

DECLARATION

I declare that the thesis entitled "EXPLORATION OF SOLVATION CONSEQUENCES OF SOME IONIC LIQUID AND BIOLOGICALLY POTENT MOLECULES PREVAILING IN DIFFERENT LIQUID ENVIRONMENTS" has been prepared by me under the proper guidance of Dr. Mahendra Nath Roy, Professor of Chemistry, University of North Bengal. No part of this thesis has formed the basis for the award of any degree or fellowship previously.

Sukdev Majumder

Sukdev Majumder

Department of Chemistry,

University of North Bengal,

Darjeeling 734013,

West Bengal

Date: 03.01.2022

UNIVERSITY OF NORTH BENGAL

Prof (Dr.) M. N. Roy,

FRSC (London)

Awardee of

UGC One Time Grant Under Basic Scientific Research

Prof. Suresh C. Ameta award from ICS

Bronze Medal from CRSI

Shiksha Ratna from the Govt. of West Bengal

Panchanan Barma Sadbhavona Sanman

and

Dewang Mehta Best Professor in Chemistry

Department of Chemistry



ENLIGHTENMENT TO PERFECTION

Phone: 0353 2776381

Mobile: 09434496154

Fax: 91 353 2699001

Darjeeling 734 013, INDIA

January, 2022

E-mail: mahendraroy2002@yahoo.co.in

CERTIFICATE

I certify that Mr. Sukdev Majumder, *M. Sc.* in *Chemistry*, has prepared the thesis entitled "EXPLORATION OF SOLVATION CONSEQUENCES OF SOME IONIC LIQUIDS AND BIOLOGICAL POTENT MOLECULES PREVAILING IN DIFFERENT LIQUID ENVIRONMENTS", for the award of *Ph. D. Degree (Doctor of Philosophy)* of the *University of North Bengal*, under my guidance. He has carried out the work at the *Department of Chemistry, University of North Bengal*.

Mahendra Nath Roy

PROF. (DR.) MAHENDRA NATH ROY,

Professor of Chemistry,

Department of Chemistry,

University of North Bengal,

Dist: Darjeeling, Pin: 734013,

West Bengal, INDIA

DATE: 03-01-2022

Prof. (Dr.) M.N. Roy
FRSC (London), UK
Department of Chemistry
University of North Bengal
Darjeeling-734013, India

UNIVERSITY OF NORTH BENGAL

Dr. Nitish Roy
Assistant Professor
Raja Rammohunpur,
Darjeeling, WB-734013 India



Email: ntu.litg@gmail.com
Mob: 91 7872808189
Website: <https://ntu.litg.wixsite.com/ntitshroy>
January, 2022

ENLIGHTENMENT TO PERFECTION

CERTIFICATE

I certify that Mr. Sukdev Majumder, *M. Sc.* in *Chemistry*, has prepared the thesis entitled “EXPLORATION OF SOLVATION CONSEQUENCES OF SOME IONIC LIQUIDS AND BIOLOGICALL POTENTMOLECULES PREVAILING IN DIFFERENT LIQUID ENVIRONMENTS”, for the award of *Ph. D. Degree (Doctor of Philosophy)* of the *University of North Bengal*, under my guidance. He has carried out the work at the *Department of Chemistry, University of North Bengal*.

Nitish Roy
DR. NITISH ROY,
(CO-SUPERVISOR)

Dr. Nitish Roy
Assistant Professor
Department of Chemistry
University of North Bengal
Raja Rammohunpur,
Darjeeling, WB-734013, India

Assistant Professor,
Department of Chemistry,
University of North Bengal,
Dist: Darjeeling, Pin: 734013,
West Bengal, INDIA

DATE: 03/01/2022

Document Information

Analyzed document Sukdev Majumder_Chemistry.pdf (D122671774)
Submitted 2021-12-16T11:42:00.0000000
Submitted by University of North Bengal
Submitter email nbuplg@nbu.ac.in
Similarity 0%
Analysis address nbuplg.nbu@analysis.arkund.com

Sources included in the report

- W URL: [https://www.geteasysolution.com/\(1/4\)0-2](https://www.geteasysolution.com/(1/4)0-2)
Fetched: 2021-11-10T20:58:18.9000000  3
- W URL: <https://socratic.org/questions/can-you-prove-that-1-2-2-2-3-2-n-2-1-6n-n-1-2n-1>
Fetched: 2021-04-27T17:57:52.7870000  1

Sukdev Majumder

Signature of candidate

03.01.2022

Nitish Roy

Signature of Co-Supervisor

03/01/2022

Dr. Nitish Roy
Assistant Professor
Department of Chemistry
University of North Bengal
Raja Ramohanpur,
Dargajing, WB-734013, India

Mahendra Nath Roy

Signature of Supervisor (03-01-2022)

Prof. (Dr.) M.N. Roy
FRSC (London), UK
Department of Chemistry
University of North Bengal
Darjeeling-734013, India

ACKNOWLEDGEMENT

Completing the Ph. D. degree has been one of the most appreciated dreams of my life right from the early days of my graduation. This Ph. D. thesis has been the most challenging academic task I have ever faced. At the juncture of this milestone achievement, I would like to express my sincere gratitude to everyone who believed in me and to whom I am indebted to for their help, support and motivation in all my accomplishments.

At the first occasion, I would like to express my profound sense of gratitude and inner attitude to my respected teacher and supervisor **Dr. Mahendra Nath Roy**, Professor in Physical Chemistry, Department of Chemistry, University of North Bengal, and Darjeeling, India for accepting me into his research group. He is an ideal role model for his professionalism in both work and personal lives. Without the opportunity, he offered I would not be where I am today! Throughout my research period, I received constant guidance, priceless suggestions, ceaseless inspirations and constructive criticism from him. He deserves special thanks since he has not only offered me his kind guidance but also motivated and encouraged me to go that extra mile during this journey. I am deeply indebted to him for his keen interest, constant enthusiasm, deep knowledge, confidence and sympathetic consideration. He gave me the freedom to pursue an intriguing and a challenging voyage although never falling behind to trust me, often more times than myself, thus tremendously boosting my confidence to explore the true capabilities of my potential. He was always there to listen and to give advice. He taught me how to ask questions and express my ideas. He showed me different ways to approach a research problem and the need to be persistent to accomplish any goal. Without his loving care, meticulous guidance and precious supervision, the formulation of my work associated with my thesis would not have been possible for me to bring the present contour. The good advice, support and encouragement that I have received from him has been invaluable on both an academic and a personal life, for which I shall ever remain very obliged.

I am also very much grateful to my co-guide Dr. Nitish Roy, Department of Chemistry, University of North Bengal, for his outstanding knowledge, sincere guidance and

Acknowledgement

Valuable advices throughout the journey of my research work.

I also put-across my profound prudence of appreciation to all of the respected faculty members of Department of Chemistry, University of North Bengal for their untiring assistance, academic, technical support and continual inspiration during the course of my research work. I am gleefully thankful to the non-teaching staff of the Department for their cooperation and help.

I am grateful to the University authority for providing laboratory and library amenities, especially Computer Centre and University Scientific Instrumentation Centre (**USIC**) of the University for serving me in my research work.

My special thanks go to Dr. Subhodip Saha, Dr. Deepak Ekka, Dr. Anuradha Singha, Dr. Lovley Sarkar, Dr. Ashutosh Dutta and lab mates of my research laboratory for their valuable assistance and cooperation throughout my research work.

I am highly grateful to my beloved father, Mr. Satya Ranjan Majumder and my mother, Mrs. Khusumbala Majumder for their irreparable contribution for all round developments in my life. I would like to give special thanks to my wife, Sabita Majumder(Sarkar), sister Rinku Majumder, son Sanay Majumder, elder brothers Sri Sujit Majumder and Sri Subrata Majumder for their constant help, support, encouragement and whole hearted cooperation and heart felt inspiration with a view to building my academic career associated with my Ph.D. thesis.

I am thankful to the Departmental Special Assistance Scheme under the University Grants Commission, New Delhi (**No. F 540/27/ DRS/2007, SAP-1**) for providing financial aid and instrumental assistance in order to continue my research work. I would also like to record my thankfulness to '**ONE TIME GRANT**' Ref No. **F.4-10/2010(BSR)** awarded to my Supervisor, **Prof. M. N. Roy**, under **Basic Scientific Research (BSR), UGC, New Delhi** for financial and instrumental assistance in connection with research work.

I am constantly aware of what a huge debt I owe to the sources of the information required for my research work: the numerous books, monographs, articles, computer website, etc. I put on record some measure of my gratitude to those whose references I have cited in this thesis.

The above list is neither complete in names, nor in deeds of all the people who have helped me towards achieving this Ph.D. degree. I would like to profusely apologize, and state that the omissions were not a meditated slight. This dissertation would not have been possible without their help.

Sukdev Majumder
Sukdev Majumder

Research Scholar

Department of Chemistry

University of North Bengal

Dist- Darjeeling, Pin-734013,

West Bengal, INDIA

PREFACE

The excellent work done in this thesis entitled “**EXPLORATION OF SOLVATION CONSEQUENCE OF SOME IONIC LIQUID AND BIOLOGICALLY POTENT MOLECULES PREVAILING IN DIFFERENT LIQUID ENVIRONMENTS**” was started in **March 2018** under the supervision of *Dr. M. N. Roy, Professor of Physical Chemistry, Department of Chemistry, University of North Bengal, and Darjeeling (NBU)*. This research became conscious within the framework of the Programme in the field of “*Ionic Liquids & Solution Thermodynamics*” and Research Group of Professor Roy.

The work is an attempt to explore the solute –solvent as well as ionic level interactions of IONIC LIQUIDS and AMINO ACIDS in aqueous solution systems by studying their thermophysical, thermodynamic, transport, optical, computational and spectroscopic properties.

I was exceedingly enthused by my listening, interacting and cooperating with renowned researchers, experts, reviewers and scientists during the course of my research work through the communicating via email, web-side in internet, with the participation in several meets and attaining, presenting in seminars/symposiums/ conferences across the country. I am even fortunate enough to publish my original research works as article enclosed in the dissertation in National and International Journals of repute.

In trusting with all-purpose perform of reporting scientific observation, due acknowledgement has been made whenever the work described was based on the finding of other investigators. I must take the responsibility of any unintentional oversights and errors, which might have crept in spite of precautions.

ABSTRACT

Ionic liquids (ILs) and amino acids are very significant molecules for our Environment system and it can be important in the field of medical application.

ILs are the salt in the liquid state/phase that consist both organic part and inorganic part. ILs have been classified those salts whose melting point generally less than 100 °C (212 °F). The ILs have some special properties like low melting point, vapour pressure, good solvent behaviour for polymeric, organic part and as well as inorganic materials, adjustable polarity. Low viscosity, over an inclusive range of potentials, high conductivity, selective catalytic effect, for this it has wide range of industrial applications, pharmaceuticals, cellulose processing, gas handling, gas treatment, solar thermal energy, nuclear fuel processing, food and by-products, waste recycling, batteries etc. In the earlier few years for sustainable environment, chemical process led to growing attention in the arena of IL for investigation and applied as a green solvent instead of very harmful organic solvents. Biological potent molecules i.e. *amino acids (AAs)* are very essential for human body, which are constructing blocks of proteins, peptides, and polypeptides. AAs are also used in nutrition enrichments, food technology, fertilizers industry, consist of the creation of biodegradable plastics, drugs, and chiral catalysts.

Physio-chemical behaviour of electrolytes take place a very crucial role in determining the solute-solute/ ion –ion, solute –solvent/ ion –solvent interactions in solution phase. For the exploration of the nature and strength of different kind of interaction, different parameter like, thermodynamic , transport properties of electrolytes, optical properties, the traditional boundaries of physical , inorganic, analytical and electrochemistry are used for this purpose.

Solution chemistry is very importance especially in the branch of physical chemistry. This branch deals with the change in properties that arise when one molecule dissolve into another molecule. ‘Solution Chemistry’, deals with broadly three types of approaches, which have been made to estimate the extent of solvation. First approaches that involves the studies of viscosity, apparent molar volume, refractive index, conductance, surface tension etc. of electrolytes and the derivation of various factors associated with ionic solvation. The second is the approach of thermodynamic by

measuring the free energies, enthalpies and entropies of solvation of ions from which factors associated with solvation can be elucidated, and the third is to use spectroscopic measurements like, UV-vis, fluorescence Study, FTIR, NMR ,where the spectral solvent shifts or the chemical shift conclude their qualitative and quantitative nature .

Ion –ion and ion –solvent interaction in solution can be understood from the computational study method, observations of transport properties of electrolytes, along with thermodynamic parameters like limiting apparent molar volume and compressibility studies. From the effect of these ion-solvent interactions is origins to cause dramatic changes in chemical reactions involving ions. The changes in ionic solvation have very significant applications in such diverse areas as organic and inorganic synthesis, studies of reaction mechanisms, in battery technology and extraction.

Solvation is the method to attraction or association of solvent molecules with solute molecules. The solute molecules surround solvent molecules when it is soluble. A solvent complex is made when a molecule or ion of solute is bounded by solvent. Solvation is the technique of rearranging solvent and also solute molecules into solvation complex and the process is so on until the solute molecules is distributed inside the solvent perfectly. The following factors like hydrogen bonding, Vander Waals forces are dependent on solvation. Insoluble solute molecules like to maintain among the interaction rather than break apart from individually and become solvated by the solvent molecules. Hydration in the way of solvation where solute molecules is surrounded by water molecules.

Mixing of different solvent or solute molecules do not have ideal solution property. This type of deviation from ideally is given in the term of thermodynamic parameter, by apparent molar properties in case of solid- liquid mixture and by excess properties in case of liquid-liquid mixture. Thermodynamic properties that are very useful to investigate the molecular interaction and arrangement of the molecule. In particular, the interaction take place between solute – solute, solvent –solvent, solute – solvent species. The modification of solute molecules has been done by the addition of solute molecules in solvent molecules. The level of interaction among molecules depends on interactions taking place between solute-solute, solute-solvent species. The ion-pairing effect of the system is explain on the basis of ionic mobility hence on the conductivity of ions in solutions. Thus, this phenomenon is the way of path for research work in solution

chemistry to deduce the nature of interaction through different experimental observation involving densitometry, viscometry, refractometry, computational study, surface tension, spectroscopy and other suitable method and explained the data collected from experiment. All-over understanding of the phenomena of solution will only reality when solute-solute, solute-solvent interaction are deduced. Thus, the present research work is intimately related to the studies of solute-solute and solute-solvent interactions in some biologically important potent molecules (amino acids) and some industrially important liquid systems.

One of the very interesting phenomena of Solution Chemistry is that the exact structure of the solvent molecule in a solution is not known with certainty. The introduction of an ion or solute modifies the solvent structure largely whereas the solute molecules are also modified as the same way. The interactions between solute-solute, solute-solvent, and solvent-solvent molecules and the resulting ion-solvation become predominant, though the isolated picture of any of the forces is still not known completely to the solution chemists.

A.1 CHOICE AND IMPORTANCE OF IONIC LIQUIDS (ELECTROLYTES) AND SOLUTE MOLECULES (NON-ELECTROLYTES) AND SOLVENTS USED

A.1.1 Ionic Liquids: - The following ionic liquid are used for my research work

1-Butyl-3-methylimidazolium octylsulphate (BMIM) (C₈SO₄), 1-Methyl-3-octylimidazolium chloride(MOIM)Cl, Benzyl tri methyl ammonium chloride, 1-Butyl pyridinium Bromide (BP) Br, Benzyl tri butyl ammonium chloride, Tetra butyl ammonium Methane sulphonate, Benzyl tri ethyl ammonium chloride

A.1.1.2 Non- Electrolytes (amino acids): following amino acids (non-electrolytes) are used for my research work.

L-tyrosine, L-phenylalanine, L-Ascorbic acid, L-Aspartic acid, L-Glutamic acid, L-Asparagine, L-Glutamine, L-methionine, L-arginine, L-histidine

A.1.2 SOLVENT: The only universal solvent, water has been carried out for my research work throughout the experiment.

The study of ionic liquid (used as an electrolyte), amino acid (non-electrolyte) and solvent is great significant due to their wide-ranging use in many industrial purposes ranging from pharmaceutical to cosmetic by means of solvent, solute and also solubilizing agents. By mixing of above mentioned solvent as a binary, ternary, quaternary etc. mixture with huge range of variation of viscosities and dielectric constants, which gives us a best array for the study.

A.2 METHODS OF INVESTIGATION:-

It is of curiosity to employ different experimental methods to develop a better vision into the behavior of solvation and different interactions prevailing in biologically potent molecules in solution systems. therefore I have tried to incorporate with some important thermophysical methods, namely, *Densitometry*, *Surface chemistry (surface tension)*; transport properties viz., *Viscometric*, *Conductometric*; optical property *Refractometric* and spectroscopic property *FTIR Spectroscopic* method, UV-visible, fluorescence study, NMR technique to examine, probing, exploring of various interactions occurring in the solution systems.

A.3 PHYSICO-CHEMICAL PARAMETERS AND THEIR IMPORTANCE:

Using experimental density values to calculate the ϕ_v^0 of the solutions. The magnitude as well as sign of limiting molar volumes provides information about the nature and magnitude of solute/ion-solvent interaction while the experimental slope (S_v^*) provides information about ion/solute-ion /solute interactions.

From experimental viscosity data the Viscosity *B*-coefficients obtained which are another tool gives the useful scheme of ion/solute-solvent interaction in solutions.

The optical property such as refractive index, spectroscopic property as FTIR, UV-visible, NMR Spectroscopy, and fluoresces are used for supporting parameters to confirm the interaction occurring in the solution systems.

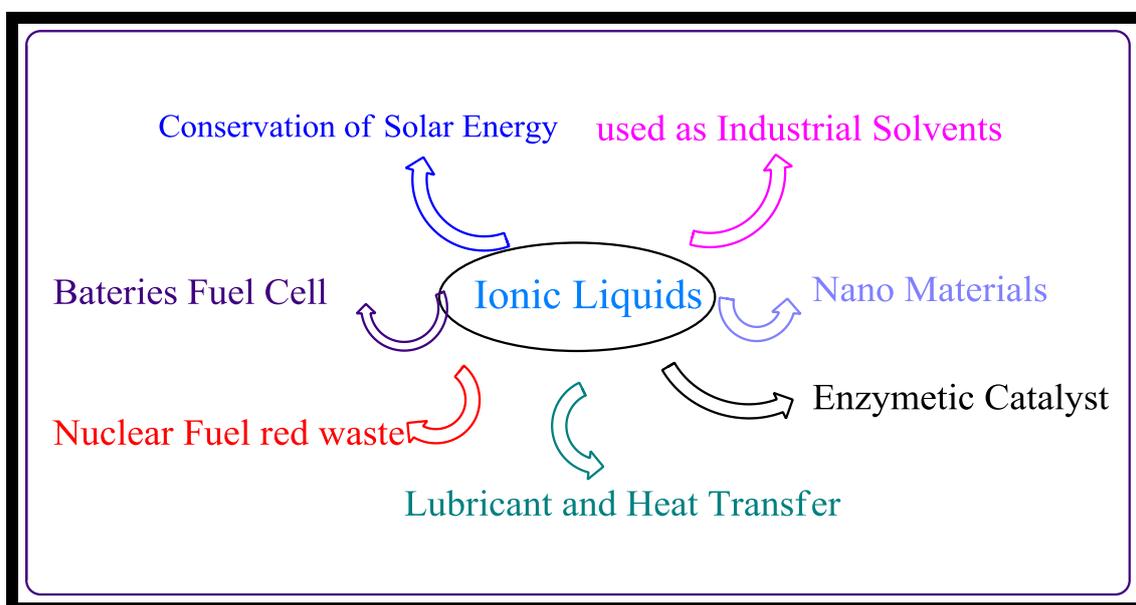
The computational study, surface tension measurement also give the type of interaction associated in molecules in solution system.

Limiting molar conductance (Λ_0) obtained from using specific conductance values and also molar conductance gives a central idea about the ion-solvent interaction in the solution mixtures. More the magnitude of molar conductance values in solution less is the ion-solvent interaction. Another important parameters that are getting from the conductance study *i.e.*, association constant, Gibbs free energy, gives an idea about the solvation properties of ions in solutions.

A.4. SUMMARY OF THE WORKS EMPHASIZE IN THE THESIS:

CHAPTER-I

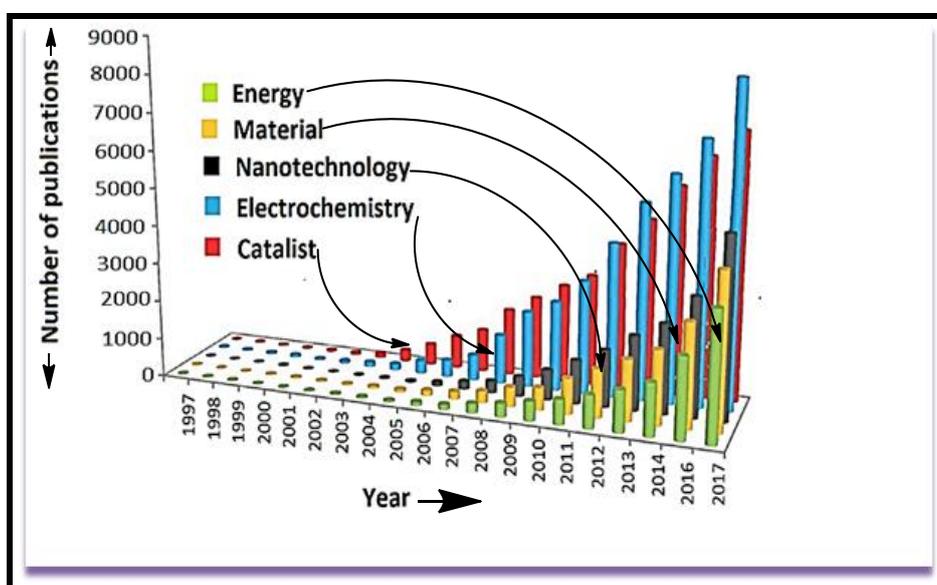
This chapter encloses the *objective, utility and applications of the research work*, the important of electrolytes/solute molecules and solvents used and methods of investigation. This also occupies the summary of the works done connected with the thesis.

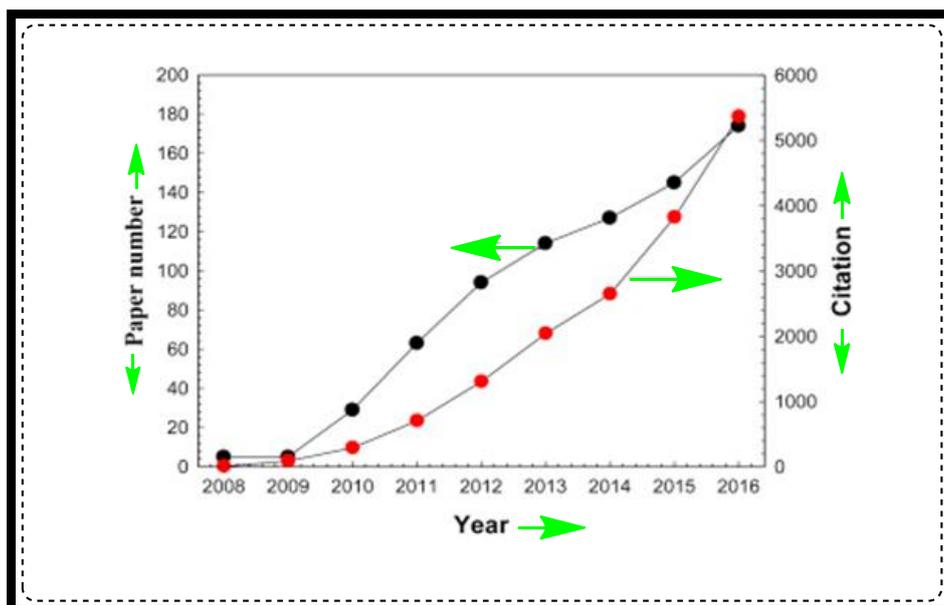


CHAPTER-II

The chapter contains *the general introduction* (Review of the Earlier Work) of the thesis and forms and the very strong background of the work embodied in the thesis. A brief criticism of remarkable works in the field of solute-solvent, solute-solute and solvent-solvent interactions has been given. In this chapter, the discussion includes the ion-solvent/solute-solvent, ion-ion/solute-solute and solvent-solvent interactions in binary, ternary mixed solvent systems and of electrolytes in pure and non-aqueous solvent

systems at various temperatures in terms of various derived parameters, estimated from the experimentally detected thermophysical properties *viz.*, *density, refractive index, viscosity and conductance*. Several semi-empirical models to approximation dynamic viscosity of binary liquid mixtures have been deliberated. Using Stokes' law and Walden rule, Ionic association and its necessity on ion-size parameters as well as relation between solution viscosity and limiting conductance of an ion has been deliberated. The molecular interactions are understood based on various derived parameters. Key assessment of different methods on the relative merits and demerits based on various types of assumptions employed from time to time of obtaining the single ion values (viscosity B coefficient and limiting equivalent conductance) and their implications have been understood. Different spectroscopic technique also discussed in this chapter. The molecular interactions are also made based on various type of equations.





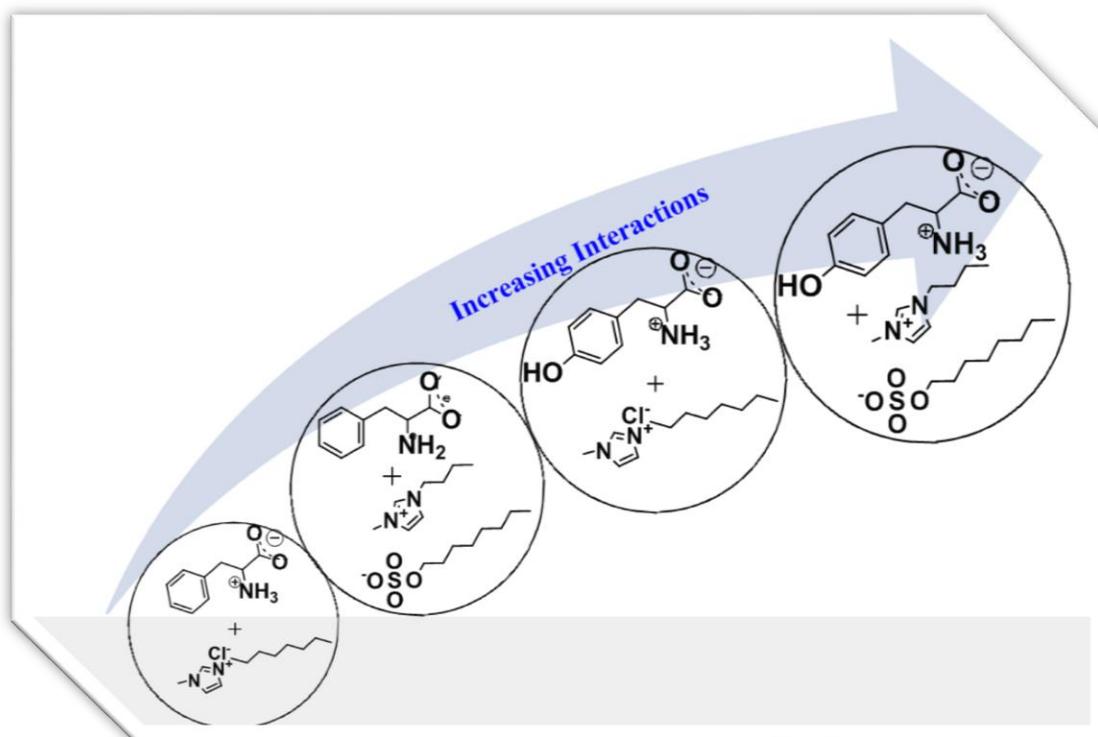
CHAPTER-III

This chapter includes *the experimental section*, which mostly contains the basic information's, structure, source, purification and uses of the ionic liquids, electrolytes/non-electrolytes or solutes, and solvents have been used throughout the whole research work. It is also confines the details of the procedure, instruments working principle and equations that are employed to know the thermophysical/thermodynamic, transport, optical and spectroscopic assets.



CHAPTER-IV

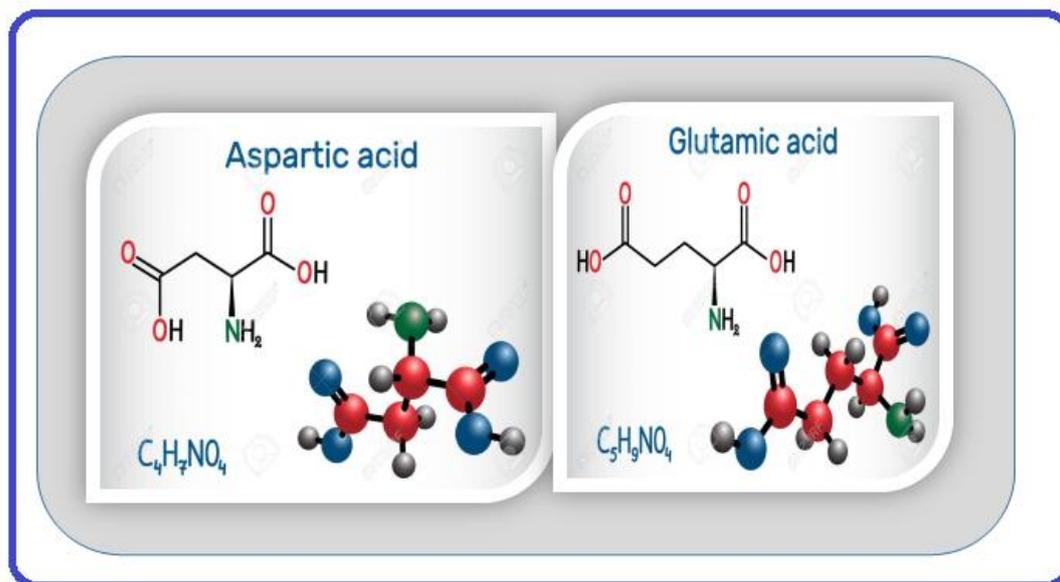
The chapter deals with the precise measurements on electrical conductance (Λ) steady state fluorescence, UV visible spectroscopy, determination of association constant, Gibbs free energy, study of proton NMR of solutions of an ionic liquid (ILs), L-Tyrosine, L-Phenyl alanine and their binary mixtures have been reported at 298.15K. From the above experiments, data reported which can explain the nature of interaction properties associated with the ionic liquids and the solute molecules. Also from the value of proton NMR, data can help the chemical environment of different protons and different types of interactions (non-covalent bond, weak pi-pi interaction).



CHAPTER-V

The chapter embraces the analysis of solute-solute and solute-solvent interactions between IL(BTAC) and two solute molecules(L-glutamic acid and L-Aspartic acid at different temperature(298.15k,303.15k,30815k) quantitatively by precise measurement of density, viscosity, refractive index, molar conductance(Λ), in the solution systems. From limiting apparent molar volume, (Φv°) experimental slopes (SV^*), viscosity B-

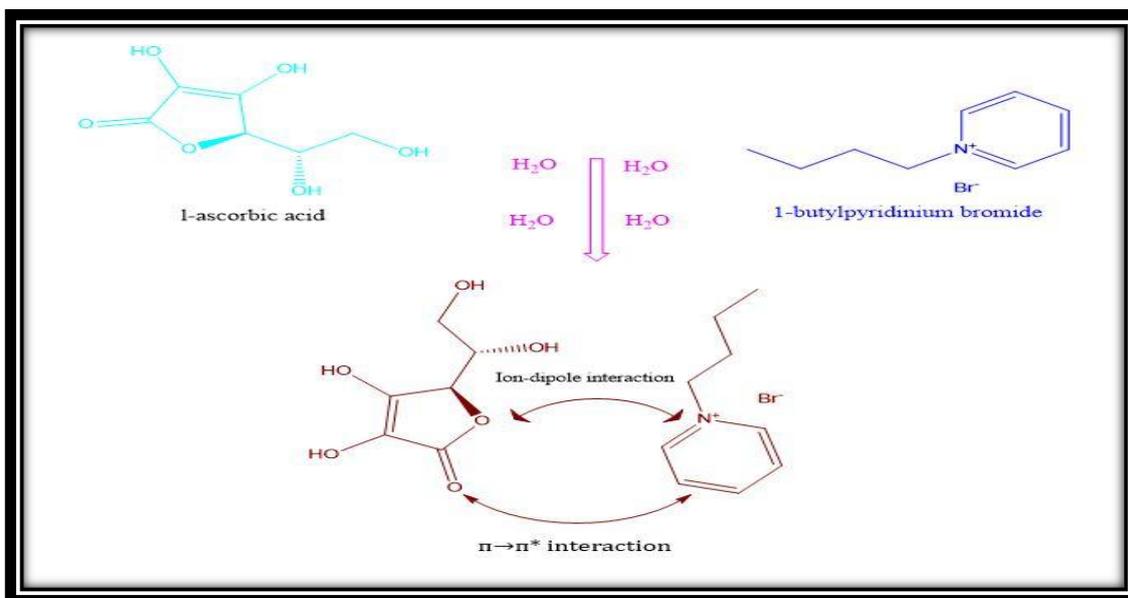
Coefficient data, molar refraction data explained the interaction phenomenon (solute-solvent and solute-solute interactions). Formation of Hydrogen bonding, Dipole-dipole interaction configurational theory, structural aspect, are the powerful forces, for the discussion of the results. The solvation behaviour is manifested by the variation of the difference parameters explained in this chapter in the presence of ionic liquids.



CHAPTER-VI

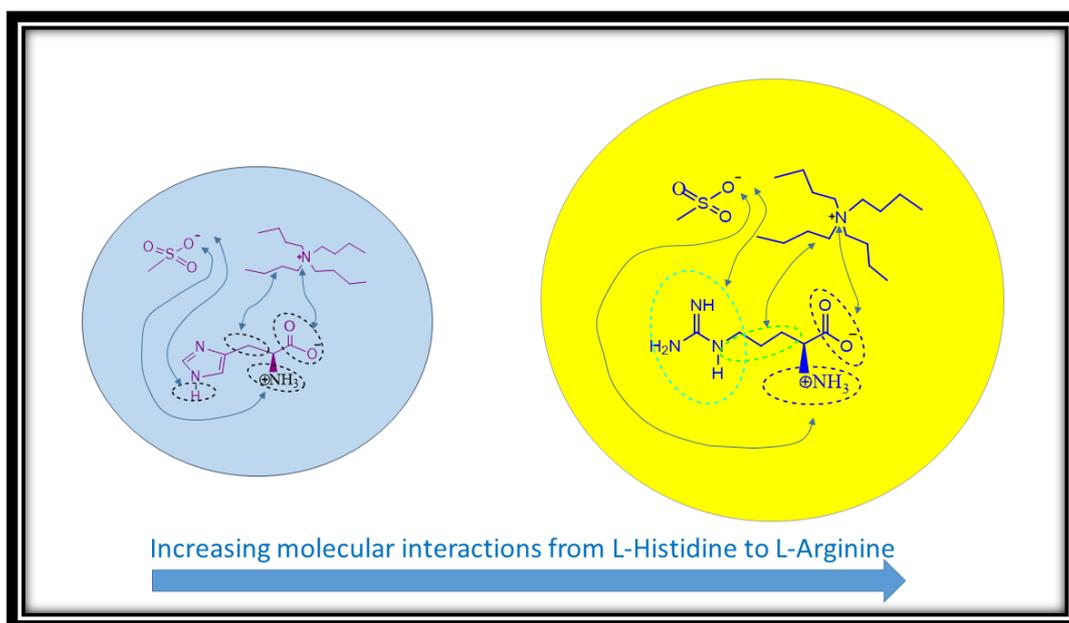
Apparent molar volumes (ϕ_v), viscosity B -coefficients, refractive index, specific conductance for L-Ascorbic acid (0.001, 0.003, and 0.005 mol.dm⁻³) in aqueous ionic liquid, 1-Butylpyridiniumbromide ($C_9H_{14}NBr$) solutions were calculated from density of solution. Also viscosity measurements at three different temperature (298.15, 308.15, and 318.15 K) and $p = 0.1$ MPa as a function of the concentration (Molality) of L-Ascorbic acid have been reported in this chapter. At infinite dilution, extrapolated of the apparent molar volumes upto zero concentration, the limiting apparent molar volumes (ϕ_v^o), obtained. Solute-solvent interactions can be explain from the different parameters obtained from the Redlich-Meyer equation. Using Jones-Dole equation, the viscosity values were discussed, and solute- solvent interactions have been explained from the resulting parameters A and B in the mixed solutions. Ability to structure making or -breaking of the electrolyte (L-Ascorbic acid) has been analyzed with the help of sign of

dB/dT . Conductance values also supported the solute-solvent interactions associated with vitamin C (L-Ascorbic acid) and ionic liquid (1-Butylpyridiniumbromide).



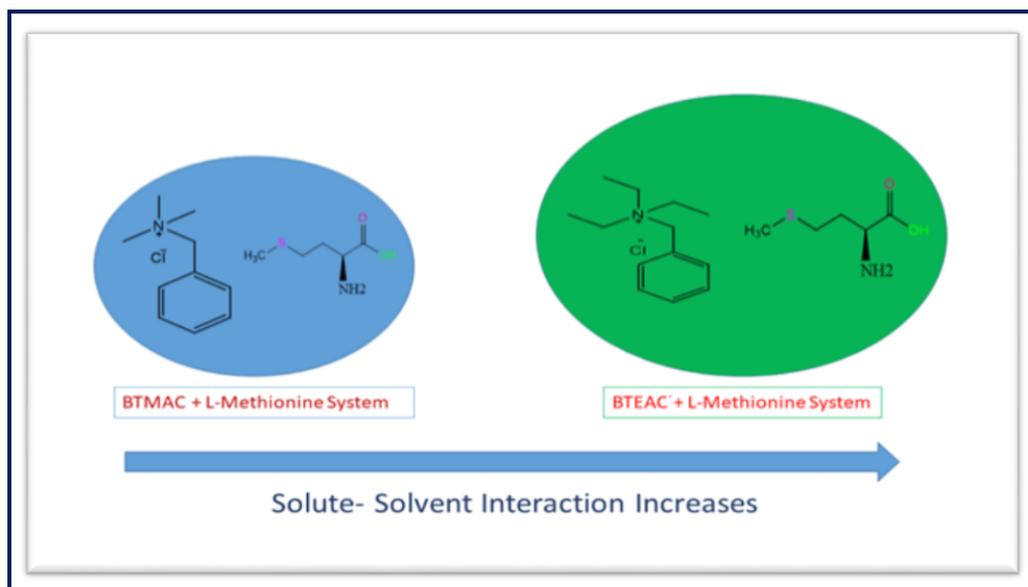
CHAPTER-VII

Custody in mind the uses of amino acids the apparent molar volume (ϕ_V), viscosity B -coefficient, Molar conductance (Λ) and molar refraction (R_M) of L-Arginine and L-Histidine have been determined in IL (Tetra butyl ammonium methane sulfonate) at 298.15 K, 303.15K, 308.15K from density (ρ), viscosity (η), Specific conductance and refractive index (n_D) respectively. Using Masson equation, the limiting values at infinite dilution are by extrapolated to zero concentration of apparent molar volumes. Interactions phenomenon of both solute-solute & solute-solvent have been understood from the slopes (S_V^*) and (ϕ_V^0), which obtained from the Masson equation. Viscosity parameter A & B which derived from Jones- Dole equation, using viscosity values have been used to interpretation the molecular interactions in solution. Applying Lorentz-Lorenz equation to evaluated the Molar refraction (R_M) values as explain the solvation behaviour of solution mixtures. Molar conductance data also explain the molecular interactions involving in solutions. Interactions properties also explain by computational study. Some thermodynamic parameters also derived by using some equations for explanation of interactions in solution.



CHAPTER-VIII

This chapter includes the study on interactions between solute-solvent and solute-solute. Here the interactions behaviour between two ionic liquids (solvent) , Benzyl tri methyl ammonium chloride and Benzyl tri ethyl ammonium chloride with one amino acid(solute)L-Methionine have been carried out by volumetric, viscometric, conductometric, refractometric, surface tension, NMR, Computational study measurements. Comparison of solute-solute and solvent-solvent interactions between ILs with amino acid can be explained with the help of some physicochemical parameter such as limiting apparent Molar volumes (Φ_v°), viscosity B-Coefficient, Molar conductance (Λ) data. In addition, proton NMR, UV-Visible and FTIR spectroscopy help to determine the interaction properties in pure as well as the solution mixtures. Variation of optimization energy calculated theoretically by Gaussian Method of pure ionic liquids and mixture with amino acid gives the same result obtained practically from above mentions of different parameters in this chapter.



CHAPTER-IX

In this chapter physicochemical properties such as density (ρ), viscosity (η), refractive index (n_D), molar conductance (Λ), surface tension measurements of ionic liquid (Benzyltributylammoniumchloride), solute molecules, Lglutamine ($C_5H_{10}N_2O_3$) & Lasparagine ($C_4H_8N_2O_3$) and their ternary mixtures (IL+AA+H₂O) have been observed at 298.15 K, 303.15K, 308.15K, respectively. Solute- solute and solute- solvent interaction have been interpreted by some very significant physicochemical parameters namely, Apparent molar volumes (ϕ_V), and viscosity B -coefficients accompanied with the data of densities and viscosities respectively. Using the Masson and Jones-Dole equation for elucidating the limiting apparent molar volumes (ϕ_V^0), slopes (S_V^*), viscosity A , B coefficients respectively. Spectroscopic technique such as ¹HNMR, UV-vis. is also applying for determination of molecular interactions. Molar expansibility factor (ΦE° and $\partial\Phi E^\circ/\partial T$) obtained by applying polynomial equation which explain the solute- solvent interactions properties. Computational study is also accompanied with the manifestations of interactions prevailing in ionic liquid with two amino acids.

CHAPTER-X

In this chapter, covers the concluding remarks of the works related or detailed described in the thesis (dissertation).

TABLE OF CONTENTS

Subject	Page No
<i>Declaration</i>	(iv)
<i>Certificate</i>	(v-vi)
<i>Antiplagiarism Report</i>	(vii)
<i>Acknowledgements</i>	(viii-x)
<i>Preface</i>	(xi)
<i>Abstract</i>	(xii-xxiii)
<i>List of Tables</i>	(xxx-xliv)
<i>List of Figures</i>	(xlv-liii)
<i>List of Schemes</i>	(liv)
<i>List of Appendices</i>	(lv)
<i>Appendix A: List of Publication(s),List of Research Publication(s)</i>	(lvi-lvii)
<i>Appendix B: List of Seminars / Symposiums / Conferences Attended</i>	(lviii)
<i>Appendix C: List of Symbols, Abbreviations and Acronyms</i>	(lix-lxiv)
CHAPTER: I	(1-14)
<i>Necessity of the Research Work</i>	
I.1. Scope, Objective and Applications of the Research Work	
I.2. Choice and Importance of Solutes and Solvent Used	
I.3. Methods of Investigation	
I.4. Summary of the Work Emphasize in the Dissertation	
CHAPTER: II	(15-79)
<i>General Introduction(Review of the Earlier Works)</i>	
II.1. Ionic liquids	
II.2. Amino acids	
II.3. Solution chemistry	
II.4. Various driving forces of interaction	
II.5. Interactions in solution systems	
II.6. Investigation on different kind of interactions	

Table of Contents

Subject	Page No
II.7. Volumetric Measurements II.8. Viscosity of liquids and liquid mixtures II.9. Refractive index II.10. Conductance II.11. FTIR spectroscopy II.12. UV-Visible-Spectroscopy II.13. Fluorescence Spectroscopy II.14. Surface Tension Measurements II.15. $^{15}\text{H}^1\text{NMR}$ Spectroscopy	
CHAPTER: III <i>Experimental Section</i>	(80-117)
III.1. Name, Structure, Physical Properties, Purification and Applications of the Chemicals used in the Research Work III.2. Experimental Methods	
CHAPTER: IV EXPLORING DIVERSE INTERACTIONS OF SOME SURFACE ACTIVE IONIC LIQUIDS WITH AMINO ACIDS PREVALENT IN AQUEOUS ENVIRONMENTS BY PHYSICOCHEMICAL CONTRIVANCE	(118-133)
IV.1. Introduction IV.2. Experimental section IV.2.1 chemicals IV.2.2 Apparatus and procedure IV.3. Results and discussion IV.3.1 Conductance study IV.3.2 UV-vis spectroscopy IV.3.3 Steady state fluorescence study IV.3.4 Determination of Association constant –spontaneity and features of interactions IV.3.5 NMR Study IV.4. Conclusions	

Subject	Page No
Tables Figures Schemes *Published in J. Adv. Chem. Sci. – Volume 5 Issue 2 (2019) 637–642	
CHAPTER: V EXPLORATION OF SOLVATION CONSEQUENCES OF SOME BIOLOGICALLY POTENT MOLECULES IN AQUEOUS IONIC LIQUID SOLUTIONS WITH THE MANIFESTATION OF MOLECULAR INTERACTIONS	(134-160)
V.1. Introduction V.2. Experimental section V.2.1 Source and purity of samples V.2.2 Apparatus and procedure V.3. Results and discussion V.3.1 Density V.3.2 Viscosity V.3.3 Refractive Index V.3.4 Electrical Conductance V.4. Conclusions Tables Figures Schemes *Published in JCBPS; Section A; November 2020 –January 2021, Vol. 11, No. 1; 091-114.	
CHAPTER: VI PHYSICOCHEMICAL INVESTIGATION OF DIVERSE INTERACTIONS OF SOME BIOLOGICALLY POTENT MOLECULES PREVALENT IN AQUEOUS IONIC LIQUID SOLUTIONS AT DIFFERENT TEMPERATURES	(161-175)
VI.1. Introduction VI.2. Experimental section VI.2.1 Source and purity of materials	

Subject	Page No
VI.2.2 Apparatus and procedure VI.3. Results and discussion VI.3.1 Apparent molar volume VI.3.2 Viscosity VI.3.3 Refractive index VI.3.4 Conductivity study VI.4 Conclusion Tables Figures Schemes *Published in IJACS 2021; 9(2):89-97	
CHAPTER: VII SUBSISTENCE OF ASSORTED MOLECULAR INTERACTIONS OF SUBSTANTIAL AMINO ACIDS PREVALENT IN AQUEOUS SOLUTIONS OF IONIC LIQUID (TBMS) PROBED BY EXPERIMENTAL AND COMPUTATIONAL INVESTIGATIONS	(176-222)
VII.1. Introduction VII.2. Experimental VII.2.1 Source and purity of samples VII.2.2 Apparatus and procedure VII.3. Results and discussion VII.3.1 Density VII.3.2 Viscosity VII.3.3 Ultrasonic speed VII.3.4 Limiting ionic apparent molar volume and ionic viscosity B-coefficient VII.4. Conclusions Tables Figures Scheme	

Subject	Page No
Communicated	
CHAPTER: VIII EXPLORATION OF DIVERSE INTERACTIONS OF L-METHIONINE IN AQUEOUS SIGNIFICANT MIXED IONIC LIQUID SOLUTIONS OPTIMIZED BY COMPUTATIONAL THEORY	(223-272)
VIII.1. Introduction VIII.2. Experimental section VIII.2.1 Chemicals VIII.2.2 Measurements VIII.3. Results and discussion VIII.4. Conclusion Tables Figures Scheme *Communicated	
CHAPTER: IX SOLVATION BEHAVIOUR OF L-ASPARAGINE AND L-GLUTAMINE PREVAILING IN AQUEOUS IONIC LIQUID SOLUTION BY PHYSICOCHEMICAL AND COMPUTATIONAL INVESTIGATIONS	(273-298)
IX.1. Introduction IX.2. Experimental IX.2.1 Source and purity of samples IX.2.2 Apparatus and procedure IX.3. Results and discussion IX.3.1 Apparent molar volume IX.3.2 Viscosity IX.3.3 Refractive Index IX.3.4 Conductivity Study IX.3.5 Surface Tension	

Table of Contents

Subject	Page No
IX.3.6 NMR Study IX.3.7 Computational Study IX.4. Conclusions Tables Figures Schemes *Communicated	
CHAPTER: X <i>Concluding Remarks</i>	(299-302)
BIBLIOGRAPHY	(303-345)
INDEX	(346-348)

LIST OF TABLES

CHAPTERS	TABLES CAPTIONS	PAGE NO.
Chapter-II	<p>Table-11.1: Comparison between organic solvents and ionic liquids.</p>	(17-18)
Chapter-IV	<p>Table-1V.1: Brief description of chemical used</p> <p>Table 1V.2: Conductivity values for the [BMIM] [C₈SO₄] and [MOIM] Cl IL with L-tyr in aqueous at three different temperatures (K^a).</p> <p>Table 1V.3: Conductivity values for the [BMIM] [C₈SO₄] and [MOIM] Cl IL with L-phe in aqueous at three different temperatures (K^a).</p> <p>Table IV.4: Data for the Benesi-Hildebrand double reciprocal plot obtained from UV-Vis spectroscopy for aqueous [BMIM] [C₈SO₄] and [MOIM] Cl ILs with L-tyr system at 298.15K^a.</p> <p>Table-1V.5: Data for the Benesi-Hildebrand double reciprocal plot obtained from UV-Vis spectroscopy for aqueous [BMIM] [C₈SO₄] and [MOIM] Cl ILs with L-phe system at 298.15K^a.</p> <p>Table IV.6: Data for the Benesi-Hildebrand double reciprocal plot obtained from fluorescence spectroscopy for aqueous [BMIM][C₈SO₄] and [MOIM]Cl ILs with L-tyr system at 298.15K</p> <p>Table 1V.7: Data for the Benesi-Hildebrand double reciprocal plot obtained from fluorescence spectroscopy for aqueous [BMIM] [C₈SO₄] and [MOIM] Cl ILs with L-phe system at 298.15K^a.</p>	(124-128)

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>Table-1V.8: 1HNMR chemical shift displacements of [BMIM] [C₈SO₄] and [MOIM] Cl in interaction with L-tyr and L-phe in D₂O at 298.15 K^a.</p>	
Chapter-V	<p>TableV.1: Experimental values of density (ρ), viscosity (η) and molar refraction (R_M) of different molality (m) of aqueous IL (BTAC) solution at 293K, 303K and 313K.</p> <p>TableV.2: : Experimental values of refractive index (n_D) and specific conductance (κ) of different molality (m) of aqueous IL (BTAC) solution at 293K, 303K and 313K.</p> <p>TableV.3: Density (ρ), viscosity (η) and molar refraction (R_M) of L-Aspartic acid in aqueous (BTAC) ionic liquid solutions at 293K, 303K and 313K.</p> <p>TableV.4: Density (ρ), viscosity (η) and molar refraction (R_M) of L-Glutamic acid in aqueous (BTAC) ionic liquid solutions at 293K, 303K and 313K.</p> <p>Table-V.5: Apparent molar volume, (Φ_v) and $(\eta/\eta^0 - 1) / \sqrt{m}$ of L-Aspartic acid solution in 0.01m, 0.03m and 0.05m aqueous BTAC solution at different temperatures (293K, 303K, 313K).</p> <p>TableV.6: Apparent molar volume, (Φ_v) and $(\eta/\eta^0 - 1) / \sqrt{m}$ of L-Glutamic acid solution in 0.01m, 0.03m and 0.05m in aqueous (BTAC) solution at different temperatures (293K, 303K, 313K)</p> <p>TableV.7: Refractive index (n_D) and specific conductance (κ) of L-Aspartic acid in aqueous IL (BTAC) solution at 293K, 303K and 313K.</p>	(145-155)

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>TableV.8: Refractive index (n_D) and specific conductance (κ) of L-Glutamic acid in aqueous IL (BTAC) solution at 293K, 303K and 313K.</p> <p>TableV.9: Limiting apparent molar volumes (Φ_{v^0}), Limiting molar refraction (R_M^0), experimental slopes (S_{v^*}), viscosity A, B-coefficients of L-Aspartic acid solution in IL at different temperatures.</p> <p>Table –V.10: Limiting apparent molar volumes (Φ_{v^0}), Limiting molar refraction (R_M^0), experimental slopes (S_{v^*}), viscosity A, B-coefficients of L-Glutamic acid solution in IL at different temperatures.</p> <p>Table-V.11: The empirical coefficient values (a_0, a_1 and a_2) of L-Aspartic acid solution & L-Glutamic acid in different concentration of the IL (0.01, 0.03m, 0.05m) at 293K, 303K and 313K.</p> <p>Table-V.12: Values of limiting molar expansibilities (Φ_E^0) for L-Aspartic acid solution in IL (BTAC) at different temperatures.</p> <p>Table-V.13: Values of limiting molar expansibilities (Φ_E^0) for L-Glutamic acid solution in IL (BTAC) at different temperatures.</p> <p>TableV.14: Viscosity B-coefficients of L-Aspartic acid along with dB/dT values in different concentrations of IL at (293, 303 and 313) K.</p>	

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>TableV.15: Viscosity B-coefficients of L-Glutamic acid along with dB/dT values in different concentrations of IL at (293, 303 and 313) K.</p> <p>TableV.16: Molar conductance (Λ) of L-Aspartic acid and L-Glutamic acid solution in (0.01m, 0.03m, 0.05m) IL at 293K, 303K and 313K.</p>	
Chapter-VI	<p>TableVI.1: Source and purity of the chemicals</p> <p>TableVI.2: Experimental values of density (ρ), viscosity (η) and refractive index (n_D) at various temperature and at pressure 1.013 bar.</p> <p>TableVI.3: Experimental values of density (ρ) and viscosity (η), L-ascorbic acid in different mass fractions of aqueous IL acid mixture (w_1) at five different temperatures and at pressure 1.013 bar*</p> <p>TableVI.4: Apparent molar volume (ϕ_V) and $(\eta_r - 1)/\sqrt{m}$ of L-Ascorbic acid in different mass fraction (w_1) of aqueous IL mixtures at five different temperatures*</p> <p>TableVI.5: Limiting apparent molar volume (ϕ_V^0), experimental slope (S_V^*), viscosity A- and B-coefficient of L-ascorbic acid in different mass fraction (w_1) of aqueous IL mixtures at five different temperatures*</p> <p>TableVI.6: Values of various coefficients and standard deviation of equation-3 for L-ascorbic acid in different aqueous IL solutions*</p>	(168-174)

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>TableVI.7: Limiting apparent molar expansibilities (φ_E^0) for L-ascorbic acid in different mass fraction of aqueous IL (w_I) at different temperature</p> <p>TableVI.8: Values of dB/dT, A_1, A_2 coefficients for the L-Ascorbic acid in different mass fraction of aqueous IL acid (w_I) at studied temperatures</p> <p>TableVI.9: Refractive index (n_D) and molar refraction (R_M) of L-ascorbic acid in different mass fraction of aqueous solutions at different temperatures and at pressure 1.013 bar *</p> <p>TableVI.10: Limiting molar refraction (R_M^0) of L-ascorbic acid in different temperatures and in different mass fraction of aqueous IL solutions at pressure 1.013 bar *</p> <p>TableVI.11: Specific conductivity (k) of L-ascorbic acid in different temperatures and in different mass fraction of aqueous IL solutions at pressure 1.013 bar *</p>	
Chapter-VII	<p>Table VII.1: Specification of chemical samples.</p> <p>TableVII. 2: Limiting apparent molar volumes (Φ_V^0) and Experimental slopes (S_V^*) of (L-ARGININE+TBMS+H₂O) and (L-HISTIDINE+TBMS+H₂O) systems in aqueous solutions of (0.001, 0.003, 0.005) m IL (TBMS) at 298.15 K, 303.15 K, 308.15 K at atmospheric pressure 0.1MPa.</p> <p>TableVII.3: Empirical coefficient values (a_0, a_1 and a_2) of L-Arginine & L-Histidine in different concentrations (0.001, 0.003, 0.005)m in aqueous IL (TBMS) solutions at 298.15 K, 303.15 K, 308.15 K and at atmospheric pressure 0.1MPa.</p>	(194-211)

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>Table VII. 4: Values of limiting molar expansivities Φ_E^0 & $(\delta\Phi_E^0/\delta T)_P$ of L-Arginine and L-Histidine of different concentrations (0.001, 0.003, 0.005) m in aqueous IL (TBMS) solutions at different temperature and pressure 0.1MPa</p> <p>Table VII. 5: Viscosity <i>B</i>-coefficients, <i>A</i>-coefficients of (L-ARGININE+TBMS+H₂O) and L-HISTIDINE+TBMS+H₂O) systems along with dB/dT values in aqueous IL(TBMS) solutions of different concentrations (0.001,0.003,0.005)m at 298.15 K, 303.15 K, 308.15 K and at atmospheric pressure 0.1MPa</p> <p>Table VII.6: Values of (B/Φ_V^0) for L-Arginine and L-Histidine in different concentrations of aqueous TBMS (IL) solutions at different temperature and atmospheric pressure 0.1MPa.</p> <p>Table VII.7: Values of $(V_1^0 - V_2^0)$, $\Delta\mu_1^{0\#}$, $\Delta\mu_2^{0\#}$, $T\Delta S_2^{0\#}$, $\Delta H_2^{0\#}$ for L-Arginine and L-Histidine in different concentrations of an aqueous solution of IL(TBMS) mixture at different temperatures and atmospheric pressure 0.1MPa.</p> <p>Table VII.8 : Limiting molar refraction $(^R_M^0)$ of L-Arginine and L-Histidine in aqueous ionic liquid IL (TBMS) solutions of different concentrations, (0.001, 0.003, 0.005) m at different temperature and atmospheric pressure 0.1MPa.</p> <p>Table VII. 9: Molar conductance (<i>A</i>) of L-Arginine and L-Histidine in aqueous IL (TBMS) solution of different concentrations, (0.001, 0.003, 0.005) m at 298.15 K, 303.15 K, 308.15 K and at atmospheric pressure 0.1MPa.</p> <p>Table VII. 10: CMC values of L-Arginine and L-Histidine in different concentrations(0.001, 0.003, 0.005)m aqueous solutions</p>	

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>of TBMS at different temperatures at atmospheric pressure 0.1MPa.</p> <p>Table VII.11:</p> <p>Surface tension (σ) of L-Arginine and L-Histidine of different molality at 298.15 K in different concentrations(0.001, 0.003, 0.005) m of IL (TBMS) solutions and at atmospheric pressure 0.1MPa</p> <p>Table VII. 12:</p> <p>Optimizations Energy of pure TBMS, L-ARG, L-HIS and (TBMS+L-ARG), (TBMS+L-HIS) systems using appropriate methodology and 6-311G (d) basis set</p> <p>Table VII.S1 Experimental values of density (ρ), viscosity (η), molar refraction (R_M) of different concentrations (0.001, 0.003, 0.005) m of aqueous solvent (TBMS) solutions at 298.15 K, 303.15 K, 308.15 K at atmospheric pressure 0.1MPa.</p> <p>Table VII. S2:</p> <p>Experimental values of refractive index (n_D), sp. conductance (κ), surface tension (σ) of different concentrations (0.001, 0.003, 0.005) m of aqueous solvent (TBMS) solution at 298.15 K, 303.15 K, 308.15 K and at atmospheric pressure 0.1MPa.</p> <p>TableVII.S3:</p> <p>Density(ρ) of (L-ARGININE+TBMS+H₂O) and (L-HISTIDINE+TBMS+H₂O) systems in aqueous TBMS solutions of different concentrations (0.001, 0.003, 0.005) m at 298.15 K, 303.15 K and 308.15 K and at atmospheric pressure 0.1MPa.</p> <p>Table VII.S4:</p> <p>Apparent Molar volume (Φ_V) of (L-ARGININE+TBMS+H₂O) and (L-HISTIDINE+TBMS+H₂O) systems in aqueous IL (TBMS) of different concentrations (0.00, 0.003, 0.005) m mass fractions, $W_1=0.001, 0.003, 0.005$ at 298.15 K, 303.15 K, 308.15 K and at atmospheric pressure0.1MPa.</p>	

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>TableVII.S5: Volume transfer/$\Delta\Phi_v^0$ for L-Arginine and L-Histidine in aqueous solutions of (0.001, 0.003, 0.005) m IL (TBMS) at 298.15 K, 303.15 K, 308.15 K at atmospheric pressure 0.1MPa.</p> <p>Table VII.S6: Viscosity (η) and $(\eta/\eta^0-1)/\sqrt{m}$ of (L-ARGININE+TBMS+H₂O)in aqueous IL(TBMS) of different concentrations (0.001, 0.003, 0.005) m at 298.15 K, 303.15 K, 308.15 K and at atmospheric pressure 0.1MPa.</p> <p>TableVII.S7: Viscosity (η) and $(\eta/\eta^0-1)/\sqrt{m}$ of(L-HISTIDINE+TBMS+H₂O) system in aqueous IL (TBMS) of different concentrations (0.001, 0.003, 0.005) m at 298.15 K, 303.15 K, 308.15 K and at atmospheric pressure 0.1MPa.</p> <p>Table VII. S8: Refractive index (n_D) and molar refraction (R_M) of (L-ARGININE+TBMS+H₂O) in aqueous IL (TBMS) solutions of different concentrations (0.001, 0.003, 0.005) m at 298.15 K, 303.15 K and 308.15 K and at pressure 0.1MPa.</p> <p>Table VII.S9: Refractive index (n_D) and molar refraction (R_M) of (L-HISTIDINE+TBMS+H₂O) in aqueous IL (TBMS) solutions of different concentrations (0.001, 0.003, 0.005) m at 298.15 K, 303.15 K and 308.15 K and at pressure 0.1MPa.</p> <p>TableVII.S10: Specific conductance (κ) of (L-ARGININE+TBMS+H₂O) and (L-HISTIDINE+ TBMS+H₂O) Systems in aqueous TBMS solutions of different concentrations (0.001, 0.003, 0.005) m at 298.15 K, 303.15 K, 308.15 K at atmospheric pressure 0.1MPa.</p>	

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>Table VII.S11 Specific conductance (κ) of (L-ARGININE+TBMS+H₂O) system in aqueous IL (TBMS) solutions of concentration 0.001m at 298.15 K, 303.15 K and 308.15 K and at atmospheric pressure 0.1MPa.</p> <p>Table VII.S12: Specific conductance (κ) of (L-ARGININE+TBMS+H₂O) system in aqueous IL (TBMS) solutions of concentration 0.003m at 298.15K, 303.15K and 308.15 K and at atmospheric pressure 0.1MPa.</p> <p>Table VII. S13 : Specific conductance (κ) of (L-ARGININE+TBMS+H₂O) system in aqueous IL (TBMS) solutions of concentration 0.005m at 298.1 K, 303.15 K and 308.15 K and at atmospheric pressure 0.1MPa.</p> <p>Table VII. S14: Specific conductance (κ) of (L-HISTIDINE +TBMS+H₂O) system in aqueous IL (TBMS) solutions of concentration 0.001m at 298.15 K, 303.15 K and 308.15 K and at atmospheric pressure 0.1MPa.</p> <p>Table VII.S15: Specific conductance (κ) of (L-HISTIDINE +TBMS+H₂O) system in aqueous IL (TBMS) solutions of concentration 0.003m at 298.15K, 303.15K and 308.15 K and at atmospheric pressure 0.1MPa.</p> <p>TableVII.S16: Specific conductance (κ) of (L-HISTIDINE +TBMS+H₂O) system in aqueous IL (TBMS) solutions of concentration 0.005m at 298.15K, 303.15 K and 308.15 K and at atmospheric pressure 0.1MPa</p>	
Chapter-VIII	<p>TableVIII.1: Specification of chemical samples</p> <p>TableVIII.2: Limiting apparent molar volumes (Φ_v^0), Limiting molar refraction (R_M^0), experimental slopes (S_v^*), viscosity A,</p>	(243-256)

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>B-coefficients of L-Methionine solution in IL (BTMAC) at different temperatures and pressure at 1.013bar*</p> <p>Table VIII. 3:</p> <p>Limiting apparent molar volumes (Φ_V^0), Limiting molar refraction (R_M^0), experimental slopes (S_V^*), viscosity A, B-coefficients of L-Methionine solution in IL (BTEAC) at different temperatures and pressure at 1.013bar*</p> <p>Table VIII. 4:</p> <p>The empirical coefficient values (a_0, a_1 and a_2) of L-Methionine solution in different concentration of the ILs (BTMAC) & (BTEAC) (0.001m,0.003m,0.005m) at 298.15K, 303.15K and 308.15K and pressure at 1.013bar*</p> <p>Table VIII. 5:</p> <p>Values of limiting molar expansibilities (Φ_E^0) for L-Methionine solutions in IL (BTMAC) at different temperatures and pressure at 1.013bar*</p> <p>Table VIII. 6:</p> <p>Values of limiting molar expansibilities (Φ_E^0) for L-Methionine solution in IL (BTEAC) at different temperatures and pressure at 1.013bar*</p> <p>Table VIII. 7:</p> <p>Viscosity B-coefficients of L-Methionine solution along with dB/dT values in different concentrations of IL (BTMAC) at (298.15, 303.15 and 308.15) K and pressure at 1.013bar*</p> <p>Table VIII. 8:</p> <p>Viscosity B-coefficients of L-Methionine solution along with dB/dT values in different concentrations of IL (BTEAC) at (298.15, 303.15 and 308.15) K and pressure at 1.013bar*</p> <p>Table VIII. 9:</p> <p>Values of ($\bar{V}_1^0 - \bar{V}_2^0$), $\Delta\mu_1^{0\#}$, $\Delta\mu_2^{0\#}$, $T\Delta S_2^{0\#}$, $\Delta H_2^{0\#}$ for L-Methionine in different molality(m) of aqueous solution of IL(BTMAC&BTEAC) mixture at different temperatures and atmospheric pressure 0.1MPa</p>	

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>Table VIII.10: Molar conductance (Λ) of L-Methionine solutions in aqueous BTMAC & BTEAC ionic liquid solution in (0.001m, 0.003m, 0.005m) at 298.15K, 303.15K and 313.15K and pressure at 1.013bar*</p> <p>Table VIII. 11: Surface Tension (γ) values of L-Methionine solutions in IL (BTMAC) and L-Methionine solutions in IL(BTEAC)at different concentration(0.001m,0.003m,0.05m) at room temperature and pressure at 1.013bar*</p> <p>Table VIII. 12: Limiting Slopes ($\partial\sigma/\partial m$) of the Surface Tension of the Aqueous Solutions of α-Amino acid</p> <p>Table VIII. 13: UV-Vis Spectroscopic data for the Benesi-Hildebrand double reciprocal plot of BTMAC+L-Met system at 298.15K.</p> <p>Table VIII.14: UV-Vis Spectroscopic data for the Benesi-Hildebrand double reciprocal plot of BTEAC+L-Met system at 298.15K.</p> <p>Table VIII.S1: Experimental values of density (ρ), viscosity (η) and molar refraction (R_M) of different molality (m) of aqueous IL (BTMAC) solution at 298.15K, 303.15K and 308.15K and pressure at 1.013bar*</p> <p>Table VIII.S2: Experimental values of density (ρ), viscosity (η) and molar refraction (R_M) of different molality (m) of aqueous IL (BTEAC) solution at 298.15K, 303.15K and 308.15K. and pressure at 1.013bar*</p> <p>Table VIII.S3: Experimental values of refractive index (n_D) and specific conductance (κ) of different molality (m) of aqueous IL</p>	

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>(BTMAC) solution at 298.15 K, 303.15 K and 308.15 K and pressure at 1.013bar*</p> <p>TableVIII.S4:</p> <p>Experimental values of refractive index (n_D) and specific conductance (κ) of different molality (m) of aqueous IL (BTEAC) solution at 298.15 K, 303.15 K and 308.15 K. and pressure at 1.013bar*</p> <p>Table VIII S5:</p> <p>Density (ρ), viscosity (η) and molar refraction (R_M) of L-Methionine in aqueous (BTMAC) ionic liquid solutions at 298.15K, 303.15K and 308.15K and pressure at 1.013bar*</p> <p>TableVIIS6:</p> <p>Density (ρ), viscosity (η) and molar refraction (R_M) of L-Methionine in aqueous (BTEAC) ionic liquid solutions at 298.15K, 303.15K and 308.15K. and pressure at 1.013bar*</p> <p>Table VIII S7:</p> <p>Apparent molar volume, (Φ_v) and $(\eta/\eta^0 - 1) / \sqrt{m}$ of L-Methionine solution in 0.001m, 0.003m and 0.005m aqueous BTMAC solution at different temperatures 298.15K, 303.15K, 308.15K and pressure at 1.013bar*</p> <p>Table VIII S8:</p> <p>Apparent molar volume, (Φ_v) and $(\eta/\eta^0 - 1) / \sqrt{m}$ of L-Methionine solutions in 0.001m, 0.003m and 0.005m in aqueous (BTEAC) solution at different temperatures 298.15K, 303.15K, 308.15K and pressure at 1.013bar*</p> <p>TableVIII.S9:</p> <p>Refractive index (n_D) and specific conductance (κ) of L-Methionine in aqueous IL (BTMAC) solution at 298.15K, 303.15K and 308.15K and pressure at 1.013bar*</p> <p>Table VIII. S10:</p> <p>Refractive index (n_D) and specific conductance (κ) of L-Methionine in aqueous IL (BTMAC) solution at 298.15K, 303.15K and 308.15K and pressure at 1.013bar*</p>	

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>Table VIII. S11: Refractive index (n_D) and specific conductance (κ) of L-Methionine in aqueous IL (BTEAC) solution at 298.15K, 303.15K and 308.15K and pressure at 1.013bar*</p>	
Chapter-IX	<p>Table IX. 1: Experimental values of density (ρ), viscosity (η) and molar refraction (R_M) of different molality (m) of aqueous IL (BTBAC) solution at 298.15K, 303.15K and 308.15K.</p> <p>Table IX.2: Experimental values of refractive index (n_D) and specific conductance (κ) of different molality (m) of aqueous IL (BTBAC) solution at 298.15 K, 303.15 K and 308.15 K.</p> <p>Table IX.3: Density (ρ), viscosity (η) and molar refraction (R_M) of L-Asparagine in aqueous (BTBAC) ionic liquid solutions at 298.15K, 303.15K and 308.15K.</p> <p>Table IX. 4: Density (ρ), viscosity (η) and molar refraction (R_M) of L-Glutamine in aqueous (BTBAC) ionic liquid solutions at 298.15K, 303.15K and 308.15K.</p> <p>Table IX. 5: Apparent molar volume, (Φ_v) and $(\eta/\eta^0 - 1) / \sqrt{m}$ of L-Asparagine solution in 0.001m, 0.003m and 0.005m aqueous BTBAC solution at different temperatures (293.15K, 303.15K, 313.15K).</p> <p>Table IX. 6: Apparent molar volume, (Φ_v) and $(\eta/\eta^0 - 1) / \sqrt{m}$ of L-Glutamine solution in 0.001m, 0.003m and 0.005m in aqueous (BTBAC) solution at different temperatures (298.15K, 303.15K, 308.15K).</p> <p>Table IX. 7(a): Limiting apparent molar volumes (Φ_v^0), Limiting molar refraction (R_M^0), experimental slopes (S_v^*), viscosity A, B-coefficients of L-Asparagine solution in IL at different temperatures.</p>	(286-294)

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>Table IX. 7(b): Limiting apparent molar volumes (Φ_V^0), Limiting molar refraction (R_M^0), experimental slopes (S_V^*), viscosity A, B-coefficients of L-Glutamine solution in IL at different temperatures.</p> <p>Table IX. 8: The empirical coefficient values (a_0, a_1 and a_2) of L-Asparagine solution & L-Glutamine solution in different concentration of the IL (0.001, 0.003m, 0.005m) at 298.15K, 303.15K and 308.15K.</p> <p>Table IX. 9(a): Values of limiting molar expansibilities (Φ_E^0) for L-Asparagine solution in IL(BTBAC) at different temperatures.</p> <p>Table IX. 9(b): Values of limiting molar expansibilities (Φ_E^0) for L-Glutamine solution in IL(BTBAC) at different temperatures.</p> <p>Table IX. 10(a): Viscosity B-coefficients of L-Asparagine solution along with dB/dT values in different concentrations of IL at (298.15, 303.15 and 308.15) K.</p> <p>Table IX. 10(b): Viscosity B-coefficients of L-Glutamine solution along with dB/dT values in different concentrations of IL at (298.15, 303.15 and 308.15) K.</p> <p>Table IX. 11: Values of $(\bar{V}_1^0 - \bar{V}_2^0)$, $\Delta\mu_1^{0\neq}$, $\Delta\mu_2^{0\neq}$, $T\Delta S_2^{0\neq}$, $\Delta H_2^{0\neq}$ for L-Asparagine and L-glutamine in different molality (0.001,0.003,0.005) of aqueous solution of IL(BTBAC) mixture at different temperatures and atmospheric pressure 0.1MPa.</p>	

CHAPTERS	TABLES CAPTIONS	PAGE NO.
	<p>Table IX. 12: Values of (B/Φ_r^0) for L-Asparagine and L-Glutamine in different molality of aqueous TBMS (IL) solutions at different temperature and atmospheric pressure 0.1MPa.</p> <p>Table IX. 13(a): Refractive index (n_D) and specific conductance (κ) of L-Asparagine in aqueous IL (BTBAC) solution at 293.15K, 303.15K and 313.15K.</p> <p>Table IX. 13(b): Refractive index (n_D) and specific conductance (κ) of L-Glutamine in aqueous IL (BTBAC) solution at 298.15K, 303.15K and 308.15K.</p> <p>Table IX. 14: Molar conductance (Λ) of L-Asparagine and L-Glutamine solution in (0.001m, 0.003m, 0.005m) IL at 298.15K, 303.15K and 308.15K.</p> <p>Table IX. 15: Surface Tension values of L-Asparagine and L-glutamine solutions in BTBAC at different concentration (0.001m, 0.003m, 0.005m) at room temperature.</p> <p>Table IX.16: Optimization energies of pure BTBAC, L-Glu, L-Asp and (BTBAC + L-Glu), (BTBAC + L-Asp), systems using UB3LYP methodology and 6-31G (d) as a basis set.</p>	

LIST OF FIGURES

CHAPTERS	FIGURE CAPTIONS	PAGE NO
Chapter-II	<p>Figure II.1: Difference between an ionic solution and an ionic liquid.</p> <p>Figure II. 2: Some commonly used ionic liquid systems.</p> <p>FigureII.3: Growth rate of ionic liquid publications, 1986-2006.</p> <p>Figure II. 4: Annual growth of ionic liquid patents, 1996-2006.</p> <p>Figure II. 5: Annual growth of ionic liquid paper and patents, up to 2010</p> <p>Figure II.6: Growth in the number of IL publications and representative areas of interest. (Data obtained from SciFinder Scholar using the search terms “ionic liquid” or “ionic liquids” and then refined by publication year. The data for total publications includes the number of patents, and the area of the particular field does not represent the number of publications in the subfield)..</p> <p>Figure II. 7: The twin concepts of ILs as solvents and green chemistry propelled a dramatic increase in publications in this field.</p> <p>Figure II. 8a: The diverse application of ionic liquids</p> <p>Figure II. 8b: Selection of applications where ionic liquids have been used.</p> <p>Figure II.9a: A diagram for the explanation of molal volume.</p> <p>Figure II.9b: A diagram to assist in the explanation of a partial molal volume</p>	(15-47)
Chapter-IV	<p>Figure1V.1: Molar conductance of (a) [BMIM] [C₈SO₄] in aqueous solution with L-tyr and (b) [MOIM] Cl in aqueous solution with L-tyr at three different temperatures.</p> <p>Figure1V.2: Molar conductance of (a) [BMIM][C₈SO₄] in aqueous solution with L-phe and (b) [MOIM]Cl in aqueous solution with L-phe at three different temperatures</p>	(129-132)

CHAPTERS	FIGURE CAPTIONS	PAGE NO
	<p>Figure1V.3: Increase in absorption spectra of (a) [BMIM][C₈SO₄] and (b) [MOIM]Cl at different concentration of L-tyrosine (1) absence of L-tyrosine, (2) 0.0004 M, (3) 0.0008 M, (4) 0.0012 M, (5) 0.0016 M, (6) 0.0018 M, (7)0.002 M respectively.</p> <p>Figure1V.4:Increase in absorption spectra of (a) [BMIM][C₈SO₄] and (b)[MOIM]Cl at different concentration of L-phenylalanine (1) absence of L-phenylalanine, (2) 0.0004 M, (3) 0.0008 M, (4) 0.0012 M, (5) 0.0016 M, (6) 0.0018 M, (7)0.002 M respectively.</p> <p>Figure1V.5: Fluorescence spectra of (a) [BMIM] [C₈SO₄] and (b) [MOIM] Cl at different concentration of L-tyrosine (1) absence of L-tyrosine, (2) 0.0003 M, (3) 0.0006 M, (4) 0.0009 M, (5) 0.0012 M, (6) 0.0015 M, (7)0.0018 M respectively.</p> <p>Figure1V.6: Fluorescence spectra of (a) [BMIM] [C₈SO₄] and (b) [MOIM] Cl at different concentration of L-phenylalanine (1) absence of L-phenylalanine, (2) 0.0003 M, (3) 0.0006 M, (4) 0.0009 M, (5) 0.0012 M, (6) 0.0015 M, (7)0.0018 M respectively.</p> <p>Figure 1V.7: Benesi-Hildebrand plot of $1/\Delta A$ vs. $1/[AA]$ in UV-vis spectroscopy for (a) [BMIM][C₈SO₄] and (b) MOIM]Cl in L-tyr and for (c)[BMIM][C₈SO₄] and (d) MOIM]Cl in L-phe at 298.15K^a ¹H NMR spectra of (a) [BMIM][C₈SO₄], (b) ([BMIM][C₈SO₄]+ L-tyr) system and (c) ([BMIM][C₈SO₄] + L-phe) system in D₂O at 298.15K.</p> <p>Figure1V.8: Benesi-Hildebrand plot of $1/\Delta A$ vs. $1/[AA]$ in fluorescence spectroscopy for (a) [BMIM] [C₈SO₄] and (b) MOIM] Cl in L-tyr and for (c) [BMIM] [C₈SO₄] and (d) MOIM] Cl in L-phe at 298.15K^a.</p> <p>Figure1V.9: ¹H NMR spectra of (a) [MOIM] Cl, (b) ([MOIM] Cl+ L-tyr) system and (c) ([MOIM] Cl + L-phe) system in D₂O at 298.15K.</p> <p>Figure1V.10: ¹H NMR spectra of (a) [BMIM] [C₈SO₄], (b) ([BMIM] [C₈SO₄] + L-tyr) system and (c) ([BMIM] [C₈SO₄] + L-phe) system in D₂O at 298.15K.</p>	

CHAPTERS	FIGURE CAPTIONS	PAGE NO
Chapter-V	<p>FigureV.1(a)Variation of limiting apparent molar volume (Φ_v^0) of L-Aspartic acid solution at 0.01m, 0.03m and 0.05m of the aqueous IL solutions at 293K(Series1), 303K(Series2) and 313K(Series3).</p> <p>FigureV.1(b)Variation of limiting apparent molar volume (Φ_v^0) of L-Glutamic acid solution at 0.01m, 0.03m and 0.05m of the aqueous IL solutions at 293K(Series1), 303K(Series2) and 313K(Series3).</p> <p>Figure V.2(a)Variation of B values of L-Aspartic acid against 0.01m IL, 0.03m IL and 0.05m IL solutions at 293K(Series1), 303K(Series2) and 313K(Series3).</p> <p>FigureV.2(b)Variation of B values of L-Glutamic acid against 0.01m IL, 0.03m IL and 0.05m IL solutions at 293K(Series1), 303K(Series2) and 313K(Series3).</p> <p>FigureV.3 (a) Variation of R_M^0 values of L-Aspartic acid solution against 293K, 303K and 313K in aqueous solution of IL at 0.01m (Series1), 0.03m (Series2) and 0.05m (Series3).</p> <p>FigureV.3 (b) Variation of R_M^0 values of L-Glutamic acid solution against 293K, 303K and 313K in aqueous solution of IL at 0.01m (Series1), 0.03m (Series2) and 0.05m (Series3).</p> <p>FigureV.4(a) Variation of molar conductance (Λ) with different concentrations of L–Aspartic acid in aqueous (0.01m,0.03m,0.05m) BTAC (IL) solution at 293K, 303K, 313K.0.01m at 293K(Series1), 0.01m at 303K(Series2), 0.01m at 313K(Series3)0.03m at 293K(Series4), 0.03m at 303K(Series5), 0.03m at 313K(Series6)0.05m at 293K(Series7), 0.05m at 303K(Series8), 0.05m at 313K(Series9)</p> <p>FigureV.4(b)Variation of molar conductance (Λ) with different concentrations of L–Glutamic acid in aqueous (0.01m,0.03m,0.05m) BTAC (IL) solution at 293K, 303K, 313K.0.01m at 293K(Series1), 0.01m at 303K(Series2), 0.01m at 313K(Series3)0.03m at 293K(Series4), 0.03m at 303K(Series5), 0.03m at 313K(Series6)0.05m at 293K(Series7), 0.05m at 303K(Series8), 0.05m at 313K(Series9)</p>	(155-159)

CHAPTERS	FIGURE CAPTIONS	PAGE NO
Chapter-VI	No figure	
Chapter-VII	<p>Figure VII.1. Variation of limiting apparent molar volumes (Φ_r^0) of L-Arginine as a function of temperature /K in aqueous TBMS solutions of different concentrations (-▲- 0.001m/mol.kg⁻¹; -■- 0.003m/mol.kg⁻¹; -◆- 0.005m/mol.kg⁻¹).</p> <p>Figure VII.2. Variation of limiting apparent molar volumes (Φ_r^0) of L-Histidine as a function of temperature /K in aqueous TBMS solutions of different concentrations (-Δ- 0.001m/mol.kg⁻¹; -□- 0.003m/mol.kg⁻¹; -◇- 0.005m/mol.kg⁻¹).</p> <p>FigureVII.3 Variation of viscosity <i>B</i>-coefficient of L-Arginine as a function of different concentrations of aqueous TBMS (IL) solutions at (-◇- 298.15K; -□- 303.15K; -Δ- 308.15K).</p> <p>Figure VII. 4 Variation of viscosity <i>B</i>-coefficient of L-Histidine as a function of different concentrations of aqueous TBMS (IL) solutions at (-◆- 298.15K; -■- 303.15K; -▲- 308.15K).</p> <p>FigureVII.5: Variation of limiting molar refraction (R_M^0) plot of L-Arginine (big size figure) and L-Histidine (small size figure) as a function of different concentrations of aqueous TBMS solutions and as a function of temperature (<i>T</i>/K).</p> <p>Figure VII.6 Variation of molar conductance (<i>A</i>) plot as a function of the concentration of L-Arginine (amino acid) in different concentrations aqueous TBMS solutions at different temperatures(<i>T</i>/K)(-◇-concentration(IL) 0.001m/mol.kg⁻¹at298.15K;-□-concentration(IL) 0.001m/mol.kg⁻¹at303.15K;-Δ-concentration(IL)0.001m/mol.kg⁻¹ at 308.15K, -x-concentration (IL) 0.003m/mol.kg⁻¹ at 298.15K; *concentration (IL) 0.003m/mol.kg⁻¹ at 303.15K; -●-concentration (IL) 0.003m/mol.kg⁻¹ at 308.15K; -+concentration (IL) 0.005 at 298.15K; — concentration</p>	(212-220)

CHAPTERS	FIGURE CAPTIONS	PAGE NO
	<p>(IL) 0.005m/mol.kg⁻¹ at 303.15K and — concentration (IL) 0.005m/mol.kg⁻¹ at 308.15K.</p> <p>Figure VII.7 Variation of molar conductance (Λ) plot as a function of the concentration of L-Histidine(Amino acid) in different concentrations aqueous TBMS solutions at different temperatures(T/K)(-◇- concentration(IL) 0.001m/mol.kg⁻¹ at 298.15K; -□- concentration(IL)0.001m/mol.kg⁻¹ at 303.15K;-△- concentration(IL)0.001m/mol.kg⁻¹ at 308.15K, -x- concentration (IL) 0.003m/mol.kg⁻¹ 0.003 at 298.15K; * concentration (IL) 0.003m/mol.kg⁻¹ at 303.15K; -●- concentration (IL) 0.003m/mol.kg⁻¹ at 308.15K; + concentration (IL) 0.005m/mol.kg⁻¹ at 298.15K; — concentration (IL) 0.005m/mol.kg⁻¹ at 303.15K and — concentration (IL) 0.005m/mol.kg⁻¹ at 308.15K.</p> <p>Figure VII.8 Variation of surface tension (σ) plot of L-Arginine as a function of different concentrations (-▲- 0.001m/mol.kg⁻¹; -■- 0.003m/mol.kg⁻¹; -◆- 0.005m/mol.kg⁻¹) of aqueous TBMS solutions at 298.15 K.</p> <p>Figure VII. 9 Variation of surface tension (σ) plot of L-Histidine as a function of different concentrations (-▲- 0.001m/mol.kg⁻¹; -■- 0.003m/mol.kg⁻¹; -◆- 0.005m/mol.kg⁻¹) of aqueous TBMS solutions at 298.15 K.</p> <p>Figure VII.S1 Variation of viscosity B-coefficient of L-Arginine against temperature in different concentrations(-◇-0.001m/mol.kg⁻¹;0.003m/mol.kg⁻¹; -△- 0.005m/mol.kg⁻¹) of aqueous IL Solution.</p> <p>Figure VII.S2 Variation of viscosity B-coefficient of L-Histidine solution against temperature in different concentrations (-◇-0.001m/mol.kg⁻¹;0.003m/mol.kg⁻¹; -△- 0.005m/mol.kg⁻¹) of aqueous solutions of IL.</p> <p>Figure VII. S3 CMC plot of conductance of L-Arginine (a, b, c) and L-Histidine (d, e, f) with addition of 0.001 m aqueous solution of TBMS IL.</p>	

CHAPTERS	FIGURE CAPTIONS	PAGE NO
	<p>Figure VII.S4 CMC plot of conductance of L-Arginine (a, b, c) and L-Histidine (d, e, f) with addition of aqueous solutions of IL (0.003 m) at different temperatures.</p> <p>Figure S5 CMC plot of conductance of L-Arginine (a, b, c) and L-Histidine (d, e, f) with addition 0.005 m aqueous solution of IL (TBMS).</p>	
Chapter-VIII	<p>Figure VIII.1 .Variation of limiting apparent molar volume (Φ_v^0) of L-methionine as a function of temperature (T/K) and different concentrations of (0.001,0.003,0.005)m aqueous BTMAC solutions.</p> <p>FigureVIII.2 Variation of limiting apparent molar volume (Φ_v^0) of L-methionine as a function of temperature (T/K) and different concentrations of (0.001,0.003,0.005)m aqueous BTEAC solutions.</p> <p>Figure VIII. 3.Variation of viscosity B-coefficient of L-methionine as a function of different temperature(T/K) and different concentrations of aqueous BTEAC (IL) and BTMAC (IL) solutions.</p> <p>FigureVIII.4.Variation of Limiting Molar refraction (R_M^0) of L-methionine as a function of temperature (T/K) and different concentrations of(0.001,0.003,0.005)m aqueous BTMAC solutions.</p> <p>FigureVIII.5.Variation of Limiting Molar refraction (R_M^0) of L-methionine methionine as a function of temperature (T/K) and different concentrations of (0.001,0.003,0.005)m aqueous BTEAC solutions.</p> <p>Figure VIII. 6.Variation of molar conductance (Λ) plot as a function of the concentration of L-Methionine (amino acid) in different concentrations of aqueous BTMAC solutions at different temperatures (T/K)</p> <p>FigureVIII. 7.Variation of molar conductance (Λ) plot as a function of the concentration of L-Methionine (amino acid) in different concentrations of aqueous BTEAC solutions at different temperatures (T/K)</p>	(256-271)

CHAPTERS	FIGURE CAPTIONS	PAGE NO
	<p>Figure A1. FTIR Spectrum of pure ILs (BTMAC & BTEAC) and AA (L-Met)</p> <p>Figure A2. FTIR Spectrum of L-Met + BTMAC Mixture (AA:IL=1:3,2:2,3:1)</p> <p>Figure A3. FTIR Spectrum of L-Met + BTEAC Mixture (AA:IL=1:3,2:2, 3:1)</p> <p>Figure B1. $^1\text{H-NMR}$ Spectrum of pure BTMAC in D_2O.</p> <p>Figure B2. $^1\text{H-NMR}$ Spectrum of pure BTEAC in D_2O.</p> <p>Figure B3. $^1\text{H-NMR}$ Spectrum of pure L-Methionine in D_2O.</p> <p>Figure B4. $^1\text{H-NMR}$ Spectrum of L-Met + BTMAC(AA:IL=4:1) in D_2O</p> <p>Figure B5. $^1\text{H-NMR}$ Spectrum of L-Met + BTEAC (AA:IL=4:1) in D_2O.</p> <p>Figure VIII.C1. UV-Vis spectra of (BTMAC+L-Met) system</p> <p>Figure VIII. C2. UV-Vis spectra of (BTEAC+L-Met) system.</p> <p>Figure VIII. C3. Benesi double reciprocal plot of BTMAC+L-Met system</p> <p>Figure VIII. C4. Benesi double reciprocal plot of BTEAC+L-Met system.</p> <p>Figure VIII. C5: Optimized geometries of the (a) L-Met-BTMAC (b) L-Met-BTEAC in aqueous solution.</p> <p>Figure VIII. C6. Electrostatic potential maps for (a) L-Met-BTMAC (b) L-Met-BTEAC in aqueous medium.</p> <p>Figure VIII. C7. Plots of reduced density gradient (RDG) for (a) L-Met-BTMAC (b) L-Met-BTEAC composites</p> <p>Figure VIII.S1. Variation of Apparent molar volume, Φ_v of L-methionine solutions with concentration, \sqrt{m} against different temperature in 0.001m, 0.003m, 0.005m aqueous IL (BTMAC) solutions.</p>	

CHAPTERS	FIGURE CAPTIONS	PAGE NO
	<p>Figure VIII.S2. Variation of Apparent molar volume, Φ_V of L-methionine solutions with concentration, \sqrt{m} against different temperature in 0.001m, 0.003m, 0.005m aqueous IL (BTEAC) solutions.</p> <p>Figure VIII. S3. Variation of Molar refraction, R_M plot (a,b,c,d,e,f,g,h,i) of L-methionine against concentration, \sqrt{c} at different temperature in 0.001m, 0.003m, 0.005m aqueous solutions of IL(BTMAC).</p> <p>Figure VIII. S4. Variation of Molar refraction, R_M plot (a,b,c,d,e,f,g,h,i) of L-methionine against concentration, \sqrt{c} at different temperature in 0.001m, 0.003m, 0.005m aqueous solutions of IL (BTEAC).</p> <p>Figure VIII. S5. Variation of surface tension plot (γ) (a ,b, c) with different conc. of L-methionine at room temperature in 0.001m, 0.003m, 0.005m aqueous solutions of ionic liquid (BTMAC).</p> <p>Figure VIII. S6. Variation of surface tension (γ) plot (a ,b, c) with different conc. of L-methionine at room temperature in 0.001m, 0.003m, 0.005m aqueous solutions of ionic Liquid(BTEAC).</p>	
Chapter-IX	<p>Figure IX.1. Variation of B values of L-Glutamine and L-Asparagine in aqueous solution of BTBAC respectively, against 0.001m IL, 0.003m IL and 0.005m IL solutions at different temperatures.</p> <p>Figure IX.2. variation of R_M° values of L-asparagine solution Against(298.15k,303.15k,308.15k) in aqueous IL at 0.001m,0.003m,0.005m.</p> <p>Figure IX .3. variation of R_M° of L-glutamine solution Against (298.15k,303.15k,308.15k) in aqueous IL at 0.001m,0.003m,0.005m.</p> <p>Figure IX. 4(1). 1HNMR Spectra of pure BTBAC in D₂O at298.15K.</p> <p>Figure IX. 4(2). 1HNMR Spectra of pure L-Asparagine in D₂O at298.15K.</p>	(294-297)

CHAPTERS	FIGURE CAPTIONS	PAGE NO
	<p>Figure IX. 4(3).1HNMR Spectra of pure L-Glutamine in D₂O at298.15K.</p> <p>Figure IX. 5(1).1HNMR Spectra of BTBAC: L-Asparagine (1:1) in D₂O at298.15K.</p> <p>Figure IX. 5(2).1HNMR Spectra of BTBAC: L-Glutamine (1:1) in D₂O at298.15K.</p>	

LIST OF SCHEMES

CHAPTERS	SCHEME CAPTIONS	PAGE NO
Chapter-IV	<p>SchemeIV.1: Ball & stick representation of (a) L-tyrosine,(b)L-phenylalanine, (c) 1-butyl-3-methyl imidazolium octylsulphate [BMIM][C₈SO₄] and (d) 1-methyl-3-octylimidazoliumchloride[MOIM]Cl respectively.</p> <p>SchemeIV.2: Schematic representation of interactions between (a) ([BMIM] [C₈SO₄] +L-tyr) (b) ([MOIM] Cl +L-tyr) (c) ([BMIM] [C₈SO₄] + L-phe) and (d) ([MOIM] Cl +L-phe) systems in aqueous solution respectively.</p>	133
Chapter-V	Scheme V.1. Molecular structure of ionic liquid and amino acid	160
Chapter-VI	SchemeV1.1. Plausible solute-co solute interaction.	175
Chapter-VII	<p>SchemeVII.1. Molecular Structure of Tetrabutylammonium Methanesulphonate and L-Arginine and L-Histidine.</p> <p>Scheme 2 (a, b) Optimized geometry of (a) (TBMS+ L-ARG) and(b) TBMS+ L-HIS Systems.</p> <p>SchemeVII.3. Schematic representation of plausible molecular interactions between amino acid and ionic liquid, a & b ion-ion interactions (→); c & d ion-hydrophobic interactions (→); e & f hydrogen bonding interactions (→); g & h hydrophobic-hydrophobic interactions (→).</p>	221 222 221
Chapter-VIII	SchemeVIII. 1. Plausible molecular interactions between the ionic liquids, BTMAC and BTEAC with the amino acid, L-Methionine.	272
Chapter-IX	Scheme IX.1.Fig.(a, b) Optimized geometry of (a) (BTBAC+ L-ASP) and(b) (BTBAC+ L-GLU Systems.	298

LIST OF APPENDICES

APPENDICES	PAGE NO
<u>APPENDIX-A</u> <i>List of Research Publication(s)</i>	(liv-lvii)
<u>APPENDIX-B</u> <i>List of Seminar/Symposium/Convention Attended</i>	(lviii)
<u>APPENDIX-C</u> <i>List of Symbol, Abbreviation and Acronyms</i>	(lix-lxiii)

APPENDIX-A

LIST OF RESEARCH PUBLICATIONS/COMMUNICATIONS

1. Investigation of Solution Behaviour of an Ionic Liquid in Diverse Cellosolves by Physicochemical Contrivance



Journal of Advanced Chemical Science-Volume 4 Issue1(2018) 543-548

2. Exploring Diverse Interactions of Some Surface Active Ionic Liquids with Amino Acids Prevalent in Aqueous Environments by Physicochemical Contrivance



Journal of Advanced Chemical Science- Volume 5 Issue 2 (2019) 637–642.

(INCLUDED IN THE THESIS)

3.Exploration of Solvation Consequences of Some Biologically Potent Molecules in Aqueous Ionic Liquid Solutions with the Manifestation of Molecular Interactions



Journal of chemical, biological and physical sciences, Section A; November 2020 – January 2021, Vol. 11, No. 1; 091-114.

(INCLUDED IN THE THESIS)

4. Physicochemical Investigation of Diverse Interactions of Some Biologically Potent Molecules Prevalent in Aqueous Ionic Liquid Solutions at Different Temperatures
(INCLUDED IN THE THESIES)



Indian journal of Advances in Chemical science 2021; 9(2):89-97

(INCLUDED IN THE THESIES)

5. Subsistence of Assorted Molecular Interactions of Substantial Amino Acids Prevalent in Aqueous Solutions of Ionic Liquid (TBMS) Probed by Experimental and Computational Investigations

(INCLUDED IN THE THESIS)

COMMUNICATE

6. Exploration of Diverse Interactions of L-Methionine in Aqueous Significant Mixed Ionic Liquid Solutions Optimized by Computational Theory

(INCLUDED IN THE THESIS)

COMMUNICATE

7. Solvation behaviour of l-asparagine and l-glutamine prevailing in aqueous ionic liquid solution by physicochemical and computational investigations

(INCLUDED IN THESIS)

COMMUNICATE

APPENDIX-B

List of Seminar/Symposium/Convention Attended

Sl. No.	Seminar/Symposium/ Convention Attended	Date	Organizer and Venue
1.	National Seminar on” Frontiers in Chemistry-2019	May,22,2019	Department of Chemistry of North Bengal& CRSI North Bengal Local Chapter
2.	SERB Sponsored National Conference on “Green Chemistry”: An Alternative Of Conventional Chemistry”	September, 20-21, 2019	DepartmentofChemistry,CBPBU,WeastBengal,I ndiaInassociationwithIndianChemicalSocietKolk ata
3.	International Seminar on” International year of the Periodic Table of Chemical Element-2019	November 22-23, 2019	Department of Chemistry, University of North Bengal
4.	National Seminar on “Frontiers in Chemistry- 2020”	March,5,2020	Department of Chemistry, University of North Bengal
5.	One Day International Seminar on “ Frontiers in Chemistry 2020(Virtual Mode)	October,01, 2020	Department of Chemistry, University of North Bengal In Collaboration with Chemical Research Society of India, North Bengal Local Chapter
6.	One Day International Seminar on” Recent Trends in Chemistry-2020(Virtual Mode)	October,16,2020	Department of Chemistry, University of North Bengal In Collaboration with Chemical Research Society of India, North Bengal Local Chapter
7.	Two Days National web- Based Conference On ”Environmental Determinism, Diverse Pollutions ,Sources, And Controlling Management Through Sciences And Humanities”	22 nd and 23 rd March, 2021	Organized by Alipurduar University

APPENDIX-C

LIST OF SYMBOL, ABBREVIATION AND ACRONYMS

ILs	Ionic liquids
RTILs	Room-temperature ionic liquids
PILs	protic ionic liquids
AILs	aprotic ionic liquids
AAs	Amino acids
[BMIM][C8SO4]	1-Butyl-3-methylimidazolium octylsulphate
[MOIM]Cl	1-Methyl-3-octylimidazolium chloride
[BTMA]Cl	Benzyltri methyl ammonium chloride
[BP] Br	1-Butyl pyridinium Bromide
[BTBA]Cl	Benzyl tri butyl ammonium chloride
TBMS	Tetra butyl ammonium Methanesulphonate
[BTEA]Cl	Benzyl tri ethyl ammonium chloride
L-tyr	L-tyrosine
L-Phe	L-Phenyl alanine
L-Asc	L-Ascorbic acid
L-Asp	L-Aspartic acid
L-Glu	L-Glutamic acid
L-Asp	L-Asparagine,
L-Glu	L-Glutamine
L-Met	L-methionine
L-Arg	L-arginine
L-His	L-histidine
<i>RPM, SMC(0.327), & TK (0.09373)</i>	Speed, spindle multiplier constant, and viscometer torque constant of DV-III pro viscometer.
<i>A</i>	molar Conductance
<i>A_o</i>	limiting molar conductance
<i>K_A</i>	association constant
<i>R</i>	association diameter

λ_o^\pm	limiting ionic conductance
c	molar concentration
κ	specific conductance
ϵ_r	relative permittivity
R_X	relaxation field effect
k^{-1}	radius of the ion atmosphere
e	electron charge
k_B	Boltzmann constant
K_S	association constant of the contact-pairs
K_R	association constant of the solvent-separated pairs
γ	fraction of solute present as unpaired ion
α	fraction of contact pairs
f	activity coefficient
T	absolute temperature
β	twice the Bjerrum distance
δ	minimum standard deviation
$a = (r_+ + r_-)$	crystallographic radii of electrolyte. i.e.; sum of the crystallographic radii of the cation (r_+) and anion (r_-)
d	average distance corresponding to side occupied by solvent molecules
M	molar mass
ρ	density of the solution
M_{av}	average molar mass by the mole fraction
w_1 & w_2	mass fraction of the first & second component of molar mass M_1 & M_2
η_o	solvent viscosity
η	Viscosity of solution
η^{-1}	fluidity
$\Lambda_o\eta$	Walden product
r_{eff}	effective solvated radius
λ_o^\pm	Limiting ionic conductance
$\lambda_o^\pm\eta$	limiting ionic Walden product
r_s	Stokes' radii

List of Appendices

r_c	crystallographic radii
w	mass fraction
ΔG°	Gibbs energy changes
R_g	Gas constant
D_{\pm}	diffusion coefficient
k_B	Boltzmann's constant
i_{\pm}	ionic mobility
z_{\pm}	ionic charge
F	Faraday constant
A_{theo} -coefficient	Ion-ion interactions from Debye-Hückel theory
V_s	Solvated volume of the ion
V_o	volume of the solvent molecules
n_s	solvation number
A_0^r	Limiting triple-ionic conductance
K_P	ion-pair formation constant
K_T	triple-ion formation constant
S	limiting Onsager coefficient
C_P	ion-pair concentrations
C_T	triple-ion concentrations
α	fraction of ion-pairs present in the solution
α_T	fraction of triple-ions present in the solution
a_{IP}	interionic distance parameter for ion-pair
$Q(b)$ and b	constant of Bjerrum's theory
a_{TI}	interionic distance parameter for triple ion
$I(b_3)$	a double integral tabulated in Bjerrum's theory
b_3 & $I(b_3)$	function of a_{TI}
ϕ_V	Apparent molar volume
B -coefficients	Viscosity B -coefficient
\sqrt{c}	square root of molar concentration
ϕ_V^0	partial molar volume at infinite dilution or limiting molar volume
A or A_V	Ion-ion or solute-solute interaction from Masson equation

B or B_V	Ion-solvent or solute-solvent interaction from Masson equation
$\eta_r = \eta/\eta_0$	Relative viscosity
\bar{V}_1^0	partial molar volumes of the solvent
\bar{V}_2^0	partial molar volumes of the solute
$\Delta\mu_1^{0\#}$ or $\Delta G_1^{0\#}$	free energy of activation per mole of solvent mixture of viscous flow
$\Delta\mu_2^{0\#}$	free energy of activation per mole of the solute of viscous flow
h	Planck's constant
N_A	Avogadro's number
$\Delta S_2^{0\#}$	Entropy of the solution
$\Delta H_2^{0\#}$	Enthalpy of the solution
m	Molality of the solution
β_s	adiabatic compressibility
ϕ_K	apparent molar adiabatic compressibility
ϕ_K^0	limiting apparent molar adiabatic compressibilities
S_K^*	experimental slopes
ϕ_{\pm}^0	limiting ionic apparent molar volumes
B_{\pm}	ionic viscosity B -coefficients
n_D	refractive index
R_M	molar refraction
c	speed of light in the medium
c_0	speed of light
$-R$	alkyl chain group of the amino acid
n_c	number of carbon atoms in the alkyl chain of the amino acid
$\phi_V^0(\text{NH}_3^+, \text{COO}^-)$	zwitterionic end group to apparent molar volume
$\phi_V^0(\text{CH}_2)$	methylene group contribution to ϕ_V^0
$\Delta\phi_V^0$	standard transfer volume for amino acid from H_2O to aqueous ionic liquids solution
ϕ_{VW}	van der Waals volume

List of Appendices

ϕ_{VS}	volume associated with voids or empty space
ϕ_S	shrinkage volume due to electrostriction
$\Delta\phi_V^0(\text{NH}_3^+, \text{COO}^-)$	standard partial molar volumes of transfer of the zwitterionic end group
$\Delta\phi_V^0(\text{R})$	standard partial molar volumes of transfer of other alkyl chain groups
n_H	hydrated to the amino acids
$\phi_V^0(\text{int})$	intrinsic partial molar volumes of the amino acids
$\phi_V^0(\text{elect})$	electrostriction partial molar volume resulting of hydration of amino acid
$\phi_V^0(\text{cryst})$	molar volume of crystal
ϕ_E^0	limiting apparent molar expansibilities
$B(\text{NH}_3^+, \text{COO}^-)$	zwitterionic end group to viscosity B -coefficient
$B(\text{CH}_2)$	methylene group to apparent molar volume
$B(\text{R})$	side chain contributions to B -coefficients
$\Delta\mu^{0\#}$	total free energy of activation of viscous flow of the solution
n_1 & n_2	number of moles of mixed solvent and solute, respectively
R^2	squared correlation coefficient or linear regression coefficient
λ	Wave length
<i>Eq.</i>	Equation
<i>Fig.</i>	figure

Some Important Dimensional Constants Used

Name of the constant	Symbol	Value
Density of the water at 298.15K	ρ_0	: $0.99713 \times 10^3 \text{ kg m}^{-3}$
Viscosity of water	η_0	: 0.890 mP s
Conductivity of water		: $<1 \times 10^{-6} \text{ S cm}^{-1}$
Relative permittivity of water	μ_0	: 78.30
Boltzmann's Constant	k_B	: $1.3806488 \times 10^{-23} \text{ m}^2 \text{ kg s}^{-2} \text{ K}^{-1}$
Faraday	F	: 96500 coulomb
Π		: 3.143
Avogadro number	N_A	: $6.023 \times 10^{23} \text{ mol}^{-1}$
Universal Gas constant	R_g	: $8.314 \times 10^7 \text{ erg mol}^{-1} \text{ K}^{-1}$
plank Constant	h	: $6.63 \times 10^{-34} \text{ J s}^{-1}$
Speed of light	c_0	: $3.00 \times 10^8 \text{ m s}^{-1}$
Permeability of free space	μ_0	: $1.256637 \times 10^{-6} \text{ Henry m}^{-1}$
Electronic charge Relative:	E	$1.60 \times 10^{-19} \text{ C}$

Useful Relations

$\rho = n \cdot m$	$N_A = n \cdot v_N$
$m = M/N_0$	$v_N = V/N$
$R_g = R_0/M$	$N = W/M$
$R_0 = N_0 k_B$	

<u>Unity</u>		
	mL : milliliter	g : gram
	eq. : equivalents	h : hour
	min. : minute	mg : milligram
	mol : mole	°C : degree Celsius
	mmol : millimole	K : degree Kelvin
	ppm : part per million	Hz : Hertz
	μmol : micromole	