alkyl descriptor. Moreover an alkyl descriptor is not strictly tied to a single source or production process and can therefore be used independent of the origin (including use of mixed sources) and the production process used.

4. OECD CHARATERISATION, FOR HAZARD ASSESSMENT PURPOSES, OF OLEOCHEMICALS

i. Qualitative descriptors

The group of oleochemicals comprises substances whose individual constituents have a common structural feature: one or more alkyl group(s) with variable C-chain attached to a functional group. Their constituents differ from each other with respect to one or more of the following alkyl-chain group characteristics:

- Length of carbon chain (carbon number)
- Saturation
- Structure (linear or branched)
- Position of the functional group

The constituents can be sufficiently and systematically characterised by using the following three descriptors:

- Functionality descriptor
- Alkyl descriptor

– Salt descriptor

Functionality descriptor

The functionality descriptor identifies the functional group of the substance, e.g. amine, ester, ammonium, sulphate.

Alkyl descriptor

The alkyl descriptor describes the number of carbon atoms in the carbon chain length(s):

- In general, the alkyl descriptor refers to saturated, linear[3] alkyl chains comprising all chain lengths, e.g. "C12–14" corresponds to "C12, C13, C14" including both even and odd numbered linear alkyl-chains;

- It should be indicated if the alkyl descriptor refers to branched-alkyl chains, e.g. "C12–14 (branched)" or branched as well as linear alkyl chains, e.g."C12–14 (linear and branched)";

- It should be indicated if the alkyl descriptor refers only to even or odd numbered alkyl chains e.g. C12-14 (even numbered)

- A narrow alkyl chain length distribution does not cover a broader one e.g. "C12–14" does not cover "C12–18". Equally a broad alkyl chain length distribution does not cover a narrower one e.g. "C12–18" does not cover "C12–14".

- In general, since the alkyl descriptor refers to saturated alkyl chains, it should be indicated if the alkyl descriptor refers (also) to unsaturated alkyl chains, e.g. fatty acids, C16-18 and C18 (unsaturated).

Salt descriptor

The salt descriptor identifies the cation/anion of any salt present in the substance, e.g. sodium (Na+), carbonate $(CO3)^{2-}$, lithium (Li+).

Even vs. Odd carbon numbers and branching

Oleochemicals derived from animal and vegetable oils and fats normally contain only even numbered and linear carbon alkyl chain lengths, by contrast, oleochemicals produced from synthetic feedstocks might contain odd carbon chain lengths at high concentrations, e.g. "C13-C15 (odd numbered)", or else, odd- as well as even-numbered chain lengths or, in some cases, just even-numbered chain lengths, in significant amounts. Some manufacturing processes where synthetic feedstock is used can lead to a high degree of branching of the final alkyl chains. In order to reflect the differences in source the naming of oleochemicals should describe the presence of branched/linear in addition to odd/even numbered alkyl chains in those constituents.

[3] In the present guidance 'linear' is defined as devoid of any branching, in accordance with standard chemical nomenclature. This is different from the internationally recognized SDA naming practice (see footnote 2) which also includes mono methyl and mono ethyl branching under the term 'linear'

UVCBs vs. Well Defined Substances

The system outlined above can be used to describe substances with variation in the carbon chain lengths. This guidance is not applicable if the variation in carbon chain length is sufficiently controlled and the substance can be defined as a well-defined substance[4].

In conclusion, the information on the alkyl descriptor, the functionality descriptor and the salt descriptor are the basis for characterising an oleochemical UVCB substance. In addition, information on the source and the process may be important to support the characterisation of the substance.

ii. Quantitative descriptors

Quantitative criteria or cut-off values for carbon chain lengths that should be considered for the characterisation of an oleochemical UVCB substance are defined below:

- Substances derived from natural fats or oils (or synthetic sources) are UVCBs due to their variation in the carbon chain length distribution. However, if one constituent with a specific and defined alkyl chain is present at a minimum concentration of 80 %, the substance is considered a well-defined substance and not as an oleochemical UVCB substance.

- For a composition based characterisation, all alkyl chains, whose concentration is above 10 % (based on the maximum concentration value of the concentration range), should be part of the characterisation. Further the sum of all the alkyl chain lengths mentioned in the characterisation must total at least 80 % (w/w) of the total substance.

- In case of constituents with alkyl chains, each present with a concentration above 10 % (based on the maximum concentration value of the concentration range), that altogether do not compose ≥ 80 % (w/w) of the substance, all alkyl chain lengths, regardless of their concentration, should be considered for the characterisation. However, if justifiable, manufacturer intent can be used to determine whether chain lengths with a concentration <10 % (based on the maximum concentration value of the concentration range) should be included as part of alkyl descriptor or not.

Establishing the typical, minimum and maximum concentration values

The typical, minimum and maximum concentration value for a given constituent should be included in the substance specification. The substance specification refers to individual manufacturers i.e. certificate of analysis used to ensure product quality. This information can be established by analysing a number of separate batches (typically five) over a period of time. The average value of this multiple batch analysis should be used to set the mean (typical value). The minimum and maximum values should be no more than 3 standard deviations from the mean/typical value.

Step-wise process to establishing alkyl descriptor:

1. Analyse substance

2. Group constituents as follows:

[4] This typically means a substance composed of molecules with particular atoms arranged in a definite, known structure which accounts for >80 % of the substance composition.

a. C_x (saturated linear)

b. $C_{x\ branched}$

c. $C_{x\ unsaturated}$

3. For each group establish the maximum concentration (% w/w)

4. Establish the name based on the rules

Example:

C14 (saturated linear) = 20 % w/w max

C16 (saturated linear) = 30 % w/w max

C18 (saturated linear) = 15 % w/w max

C18 (branched) = 20 % w/w max

C18 (unsaturated) = 15 % w/w max

Alkyl descriptor = C14–18 (even numbered) and C18 (branched) and C18 (unsaturated) alkyl

Illustrative example

The functionality descriptor is usually the most important part of the characterisation and as such it should be mentioned first followed by the alkyl descriptor e.g. Amines, C16-18 (even numbered) and C18 (unsaturated) alkyl.

"*Amines, C16-18 (even numbered) and C18 (unsaturated) alkyl*"

Functionality descriptor: "amine"; identifies the functional group of the substance.

Alkyl descriptor: "C16-18 (even numbered) and C18 (unsaturated) alkyl"; describes the linear saturated alkyl chains with a carbon number of C16 and C18 present at concentrations ≥10 % and < 80 % and identifies that the alkyl chain, C18, is also present in unsaturated form.

Salt descriptor: in this case, no salt descriptor is relevant for naming.

5. IDENTIFIERS

Identifiers are necessary to establish the overall substance characterisation in a comprehensive way. Further information on identifiers for oleochemicals is described in Appendix 1.

6. EXAMPLES

Seven examples of existing oleochemical substances are provided in appendix 2. They have been chosen to illustrate how the characterisation, described in this paper, has been applied by European oleochemicals and allied products group (APAG) and CAS registry services. They highlight how substances with broad generic names can be named more precisely.

APPENDIX 1 - IDENTIFIERS

i. Information on chemical composition

Information on chemical composition means typical concentration and concentration ranges (minimum and maximum values) for all known constituents. Consideration should be given to ensure the concentration ranges are reasonable, i.e. not overly broad, and reflect the reality i.e. the concentration ranges of constituents mirror the source in nature, unless explained. The rule specified under section 4 ii is to be followed i.e. minimum and maximum values should be no more than 3 standard deviations from the mean/typical value.

ii. Source and process description

For oleochemicals, where the composition is relatively well-defined (in terms of the identity of individual constituents), toxicological properties can be linked more directly to the chemical structure of the individual constituents rather than to the nature of the source/starting material. However, information on source and process description is important for the following reasons:

1) To understand and verify the composition profile, in particular the concentration ranges established for individual constituents.

2) Different sources e.g. vegetable/animal fats versus synthetic feedstock will have different profiles including minor constituents that may not be reported in the final substance composition but nevertheless may affect the toxicological properties of the substance.

Information on source and process description typically includes, as appropriate:

- Alkyl chain distribution with upper and lower concentration ranges and name of biological source (e.g. palm oil) if known and available.
- Ratio of starting materials
- Reaction type e.g. esterification
- Description of the manufacturing process including each individual process step (block diagrams can be a useful way to illustrate this)
- Relevant non-confidential operating parameters (pH, temperature at a particular manufacturing step) that influence or determine the composition of the manufactured substance
- Iodine numbers and other values used in the manufacture of oleochemicals

iii. Analytical information

The analytical information and spectral data provided should be sufficient to be able to verify the composition of the substance. A combination of the following spectral and chromatographic analysis is usually sufficient:

- Ultra violet (UV) spectroscopy;
- Infra-red (IR) spectroscopy;
- Nuclear Magnetic Resonance (NMR) and/or Mass spectroscopy (MS)
- Gas or High Performance Liquid Chromatography (GC or HPLC)

It should be noted that where the substance is a salt it is necessary to employ a technique to identify and quantify the relevant counter-ion.

iv. Impact on CAS identifiers

Over the years, manufacturers of UVCBs have obtained CAS Registry Numbers and Chemical Abstracts (CA) Index Names (with associated supplemental definitions where appropriate) for some of their UVCB substances and reported the chemicals with these identities under different regulatory programmes around the world.

If CAS identification is used in conjunction with the guidance on characterisation presented in this paper then it is important that the use of a CAS Registry Number and corresponding CAS name (and CAS definition) is consistent with the substance in question i.e. it does not contradict the substance identity provided by applying the guidance described in this paper.

In practice this means that first a substance name using the guidance in this paper should be assigned and then either using (a) the CAS registry lookup service, find the correct match in the existing inventory or (b) using the CAS Inventory Expert service, obtain a new CA Index name and CAS Registry Number based on the guidance in this paper.

APPENDIX 2 – EXAMPLES

The examples below have been provided by the European Oleochemicals and Allied Products Group (APAG) who are a sector group of the European Chemical Industry Council (CEFIC). The examples demonstrate how existing substances, which have existing names and CAS numbers, can be named based on the conventions in this paper. The examples also show how a second CAS entry was created based on composition which supplements rather than eliminates the original CAS entry based on source.

It must be noted that the new CAS name is not perfectly equivalent with the name derived from this convention as CAS nomenclature does not allow the use of the term ‘even-numbered’, meaning that these CAS names based on compositions refer to substances that can either contain only even-numbered alkyl chains or both even and odd alkyl chains. Consequently these CAS entries are broader in their scope than the name created based on the conventions in this paper.

Example No.	**1**	**2**	**3**	**4**	**5**	**6**	**7**
Alkyl chain distribution (%)							
C8		<10				<10	
C10		<10				<10	
C12	<5	40-60	<5			40-60	
C14	<10	10-30	<10	<10	<10	10-30	>1-10
C16	25-40	5-20	25-40	25-40	20-40	5-20	15-35
C18	49-75	>3-12	49-75	20-35	55-75	>3-12	10-30
C18 unsatd.		<10		25-45		<10	40-60
CAS Name (based on source)	(Hydrogenated tallow) amine	Cocoamine	Di(hydrogenated tallow)amine	Bis (2-hydroxyethyl) tallow alkylamine	Bis (2-hydroxyethyl) hydrogenated tallow alkylamine	Coconitrile	Tallownitrile
CAS No. (based on source)	61788-45-2	61788-46-3	61789-79-5	61791-44-4	90367-28-5	61789-53-5	61790-28-1
Name based on conventions in this paper (based on composition)	Amines, C16-18 (even numbered) alkyl	Amines, C12-18(even numbered) alkyl	Amines, di-C16-18 (even numbered) alkyl	2,2'-(C16-18 (even numbered, C18 unsaturated) alkyl imino) diethanol	2,2'-(C16-18 (even numbered) alkyl imino) diethanol	Nitriles, C12-18 (even numbered) alkyl	Nitriles, C16-18 (even numbered) and C18 (unsaturated) alkyl
Associated CAS No. (based on composition)	90640-32-7	68155-27-1	308062-60-4	1218787-32-6	1218787-30-4	1218787-29-1	164383-22-6
Associated CAS Name (based on composition)	Amines, C16-18-alkyl	Amines, C12-18-alkyl	Amines, di-C16-18-alkyl	Ethanol, 2,2'-iminobis-, N-(C16-18 and C18-unsatd. alkyl) derivs.	Ethanol, 2,2'-iminobis-, N-C16-18-alkyl derivs.	Nitriles, C12-18	Nitriles, C12-18