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The Effect of Hydrophile and Hydrophobe Part on Surface Activity of Ester Quaternary Ammonium Compounds

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Research Article

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ABSTRACT

This study deals with the synthesis of six cationic surfactants forming two groups. Using alkyl diols, bromoacetic acid, triethyl amine and triethanol amine, these surfactants were synthesized. From the analysis, it was found that the surfactants prepared are ester quaternaries. Du Nouy tensiometer has been used for obtaining the surface activity of surfactants. In terms of their hydrophilic and hydrophobic part, different surface parameters were discussed. All showed the biological features such as antimicrobial activity.

INTRODUCTION

Ester of quaternary ammonium amphiphiles are environmentally friendly surfactants of elevated biodegradability, low toxicity and outstanding active surface characteristics. These compounds also demonstrate antitumor therapy

Measurment of surface parameters

Surface tension, efficiency (PC20), surface pressure (effectiveness π_{cmc}) and Critical Micelle Concentration (CMC) were determined for two prepared groups from 1×10^{-2} to 5×10^{-8} mol/L at 25°C with Du Nouy tensiometer (Kruss K12) with a platinum ring [5-8].

RESULTS

Characterization data of ester quaternary ammonium surfactants

Compounds 2_{a-c} were confirmed before as in previous paper. The structure of the synthesized surfactants and purity were confirmed by different methods (IR, 1 H NMR, 13 C NMR and mass) (Figures 2-17) [9].

Figure 2. FTIR spectrum of compound (3a).

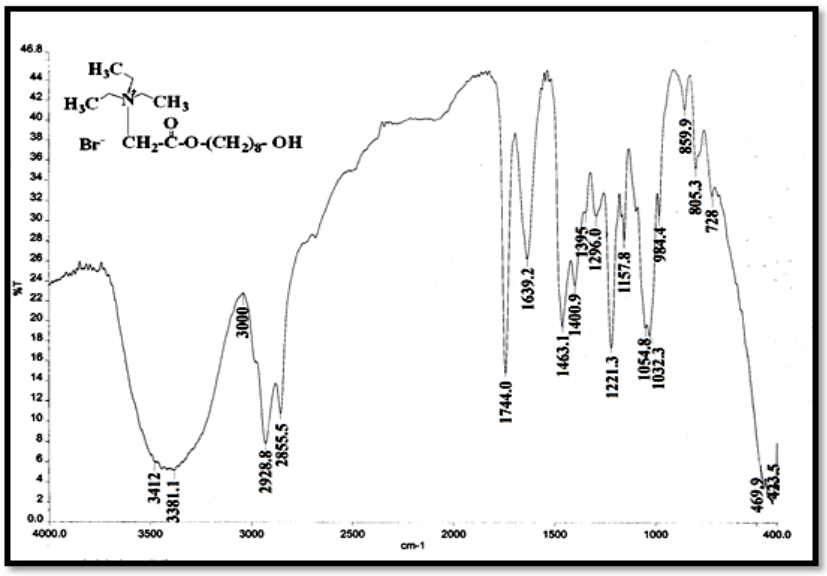

Figure 3. 1H NMR spectrum of compound (3a).

Figure 6. FTIR spectrum of compound (3b).

Figure 7. 1H NMR spectrum of compound (3b).

Figure 8. 13C NMR spectrum of compound (3b).

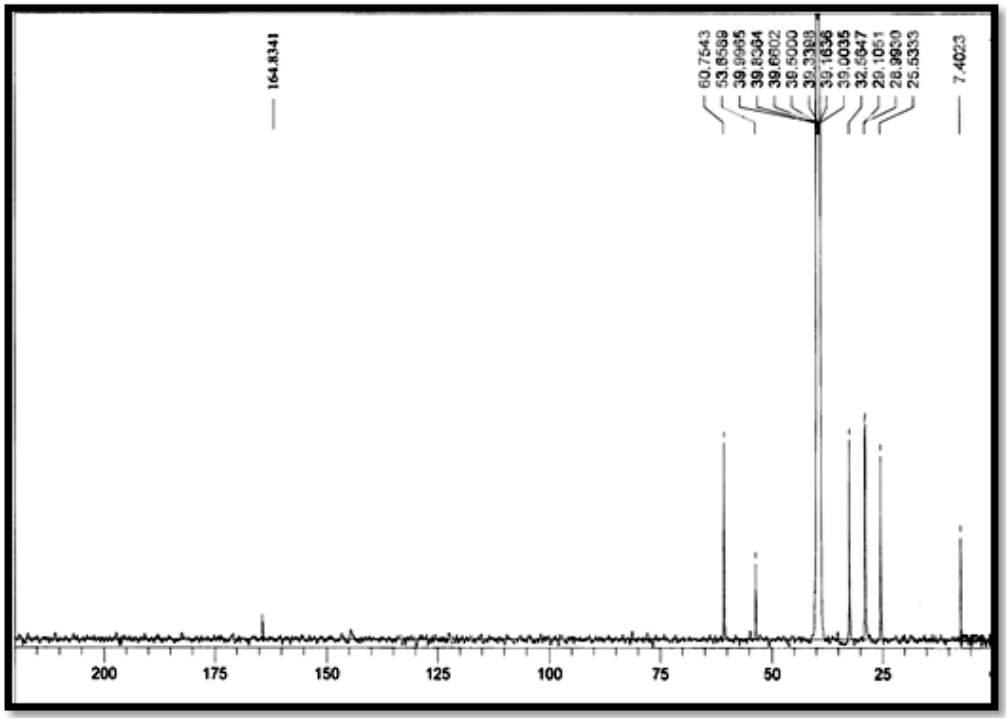

Figure 9. Mass spectrum of compound (3b).

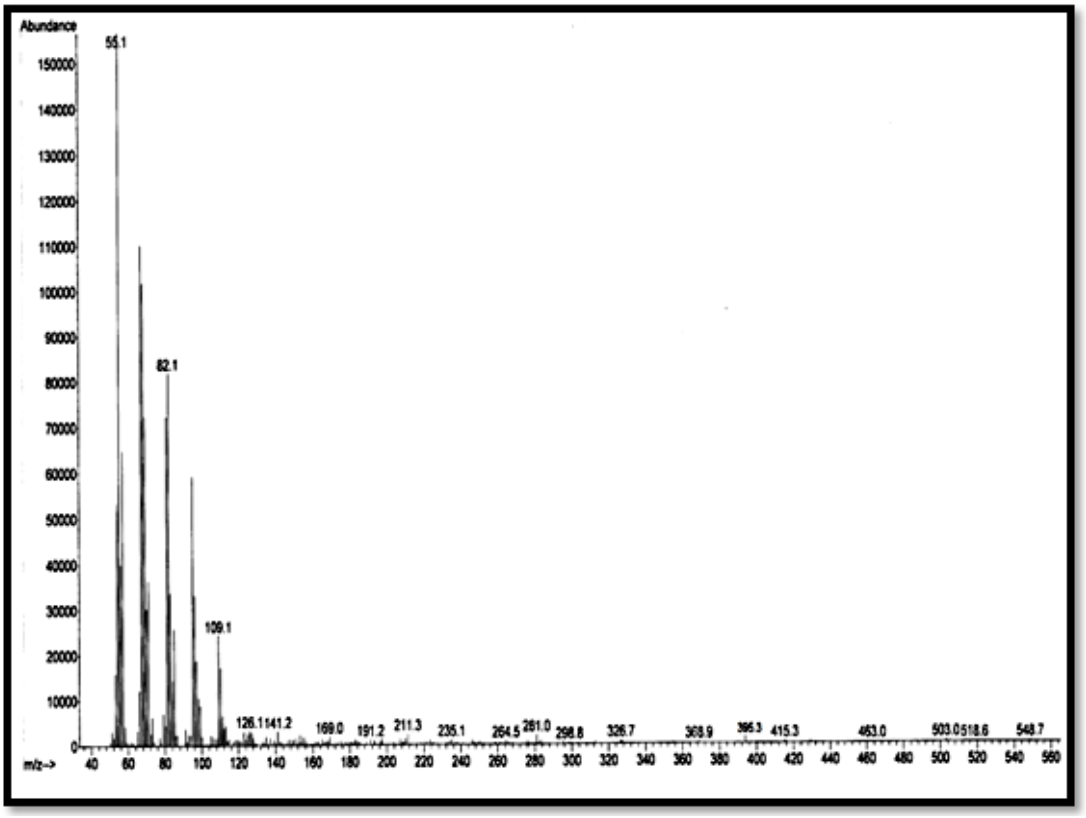

Figure 12. 13C NMR spectrum of compound (3c).

Figure 13. Mass spectrum of compound (3c).

Surface properties of cationic surfactants and thermodynamic parameters

The Critical Micelle Concentration (CMC) is a fundamental characteristic of each dissolved surfactant in the solvent. CMC can be determined by drawing a relationship between one of the properties of the surface activity material (the surface tension of the compounds under study) and the concentration of these compounds [10-14]. The relationship is linear until we reach the critical degree of concentration at which the refraction occurs in the curve as shown in Figures 18 and 19.

Figure 18. Variation in surface tension of surfactants $3_{a\text{-}c}$ *versus* concentration at 25°C. **Note:** ■3_a ●3_b ▲ 3_c.

Figure 19. Variation in surface tension of surfactants $4_{a\text{-}c}$ *versus* concentration at 25°C. **Note:** ■4_a ●4_b ▲4_c.

With rising concentration of surfactant, the surface tension reduces and then reaches a definite break point that is taken as the CMC.

One of the most important factors affecting CMC values in aqueous solutions is the structure of surface active substances, which include hydrophobic groups and hydrophilic groups [15].

Effect of the hydrophobic groups

The results of Tables 1 and 2 indicate that the number of methylene groups in the hydrophobic fraction is the variable affecting the CMC value. For the all prepared compounds, the CMC values decrease by raising the length of the hydrocarbon part is due to the increased hydrophobic properties of the molecules which are the driving force of the molecules to escape from the solution to the surface (Tables 1 to 6).

Table 1. Characterization data of compounds 3_{a-c}.

Compound code	Compound name	Mol. formula mol .weight	M.P (˚C) color	Yield (%) crystallization solvent	Elemental analysis (%) calc\found			
					C %	H %	N %	Br %
3_a	Triethyl (8-hydroxy-octyl oxy carbonyl methyl) ammonium bromide	$C_{16}H_{34}O_3NBr$	-	0.7517	52.12	9.22	3.8	21.68
		368.38	Yellow	Benzene	52.38	9.49	4.11	22.01
3_b	Triethyl (10-hydroxy-decyl oxy carbonyl methyl) ammonium bromide	$C_{18}H_{38}O_3NBr$	130	0.8512	54.54	9.66	3.53	20.16
		396.4	Paige	Benzene	54.92	9.87	3.79	20.42
3_c	Triethyl (12-hydroxy-dodecyl oxy carbonyl methyl) ammonium bromide	$C_{20}H_{42}O_3NBr$	-	0.8846	56.59	9.97	3.3	18.83
		424.46	White	Ethanol	56.88	10.33	3.68	19.17

Table 2. Characterization data of compounds 4_{a-c}.

Compound code	Compound name	Mol. formula Mol .weight	M.P (˚C) color	Yield (%) crystallization solvent	Elemental analysis (%) calc\found			
					C %	H %	N %	Br %
4_a	(8-hydroxy-octyl oxy carbonyl methyl)-tris-(2-hydroxyethyl)-ammonium bromide	$C_{16}H_{34}O_6NBr$	129	0.8311	46.16	8.23	3.36	19.19
		416.35	White	Ethanol	46.48	8.58	3.72	19.55
4_b	(10-hydroxy-decyl oxy carbonyl methyl)-tris -(2-hydroxyethyl)-ammonium bromide	$C_{18}H_{38}O_6NBr$	135	0.5788	48.64	8.55	3.15	17.97
		444.4	White	Ethanol	48.87	8.76	3.44	18.28
4_c	(12-hydroxy-dodecyl oxy carbonyl methyl)-tris-(2-hydroxyethyl)-ammonium bromide	$C_{20}H_{42}O_6NBr$	147	0.9854	50.84	8.96	2.96	16.91
		472.407	White	Ethanol	51.09	9.32	3.22	17.29

Tables 2 and 3 shows that the efficiency values of the prepared amphiphiles show its ability to behave as efficient interfaces for multiple applications requiring low surface tension.

Maximum surface excess (τ_{max}), Minimum surface area (A_{min})

The amount of adsorbed surfactant (τ) at the air-water interface can be evaluated by the Gibbs adsorption isotherm. The values of the average area occupied by surfactant molecules at the aqueous-air interface were calculated using τmax as explained in:

The increase in the values of τmax means an increase in surface concentration, increasing the number of particles of active substances adsorbed on the surface, so congestion occurs and reduces the A_{min} available space for each molecule on the surface (Tables 2 and 3).

Hence, it is concluded that rising the length of hydrophobe chain of the molecule increases the concentration of surface and reduces the available surface area of the molecule.

Micellization Standard Free Energy Change ΔG°_{mic} and Adsorption ΔG°_{ads}

Standard free energy for adsorption ΔG°_{ads} and standard free energy for ΔG°_{mic} were calculated using Rosen's methodology

$\Delta G^\circ_{mic} = -RT \ln CMC$

$\Delta G^\circ_{ads} = \Delta G^\circ_{mic} - 6.023 \times 10^{-1} \pi_{cmc} - A_{min}$

ΔG°_{mic} expresses the driving force or the tendency of the methylene group of surface active substances to move from the surrounding water into the micelle. The negative value of both ΔG°_{ads} and ΔG°_{mic} mean that both the procedures of adsorption and micellization took place spontaneously.

Note that the high negative values of ΔG°_{ads} for the surface-active compounds prepared and their high agglomeration on the surface as derived from the values of Amin, hence we can say that these compounds have a high surface activity and therefore can be applied in many fields such as emulsions, corrosion inhibitors and antibacterial.

DISCUSSION

Biological survey of prepared ester quaternary ammonium compounds was detected at 25°C using well diffusion test method against gram-positive bacteria, some fungi and yeasts, as explained in Table 7.

Table 7. Microbial activity against pathogenic microorganism.

		Inhibition zone (mm/mg)					
Comp. code.	**Concentration (ppm)**	***Escherichia coli.***	***Pseudomonas spp.***	***Staphylococcus aureus***	***Bacillus subtilis***	***Candida albicans***	
3_a	100000	0	0	0	11	0	
3_b	30000	13	14	19	21	20	

3_c	30000	11	12	0	14	0
4_a	100000	0	0	0	11	0
4_b	100000	18	0	21	17	19
4_c	100000	12	12	0	11	11
CTAB	100000	32	25	23	26	26

Cetyl Trimethyl Ammonium Bromide (CTAB) has been used as a reference compound to compare its effect on pathogenic microorganisms with the effect of prepared compounds. The compounds in question were dissolved in distilled water. The high biological activity of these cationic compounds can be explained by the electrostatic attraction forces between the positive charges (N^+) of quaternary ammonium compounds and the negative charges of phospholipids forming the cell wall. The resemblance between the hydrocarbon chains of the prepared compounds, the lipid layers and the cell membrane building blocks make adsorption easier and thus disrupts the selective permeability of the outer wall of the cell hence the biological activity of microorganisms leading to their death. We can also say that the large inhibitory diameter is due to the large volume of micelle at low concentrations, which makes it suitable for interaction with the cell membrane [21,22].

Recent studies have tended to use quaternary ammonium compounds in the field of biocides to prevent the reproduction of bacteria that cause significant damage to the petroleum sector as these quats have proven effective as inhibitors of the activity of Sulfate Reducing Bacteria (SRB) (Table 8), whose growth causes corrosion in petroleum pipelines 21. Sulfide is corrosive and toxic and causes reservoir blocking [23].

Table 8. Most probable number for SRB treated with different concentrations (10 ppm, 30 ppm, 60 ppm, 90 ppm and 120 ppm) of prepared ester quaternary ammonium compounds and CTAB as pure reference compound.

Concentration (ppm)	10	30	60	90	120
SRB (control) no biocide	10^5 (100000 cell/ml)	10^5	10^5	10^5	10^5
CTAB	$\geq 10^5$	10^4	10^2	10^1	0
3_a	$\geq 10^5$	$\geq 10^5$	$\geq 10^5$	$\geq 10^5$	$\geq 10^5$
3_b	$\geq 10^5$	10^4	10^2	10	0
3_c	$\geq 10^5$	10^4	10^2	10	0
4_a	$\geq 10^5$	$\geq 10^5$	$\geq 10^5$	$\geq 10^5$	$\geq 10^5$
4_b	$\geq 10^5$	10^4	10^2	10	0
4_c	$\geq 10^5$	10^4	10^2	10	0

Hence, we can say that increasing concentration in the biocide increases the activity of the compound towards SRB, all prepared compounds show good activity compared with reference compound.