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

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**Abstract**

Ultrasonic velocity, density and viscosity has been measured of aqueous solution for Polyethylene glycol at 1MHz frequency. Experimental values have been calculated at different range of concentration and at 45°C temperature. Different parameters have been 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:** Ultrasonic 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. Ultrasonic velocity, density and viscosity of Polyethylene glycol with acetonitrile and water mixtures was studied by V K Syal et. al. [3]. Ultrasonic velocity measurement studies in recent years, are widely used in the investigation of behaviour of molecular systems and to understand physio-chemical nature in liquid mixtures. To understand the molecular interaction between solute and solvent for binary and ternary mixtures [4-7] literature survey reveals that adiabatic compressibility and ultrasonic velocity are found useful. Ultrasonic properties of solutions of polymers have shown that ultrasonic measurement studies and its 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]. Many researchers [10-14] have calculated the ultrasonic parameters for Polyethylene glycol. The literature for Polyethylene glycol of molecular weight approximately 200 is not much. Therefore, in present investigation Polyethylene glycol of molecular weight 200 is used to elaborate the data.

1. **Experimental Detail**

In present investigation polyethylene glycol (of approximate molecular weight ≈ 200 Da) in liquid form is used with water. By adding known volume of polyethylene glycol to fixed volume of water, the solutions were prepared by stirring under reflex until a clear solution was obtained. The 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. Ultrasonic velocity measurement is made by using variable path Ultrasonic interferometer with reproducibility 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, the temperature of the solution has been kept constant through the outer jacket of the double walled measuring cell having 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 uncertainty measurement in density was found to be 0.5 kg/m3. The viscosity of the mixtures was measured by using Ostwald’s viscometer, which was kept inside a double walled jacket, in which water from thermostat water bath was circulated. To establish and maintain the thermal equilibrium, inner cylinder of this double wall glass jacket was filled with water of desired temperature. The uncertainty in each measurement was measured to be 0.01MPa.s. The acoustical parameters are calculated by using standard formulae[15-17].

1. **Result and Discussion**

In the present study the measurement of, density, viscosity and ultrasonic velocity have been measured at different concentration of Polyethylene glycol at 45º C temperature, which is shown in Table 1, 2 and 3 respectively. By using 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 well-known formulae and results have been presented in Table 4, 5 and 6 respectively. The variation of these parameters with respect to concentration have been shown in Fig. 1-Fig-6 respectively.

Table -1 and Fig. 1 represents the variation of density with concentration at 45ºC temperature. Density decreases with increase in concentration of PEG. This is because of electro striction in that solution. 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, viscosity decreases with increases concentration of PEG – 200. The variation of ultrasonic velocity with concentration have been shown in Table-3 and Fig.3. The value of ultrasonic velocity decreases by the increase in concentration of PEG. S K Syal V K et. al.3 also reports the same results of increase in velocity with increase in concentration. This indicates interaction between PEG with solvent molecules. This also shows interactions between contributing molecules. The predominant factor is Intermolecular free length because it determines the ultrasonic velocity in the condensed and fluid state. The increase in the concentration of solute leads to decrease in the gap between two species and this is also ideally seen in present study. It is observed from Fig. 4 and Table-4 that intermolecular free length decreases with increase in concentration (Fig 4) of PEG. It is found to be in similar trend of the reports by earlier researchers [18]. It is clearly seen from Table-5 and Fig5 that adiabatic compressibility decreases with increase in PEG concentration. These results are in agreement with earlier reports [9]. It 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 solvent molecule for the next incoming solute gets decreased. The variation of relaxation time with concentration is shown in Table-6, Fig. 6. Relaxation time increases with increase in PEG concentration. This may be because of the kinetic theory of fluid.

1. **Conclusion**

From 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 polymer molecules come close to solvent molecules by leaving sufficient space round them. This study also shows the behaviour of polymer at different concentration in terms of the molecular interactions. This study is found to be useful for production and uses of polymers in industries and different fields.

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**Table 1: Density (x103Kgm-3) at 45 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 45 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**