**Molecular Interaction Study of Polyethylene Glycol with Water**

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**Abstract**

Sound velocity, viscosity and density has been measured of binary solution of Polyethylene glycol with water at 1MHz frequency. Experimental values have been calculated at different range of concentration and at 45°C temperature. Different parameters are calculated like adiabatic compressibility, intermolecular free length and relaxation time of PEG solutions. These values are used to understand the behaviour of molecular interaction of solute and solvent.

**Keywords:** Sound velocity, adiabatic compressibility, intermolecular free length.

1. **Introduction**

For research related to Polymers field, for the molecular interactions and structural study ultrasonic study has become a very interesting tool for multicomponent systems. Polyethylene glycol has wide applications in textiles, leather industry, is widely used in rubber, textiles and in field of pharmaceuticals. Acree [1] and Praunitz et al. [2] explained the wide applications of liquid, liquid mixtures and solutions in the textiles, chemicals, nuclear industries. Sound velocity, density and viscosity of PEG with acetonitrile and mixtures of water was studied by Syal et. al. [3]. Sound velocity measurement studies in last few years, are widely used in the investigation of behaviour of solute- solvent systems and to understand the solute and solvent nature in mixtures of liquids. To understand the molecular interaction between solute and solvent for mixtures of binary and ternary liquids. [4-7] literature survey reveals that adiabatic compressibility and sound velocity are found useful. Ultrasonic properties of solutions of polymers have shown that volumetric measurement studies and their acoustical parameters provides much useful information on solute-solvent interaction, these are found to be production of polymer and their uses in industries and other areas [8]. Using Shio model, ultrasonic study of hydration of Polyethylene glycol was made by S Kalyanasundaram et. al. [9]. Several researchers [10-14] have studied the volumetric parameters for Polyethylene glycol. The available literature for PEG having molecular weight approximately 200 is not much. Therefore, in present investigation Polyethylene glycol of molecular weight 200 is taken to elaborate the study.

1. **Experimental Detail**

In present study polyethylene glycol (of approximate molecular weight ≈ 200 Da) in the form of liquid is used with water. Fixed known volume of polyethylene glycol is mixed with fixed volume of water, the solutions were prepared by mixing continuously until a clear solution is obtained. The study is concentration range studied in solution is 1%, 0.8%, 0.6%, 0.5%,0.4% and 0.3% in the temperature 45° C at 1 MHz frequency. The velocity of sound is measured by using variable path Ultrasonic interferometer with reliability of ± 4 m/s at 30⁰C. By the circulation of water from the electronically operated digital constant temperature having an accuracy of ± 0.1⁰ C, solution temperature is kept constant by the outer jacket of measuring cell having double wall experimental liquid. The densities of the solutions at different temperatures were measured by using 10 ml specific gravity bottle and single pan micro balance. The density was found to be with 0.5 kg/m3 reliability. Ostwald’s viscometer is used for measurement of viscosity of the mixtures, that was kept inside a double walled jacket, in which water from thermostat water bath was circulated. For providing the thermal equilibrium, inner cylinder of this double wall glass jacket was filled with water of required temperature. The intermolecular interaction parameters are calculated by using standard formulae [15-17].

1. **Result and Discussion**

In this investigation the density, viscosity and velocity of ultrasound have been measured at different concentration of Polyethylene glycol at 45º C temperature, which is shown in Table 1, 2 and 3 respectively. By the use of these experimental values for PEG-200 different acoustical parameters like intermolecular free length, relaxation time and adiabatic compressibility have been calculated by the use of standard formulae and results are presented in Table 4, 5 and 6 respectively. The variation of these parameters with concentration is shown in Fig. 1-Fig-6 respectively.

Table -1 and Fig. 1 represents the variation of density with concentration at temperature of 45ºC. Density decreases with concentration increment of PEG. Electro striction in solution may led to decrease in density . The volume decreases due to this electrostriction and results in the increases in the density as a number of solute molecules increases the electrostriction and density. It is clear from Table -2 and Fig.2 that, there is decrease in viscosity with increase of the concentration of PEG – 200. The plot of sound velocity with concentration is shown in Table-3 and Fig.3. The value of ultrasonic velocity decreases by the increase in PEG concentration. S K Syal V K et. al.3 also reports the same results of increase in velocity with concentration increase. This shows the interaction of PEG with solvent molecules. There may exists interaction with in the contributing molecules. Intermolecular free length being the predominant factor as it evaluate the ultrasonic velocity in the fluid and condensed state. As the concentration of solute increases this leads to reduce the gap in between the two species and this is also present ideally in present investigation. It is reported from Fig. 4 and Table-4 that intermolecular free length decreases with concentration increase (Fig 4) of PEG. It is found to be in similar trend of the reports by previous researchers [18]. It is clearly seen from Table-5 and Fig5 that adiabatic compressibility decreases with increase of concentration of PEG. These results are in agreement with previous reports [9]. This may be because of the movement of solute molecules towards each other by wrenching the molecules from bulk of the solvent, because of electro striction forces they attract certain solvent, because of this available molecule of solvent for the next incoming solute gets decreased. Table-6 and Fig. 6 shows the variation of relaxation time with concentration. With increase in concentration of PEG relaxation time also increases. This may be because of the kinetic theory of fluid.

1. **Conclusion**

In the present investigation it is clear that there is association between polyethylene glycol and water. The increase in the value of ultrasonic velocity and that led to effect the other acoustical parameters is due to molecular interaction between solvent and solute. This is because of the reason that molecules of polymer come near to molecules of solvents by leaving sufficient space round them. This study also depicts the behaviour of polymer at different concentration in terms of the molecular interactions. This study is found to be beneficial for production and applications of polymers in industries and different fields.

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**Table 1: Density (x103Kgm-3) at 45º C and at different concentration at MHz foe PEG**

|  |  |
| --- | --- |
| **Concentration (%)** | **Density** |
| **1.0** | **1.506** |
| **0.8** | **1.321** |
| **0.6** | **0.986** |
| **0.5** | **0.932** |
| **0.4** | **0.971** |
| **0.3** | **0.970** |

**Fig.1: variation of density with concentration at 45ºC**

**Table 2: Viscosity (Pa.s) at 45ºC temperature and concentration at 1MHz for PEG**

|  |  |
| --- | --- |
| **Concentration (%)** | **Viscosity** |
| **1.0** | **.045** |
| **0.8** | **0.029** |
| **0.6** | **0.026** |
| **0.5** | **0.018** |
| **0.4** | **0.010** |
| **0.3** | **0.007** |

**Fig.2: variation of viscosity with concentration at 45ºC**

**Table 3: Ultrasonic velocity (ms-1) at 450C temperature and concentration at 1MHz for PEG**

|  |  |
| --- | --- |
| **Concentration (%)** | **Ultrasonic velocity** |
| **1.0** | **1249.6** |
| **0.8** | **1245.2** |
| **0.6** | **1241.9** |
| **0.5** | **1189.6** |
| **0.4** | **1162.4** |
| **0.3** | **1120.4** |

**Fig.3: variation of ultrasonic velocity with concentration at 45ºC**

**Table 4: Intermolecular Free Length (x10-10m) at different temperature and concentration at 1MHz for PEG**

|  |  |
| --- | --- |
| **Concentration (%)** | **Intermolecular Free length** |
| **1.0** | **0.0026** |
| **0.8** | **0.0028** |
| **0.6** | **0.0035** |
| **0.5** | **0.0037** |
| **0.4** | **0.0038** |
| **0.3** | **0.0039** |

**Fig.4: variation of intermolecular free length with concentration at 45ºC**

**Table 5: Adiabatic compressibility(x10-10Kg-1ms2) at different temperature and concentration at 1MHz for PEG**

|  |  |
| --- | --- |
| **Concentration (%)** | **Intermolecular Free length** |
| **1.0** | **4.25** |
| **0.8** | **6.32** |
| **0.6** | **6.45** |
| **0.5** | **6.72** |
| **0.4** | **7.08** |
| **0.3** | **7.75** |

**Fig.5: variation of adiabatic compressibility with concentration at 45ºC**

**Table 6: Relaxation time (x10-12s) at different temperature and concentration at 1MHz for PEG**

|  |  |
| --- | --- |
| **Concentration (%)** | **Relaxation time** |
| **1.0** | **2.61** |
| **0.8** | **1.78** |
| **0.6** | **1.59** |
| **0.5** | **1.04** |
| **0.4** | **0.97** |
| **0.3** | **0.79** |

**Fig.6: variation of relaxation time with concentration at 45ºC**