Characterisation of Sodium Soaps and their Refractive Index Studies in Methanol

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Sodium soaps (abietate, oleate and myristate) have been prepared and their characteristics in solid state have been studied by I.R. methods to obtain structural information. The critical micelle concentration (C.M.C.) has been determined by refractive index and the values of molar refraction of soap, $[R]_2$, have been calculated.

INTRODUCTION

It is observed that sodium soaps of C(12–18) fatty acids are used in low foaming laundry detergent composition[1], in aqueous liquid detergent composition for washing fabrics[2], as hand cleaners[3], in paste for protecting and cleaning the skin[4], for preparation of flowable lubricating grease for switches which is effective at 8 to 15°C temperature[5], for high speed wire drawing[6], and as a low temperature grease for winter[7]. These soaps of synthetic fatty acids are used as sealing lubricants for threaded joints[8], and also used for casing boards or metal moulds of concrete gypsum mortar to protect their surface[9], and as aqueous rust inhibitors[10]. Due to their wide applications an attempt has been made to prepare sodium soaps (abietate, oleate, myristate) and characterize by infrared spectroscopy. Refractive indices of these soaps in methanol have been studied in order to study their micellar behaviour.

EXPERIMENTAL

The chemicals were purified and the soap prepared by the method described earlier[11]. Distilled methanol (b.p. 65°C) and freshly prepared conductivity water were used.

The soaps were analysed by IR spectra recorded in KBr pellets on a Perkin-Elmer spectrophotometer. Refractive indices were measured by an Abbe type refractometer for the D-line of sodium. The densities were determined by dilatometer.

RESULTS AND DISCUSSION

The characteristic infrared absorption frequencies of soaps (sodium abietate, oleate and myristate) are recorded in Table-1. Oleic and myristic acids display a very broad and intensive peak due to —OH stretching near 2660–2650 cm^{-1}. The

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appearance of absorption band near 1700–1680 cm^{-1}in the spectra of fatty acids indicates that the fatty acids exists as dimer[12]. One of the characteristic bands of dimeric acids results from out-of-plane bonding of the —OH group appearing near 950–930 cm^{-1}. In the spectra of abietic and oleic acids peak at 1690–1600 cm^{-1} demonstrates unsaturation.

TABLE-1

CHARACTERISTIC ABSORPTION FREQUENCIES (cm^{-1}) OF SODIUM SOAPS

Assignments	Abietate	Oleate	Myristate
CH_2, C—H antisymmetrical stretching	2930 s	2922 s	2922 s
CH_2, C—H symmetrical stretching	–	2853 ms	2849 ms
C=C stretching	1637 w	1690 w	–
COO—, C—O anti-symmetrical stretching	1554 vs	1562 vs	1560 vs
CH_2-deformation	1464 s	1446 s	1446 s
COO^-, C—O symmetrical stretching	1364 s	1400 s	1400 s
C—O stretching, O—H in-plane deformation	1460 m	–	1400 s
CH_2 (adjacent to COOH group deformation)	1396 s	1400 s	1400 s
CH_3 symmetrical deformation	1356 vs	–	–
Progressive bonds (CH_2 twisting and wagging)	1197–1155 b	–	–
CH_3 rocking	1022 w	–	1080 w
CH_2 rocking	1022 w	721 vw	723 vw
Na—O bond	534 m	540 m	540 m

The disappearance of —OH band (Table-1) in the region of 3550–3030 cm^{-1} and lower frequency of carboxylate just below 1562–1554 cm^{-1} instead of 1700 cm^{-1} indicates the formation of soap. It is further confirmed by the presence of one asymmetric stretching band near 1560–1550 cm^{-1} and weaker symmetrical band near 1400–1364 cm^{-1} for the carboxylate anion. There is no peak between 3590–3500 cm^{-1} due to the absence of water of crystallisation. It is observed that ν_{asym} (COO—) and ν_{sym} (COO—) frequencies are not shifted much in oleate and myristate; therefore the Na—O bond strength can be presumed to be approximately same but in abietate the value is much higher which shows the different bond strength.

Refractive index: Refractive index, n, increase with increase in concentration of soaps. The critical micelle concentration C.M.C. *i.e.* 0.004 M for abietate and 0.006 M for oleate and myristate have been determined from n-C plots. The refractive index data have been analysed using the Lorentz-Lorenz equation

$$[R] = \frac{n^2 - 1}{n^2 + 2} \times \frac{X_1M_1 + X_2M_2}{d}$$

where n and d are respectively the refractive index and the density of solution, X_1 is the mole fraction of solvent of molecular weight M_1 and X_2 is the mole fraction of the solute of molecular weight M_2.

The molar refraction of solution [R] is also expressed by the equation

$$R = X_1[R]_1 + X_2[R]_2$$

where $[R]_1$ and $[R]_2$ are molar refraction of the solvent and solute respectively.

The values of $[R]_2$ (Table-2) vary too much with the soap concentration below CMC due to existence of molecularly dispersed soaps. These values do not vary appreciably with concentration above C.M.C. *i.e.*, 109.8–119.0, 120.5–125.4 and 80–84 respectively for abietate, oleate and myristate.

TABLE-2
REFRACTIVE INDICES OF SODIUM SOAPS IN METHANOL AT 308 K

Concentration (mole dm^{-3})	Refractive index N	Molar refraction of the soap solution [R]	Molar refraction of the soap $[R]_2$
		ABIETATE	
0.000	1.3318	8.4402	–
0.001	1.3320	8.4426	65.96
0.002	1.3322	8.4461	79.12
0.003	1.3324	8.4497	85.26
0.004	1.3326	8.5539	91.62
0.006	1.3330	8.8652	109.82
0.008	1.3332	8.4749	113.80
0.010	1.3335	8.4861	119.94
		OLEATE	
0.001	1.3319	8.4429	73.08
0.002	1.3321	8.4485	109.03
0.003	1.3322	8.4518	102.31
0.004	1.3324	8.4579	115.60
0.006	1.3327	8.4682	121.74
0.008	1.3330	8.4771	120.53
0.010	1.3334	8.4884	125.40
		MYRISTATE	
0.001	1.3319	8.4420	50.93
0.002	1.3320	8.4443	57.51
0.003	1.3321	8.4464	57.95
0.004	1.3322	8.4487	60.14
0.006	1.3324	8.4542	64.14
0.008	1.3327	8.4634	79.99
0.010	1.3329	8.4715	84.44

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