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### Committee of Experts on the Transport of Dangerous Goods and on the Globally Harmonized System of Classification and Labelling of Chemicals

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# **Revision of names for chemical substances**

### Submitted by the expert from Spain\*

## Introduction

1. Over the last years, Spain has been carrying out a revision of the Spanish names of the UN numbers, as the Spanish translation of the UN numbers in the different regulations (Model Regulation, ICAO Technical Instructions, IMDG Code) is not coincident. In the course of doing this, different cases have appeared where it would seem reasonable to amend not only the Spanish name, but also the English and French ones. Specifically, this is the case for many chemical names.

# Analysis

2. The names of the UN numbers are long standing names that have not been amended, in most of the cases, since the UN numbers were introduced into the dangerous goods regulations.

3. The names of chemical substances, even those who belong to the first group of those defined under 2.0.2.2 (a) of the Model Regulations (single entries for well-defined substances or articles), have not been assigned following a homogenous criterion. The establishment of such a criterion would avoid ambiguities and would permit an easier identification of the correct UN number.

<sup>\*</sup> In accordance with the programme of work of the Sub-Committee for 2017–2018 approved by the Committee at its eighth session (see ST/SG/AC.10/C.3/100, paragraph 98 and ST/SG/AC.10/44, para. 14).

4. The international reference for assignment of names for chemical substances are the rules and criteria established by the International Union of Pure and Applied Chemistry (IUPAC).

5. Chemical names assigned in the Model Regulations may have been, at least partially, assigned following the IUPAC rules, but these have changed over time. The IUPAC updates its rules periodically (according to "Nomenclature of Inorganic Chemistry, IUPAC Recommendations 2005) to:

- (a) Resolve ambiguities which might have arisen;
- (b) Clarify the rules and its applications;
- (c) Describe new compounds or classes of compounds:
- (d) Make the nomenclature as systematic and uncomplicated as possible to assist less familiar users.

6. Specifically, there have been two mayor updates of the IUPAC rules in 2000 and 2005, which are subsequent to the assignment of the majority of names of the UN numbers in the Model Regulations, but are already well established and introduced in training and industry.

7. The IUPAC as the basis for assigning chemical names is also referenced as such in GHS (index and A.4.3.3.1.1). Regulation (EC) N° 1272/2008 on the classification, labelling and packaging of substances and mixtures also applies the IUPAC criteria, using the systematic IUPAC and/or admitted traditional names (admitted by IUPAC), and adds for further information, the CE and Chemical Abstracts Service (CAS) numbers, if applicable.

8. In the present Model Regulations, by not following a single criterion, deficiencies and differences can be observed in the names that have been chosen for the UN numbers.

9. Without doing a complete review of the chemical names in the Model Regulations, after consulting the Spanish, English and French chemical names, many deficiencies and defects have shown up, for example:

(a) Use of rules which IUPAC specifically recommends not to use:

Use of suffixes for the cations of inorganic salts, not following the present recommendations. For example, for UN 1466, "FERRIC NITRATE" in English and, "NITRATO FERRICO", in Spanish, should be updated to "IRON(III) NITRATE" and "NITRATO DE HIERRO(III)", respectively. The French name follows nevertheless the present recommendations. Similar examples can be found in many other cases;

(b) Incorrect or incomplete use of IUPAC rules:

(i) Incomplete use of the rules for indicating the positions of radicals or substituents. For example, for UN 1369, p-NITROSODIMETHYLANILINE, the position of the methyl group is not indicated. The complete name of this substance should be p-NITROSO-N,N-DIMETHYLANILINE, which indicates that the methyl group is attached to the nitrogen and not to the benzene ring. The French and Spanish versions have the same imprecision;

(ii) For UN 2226, the most appropriate name would be "(TRICHLOROMETHYL)BENZENE" instead of "BENZOTRICHLORIDE", which may be mistaken for trichlorbenzene. Also the parenthesis indicates that the chlorine atoms are attached to the methyl group, and not to the benzene ring. Similarly, the correct Spanish name should be "(TRICLOROMETIL)BENCENO". The French version of this UN number, "CHLORURE DE BENZYLIDYNE", is confusing because on one hand this name would be valid for trichlormethyl, dichlormethyl or chlormethil, and on the other hand the name "benzylidyne" is reserved for when the carbon of the original methyl has a triple bond;

(iii) For salts with two cations, the alphabetical order of the cations is not respected. For example, the Spanish version of UN 1419 is named "FOSFURO DE MAGNESIO Y ALUMINIO" instead of "FOSFURO DE ALUMINIO Y MAGNESIO". It may be additionally noted that a correct IUPAC denomination would be "TRIFOSFURO DE ALUMINIO Y TRIMAGNESIO";

(iv) Also for organic substances with several radicals or substituents, these should be named in alphabetical order. This rule is not respected in different cases, for example for UN 1087 and 1193:

1087	ÉTHER MÉTHYLVINYLIQUE STABILISÉ	VINYL METHYL ETHER, STABILIZED	VINIL METIL ÉTER ESTABILIZADO
1193	ÉTHYLMÉTHYLCÉTONE (MÉTHYLÉTHYLCÉTONE)	ETHYL METHYL KETONE (METHYL ETHYL KETONE)	ETILMETILCETONA (METILETILCETONA)

(c) Use of specific names which IUPAC recommends not to use, for example:

(i) The present IUPAC rules advise against the use of the names "phosphine", "arsine", "stibine" and "bismuthine", for PhH3, AsH3, SbH3 y BiH3, and its derivates, respectively. They should be correctly named as "phosphane", "arsane", "stibane" and "bismuthane". Therefore, the UN numbers 2199, 2501, 2798 and 2940, for example, should be corrected in Spanish, English and French.

(ii) Following the IUPAC rules, for inorganic substances the names "nitric oxide" for NO, and "nitrous oxide" for N2O should not be further used (similarly in French and Spanish). The terminology "nitrogen monoxide" y "dinitrogen oxide" should used instead, and the name of UN1975, for example, should be corrected.

(iii) Similarly, "mercapto" and "mercaptan" (English version, similar in French and Spanish) should be substituted by "sulfanyl" or "thiol". For example, for UN 2347, "BUTYL MERCAPTAN" should be substituted by "BUTANE-1-THIOL" (The "1" has to be added to indicated to differentiate the position of the radical "thiol").

(d) Use of outdated technical names:

In some cases, very outdated technical names have been used. This is the case for example for UN 1511 in its Spanish version, where "AGUA OXIGENADA" is used for "PERÓXIDO DE HIDRÓGENO". As a systematic review of the chemical names in English and French has not been done, no specific case has been found for these languages. Nevertheless, it would be worth to make a search for these cases also in other languages.

10. For the other types of entries defined by 2.0.2.2 (Generic entries for well-defined group of substances or articles, specific n.o.s. entries covering a group of substances or articles of a particular chemical or technical nature and general n.o.s. entries covering a group of substances or articles meeting the criteria of one or more classes or divisions), similar corrections could be analysed.

#### **Proposal**

11. Spain proposes to make a systematic review of the UN numbers which contain chemical names and designations.

12. If the Sub-Committee agrees to do so, Spain would be willing to lead a correspondence informal working group to do so, which could:

- (a) Discuss the most appropriate criteria to amend the names of the UN numbers;
- (b) Group the cases of UN numbers that should be analysed;
- (c) Make a proposal for the amended names.

13. Doing this revision would not necessarily imply the amendment of a big share of the UN numbers, but would permit updating the Model Regulations and making them more coherent and easier to apply, avoiding the use of names and designations that are no longer in use and/or are the source of ambiguities.