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FTIR study of hydrogen bonding between acyclic ester with monohydric alcohols

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ABSTRACT

Hydrogen bonding between acyclic ester Ethyle Oleate with monohydric alcohols has been studied by using the FTIR spectroscopic method. The change in Gibbs energy and Enthalpy values vary with alcohol chain length, which suggests that the proton donating ability of alcohols is in the order: Butanol < 2-Propanol < Ethanol. The FTIR explained –OH stretching frequency variation in monohydric alcohols.

Keywords: FTIR spectroscopy, acyclic ester, alcohols, hydrogen bonding.

INTRODUCTION

In addition to the thermo physical and acoustic parameters, FTIR studies also were conducted for the binary mixtures of acyclic ester Ethyl Oleate with monohydric alcohols Butanol, Ethanol and Propanol in order to estimate the intermolecular interactions between two miscible organic liquids which is for the present discussion. Hydrogen bonds constitute a very interesting class of intermolecular interactions, which are of extreme importance in many fields of chemistry and molecular biology. The study of the H-bonds of the type O–H----O=C occupies a position of considerable importance as it relates to the study of biopolymers.

MATERIALS AND METHODS

All the materials procured of Sigma-Aldrich AR grade and glassware used of Borosilicate make. Organic liquid Ethyl Oleate ($C_{20}H_{38}O_2$, 310.51g/mol), Ethanol (C_2H_6O , 40.06g/mol), Butanol ($C_4H_{10}O$, 74.12g/mol) and Isopropanol (C_3H_8O , 60.1g/mol) of AR grade were procured from Sigma-Aldrich with CAS no.111-62-6,64-17-5,64-17-5 and 67-63-0 respectively are used directly without purification. The densities and viscosities of the liquid compounds were measured with specific gravity bottle and Ostwald viscometer pre calibrated with 3D [5] water of Millipore to nearest mg/ml. The time taken for flow of viscous fluid in Ostwald viscosity meter is measured to a nearest 0.01 sec. Borosilicate glassware, Japan make Shimadzu electronic balance of sensitivity ± 0.001 gm and constant temperature water bath of accuracy ± 0.1 K were used while conducting the experiments. 2MHz ultrasonic interferometer model no. F-05 with least count of micrometer 0.001mm of Mittal Enterprises [6] was used for calculating velocities of sound waves and all the tests were conducted as per ASTM standard [7] procedures. FTIR spectra were obtained with a Bruker ALPHA FT-IR spectrometer.

Table.1. Experimental and literature values of density, viscosity and velocity of pure compounds at 323.15K and 2MHz

Parameter	Ethyl Oleate		Ethanol		Butanol		2-Propanol	
	Expt.	Lite.	Expt.	Lite.	Expt.	Lite.	Expt.	Lite.
Density(ρ) kg/m ³	848.3	848.50[1] 847.16[4]	774.3	773.90[2]	786.2	787.63[2] 786.29[3]	763.61	773.0[2]
Viscosity(η) Ns/m ²	3.4286	3.4247[1]	0.7481	0.7630[2]	1.3791	1.3631[2]	0.9833	1.0983[2]
Velocity(U) m/s	1289.6	1291.03[4]	1063.2	-	1164.1	1156.92[3]	1052.2	-

RESULTS AND DISCUSSION

Density, viscosity and velocity of ultrasonic wave in pure compounds are measured, tabulated and compared with the works of the previous scholar and presented in table.1. and for binary mixtures at various mole fractions of Ethyl Oleate in table.2. From the above table.2. of experimental data it is observed that the velocity (U), density (ρ) and viscosity (η) of all the binary mixtures of alcohols are increasing with the increase of mole fraction (X_1) of Ethyl Oleate. The derived quantities the change in

Table2: Velocity (U), Density (ρ), Viscosity (η), at 323.15K for binary mixtures of Ethyl Oleate (X_1) with Ethanol, Butanol and 2-Propanol

Mole fraction X_1	U m/sec	ρ Kg/m ³	η Nsm ⁻²	Gibbs free energy (G^E)	Enthalpy (H)
Ethyl Oleate + Butanol					
0.0000	1164.1	786.2	1.3791	0.0000	0.0000
0.0489	1185.01	812.8	1.7206	0.00960	6.8231
0.1140	1205.92	825.3	2.0621	0.01665	11.1470
0.2048	1226.83	834.2	2.4036	0.02136	13.1913
0.3399	1247.74	841.9	2.7451	0.02322	12.9294
0.5628	1268.65	847.6	3.0866	0.01960	9.5421
1.0000	1289.56	848.3	3.4281	0.0000	0.0000
Ethyl Oleate + Isopropyl alcohol					
0.0000	1052.20	763.61	0.9833	0.0000	0.0000
0.0412	1091.76	789.2	1.3908	0.0059	3.9233
0.0970	1131.32	805.3	1.7983	0.0108	6.7430
0.1769	1170.88	820.6	2.2058	0.0143	8.2345
0.3007	1210.44	833.4	2.6133	0.0156	8.1531
0.5180	1250.0	843.6	3.0208	0.0129	5.9461
1.0000	1289.56	848.3	3.4283	0.0000	0.0000
Ethyl Oleate + Ethanol					
0.0000	1063.2	774.3	0.7481	0.0000	0.0000
0.0274	1100.93	794.3	1.1948	0.0138	10.302
0.0660	1138.66	811.1	1.6415	0.0235	16.633
0.1238	1176.39	826.5	2.0882	0.0305	19.891
0.2203	1214.12	838.9	2.5349	0.0345	20.083
0.4140	1251.85	846.3	2.9816	0.0318	15.871
1.0000	1288.89	848.3	3.4283	0.0000	0.0000

Gibbs energy (G^E) and Enthalpy (H^E) values vary with alcohol chain length, which suggests that the proton donating ability of alcohols is in the order: 1-Butanol < 2-Propanol < Ethanol. The negative inductive effect of the alkyl groups increases in the order ethyl to butyl, and the electron contribution of the butyl group to the C=O group is significantly greater than that from the ethyl group. Therefore, one would expect that the strongest intermolecular hydrogen bonds formed would be between the C=O group of ethyl oleate and the OH proton of butyl alcohol, with the weakest occurring between the C=O group of ethyl oleate and the OH proton of ethyl alcohol [8]. The sign and magnitude of ΔG° indicates whether the reaction goes strongly towards the products (large negative values), towards the reactants (large positive values), or whether equal concentrations of reactants and products are present ($\Delta G = 0$). The ΔG° values for the systems studied here have been found to be negative, which indicates that the reaction goes more towards the products and the reaction is of the exothermic type [9].

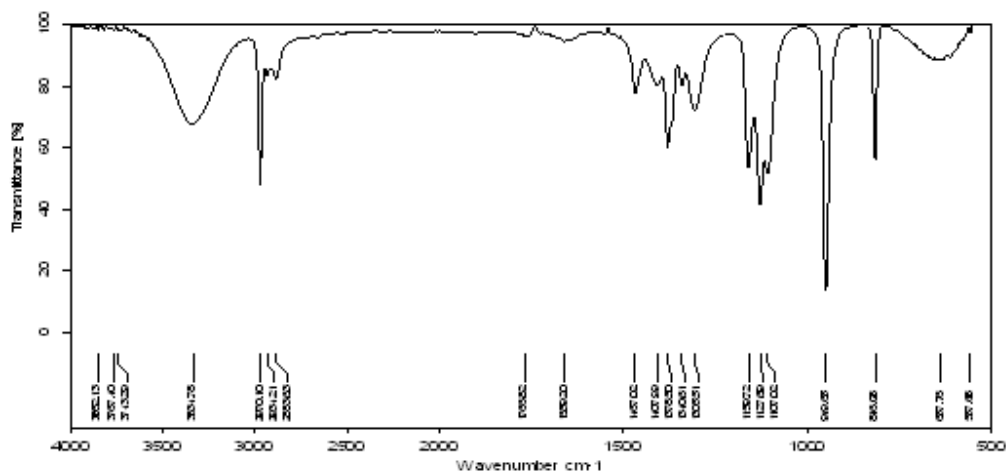


Fig.3 IR Spectra of Pure Iso Propanol

IR Spectra of pure Ethanol

The absorption band at 3324 cm^{-1} which is attributed to the stretching frequency of free O-H bond in alcohol. The band at 2973 cm^{-1} referred to the stretching frequency of C-H bond. The frequency range at 1087 and 1044 cm^{-1} belongs to C-O stretching.

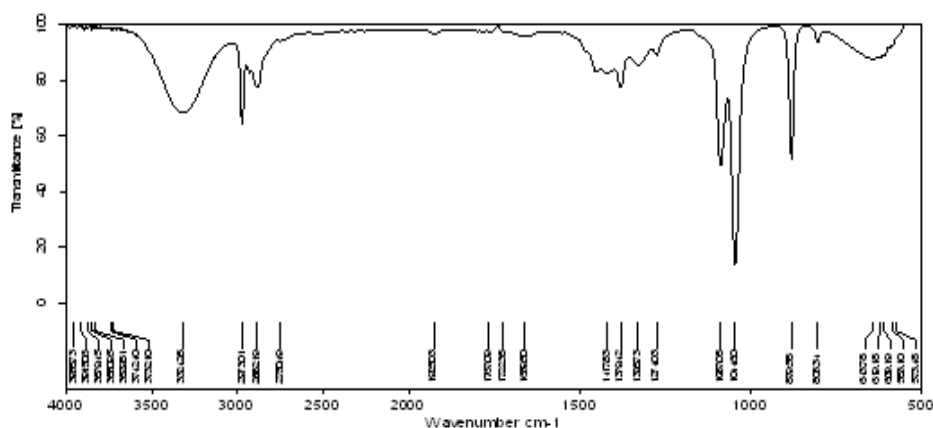


Fig. 4 IR Spectra of Pure Ethanol

IR Spectra of Ethyl Oleate + Butanol

The absorption band at 3365 cm^{-1} which is attributed to the stretching frequency of free O-H bond in alcohol. The band at 1737 cm^{-1} , which is attributed to the stretching frequency of the C=O bond of the ester. Inter molecular hydrogen bonding gives rise to broad bands. So it confirms the Ethyl oleate and Butanol are participated in inter molecular hydrogen bonding.

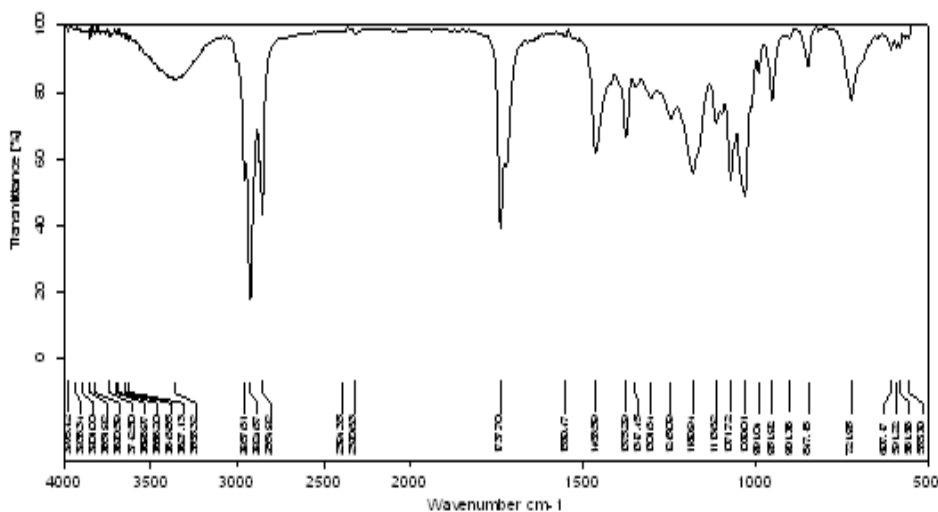
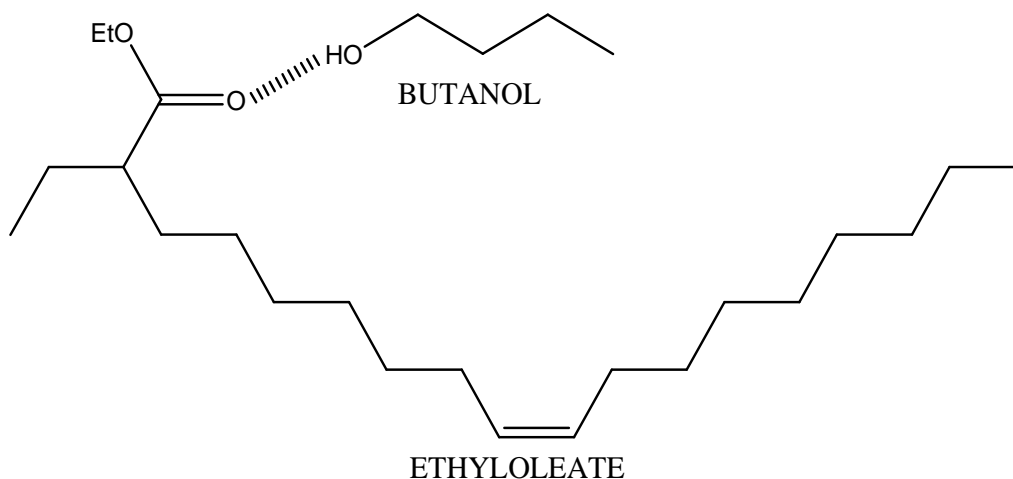


Fig 5 IR Spectra of Ethyl Oleate + Butanol

Hydrogen Bonding Interactions of Ethyloleate and Butanol

The hydrogen bond formation between the proton donor O-H of Butanol and carbonyl group(C=O) of Ethyl oleate using FTIR spectroscopy.



IR Spectra of Ethyl Oleate + Isopropanol

The absorption band at 3367cm^{-1} which is attributed to the stretching frequency of free O-H bond in alcohol. The band at 1737cm^{-1} , which is attributed to the stretching frequency of the C=O bond of the ester. Inter molecular hydrogen bonding gives rise to broad bands. So it confirms the Ethyloleate and Iso propanol are participated in inter molecular hydrogen bonding.

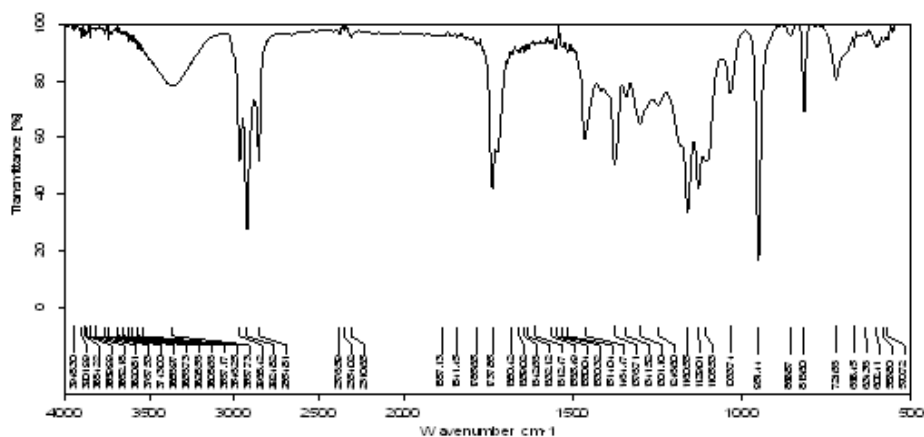


Fig 6 IR Spectra of Ethyl Oleate + Isopropanol

Hydrogen Bonding Interactions of Ethyloleate and Iso propanol

The hydrogen bond formation between the proton donor O-H of Isopropanol and carbonyl group(C=O) of Ethyl oleate using FTIR spectroscopy.

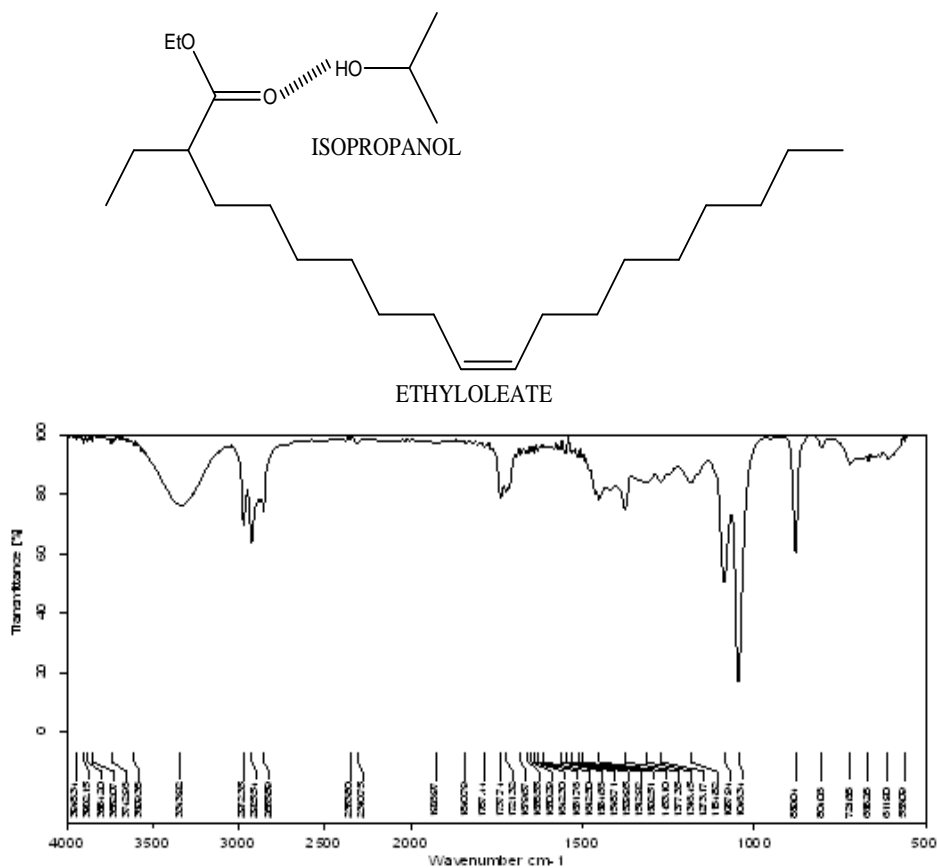


Fig 7 IR Spectra of Ethyl Oleate + Ethanol

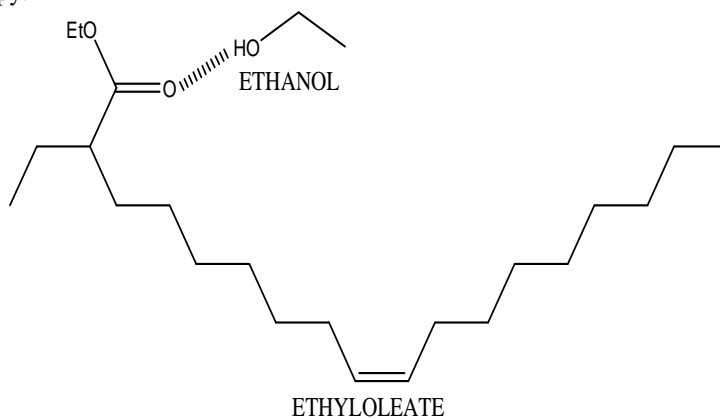
IR Spectra of Ethyl Oleate + Ethanol

The absorption band at 3337cm^{-1} which is attributed to the stretching frequency of free O-H bond in alcohol. The band at 1737cm^{-1} , which is attributed to the stretching frequency of the C=O bond of the ester. Inter molecular

hydrogen bonding gives rise to broad bands. So it confirms the Ethyloleate and Ethanol are participated in inter molecular hydrogen bonding.

Hydrogen Bonding Interactions of Ethyloleate and Ethanol

The hydrogen bond formation between the proton donor O-H of Ethanol and carbonyl group(C=O) of Ethyl oleate using FTIR spectroscopy.



CONCLUSION

The physico acoustic experiments conducted for binary mixtures of Ethyl Oleate with ethanol, butanol and isopropyl alcohol at 323.15K showed good agreements. The strength of interactions is in the order iso propanol, butanol and ethanol. Inter molecular hydrogen bonding is expected. From this study, one may conclude that the proton donating ability of alcohols and the proton accepting ability of acyclic ester vary linearly with the carbon-chain length of the alcohols.

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