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Površinsko aktivne snovi - Znanstvena klasifikacija

Surface active agents -- Scientific classification

Agents de surface -- Classification scientifique

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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 PRINCIPLE[1)]

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.

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[1)]

THE KEY HYDROPHOBIC RESIDUE IS, IN PRINCIPLE, THE HYDROCARBON RESIDUE FARTHEST FROM THE KEY HYDROPHILIC GROUP.

The need for classifying as the key hydrophobic residue that farthest 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 (*for example* 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[1)]

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

Rule 6[1)]

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

Example : C_6 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 $-CO-N(C_4H_9)_2$. 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 eight carbon atoms.

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

1) 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 ten figures divided into three groups of three figures, with at least one 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, while considerations regarding the application of the decimal classification system are given in annex D.

Some examples of the application of this classification are given in annex F.

A system of reference classification on punched cards is dealt with in annex E.

TABLE – **Scientific classification of surface active agents**

F_1 – KEY HYDROPHILIC GROUP Characteristic properties			R_1 – KEY HYDROPHOBIC PART Important descriptive characteristic properties :		
1 ANIONIC	2 CATIONIC	3 NON-IONIC	4 CONSTITUTION	5 SUBSTITUTION	6 LINKAGE OF KEY FUNCTION F_1
0 AA Absence of	0 AA Absence of	0 AA Absence of	0 AA Non-branched aliphatic group	0 AA Absence of	0 AA Non aromatic, primary
1 BB – COOH	1 BB Primary amine	1 BB Aliphatic hydroxyl group	1 BB Branched aliphatic group	1 BB Unsaturation – C = C – – C ≡ C –	1 BB Non-aromatic, secondary
2 CC – OSO_3H	2 CC Secondary amine	2 CC Alicyclic or aromatic hydroxyl group	2 CC Alicyclic group, terpenes	2 CC Alkyl group (linked to cycles)	2 CC Non-aromatic, tertiary
3 DD – SO_3H	3 DD Tertiary amine	3 DD Non-branched polyether on intermediate chain	3 DD Non-condensed benzene group	3 DD Ring group	3 DD By intermediate chain on ring, primary
4 EE – S – SO_3H	4 EE Amine oxide	4 EE Branched polyether on intermediate chain	4 EE Aromatic group with condensed cycles	4 EE Halogens, nitro, nitroso and similar substituents	4 EE By intermediate chain on ring, secondary
5 FF – SO_2H including other sulphur functions – SO_2NH (r)	5 FF Quarternary ammonium	5 FF Derivatives of sorbitan, mannitan, carbohydrates and similar	5 FF Heterocyclic group with 1 non-carbon atom on the ring	5 FF Ether hydroxyls	5 FF By intermediate chain on ring, tertiary
6 GG Orthophosphoric acid esters	6 GG Pyridinium, Quinolinium and similar	6 GG Derivatives of sorbitan, mannitan, oxy alkyl carbo-hydrates	6 GG Heterocyclic group with 2 or more non-carbon atoms on the ring	6 GG Carboxyl functions and derivatives – COO (r), – CON $(r)_2$, etc...	6 GG Direct linkage on aromatic ring
7 HH Phosphonic acids	7 HH Sulphonium	7 HH Carbonyl group	7 HH Polymer group	7 HH Sulphide and sulphate functions	7 HH Direct linkage on non-aromatic carbon ring
8 KK Per acids	8 KK Phosphonium	8 KK Ureas, ureides, polypeptides	8 KK Group containing other elements in a chain	8 KK Primary, secondary and tertiary amine functions	8 KK Direct linkage through carbon atom of a hetero-cycle
9 LL Other anionic functions	9 LL Other cationic functions	9 LL Other non-ionic functions	9 LL Other hydrophobic groups Z, Y, X	9 LL Other substitutions and substitutions not chemically designated	9 LL Direct linkage through non-carbon atom of a heterocycle

P – HYDROPHOBIC PART Supplementary characteristic properties			HYDROPHILIC PART Supplementary characteristic properties		
7 INTERMEDIATE FUNCTIONAL GROUP X_1	8 INTERMEDIATE FUNCTIONAL GROUP X_2	9 CHARACTERISTIC HYDROPHOBIC PART R_2	10/1 ANIONIC	10/2 CATIONIC	10/3 NON-IONIC
0 AA Absence of	0 AA Absence of	0 AA Absence of	0 AA Absence of	0 AA Absence of	0 AA Absence of
1 BB – COO —— F_1	1 BB – COO —— R	1 BB Part R_2 identical with part R_1	1 BB Alkaline metal salts : Li, Na, K, etc... (Group I a)	1 BB One or two hydrophobic groups. Inorganic anion	1 BB Characteristic hydroxyl function
2 CC – OOC —— F_1	2 CC – OOC —— R	2 CC Aliphatic branched or not	2 CC Alkaline earth metal salts : Mg, Ca, Sr, Ba, etc... (Group II a)	2 CC One or two hydrophobic groups. Organic anion	2 CC Characteristic ester function
3 DD – CON (r) —— F_1 – N (r) CO —— F_1 One and two intermediate functions	3 DD – CON (r) —— R – N (r) CO —— R One and two intermediate functions	3 DD Saturated cyclic hydrocarbons, olefinic cyclic or alicyclic hydrocarbons	3 DD Precious and volatile metal salts : Cu, Ag, Zn, Cd, Hg (Groups I b and II b)	3 DD One or two hydrophobic groups; Benzyl radical and similar Inorganic anion	3 DD Characteristic ether function
4 EE – SO_2N (r) —— F_1 – N (r) SO_2 —— F_1	4 EE – SO_2N (r) —— R – N (r) SO_2 —— R	4 EE Aromatic heterocyclic	4 EE Transition metal salts : Cr, Mn, Fe, Co, Ni (Groups VI a, VII a and VIII)	4 EE One or two hydrophobic groups Benzyl radical and similar Organic anion	4 EE Characteristic amide function
5 FF – O —— F_1 One, two and three intermediate functions	5 FF – O —— R One, two and three intermediate functions	5 FF Group substituted by hydroxyl or – OR_2	5 FF Salts of metals with *p* valencies : Al, In, Sn, Pb, Bi (Groups III b to V b)	5 FF Three hydrophobic groups. Inorganic anion	5 FF Characteristic sulphamide function – SO_2N (r)$_2$
6 GG – S —— F_1 – SO —— F_1 – SO_2 —— F_1	6 GG – S —— R – SO —— R – SO_2 —— R	6 GG Group substituted by $N(r)_2$ or NH(r)	6 GG Lanthanium and actinium group metal salts : La, Ce, Th, U, etc...	6 GG Three hydrophobic groups. Organic anion	6 GG
7 HH – N (r) —— F_1	7 HH – N (r) —— R	7 HH Groups with – COOH function and derived functions	7 HH Ammonium salts	7 HH Metallic complexes	7 HH
8 KK Others X —— F_1	8 KK Others – X —— R	8 KK Groups with functions such as – SO_3H, OSO_3H, and similar	8 KK Organic base salts	8 KK Trimethylglycine	8 KK Organo-metallic derivatives
Supplementary substitution characteristic properties, in the absence of : Function X_1 / Function X_2		9 LL Polymer group or group containing Si, B, and other hydrophobic groups	9 LL Salts of complex metals. Organo-metallic bases	9 LL Other specialized characteristics	9 LL Other characteristic functions
9 LL Supplementary unsaturation C = C – C ≡ C	9 LL Substitutions of column 5 on intermediate chain C				

ANNEX A

PRINCIPLE OF CLASSIFICATION AND CONSTITUTIVE DIAGRAMS

A.1 PRINCIPLE OF CLASSIFICATION

The diagrams in clause A.2, in which the notation below has been used, allow a more practical presentation of the principle of classification.

In general,

F indicates a group with hydrophilic structure;

R indicates a group with hydrophobic structure;

X indicates an intermediate functional group.

In particular,

F_1 indicates the key hydrophilic group;

F_2 indicates a secondary hydrophilic group;

R_1 indicates the key hydrophobic residue;

R_2 indicates a characteristic hydrophobic residue;

X_1 indicates the intermediate functional group closest to F_1;

X_2 indicates another intermediate functional group;

C indicates an intermediate hydrocarbon link;

S indicates a substitution of a general nature, but without solubilizing properties (including unsaturation regarded as a substitution of π electrons on the chain).

A.2 CONSTITUTIVE DIAGRAMS