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FT-IR AND ULTRASONIC STUDIES ON BINARY MIXTURES OF ETHYL OLEATE + ISOPROPANOL AT 303.15K TO 318.15K TEMPERATURES

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ABSTRACT

Density, viscosity and ultrasonic velocities in the temperature range 303K to 318K were determined for various mole fractions of two organic liquids Ethyl Oleate and Isopropanol. Thermo acoustic parameters like adiabatic compressibility, inter molecular free length, excess molar volume and internal pressure were calculated. The results were interpreted conclude intermolecular interactions between two organic liquids.

KEYWORDS: Ethyl Oleate, Isopropanol, ultrasonic speed, viscosity, density, FT-IR spectroscopy.

INTRODUCTION

There are certain intra and intermolecular interactions in any fluids and fluid mixtures to keep them as pure fluid or miscible liquid mixtures. These interactions either attractive or repulsive in toto are called as Vander Walls forces [5]. Binary mixture of organic liquids has importance of its own in various fields ranging from cosmetics to building materials, soft drinks to fuel mixtures. Certain physicochemical properties of fatty acid ethyl ester Ethyl Oleate in pure and in combination with 2-Propanol were studied keeping the possibilities of using it as bio diesel and diesel mixtures. As the fuel has to be stored at room temperatures the studies conducted were limited within the range of 303.15K to 318.15K with an increase of 5^0C.Thorough literary survey has been conducted as part of the author`s doctoral programme and identified a new organic fatty acid ethyl ester, Ethyl Oleate [4] which can used as biodiesel or bio diesel mix in combination with other compounds like alcohols, amines, ketones, hydrocarbons etc. An attempt was made to find the temperature effects on physic chemical and ultrasonic velocity for Ethyl Oleate and Isopropyl alcohol in pure form as well as in various mix proportions. The derived parameters adiabatic compressibility (β_{ad}), inter molecular free length(L_f), excess molar volume (V_m^E) and internal pressure(Π_i) were calculated in addition to experimental density (ρ),viscosity (η), and velocity (U) of 2MHz ultrasonic sound wave in order to understand the molecular interactions among the two organic liquids at 303.15K,308.15K,313.15K and 318.15K. FT-IR spectroscopy can be done by BRUKER ALPHA 400MHz spectrometer.

RESULTS AND DISCUSSION

Velocity of 2MHz ultrasonic wave in pure liquids, densities and viscosities of Ethyl Oleate and 2-Proponol were measured with pre calibrated interferometer, density bottle and viscosity meters respectively to nearest mg in the temperature range of 303.15K to 318.15K. The results were compared with available literature and shown in table.1. [4], [6], [10], [13] and [15]. The velocities, densities and viscosities of binary mixtures at said temperatures were also measured. The derived quantities from literature [14] adiabatic compressibility β_{ad}, intermolecular free length L_f, molar volume V_m, free volume (V_f) and internal pressure Π also were calculated, given in table.2. The excess values viz. $\Delta\beta_{ad}$, Π^E, V_m^E , V_f^E and L_f^E were shown in table 3.The graphs for mole fraction of Ethyl Oleate X_1 vs velocity (U), density (ρ), viscosity (η), excess adiabatic compressibility ($\Delta\beta_{ad}$), excess inter molecular free length (L_f^E), excess molar volume (V_m^E), excess free volume (V_f^E) and excess internal pressure (Π^E) were drawn and presented as Figure-1.

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Table-1: Density, viscosity and velocity of pure compounds and comparison

Compound	Temp. K	Density(ρ) kg/m^3		Viscosity(η) Ns/m^2		Velocity (U) m/s	
		Exp.	Lit.	Exp.	Lit.	Exp.	Lit.
Ethyl Oleate	**303.15**	863.50	863.20[4]	5.3101	5.3094[4]	1368.16	1360.67[15]
	308.15	859.34	859.50[4]	4.7164	4.7156[4]	1340.78	1342.98[15]
	313.15	855.62	855.80[4]	4.2163	4.2137[4]	1324.00	1325.49[15]
	318.15	852.04	852.20[4]	3.7820	3.7876[4]	1305.09	1308.17[15]
2-Proponol	**303.15**	776.25	777.47[13]	1.7659	1.7635[6]	1117.80	1132.16[13]
	308.15	772.79	773.15[13]	1.5499	1.5533[6]	1107.80	1114.33[13]
	313.15	767.29	768.45[13]	1.3162	1.3130[6]	1091.40	1096.18[13]
	318.15	765.40	767.10[10]	1.1694	1.1624[6]	1074.80	1075.50[6]

The densities of Ethyl Oleate and Isopropyl alcohol are decreasing with the increase of temperature as usually. Viscosity and velocity of ultrasonic wave are also decreasing with the increase of temperature. Ultrasonic velocity **(U)** is increasing with the increase in mole fraction X_1 of Ethyl Oleate. Adiabatic compressibility (β_{ad}) is decreasing with the with the increase of mole fraction and increasing with increase of temperature at a constant mole fraction. Inter molecular free length (L_f) also follows the same trend as adiabatic compressibility. Internal pressure (Π_i) is enormously increasing with the increase of mole fraction. Negative excess molar volume (V_m^E) represents the considerable interactions among the molecules of the binary mixtures [6].

*Table-2. **Mole fraction, velocity (U), density (ρ), viscosity (η), adiabatic compressibility (β_{ad}), inter molecular free length (L_f), molar volume (V_m), free volume (V_f) and internal pressure (Π) for binary mixture of Ethyl Oleate (X_1) + 2-propanol (X_2) at various temperatures.***

Mole fraction (X_1)	Mole fraction (X_2)	Velocity m/sec (U)	Density Kg/m^3 (ρ)	Viscosity Nsm^{-2} (η)	Ad. Comp. 10^{-10} N^{-1}.m^2 (β_{ad})	Int. Mol. Free length 10^{-10} m (L_f)	Mol. Vol. (V_m)	Free Volume (V_f)	Internal pressure (π)
T= 303.15 K									
0.0000	1.0000	1117.8	776.25	1.7659	10.310	6.6627	77.423	0.2649	930.89
0.0412	0.9587	1159.5	793.16	2.3559	9.3770	6.3540	88.806	0.2304	889.92
0.0971	0.9028	1201.2	807.70	2.9459	8.5794	6.0778	104.54	0.2281	800.96
0.1771	0.8228	1243.0	822.25	3.5359	7.8711	5.8215	127.04	0.2512	681.03
0.3009	0.6990	1284.7	837.02	4.1259	7.2380	5.5824	161.85	0.3093	540.70
0.5184	0.4815	1326.5	851.24	4.7159	6.6762	5.3614	223.11	0.4408	387.92
1.0000	0.0000	1368.2	863.50	5.3059	6.1860	5.1608	359.60	0.8089	230.49
T=308.15 K									
0.0000	1.0000	1107.8	772.79	1.5499	10.5442	6.8028	77.770	0.3178	887.84
0.0412	0.9587	1146.6	789.2	2.0779	9.6375	6.5038	89.247	0.2735	851.53
0.0971	0.9028	1185.4	803.62	2.6059	8.8547	6.2340	105.06	0.2687	768.34
0.1771	0.8228	1224.2	818.04	3.1339	8.1556	5.9829	127.68	0.2942	654.56
0.3009	0.6990	1263.1	832.66	3.6619	7.5273	5.7478	162.67	0.3605	520.49
0.5184	0.4815	1301.9	846.88	4.1899	6.9660	5.5294	224.23	0.5117	373.94
1.0000	0.0000	1340.7	859.30	4.7179	6.4735	5.3303	361.36	0.9359	222.45
T=313.15 K									
0.0000	1.0000	1091.4	767.29	1.3162	10.941	6.9959	78.327	0.3971	833.68
0.0412	0.9587	1130.1	783.70	1.7992	9.9895	6.6847	89.918	0.3324	806.82

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0.0971	0.9028	1168.9	798.62	2.2822	9.1631	6.4022	105.81	0.3215	731.99
0.1771	0.8228	1207.7	813.44	2.7652	8.4276	6.1399	128.56	0.3485	625.82
0.3009	0.6990	1246.5	828.36	3.2482	7.7688	5.8950	163.74	0.4239	498.93
0.5184	0.4815	1285.3	843.08	3.7312	7.1794	5.6670	225.50	0.5983	359.34
1.0000	0.0000	1324.14	856.20	4.2142	6.6612	5.4586	362.67	1.0880	214.47
T=318.15 K									
0.0000	1.0000	1074.8	765.40	1.1694	11.309	7.1800	78.521	0.4634	803.18
0.0412	0.9587	1113.1	780.92	1.6054	10.333	6.8631	90.208	0.3854	778.64
0.0971	0.9028	1151.5	795.72	2.0414	9.4765	6.5723	106.13	0.3712	707.43
0.1771	0.8228	1189.9	810.21	2.4774	8.7162	6.3032	128.97	0.4014	605.27
0.3009	0.6990	1228.3	824.82	2.9134	8.0350	6.0519	164.29	0.4875	482.73
0.5184	0.4815	1266.7	839.09	3.3494	7.4269	5.8183	226.40	0.6875	347.63
1.0000	0.0000	1305.1	852.12	3.7854	6.8894	5.6039	364.40	1.2506	207.35

*Table-3: Excess parameters of **adiabatic compressibility (β_{ad}), inter molecular free length (L_f), molar volume (V_m), free volume (V_f) and internal pressure (Π).***

(X_1)	$\Delta\beta_{ad}$	L_f^E	V_m^E	V_f^E	Π^E
303.15K					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0412	-0.7629	-0.2466	-0.2659	-0.0569	-12.055
0.0971	-1.3299	-0.4384	-0.3072	-0.0896	-61.861
0.1771	-1.7084	-0.5758	-0.3680	-0.1100	-125.77
0.3009	-1.8308	-0.6282	-0.5049	-0.1193	-179.37
0.5184	-1.4959	-0.5226	-0.5996	-0.1061	-179.87
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
308.15K					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0412	-0.7387	-0.2382	-0.2257	-12.0551	-8.8402
0.0971	-1.2940	-0.4257	-0.2612	-61.8612	-54.852
0.1771	-1.6677	-0.5591	-0.3121	-125.775	-115.43
0.3009	-1.7919	-0.6119	-0.4302	-179.378	-167.12
0.5184	-1.4682	-0.5102	-0.5303	-179.871	-169.01
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
313.15K					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0412	-0.7745	-0.2475	-0.1829	-0.0932	-1.2196
0.0971	-1.3610	-0.4438	-0.2248	-0.1430	-41.339
0.1771	-1.7535	-0.5829	-0.2684	-0.1713	-97.879
0.3009	-1.8814	-0.6371	-0.3559	-0.18157	-147.96
0.5184	-1.5397	-0.5307	-0.4551	-0.1574	-152.84
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
318.15K					
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0412	-0.7935	-0.2517	-0.1233	-0.1105	0.0739
0.0971	-1.4033	-0.4543	-0.1888	-0.1687	-37.8062
0.1771	-1.8099	-0.5973	-0.2312	-0.2015	-92.2881
0.3009	-1.9435	-0.6534	-0.3206	-0.2129	-141.009
0.5184	-1.5903	-0.5442	-0.3846	-0.1841	-146.536
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000

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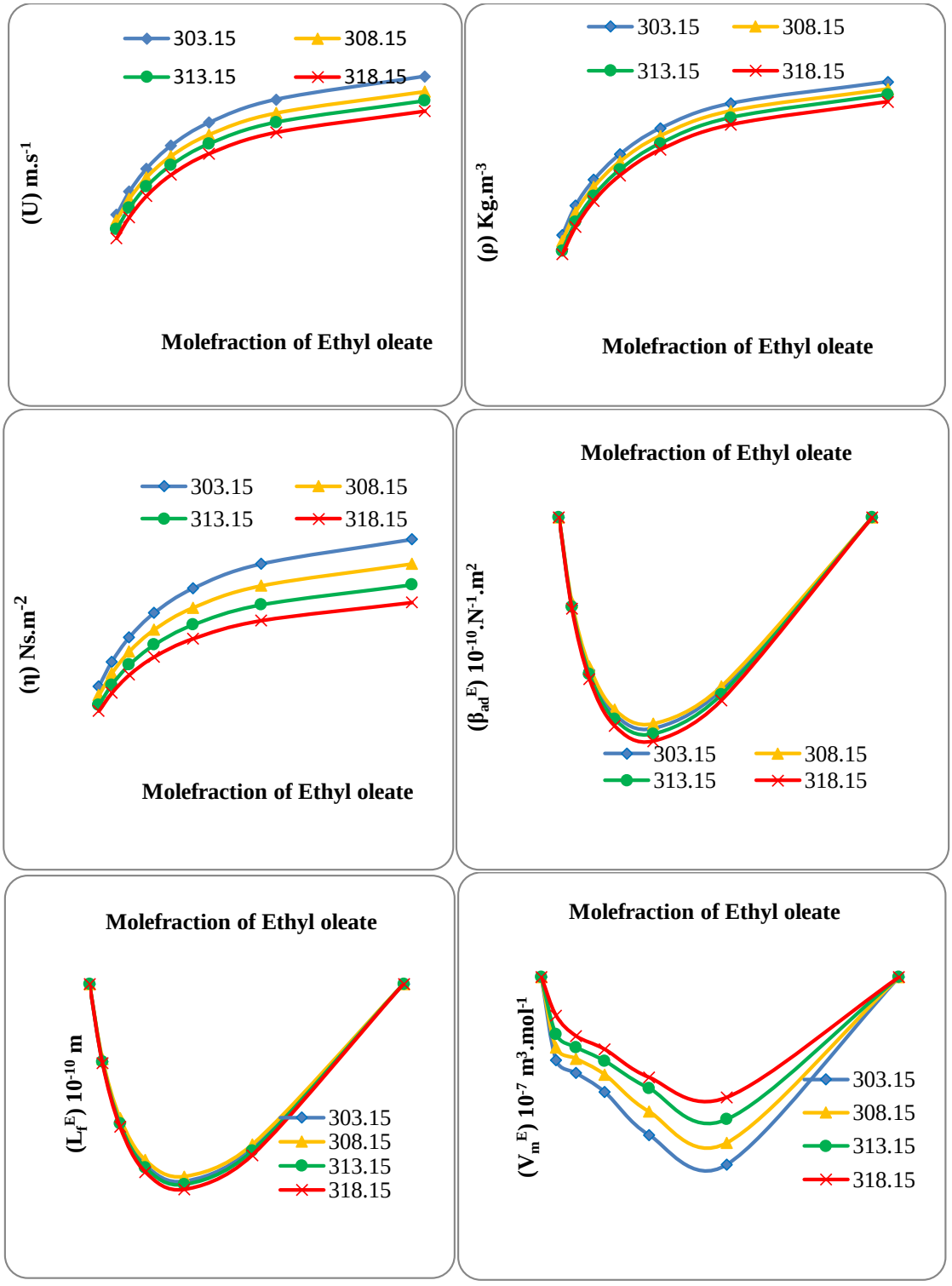

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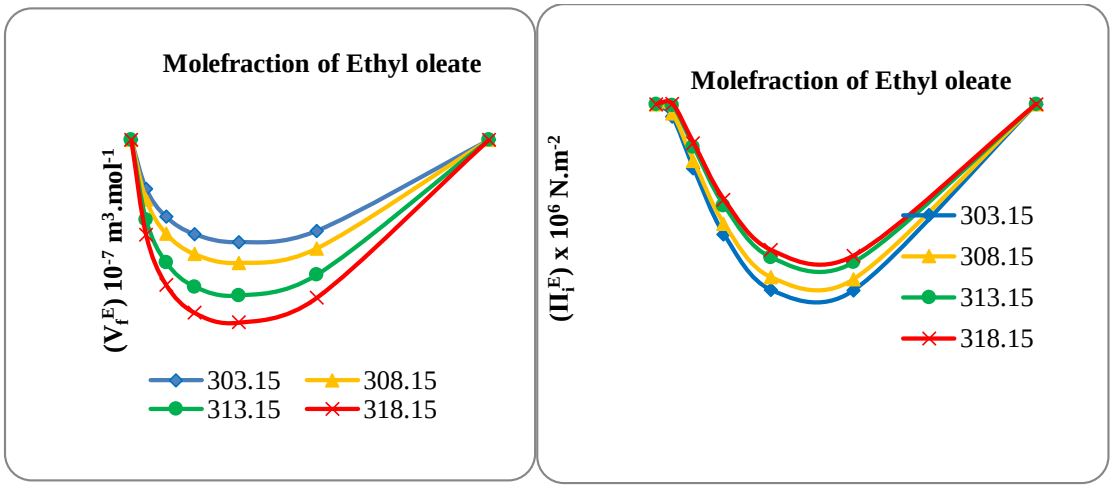

Figure-1: The plots of Ethyl oleate mole fraction verses Velocity(U), Density(ρ), Viscosity(η), Excess intermolecular free length (Lf^E), deviation in adiabatic compressibility ($\Delta\beta_{ad}$), Excess free volume (Vf^E), Excess internal Pressure (Π^E).

IR Spectra of Pure Iso Propanol

The absorption band at 3334 cm^{-1}which is attributed to the stretching frequency of free O-H bond in alcohol. The band at 2970 cm^{-1} referred to the stretching frequency of C-H bond. The frequency range at 1127 and 1107cm^{-1} belongs to C-O stretching.

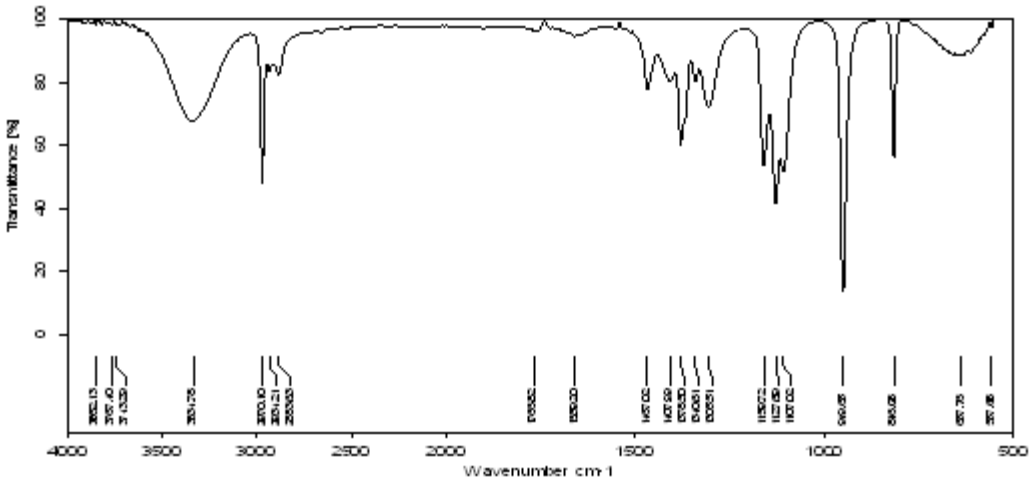

Fig .2 IR Spectra of Pure Iso Propanol

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.

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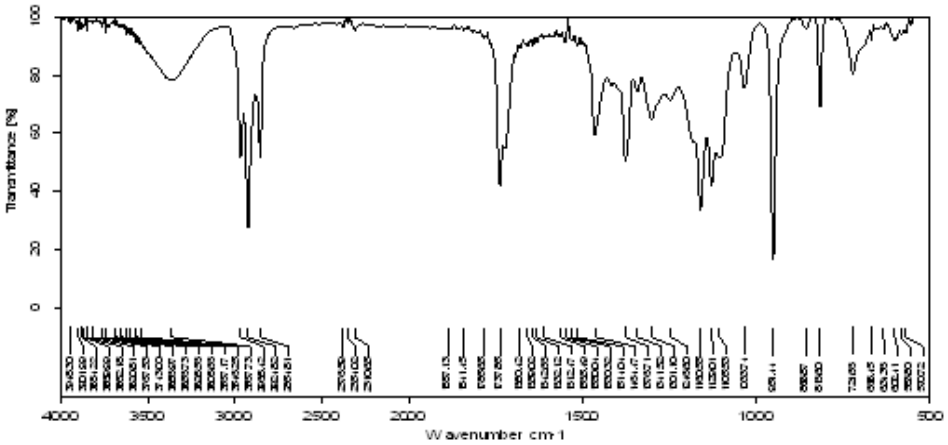

Fig 3 IR Spectra of Ethyl Oleate + Isopropanol

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.

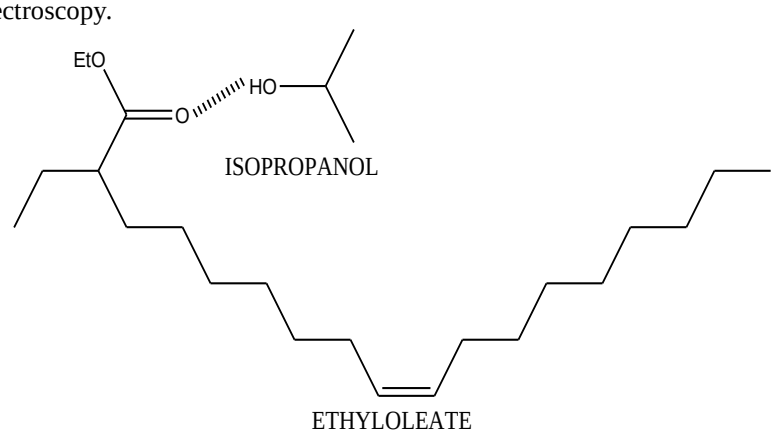

Fig.4 Hydrogen Bonding Interactions of Ethyloleate and Iso propanol

CONCLUSIONS

The miscible organic compounds Ethyl Oleate and Isopropyl alcohol are showing negative values of Excess intermolecular free length (Lf^E), deviation in adiabatic compressibility ($\Delta\beta_{ad}$), Excess free volume (Vf^E), Excess internal Pressure (Π^E), this may give an information about strong interactions between this binary mixture. So we concluded that inter molecular hydrogen bonding interactions observed.

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