



ISO Technical Reports are subject to review within three years of publication, with the aim of achieving the agreements necessary for the publication of an International Standard.

Surface active agents — Scientific classification

Agents de surface — Classification scientifique

ISO Recommendation R 896, *Surface active agents — Scientific classification*, was published in December 1968. In June 1972, an enquiry carried out with a view to transformation of ISO/R 896 into an International Standard showed that it was necessary to bring its contents up to date. In 1973 and 1974, member bodies were requested to submit their proposals for revision to Technical Committee ISO/TC 91, *Surface active agents*, but the majority replied that they were not able to provide the information likely to bring an effective contribution to this work. Therefore, in December 1974, ISO/TC 91 decided not to transform this ISO Recommendation immediately into an International Standard but approved, in October 1975, its publication as a Technical Report. This decision was taken for the following reasons :

- on the one hand, the proposed scientific classification, despite its imperfections, still offers a certain interest as a basis for a system of decimal classification which can be used to identify a surface active agent, considered in isolation, according to its chemical formula;
- on the other hand, it is estimated that the revision which at the present time is being undertaken by the Comité international des dérivés tensio-actifs (CID) will not be completed for three or four years. Consequently, during this interim period, it is desirable that the existing classification, although not widely known, should still be available to persons concerned in the establishment of the classification index number of a surface active agent. This will enable definite examples to be given, which could be pointed out as giving rise to difficulties for classification and which accordingly may be useful for modifying the rules of classification in order to perfect and to complete it.

Thereafter, ISO/TC 91, as soon as it has received proposals for revision, either from member bodies or from interested international organizations, will examine the possibility of reviewing the existing classification system and publishing an International Standard.

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0 INTRODUCTION

The classification of surface active agents is intended to provide a clear and logical designation of the structural chemical groups of a surface active agent, in the form of a decimal notation. Its aim is to describe a surface active agent, considered in isolation, according to its chemical formula.

The classification is based on the polar/non-polar structure of surface active agents, which determines their hydrophilic and lipophilic properties.

The traditional importance of water-soluble surface active agents leads to separate consideration of the hydrophilic part and the hydrophobic part of the molecule. A surface active agent can be characterized by indicating these parts; however, the extremely numerous possibilities of variation in the structure of the hydrophobic part make it necessary to specify this part in some detail; the hydrophilic part, though structurally simpler, still needs to be defined by certain of its characteristics, especially those responsible for solubility in water or in organic media.

The subdivision of the classification is, however, not taken far enough to enable one classification index number to be considered as necessarily corresponding to a specific product (the classification is not a precise chemical nomenclature). On the contrary, it may be considered that in general, several products having chemical structures and practical characteristics that are of necessity closely similar will be designated by the same classification index number. Moreover, the classification index number would enable one to reconstruct a molecular structure, which is approximate but nevertheless sufficiently precise.

The application of the decimal classification is a matter for judgment, which is within the capacity of technicians with an ordinary knowledge of the chemistry and technology of surface active agents. Rigorous application of the rules of classification and detailed study of the classification table are indispensable for establishing the classification index number of a surface active agent, which should be obtained without any ambiguity.

1 SCOPE

This Technical Report sets out a scientific classification of surface active agents.

2 FIELD OF APPLICATION

This classification is applicable both to surface active agents which are preferably used in an aqueous medium and to those used in organic media.

3 DEFINITIONS

3.1 key hydrophilic group : A group embodying one and only one function which is considered as the most important for the hydrophilic behaviour of the surface active agent.

3.2 secondary hydrophilic groups : Groups embodying functions with solubilizing properties other than those of the key hydrophilic group; these serve only in a secondary manner to characterize further the surface active agent.

3.3 key hydrophobic residue (determining the hydrophobic behaviour of the surface active agent) : A residue comprising a radical of the hydrophobic type considered as a whole, along with direct substitutions. It should be linked to the key hydrophilic group in a clearly definable way.

3.4 characteristic hydrophobic residues : Chemical groups which are not more hydrophobic than the key hydrophobic residue to which they are *functionally linked*. They constitute either an intermediate connecting link within the molecule itself or appear as a secondary hydrophobic residue attached to the rest of the molecule.

3.5 intermediate functional groups : Groups occurring between the hydrophobic residue(s) and the key hydrophilic group and joined to the latter either by a hydrocarbon link or a characteristic hydrophobic residue. They provide supplementary characteristics for the hydrophobic part.

3.6 supplementary properties of the hydrophilic part : Properties which make it possible to provide a fuller description of the hydrophilic part and to give details either of its solubilizing properties in an aqueous medium, or of its preferential behaviour of insolubility in water, for special use in organic media.

4 PRINCIPLE¹⁾

The classification of surface active agents enables them to be specified by the following characteristics defined in clause 3 :

- a) the *key hydrophilic group*;
- b) possibly, *secondary hydrophilic groups*;
- c) the *key hydrophobic residue*;
- d) possibly, *characteristic hydrophobic residues*;
- e) *intermediate functional groups*;
- f) *supplementary properties of the hydrophilic part*.

5 RULES OF CLASSIFICATION

5.1 The classification of a surface active agent is governed by the determination of the key hydrophilic group, followed by the key hydrophobic residue. In order to avoid any ambiguity, these two elements should be determined in accordance with the following rules :

Rule 1

THE KEY HYDROPHILIC GROUP IS THE FIRST PART CONSIDERED IN THE PREPARATION OF THE CLASSIFICATION INDEX NUMBER CHARACTERIZING A SURFACE ACTIVE AGENT.

5.2 Hydrophilic groups can be classified in three groups :

- hydrophilic groups with anionic properties;
- hydrophilic groups with cationic properties;
- hydrophilic groups with non-ionic properties.

Rule 2

THE CLASSIFICATION OF A SURFACE ACTIVE AGENT INTO ONE OF THE THREE FOREGOING GROUPS IS EFFECTED BY MEANS OF THE FIRST THREE FIGURES :

- the first relating to groups with anionic properties;
- the second to groups with cationic properties;
- the third to groups with non-ionic properties.

5.3 Where the surface active agents contain only one hydrophilic group, there is no possibility of ambiguity. Where they contain several of these groups, the following rules should be applied :

Rule 3

If the molecule contains more than one hydrophilic group,

1) THE KEY HYDROPHILIC GROUP IS THE ONE WHICH APPEARS FIRST. THE ORDER IN WHICH FUNCTIONS SHOULD BE SELECTED IS AS FOLLOWS (see the table) :

- a) a cationic group from column 2, indicated in boxes 5, 6, 7, 8 and possibly 9, if the function is sufficiently basic;
- b) an anionic group from column 1, indicated in boxes 2, 3, 4, 5, 6, 7, 8 and possibly 9, if the function is sufficiently acid;
- c) a non-ionic group from column 3, indicated in boxes 3, 4, 5 and 6;
- d) a cationic group from column 2, indicated in boxes 1, 2, 3, 4 and possibly 9, if the function is slightly basic;
- e) an anionic group from column 1, indicated in box 1, and possibly box 9, if the function is slightly acid;
- f) the other non-ionic groups from column 3, indicated in boxes 1, 2, 7, 8 and 9.

The figure corresponding to the key group should be underlined.

1) See, in annex A, diagrams giving practical details of the principle of the classification.