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An Insight into the Physico-Acoustical Properties of Biologically Active heterocycles: Chalcones in Different Solvents at Various Temperatures

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Abstract: *The density, viscosity and ultrasonic velocity have been measured for synthesized (2E)-3-(4-Chlorophenyl)-1-(4-fluorophenyl) propenone (FCC) in DMF, THF and $CHCl_3$solutions of various concentrations at 300.15K with a view to understand the molecular interactions in these solutions. The experimental data have been used to calculate various acoustical parameters, which are interpreted in terms of solute-solute and solute-solvent interactions in different solvents.*

Keywords: FCC**,** Density, Viscosity, Ultrasonic Velocity, DMF, THF, $CHCl_3$, Acoustical Parameters.

I. INTRODUCTION

Chalcones are unsaturated ketones containing the reactive keto and ethylenic group –CO –CH=CH – and are colored compounds due to presence of the chromophore and auxochromes [1, 2].Chemically they are open-chain flavonoids in which the two aromatic rings are joined by a three carbon α, βunsaturated carbonyl system.Chalcones are characterized by their possession of a structure in which two aromatic rings are linked by an aliphatic three carbon chain. The presence of different substituents around the chalcone ring system shows very different physical and chemical characteristics which are reflected in their biological activities[3-8]. The chemistry of chalcones has generated intensive scientific studies throughout the world, due to their biological and industrial applications. Chalcones are characterized by their possession of a structure in which two aromatic rings are linked by an aliphatic three carbon chain. Different methods are available in the literature for the synthesis of chalcones. The most convenient method is the one, which involves the Claisen-Schimidt condensation of equimolar quantities of aryl methyl ketones with aryl aldehyde in presence of alcoholic alkali [9-13].The chalcones have been found to be useful for the synthesis of variety of heterocyclic compounds and are associated with different biological activities.

Now a days, lots of interest has been generated on the use of ultrasound radiation in synthetic organic chemistry, which includes decrease of reaction time, increase of yield, lower reaction temperature etc. [14-17]. By ultrasonic sound velocity measurements, the molecular interactions in pure liquid[18], aqueous solutions[19-21] and liquid mixtures[22]have also been studied.

Several physico-chemical parameters are available in the list and few of them are of much interest. It was well understood by the literature that physico-chemical properties such as acoustical properties, density, viscosity, ultrasonic sound velocity, etc.of the organic as well as heterocyclic compounds. These properties have contributed advancement in the physical sciences and also in daily human life.The study of physico-chemical properties of compounds in solutions gives complete understanding of the behavior of compounds in different solvents. These properties are the sensitive indicators for understanding molecular interactions.

Thus, in the present work, (2E)-3-(4-Chlorophenyl) -1-(4-fluorophenyl) propenone (FCC)was synthesized and characterized by IR and NMR spectra.Various physico-chemical properties and acoustical properties such as density, viscosity and ultrasonic sound velocity have been studied in dimethylformamide (DMF), tetrahydrofuran (THF) and Chloroform ($CHCl_3$) for different concentrations of 3-(4-Chloro-phenyl) -1-(4-fluorophenyl) propen-1-one (FCC)solution were done at 300.15K, 305.15K and 310.15K with a view to understand the molecular interactions in these solutions. From these experimental data, various acoustical parameters such as isentropic compressibility, Rao's molar sound function, specific acoustical impedance, internal pressure, Vander Waals constant, free volume etc. were evaluated and results are discussed.

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II. Materials and Methods

2.1. Preparation of (2E)-3-(4-Chlorophenyl)-1-(4-fluorophenyl) propenone (FCC)

Chalcones are usually synthesized in the laboratory by various synthetic methods.The present compound was synthesized by Claisen-Schmidt condensation using ethanol as reaction medium. Melting points (°C) were determined with a MELTEMP II capillary apparatus (LAB Devices, Holliston, MA, USA) without correction. IR spectra were recorded on FT-IR spectrometer (Perkin Elmer) using KBr disc method. ^{1}H NMR spectra were recorded on Bruker 400 MHz spectrometer in $CDCl_3$ as a solvent. TLC was performed on silica gel coated plates for monitoring the reactions.

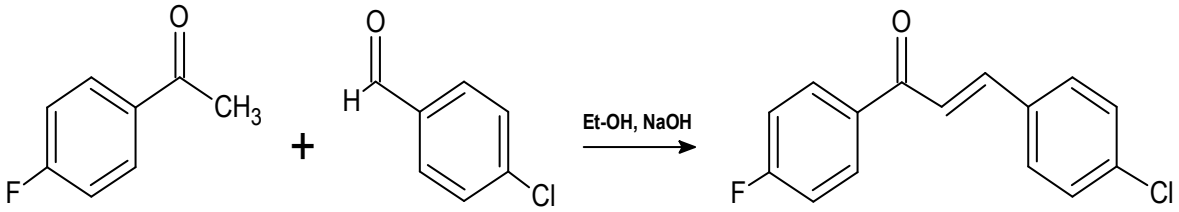
2.2 Evaluation

The general procedure for the synthesis of (2E)-3-(4-Chlorophenyl) -1-(4-fluorophenyl) propenone (FCC)

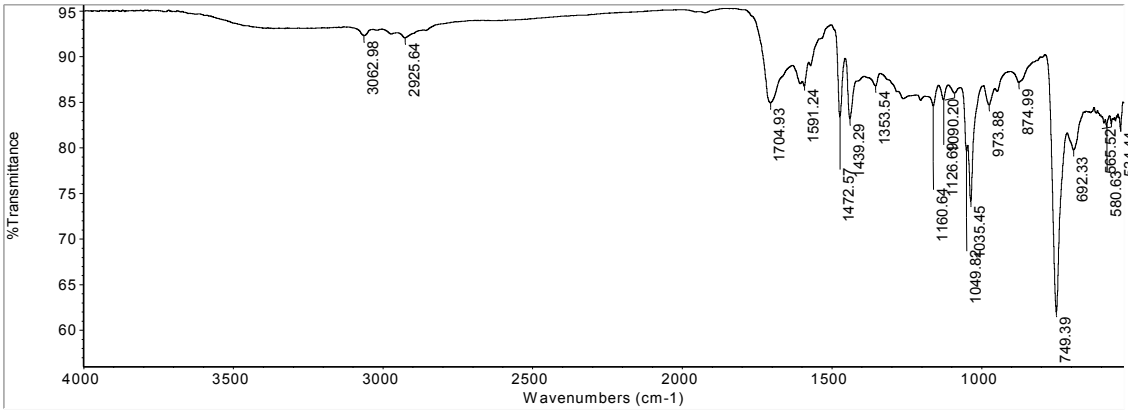
A mixture of 4-methyl benzaldehyde (1 mmol) and 4-chloroacetophenone (1 mmol) was dissolved in 15 mL ethanol. To this mixture, sodium hydroxide (20%, 1mL) was added and the reaction mixture was stirred at room temperature for 12hr. After completion of the reaction (monitored by TLC), the crude mixture was worked up in ice-cold water (100 mL). The product which separated out was filtered and recrystallized from ethanol to afford title compound.

Melting points were determined by Deep Vision instrument. The purity of the compound was checked by TLC using silica gel coated plates and spots were visualized by exposing the dry plates in iodine vapour chamber. IR spectra were recorded in the solid state, use of the FT-IR-Spectrometer. The ^{1}HNMR spectra of the compounds were carried out in Bruker AMX 400 MHZ. NMR instrument using $CDCl_3$ as a solvent and TMS as internal reference (chemical shift in δ ppm). The mass spectra of the compounds were carried out in ESI Mass.

Scheme: Synthesis of*(2E)*-3-(4-Chloro-phenyl)-1-(4-fluorophenyl) propen-1-one (FCC)



2.2.1 Infrared Spectra: (FCC)



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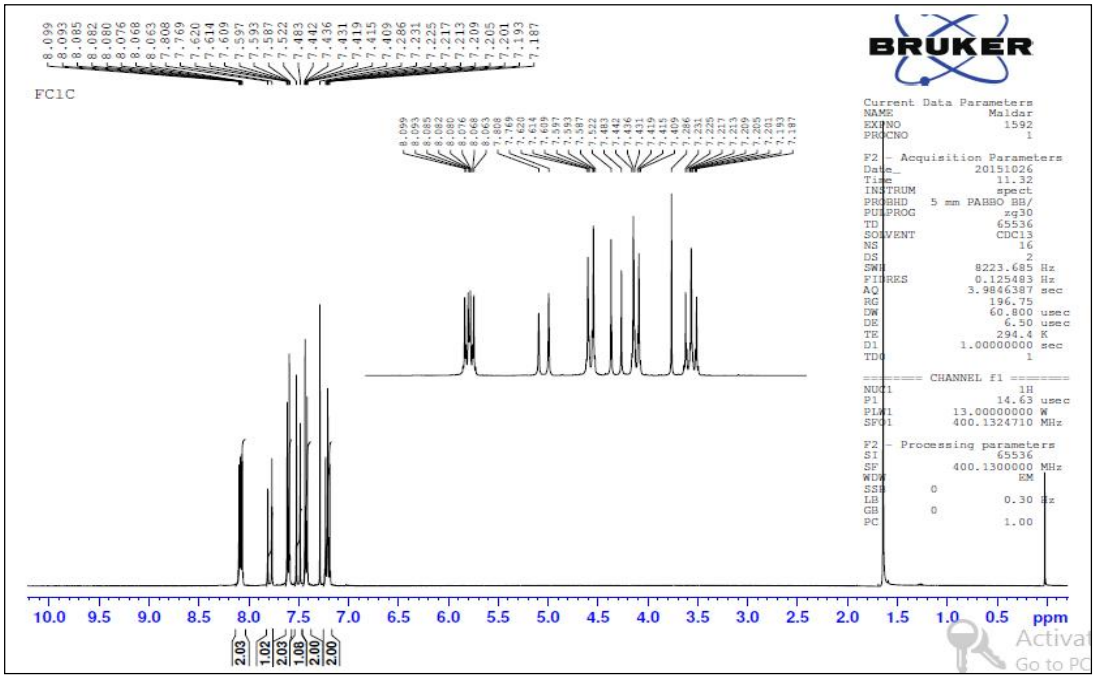
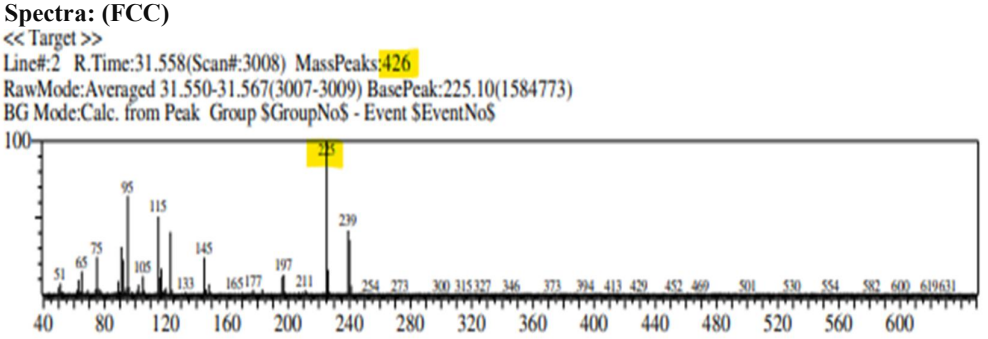
2.2.2 ^{1}H NMR SPECTRA: (FCC)



2.2.3 Mass Spectra: (FCC)



2.3 Spectral Characterization

Yield: 58 %; **M. F.**: $C_{15}H_{10}ClFO$**; Mol. Wt.**: 260.69; **Colour:** light pink**; M. P.:** 140 ºC

IR (cm^{-1})

2930.37, 1665.50, 1597.61, 1320.85, 1219.23, 840.58.

^{1}H NMR

(400 MH_z, $CDCl_3$) δ: 7.18 – 7.23 (2H, m), 7.41 – 7.45 (2H, m), 7.51 (1H, d, J = 16 Hz), 7.59 – 7.62 (2H, m), 7.78 (1H, d, J = 16 Hz), 8.06 – 8.09 (2H, m).

GCMS (ESI)

m/z [M] calcd. $C_{15}H_{10}OClF$, for: 260.69; found: 260

2.4 Choice of Solvents

N,N-Dimethylformamide (DMF),Tetrahydrofuran (THF) and Chloroform ($CHCl_3$) have been chosen as solvents in the present article. The densities, viscosities and ultrasonic velocities of solvents and solutions of different concentration were measured at 300.15, 305.15, 310.15K by using pycnometer, an Ubbelohde suspended level viscometer and ultrasonic interferometer[18].

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2.5 Experimental

The densities, viscosities and ultrasonic velocities of solvents and solutions of different concentration in DMF, THF and $CHCl_3$were measured at 300.15K, 305.15K and 310.15K by using pycnometer, an Ubbelohde suspended level viscometer and single frequency ultrasonic interferometer operating at 2 MHz, with the uncertainties of 0.0001g/cm3, + 0.06 % and 0.01% respectively.

Density Measurements (ρ)

The density, of a substance is its mass per unit volume.

$$\textbf{Density } (\rho) = \frac{Mass(M)}{Volume(V)}$$

The experimentally densities were evaluated by using following equation,

$$\textbf{Density}(\rho) = \frac{(\textbf{wt. of solvent or solution})(\textbf{densityo f water})}{(\textbf{wt. of water})}\ \textbf{g/cm}^3$$

Viscosity Measurement (η)

The determination of the viscosity of liquids or solutions are more accurately carried out by using Ubbelohde viscometer.Using the time taken for the distilled water and solution, the viscosity of unknown solutions is determined.

$$\frac{\eta_s}{\eta_w} = \frac{t_s\rho_s}{t_w\rho_w}$$

Where η_w, ρ_w and t_w are the viscosity, density and time flow of distilled water respectively and η_s, ρ_s and t_s are the viscosity, density and time flow of unknown liquid or solution respectively.

Ultrasonic Velocity Measurement (U)

The solvent/solution were filled in the measuring cell with quartz crystal and then micrometer was fixed. The circulation of water from the thermostat of required temperature was started and test solvent/solution in the cell is allowed to thermally equilibrate. The micrometer was rotated very slowly so as to obtain a maximum or minimum of anode current (n). A number of maximum reading of anode current were counted. The total distance (d) travel by the micrometer for n=10, was read. The wave length (λ) is determined by using the equation,

$$\lambda = \frac{2d}{n}$$

The sound velocity (U) of solvent and solutions were calculated from the wavelength and frequency (F) according to equation

$$U = \lambda F$$

From the experimental data of density, viscosity and ultrasonic sound velocity, various acoustical parameters are evaluated using standard equations [23-26].

Initially, all required concentrations of solutions for synthesized compounds were prepared in different solvents using calibrated volumetric flasks. All the prepared samples were retained at the desired temperature for 24 hr. to ensure their solubility at the temperature.

The experimentally calculated data of density (ρ), viscosity (η) and ultrasound velocity (U) of pure solvents and solutions of synthesized compounds in DMF, THF and $CHCl_3$ at three different temperatures are reported in tabular form (tables: 1 to 9) as follows:

Table: 1. Experimental data of density (ρ), viscosity (η) and ultrasonic velocity (U) of FCC with different concentrations in DMF at 300.15 K**.**

Sr. No.	Conc. ($x\ 10^{-3}$ M)	Density ($x\ 10^{-3}$ kgm^{-3})	Viscosity ($x\ 10^{-3}$ Nsm^{-2})	Sound velocity (ms^{-1})
1	00	0.9349	0.6596	1401.5
2	2.0	0.9361	0.6843	1408. 7

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3	4.0	0.9366	0.7143	1419.4
4	6.0	0.9370	0.7235	1428.2
5	8.0	0.9377	0.7391	1436.7
6	10	0.9380	0.7596	1448.2

Table 2: Experimental data of density (ρ), viscosity (η) and ultrasonic velocity (U) of FCC with different concentrations in DMF at 305.15 K.

Sr. No.	Conc. ($x 10^{-3}$ M)	Density ($x 10^{-3}$ kgm^{-3})	Viscosity ($x 10^{-3}$ Nsm^{-2})	Sound velocity (ms^{-1})
1	00	0.9343	0.6056	1383.3
2	2.0	0.9344	0.6515	1390.1
3	4.0	0.9349	0.6868	1389.5
4	6.0	0.9363	0.7037	1409.7
5	8.0	0.9358	0.7202	1427.0
6	10	0.9374	0.7427	1429.8

Table 3: Experimental data of density (ρ), viscosity (η) and ultrasonic velocity (U) of FCC with different concentrations in DMF at 310.15 K.

Sr. No.	Conc. ($x 10^{-3}$ M)	Density ($x 10^{-3}$ kgm^{-3})	Viscosity ($x 10^{-3}$ Nsm^{-2})	Sound velocity (ms^{-1})
1	00	0.9337	0.5739	1363.9
2	2.0	0.9347	0.6235	1370.9
3	4.0	0.9353	0.6531	1379.5
4	6.0	0.9360	0.6720	1391.3
5	8.0	0.9364	0.6821	1397.3
6	10	0.9370	0.7016	1409.5

Table 4: Experimental data of density (ρ), viscosity (η) and ultrasonic velocity (U) of FCC with different concentrations in THF at 300.15 K.

Sr. No.	Conc. ($x 10^{-3}$ M)	Density ($x 10^{-3}$ kgm^{-3})	Viscosity ($x 10^{-3}$ Nsm^{-2})	Sound velocity (ms^{-1})
1	00	0.8684	0.8505	1256.3
2	2.0	0.8689	0.8580	1265.3
3	4.0	0.8690	0.8627	1268.8
4	6.0	0.8698	0.8670	1273.2
5	8.0	0.8711	0.8720	1276.4
6	10	0.8701	0.8766	1279.6

Table: 5. Experimental data of density (ρ), viscosity (η) and ultrasonic velocity (U) of FCC with different concentrations in THF at 305.15 K.

Sr. No.	Conc. ($x 10^{-3}$ M)	Density ($x 10^{-3}$ kgm^{-3})	Viscosity ($x 10^{-3}$ Nsm^{-2})	Sound velocity (ms^{-1})
1	00	0.8679	0.8383	1234.2
2	2.0	0.8684	0.8450	1241.0
3	4.0	0.8690	0.8546	1244.7
4	6.0	0.8691	0.8605	1247.6
5	8.0	0.8693	0.867	1253.7
6	10	0.8702	0.8702	1258.8

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Table 6: Experimental data of density (ρ), viscosity (η) and ultrasonic velocity (U) of FCC with different concentrations in THF at 310.15 K.

Sr. No.	Conc. (x 10^{-3} M)	Density (x 10^{-3} kgm^{-3})	Viscosity (x 10^{-3} Nsm^{-2})	Sound velocity (ms^{-1})
1	00	0.8675	0.8256	1208.0
2	2.0	0.8677	0.8320	1215.2
3	4.0	0.8680	0.8388	1219.3
4	6.0	0.8687	0.8470	1223.0
5	8.0	0.8690	0.8523	1227.1
6	10	0.8695	0.8585	1234.1

Table 7: Experimental data of density (ρ), viscosity (η) and ultrasonic velocity (U) of FCC with different concentrations in CLF at 300.15 K.

Sr. No.	Conc. (x 10^{-3} M)	Density (x 10^{-3} kgm^{-3})	Viscosity (x 10^{-3} Nsm^{-2})	Sound velocity (ms^{-1})
1	00	1.4773	0.5303	986.65
2	2.0	1.4783	0.5340	988.97
3	4.0	1.4790	0.5361	990.58
4	6.0	1.4791	0.5371	992.33
5	8.0	1.4799	0.5380	994.00
6	10	1.4803	0.5383	995.62

Table 8: Experimental data of density (ρ), viscosity (η) and ultrasonic velocity (U) of FCC with different concentrations in CLF at 305.15 K.

Sr. No.	Conc. (x 10^{-3} M)	Density (x 10^{-3} kgm^{-3})	Viscosity (x 10^{-3} Nsm^{-2})	Sound velocity (ms^{-1})
1	00	1.4714	0.5111	965.64
2	2.0	1.472o	0.5131	967.90
3	4.0	1.4737	0.5140	969.64
4	6.0	1.4739	0.5155	971.36
5	8.0	1.4745	0.5164	972.80
6	10	1.4756	0.5190	974.45

Table 9: Experimental data of density (ρ), viscosity (η) and ultrasonic velocity (U) of FCC with different concentrations in CLF at 310.15 K.

Sr. No.	Conc. (x 10^{-3} M)	Density (x 10^{-3} kgm^{-3})	Viscosity (x 10^{-3} Nsm^{-2})	Sound velocity (ms^{-1})
1	00	1.4684	0.4966	943.46
2	2.0	1.4690	0.4987	945.63
3	4.0	1.4700	0.4993	947.09
4	6.0	1.4705	0.4995	948.73
5	8.0	1.471	0.5001	950.43
6	10	1.4720	0.5020	952.01

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2.6 Graphs

Fig.: 1. Variation of density with temperature concentrations of FCC in DMF

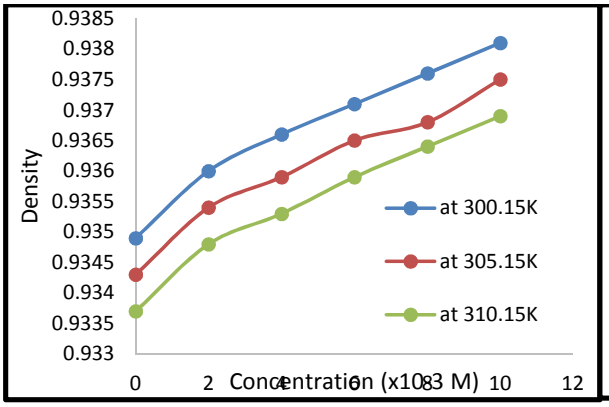

Fig.: 2.Variation of density with temperature at different at different concentrations of FCC in THF:

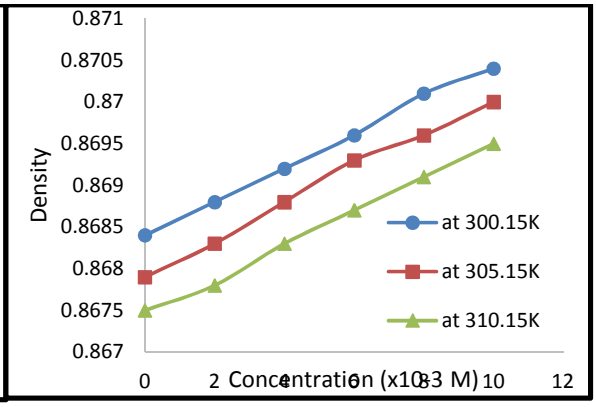

Fig.: 3. Variation of density with temperature at different concentrations of FCC in CLF

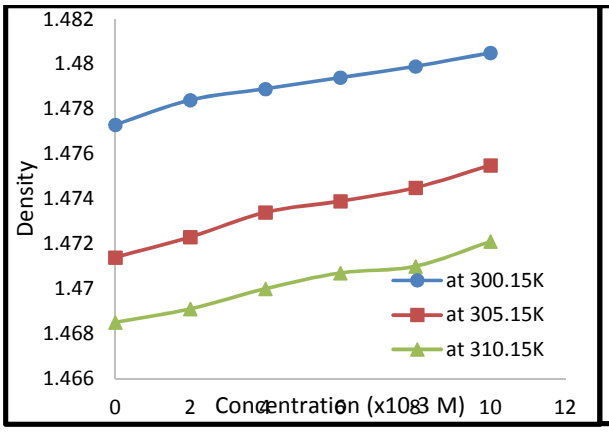

Fig.: 4. Variation of viscosity with temperature different concentrations of FCC in DMF:

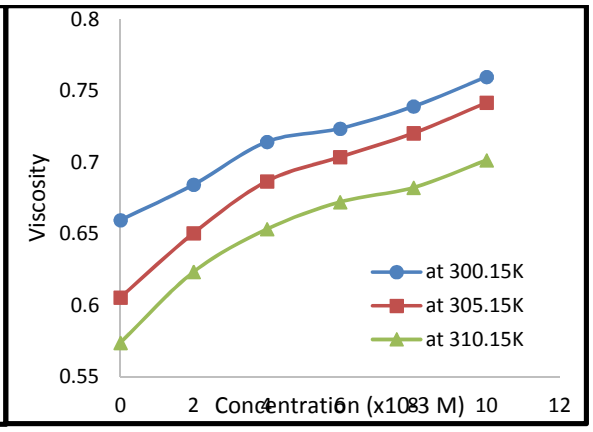

Fig.: 5. Variation of density with temperature at different concentrations of FCC in THF

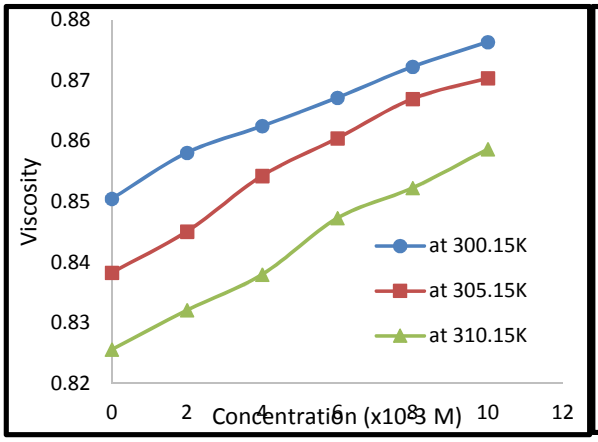

Fig.: 6. Variation of viscosity with temperature at different concentrations of FCC in $CHCl_3$

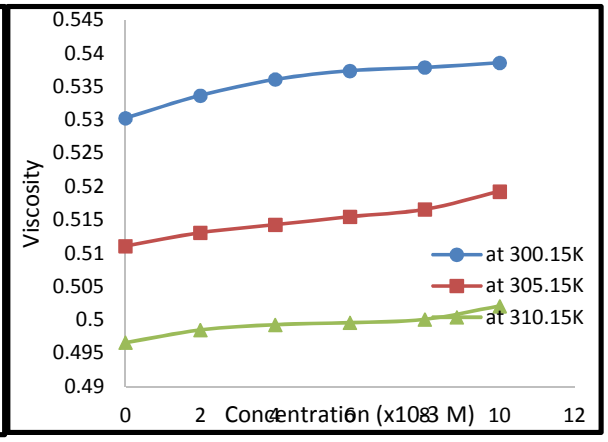

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Fig.: 7. Variation of ultrasonic velocity with temperature at different concentrations of FCC in DMF:

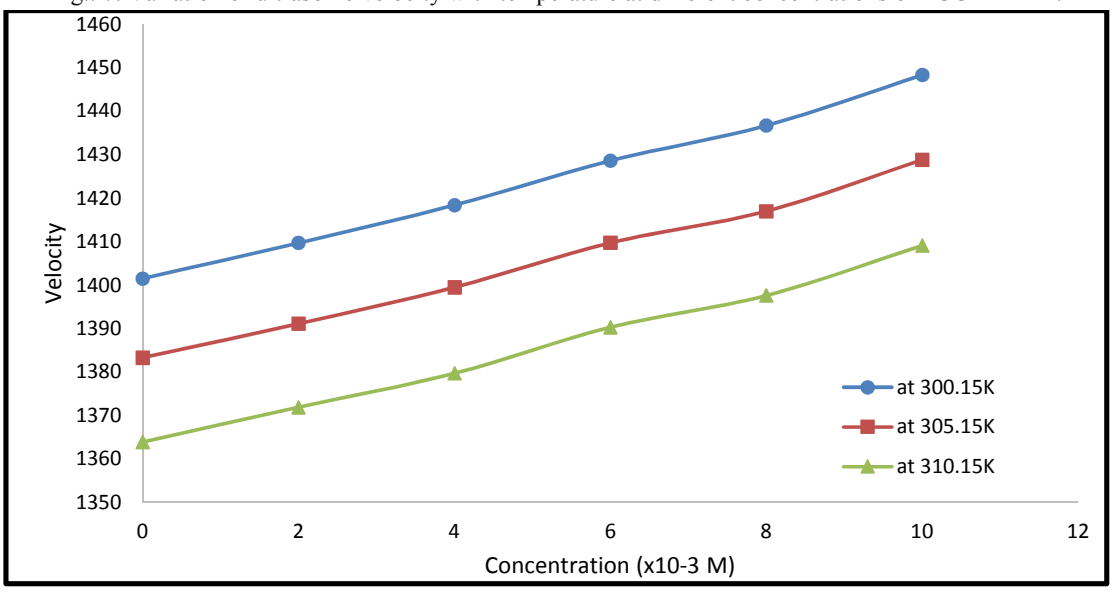


Fig.: 8. Variation of ultrasonic velocity with concentrations of FCC

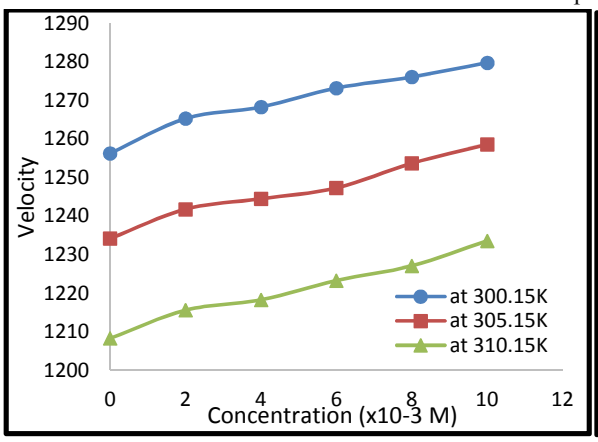
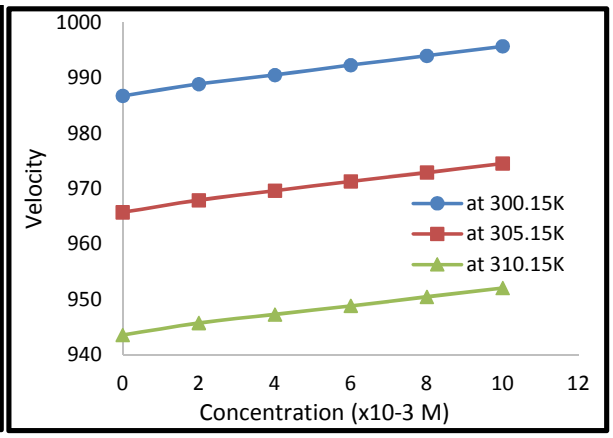


Fig.: 9. Variation of ultrasonic velocity with temperatureat different temperature at different concentrations of FCC in $CHCl_3$ in THF



2.7 Biological Activity:

In the present article, In Vitro Anti-oxidant activity and Anti-inflammatory activity of synthesized compound ***(2E)*-3-(4-Chloro-phenyl)-1-(4-fluorophenyl) propen-1-one**was studied.

Table 10: In vitro anti-oxidant activity FCC:

1	FCC	25	0.919 0.861 0.878	0.886	-
		50	1.004 0.764 0.918	0.895	-
		100	0.674 0.501 0.516	0.564	**33.88**

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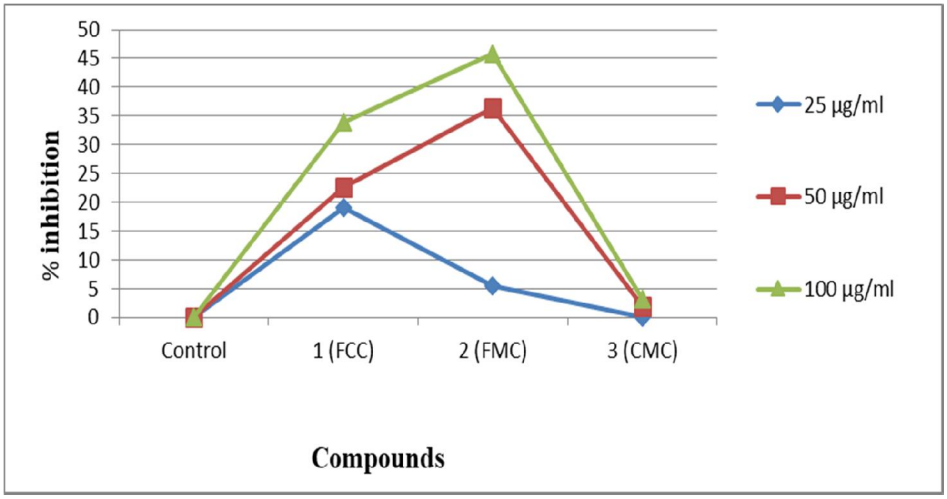

Figure 10: In vitro anti-oxidant activity

The ***(2E)***-3-(4-Chloro-phenyl)-1-(4-fluorophenyl) propen-1-one (FCC) compound have been synthesized and evaluated for antibacterial activity against specifically ***Bacillus Subtilis and Pseudomonas aerogenosa*** bacteria by Biofilm formation assay method. Among the synthesized compounds, the compounds **FCC**have shown the excellent activity showing significant inhibition which may lead to the development of the new drug.

Table 11: In vitro anti-inflammatory activity FCC:

1	FCC	10	0.26	03.70	125.30
		30	0.25	07.40	
		100	0.17	**37.03**	

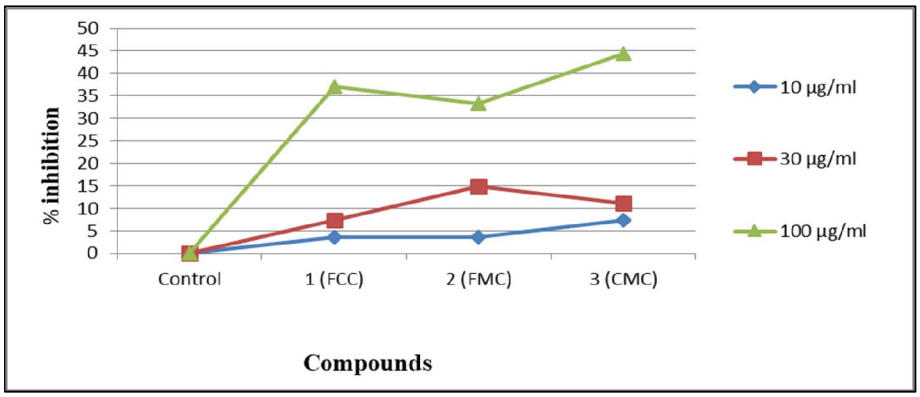

Figure 11: Anti-inflammatory activity

The ***(2E)*-3-(4-Chloro-phenyl)-1-(4-fluorophenyl) propen-1-one** was synthesized and evaluated for their anti-inflammatory activity by Membrane Lysis Assay. The result of anti-inflammatory activity reveals that all compounds were found to possess significant activity. Thus, this compound constitute an interesting template for the evaluation of new anti-inflammatory agents and may be helpful for the design of new therapeutic tools.

III. Results and Discussion

Physicochemical properties of pure and mixtures of solute and solvent are having great importance in the field of science and industrial engineering. In particular tension on the surface of film caused by some attraction, density affects some important steps in the production process such as absorption on surface and separation from the mixtures (extraction). The

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need of viscosity can useful to detect various types of fluids mainly liquids on molecular and atomic basis. Temperature dependence of viscous/sticky behavior of inorganic mixture were play on important role for characteristics the materials
In the present work, density, viscosity and ultrasonic sound velocity have been studied in DMF, THF and $CHCl_3$for different concentrations of FCC at 300.15,305.15 and 310.15K.From the experimental data (Table 1 to 9) and figures from 1 to 9 shows variation in density(P), viscosity(η) and ultrasonic sound velocity(U) of pure solvents (DMF, THF and $CHCl_3$) and the solutions of synthesized compound. It is observed that density, viscosity and ultrasonic velocity (U) increases with increase in concentration of the compound due increase in amount of compounds. The increase in temperature a solution causes molecules to speed up and causes slightly further apart, occupying a larger volume that results in a decrease in density. The increase in temperature causes the kinetic or thermal energy to increase and the molecules become more mobile, due which attractive binding energy is reduced and therefore the viscosity is reduced. The temperature variation of the solutions indicates that the strength of intermolecular nitration increases with increase in temperature.

IV. CONCLUSION

In summary, the ultrasonic velocity, density and viscosity measurements of titled (FCC) compound are carried out in various organic solvents at various temperatures. The strong molecular interactions are confirmed. The trends and deviations in derived parameters were confirmed further the existence of strong interactions and dipole-dipole interaction. The linearity in properties concluded the specific interaction between the solute and solvent molecules. At lower values the strong molecular interaction through *H*-bonding. It is confirmed that at low value of concentrations shows the weak interaction among the solute-solvent interaction. This suggests that interactions exist among solute-solute and solute-solvent in these systems.

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