**Molecular interaction Study of Polyvinyl chloride in dimethylformamide**

Richa Saxena1\*, S C Bhatt2, Manish Uniyal3

1IFTM University, Lodhipur, Rajput, Moradabad-244001, (Uttar Pradesh) India.

2Ultrasonic and Dielectric Laboratory, Department of Physics, H.N.B. Garhwal University, Central University, Srinagar, Garhwal - 246174, (Uttarakhand) India.

3Department of Physics, BGR Campus, Pauri, H N B Garhwal University, Central University, Srinagar, Garhwal

Corresponding author: Richa Saxena\*

E-mail id-saxena.richa23@gmail.com

**Abstract**

In present investigation values of density, viscosity and ultrasonic velocity are experimentally measured of polyvinylchloride in dimethylformamide at different concentration and temperatures at frequency of 1MHz. Using these measured values various acoustical parameters of solute- solvent have been calculated to understand molecular interactions between solute and solvent. This study is helpful to understand the interaction between polymer and solvent. The change of temperature and concentration on various parameters have been studied.

**Keywords:** ultrasound sound velocity, adiabatic compressibility, Ultrasonic absorption

**I Introduction**

In last few years the ultrasonic studies of solution of polymers and in solid polymers have been the become the area of interest for research [1-5]. A literature review on volumetric studies on liquid solution reveals that measurement studies of ultrasonic velocity are helpful to understand the kind of molecular interactions in solute and solvent [6-9]. As compared to other plastics, the third most widely used plastic of synthetic polymer is Polyvinylchloride (PVC). Polyvinyl Chloride has many advantages and is generally known to be used to have advantages of least ingredient cost, wide processing adaptability, high ornamental potential and is used to produce different types of products having different range from extremely flexible to highly rapid. Using ultrasonic techniques, a revolutionary work has been done by many researchers [10-11] on polymer and polymer compatibility. As PVC is an major polymer for industry therefore it is chosen to investigate the behaviour of interactions of polyvinylchloride in dimethylformamide.

Takeda and Endo [12] observed the viscosity study of solution of polyvinylchloride in dilute form. B. Thapa et. al. studied the volumetric studies of polyvinylchloride with solution of cyclohexanone and 1, 4-Dioxane. During Polyvinyl chloride plastisol’s gelation and fusion with light scattering at small angle, Xiang et. al. [13] survey an effective means for the characterization of structural changes in Polyvinyl chloride particles. From the density, viscosity and viscometric measurement, the compatibility study of blend system of PVC and starch acetate in 1, 4 dioxane studied by Thakore et. al. [14]. In interest of observing the outcome of temperature and concentration, experiment was carried out at different concentration and temperature. Very limited literature is available on polyvinylchloride so it is interesting to study molecular interaction in polyvinylchloride. In present investigation various interaction parameters at different range of concentration and temperature of polyvinylchloride in dimethylformamide have been measured and the analysis are described in terms of molecular interaction between solute and solvent. Ultrasonic parameters are very important to understand the physio-chemical behavior of PVC and dimethyl formamide and for production, their applications in different field.

1. **Experimental Details**

## In present study Polyvinyl chloride (of molecular weight ≈ 134.5 Da) in form of liquid is used with dimethylformamide. By mixing the fixed volume of polyvinyl chloride to known volume of dimethylformamide, solutions were prepared and it were stirred spontaneously till a clear solution was obtained. The studied range of concentration in solution is 1%, 0.8%, 0.6%, 0.5%,0.4% and 0.3% in the temperature range 30°C, 35°C, 40° C, 45° C, 50°C, 55°C, 60°C, 65°C at 1 MHz frequency. Ultrasound velocity is measured by using Ultrasonic interferometer having a reliability of ± 4 m/s at 30⁰C. specific gravity bottle of 10 ml capacity and single pan micro balance is used for density measurements with the reliability of 0.5 kg/m3. Ostwald’s viscometer is used for measuring the viscosity of the solution that was kept inside a double walled jacket, in which water was flowed from thermostat water bath. Water of required temperature was used to fill the inner cylinder of this double wall glass jacket so as to initiate and keep up the thermal equilibrium. In uncertainty in each measurement was measured to be 0.01MPa.s. By the use of standard formulae [15-17] the different acoustical parameters are calculated.

1. **Results and discussion**

In the present study, the mixtures property parameters, namely, ultrasonic velocity, viscosity, density and its related parameters like adiabatic compressibility, acoustic impedance, intermolecular free length, relaxation time and ultrasonic absorption for polyvinyl chloride with dimethylformamide in different temperature range 30° C, 35°C, 40° C, 45° C, 50°C, 55°C, 60°C, 65°C and concentration range 1.0%, 0.8%, 0.6%, 0.5%,0.4% and 0.3% have been presented in Table 1 to Table 8 respectively.

The experimental values of density, viscosity and ultrasonic velocity have been presented in Table 1, 2 and 3 and their variation with temperature and concentration is presented in Figure 1 to 6 respectively. Table 1, Fig. 1 and Fig.2 indicates the variation of density with different temperature and concentration respectively. It is reported that density decreases with increase in the value of temperature and increases with increase in concentration of polyvinylchloride in the solution. Increase in the value of density is because of the reason that number of polymer chains increases in addition in the solution with increase in concentration of the PVC. As compared to solvent, polymer have large molecular weight that also contributes in the increase in density. The result reported in the present investigation are in good agreement with the results reported by earlier researchers [18, 19]. Viscosity is an important property and it depends on the molecular size, shape and intermolecular attraction. The measurement of viscosity provides useful information for study of solute- solvent interaction and for interaction of solute-solute. Table 2 and Fig.3 and Fig.4 reports the variation of viscosity with temperature and concentration respectively. It is observed that viscosity measurements decrease with temperature increase and increases with increment in concentration of polyvinylchloride in the solution. The solution becomes more and more viscous as the solute is added`, less fluidity thus led to increase in the viscosity. With the increase in the concentration, the fractional resistance between the medium layers increases and that led to increase in the viscosity. A similar behavior was made by previous authors [20]. Ultrasonic velocity decreases with increase in temperature due to weakening of intermolecular force and increases with increase in concentration of polyvinyl chloride as presented in Table 3, Fig. 5 and Fig.6 respectively. This may be due to increase in mobility of the molecules which may further increase the cohesion between molecules and thus filling all the available free spaces between it. This behaviour in the ultrasonic velocity may be because of changes in the structure in the mixture may be because of increasing intermolecular forces. Similar trend is observed by earlier authors [21]. A V Narasimham et al. have concluded the similar results for polyvinyl chloride solutions [22]. Table 4 and Fig. 7 shows that intermolecular free length increases with increase in range of temperature and decreases with increase in the concentration of Polyvinylchloride as presented in Table 4 and Fig.8. The variation of ultrasonic velocity in solution depends on intermolecular free length. According to Eyring and Kincaid model [23], ultrasonic velocity is inversely proportional to intermolecular free length, ultrasonic velocity should decrease with the increase of intermolecular free length and inverse is also true. The results reported in present study are in similar trends with proposed model. Variation of adiabatic compressibility with temperature and concentration are shown in Table 5 and Fig. 9 and 10 respectively. It is reported that adiabatic compressibility increases with increase in temperature and decreases with increase in concentration of polyvinyl chloride in solution. This decrease in value suggests the weakening of molecular interactions in the liquid mixtures. This can be explained in terms of the electrostatic effects of the polymer on the solvent molecules surrounding. The results also indicates that the medium become more compressible. The adiabatic compressibility is inversely proportional to ultrasonic velocity square value, therefore the trend in the adiabatic compressibility is reverse of the trend of ultrasonic velocity with temperature and concentration. With the increase in the velocity with concentration and the density also increases, the compressibility must decrease with increase in concentration of PVC. Some earlier workers have also reported similar behavior of adiabatic compressibility [24]. Acoustic impedance is an important property as it is related to elastic properties of the medium. Therefore, its variation with temperature and concentration is studied. Table 6 and Fig.11 and Fig. 12 shows the variation of acoustic impedance with temperature and concentration. It is found that acoustic impedance decreases with increase in temperature of solution and increases as concentration of polyvinylchloride in solution increases. This is the resistance of the medium to the longitudinal wave motion. Due to the prominent interaction among the molecules, there is more resistance that results in increase in the value. This may be also due to increase in density and viscosity in solution and also because increase in elasticity of the medium. Table 7, Fig. 13 and Fig. 14 represents the variation of relaxation time with different temperature and concentration range respectively. It is observed from Table 7 and Fig.13 that relaxation time decreases with increase in the value of temperature and increases with increase in polyvinylchloride concentration in the solution (Table 7 and Fig.14). The relaxation time takes place due to structural relaxation process and it is presumed that because of the cooperative process, the molecules get rearranged. Variation of ultrasonic absorption with temperature and concentration is presented in Table 8 and Fig. 15 and Fig.16 respectively. It is clear that ultrasonic absorption decreases with increase in temperature and increases with increase in concentration of polyvinyl chloride in solution. The increase in the value of relaxation time and ultrasonic absorption with increase in concentration can be understand in terms of macromolecular interchain forces motion, which are influenced by density, viscosity and ultrasonic velocity.

1. **Conclusion**

Density, viscosity and velocity of ultrasound have been measured for PVC in dimethylformamide at different concentration and temperature. Using these values different acoustical parameters like adiabatic compressibility, acoustic impedance, intermolecular free length, relaxation time and ultrasonic absorption have been calculated. Effect of temperature and concentration have been studied on these parameters can lead to structural investigation of the medium. The results shows that there is strong molecular interaction between polymer and the solvent with the increase in concentration. This study is helpful in understanding the nature of polymer, their production and uses.

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**Table -1: Density(x103kg/m3) of PVC at different temperature and concentration**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Temperature****Concentration** | **30°C** | **35°C** | **40°C** | **45°C** | **50°C** | **55°C** | **60°C** | **65°C** |
| **1.0%** | **1.053** | **1.036** | **1.031** | **0.989** | **0.979** | **0.964** | **0.948** | **0.942** |
| **0.8%** | **1.042** | **1.034** | **1.028** | **0.981** | **0.967** | **0.951** | **0.944** | **0.941** |
| **0.6%** | **0.964** | **0.937** | **0.918** | **0.867** | **0.840** | **0.831** | **0.827** | **0.825** |
| **0.5%** | **0.917** | **0.904** | **0.893** | **0.843** | **0.832** | **0.818** | **0.811** | **0.81** |
| **0.4%** | **0.891** | **0.868** | **0.855** | **0.808** | **0.796** | **0.783** | **0.777** | **0.776** |
| **0.3%** | **0.854** | **0.803** | **0.789** | **0.745** | **0.735** | **0.722** | **0.722** | **0.716** |

**Table -2: Viscosity (x10-2 MPas) of PVC at different temperature and concentration -**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Temperature****Concentration** | **30°C** | **35°C** | **40°C** | **45°C** | **50°C** | **55°C** | **60°C** | **65°C** |
| **1.0%** | **0.0029** | **0.0024** | **0.0022** | **0.0021** | **0.00195** | **0.0018** | **0.0017** | **0.0016** |
| **0.8%** | **0.0027** | **0.0024** | **0.0022** | **0.0021** | **0.0019** | **0.0018** | **0.0017** | **0.0016** |
| **0.6%** | **0.0027** | **0.0023** | **0.0020** | **0.0019** | **0.0017** | **0.00169** | **0.0016** | **0.0015** |
| **0.5%** | **0.0023** | **0.0021** | **0.0019** | **0.0018** | **0.0016** | **0.0015** | **0.0015** | **0.0014** |
| **0.4%** | **0.0023** | **0.0020** | **0.0019** | **0.0017** | **0.0016** | **0.0015** | **0.0015** | **0.0014** |
| **0.3%** | **0.0022** | **0.0019** | **0.0018** | **0.0017** | **0.0016** | **0.0015** | **0.0014** | **0.0013** |

**Table -3: Ultrasonic velocity (m/s) of PVC at different temperature and concentration-**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Temperature****Concentration** | **30°C** | **35°C** | **40°C** | **45°C** | **50°C** | **55°C** | **60°C** | **65°C** |
| **1.0%** | **1264.1** | **1258.3** | **1210.8** | **1197.5** | **1189.8** | **1160.8** | **1153.9** | **1143.6** |
| **0.8%** | **1242.8** | **1238.6** | **1207.3** | **1190.6** | **1187.6** | **1154** | **1143** | **1138.5** |
| **0.6%** | **1240.6** | **1210.4** | **1204.6** | **1188.3** | **1177.3** | **1150.6** | **1142.6** | **1136** |
| **0.5%** | **1224.2** | **1206** | **1181.6** | **1178** | **1150.7** | **1148.4** | **1142** | **1132.2** |
| **0.4%** | **1187** | **1181.8** | **1172.5** | **1165.2** | **1150.4** | **1146.7** | **1142** | **1131.6** |
| **0.3%** | **1177.6** | **1168.1** | **1156.8** | **1152** | **1146** | **1136.6** | **1131.2** | **1130.6** |

**Table – 4: Intermolecular Free Length (x10-13m) of PVC at different temperature and concentration-**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Temperature****Concentration** | **30°C** | **35°C** | **40°C** | **45°C** | **50°C** | **55°C** | **60°C** | **65°C** |
| **1.0%** | **3.3** | **3.341** | **3.481** | **3.596** | **3.637** | **3.756** | **3.809** | **3.855** |
| **0.8%** | **3.374** | **3.396** | **3.496** | **3.629** | **3.665** | **3.803** | **3.855** | **3.875** |
| **0.6%** | **3.514** | **3.653** | **3.708** | **3.868** | **3.967** | **4.056** | **4.123** | **4.24** |
| **0.5%** | **3.65** | **3.795** | **3.834** | **3.957** | **4.087** | **4.122** | **4.148** | **4.2** |
| **0.4%** | **3.819** | **3.887** | **3.948** | **4.087** | **4.17** | **4.218** | **4.252** | **4.266** |
| **0.3%** | **3.933** | **4.164** | **4.164** | **4.305** | **4.344** | **4.431** | **4.452** | **4.475** |

**Table – 5: Adiabatic compressibility(x10-10kg-1m4s2) of PVC at different temperature and**

**concentration-**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Temperature****Concentration** | **30°C** | **35°C** | **40°C** | **45°C** | **50°C** | **55°C** | **60°C** | **65°C** |
| **1.0%** | **5.95** | **6.09** | **6.62** | **7.06** | **7.22** | **7.7** | **7.92** | **8.11** |
| **0.8%** | **6.21** | **6.30** | **6.67** | **7.19** | **7.33** | **7.89** | **8.11** | **8.20** |
| **0.6%** | **6.74** | **7.28** | **7.51** | **8.17** | **8.59** | **8.98** | **9.28** | **9.58** |
| **0.5%** | **7.27** | **7.86** | **8.02** | **8.55** | **9.08** | **9.28** | **9.39** | **9.63** |
| **0.4%** | **7.96** | **8.25** | **8.51** | **9.12** | **9.49** | **9.71** | **9.87** | **9.94** |
| **0.3%** | **8.44** | **9.13** | **9.47** | **9.51** | **9.53** | **9.77** | **9.88** | **9.96** |

**Table -6: Acoustic impedance (x103kgm2s-1) of PVC at different temperature and concentration-**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Temperature****Concentration** | **30°C** | **35°C** | **40°C** | **45°C** | **50°C** | **55°C** | **60°C** | **65°C** |
| **1.0%** | **1330.6** | **1304.1** | **1248.2** | **1183.1** | **1164.2** | **1118.9** | **1094.0** | **1077.6** |
| **0.8%** | **1294.9** | **1282.2** | **1241.6** | **1168.2** | **1148.5** | **1097.7** | **1078.7** | **1071.7** |
| **0.6%** | **1195.8** | **1134.4** | **1105.9** | **1030.5** | **988.6** | **962.0** | **944.1** | **920.1** |
| **0.5%** | **1123.1** | **1072.4** | **1054.9** | **993.3** | **957.2** | **938.8** | **928.8** | **917.2** |
| **0.4%** | **1057.9** | **1026.0** | **1002.3** | **941.4** | **915.6** | **897.9** | **887.2** | **883.6** |
| **0.3%** | **1005.7** | **937.5** | **913.2** | **903.2** | **858.0** | **821.0** | **817.0** | **809.2** |

**Table – 7: Relaxation time (x10-12s) of PVC at different temperature and concentration-**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Temperature****Concentration** | **30°C** | **35°C** | **40°C** | **45°C** | **50°C** | **55°C** | **60°C** | **65°C** |
| **1.0%** | **2.720** | **2.520** | **2.460** | **2.455** | **1.970** | **1.920** | **1.838** | **1.764** |
| **0.8%** | **2.680** | **2.498** | **2.420** | **2.394** | **1.950** | **1.876** | **1.860** | **1.700** |
| **0.6%** | **2.640** | **2.420** | **2.391** | **2.351** | **1.868** | **1.830** | **1.82** | **1.976** |
| **0.5%** | **2.610** | **2.380** | **2.330** | **2.251** | **1.780** | **1.942** | **1.726** | **1.605** |
| **0.4%** | **2.560** | **2.332** | **2.290** | **2.227** | **1.750** | **1.730** | **1.690** | **1.62** |
| **0.3%** | **2.454** | **2.310** | **2.234** | **2.180** | **1.72** | **1.690** | **1.620** | **1.600** |

**Table -8: Ultrasonic absorption (x10-15s2m-1) of PVC at different temperature and concentration-**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Temperature****Concentration** | **30°C** | **35°C** | **40°C** | **45°C** | **50°C** | **55°C** | **60°C** | **65°C** |
| **1.0%** | **3.56** | **3.52** | **3.47** | **3.44** | **3.40** | **3.34** | **3.31** | **3.20** |
| **0.8%** | **3.55** | **3.50** | **3.45** | **3.41** | **3.38** | **3.28** | **3.22** | **3.16** |
| **0.6%** | **3.51** | **3.47** | **3.42** | **3.38** | **3.35** | **3.25** | **3.20** | **3.05** |
| **0.5%** | **3.48** | **3.45** | **3.38** | **3.35** | **3.33** | **3.21** | **3.18** | **3.03** |
| **0.4%** | **3.45** | **3.41** | **3.35** | **3.32** | **3.29** | **3.18** | **3.15** | **3.01** |
| **0.3%** | **3.42** | **3.39** | **3.32** | **3.30** | **3.25** | **3.21** | **3.14** | **3.01** |

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**Fig.-1: Variation of density with temperature at different concentration of PVC**

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**Fig.-2: Variation of density with concentration at different temperature of PVC**

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 **Fig.-3: Variation of Viscosity with temperature at different concentration of PVC**

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**Fig.-4: Variation of Viscosity with concentration at different temperature of PVC **

**Fig.-5: Variation of ultrasonic velocity with temperature at different concentration of PVC**

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**Fig.-6: Variation of ultrasonic velocity with concentration at different temperature of PVC**

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**Fig. -7: Variation of intermolecular free length with temperature at different concentration of PVC**

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**Fig.- 8: Variation of intermolecular free length with concentration at different temperature of PVC**

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**Fig. -9: Variation of adiabatic compressibility with temperature at different concentration of PVC**

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**Fig.-10: Variation of adiabatic compressibility with concentration at different temperature of PVC**

****

**Fig. -11: Variation of acoustic impedance with temperature at different concentration of PVC**

****

**Fig. -12: Variation of acoustic impedance with concentration at different temperature of PVC**

**1.5**

**1.7**

**1.9**

**2.1**

**2.3**

**2.5**

**2.7**

**2.9**

**30**

**35**

**40**

**45**

**50**

**55**

**60**

**65**

**Temperature (**

**0**

**C)**

**Relaxation time(x10-12s)**

1

0.8

0.6

0.5

0.4

0.3

**Fig.-13: Variation of relaxation time with temperature at different concentration of PVC**

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**Fig.-14: Variation of relaxation time with concentration at different temperature of PVC**

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**Fig.-15: Variation of ultrasonic absorption with temperature at different concentration of PVC**



**Fig.-16: Variation of ultrasonic absorption with concentration at different temperature of PVC**