

ISO

INTERNATIONAL ORGANIZATION FOR STANDARDIZATION



ISO RECOMMENDATION R 896

SURFACE ACTIVE AGENTS
SCIENTIFIC CLASSIFICATION

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BRIEF HISTORY

The ISO Recommendation R 896, *Surface active agents – Scientific classification*, was drawn up by Technical Committee ISO/TC 91, *Surface active agents*, the Secretariat of which is held by the Association Française de Normalisation (AFNOR).

Work on this question led, in 1963, to the adoption of a Draft ISO Recommendation.

In June 1965, this Draft ISO Recommendation (No. 817) was circulated to all the ISO Member Bodies for enquiry. It was approved, subject to a few modifications of an editorial nature, by the following Member Bodies :

Argentina	France	Portugal
Australia	Germany	South Africa, Rep. of
Austria	Hungary	Spain
Belgium	Ireland	Switzerland
Brazil	Israel	U.A.R.
Canada	Italy	United Kingdom
Chile	Korea, Rep. of	Yugoslavia
Colombia	Netherlands	
Czechoslovakia	Poland	

One Member Body opposed the approval of the Draft :

Romania

The Draft ISO Recommendation was then submitted by correspondence to the ISO Council, which decided, in December 1968, to accept it as an ISO RECOMMENDATION.

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FOREWORD

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.

SURFACE ACTIVE AGENTS

SCIENTIFIC CLASSIFICATION

1. SCOPE

The purpose of this ISO Recommendation is to set out a scientific classification of surface active agents.

2. FIELD OF APPLICATION

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

3. TERMINOLOGY

- 3.1 *Key hydrophilic group*. 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). 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. PRINCIPLE*

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

- (1) *the key hydrophilic group*;
- (2) possibly, *secondary hydrophilic groups*;
- (3) *the key hydrophobic residue*;
- (4) possibly, *characteristic hydrophobic residues*;
- (5) *intermediate functional groups*;
- (6) *supplementary properties of the hydrophilic part*.

* See in Annex A, diagrams giving practical details of the principle of the classification.

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 and
- 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 Table, pages 10 and 11) :

- (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 acidic;
- (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 acidic;
- (f) The other non-ionic groups from column 3, indicated in box 1, 2, 7, 8 and 9.

The figure corresponding to the key group should be underlined.

- (2) THE SECONDARY HYDROPHILIC GROUP SHOULD BE SELECTED USING THE SAME ORDER OF FUNCTIONS. The figure chosen for this secondary hydrophilic group cannot be quoted if it is in the same column as that of the key hydrophilic group.

- 5.4 The hydrophobic part of a surface active agent has a more or less complex chemical structure, as it may consist of various hydrocarbon residues with hydrophobic properties, intermediate hydrocarbon functions or substituents.

The choice of a key hydrophobic residue is an essential factor in the classification of a surface active agent. The following rules should make it possible to make an unambiguous choice :

Rule 4*

THE KEY HYDROPHOBIC RESIDUE IS IN PRINCIPLE THE HYDROCARBON RESIDUE, AS FAR AWAY AS POSSIBLE FROM THE KEY HYDROPHILIC GROUP.

The need in classifying the key hydrophobic residue as far away as possible from the key hydrophilic group is to make it possible to include the maximum amount of information in the supplementary characterization of the surface active agent.

Substituents occurring on the key hydrophobic residue do not affect the choice of the latter.

IN THE CASE WHERE THE HYDROPHOBIC RESIDUE CHOSEN AS THE KEY RESIDUE COMPRISES STRUCTURAL ELEMENTS OF BOTH ALIPHATIC AND RING (e.g. AROMATIC) TYPES, ACCOUNT SHOULD BE TAKEN OF THE LENGTHS OF THE ALIPHATIC CHAINS IN ORDER TO DEFINE THE RING CHARACTER OF THE HYDROPHOBIC RESIDUE.

Rule 5*

THE ALIPHATIC HYDROCARBON CHAIN SHOULD BE CONSIDERED SUFFICIENTLY LARGE, WITHIN THE MEANING OF RULE 4, IF IT CONTAINS A CHAIN OF AT LEAST 8 CARBON ATOMS.

Rule 6*

IN THE ABSENCE OF ALIPHATIC HYDROCARBON CHAINS WITH 8 OR MORE CARBON ATOMS, THE RING RESIDUE WITHIN THE MEANING OF RULE 4 SHOULD BE REGARDED AS THE KEY PART.

Rule 7

IN THE ABSENCE OF AN ALIPHATIC HYDROCARBON CHAIN WITH 8 OR MORE CARBON ATOMS, AND IN THE ABSENCE OF ANY RING RESIDUE, THE LARGEST HYDROPHOBIC PART SHOULD BE REGARDED AS THE KEY HYDROPHOBIC RESIDUE.

For example : C₆ chain of sodium hexyl sulphate.

- 5.5 A hydrophobic residue other than the key hydrophobic residue, and functionally linked to it, may affect the behaviour of a surface active agent, if it is sufficiently hydrophobic; it should then be regarded and described as a characteristic hydrophobic residue.

Rule 8

A CHARACTERISTIC HYDROPHOBIC RESIDUE SHOULD SATISFY RULES 5 OR 6 DEFINING THE KEY HYDROPHOBIC RESIDUE.

However, a secondary function may make it possible to include in the molecule two radicals which are not very important when considered separately, but which are linked to each other, for example, the dibutylamide function $-\text{CO}-\text{N}(\text{C}_4\text{H}_9)_2$. In this case, these secondary radicals should be added together, and the group should be regarded as a characteristic hydrophobic radical, provided that it contains at least 8 carbon atoms.

IN ACCORDANCE WITH RULE 6, AN AROMATIC INTERMEDIATE LINK, EVEN WHEN NOT SUBSTITUTED, SHOULD BE REGARDED AS A CHARACTERISTIC HYDROPHOBIC RESIDUE.

* See Annex B for examples illustrating the application of rules 4, 5 and 6 in the case of surface active agents the hydrophobic part of which comprises both aliphatic chains and rings.

6. CLASSIFICATION

This classification system operates on the decimal system, with a minimum of 10 figures divided into 3 groups of 3 figures, with at least 1 additional figure, so that the key hydrophilic groups may be defined.

The groups of figures are arranged in columns, according to the constitutive sequence of relative positions described above.

Each column contains subdivisions numbered from 0 to 9, 0 usually indicating (unless otherwise stated) the absence of functions, groups or characteristics according to the specific designations of the various columns.

The detailed description of the elements used in the classification is given in Annex C.

Some examples of the application of this classification are given in the Appendix, page 26.