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R 896

SURFACE ACTIVE AGENTS

SCIENTIFIC CLASSIFICATION

1st EDITION

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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.

ISO Recommendation | R 896 | December 1968

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 : 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 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.

TABLE – Scientific classification of surface active agents

F_1 – KEY HYDROPHILIC GROUP Characteristic properties			R_1 – KEY HYDROPHOBIC RESIDUE 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, Quinilinium 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 functions 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 Betaines	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

A.1 PRINCIPLE OF CLASSIFICATION

The following diagrams 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

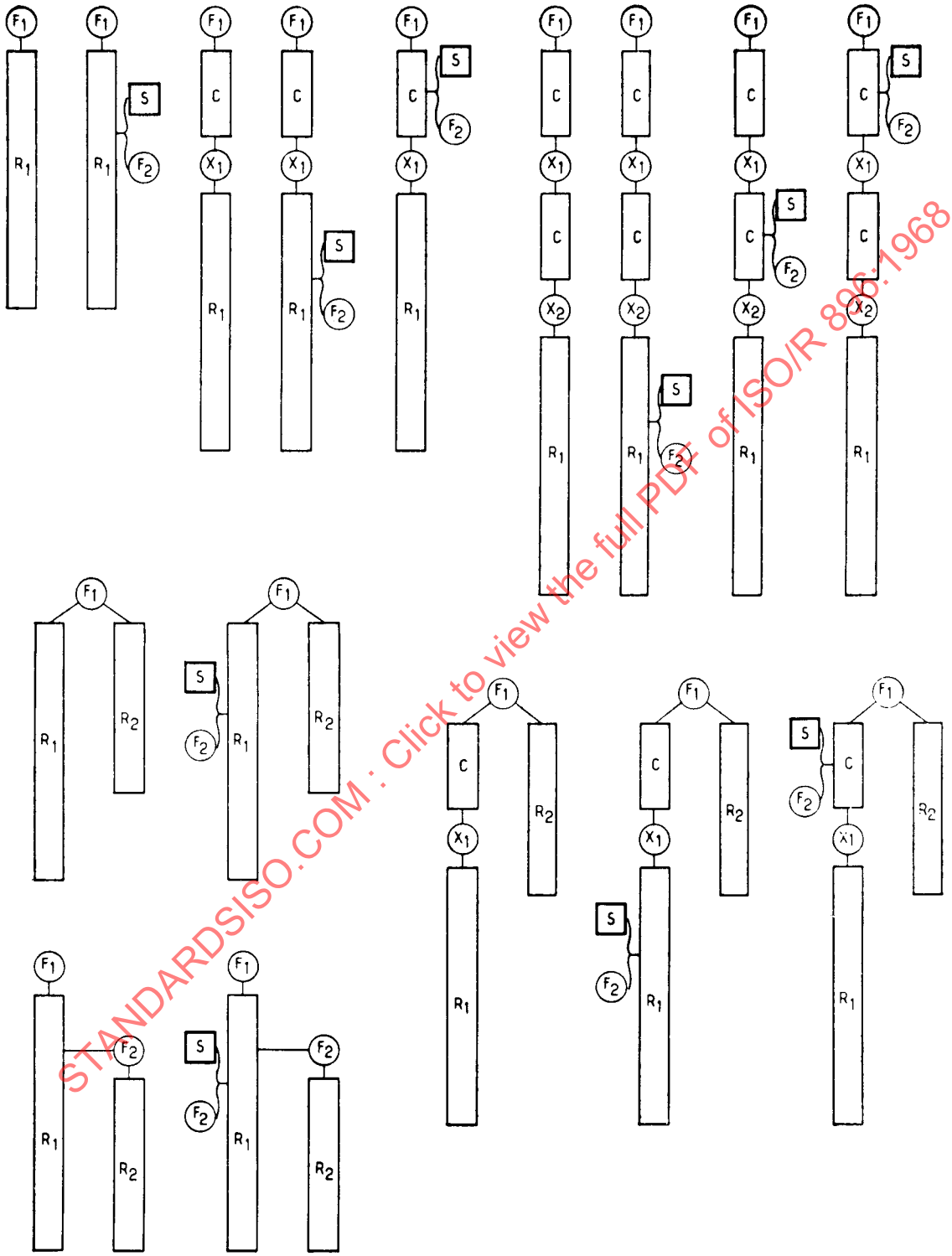
X_1 indicates the intermediate functional group closest to F_1

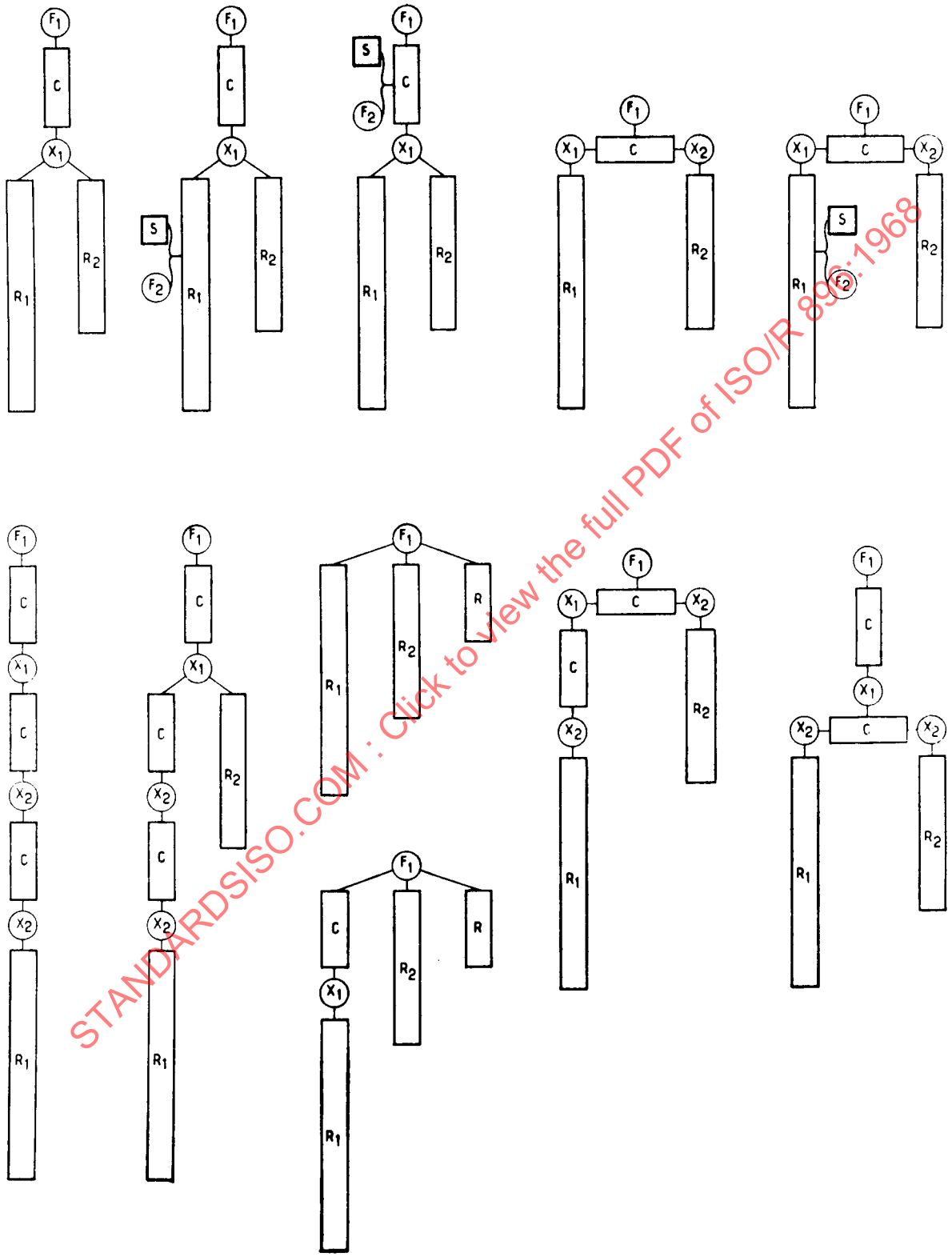
X_2 indicates another intermediate functional group

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





ANNEX B

RULES OF CLASSIFICATION

The case of surface active agents whose hydrophobic part comprises both aliphatic chain structures and rings is particularly important. The following examples illustrate the application of rules 4, 5 and 6, Θ designating a ring residue :

For the substances

$$\Theta - (CH_2)_8 - F_1$$

$$\Theta - (CH_2)_3 - \underset{\displaystyle (CH_2)_3 - CH_3}{\underset{|}{CH}} - F_1$$

$$\Theta - (CH_2)_2 - \underset{\displaystyle (CH_2)_3 - CH_3}{\underset{|}{CH}} - CH_2 - F_1$$

$$CH_3 - (CH_2)_5 - \underset{\displaystyle \Theta}{\underset{|}{CH}} - CH_2 - F_1$$

the aliphatic chain with 8 carbon atoms constitutes the key hydrophobic residue, while the ring residue Θ is regarded as a substitution on this key hydrophobic residue.

On the other hand, for the substances

$$\Theta - (CH_2)_7 - F_1$$

$$CH_3 - (CH_2)_6 - \Theta - F_1$$

the ring residue Θ constitutes the key hydrophobic residue, and the aliphatic chain is regarded as an intermediate chain in the first case, and as a substituent in the second.

Moreover, in order to ensure the best possible designation for products of the following types,

$$CH_3 - (CH_2)_n - \Theta - F_1$$

$$CH_3 - (CH_2)_n - \Theta - (CH_2)_p - F_1$$

the ring residue Θ should be chosen as the key hydrophobic residue, whatever the values of n and p. The presence of intermediate functional groups has the following effect in the case of these compounds :

for the substances

$$CH_3 - (CH_2)_7 - X_1 - \underset{\displaystyle R}{\underset{|}{\Theta}} - F_1$$

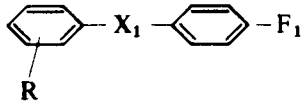
$$CH_3 - (CH_2)_4 - \underset{\displaystyle CH_2 - CH_3}{\underset{|}{CH}} - X_1 - \underset{\displaystyle R}{\underset{|}{\Theta}} - F_1$$

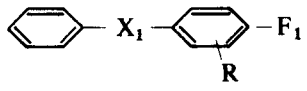
the aliphatic chain constitutes the key hydrophobic residue, whatever R may be. On the other hand, for the substance

$$CH_3 - (CH_2)_6 - X_1 - \underset{\displaystyle R}{\underset{|}{\Theta}} - F_1$$

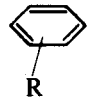
the key hydrophobic residue is the structural unit Θ – R, or Θ, when R is not present.

In the two cases below,





the key hydrophobic residue is the group



ANNEX C

DETAILED DESCRIPTION OF THE ELEMENTS USED IN THE CLASSIFICATION*

C.1 FIRST GROUP OF 3 COLUMNS : COLUMNS 1, 2, 3

"Key hydrophilic group : properties"

This group of figures provides an identification of the polar group in the classification, i.e. the key hydrophilic function or the group of hydrophilic functions. On the first figure depends the order in which the remaining parts of the molecule are to be classified.

Column 1 designates the acid functions (anionic type), or functions classified as such, in the case of salts.

Column 2 designates the basic functions (cationic type), or functions classified as such, in the case of salts.

Column 3 designates those functions or functional groups which have no ionic properties, or those classified as such, in the case of functional groups of a non-ionic type. For example, a simple ether derived from an alcohol function.

The designation of key functions by means of figures in columns 1, 2 and 3 should be limited to a strict minimum, and those indicated should be given in the order of their relative importance as laid down in the rules already given.

The designation of supplementary functions of lesser importance should be found in column 5 of the classification. For example the hydroxyl group of ricinoleic acid should not be designated as a key function, but as a substituent in column 5.

C.2 SECOND GROUP OF 3 COLUMNS : COLUMNS 4, 5, 6

"Key hydrophobic residue : important descriptive properties"

This group is intended to classify elements of the key hydrophobic residue (generally that farthest away from the key hydrophilic function) and the linkage of the key functional group determining the polar/non-polar structural relations of the molecule.

Column 4 describes the constitution of the key hydrophobic radical or residue R_1. It is arranged in such a way that it shows constitutive elements of the hydrophobic radicals, carefully distinguished one from the other so that the clearest possible classification is obtained.

Column 4, although taken as a key, is more often a factor deciding the entire character of the hydrophobic residue in question. An isododecyl benzene sulphonate is classified under subdivision 3 of column 4 : "non-condensed benzene residue". Alkylbenzimidazol derivatives are classified under subdivision 6 of column 4 : "Hetero-cyclic residue with 2 or more non-carbon atoms in the ring".

Column 5 describes the substitution which may occur in the *hydrophobic part*, and in particular in the key hydrophobic residue designated in column 4.

Since several different substitutions may occur on the same hydrophobic residue, it is advisable, in the decimal classification, to designate one single substituent, i.e. the one which will most clearly differentiate the molecule which is being classified. Failing any decisive observation to this effect, the following should be designated, in order of their importance : the main carbon substituent (chain or ring); then a substituent secondary function F_2, the most polar substituent; and lastly the degree of unsaturation (substitution by π electrons).

Column 6 indicates the way in which the key hydrophilic group F_1 is linked with the rest of the molecule; this column can be arranged in such a way that it provides additional information about the molecular constitution.

For example, the use of a figure in column 4 corresponding to ring constitutive elements, in combination with a designation for a functional bond not directly linked to the ring, indicates the existence of a carbon chain separating the ring from the function.

* See Table, pages 10 and 11.

C.3 THIRD GROUP OF 3 COLUMNS : COLUMNS 7, 8 AND 9

"Hydrophobic part : supplementary properties"

In subdivisions 0 to 8, columns 7 and 8 describe the intermediate functions which may separate the key hydrophilic function F_1 either from the key hydrophobic residue or from a characteristic hydrophobic residue. These separations also imply the existence of intermediate carbon links C (or X).

Column 7 designates (from 0 to 8) *the intermediate function* X_1 closest to the key hydrophilic function F_1.

Column 8 designates (from 0 to 8) a *second intermediate function* X_2 which may either separate the key hydrophobic radical R_1 from the function F_1 by means of an extra link C (or X), or introduce a supplementary characteristic hydrophobic radical R_2.

In complex cases, where several intermediate functions X_2 may exist together in the same molecule, column 8 should first show the function which introduces a supplementary characteristic hydrophobic radical R_2. If no such radical is present, the intermediate function X_2 designated should be the one closest to the key residue R_1.

In connection with the functional specifications of columns 7 and 8, special mention should be made of the indications given in subdivisions 3 and 5.

In these cases, provision has been made for groups of intermediate polyfunctional links, which may comprise up to 3 intermediate similar functions and grouped as such. The number 3 is the maximum, as above this number functional groups of this kind become hydrophilic groups, which is sufficient to justify the designation of non-ionic hydrophilic group in column 3 of the first group of 3 columns.

NOTE. – The foregoing is applicable only in the case of simple intermediate links, such as $O - CH_2 - CH_2 - O$ of polyethylene oxides.

The figures 9 of columns 7 and 8 provide further supplementary characteristics of the *hydrophobic part P*; these caracteristics are included here to increase the flexibility of the classification and greatly extend (as is necessary) the possibility of combinations :

- In the absence of an intermediate function X_1 (i.e. an intermediate connecting link C), figure 9 of column 7 makes provision for the possibility of designating a supplementary unsaturation in the carbon chain of the key hydrophobic residue; this information is important for the classification of linoleic or ricinoleic derivatives. This supplementary information can also be extended to cover the case of derivatives comprising the intermediate functions X and the intermediate links C, on the assumption that the designations of column 8, which generally represent the intermediate functions X_2, are now being used to designate the intermediate functions X_1.
- Figure 9 of column 8 is used only in the absence of an intermediate function X_2; the use of figure 9 in the classification then means that the indications of substitutions found in column 5 of the second group of 3 columns refer exclusively to substitutions occurring on, and more characteristic of, the intermediate link C. This arrangement makes it possible to classify clearly such products as sulphated glycerol laurate.

Column 9 of the group describes a characteristic hydrophobic residue R_2, appearing by functional bonds in the molecule, or functionally linked, as a secondary hydrophobic residue, to the rest of the molecule.

A characteristic hydrophobic residue R_2 of this kind is included in the molecule by functional bonds X_1 and X_2. It is then characteristic, in the sense that it designates in particular an *aromatic or aliphatic supplementary property of the molecule, which will become apparent a priori*.

On the other hand, column 9 also designates a characteristic hydrophobic residue R_2, which appears as an adequate, hydrophobic, supplementary, radical. A functionally linked residue of this kind can be attached to the whole molecule by an intermediate function X_2, (as in the case of sulphonated succinic diesters), by a substituent function F_2, or even by any intermediate functions X or key function F_1, provided that these functions are polyvalent : amine functions for example, secondary or tertiary amines – quaternary ammoniums, etc.

The figure 1 of column 9 is used only in the case of a characteristic radical of a supplementary nature. Designating a residue R_2, which is identical according to the classification with the residue R_1, figure 1 is intended in particular to distinguish the polyglycerides, dialkylamines, etc.

C.4 FOURTH GROUP OF 3 COLUMNS : COLUMNS 10/1, 10/2, 10/3

"Hydrophilic part : supplementary properties"

This section can be used in the decimal classification as either 1 or 2 supplementary figures.

The supplementary properties of the polar grouping, thus designated, relate in particular to the salt-forming elements of ionic functions and transformations of non-ionic functions. They provide additional descriptions of complex functions and make it possible to assess the solubilization properties.

Column 10/1 describes the anionic compounds, by providing a systematic table of salt-forming cations. The complex cations, described under box 9 of this column, are cations of metallic co-ordinations with simple molecules in which hydrophobic properties do not predominate (NH_3, ethylene diamine, aniline, etc.) or cations of true organo-metallic bases.

Column 10/2 describes the cationic compounds, by characterizing more accurately the state of multiple functional valency of the hydrophilic group (see also column 9 of the third group of 3 columns, which covers part of this functional diversification). It emphasizes the important part played by the salt-forming anion.

The metallic complexes described under box 7 of column 10/2 are metal salts co-ordinated with molecules which can form complexes, and which in themselves have the constitution of surface active agents, being in consequence the basis for classification, by application of the designations of the preceding groups of columns. For example, copper chloride complex with 2 molecules of lauryl propylene diamine.

Column 10/3 gives details of the derived non-ionic functions which have not been explicitly described in column 3 of the first group of 3 columns.

Box 8 of column 10/3 covers organo-metallic derivatives which are regarded as non-ionic, and which cannot be more accurately described in the preceding classification groups. For example, trialkyl aluminium.

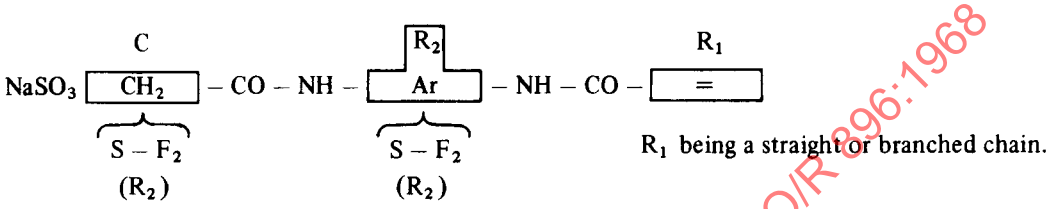
D.2 It can easily be seen that any other method of distinguishing between the elements of the above formula would provide less information about its constitution.

Having said this, it should be admitted that it has not been possible to designate

(*a*) the substituent function – O – on the characteristic benzene residue;

(*b*) the octyl hydrophobic residue, which is also characteristic but is of secondary importance.

D.3 The preceding classification index-number allocated does however correspond to a synthesis diagram, which would (probably) be as follows :



R_1 being a straight or branched chain.

The classification is specific for one molecule, in that it is possible to designate any chemically defined molecule, but not a mixture.

It is possible to classify a mixture of two surface active agents with different chemical constitutions by giving the mixture the two series of classification figures corresponding to the two products mixed.

On the other hand, the classification cannot make provision for the uncertain molecular constitution of the main hydrophobic radical, which frequently occurs as a result of the transformation of natural fatty substances or the processing of synthetic raw materials.

For example :

– a mixture of $C_{12} - C_{14} - C_{16}$ chains obtained from natural fatty acids;

– constitution of complex mixtures of OXO synthetic alcohols;

– mixtures of various structural tetra-propylenes, etc.

ANNEX E

REFERENCE CLASSIFICATION ON PUNCHED CARDS

The foregoing considerations regarding the application of the decimal classification stress the importance of the work of the technicians applying the system and the supplementary information which would be desirable, but which cannot be included satisfactorily within the framework of a simple decimal system.

It is apparent that there is an immediate need for classification, preferably on *punched cards*, which can be used for reference purpose by all technicians.

If this system of reference classification on punched cards is to be of any value, it should fulfil the following conditions :

(1) It should not entail any alteration to the basic elements of classification reflected in the decimal classification.

(2) It should abide by the rules of classification sequence proposed for the decimal classification.

(3) It should provide in more detail for the very large number of elements in the classification system : key functions, hydrophobic residues, intermediate functions, intermediate links, substitutions and other characteristics.

(4) It should make provision for the constitution of hydrophobic residues of different origins in complex mistures.

(5) Finally, it should be possible to superimpose the punched cards system on the decimal classification system without any alteration in the method of presentation.

A reference classification, on punched cards, of this kind, has been worked out and is described below; it has been superimposed on the decimal classification system described above. It makes use of letters, either in columns or in addition to the classification; these letters correspond to the perforations on the punched cards.

The reference classification can only be established by a specialist, in conformity with its use as a classification reference.

The general appearance of the reference classification, in four groups of 3 columns, is the same as that of the decimal classification.

In each column of the classification, in addition to the figure of the decimal classification, there are two reference letters, which indicate the supplementary perforations corresponding to the figures on the punched card.