Chalcones: A Physicochemical Study

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Abstract— *Some physicochemical properties such as density, refractive index, solubility, conductance, dissociation constant etc. have been studied for some newly synthesized chalcones in different solvents at 308.15 K.*
Keywords—Chalcones, Density, Refractive Index, solubility, Conductance, dissociation constant.

I. INTRODUCTION

The synthesis of chalcones continues to attract much interest in organic chemistry due to its various therapeutic properties [1-8]. These compounds have applications in various other fields also [9, 10]. However, best of our knowledge, very little work is known for their physicochemical properties such as density, refractive index, solubility, conductance, dissociation constant etc.

Refractive Index along with density, molecular mass and specific volume is very useful in the evaluation of various thermodynamics properties of chemical materials. The number of atoms, groups, radicals and bonds present in the compound can also be calculated by refractive index measurement. It has applications in separation techniques, e.g., in ion exchange chromatography of inorganic and organic ionic species [11], for development and test of an integrated micro system for HPLC separation and detection [12, 13] etc. Conductometry method is useful to various biological processes [14-19]. Solubility is one of critical physicochemical properties for pharmaceutical compounds. Further, solution crystallization is a key step for industrial purification process, which control product quality such as purity, yield, and crystal size distribution [20-22]. The dissociation constant plays an important role in various analytical processes and is used to determine stereo-chemical and conformational structures, directions of nucleophilic and electrophilic attack, stability of intermediates etc.[23,24] The knowledge of dissociation constant is important to understand transport behavior, solubility, binding to receptors, lipophilicity and mechanism of action of certain pharmaceutical samples [25].

Thus, the present work was undertaken to study some physicochemical properties such as density, refractive index, dissociation constant and conductance of some newly synthesized chalcones in solutions of different solvents.

II. EXPERIMENTAL

Overall, ten different chalcones have been synthesized and their general structure is given in Figure 1. The structures of all the synthesized compounds were confirmed by IR, 1H NMR and mass spectral data. Table 1 shows the physical parameters of synthesized chalcones.

Physicochemical studies: All the synthesized chalcones were recrystallized from DMF. The solvents dimethyl formamide (DMF), 1, 4-dioxane (DO), chloroform ($CHCl_3$) and dimethyl sulfoxide (DMSO) were used for the physicochemical studies. All these solvents were purified by standard methods [26]. The purity of DMF was confirmed by GC-MS (SHIMADZU-Model No.-QP-2010) equipped with column (DB-5MS, 25 m in length, 0.20 mm internal diameter and 0.33μm film) and was found to be 99.99%. For the determination of dissociation constant, DMF: water binary mixture was used. The selection of solvents in different physicochemical study is due to solubility and other practical problems.

2.1. Density and refractive index: Solutions of different concentrations were made in DMF and DMSO of all the synthesized compounds. The density and refractive index of pure solvents and of solutions were measured at 308.15 K by pyknometer and Abbe refractometer respectively. The temperature was maintained by circulating water through jacket around the prisms of refractometer from an electronically controlled water bath (NOVA NV-8550 E). The uncertainty of temperature was $\pm$ 0.1^{0}C and that of density and refractive index was $\pm$ 0.0001 g/cm^3 and 0.0005 respectively.

2.2. Conductance: Solutions of different concentrations were made in DMF and $CHCl_3$ of all the synthesized compounds. The conductance of pure solvents and of solutions was measured using Equip-tronics conductivity meter (Model No. 664) at 308.15 K. The cell constant was 0.85 cm^{-1} at 308.15 K.

2.3. Solubility: The solubility measurement was carried out by gravimetric method. An excess mass of synthesized

compound were added to a known mass of solvent. The solution was heated at constant temperature with continuous stirring until equilibrium established. After few hours the stirring was stopped and the solution was kept at constant temperature for 2 hours. After 2 hours the change in concentration was less than 1%. So this solution was filtered and 2 ml of the solution was taken in pre weighted measuring vial. This vial was instantly weighted to determine the mass of the sample and then kept in vacuum oven at 318.15 K to evaporate solvent present in it. When in the vial mass of residue reached to the constant value then the final mass of residue was recorded. The weights were taken in electronic balance (Mettler Toledo AB204-S, Switzerland) with uncertainty of ±0.0001 g. During the whole experiment, at each temperature the measurement was conducted three times and average value was used to determine the mole fraction solubility of solute (x_i) in solvents by using equation 1 and given in Table 4.

$$x_i = \frac{m_2/M_2}{m_1/M_1 + m_2/M_2}$$

where, M_1 and M_2 is the molecular weight of solvent and compound respectively. m_1 and m_2 are weights of solvent and synthesized compound in the solution respectively.

2.4. Dissociation constant: 100 ppm solution of sample was prepared in DMF. This solution known as standard solution was used to determine λ_{max} using UV spectrophotometer (SHIMADZU PHARMA SPEC-1700 UV VISIBLE) equipped with 1 cm path length cell, controlled by computer. The instrument was calibrated by usual procedure.

For all the synthesized compounds, following two sets of mixtures were prepared.
(1) 2 ml HNO_3 (0.01 M) + 4 ml $NaNO_3$ (0.01 M) + 19 ml DMF
(2) 2 ml HNO_3 (0.01 M) + 4 ml $NaNO_3$ (0.01 M) + 2 ml ligand solution (15 ppm) + 17 ml DMF

Thus, total volume of each set of solution was 25 ml and DMF: water ratio was 90:10(v/v).

For each set of solution, pH and absorbance were measured after each addition of 0.1 ml NaOH till there was no change in absorbance. A Systronic pH meter (Model No. EQ 664) was used for the pH determination. pH meter was calibrated by known buffer solutions. The glass electrode and a saturated calomel electrode were used as indicator and reference electrodes respectively.

III.   RESULTS AND DISCUSSION

Table 1 shows physical constants such as molecular formula, molecular weight, melting point, % yield, R_f values etc. of all the synthesized compounds.

3.1. Density and Refractive index: The density of each compound was evaluated using the following relation:

$$1/\rho_{12} = g_1/\rho_1 + g_2/\rho_2$$

where ρ_1, ρ_2 and ρ_{12} are the density of pure solvent, pure solute (i.e., synthesized compound) and solution respectively. g_1 and g_2 are the weight fractions of solvent and solute respectively. The slope of plot of $1/g_1\rho_{12}$ versus g_1/g_2 gives $1/\rho_2$.

Theoretically also, density of compounds can be evaluated using the equation:

$$\rho = KM/N_A\sum\Delta V_i$$

where ρ the density of the compound, K is packing fraction (0.599), M is the molecular weight of the compound, N_A is the Avogadro's number and ΔV_i is the volume increment of the atoms and atomic groups present in the compound. Table 2 shows the experimental and theoretical values of density.

It is observed that there is deviation between experimental and theoretical density values. Further, for the same compound, density in the two solvents is different. The values are much higher in chloroform than in DMF. The different values in different solvents suggest that interactions play an important role. In solutions, molecular interactions exist which differ in different solvents. Further, these interactions differ due to different substitutions in compounds. Due to these interactions, there may be some changes in volume, which affects density. Thus, different density values in different solvents and deviation between experimental and theoretical density values suggest the presence of intermolecular interactions between solute and solvent molecules.

Further, using Lorentz and Lorentz equations [27], molar refraction of pure liquid and solutions can be determined.
For pure liquid:

$$(MRD) = [(n^2-1)/(n^2+2)].M/\rho$$

where n, M and ρ are refractive index, molecular weight and density of pure liquid respectively.

For solutions:

$$(MRD)_{12} = [(n^2_{12}-1)/(n^2_{12}+2)].(X_1M_1+X_2M_2)/\rho_{12}$$

where n_{12} and ρ_{12} are refractive index and density of the solution respectively. X_1 and X_2 are the mole fractions and

M_1 and M_2 are the molecular weight of the solvent and compound respectively.

From these values of molar refraction of solutions and pure solvents, molar refractions of solid compounds were calculated by the following equation:

$$(MRD)_{12} = X_1(MRD)_1 + X_2(MRD)_2$$

From the density and molar refraction data, the refractive indexes of all the compounds were calculated using above equation and are given in Table 3.

It is observed that both $(MRD)_2$ and refractive index of compounds are different in each solvent. This again proves that in different solvents, inter molecular interactions are different which affects these parameters. In some solvents, aggregation or hydrogen bonding takes place whereas in others, breakage of bonds takes place. As refractive index and molar refraction depends not only upon atomic refraction but also on single, double or triple bonds, these parameters are affected by the type of interactions taking place in solution.

3.2. Conductance: The measured conductance of all the compounds in studied solvents was corrected by subtracting the conductance of pure solvent. Using corrected conductance (k), specific conductance (κ) and equivalent conductance (λ_C) were evaluated. The equations used for calculating specific conductance (κ) and equivalent conductance (λ_C) are:

$$\kappa = k\theta$$
$$\lambda_C = \frac{1000.\kappa}{C}$$

where θ is the cell constant and c is the concentration (g. equi./lit) of solution. Table 4 shows equivalent conductance for all the chalcone compounds in DMF and chloroform solutions.

Figure 1 shows the variation of conductance with concentration for both the solvents. It is observed that for all the systems studied, conductance increases with concentration and values are less in $CHCl_3$ than that in DMF. Further, at low concentrations, as concentration increases, there is linear increase in conductance with concentration. However, at higher concentration, increase is non-linear.

Figure 2 shows variation of equivalent conductance against square root of concentration for $CHCl_3$ and DMF. It is obvious from these figures that for compounds exhibit different nature in different solvents. Some chalcones (AKFC-05, AKFC-06 and AKFC-10) exhibit weak electrolytic in nature in DMF. However, in $CHCl_3$ strong electrolytic behavior is observed. For weak electrolytes, it is difficult to determine λ_0. However, in the studied solutions of compounds, λ_0 values are evaluated approximately by extrapolation method and are given in Table 5. In some compounds, λ_0 values could not be evaluated by extrapolation due to weak electrolytic nature of compound.

3.3. Solubility: The solubility (x) of synthesized compounds in DMF and 1, 4-dioxane is shown in Figure 3. It is evident that the solubility increases with temperature in both the solvents. Comparison of solubility in the two solvents shows that overall solubility is greater in DMF than that in 1, 4-dioxane. This is expected because the dielectric constant and dipole moment of DMF (36.71, 3.86) are greater than that of 1, 4-dioxane (2.209, 0). Thus, these properties of solvent play an important role on the solubility.

The temperature dependence solubility in solvents is described by the modified Apelblat equation [28]:

$$ln\ x_i = A + B/T + C\ ln(T)$$

where x_i is the solubility of compounds; T is the absolute temperature and A, B and C are the coefficients. The values of these coefficients were evaluated from the ln x verses T and are given in Table 4. Using these values of A, B and C, calculated solubility were evaluated and are plotted in figure 3 along with experimental solubility data. It is observed from figure 3 that there is good agreement between experimental and calculated values.

According to van't Hoff analysis [29], the standard enthalpy change of solution is obtained from the slope the *ln x* versus *1/T* plot. However, in recent thermodynamic treatment, some modifications have been introduced in the van't Hoff equation to diminish the propagation of errors and consequently to separate the chemical effects from those due to statistical treatment used when enthalpy-entropy compensation plots are developed [30]. For this reason, the The mean harmonic temperature (T_{hm}) is used in van't Hoff analysis, which is calculated by the following equation:

$$T_{hm} = \frac{n}{\sum_{i=1}^{n}\left(\frac{1}{T}\right)}$$

where *n* is the number of experimental temperatures studied. The T_{hm} value calculated by this equation is found to be 307.93 K.

So, the modified Van't Hoff equation is [31]:

$$\left(\frac{\partial\ ln\ x_i}{\partial\left(\frac{1}{T} - \frac{1}{T_{hm}}\right)}\right)_P = -\frac{\Delta H_{sol}}{R}$$

where ΔH_s is the heat of solution and R is the gas constant. The change in Gibb's free energy during solubility process can be calculated by intercept of the plot of lnx_i versus ($1/T$ - $1/T_{hm}$) by following equation:

$$\Delta G_{sol} = -R \times T_{hm} \times Intercept$$

Finally, the entropy of solution (ΔS_{sol}) was obtained from these evaluated ΔH and ΔG values at T_{hm} [31].

$$\Delta S = \frac{(\Delta H - \Delta G)}{T_{hm}}$$

All the thermodynamic parameters are given in Table 5. It is evident from tablets that for all the compounds ΔH_s and ΔG values are positive whereas ΔS values are negative. When stronger bonds are broken and weaker bonds are formed, energy is consumed and so, ΔH_s become positive [32]. This indicates endothermic dissolution of compounds where the enthalpy term contributes to an unfavorable positive value of ΔG. Thus, positive values of ΔG indicate that the dissolution process is not spontaneous [32]. The negative entropy indicates less randomness in solutions [32].

3.4. Dissociation constant: The dissociation constant or pK_a of a compound is determined by the equation:

$$pK_a = pH + log\frac{[BH^+]}{[B]}$$

Rearrangement of above equation gives:

$$log\frac{[BH^+]}{[B]} = pH - pK_a$$

A plot of left hand side versus pH will yield a straight line and $pH = pK_a$ when ratio of log $[BH^+]/[B] = 0$. [33].
The concentrations of BH^+ and B can be determined spectrophotometrically by measuring the absorbance at particular wavelength.
Table 6 shows the pK_a values for the studied compounds. It is observed that substitution group affects the dissociation constant as expected. It is observed that the NH_2 groups at para position of the phenyl ring makes AKFC-4 the least acidic or most basic one, whereas AKFC-5 is found to be most acidic due to the halogen (Cl).

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Table.1: Physical constants and substitutions groups of synthesized Chalcones.

S. No.	Compd. Code	R	Mol. Wt (g.mol^{-1})	R_f* value	Melting point (^{0}C)	Yield %
1	AKFC-1	4-OCH$_3$-C$_6$H$_6$	349.33	0.48	141	58
2	AKFC-2	4-Cl-C$_6$H$_6$	353.75	0.42	170	60
3	AKFC-3	4-Br-C$_6$H$_6$	398.20	0.48	160	68
4	AKFC-4	--C$_6$H$_6$	319.31	0.47	142	60
5	AKFC-5	4-OH-C$_6$H$_6$	335.31	0.51	152	56
6	AKFC-6	2-Furan	309.27	0.57	178	55
7	AKFC-7	3-coumarin	387.34	0.48	172	62
8	AKFC-8	4-NO$_2$-C$_6$H$_6$	364.30	0.50	218	54
9	AKFC-9	3-NO$_2$-C$_6$H$_6$	364.30	0.54	180	62
10	AKFC-10	4-NH$_2$-C$_6$H$_6$	334.32	0.44	171	58

*Hexane:Ethyl acetate-8:2

Table.2: Experimental and theoretical values of density of synthesized Chalcones.

Compound Code	Experimental density, g. cm^{-3}		Theoretical density, g. cm^{-3}
	DMF	CHCl$_3$	
AKFC-1	1.2235	1.5172	1.2504
AKFC-2	1.2918	1.5270	1.2628
AKFC-3	1.2593	1.5494	1.4439
AKFC-4	1.2255	1.5962	1.2760
AKFC-5	1.3077	1.5530	1.2314
AKFC-6	1.1766	1.5773	1.3345
AKFC-7	1.1660	1.5579	1.3469

Table.3: Molar refraction ((MRD)$_2$) and refractive index (R.I) of synthesized Chalcones.

Compound Code	Solvents			
	DMF		CHCl$_3$	
	(MRD)$_2$	R.I	(MRD)$_2$	R.I
AKFC-01	113.11	1.3653	0.2912	1.7241
AKFC-02	125.92	1.4125	118.12	1.6905
AKFC-03	142.11	1.4145	120.37	1.5961
AKFC-04	115.25	1.4190	104.22	1.6662
AKFC-05	117.90	1.4066	107.18	1.6477
AKFC-06	103.57	1.3803	97.26	1.3745
AKFC-07	118.15	1.3393	100.44	1.4822

Table.4: The Apelblat parameters for synthesized Chalcones in DMF and 1,4-dioxane.

Compound Code	DMF			1,4-dioxane		
	A	B	C	A	B	C
AKFC-1	-3.9669	-222.3388	0.0377	-4.2285	-99.8093	-0.0623
AKFC-2	-4.0239	-346.9540	-0.0380	-4.4852	-245.88	-0.1053
AKFC-3	-4.1932	-151.6230	0.0446	-4.3198	-154.4350	-0.0850

AKFC-4	-3.9961	-160.5220	-0.0156	-4.2347	-184.304	-0.0602
AKFC-5	-4.23	-181.9430	-0.0304	-4.3119	-157.306	-0.0565
AKFC-6	-4.0991	-105.2370	-0.0377	-4.2678	-80.412	-0.0732
AKFC-7	-4.1311	-181.4310	-0.0399	-4.3261	-102.692	-0.0732
AKFC-8	-4.5444	-240.0877	-0.1215	-4.3797	-357.6174	-0.0873
AKFC-9	-4.2338	-151.5785	-0.0645	-4.2988	-122.9682	-0.0724
AKFC-10	-4.7482	-61.5130	-0.1726	-4.5330	-230.727	-0.1238

Table.5: Thermodynamic parameters for synthesized chalcones in DMF and 1,4-dioxane.

Compound Code	DMF			1,4-dioxane		
	ΔH_{Sol} (cal.mol^{-1})	ΔG_{Sol} (kcal.mol^{-1})	ΔS_{Sol} (cal.mol^{-1}.K^{-1})	ΔH_{Sol} (cal.mol^{-1})	ΔG_{Sol} (kcal.mol^{-1})	ΔS_{Sol} (cal.mol^{-1}.K^{-1})
AKFC-1	189.53	2.7447	-8.2977	158.08	3.0040	-9.2422
AKFC-2	421.38	3.6022	-10.3296	421.38	3.6022	-10.3296
AKFC-3	275.29	3.0234	-8.9245	240.22	3.2478	-9.7672
AKFC-4	297.27	2.8185	-8.1877	332.64	3.1681	-9.2082
AKFC-5	370.33	3.0562	-8.7224	303.53	3.1488	-9.2401
AKFC-6	184.46	2.8493	-8.6540	114.44	3.0276	-9.4606
AKFC-7	342.10	3.0281	-8.7229	172.29	3.1077	-9.5326
AKFC-8	403.99	3.6836	-10.6504	644.44	3.6966	-9.9120
AKFC-9	258.92	3.1176	-9.2837	196.67	3.1283	-9.5204
AKFC-10	18.15	3.6324	-11.7373	371.78	3.6658	-10.6974

Table.6: The pK$_a$ values for the studied chalcone compounds.

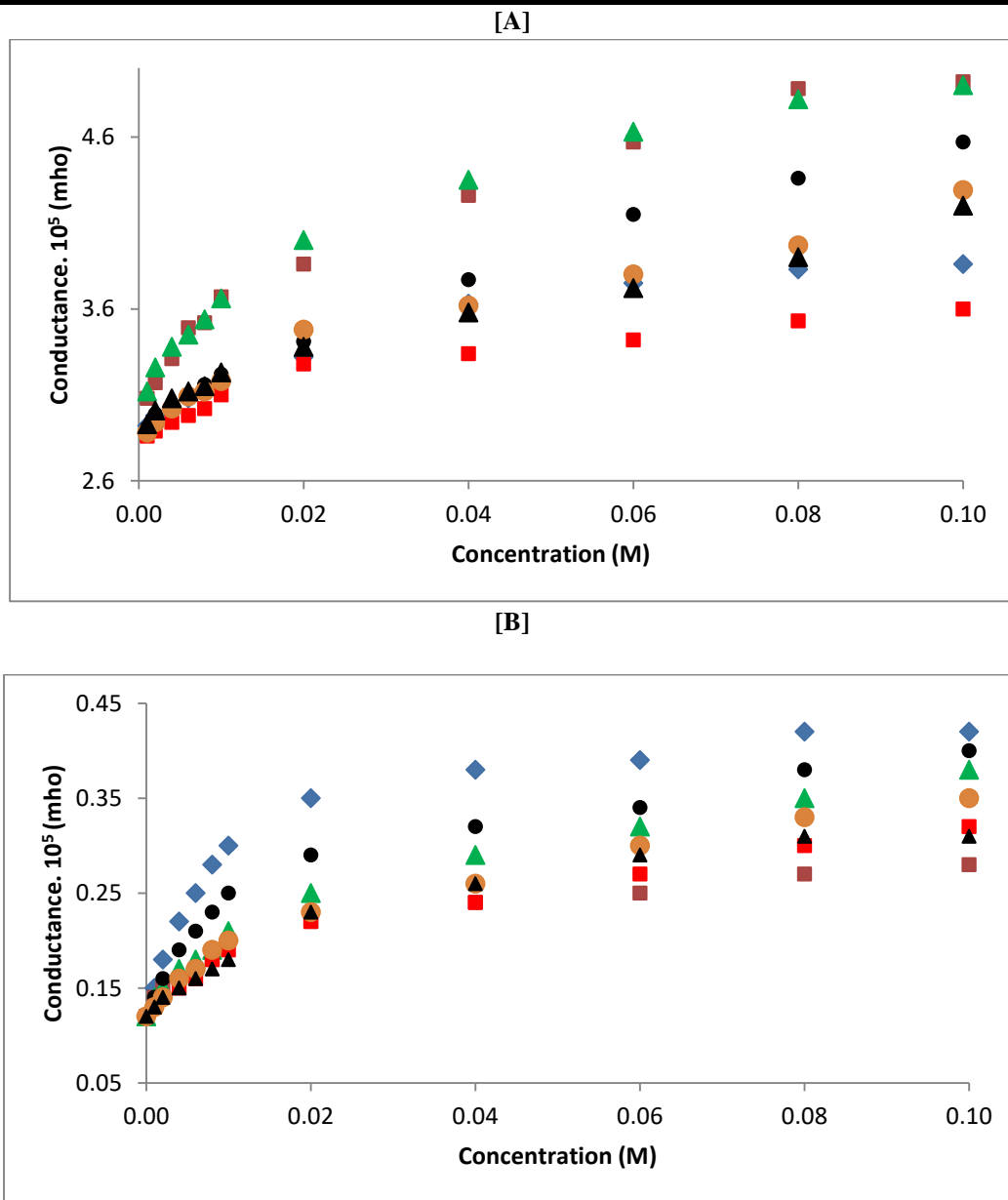| Compound Code	Average pK$_a$
AKFC-1	9.22
AKFC-2	9.31
AKFC-3	9.23
AKFC-4	9.14
AKFC-5	8.87
AKFC-6	8.58
AKFC-7	8.50
AKFC-8	9.21
AKFC-9	8.63
AKFC-10	8.93

[A]

[B]

Fig. 1: Variation of Conductance of Chalcone compounds with concentration in [A]DMF and [B] Chloroform solutions.
(◆): AKFC-1, (■): AKFC-2, (▲):AKFC-3, (●):AKFC-4, (■):AKFC-5, (●):AKFC-6, (▲):AKFC-7
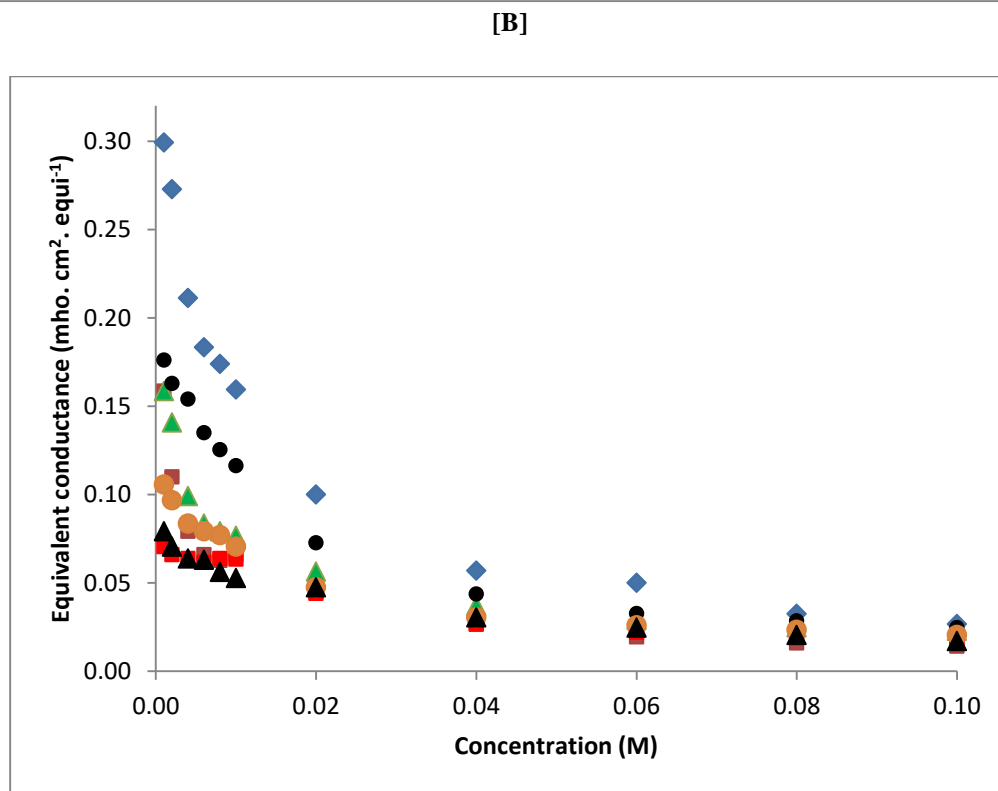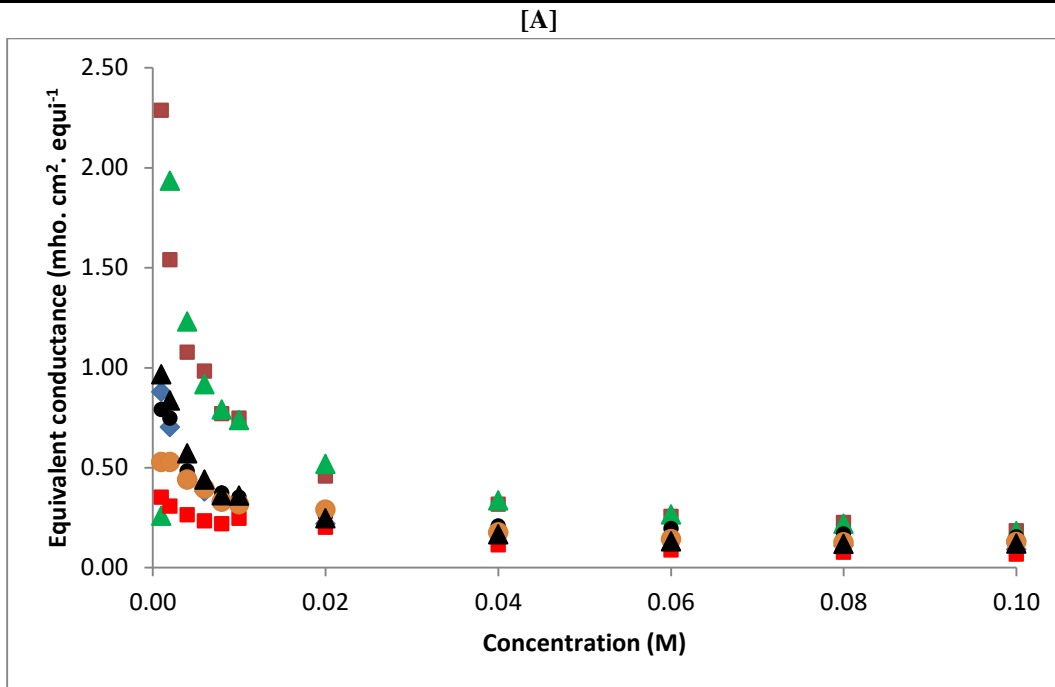
[A]

[B]

Fig. 2: Variation of equivalent conductance of Chalcone compounds with concentration in [A] DMF and [B] Chloroform solutions.

(♦): AKFC-1, (■): AKFC-2, (▲):AKFC-3, (●):AKFC-4, (■):AKFC-5, (●):AKFC-6, (▲):AKFC-7
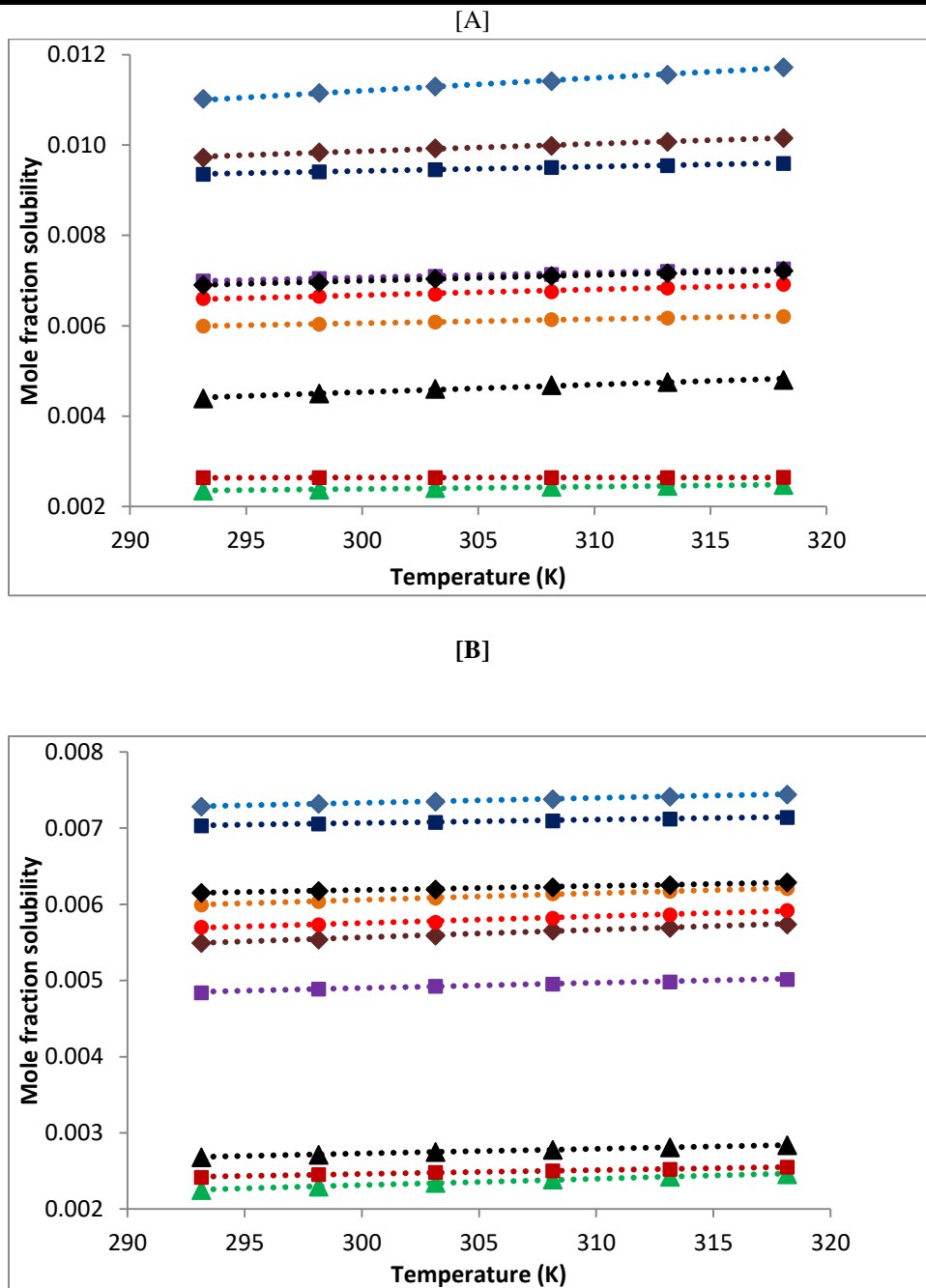
[A]

[B]

Fig. 3: The variation of experimental mole fraction solubilities with temperature for studied compounds in [A] DMF and [B] 1,4-dioxane. Symbols for experimental points and corresponding dotted lines (……) are for calculated mole fraction solubilities by Apelblat equation.
(♦):AKFC-1, (▲):AKFC-2, (■):AKFC-3, (♦):AKFC-4, (●):AKFC-5, (■):AKFC-6, (♦):AKFC-7, (▲):AKFC- 8, (●):AKFC-9,
(■):AKFC-10.