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Synthesis and acoustical studies of some chalcones of furaldehyde in different solvents at 308.15K

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ABSTRACT

Some new chalcones of 2-Furaldehyde have been synthesized and their characterization was done by IR, ^1H NMR, and mass spectral data. Ultrasonic velocities of various solutions of different concentrations of these synthesized compounds in dimethyl formamide and chloroform have been measured at 308.15 K by using single crystal interferometer at a frequency of 2 MHz. The density and viscosity have also been measured by pycnometer and Ubbelhode viscometer. Using these experimental data, various acoustical parameters are calculated, which are interpreted in terms of solute-solute and solute-solvent interactions in different solutions.

Keywords: 2-Furaldehyde, chalcone, Ultrasonic velocities, chloroform, dimethylformamide.

INTRODUCTION

Literature survey shows synthesis of chalcones by a number of workers [1-6]. Many Chalcones are known to exhibit various biological properties such as antimalarial, antifungal, antibacterial activity [7-9]. In our previous publications, we have studied acoustical studied of some Schiff bases [10, 11]. In continuation, in the present paper, acoustical properties of some chalcones have been studied in DMF and chloroform 308.15 K to understand the molecular interactions in these solutions.

MATERIALS AND METHODS

Synthesis:

A mixture of 2-Furaldehyde derivative (0.01 M) and substituted acetophenone (0.01 M) was stirred for 24 hours in presence of NaOH as catalysis. The product was isolated and crystallized from ethanol. All the synthesized compounds were recrystalized from ethanol. The purity of compounds was checked by thin layer chromatography. The characterizations of all the synthesized compounds were done by IR, ^1H NMR and Mass spectral data.

Reaction scheme

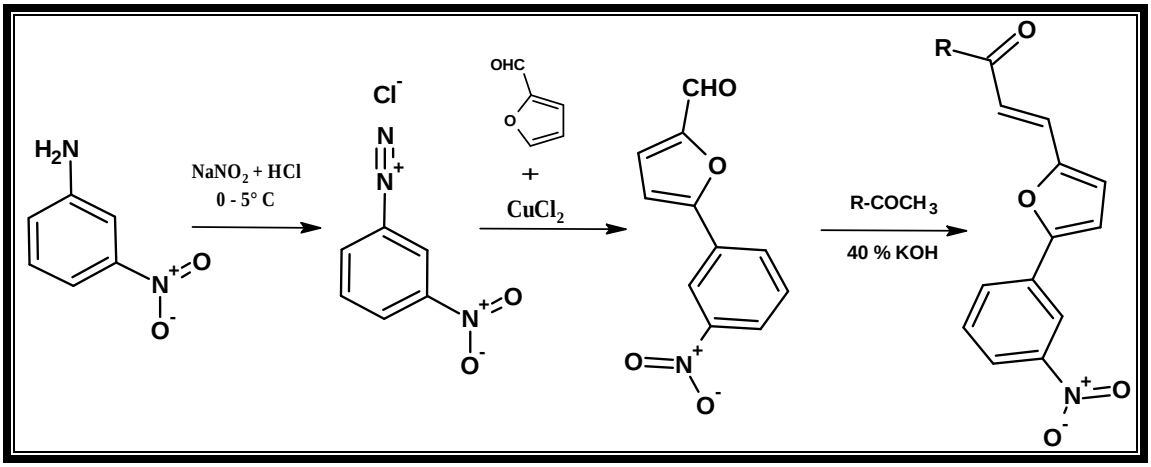


Figure 1 shows the structure of these synthesized compounds along with their IUPAC names. The physical properties of these synthesized compounds are given in Table 1.

Acoustical properties:

The solvents DMF and chloroform used in the present work were of AR grade and were purified according to the standard procedure described in the literature [12]. The computation of ultrasonic and thermodynamic properties require the measurements of ultrasonic velocity (U), viscosity (η) and density (ρ).

The densities of pure solvents and their solutions were measured by using a single capillary Pyknometer, made of borosil glass havinρg a bulb capacity of 10 ml. The ultrasonic velocity of pure solvents and their solutions were measured by using Single Crystal Variable Path Ultrasonic Interferometer operating at 2 MHz. The accuracy of density and velocity are ± 0.0001 g/cm^3 and ± 0.1% cm/sec respectively. Viscosity of pure solvents and solutions were measured by an Ubbelohde viscometer with an accuracy of 0.05%. All the measurements were carried out at 308.15 K. The uncertainty of temperature is ± 0.1 K and that of concentration is 0.0001 moles /dm^3.

The experimental data of ultrasonic velocity, density and viscosity are given in Table 2.

RESULTS AND DISCUSSION

From the experimental data of density, viscosity and ultrasound velocity of pure solvent and solutions, various acoustical parameters were calculated using following standard equations.

Isentropic compressibility (κ_S): $\kappa_S = 1/ (U^2\rho)$

Intermolecular free path length (L_f): $L_f = K_J \kappa_S^{1/2}$

where K_J is Jacobson constant (= 6.0816 x 10^4).

Rao's molar sound function (R_m): $R_m = (M/\rho)\, U^{1/3}$
where M is the molecular weight of solution.

Van der Waal's Constant (b): $b = (M/\rho)\,(1-RT/MU^2\,(\sqrt{(1+MU^2/3RT)}-1))$
where R is gas constant and T is absolute temperature.

Molar Compressibility (W): $W = (M/\rho)\,\kappa_S^{-1/7}$

Solvation number (S_n): $S_n = M_2/M_1\,[1-\kappa_S/\kappa_{S\,1}]\,[(100-X)/X]$
where X is the number of grams of solute in 100 gm of the solution. M_1 and M_2 are the molecular weights and κ_{S1} and κ_S are isentropic compressibility of solvent and solute respectively.

Apparent Molar Volume (Φ_V): $\Phi_V = [M/\rho]-[(1000\{\rho-\rho_o\})/(\rho C)]$
where ρ and ρ_o are the densities of solutions and solvent respectively and C is the concentration of the solution in molarity.

Apparent Molar Compressibility(Φ_k):
$\Phi_k = [(\rho_o\kappa_S - \rho\kappa_{S1})\,(1000/C\rho_o)] + [\kappa_{S1}\,M_2/\rho_o]$
where M_2 is the molecular weight of the compounds.

Some of these acoustical parameters are given in Table 3. In both DMF and chloroform solutions, density (ρ), ultrasonic velocity (U) and viscosity (η) values increase with concentration for all the compounds. Figure 2 shows the variation of Ultrasonic velocity (U) of Chalcones in DMF and chloroform at 308.15 K. It is clear from Figure 2 that the increase is less pronounced in chloroform than DMF. The increase in velocity is reverse of intermolecular free path length (L_f). In a solution, when molecules of solute and solvent come close to each other, the intermolecular free path length L_f decreases. This causes an increase in ultrasonic velocity. The decrease of L_f values with concentration in both the solvents is shown in Figure 3. Further, in Figure 4, the isentropic compressibility (κ_S) also observed to decrease with concentration in both solvents. The decrease in compressibility is due to aggregation of solvent molecules around solute molecules. Thus, the increase in ultrasonic velocity and decrease in κ_S, L_f and r (in Table 3) with increase in concentration values suggest predominance of solute-solvent interactions in all these systems.

Table 3 shows that molar sound function (R_m), molar compressibility (W), and Vander Waals constant (b) are observed to increase linearly with concentration in all the systems in both the solvents. The linear variation of these acoustical properties indicates the absence of complex formation in these systems. The correlation coefficients along with their correlation equations of these parameters are given in Table 4.

Further, isentropic compressibility, apparent molar compressibility and apparent molar volume of solutions is fitted to Bachem's , Gucker's and Masson's relations:

Bachem's relation : $\kappa_S = \kappa_{S1} + AC + BC^{3/2}$

Gucker's relation : $\phi_k = \phi^\circ_k + S_kC^{1/2}$

Masson's equation: $\phi_v = \phi°_v + S_v C^{1/2}$

Using these equations, values of intercept and slopes were evaluated from their respective plots. Table 5 shows the values of these constants in both the solvents. For DMF, values of A, $\phi°_k$ and $\phi°_v$ are negative for first four compounds, whereas for AKFC-05, these values are positive. The negative A, $\phi°_k$ and $\phi°_v$ again proves predominance of solute-solvent interactions whereas positive values suggest the existence of solute-solute interactions in the system. This is further supported by low values of B in AKFC-05. For other four systems in DMF, B values are high. Similarly, higher S_k and S_v values also suggest predominance of solute-solvent interactions of first four compounds in DMF. In chloroform, all the constants suggest solute-solute interactions for all the compounds. Thus, in chloroform both solute-solute and solute-solvent interactions exist whereas in DMF, mostly solute-solvent interactions predominate.

Figure 1: Structures of synthesized Chalcones along with their IUPAC names

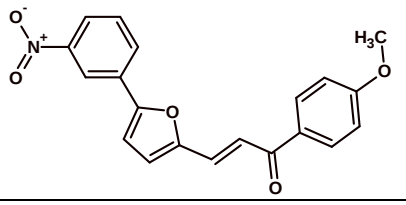
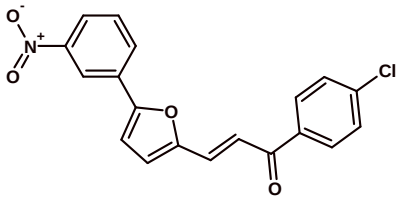
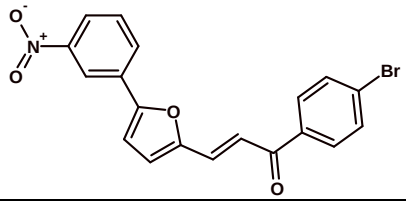
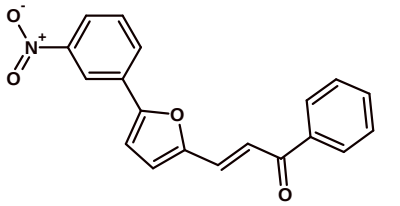
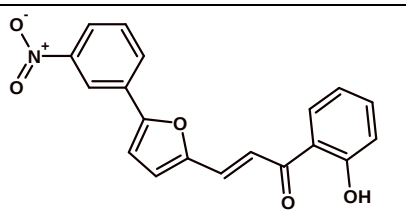
CODES	IUPAC NAME	STRUCTURE
AKFC-01	(2*E*)-1-(4-methoxyphenyl)-3-[5-(3-nitrophenyl)furan-2-yl]prop-2-en-1-one	
AKFC-02	(2*E*)-1-(4-chlorophenyl)-3-[5-(3-nitrophenyl)furan-2-yl]prop-2-en-1-one	
AKFC-03	(2*E*)-1-(4-bromophenyl)-3-[5-(3-nitrophenyl)furan-2-yl]prop-2-en-1-one	
AKFC-04	(2*E*)-3-[5-(3-nitrophenyl)furan-2-yl]-1-phenylprop-2-en-1-one	
AKFC-05	(2*E*)-1-(2-hydroxyphenyl)-3-[5-(3-nitrophenyl)furan-2-yl]prop-2-en-1-one	

Table 1: Physical properties of synthesized chalcones

Sr. No.	Code	R	M.F	M. Wt (g/mol)	R_f	M.P °C	Yield %
1	AKFC-01	$-4C_6H_4-OCH_3$	$C_{20}H_{15}NO_5$	349	0.55	130	75
2	AKFC-02	$-4C_6H_4-Cl$	$C_{19}H_{12}ClNO_4$	353	0.81	170	69
3	AKFC-03	$-4C_6H_4-Br$	$C_{19}H_{12}BrNO_4$	398	0.88	175	72
4	AKFC-04	$-C_6H_5$	$C_{19}H_{13}NO_4$	319	0.54	110	77
5	AKFC-05	$2C_6H_4-OH$	$C_{19}H_{13}NO_5$	335	0.48	142	68

Table-2: Experimental data of density, velocity and viscosity of Chalcones in solutions of different concentrations in DMF and chloroform at 308.15 K

Conc. (M)	Density g. cm^{-3}	Velocity x 10^{-5} cm/s	Viscosity x 10^3 poise	Density g. cm^{-3}	Velocity x 10^{-5} cm/s	Viscosity x 10^3 poise
AKFC-01	**DMF**			**Chloroform**		
0.00	0.9632	1.4448	7.9668	1.4402	0.9941	6.3929
0.01	0.9637	1.4500	7.9532	1.4404	0.9536	6.4693
0.02	0.9653	1.4504	8.0754	1.4406	0.9554	6.5232
0.04	0.9675	1.4533	8.1979	1.4410	0.9568	6.6310
0.06	0.9682	1.4534	8.3055	1.4413	0.9584	6.6401
0.08	0.9703	1.4540	8.4865	1.4416	0.9608	6.7019
0.10	0.9722	1.4555	8.7635	1.4420	0.9655	6.7490
AKFC-02	**DMF**			**Chloroform**		
0.01	0.9643	1.4446	7.9962	1.4405	0.9518	6.4962
0.02	0.9649	1.4450	8.0341	1.4407	0.9532	6.5087
0.04	0.9655	1.4454	8.1050	1.4412	0.9556	6.5901
0.06	0.9677	1.4457	8.2733	1.4416	0.9592	6.6260
0.08	0.9715	1.4463	8.3899	1.4419	0.9616	6.7413
0.10	0.9743	1.4464	8.4883	1.4422	0.9642	6.7877
AKFC-03	**DMF**			**Chloroform**		
0.01	0.9642	1.4402	7.9903	1.4408	0.9502	6.4637
0.02	0.9648	1.4405	8.0231	1.4413	0.9512	6.5493
0.04	0.9654	1.4407	8.1117	1.4418	0.9539	6.6120
0.06	0.9674	1.4413	8.2631	1.4423	0.9578	6.6674
0.08	0.9714	1.4418	8.3814	1.4428	0.9594	6.7110
0.10	0.9744	1.4430	8.4943	1.4431	0.9622	6.8451
AKFC-04	**DMF**			**Chloroform**		
0.01	0.9655	1.4421	8.0188	1.4423	0.9510	6.4743
0.02	0.9663	1.4448	8.0914	1.4426	0.9531	6.5059
0.04	0.9675	1.4464	8.1903	1.4431	0.9554	6.5610
0.06	0.9694	1.4490	8.3362	1.4435	0.9578	6.5780
0.08	0.9704	1.4498	8.4747	1.4439	0.9604	6.6859
0.10	0.9728	1.4518	8.7050	1.4441	0.9644	6.9144
AKFC-05	**DMF**			**Chloroform**		
0.01	0.9230	1.4404	7.6491	1.4412	0.9504	6.4804
0.02	0.9237	1.4402	7.6965	1.4414	0.9529	6.5536
0.04	0.9240	1.4417	7.7252	1.4419	0.9546	6.6163
0.06	0.9241	1.4434	7.8061	1.4423	0.9571	6.6787
0.08	0.9263	1.4437	7.8855	1.4427	0.9595	6.7182
0.10	0.9287	1.4446	7.9886	1.4429	0.9623	6.7496

Table 3: Variation of some acoustical parameters with concentration of Chalcones in DMF and Chloroform at 308.15 K.

Compounds	Conc. (M)	DMF				Chloroform			
		R	b ($cm^3.mol^{-1}$)	$R_m.10^{-3}$ ($cm^{-8/3}.sec^{-1/3}$)	$W.10^{-3}$ ($cm^{-1}.dyn^{-1}$)	r	b ($cm^3.mol^{-1}$)	$R_m.10^{-3}$ ($cm^{-8/3}.sec^{-1/3}$)	$W.10^{-3}$ ($cm^{-1}.Dyn^{-1}$)
AKFC-01	**0.00**	0.1845	75.8806	3.9817	2.2492	0.6140	82.9706	3.8437	2.3410
	0.01	0.1787	76.8804	4.0390	2.2814	0.6448	83.3471	3.8080	2.3239
	0.02	0.1782	77.7869	4.0870	2.3090	0.6434	83.7218	3.8275	2.3357
	0.04	0.1749	79.6672	4.1886	2.3669	0.6424	84.4699	3.8636	2.3576
	0.06	0.1749	81.6655	4.2937	2.4266	0.6412	85.2237	3.9003	2.3799
	0.08	0.1741	83.5254	4.3922	2.4830	0.6394	85.9793	3.9381	2.4028
	0.10	0.1724	85.3882	4.4916	2.5398	0.6358	86.7287	3.9789	2.4272
AKFC-02	**0.01**	0.1848	76.8618	4.0330	2.2786	0.6461	83.3543	3.8059	2.3229
	0.02	0.1843	77.8797	4.0869	2.3092	0.6451	84.7384	3.8253	2.3346
	0.04	0.1838	79.9600	4.1964	2.3713	0.6433	84.5105	3.8639	2.3580
	0.06	0.1835	81.8890	4.2979	2.4294	0.6406	85.2841	3.9041	2.3822
	0.08	0.1829	83.6478	4.3908	2.4832	0.6388	86.0580	3.9428	2.4056
	0.10	0.1828	85.4751	4.4868	2.5386	0.6368	86.8412	3.9822	2.4294
AKFC-03	**0.01**	0.1897	77.1293	4.0430	2.2848	0.6473	83.4688	3.8090	2.3251
	0.02	0.1894	78.5026	4.1152	2.3257	0.6465	83.9727	3.8334	2.3399
	0.04	0.1892	81.2638	4.2602	2.4076	0.6445	85.0120	3.8844	2.3709
	0.06	0.1885	83.8510	4.3964	2.4853	0.6417	86.0474	3.9370	2.4027
	0.08	0.1879	86.2155	4.5209	2.5572	0.6404	87.0877	3.9870	2.4330
	0.10	0.1866	88.6433	4.6495	2.6310	0.6384	88.1332	4.0386	2.4643
AKFC-04	**0.01**	0.1876	76.5433	4.0140	2.2684	0.6467	83.1535	3.7957	2.3172
	0.02	0.1845	77.3212	4.0573	2.2930	0.6452	83.4439	3.8117	2.3268
	0.04	0.1827	78.9030	4.1419	2.3411	0.6434	84.0292	3.8416	2.3449
	0.06	0.1797	80.4150	4.2238	2.3878	0.6416	84.6179	3.8717	2.3631
	0.08	0.1788	81.9968	4.3077	2.4355	0.6397	85.2066	3.9021	2.3814
	0.10	0.1766	83.4396	4.3854	2.4802	0.6367	85.8051	3.9350	2.4010
AKFC-05	**0.01**	0.1895	80.2128	4.2048	2.3612	0.6471	83.2617	3.7998	2.3195
	0.02	0.1897	81.1758	4.2551	2.3897	0.6453	83.5929	3.8183	2.3305
	0.04	0.1881	83.2085	4.3631	2.4504	0.6440	84.2598	3.8510	2.3505
	0.06	0.1861	85.2539	4.4721	2.5115	0.6422	84.9301	3.8850	2.3710
	0.08	0.1858	87.0818	4.5683	2.5663	0.6404	85.6020	3.9190	2.3916
	0.10	0.1847	88.8723	4.6633	2.6206	0.6383	86.2820	3.9540	2.4126

Table 4: The correlation coefficient (γ) and correlation equations between some acoustical parameters and concentration (C) of Chalcones in DMF and Chloroform at 308.15 K

Parameter	Compounds	DMF		Chloroform	
		γ	Correlation equation	γ	Correlation equation
$R_m.10^{-3}$ ($cm^{-8/3}.sec^{-1/3}$)	**AKFC-01**	0.9998	R_m-5.0844C=3.9854	0.9996	R_m-1.8822C=3.7888
	AKFC-02	0.9991	R_m-5.0751C=3.9858	1.0000	R_m-1.961C=3.7860
	AKFC-03	0.9993	R_m-6.7423C=3.9825	0.9999	R_m-2.5569C=3.7828
	AKFC-04	0.9998	R_m-4.1463C=3.9740	0.9998	R_m-1.5358C=3.7803
	AKFC-05	0.9994	R_m-5.187C=4.1549	0.9999	R_m-1.7027C=3.7832
$W.10^{-3}$ ($cm^{-1}.dyn^{-1}$)	**AKFC-01**	0.9999	W-2.8828C=2.2522	0.9997	W-1.1388C=2.3123
	AKFC-02	0.9992	W-2.8882C=2.2525	1.0000	W-1.1843C=2.3109
	AKFC-03	0.9993	W-3.8453C=2.2499	1.0000	W-1.5499C=2.3092
	AKFC-04	0.9998	W-2.3575C=2.2459	0.9998	W-0.9246C=2.3079

	AKFC-05	0.9994	W-2.9029C=2.3333	0.9999	W-1.0293C=2.3094
b ($cm^3 . mol^{-1}$)	**AKFC-01**	0.9990	b-127.9303C=75.9911	1.0000	b-37.5939C=82.9693
	AKFC-02	0.9990	b-95.6866C=76.0084	1.0000	b-38.7234C=82.9637
	AKFC-03	0.9999	b-95.0371C=75.9086	1.0000	b-51.8644C=82.9406
	AKFC-04	0.9998	b-76.9218C=75.7955	1.0000	b-29.4448C=82.8547
	AKFC-05	0.9993	b-96.9416C=79.2921	1.0000	b-33.5441C=82.9216

Table 5: Bachem's, Gucker's and Masson's constants of Chalcones in DMF and Chloroform at 308.15 K.

Compounds	**A x 10^{11} $dyn^{-1} cm^{-3} .mol^{-1}$**	**B x 10^{11} $dyn^{-1} cm^{-1/2} .mol^{-3/2}$**	**$\phi°_K$ x 10^8 $dyn^{-1}.mol^{-1}$**	**S_K x 10^8 $dyn^{-1} cm^{-3/2} .mol^{-3/2}$**	**$\phi°_v$ $cm^3.mol^{-1}$**	**S_v $cm^3.mol^{-1}$**
DMF						
AKFC-01	-14.00	33.33	-26.00	70.00	-2220.00	5777.77
AKFC-02	-11.40	28.00	-28.00	60.00	-2060.00	5200.00
AKFC-03	-9.20	21.80	-17.50	45.45	-2020.00	5333.33
AKFC-04	-11.40	26.60	-23.00	60.00	-2180.00	5600.00
AKFC-05	1.70	6.42	4.10	8.30	126.00	300.00
Chloroform						
AKFC-01	30.00	80.00	33.00	90.36	68.50	16.66
AKFC-02	32.00	90.90	40.00	100.00	59.50	54.54
AKFC-03	31.00	88.88	35.00	100.00	23.50	142.85
AKFC-04	32.00	88.88	33.00	88.88	6.00	120.00
AKFC-05	33.00	90.90	33.00	90.90	31.50	116.66

Figure 2: Variation of Ultrasonic velocity (U) of Chalcones in [A] DMF and [B] Chloroform at 308.15 K.

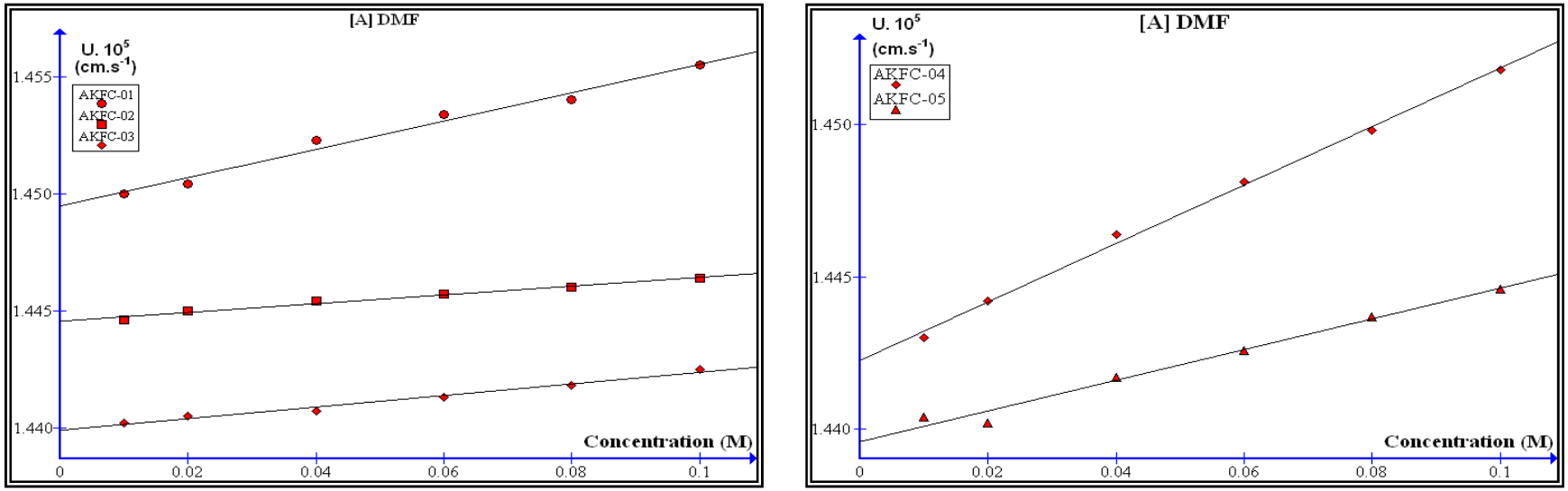
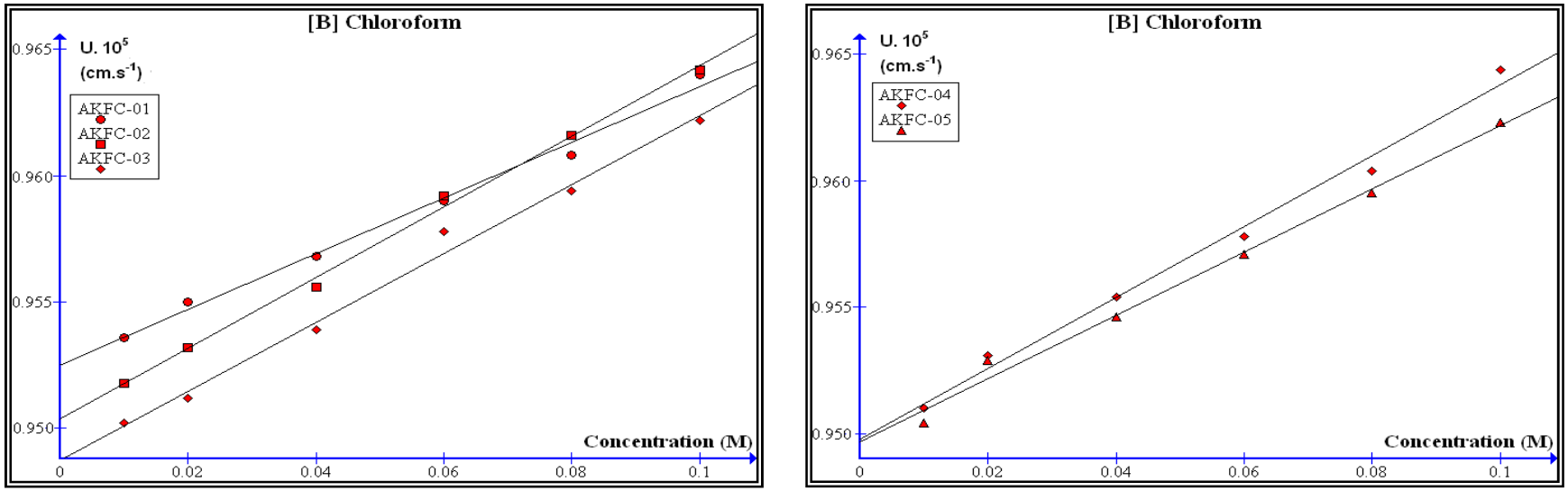


Figure 3: Variation of Intermolecular free length (L_f) of Chalcones in [A] DMF and [B] Chloroform at 308.15 K.



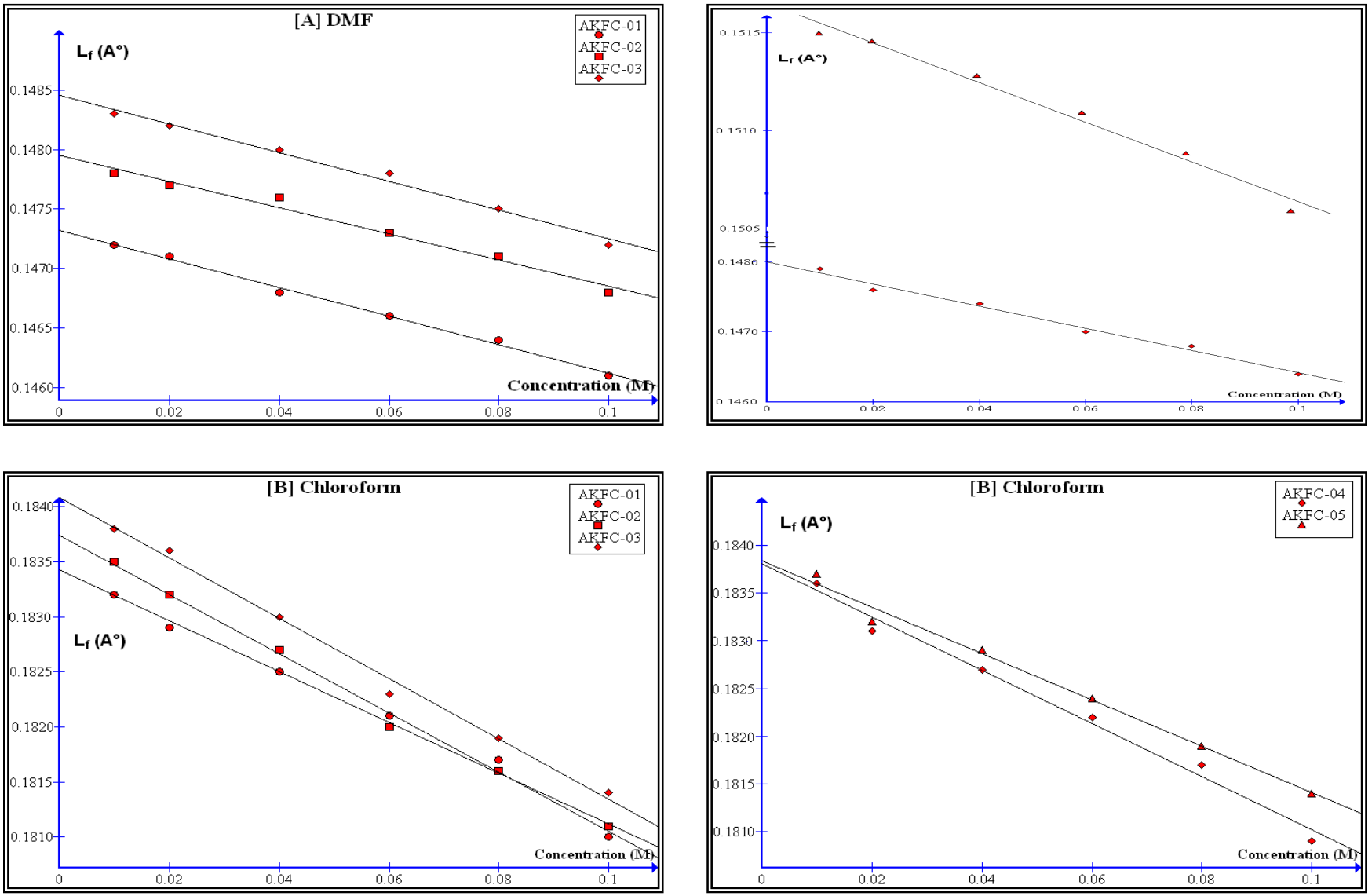
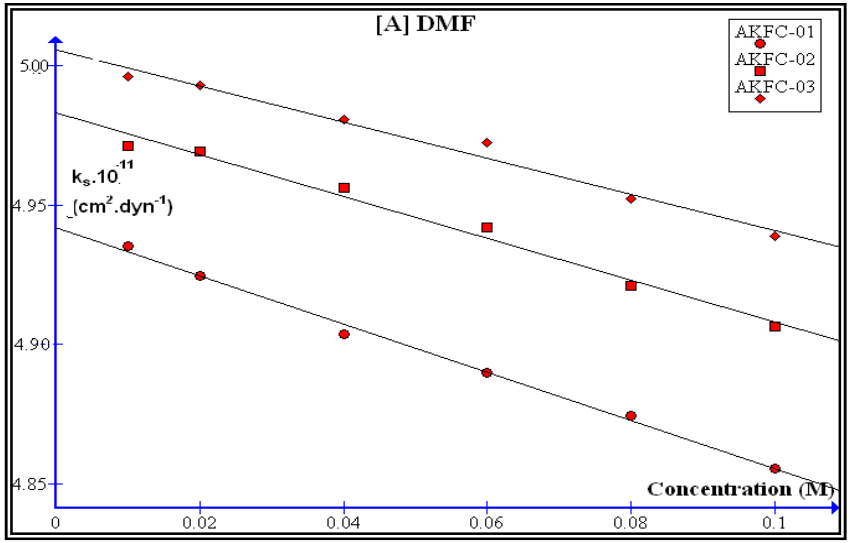
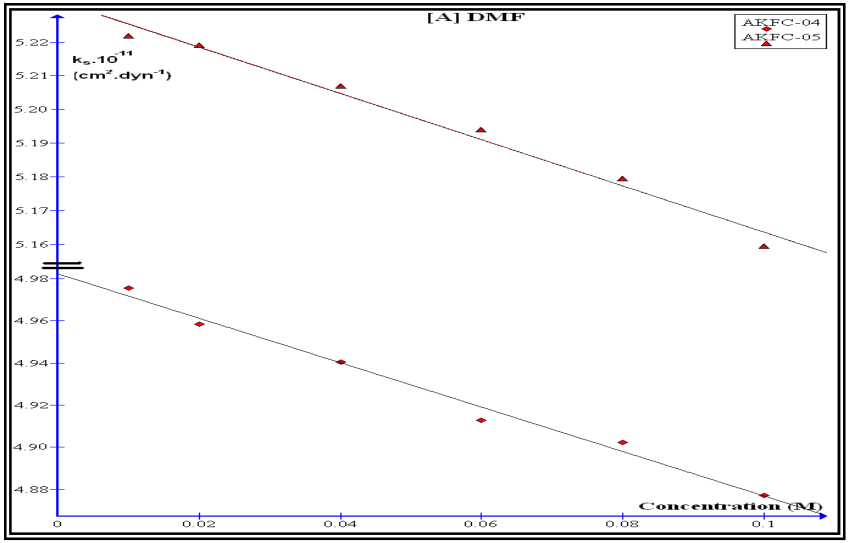
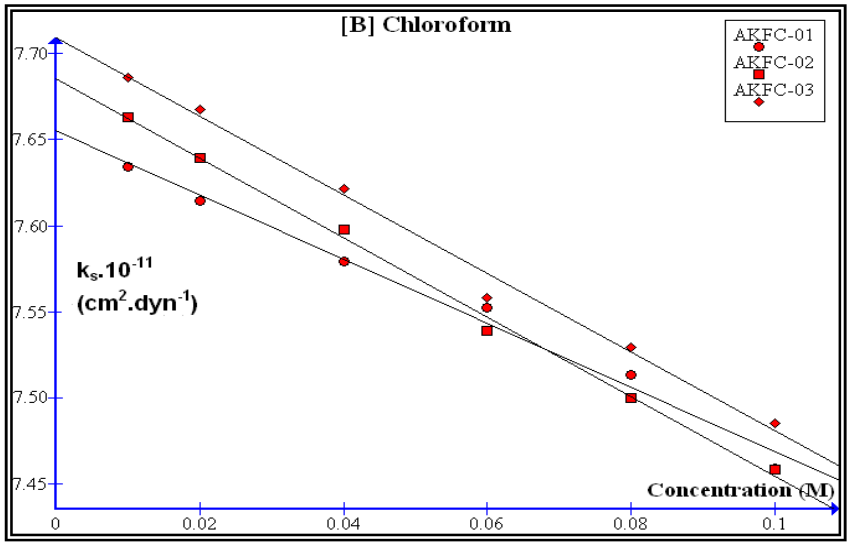
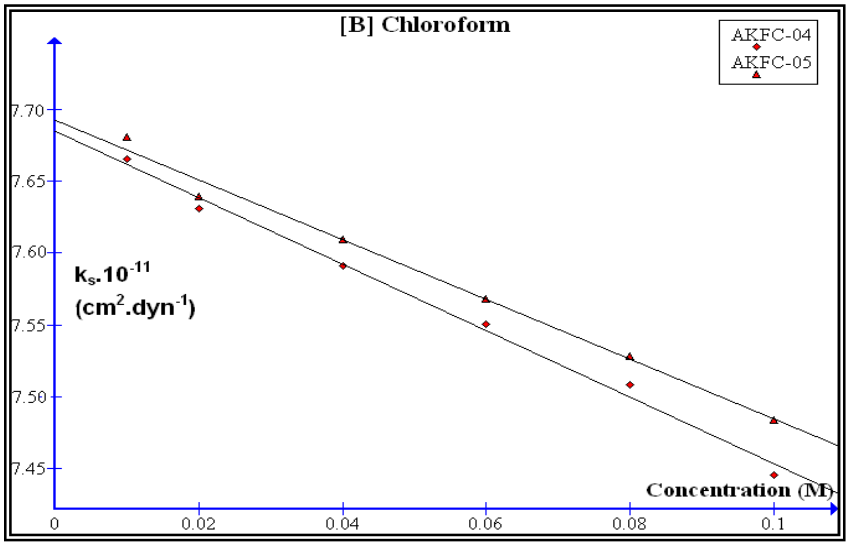


Figure 4: Variation of Isentropic compressibility (κ_s) of Chalcones in [A] DMF and [B] Chloroform at 308.15 K.


[A] DMF
AKFC-01
AKFC-02
AKFC-03
$k_s.10^{-11}$
$(cm^2.dyn^{-1})$
Concentration (M)
5.00
4.95
4.90
4.85
0
0.02
0.04
0.06
0.08
0.1


[A] DMF
AKFC-04
AKFC-05
$k_s.10^{-11}$
$(cm^2.dyn^{-1})$
Concentration (M)
5.22
5.21
5.20
5.19
5.18
5.17
5.16
4.98
4.96
4.94
4.92
4.90
4.88
0
0.02
0.04
0.06
0.08
0.1


[B] Chloroform
AKFC-01
AKFC-02
AKFC-03
$k_s.10^{-11}$
$(cm^2.dyn^{-1})$
Concentration (M)
7.70
7.65
7.60
7.55
7.50
7.45
0
0.02
0.04
0.06
0.08
0.1


[B] Chloroform
AKFC-04
AKFC-05
$k_s.10^{-11}$
$(cm^2.dyn^{-1})$
Concentration (M)
7.70
7.65
7.60
7.55
7.50
7.45
0
0.02
0.04
0.06
0.08
0.1

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