

RESEARCH ARTICLE

Spectral and Ultrasonic Investigation of Hydrogen Bonded Complexes of Cyclohexanol and Aryl Ketones in DMSO Medium

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Received- 23 January 2018, Revised- 20 March 2018, Accepted- 3 April 2018, Published- 10 April 2018

ABSTRACT

UV spectral studies and ultrasonic method are used to investigate the presence of associative interaction between cyclohexanol (CHL) and two aromatic ketones (acetophenone (ACP) and p-nitroacetophenone (PNA)) in DMSO medium. The variation of acoustic parameters with concentration establishes the molecular association in this ternary liquid mixture. The effect of temperature on H-bonding is also studied using acoustic method by determining the acoustical properties at three different temperatures. UV-visible spectral studies are carried out at room temperature (303 K). Ultrasonic velocity plots show the concentrations at which the interaction is strong, and UV spectra are recorded at these specific concentrations. The appearance of new absorptions in UV-visible spectra in the two systems confirms the presence of intermolecular hydrogen bond between CHL and the two aryl ketones.

Keywords: Hydrogen bonded interaction, Cyclohexanol-acetophenone, Cyclohexanol-p-nitroacetophenone, Adiabatic compressibility, Free length, Internal pressure.

1. INTRODUCTION

Hydrogen bond, the most important interactive force among the various types of molecular interactions plays an important role in biological and chemical process. For example water, proteins and DNA, which are the vital factors in biosystems are held together by H-bond networks. The energy of H-bond varies from 10 to 40 k J/mol. With respect to the surroundings, H-bonds form and break easily and hence have on or off biological functions [1]. It is possible to design the novel functional molecules, nanomaterials, and molecular devices both theoretically and experimentally depending on such interactive forces [2]. Dielectric relaxation studies, infrared and UV-visible

spectral techniques and microwave absorption studies are extensively used to explore the molecular structures containing X---H-Y (X and Y are electronegative atoms) bonds in dilute solutions [2, 3]. The sound velocity approach related to the qualitative determination of degree of association in liquid has been specified in [4]. Recently, it is studied that the low amplitude ultrasonic waves can be used to explore the molecular interactions and physico-chemical behaviours of pure, binary, ternary liquid mixtures and suspensions [5-11]. Characterization of the process state can also be done by measuring the velocity of an ultrasonic pulse travelling along a fermentation tank [12]. The molecular association of ternary

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Double blind peer review under responsibility of DJ Publications

<https://dx.doi.org/10.18831/djchem.org/2018011004>

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liquid mixtures containing phenol and o-cresol with dimethyl sulphoxide (DMSO) in CCl_4 has been investigated ultrasonically and studied at different temperatures [13-15]. IR spectral studies support the complex formation and are explained based on the acoustical parameters. [16] has reported the H-bonded interaction between the aromatic amines and aryl ketones in hexane. The complex formation is established by spectrophotometric method and is reported that it can be identified by computing excess parameters in ultrasonic velocity method. Negative values of excess parameters indicate complex formation [17-19]. In this study, an effort has been taken to use UV-visible spectroscopy and ultrasonic method to investigate H-bonded interactions in two ternary systems namely, cyclohexanol-acetophenone and cyclohexanol-p-nitroacetophenone in DMSO medium. The temperature effect on the strength of H-bonded interaction is also studied by measuring density, viscosity and ultrasonic velocity of two systems at different concentrations and varying temperatures at 303, 308 and 313 K.

2. MATERIALS AND METHODS

2.1. Materials

Cyclohexanol, acetophenone, p-nitroacetophenone and DMSO samples are of AnalaR grade, procured from Merck. After checking the boiling point, the samples are used as such. The required concentrations (0.01 M-0.1 M) of the solutions containing equal molar concentration of cyclohexanol and aryl ketone, which are freshly prepared from stock solutions of CHL and aryl ketone (0.2 M) are used.

2.2. Methods

The ultrasonic interferometer supplied by Mittal Enterprises, New Delhi operating at 2 MHz frequency (model F-05) and $\pm 0.1 \text{ m s}^{-1}$ accuracy is used to measure the ultrasonic velocities of pure liquids and mixtures. 10 ml specific gravity bottles are used to measure the accurate densities of pure compounds and their solutions. An electronic balance is used to determine the weight of the samples. Ostwald's viscometer is employed for viscosity measurements.

Thermostat is used to maintain the constant temperature of test solutions. The UV-visible spectra for both the ternary systems are recorded using Systronics smart DBS 2303 spectrophotometer, and quartz cell of optical length 1 cm is used. The relevant equations to compute the adiabatic compressibility, free length and internal pressure are given [20].

3. RESULTS AND DISCUSSION

3.1. UV-visible spectra

The UV-visible absorption spectrum of individual components in DMSO solution and that of the complexes are shown in figure 1 for cyclohexanol-acetophenone system, and in figure 2 for cyclohexanol-p-nitroacetophenone system. The interaction of proton donor (CHL) with proton acceptor (ACP or PNA) is characterized by the appearance of a new absorption band. It may be seen from figure 1 that pure CHL absorbs at 260 nm and 310 nm while pure ACP absorbs at 330 nm and 380 nm. However, the solution containing both CHL and ACP has additional absorption at 310 nm (H-bond complex in figure 1). This additional weak absorption occurs due to the formation of hydrogen bonded complex between CHL and ACP. The characteristic absorption of visible or ultra violet radiation by the H-bonded complex is greater than the wavelength of absorptions by the individual components.

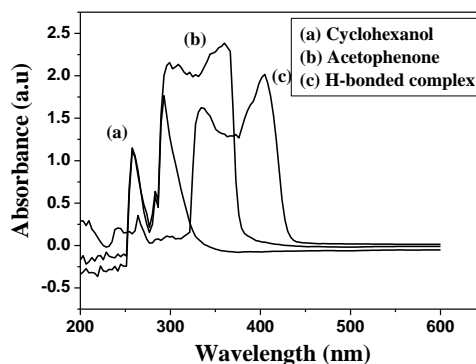


Figure 1. UV-V is absorption spectral (absorbance in absolute unit vs wavelength) of pure components (cyclohexanol, acetophenone) and that of H-bonded complex in DMSO

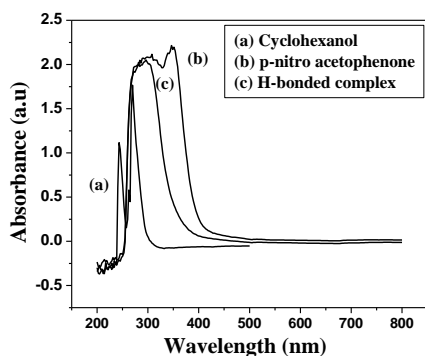


Figure 2. UV-Vis absorption spectra (absorbance in absolute unit vs wavelength) of the pure components (cyclohexanol, p-nitroacetophenone) and that of hydrogen bonded complex in DMSO

Similarly in case of CHL-PNA system, additional peak absorption is obtained at 310-315 nm, and it is relatively a stronger one when compared to the absorption of CHL-ACP system. This suggests that PNA may form relatively stronger hydrogen bonded complex with CHL than ACP.

3.2 Ultrasonic studies

The experimentally measured values of ultrasonic velocity, density and viscosity and acoustic parameters such as adiabatic compressibility, free length and internal pressure for CHL-ACP and CHL-PNA system in DMSO medium at varying temperatures 303 K, 308 K and 313 K are presented in tables A1 and A2 respectively. Figures 3(a) and 3(b) show the plot of ultrasonic velocity vs concentration of cyclohexanol-acetophenone and cyclohexanol-p-nitroacetophenone in DMSO medium. It is seen from the table A1 that the ultrasonic velocity for cyclohexanol-acetophenone system initially decreases and there is a sharp increase above the concentration of 0.03 M. Ultrasonic velocity reaches a maximum value at a specific concentration of 0.06 M with a temperature of 303 K. Similar trend is observed at the other two investigated temperatures, but the peak is shifted towards lower concentration (0.05 M at 308 K and 0.04 M at 313 K). Initial decrease in ultrasonic velocity indicates the breaking of cyclohexanol structure associated with intermolecular hydrogen bond. The structural breaking may be due to the interaction of

molecules of DMSO and ACP with those of CHL.

The maximum velocity indicates the strong molecular interaction hydrogen bond between CHL and ACP at specific concentration. [21] has shown that complex formation between unlike molecules is indicated by the non-linear variation of ultrasonic velocity with concentration. But in the system of cyclohexanol-acetophenone in DMSO, the interaction is found to be H-bonding as shown by UV-visible spectral studies. The spectra are recorded at the concentration, where U is maximum. In case of CHL-PNA system also, similar trend is observed. However, it may be noted that the increase in velocity is not significant above the specific concentration observed in CHL-ACP system. This indicates that the interaction is similar to this system also, but the intermolecular hydrogen bond between CHL and PNA is not as strong as that present in CHL-ACP system. In both the systems, ultrasonic velocity decreases with increase in temperature at a given concentration thereby specifying the decrease in strength of hydrogen bond due to thermal agitation.

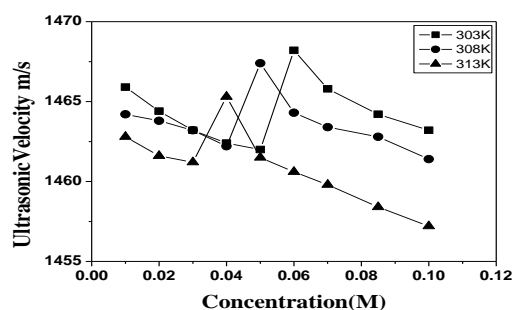


Figure 3(a). Plots of ultrasonic velocity vs concentration of cyclohexanol or acetophenone in DMSO at different temperatures

The adiabatic compressibility (κ) and free length (L_f) are the measures of intermolecular association between the hydrogen donor and acceptor. The non-linear variations in these two parameters indicate strong interaction between solute molecules. The plot of adiabatic compressibility against concentration at different temperatures is depicted in figures 4(a) and 4(b) for the two systems. It is found that these plots

are reverse when compared to the plot in figure 3.

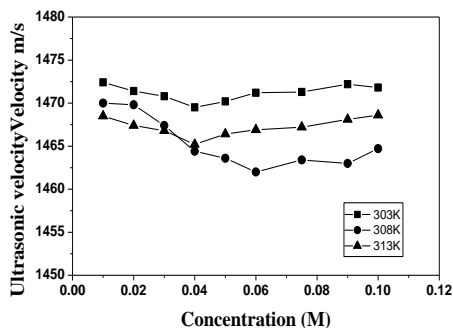


Figure 3(b). Plots of ultrasonic velocity vs concentration of cyclohexanol or p-nitroacetophenone in DMSO at different temperatures

At each temperature, the κ value reaches minimum at specific concentration (figures 4(a) and 4(b)). The adiabatic compressibility shows a decreasing trend with increasing concentration at all three temperatures suggesting that the molecules are more compressible as there is strong interaction between unlike molecules due to H-bonding. The compressibility values are higher at higher temperatures. This is because as temperature increases, the H-bond becomes weaker and the solute molecules are less compact. A minimum in compressibility is observed at 0.06 M for the CHL-ACP system (figure 4(a)) at 303 K but at 308 K and 313 K, the minimum value in the curve is shifted towards lower concentration (0.05 M and 0.04 M respectively). From figure 4, U maxima and κ minima occur at the same concentrations, which specify that there exists a significant interaction between the two solute molecules [22].

Due to these structural characteristics, the compressibility factor changes, thus leading to a change in ultrasonic velocity. In case of liquid mixtures, minimum value of κ indicates the increase in the compactness of the system due to the approach of unlike molecules as a consequence of strong molecular attraction or complex formation [23]. In case of ternary system containing p-nitroacetophenone, there is increase in compressibility at lower concentrations, but as concentration increases, the compressibility decreases slightly (figure 4(b)). This parameter confirms lack of strong interaction between the solute molecules.

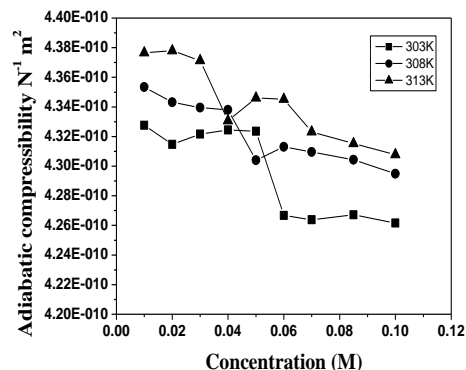


Figure 4(a). Plots of adiabatic compressibility vs concentration of cyclohexanol or acetophenone in DMSO at different temperatures

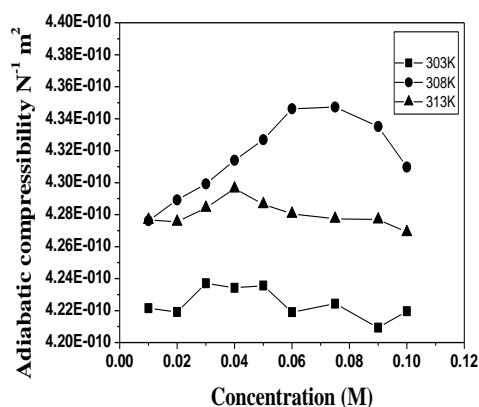


Figure 4(b). Plots of adiabatic compressibility vs concentration of cyclohexanol or p-nitroacetophenone in DMSO at different temperatures

The trend in the variation of κ with concentration is similar at the three temperatures. The variation in κ values with concentration in the two systems also suggests that there is stronger hydrogen bond between CHL and ACP rather than between CHL and PNA. In PNA molecule, the nitro group at para position withdraws electron from the carbonyl oxygen and hence the oxygen in PNA is less electronegative than that in ACP molecule. The internal pressure (π_i) in liquid mixtures is found to be the estimated measure of intermolecular attraction between the components. The values of internal pressure for the two systems are computed and they are listed in tables A1 and A2 respectively.

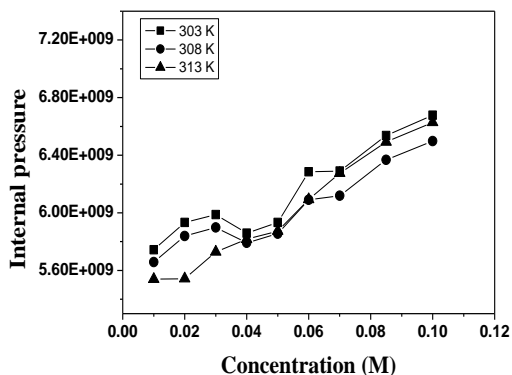


Figure 5(a). Plots of internal pressure (π_i) vs concentration of cyclohexanol or acetophenone in DMSO at 303, 308 and 313 K

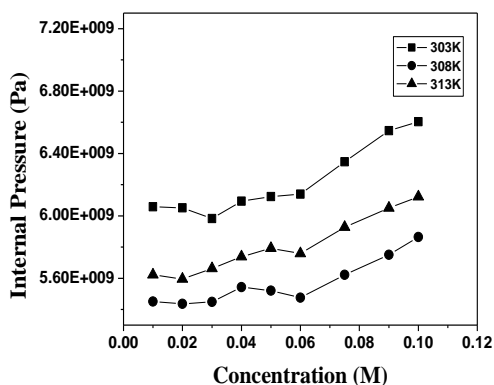


Figure 5(b). Plots of internal pressure (π_i) vs concentration of cyclohexanol or p-nitroacetophenone in DMSO at 303, 308 and 313 K

The plots of internal pressure against concentration for both the systems in DMSO at three different temperatures are given in figures 5(a) and 5(b). The internal pressure shows increasing trend at all three temperatures for both the systems. This indicates that there is a strong solute-solute interaction between the molecules in the two ternary mixtures. The growing affinity between the solute molecules results in H-bonded interaction, which may increase the viscous force, and it is well established by the increasing trend in the internal pressure. Since, H-bonded interaction between the -OH hydrogen and carbonyl oxygen is less significant at higher temperatures, the π_i values decrease with temperature.

4. CONCLUSION

The presence of associative interaction between cyclohexanol and two structurally different aryl ketones is investigated by ultrasonic velocity measurements at different concentrations. The trend in the acoustical parameters with concentration establishes the formation of hydrogen bonded complexes between CHL and the two ketones. The effect of temperature on H-bonding and its influence on ultrasonic velocity is also studied. UV-visible spectral studies are carried out at room temperature (303 K). The spectra are recorded at specific concentrations (at the ultrasonic velocity peaks). The formation of hydrogen bonded complexes in the two systems is established from the appearance of new peaks at characteristic wavelength for the two systems. It is also observed that the hydrogen bond between CHL and aryl ketone is not favoured when an electronegative group like -NO₂ is present at the 4-position of acetophenone.

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APPENDIX

Table A1. Ultrasonic velocity(U), density(ρ), viscosity co-efficient(η), adiabatic compressibility(κ), free length(L_f) and internal pressure (π_i) of cyclohexanol – acetophenone system at different temperatures

Solvent: DMSO

[CHL] = [ACP]

Concentration mol dm ⁻³	U M s ⁻¹	ρ kg m ⁻³	$\eta/10^{-4}$ m Pa s	$\kappa/10^{-10}$ kg ⁻¹ ms ²	$L_f/10^{-11}$ m	$\pi_i/10^9$ Pa
303 K						
0.01	1465.9	1075.3	1.55	4.33	4.316	5.74
0.02	1464.4	1077.8	1.63	4.29	4.297	5.93
0.03	1463.2	1080.8	1.65	4.32	4.312	5.96
0.04	1462.4	1081.6	1.57	4.32	4.312	5.99
0.05	1462.0	1082.1	1.60	4.32	4.312	6.13
0.06	1468.2	1087.3	1.77	4.29	4.297	6.19
0.07	1463.4	1089.4	1.74	4.29	4.297	6.21
0.08	1465.8	1091.6	1.80	4.27	4.287	6.29
0.09	1464.2	1093.1	1.86	4.26	4.282	6.54
0.10	1461.4	1095.2	1.90	4.26	4.282	6.68
308 K						
0.01	1464.2	1071.5	1.51	4.35	4.365	5.66
0.02	1463.8	1074.6	1.59	4.34	4.360	5.89
0.03	1463.2	1076.3	1.61	4.35	4.365	5.93
0.04	1462.2	1078.2	1.54	4.35	4.365	5.96
0.05	1465.6	1079.0	1.57	4.34	4.360	6.06
0.06	1467.4	1080.6	1.62	4.31	4.345	6.09
0.07	1464.7	1081.3	1.67	4.32	4.350	6.18
0.08	1463.4	1083.5	1.72	4.31	4.345	6.28
0.09	1462.8	1085.8	1.77	4.31	4.345	6.49
0.10	1461.4	1090.2	1.81	4.30	4.340	6.63
313 K						
0.01	1462.8	1067.8	1.45	4.38	4.424	5.54
0.02	1461.6	1069.2	1.43	4.38	4.424	5.56
0.03	1461.2	1071.5	1.51	4.37	4.420	5.73
0.04	1465.3	1073.6	1.54	4.34	4.402	5.82
0.05	1463.8	1075.5	1.55	4.34	4.402	5.87
0.05	1461.5	1077.2	1.59	4.33	4.396	5.96
0.06	1460.5	1078.8	1.63	4.35	4.411	5.84
0.07	1459.8	1083.4	1.67	4.33	4.396	5.90
0.08	1459.0	1085.5	1.74	4.33	4.396	6.14
0.09	1458.4	1089.4	1.76	4.32	4.390	6.22
0.10	1457.2	1093.2	1.79	4.31	4.385	6.36

Table A2. Ultrasonic velocity(U), density(ρ), viscosity co-efficient(η), adiabatic compressibility(κ), free length(L_f) and internal pressure (π_i) of cyclohexanol – p-nitroacetophenone system at different temperatures

Solvent: DMSO [CHL] = [PNA]						
Concentration Mol dm ⁻³	U M s ⁻¹	ρ kg m ⁻³	$\eta / 10^{-4}$ m Pa s	$\kappa / 10^{-10}$ kg ⁻¹ ms ²	$L_f / 10^{-11}$ m	$\pi_i / 10^9$ Pa
303 K						
0.01	1472.4	1092.6	1.69	4.22	4.262	6.05
0.02	1471.4	1094.7	1.66	4.22	4.262	6.06
0.03	1470.8	1091.0	1.62	4.24	4.272	6.09
0.04	1469.5	1093.6	1.66	4.24	4.272	6.11
0.05	1470.2	1092.2	1.66	4.23	4.267	6.13
0.06	1471.2	1095.0	1.63	4.22	4.262	6.15
0.07	1471.5	1093.5	1.68	4.23	4.267	6.25
0.08	1471.8	1094.4	1.72	4.22	4.262	6.34
0.09	1472.2	1096.0	1.78	4.21	4.257	6.55
0.10	1471.8	1096.3	1.79	4.23	4.267	6.60
308 K						
0.01	1470.0	1084.3	1.47	4.28	4.330	5.62
0.02	1469.8	1086.2	1.43	4.29	4.335	5.59
0.03	1467.4	1084.9	1.46	4.26	4.320	5.66
0.04	1464.4	1084.2	1.48	4.31	4.345	5.73
0.05	1463.6	1084.9	1.50	4.33	4.355	5.79
0.06	1462.0	1085.6	1.45	4.35	4.365	5.85
0.07	1463.4	1086.0	1.48	4.35	4.365	5.93
0.08	1463.2	1085.2	1.51	4.35	4.365	6.05
0.09	1463.0	1084.8	1.54	4.35	4.365	6.09
0.10	1464.7	1086.0	1.56	4.35	4.365	6.14
313 K						
0.01	1468.5	1082.2	1.39	4.29	4.375	5.45
0.02	1467.4	1079.2	1.37	4.29	4.375	5.46
0.03	1466.8	1080.2	1.36	4.30	4.380	5.46
0.04	1465.2	1080.9	1.39	4.31	4.385	5.48
0.05	1466.4	1078.9	1.37	4.29	4.375	5.52
0.05	1466.9	1076.4	1.32	4.29	4.375	5.54
0.06	1467.2	1074.1	1.34	4.31	4.385	5.62
0.07	1467.9	1075.6	1.37	4.31	4.385	5.75
0.08	1468.1	1076.7	1.40	4.31	4.385	5.80
0.09	1468.4	1077.8	1.41	4.30	4.380	5.86
0.10	1468.8	1081.5	1.43	4.30	4.380	5.94