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"MOLECULAR INTERACTION STUDIES OF SOME AMIDES WITH ASSOCIATIVE MOLECULES"

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In

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By

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Under the Supervision of

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"MOLECULAR INTERACTION STUDIES OF SOME AMIDES WITH ASSOCIATIVE MOLECULES"

Introduction

Interaction take place among two or more objects have an effect upon one another. Molecular interaction occurs with the attractive or repulsive forces between molecules of same or different group. Molecular interactions are important in material science, drug design, sensors, diverse fields of protein folding, and nanotechnology and so on. The interaction can take place in solid, liquid and gas. Among these interactions, liquid interaction gives effective information about the molecular interaction. Liquids owe their fascinating features to the balanced effects of molecular interactions and thermal agitation. The knowledge of molecular interaction in binary liquid mixtures is of considerable importance in the elucidation of the structure and dynamics of the molecules [1]. The study of molecular interaction provides some understanding of the fundamental problems concerned with the mechanisms of chemical and biological catalysis and path of the chemical reactions [2-4]. Molecular interactions can also throw light on energy transfer in enzymes, phase transition etc [4-6]. In transport and chemical industries attribution of molecular science is indispensable one [4,7]. Study of liquid materials and its variation in terms of interaction in different polar and nonpolar solvent environments can be done by various experimental spectroscopic techniques such as NMR, FTIR, Raman spectroscopy, dielectric relaxation spectroscopy, infrared spectroscopy etc [8–17]. One of the most powerful techniques to study the molecular response of the liquids in pure and mixed state is dielectric relaxation spectroscopy (DRS). Dielectric relaxation spectroscopy (DRS) study of polar liquids and their binary mixtures has drawn attention of many researchers because it gives fruitful information about the inter-intra molecular interactions, different relaxation processes, dielectric polarization and electrical conduction. The low frequency dielectric dispersion study of liquid provides detailed insight into the charge dynamics and electrical conduction mechanism, which are directly correlated to their dielectric polarization strength and molecular structure [18]. For better understanding of dielectric and electrical properties in lower frequency region complex conductivity, complex modulus and complex impedance formalism are used [19–28]. In Microwave frequency region it provides information about dipolar relaxation process. If the study is conducted at different temperatures, different thermodynamical parameters can be determined [29–36]. Apart from this, dielectric spectroscopy technique has great potential in understanding the H-bond interactions, dipolar

alignment and hydrogen bond connectivity [36-39]. Dielectric relaxation spectroscopy is a versatile tool for the study of conducting fluids which discover the structural dynamics in liquid samples. Further, it gives information about not only molecular interactions in the system but also the formation of monomers and multimers [1]. The concentration and temperature dependent dielectric parameters are related to the formation of aggregated complex structures in the mixture. Broad band DRS technique involves the complex permittivity measurements of the material under study in the frequency range spanning from 1 μHz to several THz. Broad band dielectric spectroscopy data provides significant information about the molecular and collective dipolar fluctuations, as well as about charge transport and polarization effects that occur in the material under study [40]. In the frequency range starting from 1 μHz to 10^7 Hz the effect of electrode polarization and ionic conduction relaxation mechanisms were found in most of the polar liquid materials. Further, in the frequency range of few tens of kHz to hundreds of MHz the real part of complex permittivity (dielectric constant) provides the static dielectric region. Dipolar relaxation process in most of the polar liquids is observed in the microwave frequency region ranging from hundreds of MHz to 300 GHz [41-42]. In this frequency range, most liquid polar molecules have high orientation polarizations and there is appreciable dielectric loss, which corresponds to various dielectric relaxation (α, β and γ). Beyond the microwave frequency range to several terahertz (THz), the material under test shows the collective molecular motions corresponding to existence of energy-level spacings in this region [43].

The study of physico-chemical properties, such as density, and viscosity, and other related parameters of liquid binary mixtures under varying condition of concentrations and temperatures, is significantly important in both industry and academia in order to gain extensive information about the physico-chemical and thermodynamic behaviour [44]. For a variety of industrial operations, particularly those in the chemical engineering industries, a whole information of the physico-chemical characteristics of multicomponent is necessary [45-48]. These are important to the emerging models for engineering applications or simulation procedures. They are also essential to the investigation of further thermodynamic and transport aspects of solutions [46,47,49]. In order to understand the nature of molecular interactions, the creation and deformation of hydrogen bonds, dipole-dipole interactions, dipole-induced dipole interactions, etc., it is significant to examine the physico-chemical properties of liquid materials [50]. Additionally, optical and acoustical characteristics of liquid materials, such as their

refractive index and ultrasonic velocity data, can be used to learn more about the physical nature and force between the constituent molecules [44].

Materials and Objectives of the Study

Alcohols are self-associated liquids that form a three-dimensional network of hydrogen bonds, allowing them to interact with other polar chemical groups. This property has attracted significant attention from many researchers [1,4,20,44]. Specifically, n-Hexanol and n-Octanol have been chosen for their diverse applications. n-Hexanol is commonly used as an antibacterial agent in medicine, an insecticide in agriculture, and a flavoring additive in the chemical industry. n-Octanol, on the other hand, is recognized as a potential biofuel derived from biomass and is important in synthesizing 1-octene, a crucial component in polyethylene production and various petrochemical processes [51-53]. DMF, belonging to the amide group, is notable for its high polarity and strong solvating power. It is widely used in the petrochemical, agricultural, and pharmaceutical industries. Additionally, DMF has garnered considerable interest due to its interactions with proteins and peptides, making it an important solvent in biochemical studies [54-55].

Main objectives of the present investigation are as follows:

- To study of dielectric and electrical properties of binary mixtures of n-Hexanol+DMF and n-Octanol+DMF at different temperatures (293.15 K →313.15 K) in frequency range 20 Hz to 2 MHz (Using LCR meter).
- To study dielectric properties of binary mixtures of n-Hexanol+DMF and n-Octanol+DMF at different temperatures in frequency range 200 MHz to 20 GHz (Using VNA).
- To study of Acoustical and Physico-chemical properties of the mixtures of n-Hexanol+DMF and n-Octanol+DMF at different temperatures.
- To analyze the dielectric, physicochemical and acoustical parameters to gain information about the solute-solvent interactions and molecular structures.
- An attempt is also made to identify the functional groups that will involve in interactions by FTIR analysis. The FT-IR study has been carried out for understanding inter or intra molecular hydrogen bonding between these binary mixtures.

- ❖ Various empirical/semi-empirical mixing models for static dielectric constant, refractive index, ultrasonic velocity and viscosity are tested and validated for the studied binary mixture systems.

Outline of Thesis

The Thesis will be presented in the form of the nine following chapters:

Chapter-1	Introduction
Chapter-2	Theoretical Backgrounds
Chapter-3	Experimental Procedures and Evaluation of Different Parameters
Chapter-4	Dielectric Relaxation Study of Binary Mixtures (n-Hexanol+ N, N-Dimethylformamide)
Chapter-5	Dielectric Relaxation Study and Electrochemical Impedance Spectroscopy (EIS) of Binary Mixtures (n-Octanol+ N, N-Dimethylformamide)
Chapter-6	Acoustic, Volumetric and IR spectra study of Binary Mixtures of n-Hexanol and N, N-Dimethylformamide
Chapter-7	Acoustic, Volumetric and Thermodynamics study of Binary Mixtures of n-Octanol and N, N-Dimethylformamide
Chapter-8	Study of Refractometric and various mixing relations of Binary Mixtures (n-Hexanol +N, N-Dimethylformamide, n-Octanol + N, N-Dimethylformamide)
Chapter-9	Summary of the investigation and future scope

Chapter-1: Introduction

The importance of study of dielectric relaxation spectroscopy and physico-chemical properties of liquid materials is given in this chapter. An overview of dielectric spectroscopy (BDS), refractometric and physiochemical methods are also discussed in this chapter. Major findings from the work done by various researchers on dielectric, refractometric, acoustic and volumetric study of various liquid systems have been given in brief. Applications of the studied compound (n-Hexanol, n-Octanol and N, N-Dimethylformamide (DMF)) in different areas and their some basic physico-chemical properties is provided in it. The aim and objective of the present study is also elaborated in this present chapter.

Chapter-2: Theoretical Backgrounds

This chapter mainly includes the fundamental theory of dielectrics, exploring dielectric properties such as dipole moments and types of polarization, as well as the theory of dielectric relaxation, permittivity, and the Clausius-Mossotti equation. It encompasses static permittivity theories like Debye, Onsager, Kirkwood, and Frohlich, along with dynamic permittivity theories, detailing various relaxation models including Havriliak-Negami, Cole-

Cole, Debye and Cole- Davidsons. The chapter examines the relationship between dielectric parameters and molecular behavior, alongside thermodynamic and physico-chemical properties such as ultrasonic velocity (u), density (ρ), refractive index (n) and viscosity (η), and other related parameters. Basic theory of electrochemical impedance spectroscopy are also dissection in this chapter.

Chapter-3: Experimental Procedures and Evaluation of Different Parameters

This chapter provides detailed information on the materials and sample preparation processes. It describes the experimental methods and setups for measuring various dielectric and physico-chemical properties. Techniques for determining the complex permittivity (ε*) of liquid samples across different frequency ranges are explained, including the use of a Precision LCR meter in the frequency span 20 Hz to 2 MHz and a Vector Network Analyzer (VNA) for the 200 MHz to 20 GHz range. The chapter also covers methods for measuring ultrasonic velocity (U) using an ultrasonic interferometer (2 MHz), density (ρ) using a specific gravity bottle, refractive index using Abb's refractometer, and viscosity (η) using an Ostwald viscometer. From the experimentally determined values of complex permittivity, refractive index, ultrasonic velocity, density, and viscosity of liquid mixtures, various other dielectric, electrical, physico-chemical, and thermodynamic parameters are evaluated. Brief details about the evaluation of these parameters are also provided in this chapter.

Chapter-4: Dielectric Relaxation Study of Binary Mixtures (n-Hexanol+ N, N-Dimethylformamide)

The detailed study of the dielectric relaxation spectroscopy (DRS) study conducted over broad range of frequencies (20 Hz to 2MHz) and (200 MHz to 20 GHz) at different temperatures (293.15 K, 303.15 K, 313.15 K) for binary mixture of n-Hexanol with N, N-Dimethylformamide is given in this chapter. In this chapter, dielectric and electrical properties of the binary mixtures of n-Hexanol and N, N-Dimethylformamide have been studied in the frequency range 20 Hz to 2 MHz at various temperature. Different electrical parameters such as electrical modulus (M*(f)), electrical conductivity (σ*(f)) and complex impedance (Z*(f)) were derived from the complex permittivity spectra (ε*(f)). Ionic polarization relaxation time (τ_σ) and DC conductivity (σ_{dc}) were calculated from different dielectric and electrical formalism. With the help of dielectric parameters and DC conductivity, different parameters such as Debye length (λd), ion mobility (μ), mobile ion concentration (P_0) and ion diffusivity

(D) have been determined. Complex impedance spectra were also fitted to RC equivalent circuit using EC-Lab software. The Complex permittivity (ε*) spectra of liquid samples are obtained in frequency span (200 MHz to 20 GHz) using vector network analyser (VNA) at three different temperatures. The frequency dependence complex permittivity spectra of liquid samples were analysed in the framework of Debye (DB), Cole-Cole and Cole-Davidson dielectric models using complex nonlinear least squares (CNLS) fitting (LEVMW Software) techniques. The critical comparison of the dielectric spectra obtained from these models are discussed and the best fit relaxation model is determined. Chosen for evaluated of dielectric parameters of static dielectric permittivity (ε_0) and permittivity at optical frequency (ε_∞) of binary mixtures of n-Hexanol and DMF is determined at different temperatures. From the determined values, its excess static permittivity $(\varepsilon_0)^E$ and excess permittivity at optical frequency $(\varepsilon_\infty)^E$ are calculated and fitted to the Redlich-Kister equation. Effective correction factor (g^{eff}) and corrective correlation factor (g^f) are evaluated from the modified Kirkwood equation. Additionally, experimental data of static permittivity are fitted to the modified Bruggman equation to find Bruggman factor (F_B). The variations of these parameters are discussed in terms of molecular structures, inter molecular and dipole-dipole interactions. Further, the determined relaxation time at different temperatures were used to evaluate thermodynamic parameters, and these parameters are interpreted in terms of the force of hindrance experienced by the molecules and their orientation in the liquid mixtures.

Chapter-5: Dielectric Relaxation Study and Electrochemical Impedance Spectroscopy (EIS) of Binary Mixtures (n-Octanol+ N, N-Dimethylformamide)

In this chapter, results of the DRS study conducted over broad range of frequencies (20 Hz to 2MHz) and (200 MHz to 20 GHz) at different temperatures for binary mixtures of n-Octanol and N, N-Dimethylformamide are reported. Complex permittivity spectra of the n-Octanol, N, N-Dimethylformamide and their binary mixtures are obtained over frequency range 20 Hz to 2 MHz. Different dielectric and electrical properties such as complex permittivity ε*(ω), loss tangent (tan δ), complex electric modulus M*(ω), complex conductivity σ*(ω) and complex impedance Z*(ω) have been investigated at different temperatures. Using these properties different parameters such as electrode polarization relaxation time (τ_{EP}), ionic conductivity relaxation time (τ_σ) and D.C conductivity (σ_{dc}) have been calculated. Complex impedance spectra have been fitted to RC equivalent circuit using EC-Lab software. Different equivalent circuit model parameters such as R_1, R_2, C_1 and C_2

were determined and reported. Geometric relaxation time (τ_g) was determined from different fitting parameters. Complex permittivity spectra for binary mixtures of n-Octanol and N, N-Dimethylformamide with varying concentration (0.0→1.0) in microwave frequency range (200 MHz to 20 GHz) at different temperatures are also studied. Using CNSL fitting method, the complex permittivity data are fitted to different model (Debye (DB), Cole-Cole and Cole-Davidson). Dipolar relaxation time for the mixtures was determined from the fitted parameters for all mixture concentrations. Static dielectric permittivity (ε_0) and permittivity at optical frequency (ε_∞) of binary mixtures of n-Octanol and N, N-Dimethylformamide (DMF) is determined at various temperatures (293.15 K, 303.15 K, 313.15 K). From these measured values, the critical comparison of the dielectric spectra obtained from these models are discussed and the best fit relaxation model is determined. The static dielectric constant (ε_0) and relaxation time (τ_0) are obtained. Dielectric constant at optical frequency (ε_∞) of liquid samples are determined. From these various parameters namely; excess static dielectric constant $(\varepsilon_0)^E$, excess dielectric constant at optical frequency $(\varepsilon_\infty)^E$, Kirkwood parameters (g^{eff} and g^F) and Bruggeman parameter (F_B) are determined. Furthermore evaluated microwave radiation heating parameters like power reflected (pr), power transmitted (pt) and penetration depth (dp) at different temperature are investigated at general purpose and commercial microwave radiation 2.45 GHz. Variation of these parameters are discussed in light of molecular interaction between molecular species. Further, the determined relaxation time at different temperatures were used to evaluate thermodynamic parameters, and these parameters are interpreted in terms of the force of hindrance experienced by the molecules and their orientation in the liquid mixtures.

Chapter-6: Acoustic, Volumetric and IR spectra study of Binary Mixtures of n-Hexanol and N, N-Dimethylformamide

In this chapter experimentally measured values of ultrasonic velocity (u), Density (ρ), Viscosity (η) over temperature range of 293.15 K to 313.15 K (interval of 10 K) are reported. From the experimental data the physiochemical (Acoustic and Volumetric) parameters such as molar volume (Vm), adiabatic compressibility (β), intermolecular free length (L_f), acoustic impedance (Z), molar sound velocity (R), molar compressibility (B), surface tension (σ), internal pressure (P_{int}) and relaxation time (τ) were calculated, which are more useful to predict and confirm the molecular interaction in the binary liquid mixtures. Excess of measured acoustic parameters have been estimated and fitted in Redlich -Kister polynomial.

Variations of these parameters are discussed in the light of molecular interaction in the mixture species. Their conformational study is supported by Fourier Transform Infrared (FTIR). The effect of concentration and temperature variation on the acoustical and volumetric parameters of the binary mixture of n-Hexanol and N, N-Dimethylformamide are investigated.

Chapter-7: Acoustic, Volumetric and Thermodynamics study of Binary Mixtures of n-Octanol and N, N-Dimethylformamide

This chapter contains experimentally measured values of ultrasonic velocity (u), Density (ρ) and Viscosity (η) for binary mixtures of n-Octanol and N, N-Dimethylformamide at different temperatures (293.15 K, 303.15K, 313.15 K) are reported. From the experimental data the physiochemical parameters such as molar volume (Vm), adiabatic compressibility (β), intermolecular free length (Lf), acoustic impedance (Z), molar sound velocity (R), molar compressibility (B), relaxation strength (r), surface tension (σ), internal pressure (Pint), free volume (V_f) and relaxation time (τ), enthalpy (ΔH), entropy (ΔS), Gibbs free energy (ΔG) were calculated, which are more useful to predict and confirm the molecular interaction in the binary liquid mixtures. The Redlich-Kister equation has been associated with the excess and deviation functions that have been computed from experimental data. These functions were further discussed in terms of molecular interactions existing in the mixtures as well as the temperature influence on them.

Chapter-8: Study of Refractometric and various mixing relations of Binary Mixtures (n-Hexanol +N, N-Dimethylformamide, n-Octanol + N, N-Dimethylformamide)

This chapter deals with the present study we report the refractive index (n) and density (ρ) of binary mixtures of n-Hexanol with N, N-Dimethylformamide over varying concentration of composition at different temperature (293.15K, 303.15 K, 313.15K). The measured data are utilized to evaluate various refractometric parameters namely, molar volume (Vm), molar refraction (Rm), atomic polarization (P_A), polarizability (α), molecular radii (r) and internal pressure (P_{int}) of the liquids and their mixtures. Deviation of molar volume (Δm), reduced free volume (Δ(Vm/Rm)), molecular radii (Δr) and internal pressures (ΔP_{int}) are determined and fitted with Redlich-Kistler polynomial to derive the binary coefficients and correlation coefficient. The nature of deviations of these parameters are

discussed in light of hetero-molecular interactions between the participating molecules. Furthermore, in this chapter deals with the validation of static dielectric constant (ε_0), refractive index (n), ultrasonic velocity (Uv) and viscosity (η) of binary mixtures of (n-Hexanol +N, N-Dimethylformamide, n-Octanol + N, N-Dimethylformamide) systems.

A comparison of the predicted values of static dielectric constant (ε_0), refractive index (n), ultrasonic velocity (v) and viscosity (η) of the liquid mixtures using various mixing relations with the experimentally determined values have been assessed in terms of Average Percentage Deviation (APD).

Chapter-9: Summary of the investigation and future scope

The comprehensive summary of the research work is provided in this chapter. The investigation's major findings are reported. The scope for further investigation based on findings and experience of the current study is given in these chapter.

References.

1. S. C. Mehrotra, A. C. Kumbharkhane, A. Chaudhari, Binary polar liquids: structural and dynamic characterization using spectroscopic methods, Elsevier, 2017.
2. M. B. J. Roeffaers, G. De Cremer, H. Uji-i, B. Muls, B. F. Sels, P. A. Jacobs, F. C. De Schryver, D. E. De Vos, J. Hofkens, Single-molecule fluorescence spectroscopy in (bio) catalysis, Proc. Natl. Acad. Sci. 104 (2007) 12603–12609.
3. Z. Feng, T. Zhang, H. Wang, B. Xu, Supramolecular catalysis and dynamic assemblies for medicine, Chem. Soc. Rev. 46 (2017) 6470–6479.
4. G. Parthipan, Liquid state dielectric studies on molecular interaction and fluid structure of binary mixture of anisole with some acids, alcohol and amines, Ph.D. Thesis, Alagappa University, (2008).
5. R. Karan, M. D. Capes, S. DasSarma, Function and biotechnology of extremophilic enzymes in low water activity, Aquat. Biosyst. 8 (2012) 1–15.
6. S. Boeynaems, S. Alberti, N.L. Fawzi, T. Mittag, M. Polymenidou, F. Rousseau, J. Schymkowitz, J. Shorter, B. Wolozin, L. Van Den Bosch, Protein phase separation: a new phase in cell biology, Trends Cell Biol. 28 (2018) 420–435.
7. P. Jena, Physics and chemistry of small clusters, Springer Science & Business Media, 2013.

8. S. A. Ingole, A. R. Deshmukh, R. V. Shinde, A. C. Kumbharkhane, Dielectric relaxation study of aqueous tetraethylene glycol using time domain reflectometry technique in the frequency range 10 MHz to 50 GHz, J. Mol. Liq. 272 (2018) 450–455.
9. T. Vishwam, S. Shihab, V. R. K. Murthy, H. S. Tiong, S. Sreehari Sastry, Microwave dielectric relaxation spectroscopy study of propylene glycol/ethanol binary mixtures: Temperature dependence, Spectrochim. Acta - Part A Mol. Biomol. Spectrosc. 179 (2017) 74–82.
10. V. A. Rana, D. P. Shah, C. M. Trivedi, Orientational and dielectric behaviour of N, N-dimethylformamide in different non-polar solvents, Indian J. Pure Appl. Phys. 56 (2018) 677–683.
11. G. Arivazhagan, A. Elangovan, R. Shanmugam, R. Vijayalakshmi, P. P. Kannan, Spectroscopic studies, NBO analysis and dielectric studies on the behaviour of acetone molecules in non-polar solvent environment, Chem. Phys. Lett. 627 (2015) 101–106.
12. J. Kiefer, S. Wagenfeld, D. Kerle, Chain length effects on the vibrational structure and molecular interactions in the liquid normal alkyl alcohols, Spectrochim. Acta Part A Mol. Biomol. Spectrosc. 189 (2018) 57–65.
13. V. Manjula, T. V. Prasad, K. Balakrishna, K. C. J. Raju, T. Vishwam, Investigation of temperature dependent dielectric relaxation studies of 1, 4- Butanediol/DMSO binary mixtures at the microwave frequency, J. Mol. Liq. 299 (2020) 112190.
14. R. K. Chaudhary, R. Kumar, V. S. Rangra, An investigation on molecular dynamics of binary mixtures of N-methylacetamide and tetramethylurea in microwave region, Indian J. Pure Appl. Phys. 56 (2018) 896–901.
15. F. Li, Z. Men, S. Li, S. Wang, Z. Li, C. Sun, Study of hydrogen bonding in ethanol-water binary solutions by Raman spectroscopy, Spectrochim. Acta Part A Mol. Biomol. Spectrosc. 189 (2018) 621–624.
16. M. Matsugami, R. Yamamoto, T. Kumai, M. Tanaka, T. Umecky, T. Takamuku, Hydrogen bonding in ethanol–water and trifluoroethanol–water mixtures studied by NMR and molecular dynamics simulation, J. Mol. Liq. 217 (2016) 3–11.
17. D. Checinska-Majak, A. Bald, R. J. Sengwa, Static permittivities of n-propanol mixtures with ethanol, isomers of propanol, and butanol at temperature (288.15–308.15) K, J. Mol. Liq. 179 (2013) 72–77.
18. R. J. Sengwa, S. Choudhary, P. Dhatarwal, Dielectric and electrical behaviour over the static permittivity frequency regime, the refractive indices and viscosities of PC–PEG binary mixtures, J. Mol. Liq. 252 (2018) 339–350.

19. R. J. Sengwa, S. Choudhary, S. Sankhla, Low frequency dielectric relaxation processes and ionic conductivity of montmorillonite clay nanoparticles colloidal suspension in poly (vinyl pyrrolidone)-ethylene glycol blends, Express Polym. Lett. 2 (2008) 800–809.
20. V. P. Pawar, S. C. Mehrotra, Dielectric relaxation study of liquids having chloro group with associated liquids. I. Chlorobenzene with methanol, ethanol, and 1-propanol, J. Solution Chem. 31 (2002) 559–576.
21. H. A. Chaube, Dielectric, Ultrasonic and Physical Properties of Binary Mixtures of Some Associative Polar Molecules, Ph. D. Thesis, Gujarat University, (2016), (n.d.).
22. D. K. Barot, Dielectric properties of solutions of 1-Butyl-3-Methyl Imidazolium chloride in polar solvents, Ph.D. Thesis, Gujarat University, (2019).
23. R. J. Sengwa, S. Sankhla, N. Shinyashiki, Dielectric parameters and hydrogen bond interaction study of binary alcohol mixtures, J. Solution Chem. 37 (2008) 137–153.
24. A. D. Vyas, V. A. Rana, D. H. Gadani, Dielectric properties of mixtures of some rigid polar molecules with some primary alcohols, (2011).
25. H. A. Chaube, Dielectric, Ultrasonic and Physical Properties of Binary Mixtures of Some Associative Polar Molecules, Ph.D., Gujarat University., 2016.
26. R. J. Sengwa, P. Dhatarwal, S. Choudhary, Role of preparation methods on the structural and dielectric properties of plasticized polymer blend electrolytes: correlation between ionic conductivity and dielectric parameters, Electrochim. Acta. 142 (2014) 359–370.
27. V. A. Rana, T. R. Pandit, Dielectric spectroscopic and molecular dynamic study of aqueous solutions of paracetamol, J. Mol. Liq. 290 (2019) 111203.
28. K. N. Shah, V. A. Rana, Dielectric spectroscopic study of solutions of amino silicone oil in the polar solvent mixtures of methyl ethyl ketone and methyl iso butyl ketone, J. Mol. Liq. 288 (2019) 111078.
29. A. Chaudhari, P. Khirade, R. Singh, S. N. Helambe, N. K. Narain, S. C. Mehrotra, Temperature dependent dielectric relaxation study of tetrahydrofuran in methanol and ethanol at microwave frequency using time domain technique, J. Mol. Liq. 82 (1999) 245–253.
30. T. Vishwam, V. R. K. Murthy, Microwave dielectric relaxation studies of hydrogen bonded polar binary mixtures of isobutanol and aniline, J. Mol. Struct. 1035 (2013) 46–53.

31. V. A. Rana, T. R. Pandit, Microwave dielectric relaxation spectroscopy of paracetamol and its aqueous solutions, J. Mol. Liq. 314 (2020) 113673.
32. J. Bao, M. L. Swicord, C. C. Davis, Microwave dielectric characterization of binary mixtures of water, methanol, and ethanol, J. Chem. Phys. 104 (1996) 4441–4450.
33. T. Vishwam, S. Shihab, V. R. K. Murthy, H. S. Tiong, S. S. Sastry, Microwave dielectric relaxation spectroscopy study of propylene glycol/ethanol binary mixtures: Temperature dependence, Spectrochim. Acta Part A Mol. Biomol. Spectrosc. 179 (2017) 74–82.
34. H. A. Chaube, V. A. Rana, D. H. Gadani, Dielectric absorption in mixtures of anisole with some primary alcohols at microwave frequency, Philos. Mag. 91 (2011) 4465–4473.
35. A. N. Prajapati, A. D. Vyas, V. A. Rana, S. P. Bhatnagar, Dielectric relaxation and dispersion studies of mixtures of 1-propanol and benzonitrile in pure liquid state at radio and microwave frequencies, J. Mol. Liq. 151 (2010) 12–16.
36. H. P. Vankar, V. A. Rana, S. Dey, H. D. Patel, V. K. Jain, Molecular interaction in binary mixtures of 3-Bromoanisole and methanol: A microwave dielectric relaxation spectroscopy and molecular dynamic simulation study, J. Mol. Liq. (2020) 115186.
37. T. S. Thakur, M. T. Kirchner, D. Blaser, R. Boese, G. R. Desiraju, Nature and strength of C–H···O interactions involving formyl hydrogen atoms: computational and experimental studies of small aldehydes, Phys. Chem. Chem. Phys. 13 (2011) 14076–14091.
38. O. W. Kgagodi, F. Mbaiwa, Molecular dynamics study of 2, 2′-difurylmethane and n-propanol binary mixture, J. Mol. Liq. 227 (2017) 366–372.
39. V. V Chaban, Binary mixtures of novel sulfoxides and water: intermolecular structure, dynamic properties, thermodynamics, and cluster analysis, Phys. Chem. Chem. Phys. 20 (2018) 23754–23761.
40. R. Raihan, M. R. P. Elenchezhian, V. Vadlamudi, Durability of bonded composite systems, in: Durab. Compos. Syst., Elsevier, 2020: pp. 383–401.
41. R. T. Hitchcock, Radio-frequency and microwave radiation, AIHA, 2004.
42. S. Tabassum, Microwave dielectric properties in binary mixture of polar liquids using microwave techniques, Ph.D. Thesis, Swami Ramanand Teerth Marathwada University, (2019).
43. J. F. Federici, D. Gary, R. Barat, Z. H. Michalopoulou, Detection of explosives by terahertz imaging, in: Counterterrorist Detect. Tech. Explos., Elsevier, (2007) 323–366.

44. H. P. Vankar, Dielectric and physico-chemical properties of binary mixtures of 3-Bromoanisole and some associative polar liquids, Ph.D. Thesis, Gujarat University., 2021.
45. A. Estrada-Baltazar, M. G. Bravo-Sanchez, G. A. Iglesias-Silva, J. F. J. Alvarado, E. O. Castrejon-Gonzalez, M. Ramos-Estrada, Densities and viscosities of binary mixtures of n-decane+ 1-pentanol, + 1-hexanol,+ 1-heptanol at temperatures from 293.15 to 363.15 K and atmospheric pressure, Chinese J. Chem. Eng. 23 (2015) 559–571.
46. E. Vercher, F. J. Llopis, V. Gonzalez-Alfaro, P.J. Miguel, V. Orchillés, A. Martínez-Andreu, Volumetric properties, viscosities and refractive indices of binary liquid mixtures of tetrafluoroborate-based ionic liquids with methanol at several temperatures, J. Chem. Thermodyn. 90 (2015) 174–184.
47. A. Luzar, J. Stefan, Dielectric behaviour of DMSO-water mixtures. A hydrogen bonding model, J. Mol. Liq. 46 (1990) 221–238.
48. J. A. Al-Kandary, A. S. Al-Jimaz, A. H. M. Abdul-Latif, Densities, viscosities, and refractive indices of binary mixtures of anisole with benzene, methylbenzene, ethylbenzene, propylbenzene, and butylbenzene at (293.15 and 303.15) K, J. Chem. Eng. Data. 51 (2006) 99–103.
49. F. Sha, T. Zhao, B. Guo, X. Ju, L. Li, J. Zhang, Density, viscosity and spectroscopic studies of the binary system 1, 2-ethylenediamine+ 1, 4-butanediol at T= (293.15 to 318.15) K, J. Mol. Liq. 208 (2015) 373–379.
50. P. S. Nikam, M.C. Jadhav, M. Hasan, Density and viscosity of mixtures of dimethyl sulfoxide+ methanol, + ethanol, + propan-1-ol,+ propan-2-ol,+ butan-1-ol,+ 2-methylpropan-1-ol, and+ 2-methylpropan-2-ol at 298.15 K and 303.15 K, J. Chem. Eng. Data. 41 (1996) 1028–1031.
51. H. Yaman, B. Dogan, M. K. Yesilyurt, D. Erol, Application of Higher-Order Alcohols (1-Hexanol-C6 and 1-Heptanol-C7) in a Spark-Ignition Engine: Analysis and Assessment. Arab. J. Sci. Eng 46(12) (2021) 11937-11961.
52. L. Cai, Y. Uygun, C. Togbe, H. Pitsch, H. Olivier, P. Dagaut, S. M. Sarathy, An experimental and modeling study of n-octanol combustion, Proceedings of the Combustion Institute, 35 (2015) 419-427.
53. J. Julis and W. Leitner, Synthesis of 1-Octanol and 1,1-Dioctyl Ether from Biomass-Derived Platform Chemicals, Angewandte Chemie International Edition, 51 (2012) 1-6.

54. R. J. Sengwa, V. Khatri, S. Sankhla, Static Dielectric Constants and Kirkwood Correlation Factor of the Binary Mixtures of N-Methylformamide with Formamide, N, N-Dimethylformamide and N, N-Dimethylacetamide. J. Sol. Chem 38 (2009) 763-769.
55. A. N. Prajapati, S. P. Patel, V. A. Rana, Study of short range and long range molecular interactions in binary liquid mixtures of N, N-dimethylformamide (DMF) and 1-propanol. J. Mol. Liq. 354 (2022) 118832.

Publications

Publications Related to Thesis

1. **N. A. Chaudhary**, K. N. Shah, C. R. Vaja, V. A. Rana, and A. N. Prajapati, Dielectric spectroscopic study of the binary mixtures of N-Hexanol with N, N-Dimethylformamide in the frequency range of 20 Hz to 2 MHz, International Journal of Modern Physics B, 2024, 2540033 (16 page) DOI: 10.1142/S0217979225400338.
2. **N. A. Chaudhary**, S. P. Patel, C. R. Vaja, N. K. Acharya, V. A. Rana and A. N. Prajapati, Study of dielectric properties of binary mixtures of n-Octanol and N, N Dimethylformamide in lower microwave radiation, Journal of Electronic Materials, (Article in Press) 2024.
3. **N. A. Chaudhary**, S. P. Patel, N. K. Acharya, M. K. Prajapati, A. N. Prajapati, Refractive index, Density, Excess properties and IR spectra study of 2 binary liquid mixture (n-Hexanol + N, N-Dimethylformamide), Journal of Electronic Materials, (Article in Press) 2024.
4. **N. A. Chaudhary**, C. R. Vaja, K. J. Agheda, K. N. Shah, V. A. Rana, A. N. Prajapati, Insights into Molecular Interactions: Dielectric Relaxation and DFT based studies on n-Hexanol/N, N-Dimethylformamide Binary Mixtures, Journal of Molecular Liquids, (Manuscript under review) 2024.
5. **N. A. Chaudhary**, K. N. Shah, C. R. Vaja, V. A. Rana, Deepak Kumar, A. N. Prajapati, Frequency-Dependent Electrode Polarization and Ionic Conduction Relaxation in n-Hexanol and DMF Mixtures at 303.15 K: Insights into Electrochemical Dynamics, Ionics, (Manuscript under review) 2024.
6. **N. A. Chaudhary**, K. N. Shah, S. P. Patel, A. N. Prajapati, Investigation of Some Physicochemical Properties of Binary Liquid Mixtures (n-Octanol + N, N-Dimethylformamide) at Different Temperatures, Journal of Electrical System (Manuscript communicated) 2024.
7. **N. A. Chaudhary**, Deepak Kumar, A. N. Prajapati, Application of refractometric properties and their mixing rules in binary systems of n-Hexanol with N, N-Dimethylformamide at 293.15 K, Recent Advances in Functional Materials, Volume 1 - Select Proceedings of RAFM 2024, Springer Nature (Manuscript communicated).
8. **Navin A. Chaudhary,** Shivani P. Patel and Ashvin N. Prajapati, Refractive indices, density and their related properties for several binary mixtures of n-Hexanol with N, N-Dimethylformamide at constant temperature 303.15K, Proceedings of International

Conference RAISE 2023: Vol. III Computer Science & Engg., Applied Mathematics, Electrical Engineering, Applied Physics, Publisher: RRRNA GOI;2023, Page NO:248-257, ISBN Number:978-81-962938-3-3.

Publications Non-related to Thesis

1. Maitri Patel, **N. A. Chaudhary**, Deepak Kumar, Kuldeep Mishra, Neeladri Das, A. N. Prajapati, Effect of introducing different molecular liquid solvents on electrochemical 2 and physical properties of sodium ion conducting polymer gel electrolytes, Journal of Molecular Liquids, (Accept) 2024.
2. K. J. Agheda, **N. A. Chaudhary**, N. Garad, S. N. Bariya, S. S. Soni, A. C. Kumbharkhane, B. S. Chakraborty, A. N. Prajapati, Dielectric, Acoustic and Refractometric Study of Binary Mixtures of Methanol with Bromoethane, International Journal of Modern Physics B, (Manuscript under review) 2024.
3. S. P. Patel, **N. A. Chaudhary**, K. N. Shah, N. S. Shah, C. R. Vaja, V. A. Rana and A. N. Prajapati, Concentration Dependent Study of Dielectric Dispersion and Microwave Heating Parameters of Binary Mixtures of Lower Order Alcohol with Valeronitrile, Journal of Microwave Power and Electromagnetic Energy, (Manuscript under review) 2024.
4. S. P. Patel, **N. A. Chaudhary**, N. S. Shah, C. R. Vaja, V. A. Rana, A. N. Prajapati, study of concentration dependent dielectric properties of n-heptanol, propionitrile and their binary liquid mixtures at constant temperature, Title: Proceedings of International Conference RAISE 2023: Vol. III Computer Science & Engg., Applied Mathematics, Electrical Engineering, Applied Physics, Publisher: RRRNA GOI;2023, Page NO:371-379, ISBN Number:978-81-962938-3-3.
5. K. J. Agheda, **N. A. Chaudhary**, N. Garad, A. C. Kumbharkhane, B. S. Chakraborty, A. N. Prajapati, Molecular interaction through dielectric relaxation study of methanol bromopropane mixtures as a function of composition, Journal of Electric System (Manuscript communicated) 2024.
6. S. P. Patel, **N. A. Chaudhary**, C. R. Vaja, N. S. Shah, K. N. Shah, Sanketsinh Thakor, V. A. Rana and A. N. Prajapati, Concentration depended dielectric and electric study of n-Heptanol and Propionitrile at different temperatures, Journal of Macromolecular Science, Part B, (Under review) 2024.

7. Maitri Patel, Kuldeep Mishra, **N. A. Chaudhary**, Vaishali Madhani, J. J. Chaudhari and Deepak Kumar, A sodium ion conducting gel polymer electrolyte with counterbalance between 1-ethyl-3- methylimidazolium tetrafluoroborate and tetra ethylene glycol dimethyl ether for electrochemical applications, RSC Advances, 2024, 14, 14358.
8. K. J. Agheda, N. B. Jani, **N. A. Chaudhary**, B. S. Chakrabarty and A. N. Prajapati, Investigation of volumetric and refractometric properties of a binary Mixture of tetrachloromethane with primary alcohol at constant, Title: Proceedings of International Conference RAISE 2023: Vol. III Computer Science & Engg., Applied Mathematics, Electrical Engineering, Applied Physics, Publisher: RRRNA GOI;2023,Page NO:11-20, ISBN Number:978-81-962938-3-3.
9. A. K. Patel, V. S. Patel, U. D. Raval, **N. A. Chaudhary**, K. N. Shah, A. N. Prajapati, Frequency and Concentration Dependent Dielectric and Electrical Properties of N, N-Dimethylacetamide and n- Nonanol, Journal of Electrical System (Manuscript communicated) 2024.
10. U. D. Raval, V. S. Patel, A. K. Patel, **N. A. Chaudhary**, K. J. Agheda, M. K. Prajapati, K. N. Shah and A.N. Prajapati, Physiochemical, electrochemical and DFT characterization of n-butanol and benzonitrile binary mixtures, Journal of Electrical System (Manuscript communicated) 2024.
11. V. S. Patel, A. K. Patel, U. D. Raval, **N. A. Chaudhary**, K. N. Shah, A. N. Prajapati, Dielectric spectroscopic study of Chlorobenzene With n-Butanol at different temperature, Journal of Electrical System (Manuscript communicated) 2024.

Papers presented in the conferences

1. Study of various acoustics parameters for binary mixtures (DMF + 1-PROPANOL)
   Navin A. Chaudhary, Shivani P. Patel, Ashvin N. Prajapati,
   International Science Symposium 2021 on Recent Trends in Science and Technology, Christ College, Rajkot, 08/04/2021 To 09/04/2021.
2. Study of acoustic and volumetric properties of the binary mixtures of N, N Dimethylformamide +1- Propanol
   Navin A. Chaudhary, Shivani P. Patel, Ashvin N. Prajapati,
   National Conference on Advances in materials science: Challenges and Opportunities (AMSCO-2021),
   Department of Physics, MKBU, Bhavnagar 21/09/2021.

3. Study of molecular interaction of binary mixtures (DMF+1- Propanol) using refractometric Properties

   N. A. Chaudhary, A. N. Prajapati, S. P. Patel,

   International e-Conference on Frontline Areas in Chemical Sciences,

   Department of PG studies and Department of Chemistry Pacific University Udaipur, 03/10/2021 To 04/10/2021.

4. Dielectric Study of Binary Mixture Of n-Octanol And N, N-Dimethylformamide At Constant Temperature 293.15 K

   N. A. Chaudhary, S. P. Patel, C. R. Vaja, N. S. Shah, A. N. Prajapati, V. A. Rana

   International Seminar on Advanced materials and Applications,

   Applied Physics Department, FTE, The M. S. University of Baroda, Vadodara, 18/07/2022.

5. Study of refractometric properties of binary mixtures of n-Hexanol with N, N-Dimethylformamide at 293.15K

   N. A. Chaudhary, S. P. Patel, A. N. Prajapati

   National Conference on Advances in Physical Sciences for Sustainable Development (NCAPSSD-2022),

   IITE Gandhinagar, 25/08/2022.

6. Study of Molecular Interaction in Binary Liquid Mixtures of n-Hexanol with N, N-Dimethylformamide Using refractometric and acoustic data at 303.15 K

   N. A. Chaudhary, S. P. Patel, A. N. Prajapati

   National Research Scholars' Meet on Condensed Matter Physics and Materials Science (CMPMS-23),

   Department of Physics, School of Sciences, Gujarat University, Ahmedabad, 04/03/2023.

7. Study of Complex Dielectric Properties of n-Butanol, Valeronitrile and their binary mixtures at 313.15K

   S. P. Patel, **N. A. Chaudhary**, H. P. Vankar, A. N. Prajapati, V. A. Rana,

   International Seminar on Advanced materials and Applications,

   Applied Physics Department, FTE, The M. S. University of Baroda, Vadodara, 18/07/2022.

8. Concentration dependent study of dielectric dispersion and microwave heating parameters of binary mixtures of lower order alcohol with Valeronitrile,

   S. P. Patel, **N. A. Chaudhary**, N. K. Acharya, C. R. Vaja, A. N. Prajapati, V. A. Rana,

28th International Conference on Nuclear Track and Radiation Measurements, Faculty of Science, Gurugram University Gurugram 06/11/2023 TO 10/11/2023.

9. A Comparative electrochemical impedance spectroscopic investigation on sodium ion conducting gel polymer electrolyte containing EMITf and TEGDME as molecular liquids
   Pinakin Bhatt, Nimisha Pathak, **Navin Chaudhary**, Ashvin Prajapati, Deepak Kumar, International Conference on Energy Materials & Rechargeable Batteries, Manav Rachna University, Faridabad 19/12/2023 TO 22/12/2023.
10. Excess Helmholtz Energy and Kirkwood Correlation Factor in Acetophenone-Methanol Binary Mixtures: Insights into Molecular Interaction
    A. N. Prajapati and **N. A. Chaudhary**
    International Conference on Material Physics and Electronics For Sustainable Development,
    Government Vidarbha Institute of Science and Humanities, Amravati 01/07/2024 TO 02/07/2024.
11. Excess Helmholtz Energy and Kirkwood Correlation Factor in Acetophenone-Methanol Binary Mixtures: Insights into Molecular Interaction
    A. N. Prajapati and **N. A. Chaudhary**
    International Conference on Material Physics and Electronics For Sustainable Development,
    Government Vidarbha Institute of Science and Humanities, Amravati 01/07/2024 TO 02/07/2024.

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