

PHYSICOCHEMICAL STUDIES ON SCANDIUM SOAPS IN SOLID STATE

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RECEIVED : 18 January, 2017

The physicochemical studies were used to determine the structure of scandium soaps (palmitate and stearate) in solid state by the IR absorption spectra. The IR results reveal that the fatty acids exist in dimeric structure through intermolecular hydrogen bonding and scandium soaps (palmitate and stearate) were ionic in nature.

KEYWORDS: Metal soaps, IR, Scandium.

INTRODUCTION

The transition metal soaps are being widely used in industry, technology and allied sciences. The uses of metal soaps largely depend on their physical state, stability, chemical reactivity and solubility in polar and non polar solvents. These metal soaps has been a subject intense investigation in the recent past on account of its role in such diversified field as medicine, cosmetic emulsifier, lubricant, germicides and anti oxidant. The methods of preparation of potassium soaps and metal soaps were described by several workers [1-6]. The infrared absorption spectra, x-ray diffraction studies and thermal behavior of cerium and thorium laurate were studied by Gupta *et al.* [7]. The thermal decomposition kinetics of nickel and manganese soaps were studied by Mehrotra *et al.* [8]. The thermogravimetric analysis of yttrium soaps in solid state was studied by Khirwar [9]. The physicochemical studies on erbium soaps of saturated higher fatty acids in solid state studied by Rajesh *et al.* [10]. The viscometric and spectral studies of copper soap in benzene and methanol mixture were studied by Rawat [11]. The studies on miceller properties of scandium and yttrium metal soaps was studied by Khirwar [12]. The studies of ultrasonic velocity and allied properties of magnese, cobalt and copper soaps in non aqueous medium Rawat [13]. In the present work attempts have been made to determine the structure of scandium soaps (palmitate and stearate) in solid state through the infrared absorption spectra studies.

EXPERIMENTAL

The scandium soaps (palmitate and stearate) were synthesized by direct metathesis of corresponding potassium soaps with the required amount of aqueous solution of scandium nitrate at 50-55°C under vigorous stirring. The precipitated soaps were washed several times with distilled water and then acetone to remove the fatty acid and metal nitrate. The soaps were purified by recrystallization with the benzene and DMSO mixture, dried in an air oven at 50-60°C and the finally drying of the soaps were carried out under reduced pressure.

The IR absorption spectra of palmitic acid and stearic acid and their corresponding potassium, and scandium soaps (palmitate and stearate) were recorded with Perkin Elmer: 577

model grating spectrophotometer in the region of $4000\text{-}400\text{ cm}^{-1}$ using potassium bromide disc method.

RESULT AND DISCUSSION

The IR spectra of scandium soaps (palmitate and stearate) with their assignments are recorded (Fig. 1-2) compared with the results of corresponding fatty acid and potassium soap (Table 1). The absorption maxima characteristic of the aliphatic portion of the acid molecule remain unchanged on the formation of corresponding potassium and scandium soaps. The symmetrical vibration of CH_2 at $2840\text{-}2850\text{ cm}^{-1}$, the asymmetrical stretching vibration of CH_2 at $2910\text{-}2930\text{ cm}^{-1}$, the asymmetrical stretching vibration of CH_3 at $2960\text{-}2970\text{ cm}^{-1}$ and the deformation of CH_3 at $1310\text{-}1380\text{ cm}^{-1}$ are observed in spectra of potassium, scandium and as well as in corresponding fatty acid.

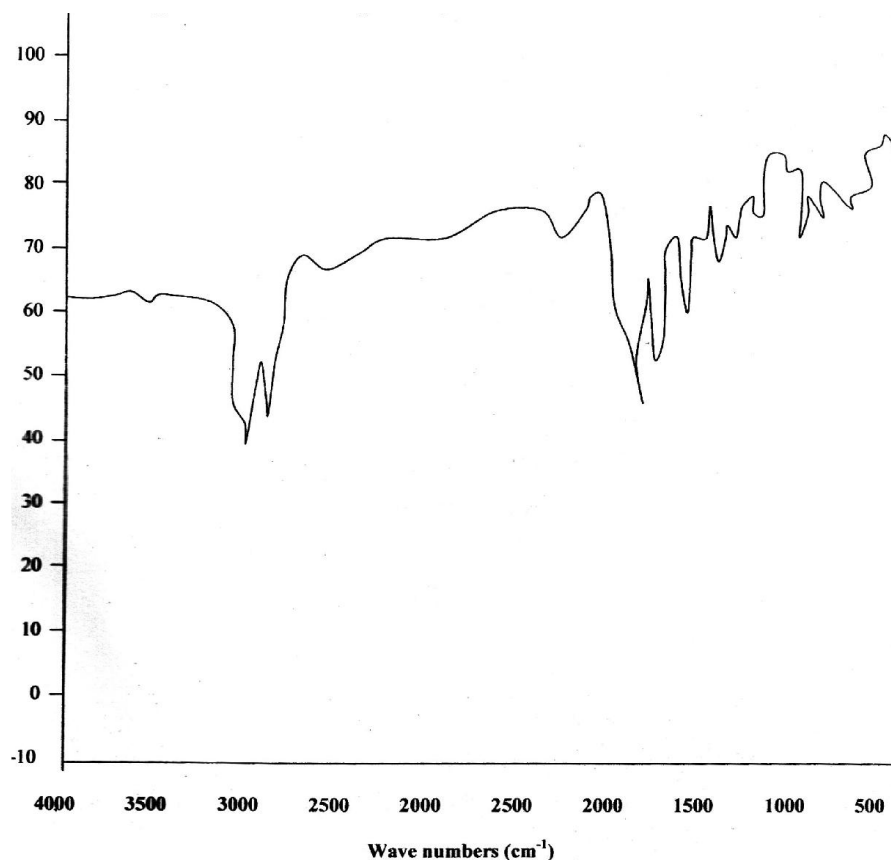


Fig. 1. Infrared Absorption Spectra of scandium Palmitate

The absorption bands observed near $2630\text{-}2640$, $1680\text{-}1690$, $1400\text{-}1450$, $920\text{-}930$, $670\text{-}680$, 540 cm^{-1} in spectra of fatty acids have identified the presence of localized COOH group in the form of dimeric structure and the existence of intermolecular hydrogen bonding between two molecules of the acid.

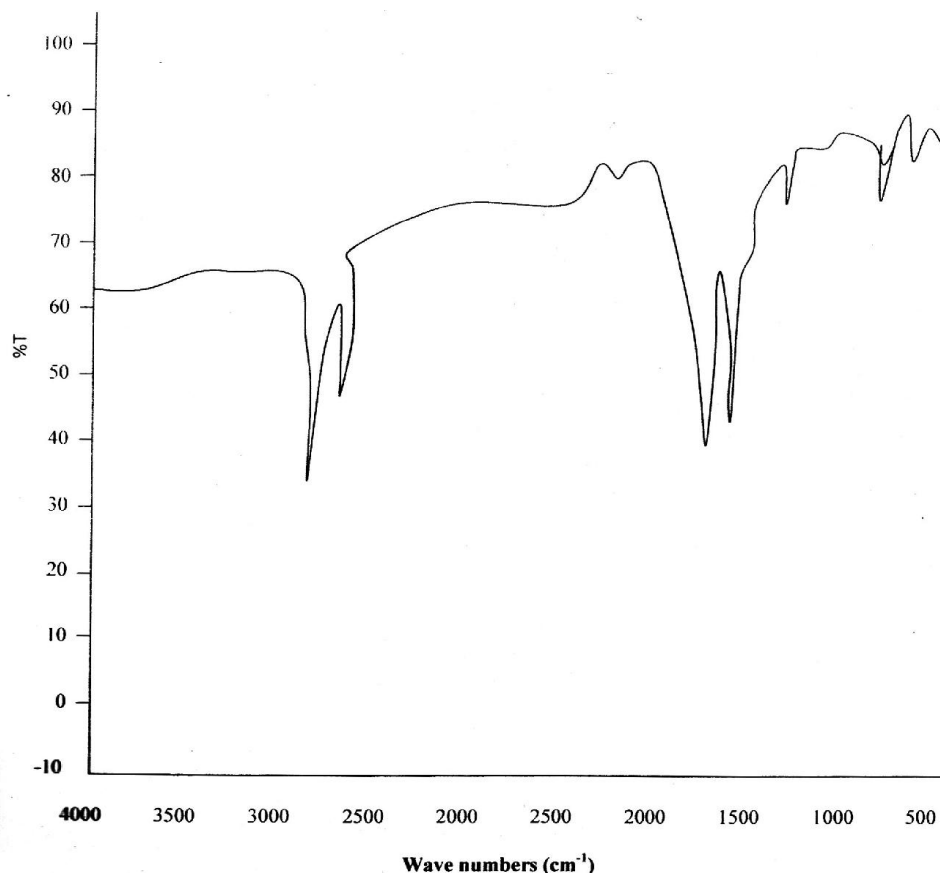


Fig. 2. Infrared Absorption Spectra of scandium Stearate

The absorption bands observed near 2630-2640, 1680-1690 and 920-930 cm^{-1} corresponding to the $-\text{OH}$ group in the spectra of fatty acids have disappeared in the spectra of corresponding potassium and scandium soaps. The absorption maxima corresponding to 670-680 and 540 cm^{-1} in the spectra of fatty acids have been assigned to the bending and wagging modes of the vibrations of the carbonyl group of the acid molecules, respectively.

The IR spectra of potassium soaps and scandium soaps show marked difference with the spectra of corresponding fatty acids in some spectral regions. The characteristic vibrations of free acids were found completely absent in the spectra of corresponding potassium and scandium soaps. The complete disappearance of the carbonyl frequency in the region of 1680-1690 cm^{-1} and appearance of two absorption bands of carboxyl group corresponding to the symmetrical and asymmetrical vibrations carboxylate ion near 1460-1470 cm^{-1} and 1540-1550 cm^{-1} respectively in the spectra of scandium soaps indicate that there is a complete resonance in the $\text{C}-\text{O}$ bonds of carboxyl groups of the soap molecules and the two bonds become identical with their force constants assuming an intermediate value between those of normal double and single bonds.

It is therefore, concluded that the resonance character of the ionized carboxyl group is retained in scandium soaps. The fatty acids exist with dimeric structure through intermolecular hydrogen bonding between carboxyl groups of two acid molecules whereas metal-to-oxygen bonds in scandium soaps are ionic in nature.

The IR spectra of scandium soaps (palmitate and stearate) do not show any absorption maxima in the region of 3500-3000 cm^{-1} which confirms that the absence of any co-ordinated water molecule in these soaps.

Table 1. Frequencies (cm^{-1}) of Absorption maxima with their Assignments of Acids and their Soaps.

Sr. No.	Assignments	Palmitic acid	Potassium Palmitate	scandium Palmitate	Stearic acid	Potassium Stearate	scandium Stearate
1.	CH ₃ , C-H Asym. Stretch.	2960VS	2950W	2970MS	2960S	2960MS	2970W
2.	CH ₂ , C-H Asym. Stretch.	2900S	2920S	2930S	2900VS	2910VS	2920VS
3.	CH ₂ , C-H Sym. Stretch.	2840S	2850S	2850S	2840S	2840S	2850VS
4.	O-H, Stretch.	2640W	-	-	2640W	-	-
5.	C = O, Stretch.	1690VS	-	-	1690VS	-	-
6.	COO, C-O Asym. Stretch.	-	1560VS	1550S	-	1550VS	1550VS
7.	COO, C-O Sym. Stretch.	-	1420MS	1460S	-	1420M	1460VS
8.	C-O Strech. + O-H in plane deformation	1450W	-	-	1422VS	-	-
9.	CH ₂ (adjacent to COOH group) deformation	1400W	1360W	-	1402M	-	-
10.	CH ₃ , Sym. deformation	1345W	1380W	1320S	1340W	1370MS	1330M
11.	Progressive bands (CH ₂ , twisting and wagging)	1340 - 1090W	1190 M	1290 - 1180B	1340 - 1090M	1315- 1180M	1250 - 1290M
12.	CH ₃ , rocking	1100W	1110W	1100W	100W	1100W	1100W
13.	OH, out-of-plane deformation	920W	-	-	930W	-	-
14.	CH ₂ , rocking	710M	720MS	720M	620S	710MS	720S
15.	COOH, bending mode	670W	-	-	679W	-	-
16.	COOH, wagging mode	540W	-	-	540W	-	-
17.	Y-O, bond	-	-	440M	-	-	390W

KEY TO ABBREVIATIONS

VS = very strong, MS = medium strong, W = weak, S = strong, M = medium, VW = very weak.

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