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 Sadbhabona Sanman
and
Dewang Mehta Best Professor in Chemistry
Department of Chemistry

ENLIGHTMENTTOPERFECTION

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 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***.

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
Darjeeiing-734013, India

UNIVERSITY OF NORTH BENGAL

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

Email: nitu.iitg@gmail.com
Mob: 91 7872808189
Website:https://nituiitg.wixsite.com/nitishroy
January, 2022

ENLIGHTENMENT TO PERFECTION

CERTIFICATE

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Nitish Roy

DR. NITISH ROY,

(CO-SUPERVISOR)

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

Assistant Professor,

Department of Chemistry,

University of North Bengal,

Dist: Darjeeling, Pin: 734013,

West Bengal, INDIA

DATE: 03/01/2022

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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 Rammohanpur,
Darjeeling, 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
Darjeeiing-734013, India

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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

Valuable advices throughout the journey of my research work.

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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 ^{o}C (212 ^{o}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 a electrolyte), amino acid (non - electrolytes) and solvent is great significant due to their wide-ranging use in many industrial purpose 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 incorporates 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.

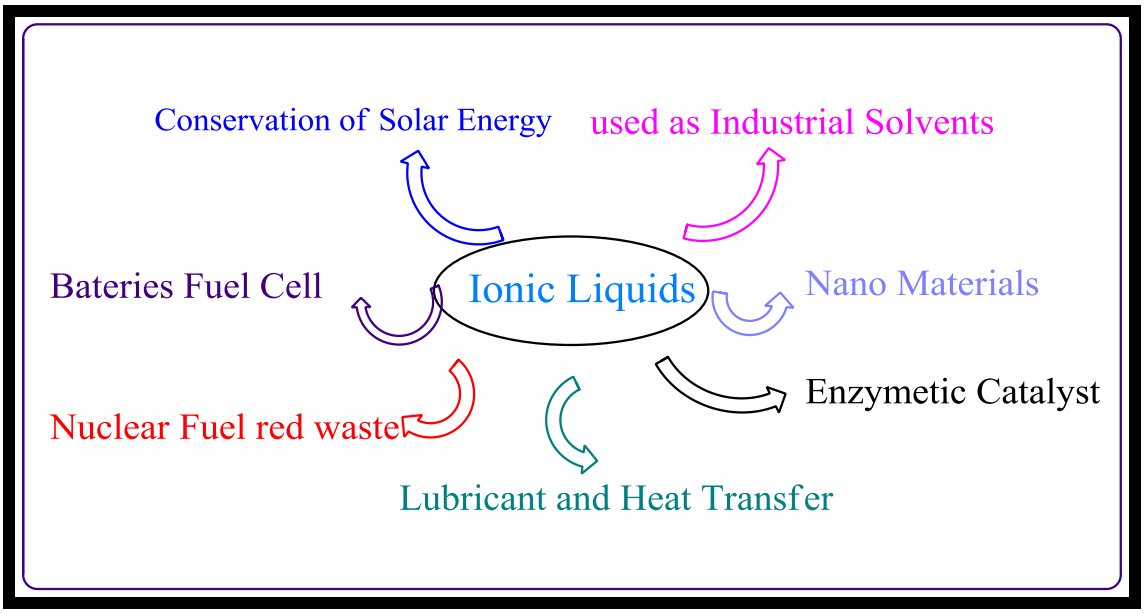
The computational study, surface tension measurement also give the type of interaction associated in molecules in solution system.

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

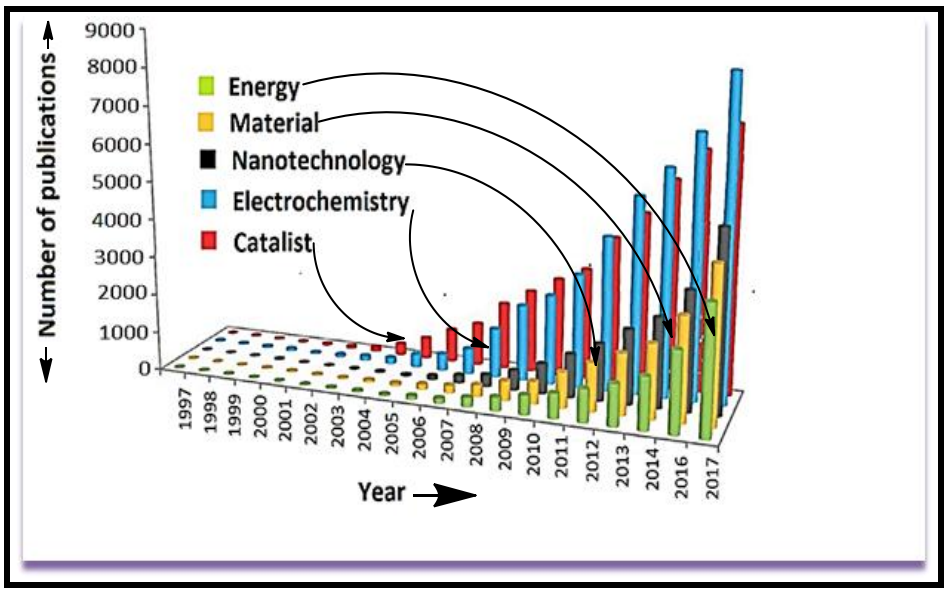
This chapter encloses the *objective, utility and applications of the research work*, the important of electrolytes/solute molecules and solvents used and methods of investigation. This also occupies the summary of the works done connected with the thesis.

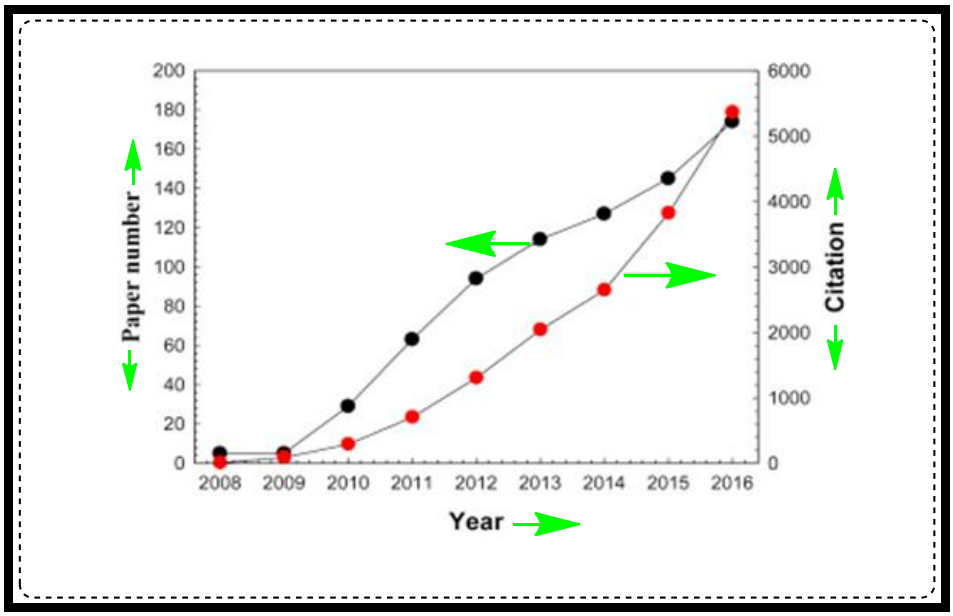


CHAPTER-II

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.



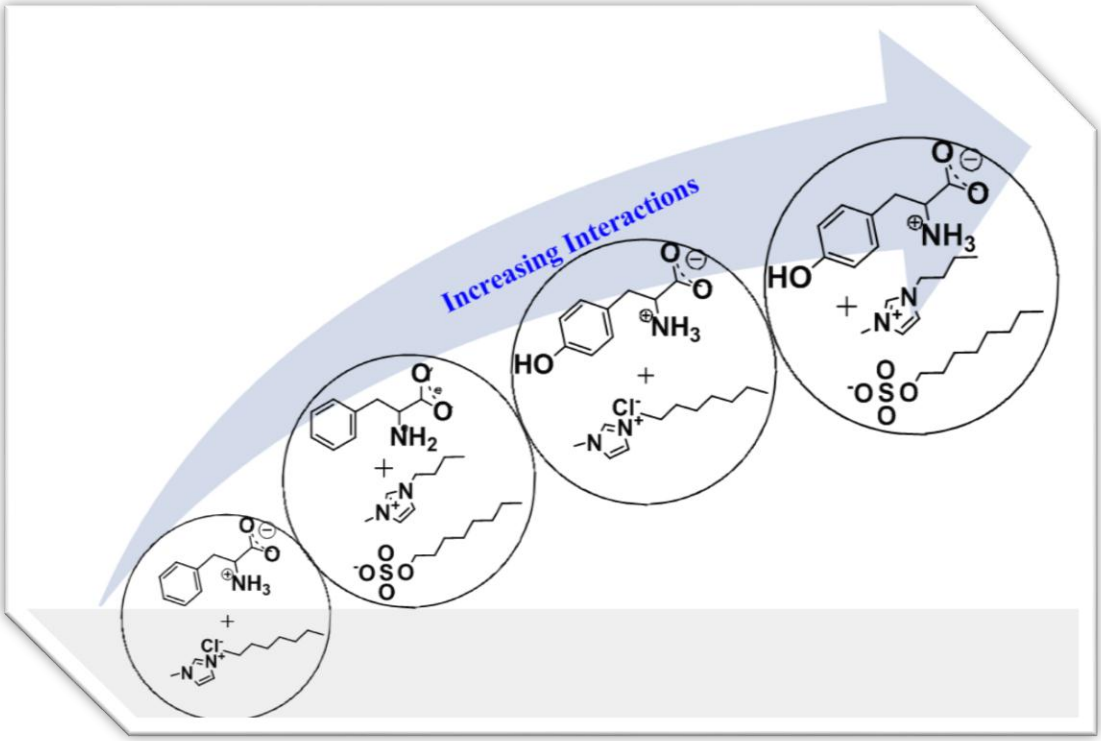


CHAPTER-III

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

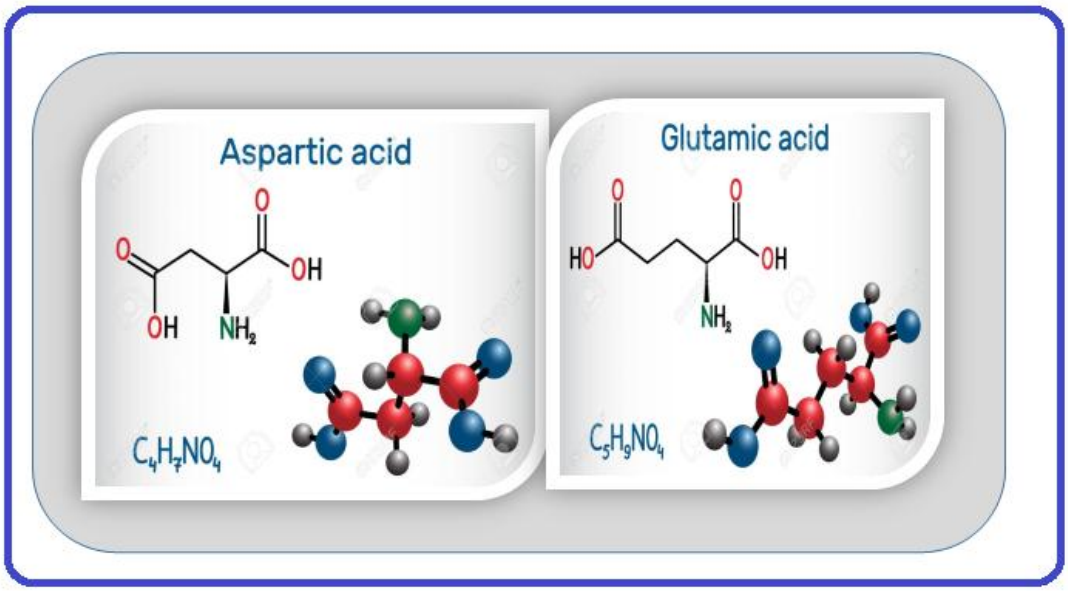
The chapter deals with the precise measurements on electrical conductance (Λ) steady state fluorescence , UV visible spectroscopy, determination of association constant , Gibbs free energy ,study of proton NMR of solutions of an ionic liquid (ILs) , L-Tyrosine, L-Phenyl alanine and their binary mixtures 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, ($\Phi v°$) experimental slopes (SV*), viscosity B-

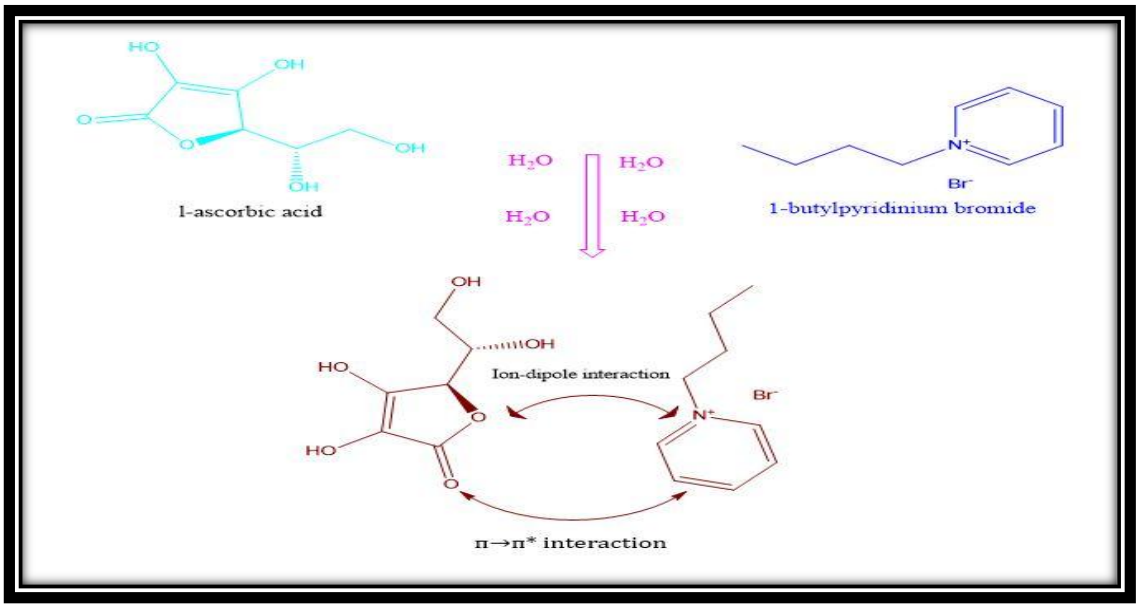
Coefficient data, molar refraction data explained the interaction phenomenon (solute-solvent and solute-solute interactions). Formation of Hydrogen bonding, Dipole-dipole interaction configurational theory, structural aspect, are the powerful forces, for the discussion of the results. The solvation behaviour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



CHAPTER-VI

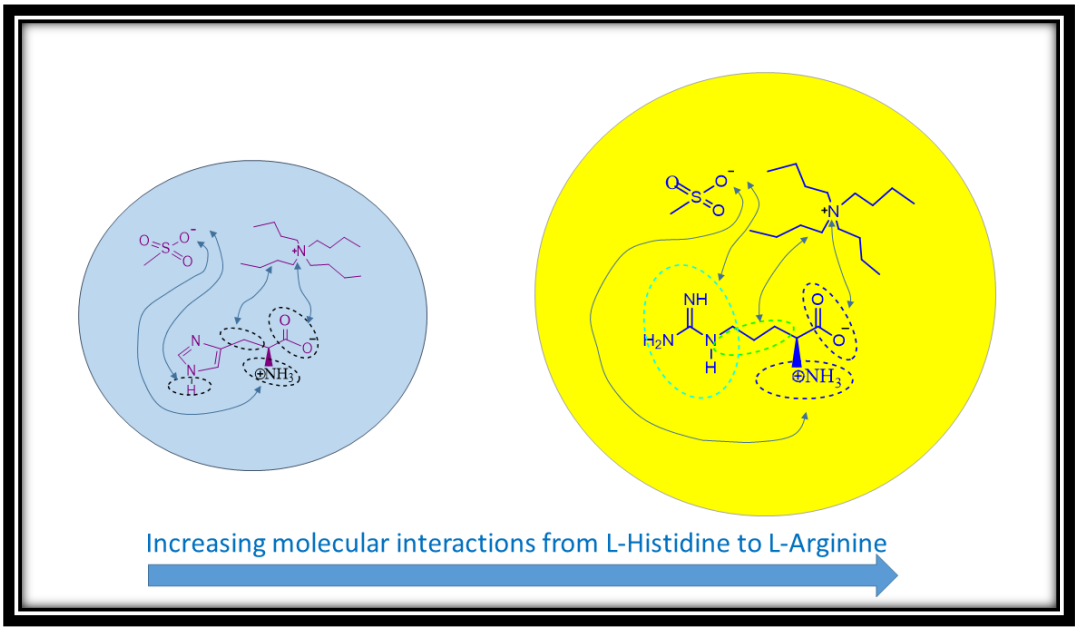
Apparent molar volumes (ϕ_V), viscosity *B*-coefficients, refractive index, specific conductance for L-Ascorbic acid (0.001, 0.003, and 0.005 mol.dm^{-3}) in aqueous ionic liquid, 1-Butylpridiniumbromide ($C_9H_{14}NBr$) solutions were calculated from density of solution. Also viscosity measurements 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-Butylpridiniumbromide).



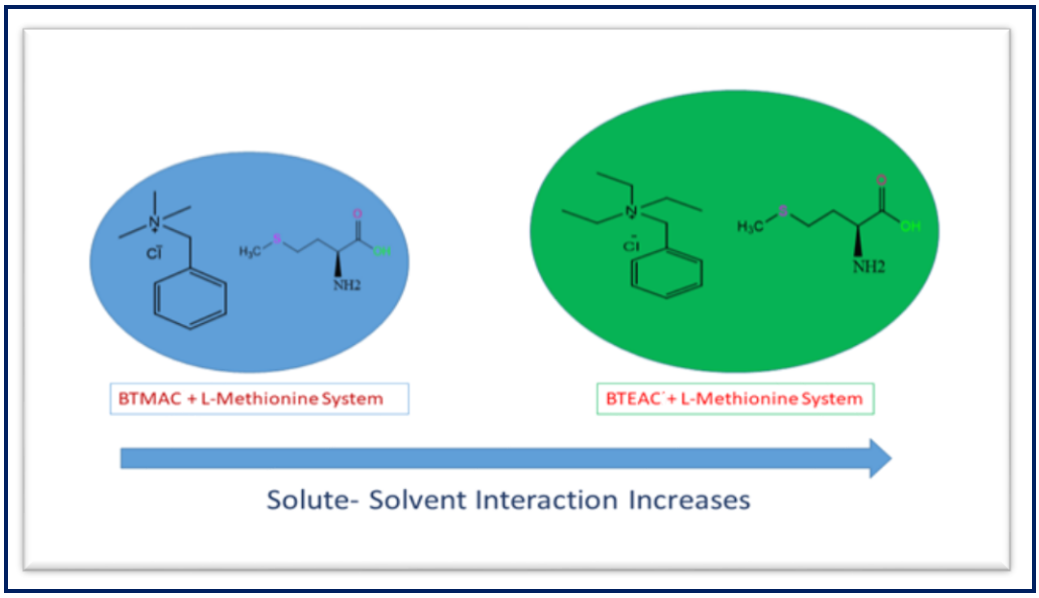
CHAPTER-VII

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, refractmetric, 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 ($\Phi v°$), 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),solutemolecules,Lglutamine(C5H10N2O3)&Laspa ragine(C4H8N2O3) 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 ^{1}HNMR , UV-vis. is also applying for determination of molecular interactions. Molar expansibility factor ($\Phi E° \; and \partial \Phi E°/\partial T$) 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).

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	(IL) 0.005m/mol.kg^{-1} at 303.15K and ▬ concentration (IL) 0.005m/mol.kg^{-1} at 308.15K. **Figure VII.7** Variation of molar conductance (Λ) plot as a function of the concentration of L-Histidine(Amino acid) in differentconcentrations 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;-Δ- 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. **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. **FigureVII. 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. **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}; -Δ- 0.005m/mol.kg^{-1}) of aqueous IL Solution. **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};-Δ- 0.005m/mol.kg^{-1}) of aqueous solutions of IL. **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.	

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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,IndiaInassociationwithIndianChemicalSocietKolkata
3.	International Seminar on" International year of the Periodic Table of Chemical bElement-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"	22nd and 23rd 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] [MOIM]Cl	1-Butyl-3-methylimidazolium octylsulphate 1-Methyl-3-octylimidazolium chloride
[BTMA]Cl	Benzyltri methyl ammonium chloride
[BP] Br	1-Butyl pryidinium 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
RPM, *SMC*(0.327), & *TK* (0.09373)	Speed, spindle multiplier constant, and viscometer torque constant of DV-III pro viscometer.
Λ	molar Conductance
Λ_o	limiting molar conductance
K_A	association constant
R	association diameter

$\lambda_o^{\pm}$	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
$\lambda_o^{\pm}$	Limiting ionic conductance
$\lambda_o^{\pm}\eta$	limiting ionic Walden product
r_s	Stokes' radii

r_c	crystallographic radii
w	mass fraction
ΔG^o	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
Λ_0^T	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
$\phi_\pm^0$	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
$\phi_V^0(NH_3^+, COO^-)$	zwitterionic end group to apparent molar volume
$\phi_V^0(CH_2)$	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

ϕ_{VS}	volume associated with voids or empty space
ϕ_S	shrinkage volume due to electrostriction
$\Delta\phi_V^0(NH_3^+, COO^-)$	standard partial molar volumes of transfer of the zwitterionic end group
$\Delta\phi_V^0$ (R)	standard partial molar volumes of transfer of other alkyl chain groups
n_H	hydrated to the amino acids
ϕ_V^0 (int)	intrinsic partial molar volumes of the amino acids
ϕ_V^0 (elect)	electrostriction partial molar volume resulting of hydration of amino acid
ϕ_V^0 (cryst)	molar volume of crystal
ϕ_E^0	limiting apparent molar expansibilities
$B(NH_3^+, COO^-)$	zwitterionic end group to viscosity *B*-coefficient
$B(CH_2)$	methylene group to apparent molar volume
$B(R)$	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
Eq.	Equation
Fig.	figure

Some Important Dimensional Constants Used

Name of the constant	Symbol	Value
Density of the water at 298.15K	ρ_0	: 0.99713×10^{3} kg m^{-3}
Viscosity of water	η_0	: 0.890 mP s
Conductivity of water		: $<1\times10^{-6}$ S cm^{-1}
Relatative permittivity of water	μ_0	: 78.30
Boltzmann's Constant	k_B	: 1.3806488×10^{-23} m^2 kg s^{-2} K^{-1}
Faraday	F	: 96500 coulomb
Π		: 3.143
Avogardo number	N_A	: 6.023×10^{23} mol^{-1}
Universal Gas constant	R_g	: 8.314×10^{7} erg mol^{-1} K^{-1}
plank Constant	h	: 6.63×10^{-34} J s^{-1}
Speed of light	c_o	: 3.00×10^{8} m s^{-1}
Permeability of free space Electronic charge Relative**:**	μ_0 E	: 1.256637 × 10-6 Henry m^{-1} 1.60×10^{-19} C

Useful Relations	
$\rho = n\cdot m$	$N_A = n\cdot\upsilon_N$
$m = M/N_0$	$\upsilon_N = V/N$
$R_g = R_0/M$	N = W/M
$R_0 = N_0\, k_B$	

Unity	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	