

Ultrasonic Study of Molecular Interactions in Polymeric Solution of Polypropylene Glycol-400 and Ethanol at 303 K

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Summary

A comprehensive ultrasonic investigation of molecular interactions in the polymeric solution of polypropylene glycol (PPG)-400 and ethanol at 303 K has been performed using the data available in literature. Several acoustic parameters such as acoustic impedance, isothermal compressibility, molar sound velocity, molar adiabatic compressibility, internal pressure, free volume, van der Waals constants, molar cohesive energy and relaxation time have been explored. Thermo-dynamical parameters viz.: available volume, intermolecular free length, relative association, surface tension, pseudo-Grüneisen parameter, Debye temperature, diffusion constant, coefficient of thermal conductivity and latent heat of melting have been evaluated. Several thermo-elastic parameters such as Young modulus, shear modulus, bulk modulus and Poisson's ratio are also determined. Excess parameters are computed to study the relative molecular interactions and strength of interaction between the constituents of the polymer mixture. The volume expansivity data is used to evaluate Moelwyn-Hughes parameter, reduced volume, reduced isothermal bulk modulus, Sharma's constants, Huggins parameter, isobaric, isochoric, and isothermal lattice Grüneisen parameters, fractional free volume, repulsive exponent, Bayer's non-linear parameter, cohesive energy density and characteristic temperature. Schaaff's collision factor theory, Jacobson's free length theory, Nomoto's relation, Van Dael-Vangeel relation, impedance dependence relation, Junjie relation and ideal mixing relation have been used to evaluate ultrasonic velocities in the system under study. The obtained results have been compared with earlier experimental results. The non-ideal behaviour of the mixture has been explained in terms of its composition and variation of its acoustical and thermo-dynamical parameters.

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1. Introduction

The extensive applications of polymeric materials in technology have imparted a significant impetus to the study of molecular interactions of polymers with solvents [1, 2, 3, 4, 5]. Polypropylene glycol (PPG) is widely used in industry in the formulation of polyurethanes. It also finds applications as a rheology modifier, in automobile seats, in foams, and in membranes. It is a prime ingredient in the manufacture of paintballs. The ultrasonic investigations of the PPG have been reported by many workers [6, 7, 8, 9, 10]. Zafarani-Moattar *et al.* [6] studied the aqueous polymer solutions of PPG for different concentrations in the temperature range 283.15 K–313.15 K and reported the polymer-solvent and polymer-polymer interactions in the system. The study also indicated the weakening of hydrogen bond interactions at higher temperatures,

leading to decrease in the molecular order in the system. Yasmin *et al.* [7] depicted the nature of polymer solutions by computing acoustical parameters from ultrasonic velocity and density data for the binary mixtures of PEG-400 + methanol, PEG-400 + ethanol, PPG-400 + ethanol and PPG-400 + 2-propanol systems at 298.15 K. Venktramanan *et al.* [8] studies the molecular interactions of the blend of PPG-400 with PPG-3000 at 303 K. Gayathri *et al.* [9] measured the ultrasound velocity, using interferometric technique, in PPG-400 and PPG-4000 in toluene for different concentrations at 303 K. Recently, Raju *et al.* [10] have investigated some acoustical parameters of PPG-400. A review of literature [6, 7, 8, 9, 10] reveals that an only a limited study is available about the nature and type of molecular interactions in PPG-400 and ethanol solution at 303 K.

In the present study, a detailed theoretical analysis of several acoustical, thermo-dynamical, elastic and solid state parameters of the polymer solution of PPG-400 and ethanol at 303 K have been investigated. The requisite data

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