



SLOVENSKI STANDARD
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Površinsko aktivne snovi - Poenostavljena klasifikacija

Surface active agents -- Simplified classification

Agents de surface -- Classification simplifiée

Ta slovenski standard je istoveten z: ISO 2131:1972

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INTERNATIONAL STANDARD



2131

INTERNATIONAL ORGANIZATION FOR STANDARDIZATION • МЕЖДУНАРОДНАЯ ОРГАНИЗАЦИЯ ПО СТАНДАРТИЗАЦИИ • ORGANISATION INTERNATIONALE DE NORMALISATION

Surface active agents — Simplified classification

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FOREWORD

ISO (the International Organization for Standardization) is a worldwide federation of national standards institutes (ISO Member Bodies). The work of developing International Standards is carried out through ISO Technical Committees. Every Member Body interested in a subject for which a Technical Committee has been set up has the right to be represented on that Committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work.

Draft International Standards adopted by the Technical Committees are circulated to the Member Bodies for approval before their acceptance as International Standards by the ISO Council.

International Standard ISO 2131 was drawn up by Technical Committee ISO/TC 91, *Surface active agents*.

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It was approved in June 1971 by the Member Bodies of the following countries :

Australia	Japan	Spain
Austria	Korea, Rep. of	Switzerland
Belgium	New Zealand	Thailand
Egypt, Arab Rep. of	Poland	Turkey
France	Portugal	United Kingdom
Germany	Romania	U.S.A.
Israel	South Africa, Rep. of	U.S.S.R.

No Member Body expressed disapproval of the document.

Surface active agents – Simplified classification

1 SCOPE AND FIELD OF APPLICATION

This International Standard establishes a simplified classification of surface active agents, in conformity, regarding the arrangement of radicals, with the scientific classification (ISO/R 896).

2 PRINCIPLE

The simplified classification of surface active agents enables their characteristics to be expressed by an abbreviated lettering and numbering system, consisting of a letter and four figures (five in the case of compounds comprising several hydrophilic groups), for the main structural elements of the molecule, using:

- 1) the letter to designate the ionic character;
- 2) the 1st figure to designate the hydrophilic group;
- 3) the 2nd figure to designate the hydrophobic group;
- 4) the 3rd figure to designate an intermediate functional group;
- 5) the 4th figure to designate a supplementary property of the hydrophilic group;
- 6) the 5th figure (in parentheses between the 1st and 2nd) to designate the second hydrophilic group of compounds comprising several hydrophilic groups of different ionic characters.

The operation is carried out by determining, from the classification Table given in the Annex arising from the general scientific classification, the figures which correspond to the groups present in the molecule, by the application of the rules defined in section 3.

3 RULES OF CLASSIFICATION

3.1 Choice of the hydrophilic group

Rule 1

The hydrophilic group is the point of departure for the classification. Its ionic character shall be designated by one of the following letters :

- A for anionic hydrophilic groups;
- C for cationic hydrophilic groups;
- N for non-ionic hydrophilic groups;
- Z for true ampholytic compounds.

Rule 2

In the presence of several hydrophilic groups with identical ionic characters, select as the principal hydrophilic group that which is designated first in the following numbering order, with reference to the divisions in the Table in the Annex :

for groups which are

- anionic : 2 – 3 – 4 – 5 – 6 – 7 – 8 – 9 – 1
- cationic : 5 – 6 – 7 – 8 – 9 – 1 – 2 – 3 – 4
- non-ionic : 3 – 4 – 5 – 6 – 1 – 2 – 7 – 8 – 9

Rule 3

In the presence of several hydrophilic groups with different ionic characters, two alternatives must be considered :

- a) in the presence of anionic and cationic groups (ampholytic compounds), use the letter Z. Designate the cationic group first and the anionic group second, in parentheses, applying Rule 2 if necessary;
- b) in the presence of an ionic group and a non-ionic group, use as the letter that which characterises the ionic group. Designate this first and the non-ionic group second, in parentheses, applying Rule 2 if necessary.

3.2 Choice of the hydrophobic group

Rule 4

The determinant hydrophobic group is the most important radical for the hydrophobic behaviour; in general, it is usually the longest hydrocarbon chain (including rings), as far removed as possible from the principal hydrophilic group.

Rule 5

An aliphatic hydrocarbon chain shall be regarded as sufficiently long, in the terms of Rule 4, if it consists of at least 8 carbon atoms.

Rule 6

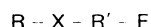
If the surface active agent does not contain a hydrocarbon chain with at least 8 carbon atoms, take a cyclic residue as the determinant hydrophobic group.

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3.3 Choice of the intermediate functional group**Rule 7**

Choose as the intermediate functional group the one which is nearest to the principal hydrophilic group.

NOTE — The most important surface active agents correspond to the formula



in which the letters F, R', X in the Table given in the Annex have the following meaning :

R indicates the principal hydrophobic group;

X indicates an intermediate function;

R' indicates a short hydrocarbon chain;

F indicates the principal hydrophilic group.

The letters F, R', X in the Table given in the Annex have the same meaning; on the other hand the letter r, used also in the table, indicates a hydrogen or alkyl residue.

3.4 Choice of the supplementary property of the hydrophilic group**Rule 8**

The supplementary property of the hydrophilic group shall be that of the principal hydrophilic group; it shall be selected in accordance with the numbering order in the Table.

3.5 Note

Should it appear necessary to record the classification on punched cards or a computer, any parentheses there may be should disappear. In the case of compounds having two or more hydrophilic groups with identical ionic characters, insert 0 between the first and second figures obtained. In the case of compounds having several groups of different ionic characters, merely omit the parentheses.

Example A 1031 (see Appendix, section Z.1) becomes A 10031 and example Z 2(1)002 (see Appendix, section Z.4) becomes Z 21002.

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ANNEX

TABLE — Simplified classification of surface active agents

Hydrophilic group		Determinant hydrophobic group	Intermediate functional group	Supplementary properties of the hydrophilic group		
anionic	cationic			non-ionic	anionic	cationic
1	-COOH	Aliphatic hydroxyl group	0	0	0	0
1	Primary amine	Branched aliphatic residue	1	1	1	1
2	Secondary amine	Alicyclic or aromatic hydroxyl group	2	2	2	2
3	Tertiary amine	Non-condensed benzene residue	3	3	3	3
4	Amino oxide	Aromatic residue with condensed rings	4	4	4	4
5	Quaternary ammonium	Heterocyclic residue with 1 non-carbon atom on the ring	5	5	5	5
6	Pyridinium imidazolium and similar	Heterocyclic residue with 2 or more non-carbon atoms on the ring	6	6	6	6
7	Sulphonium	Polymer residue	7	7	7	7
8	Phosphonium	Residue containing other elements in chain	8	8	8	8
9	Other cationic functions	Other hydrophobic residues	9	9	9	9
1	-OSO ₃ H	Aliphatic hydroxyl group	0	0	0	0
1	-SO ₃ H	Branched aliphatic residue	1	1	1	1
1	-SO ₃ H	Alicyclic or aromatic hydroxyl group	2	2	2	2
1	-SO ₃ H	Non-condensed benzene residue	3	3	3	3
1	-SO ₃ H	Aromatic residue with condensed rings	4	4	4	4
1	-SO ₃ H	Heterocyclic residue with 1 non-carbon atom on the ring	5	5	5	5
1	-SO ₃ H	Heterocyclic residue with 2 or more non-carbon atoms on the ring	6	6	6	6
1	-SO ₃ H	Polymer residue	7	7	7	7
1	-SO ₃ H	Residue containing other elements in chain	8	8	8	8
1	-SO ₃ H	Other hydrophobic residues	9	9	9	9
0	Absence of	Absence of	0	0	0	0
1	Alkaline metal salts Li, Na, K etc. (Group Ia)	-COO - R' - F	1	1	1	1
2	Alkaline earth metal salts Mg, Ca, Sr, Ba etc. (Group IIa)	-OOC - R' - F	2	2	2	2
3	Salts of metal Cu, Ag, Zn, Cd, Hg (Groups Ib and IIb)	-CON(r) - R' - F -N(r)CO - R' - F 1 and 2 intermediate functions	3	3	3	3
4	Transition metal salts Cr, Mn, Fe, Co, Ni (Groups VIa, VIIa, VIII)	-SO ₂ N(r) - R' - F -N(r)SO ₂ - R' - F	4	4	4	4
5	Salts of metals Al, In, Sn, Pb, Bi (Groups IIIb to Vb)	-O - R' - (O - R') _n F 1, 2 and 3 intermediate functions	5	5	5	5
6	Lanthanum and actinium group metal salts La, Ce, Th, U etc.	-S - R' - F -SO - R' - F -SO ₂ - R' - F	6	6	6	6
7	Ammonium salts	-N(r) - R' - F	7	7	7	7
8	Organic base salts	Others - X - R' - F	8	8	8	8
9	Salts of complex metals. Organo-metallic bases		9	9	9	9
0	Absence of		0	0	0	0
1	1 or 2 hydrophobic residues. Inorganic anion		1	1	1	1
2	1 or 2 hydrophobic residues. Organic anion		2	2	2	2
3	1 or 2 hydrophobic residues. Benzyl radical and similar. Inorganic anion		3	3	3	3
4	1 or 2 hydrophobic residues. Benzyl radical and similar. Organic anion		4	4	4	4
5	Three hydrophobic residues. Inorganic anion		5	5	5	5
6	Three hydrophobic residues. Organic anion		6	6	6	6
7	Metallic complexes		7	7	7	7
8	Betaines		8	8	8	8
9	Other specialized characteristics		9	9	9	9
0	Absence of		0	0	0	0
1	Characterising hydroxyl function		1	1	1	1
2	Characterising ester function		2	2	2	2
3	Characterising ester function		3	3	3	3
4	Characterising amide function		4	4	4	4
5	Characterising sulphamide function		5	5	5	5
6	-SO ₂ N(r) ₂		6	6	6	6

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APPENDIX

EXAMPLES OF APPLICATION OF THE SIMPLIFIED CLASSIFICATION

Z.1 ANIONIC SURFACE ACTIVE AGENTS

Sodium stearate	$C_{17}H_{35}COONa$	A 1001
Sodium lauroyl sarcosinate	$C_{11}H_{23}-CO-N(CH_3)-CH_2-COONa$	A 1031
Sodium laurylsulphate	$C_{12}H_{25}-OSO_3Na$	A 2001
Sodium lauryl ethoxy-ether sulphate	$C_{12}H_{25}-OCH_2-CH_2-OCH_2-CH_2-OSO_3Na$	A 2051
Sodium salt of the sulphuric ester of lauroyl ethanolamide	$C_{11}H_{23}-CO-NH-CH_2-CH_2-OSO_3Na$	A 2031
Sodium alkylsulphonate	$C_{11}H_{23}-CH(C_2H_5)-SO_3Na$	A 3001
Sodium oleyl-oxyethane sulphonate	$C_{17}H_{33}-COO-CH_2-CH_2-SO_3Na$	A 3011
Sodium salt of oleyl-methyltauride	$C_{17}H_{33}-CO-N(CH_3)-CH_2-CH_2-SO_3Na$	A 3031
Sodium alkylaryl-sulphonate	$C_{12}H_{25}-C_6H_5-SO_3Na$	A 3301
Sodium mono-alkylphosphate	$C_{12}H_{25}-O-P(=O)(ONa)_2$	A 6001
Sodium dioctylsulphosuccinate	$C_8H_{17}-OOC-CH_2-CH(C_8H_{17}-OOC)-SO_3Na$	A 3021

Z.2 CATIONIC SURFACE ACTIVE AGENTS

Stearyl-dimethyl-benzyl-ammonium chloride	$\left[C_{18}H_{37}-N(CH_3)_2-CH_2-C_6H_5 \right]^+ Cl^-$	C 5003
Imidazoline acetate alkyl substituted	$C_{17}H_{33}-C(=N-CH_2)-N(CH_2-CH_2OH)-CH_2-CH_2OH$, $HOOC-CH_3$	C 6002
Stearoyl-amidoethyl-trimethylammonium methosulphate	$\left[C_{17}H_{35}-CO-NH-CH_2-CH_2-N(CH_3)_3 \right]^+ OSO_3CH_3^-$	C 5031