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The Antielectrostatic Effect of N-Alkanol-N-alkoxymethyl-N,N-dimethylammonium Chlorides and Their Ester Derivatives

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Several new quaternary ammonium chlorides, analogues of choline, were prepared by reaction of 2-(dimethylamino)ethanol and its derivatives with chloromethyl alkyl ethers. The obtained chlorides were examined in respect to their antielectrostatic effects: the surface resistance and half decay time on polyethylene film were measured. Application of rough set theory permitted to perform a comprehensive analysis of data and detection of structural-activity relationships. The obtained chlorides showed high antielectrostatic properties. The most active were quaternary ammonium chlorides with 11 and 12 carbon atoms in alkyl chain.

Key words: quaternary ammonium salts, antielectrostatic effect, rough set theory, SAR

Prevention against development of electric charge in plastics most frequently involves attempts to decrease their surface resistance by their supplementation with specific compounds, the so-called antielectrostatic agents. These agents include chemical substances of a specific structure. Coating with them of a polymer surface or their introduction to the polymer mass during its synthesis or its processing affects the surface conductance and polarizing capacity of the plastic. Thus, they help to refine the materials and to broaden their application potential. Quaternary ammonium compounds (QACs) belong to the most efficient and, therefore, most frequently applied groups of antielectrostatic agents. Choline is an example of QACs of natural origin, found in many plants and animal organisms. Certain salts of the strong base, choline, the almost non-toxic substance, have proven to be even less toxic than their parent compound [1].

Our study aimed the synthesis of specifically designed new QACs, choline derivatives, and at subsequent examination of antielectrostatic properties of these compounds. The applied statistical and nonstatistical SAR analysis proved very useful for processing of the voluminous data on sets of synthesized compounds. In this paper we present application of rough set theory for analysis of the data. The subject of rough set theory, the required software and its application in analysis of QACs structure-antielectrostatic are well summed up in [2–6].

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EXPERIMENTAL

Melting points were measured on Büchi Melting Point B-540. ^{1}H-NMR spectra were recorded with a Varian Model XL 300 spectrometer at 300 MHz with TMS as standard. ^{13}C-NMR spectra were recorded on the same instrument at 75 MHz. Elemental analyses were performed at the University of A. Mickiewicz, Poznań, Poland. Satisfactory elemental analyses of CHN for QACs were acquired with 0.35% tolerance between the calculated and experimental values. Chloromethyl alkyl ether was prepared by passing HCl-gas through a mixture of formaldehyde and appropriate alcohol.

Preparation of quaternary N-alkanol-N-alkoxymethyl-N,N-dimethylammonium chlorides and their ester derivatives. General procedure. Amine (0.05 mol) was placed in a 20 mL anhydrous hexane and chloromethyl alkyl ether (0.055 mol) was added in equimolar amount at rt. The product precipitated immediately from a reaction mixture and was separated and washed with hexane. Then quaternary ammonium chloride was crystallized from acetone or ethyl acetate.

N-(2-Hydroxyethyl)-N,N-dimethyl-N-tetradecyloxymethylammonium chloride (11). ^{1}H-NMR ($CDCl_3$), δ ppm = 4.93 (s, 2H), 4.08 (s, J = 4.7 Hz, 2H), 3.83 (t, J = 6.6 Hz, 2H), 3.67 (t, J = 4.7 Hz, 2H), 3.30 (s, 6H), 1.62 (q, J = 7.0 Hz, 2H), 1.26 (m, 22H), 0.88 (t, J = 6.7 Hz, 3H). ^{13}C-NMR ($CDCl_3$), δ ppm = 91.2, 73.5, 62.7, 55.5, 48.2, 31.8, 29.4, 29.5, 25.7, 22.5, 13.9.

N-[2-(Benzoyloxy)ethyl]-N,N-dimethyl-N-undecyloxymethylammonium chloride (23). ^{1}H-NMR ($CDCl_3$), δ ppm = 8.00 (d, J = 7.1 Hz, 2H), 7.60 (t, J = 7.4 Hz, 1H), 7.46 (t, J = 7.6 Hz, 2H), 5.22 (s, 2H), 4.84 (t, J = 4.5 Hz, 2H), 4.19 (t, J = 4.5 Hz, 2H), 3.84 (t, J = 6.6 Hz, 2H), 3.52 (s, 6H), 1.55 (q, J = 6.6 Hz, 2H), 1.23 (m, 16H), 0.88 (t, J = 6.7 Hz, 3H). ^{13}C-NMR ($CDCl_3$), δ ppm = 165.5, 133.6, 129.5, 128.7, 128.5, 90.9, 73.7, 59.4, 58.1, 48.0, 31.6, 29.4, 29.3, 29.2, 29.1, 25.5, 22.4, 13.9.

N-Cyclododecyloxymethyl-N-(3-hydroxypropyl)-N,N-dimethylammonium chloride (42). ^{1}H-NMR ($CDCl_3$), δ ppm = 4.88 (s, 2H), 3.92 (t, J = 6.6 Hz, 1H), 3.69 (dt, 4H), 3.24 (s, 6H), 2.05 (m, J = 5.5 Hz, 2H), 1.72 (t, J = 6.9 Hz, 2H), 1.57 (m, 2H), 1.33 (m, 18H). ^{13}C-NMR ($CDCl_3$), δ ppm = 88.4, 81.3, 59.2, 58.0, 47.2, 28.3, 25.5, 24.9, 24.6, 22.5, 22.3, 19.7.

N-Cyclododecyloxymethyl-N-(2-hydroxypropyl)-N,N-dimethylammonium chloride (56). ^{1}H-NMR ($CDCl_3$), δ ppm = 4.97 (s, 2H), 4.48 (m, J = 6.6 Hz, 1H), 3.95 (t, J = 6.6 Hz, 1H), 3.49 (m, 2H), 3.36 (s, 3H), 3.33 (s, 3H), 1.70 (t, J = 6.6 Hz, 2H), 1.56 (m, 2H), 1.33 (m, 18H), 1.29 (d, J = 6.0 Hz, 3H). ^{13}C-NMR ($CDCl_3$), δ ppm = 89.8, 81.3, 66.2, 61.3, 48.5, 48.2, 28.6, 28.5, 24.8, 24.5, 22.64, 22.59, 22.51, 22.4, 22.3, 22.23, 21.97, 19.8.

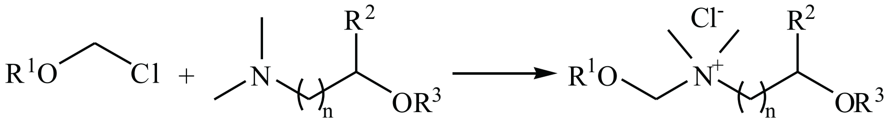
N-[2-(Decanoyloxy)ethyl]-N-dodecyloxymethyl-N,N-dimethylammonium chloride (66). ^{1}H-NMR ($CDCl_3$), δ ppm = 5.17 (s, 2H), 4.55 (t, J = 4.8 Hz, 2H), 4.01 (t, J = 4.9 Hz, 2H), 3.89 (t, J = 6.6 Hz, 2H), 3.45 (s, 6H), 2.34 (t, J = 7.7 Hz, 2H), 1.62 (dq, J = 6.9, 4H), 1.26 (m, 30H), 0.88 (t, J = 6.9 Hz, 6H). ^{13}C-NMR ($CDCl_3$), δ ppm = 172.4, 90.8, 73.7, 59.3, 57.3, 47.9, 33.9, 31.8, 31.7, 29.6, 29.53, 29.51, 29.48, 29.42, 29.26, 29.25, 29.23, 29.1, 29.0, 25.7, 24.61, 22,58, 22.55, 14.03, 14.02.

Antielectrostatic properties: In this study, the antielectrostatic effect of the prepared chlorides was measured on a polyethylene film (LDPE II 003/GO), which did not contain any lubricants or antioxidants. Thin films of QACs were deposited on disks of PE film. The PE disks of 0.125 m diameter were washed in acetone, then dried by placing them in an air-conditioned room. The disks were then immersed in 0.5% chloroform solution of QAC for 60 s. Then, they were hung up, so that the solvent could evaporate. The discs were rubbed on the surface with a cotton pad soaked with the solution of QAC to assure that the surface was covered thoroughly. The disks were stored for 24 h in an air-conditioned room at 20°C and relative humidity of 65%. Finally, the surface resistance, charge decay half time and the maximum voltage induced on the film surface were examined. The measuring apparatus, the method and the measurement conditions were described in [7].

RESULTS AND DISCUSSION

The synthesis was performed using Menschutkin's reaction (Scheme 1). We obtained crystallic salts or oil, depending upon the length of R^1 substituent and on the kind of R^3 substituent. Chlorides with alkoxymethyl substituent, containing between 3 and 11 carbon atoms proved to be strongly hygroscopic. The obtained crystals immediately absorbed water, in which they became dissolved and therefore in some cases the melting temperature could not be determined. If chloride anion was exchanged by BF_4^- or PF_6^- or $(CF_3SO_2)_2N^-$, crystalline salts were obtained. For example, substitution of chloride anion in compound **15** yielded salts poorly soluble in water of the melting temperatures: for BF_4^- 53–55°C, for $(CF_3SO_2)_2N^-$ 64–64.5°C or for PF_6^- 82–82.5°C. All these compounds are new and obtained in high yields (Table 1).

Scheme 1



(**1-70**)

Table 1. The prepared QACs and their antielectrostatic properties.

Chloride number	R^2	R^3	n	R^1	Melting point (°C)	Yield (%)	Surface resistance (Ω)	Half charge decay time (s)	Maximum voltage induced (V)	Antistatic effect
1	H	H	1	C_3H_7	oil	90	$>10^{13}$	600	957	lack
2	H	H	1	C_4H_9	oil	89	$>10^{13}$	600	971	sufficient
3	H	H	1	C_5H_{11}	oil	90	$8\cdot10^{11}$	600	943	very good
4	H	H	1	C_6H_{13}	oil	94	$7\cdot10^{9}$	600	961	excellent
5	H	H	1	C_7H_{15}	hygroscopic	91	$8\cdot10^{8}$	0.3	435	very good
6	H	H	1	C_8H_{17}	hygroscopic	89	$9\cdot10^{9}$	0.2	51	excellent
7	H	H	1	C_9H_{19}	49–51	94	$1\cdot10^{9}$	0.2	38	sufficient
8	H	H	1	$C_{10}H_{21}$	66.5–68.5	86	$6\cdot10^{11}$	0.2	67	excellent
9	H	H	1	$C_{11}H_{23}$	68.5–70	88	$7\cdot10^{8}$	0.3	12	excellent
10	H	H	1	$C_{12}H_{25}$	69.5–71.5	88	$2\cdot10^{7}$	0.15	21	excellent
11	H	H	1	$C_{14}H_{29}$	60–63	90	$6\cdot10^{7}$	0.25	13	excellent
12	H	H	1	$C_{16}H_{33}$	71–73.5	87	$4\cdot10^{6}$	0.2	7	excellent
13	H	H	1	$C_{18}H_{37}$	85–87	85	$8\cdot10^{6}$	0.2	4	excellent
14	H	H	1	$C_{12}H_{23}$ (cyclic)	130–133	90	$3\cdot10^{7}$	0.2	20	lack
15	H	OCPh	1	C_3H_7	hygroscopic	80	$3\cdot10^{13}$	600	983	lack
16	H	OCPh	1	C_4H_9	hygroscopic	84	$>10^{13}$	600	939	lack
17	H	OCPh	1	C_5H_{11}	hygroscopic	87	$>10^{13}$	600	977	lack
18	H	OCPh	1	C_6H_{13}	hygroscopic	88	$>10^{13}$	600	976	very good
19	H	OCPh	1	C_7H_{15}	hygroscopic	89	$1\cdot10^{9}$	0.2	56	insufficient
20	H	OCPh	1	C_8H_{17}	hygroscopic	87	$4\cdot10^{12}$	600	512	excellent

Table 1 (continuation)

21	H	OCPh	1	C_9H_{19}	hygroscopic	86	$3\cdot 10^{7}$	0.1	6	excellent
22	H	OCPh	1	$C_{10}H_{21}$	54–58	88	$6\cdot 10^{6}$	0	–	excellent
23	H	OCPh	1	$C_{11}H_{23}$	71–74	88	$9\cdot 10^{6}$	0	–	excellent
24	H	OCPh	1	$C_{12}H_{25}$	76–79	89	$8\cdot 10^{6}$	0	–	excellent
25	H	OCPh	1	$C_{14}H_{29}$	84–86	85	$7\cdot 10^{6}$	0	–	excellent
26	H	OCPh	1	$C_{16}H_{33}$	86–88	87	$6\cdot 10^{6}$	0	–	excellent
27	H	OCPh	1	$C_{18}H_{37}$	87–90	80	$9\cdot 10^{6}$	0	–	excellent
28	H	OCPh	1	$C_{12}H_{23}$ (cyclic)	135–136	88	$8\cdot 10^{7}$	0.15	183	sufficient
29	H	H	2	C_3H_7	oil	83	$1\cdot 10^{11}$	600	972	good
30	H	H	2	C_4H_9	oil	86	$5\cdot 10^{10}$	600	866	very good
31	H	H	2	C_5H_{11}	oil	85	$4\cdot 10^{9}$	600	844	sufficient
32	H	H	2	C_6H_{13}	oil	85	$3\cdot 10^{11}$	600	931	good
33	H	H	2	C_7H_{15}	hygroscopic	84	$1\cdot 10^{10}$	600	738	good
34	H	H	2	C_8H_{17}	hygroscopic	81	$1\cdot 10^{10}$	600	851	excellent
35	H	H	2	C_9H_{19}	hygroscopic	87	$9\cdot 10^{6}$	0	–	excellent
36	H	H	2	$C_{10}H_{21}$	63.5–66	84	$8\cdot 10^{6}$	0	–	excellent
37	H	H	2	$C_{11}H_{23}$	66.5–69	82	$5\cdot 10^{6}$	0	–	good
38	H	H	2	$C_{12}H_{25}$	69–71	84	$2\cdot 10^{10}$	0.15	9	good
39	H	H	2	$C_{14}H_{29}$	73–76	85	$9\cdot 10^{10}$	0.15	40	excellent
40	H	H	2	$C_{16}H_{33}$	83–85	84	$5\cdot 10^{8}$	0.2	18	excellent
41	H	H	2	$C_{18}H_{37}$	89–91	85	$2\cdot 10^{7}$	0.2	53	excellent
42	H	H	2	$C_{12}H_{23}$ (cyclic)	128–129	76	$2\cdot 10^{7}$	0.15	83	excellent
43	CH_3	H	1	C_3H_7	oil	83	$8\cdot 10^{7}$	0.3	332	sufficient
44	CH_3	H	1	C_4H_9	oil	86	$1\cdot 10^{11}$	600	798	sufficient
45	CH_3	H	1	C_5H_{11}	oil	85	$1\cdot 10^{11}$	600	698	sufficient
46	CH_3	H	1	C_6H_{13}	oil	84	$2\cdot 10^{11}$	600	605	good
47	CH_3	H	1	C_7H_{15}	oil	81	$6\cdot 10^{10}$	0.15	54	excellent
48	CH_3	H	1	C_8H_{17}	oil	87	$5\cdot 10^{7}$	0.15	14	good
49	CH_3	H	1	C_9H_{19}	oil	86	$7\cdot 10^{10}$	0.15	66	good
50	CH_3	H	1	$C_{10}H_{21}$	hygroscopic	87	$3\cdot 10^{10}$	0.2	35	excellent
51	CH_3	H	1	$C_{11}H_{23}$	hygroscopic	84	$3\cdot 10^{7}$	0.1	2	excellent
52	CH_3	H	1	$C_{12}H_{25}$	35–38	82	$2\cdot 10^{8}$	0.2	56	excellent
53	CH_3	H	1	$C_{14}H_{29}$	41–44	85	$1\cdot 10^{7}$	0.1	16	excellent
54	CH_3	H	1	$C_{16}H_{33}$	44–47	84	$2\cdot 10^{7}$	0.15	19	excellent
55	CH_3	H	1	$C_{18}H_{37}$	48–51	85	$2\cdot 10^{7}$	0.2	17	excellent
56	CH_3	H	1	$C_{12}H_{23}$ (cyclic)	128–129	78	$2\cdot 10^{7}$	0.3	68	lack
57	H	OCC_9H_{19}	1	C_3H_7	oil	85	$>10^{13}$	600	944	excellent
58	H	OCC_9H_{19}	1	C_4H_9	oil	81	$2\cdot 10^{7}$	0.15	52	excellent
59	H	OCC_9H_{19}	1	C_5H_{11}	oil	79	$3\cdot 10^{6}$	0	–	excellent
60	H	OCC_9H_{19}	1	C_6H_{13}	hygroscopic	85	$4\cdot 10^{6}$	0.1	19	excellent
61	H	OCC_9H_{19}	1	C_7H_{15}	50–54	88	$1\cdot 10^{7}$	0	–	excellent
62	H	OCC_9H_{19}	1	C_8H_{17}	57–60	83	$1\cdot 10^{7}$	0	–	excellent
63	H	OCC_9H_{19}	1	C_9H_{19}	62.5–64	86	$7\cdot 10^{6}$	0	–	excellent
64	H	OCC_9H_{19}	1	$C_{10}H_{21}$	65–67	87	$2\cdot 10^{7}$	0	–	excellent
65	H	OCC_9H_{19}	1	$C_{11}H_{23}$	67–69	85	$1\cdot 10^{7}$	0.15	56	excellent
66	H	OCC_9H_{19}	1	$C_{12}H_{25}$	75–76	87	$1\cdot 10^{7}$	0.15	38	excellent
67	H	OCC_9H_{19}	1	$C_{14}H_{29}$	70–72	88	$3\cdot 10^{7}$	0.2	686	excellent
68	H	OCC_9H_{19}	1	$C_{16}H_{33}$	72–73	84	$1\cdot 10^{8}$	0.2	232	excellent
69	H	OCC_9H_{19}	1	$C_{18}H_{37}$	81–83	86	$9\cdot 10^{8}$	0.3	689	very good
70	H	OCC_9H_{19}	1	$C_{12}H_{23}$ (cyclic)	110–112	85	$2\cdot 10^{9}$	0.2	413	excellent

The product of quaternization reaction was controlled by TLC on silicagel 60, where the mobile phase was 9:1 chloroform-methanol solution. The structure of new QACs was established by ^{1}H-NMR and ^{13}C-NMR and elemental analysis. The results of elemental analysis were in agreement with the theoretical values. Generally, the most important signals, characteristic for the chlorides, came from protons of N^+CH_2O, which in chlorides **1–14** and **29–56** were observed as a singlet at 4.8–5.0 ppm and in **15–28** and **57–70** as a singlet at 5.1–5.2 ppm. In the ^{13}C-NMR spectra, the chemical shift of the carbon of N^+CH_2O appeared at 90–91 ppm, however for cyclododecyl derivatives (**14**, **28**, **42**, **56**) the carbon appeared at 88–90 ppm. The synthesized QACs were proven to exhibit antielectrostatic properties. The antielectrostatic properties of the obtained chlorides, used in the experiments, result from two quantities: the surface resistance and the charge decay half time. The surface resistance R was calculated from the formula:

$$R = \frac{U \cdot l}{i \cdot s}[\Omega]$$

where U is the measured voltage, l the length of electrodes (l = 100 mm), i the electric current and s the distance between the electrodes (s = 10 mm). The obtained surface resistance values for 70 quaternary ammonium chlorides are presented in Fig. 1. The surface resistance for LDPE II 003/GO polyethylene film was $\log R = 13$. The charge decay half time was found from:

$$\tau = \sqrt{\frac{\tau_+^2 + \tau_-^2}{2}}[\mathrm{s}]$$

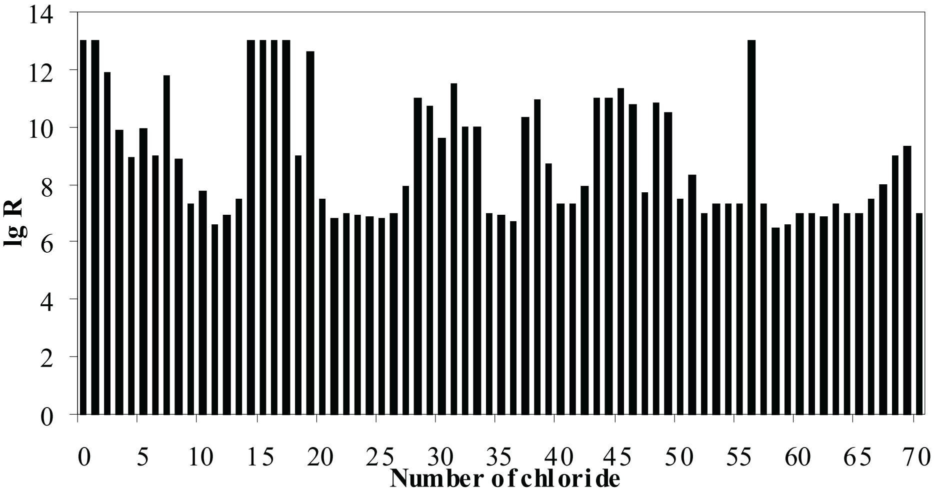


Figure 1. Values of logarithm of the surface resistance for the examined QACs and for LDPE II 003/GO polyethylene – 0.

where τ_+ and τ_- are the mean decay half times of positive and negative charges, respectively. The results obtained are shown in Fig. 2. The charge decay half time for LDPE II 003/GO polyethylene film was 600 s. The maximum voltage induced on the surface of the air-conditioning disks:

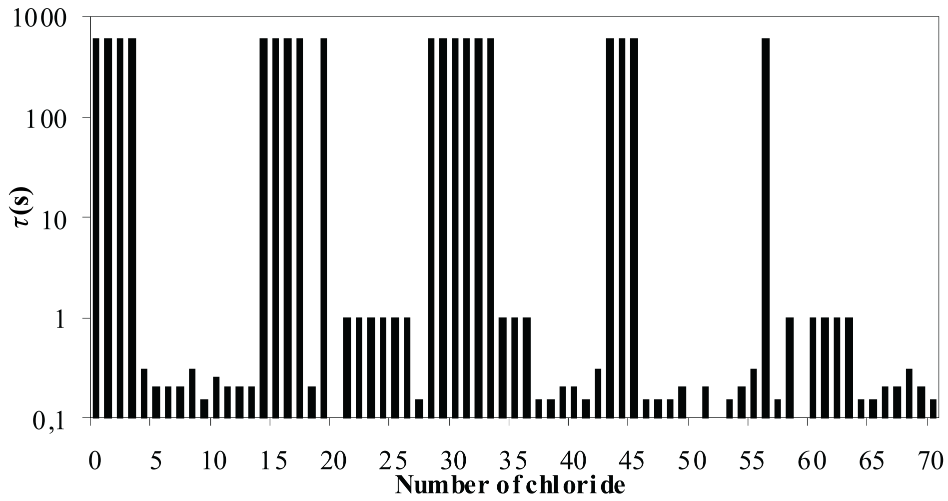


Figure 2. Values of half charge decay time for the examined QACs and for LDPE II 003/GO polyethylene – 0.

$$U = \sqrt{\frac{U_+^2 + U_-^2}{2}}\,[\mathrm{V}]$$

where U_+ and U_- are the voltages induced by positive and negative charges, respectively. Values of charge decay half time and surface resistance depended each other and were reciprocally linked by the following relation:

$$U_\tau = U_o \cdot \exp\left(\frac{-\tau}{R \cdot C}\right)[\mathrm{V}]$$

where U_τ is the measured voltage induced after time, U_o measured initial voltage induced, τ decay time, R surface resistance and C capacity. The antielectrostatic effect was determined following the criteria given by Bukała *et al.* [8], modified later [9] and listed in Table 2.

Table 2. Criteria for the estimation of the antielectrostatic effect based on the surface resistance, half decay time and decision attribute for rough set analysis.

Half charge decay time (s)	Surface resistance log R	Antielectrostatic effect	Decision attribute
< 0.5	< 9	excellent	1
1	9–9.99	very good	2
2–10	10–10.99	good	3
10–100	11–11.99	sufficient	4
> 100	12–12.99	insufficient	5
lack of antielectrostatic properties	≥ 13	lack of antielectrostatic properties	6

Generally, N-alkanol-N-alkoxymethyl-N,N-dimethylammonium chlorides and their ester derivatives have presented highly pronounced antielectrostatic activity. Naturally, there have been some departures. The effect has reflected the length of R^1 substituent and the kind of R^3 substituent. The chlorides with short alkoxy substituents for all series beside choline derivatives have shown a very slight or none antielectrostatic activity. In the case of N-alkoxymethyl-N-[2-(decanoyloxy)ethyl]-N,N-dimethylammonium chlorides, the presence of ester chain containing ten carbon atoms has compensated the short alkoxy substituents. Therefore, almost the entire series manifested excellent antielectrostatic properties.

The length of alkyl chain has proven to be the principal determinant of the intensity of antielectrostatic activity. The best properties have been revealed by compounds with 11 and 12 carbon atoms in alkyl groups, due to easy adsorption and chemical similarity of the polyethylene film. Hydroxyl group in position 2 has been capable to improve the activity, because it has absorbed water from atmosphere and has facilitated the charge outflow. The lowest activity has been manifested by compounds with cyclododecyloxy substituents (**14, 28, 56**), beside **70**, because this compound contained of the 10 carbon atoms chain. Presence of three oxygen atoms in QAC molecule has caused that compounds of high molecular weight and containing two long substituents (with total number of carbon atoms exceeding sometimes 31) exhibit an excellent antistatic effect. In this case, the hydrophilic portion of the molecule includes a quaternary nitrogen atom and its vicinity with oxygen atoms. The so pronounced increase in the hydrophilic portion promotes the adsorption of water vapour from the environment and, therefore, charge outflow.

In order to find a more comprehensive relationship and for comparison and confirmation of the “classical” analysis, we have performed of analysis results with the aid of the rough sets theory. This method, introduced by Pawlak [2], can be applied to structure activity relationships of antielectrostatic properties. In general, in this analysis we have created an information system as a representation of decision situation in the form of a decision table (Table 4). The information system contains information about particular cases (object, states, observations, events, compounds, *etc.*) in terms of their *attributes* (features, variables, characteristics, symptoms, *etc.*). A set of attributes is split into two groups:

- *Conditional attributes* which are the results of some tests or measurements, data from observations, anamnesis, symptoms of cases, states *etc*. In our case, this has involved types of compound fragments, for example alkyl group (attribute-columns of Table 3). The numbers of code have pointed to a specific fragment, *e.g.*, butyl (object-rows of Table 3). As an example, the structure of N-(2-hydroxyethyl)-N-dodecyloxymethyl-N,N-dimethylammonium chloride (**10**) can be described as 1,11,1,1,1,1 (see Table 3).
- *Decision attributes* which involve some expert's decisions, diagnoses, classified results of studies *etc.* Decision attributes divide all objects-compounds into decision classes (see Table 2).

Table 3. Condition attributes.

Code	1	2	3	4	5	6
	Kind of R^1	Kind of alkyl in R^1	Kind of cycloalkyl in R^1	Kind of R^2	Kind of R^3	n
1	alkyl	without	without	H	H	1
2	cycloalkyl	propyl	cyclododecyl	methyl	decanoyl	2
3		butyl			benzoyl	
4		pentyl				
5		hexyl				
6		heptyl				
7		octyl				
8		nonyl				
9		decyl				
10		undecyl				
11		dodecyl				
12		tetradecyl				
13		hexadecyl				
14		octadecyl				

The information system is fed to a computer and the data are processed using ROSE [10] or ROSSETA [11] software. In the first step, insignificant condition attributes are eliminated without losing quality of classification, which are equal 1. The rest of the condition attributes create the *core*. In our case the *core* is formed by 2, 4, 5 and 6 condition attributes. However, the subset of the attributes can be reduced, even more with insignificant decline of the quality of classification. After removing attributes 1, 3 and 4, the classification still has shown high quality and has equalled 0.829. Further reduction of the attributes or replacing attribute 4 by other one has caused a rapid decline in the quality of classification (Fig. 3).

Table 4. Information system of studied QACs (**1-70**).

Chloride number	Condition attributes						Decision attribute
	1	2	3	4	5	6	
1	1	2	1	1	1	1	6
2	1	3	1	1	1	1	4
3	1	4	1	1	1	1	2
4	1	5	1	1	1	1	1
5	1	6	1	1	1	1	2
6	1	7	1	1	1	1	2
7	1	8	1	1	1	1	4
8	1	9	1	1	1	1	1
9	1	10	1	1	1	1	1
10	1	11	1	1	1	1	1
11	1	12	1	1	1	1	1
12	1	13	1	1	1	1	1
13	1	14	1	1	1	1	1
14	2	1	2	1	1	1	6
15	1	2	1	1	3	1	6
16	1	3	1	1	3	1	6
17	1	4	1	1	3	1	6
18	1	5	1	1	3	1	2
19	1	6	1	1	3	1	5
20	1	7	1	1	3	1	1
21	1	8	1	1	3	1	1
22	1	9	1	1	3	1	1
23	1	10	1	1	3	1	1
24	1	11	1	1	3	1	1
25	1	12	1	1	3	1	1
26	1	13	1	1	3	1	1
27	1	14	1	1	3	1	1
28	2	1	2	1	3	1	4
29	1	2	1	1	1	2	2
30	1	3	1	1	1	2	2
31	1	4	1	1	1	2	4
32	1	5	1	1	1	2	3
33	1	6	1	1	1	2	3
34	1	7	1	1	1	2	1
35	1	8	1	1	1	2	1
36	1	9	1	1	1	2	1
37	1	10	1	1	1	2	3
38	1	11	1	1	1	2	3
39	1	12	1	1	1	2	1
40	1	13	1	1	1	2	1
41	1	14	1	1	1	2	1
42	2	1	2	1	1	2	1
43	1	2	1	2	1	1	4
44	1	3	1	2	1	1	4
45	1	4	1	2	1	1	4
46	1	5	1	2	1	1	3
47	1	6	1	2	1	1	1
48	1	7	1	2	1	1	3
49	1	8	1	2	1	1	3
50	1	9	1	2	1	1	1
51	1	10	1	2	1	1	1
52	1	11	1	2	1	1	1
53	1	12	1	2	1	1	1
54	1	13	1	2	1	1	1
55	1	14	1	2	1	1	1
56	2	1	2	2	1	1	6
57	1	2	1	1	2	1	1
58	1	3	1	1	2	1	1
59	1	4	1	1	2	1	1
60	1	5	1	1	2	1	1
61	1	6	1	1	2	1	1
62	1	7	1	1	2	1	1
63	1	8	1	1	2	1	1
64	1	9	1	1	2	1	1
65	1	10	1	1	2	1	1
66	1	11	1	1	2	1	1
67	1	12	1	1	2	1	1
68	1	13	1	1	2	1	1
69	1	14	1	1	2	1	2
70	2	1	2	1	2	1	1

As demonstrated in Fig. 3, removal of attribute 2 dramatically reduces the quality to 0.071. This fact has assured us that the kind of alkyl in R^1 is crucial to the analysis and to antielectrostatic properties. Therefore, for high quality of classification the most important and essential attributes are: attribute 2 – length of alkyl chain in

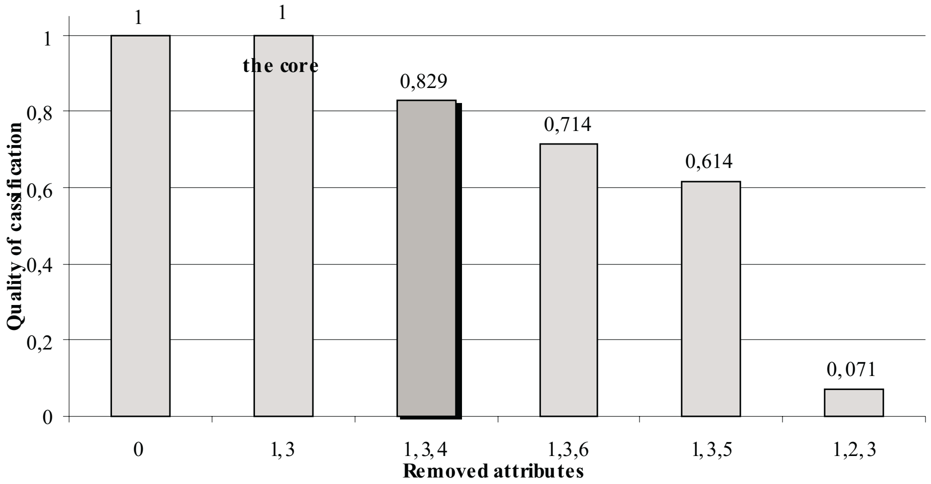


Figure 3. Reduction of condition attributes and quality of classification.

alkoxy substituents of QACs; 5 – kind of *O*-substituents in alcohol chain of QACs; attribute 6 – quantity of CH_2 groups in alcohol chain.

In the second step, *minimal set covering algorithm* (LEM2) [12], which is included in the ROSE software packet, creates *decision rules*. The decision rules portray the relationship between structures of QACs and antielectrostatic properties of QACs. Table 5 presents the decision rules obtained from the information system (Table 4) upon removal of insignificant condition rules (1, 3, 4). During the analysis, 42 decision rules have been obtained, but the most significant, strongest and backed by at least two objects (strength column in Table 5) are 8 decision rules. Deterministic (strong) ones are those, which indicate the best and worst compounds and are backed by a large number of objects. The obtained decision rules shows that the strategy for synthesis of the most active compounds (class 1) should include attachment of alkoxy substituents with 10–16 carbon atoms in alkyl chain, independently of the kind of amine: alcoholamine or esteramine. In addition to 11 and 12 carbon atom chain, the compounds should have oxy group in position 2 in alcohol original chain. The best compounds have included also alcohols with 18 carbon atoms in the chain. The worst compounds (class 6) have included chlorides, which are obtained from alcoholamine and chloromethyl cyclododecyl ether. All the data obtained from the rough set analysis have confirmed prior “classical” observation and analysis.

Table 5. Strong decision rules for significant condition attributes.

No. of rule	Condition attributes			Class	Strength
	2	5	6		
1	9			1	5
2	10		1	1	4
3	11		1	1	4
4	12			1	5
5	13			1	5
…	…	…	…	…	…
11	14	1		1	3
…	…	…	…	…	…
29	3	1	1	4	2
…	…	…	…	…	…
34	1	1	1	6	2

CONCLUSIONS

A study of the antielectrostatic properties of N-alkanol-N-alkoxymethyl-N,N-dimethylammonium chlorides and their ester derivatives has indicated, that the type of substitutent and the length of carbon chains have been reflected by various properties of the compounds.

1. In order to exhibit satisfactory antielectrostatic properties, the compound should contain 6 or more carbon atoms in the chain to adsorb on surface of the polymer. The origin of the substituents: ester alkyl part or alkoxy part has been irrelevant.
2. The optimum of activity has been revealed by the compounds with 11 and 12 carbon atoms in chain substituents.
3. The rough set theory is useful for SAR analysis and has confirmed the observed relations. In particular, multiobject sets can be analyzed by applying the theory to accelerate analysis of data and to detect vague relationships between structure and activity.

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