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“Imagination is more important than knowledge. Knowledge is limited. Imagination encircles the world”

Albert Einstein.

Introduction
1.0. Introduction

Research area of molecular sciences in the last decade of the 20\textsuperscript{th} century has robustly entered into another frontier part in the science. The number of properties investigation associated with molecules has been increasing so rapidly that many new branches of sciences have been started. The art of interaction between different molecules of the substance and recognizing different constituents of the substance, takes a prominent role in the application of science. The interaction of molecules is a very curious subject to known constitute of interacting substance. Interaction of molecules drive much technology based on thermodynamics [1]. Understanding interaction between molecules allows exploiting and predicting behavior of molecules for synthesis.

Molecular interaction implies the study of structure and functions of living systems in terms of physics of constituent molecules. It can be understand in terms of interaction between various biological molecules and their subsequent dynamics. It is mainly used to understand physical architecture of biological molecules and their functional properties.

Basic building blocks of all matter, living or non living are atoms. All living matter consists of small variety of atoms. Carbohydrates and lipids are made up of elements Hydrogen, Carbon and Oxygen, Proteins and nucleic acids are made of elements Hydrogen, Carbon, Oxygen, Nitrogen, Sulphur / Phosphorus. Ions play critical role in the entire cellular activity. Important ions present are Ca, K, S and Mg. Some of ions traces found are Fe, Cu, Zu, Co, Mu and Mo etc. The physical interaction which gives rise to a ideal structures of large bio-molecules.
Molecular interactions play an important key role in many chemical and biological processes such as protein folding and function, peptide aggregation and enzymatic reactions or the stabilization of reactive species. Molecular interaction mainly used to explore properties, reactivity and applications of complex systems consisting a large number of interacting molecules. Intermolecular interactions between solvent and solute molecules determine aggregation of proteins into many biological processes. This gives an art of computational tools to construct new models of complex systems to investigate interactions of proteins, organic molecules, solvents and co-solvents.

Molecular interactions can occur between molecules belonging to different or within chemical families. Whenever such molecules are connected by physical interactions they form molecular interaction networks which are generally classified by nature of compounds involved. The information stored in the structure of molecules is a function of their physical and chemical properties. The ability to manipulate this information leads to virtue of change in the structure of molecules. The properties directly depend on Physico-chemical behaviors of interaction; strength of interaction depends on complementarities of Physico-chemical properties of atoms.

The investigations on Physico-chemical properties of solute and solvent mixture have been found to give useful information of physical nature and strength of molecular interaction. Since liquid state poses a fascinating characteristic and challenging problem to both theoreticians and experimentalists. Physico-chemical studies of binary and ternary liquid mixtures are of considerable theoretical and technological importance as they provide a wide range of interaction between solute and solvents of varying composition.
Molecular interaction studies with varying dielectric constants are increasingly being used for study of kinetics of various reactions in different solvents. Thermodynamic studies are particular significance owing to practical applications of mixture in various analytical techniques. Therefore a deeper knowledge of solution structure and intermolecular interactions between components of binary and ternary mixtures will be important to understand many chemical and biological processes in mixed solvent media.

Bio-molecular interaction and Cellular function is emerging field in the biophysics research which provides a valuable resource for the elucidation by molecular interaction. Physics discovers the “mechanisms that interconnect many different aspect of nature”. Interactions between bio-molecules to a large extent determine by their molecular structures [2].

A structural formula for a compound conveys which atom is linked to which atoms. However it doesn’t give shape of molecules, but indicate groups of elements present. It gives clues to properties of substance. In material science molecular structures are important and responsible for all chemical process including phase behaviors [3, 4, 5].

The physical and chemical properties are different as we consider as individual then as a groups. The characteristic of molecules are generally distinct from their constituent atoms. A water molecule consists’ two hydrogen and an oxygen atom bonded together, but their physical and chemical properties are different as we consider individual then as a group. A molecule is smallest unit of compound that retains properties of the compound. To study interactions within, between, and among bio-molecules, it is highly desirable to use tools of experimental and theoretical physics or preferably a combination [6].
1.1. Molecular Interaction

The interactions between molecules are called Molecular interaction. The strength of these interaction i.e. force among atoms can be characterized according into their thermodynamic and kinetic behavior and is directly dependent on the Physico-chemical properties of organic compounds.

Molecular interaction can be classified into two types. They are Inter molecular interaction and Intra molecular interaction.

**Intra molecular interaction**

The interactions or force (attraction or repulsion) between the atoms within molecules are called intra molecular interactions.

**Inter molecular interaction**

The interactions or force (attraction or repulsion) between the two or more similar or different molecules are called inter molecular interactions.

Inter molecular interaction is particularly important in terms of how molecules interact and form biological molecules. The strength of interaction can be measured by molecular interaction. Inter molecular forces are responsible for intermolecular interaction.

The structure of bio-molecules arises out from interactions between their constituent atoms. It is necessary to know nature of force which binds atoms to understand the structure of the biological molecules. Large biological molecules like proteins and nucleic acids exhibit basic primary structure and then a number of secondary structures.
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The structure of biological molecules determines its function. In turns, the forces between atoms in molecules determine its structure. Thus structure of biological molecules can described in terms of two interaction *strong and weak interaction*. The primary structure of biological molecules is made of strong interaction. Higher order structures like secondary, tertiary and quaternary are governed by weak interaction. Strong interactions are implicated mainly in formation of chemical structure and to some extent in the formation of molecular structure. Weak interaction, on the other hand not only helps to determine three dimensional structures but also involved in the interaction between different molecules. The strength and dynamics of molecular binding is determining factors such as bioactivity and target specificity of legends [7].

Energetically, a molecule is a stable arrangement of two or more atoms. A molecule exists because energy of combined systems of atoms is less than that of separate atoms. Whenever a bond between two interacting units is broken and they are separated by supply energy. Conversely, energy is released when two atoms combines together to form a molecules.

Any interaction within molecules or between molecules can be understood as a sum of interaction between pairs of atoms. When two atoms come close to each other a potential energy is associated with systems. This potential energy is a minimum when force of attraction between atoms equals to force of repulsion, and is zero when two atoms are separated by an infinitely large distance. The system as whole tries to attain equilibrium minimum energy state and final equilibrium distance between two interacting atoms is a resultant of all different forces.
The intermolecular interaction can be described into two types, one is strong interaction or short range interaction and other is weak interaction or long range interaction [8].

**Strong interaction or short range forces**

Short range forces are known as “Chemical forces” or “Valence forces” arise when molecules come closer together with the overlap of their electron clouds.

Strong force also refers to the short range attractive force responsible for covalent bond between atoms. Strong forces determine the primary chain structure of biological molecules. Example peptide bonds in proteins, nucleotide units bonds in DNA or RNA etc.

Strong force has quantum mechanical origin; it is Pauli Exclusion Principle which determines strong binding between two atoms. For example hydrogen molecules is formed when two hydrogen atoms comes with their electron having anti-parallel spins. It is the coupling between electrons with opposite spins which overcome electrostatic repulsion between them and leads to an attractive force. These forces include covalent and ionic are classified in this category.

**Covalent bond**

When two identical atoms form a covalent bond the shared electrons move symmetrically about the center of the molecules. Quantum mechanically, electrons probability amplitude is symmetric about the center, with a maximum at the center, so that both the electrons are mostly found in between of atoms. Examples are H$_2$, O$_2$ atoms.
### Ionic bond

An ionic bond is formed due to electrostatic attraction between two opposite charged ions. In an ionic compound an electron is transferred from an electropositive to an electronegative element in order to achieve a stable electron configuration. I.e., if atoms are different, electron density shifts towards one of the nuclei. This asymmetric distribution of negative and positive charge density about the center of molecule gives rise to an effective electric dipole moment of the molecules.

The distinction between ionic and covalent bonding is done in terms of dipole moment. If dipole moment of molecules is less than 0.1Debye then the bond is referred to as pure covalent bond. If the dipole moment is more than 1Debye then it is called ionic covalent bond.

### Weak interaction or Long range interaction

They are known as “Long range forces” or “Weak forces”, arise when interacting molecules come closer together without overlap of their electron clouds. These forces are generally dependent on intermolecular separation and have no directional effect.

These forces acts between molecules like proteins, carbohydrates, fats and nucleic acids etc., give them their secondary structures. In biological systems week interaction play more important role in the sense that strong forces give rise to rather rigid or less flexible structures. The kind of flexibility or mobility that is required by biological molecules to perform their diverse function is possible only if the corresponding forces are weak.

The molecular interactions are electrostatic in nature. The strength of these interactions, the forces among atoms, can be categorized according to their
thermodynamic and kinetic behavior and is defined as affinity. Both properties are
directly dependent on Physico-chemical properties of the organic compounds.

The electrostatic interaction between two molecules arises from static charge
distributions of interacting molecular species. It is also referred as orientation
interaction. The electrostatic interactions are pair wise additive and may be attractive
as well as repulsive. This type of interaction arises as a point charge without any
deformation or polarization.

They are several types of weak long range interaction. Some of them are
simply of classical electrostatic nature and others due to quantum nature of interacting
systems. Weak interactions are mainly classified in to Van der Waals interaction and
Hydrogen interaction.

Van der Waals interaction is a weak interaction relatively short range. This
type of interaction plays an important role in their stability. It acts between all
molecules and ions, but the effect cannot be felt in presence of strong interactions like
covalent or ionic bonds. They involve interactions between electric dipoles. Van der
Waals interaction is a cumulative effect. There are several types of interaction
between molecules, which together constitutes Van der Waals interaction. Normally
there are four prominent types of interactions;

- Electrostatic interaction
- Dipole – dipole interaction or Keesam interaction
- Inductive interaction or Debye interaction
- Dispersion interaction
**Electrostatic interaction**

The electrostatic interaction between two molecules arises from static charge distribution of interacting molecular species. It is referred as orientation interaction. The electrostatic interactions are pair-wise additive and may be attractive as well as repulsive. This type of interaction arises as a point charge without any deformation or polarization. Example of electrostatic interaction is Coulomb and charge dipole interaction.

**Dipole – dipole interaction**

Willem Hendrik Keesom gave the first mathematical description in 1921 for dipole-dipole interaction; it is also called as Keesom interaction. This type of interaction is formed between two molecules with permanent dipoles. This interaction is weaker than ionic interaction because only partial charges are involved.

When two bonded atoms have a difference in their ability to attract electron, they form an electric dipole and hence possess a dipole moment. All polar molecules possess a permanent electric dipole moment. The electric dipole produces its own dipole field in which other dipoles would tend to linearly align themselves. The typical value of dipole-dipole interaction is of the order of thermal energy at normal temperature. Hence dipole-dipole interaction is not strong enough to lead to any strong alignment of molecules in a solution. Because of thermal energy, the orientation of dipoles constantly fluctuates. The strength of the interaction depends directly on the square of dipole moments.

**Inductive interaction**

This type of interaction arises when molecules experience an electric field created by electric charge distribution of another and vice versa. When molecules experience force in one direction and nuclei experience a force in other direction, it
creates an induced dipole moment in molecule and vice versa. The permanent
distribution of charge clouds gives rise to delocalization effect. Delocalized
interactions are created from distortion of the individual molecular charge distribution
in electric fields created by surrounding molecules which is attractive.

An ion or polar molecules interacts with non-polar molecules by inducing a
dipole moment in the latter. The ion or polar molecule produces its own electric field
around it. In this electric field, the electron density of the non-polar molecules shifts
slightly with respect to its centre of charge density. This results in a dipole moment
being induced within the non-polar molecule.

The strength of induction interaction is less than dipole-dipole interaction
between two polar molecules. The interaction therefore is not strong enough to
mutually orient the molecules.

**Dispersion interaction**

This type of interaction is also called Van der Waals force is due to
instantaneous dipole effects. These involve attraction between temporarily induced
dipoles in non-polar molecules. The polarization can be induced either by
polar molecules or by repulsion of negatively charged electron clouds in non-polar
molecules.

The most remarkable is intermolecular force which acts even between two
non-polar neutral molecules besides between any other types of molecules. This
interaction is responsible for interaction between atoms of inert gases or between
homo-polar molecules like H₂, O₂, etc. This is called dispersion interaction. It is a non
electrical and exact nature can be understood only in terms of quantum mechanics.
Dispersion interaction is strong enough not only bring molecules together, but also
tends to mutually orient these molecules. It is a long range force, the intermolecular separation may range from 0.2 nm to 10 nm or more.

The contribution of all the interaction viz., electrostatic, dipole-dipole, induced dipole-dipole and dispersion interaction results in a weak interaction between molecules whose potential energy of interaction. However between two molecules, the contribution to Van der Waals interaction may not come from all the parts.

In fact, between two non-polar molecules, only dispersive interaction is present; between a polar and non-polar, both inductive and dispersive interaction operate; while between polar and polar molecules, all the three interaction are present.

1.2. **Hydrogen bond interaction**

Molecular hydrogen bonding plays a decisive role in conformational changes in biologically important compounds. The hydrogen bond significance is quite different in spheres of physics, chemistry and biology its consequence such as the properties of liquid and solid [9]. A hydrogen bond is an important factor to determine physical, chemical and biology properties of many class of substances [10]. It is a specific interaction between a proton donor and proton acceptor. Because of small size of hydrogen atom and its large electrostatic field it can move in close to electronegative atom and form an electrostatic type of union known as hydrogen bond or hydrogen bridge. Moore T S and Winmill T F [11] were the first to give the concept of hydrogen bond in molecular interaction studies.

The hydrogen bond occurs between certain molecules containing hydrogen atom. Hydrogen bond is of great interest in biology, because it occurrence in biological system like protein and nucleic acid [12]. Though it is a weaker than covalent or ionic bonds, hydrogen bond is stronger than Van der Waals. The hydrogen
bond length is larger than covalent bond length between two atoms and smaller than the sum of their Van der Waals radii. Hydrogen bond may therefore be called a medium strong range interaction. This bond is very common in large biological molecules and is responsible for secondary structure like helical coiling of proteins and nucleic acids.

Hydrogen bond is invariably formed between two electronegative atoms X and Y. One of the atoms, say X, is called acceptor while other atom Y is called donor. There is a hydrogen atom attached to acceptor atom X. The electro-negativity of acceptor atom X must be enough so that it pull most of the electron cloud towards itself and hydrogen atom becomes almost a naked proton. Typical example of acceptor atoms are F, O and N. The donor atom Y must have an excess negative charge and a free non-bonding electron pair which it can donate. Typical examples of donor atoms are F, O, N and Cl. The bonding between X and Y through a hydrogen bridge is called hydrogen bond and is denoted as X – H…..Y. This is effectively a donor-acceptor interaction through hydrogen atom.

Hydrogen bonding in general results from an inter play of electrostatic and quantum mechanical forces. If electrostatic interactions dominate then H-bond is weak, if quantum mechanical interaction occurs then H-bond is strong. They are two types of hydrogen bonding. They are *Intra molecular hydrogen bond* and *Inter hydrogen bonding interaction* [13, 14].

**Intra molecular hydrogen bonding**

Hydrogen bonding which occurs within molecules is called intra molecular hydrogen bonding. It gives rise to chelating or ring formation.

Examples: Ethyl aceto acetate
Inter molecular hydrogen bonding

Hydrogen bonding which occurs between two or more similar or different molecules is called inter molecular hydrogen bonding. This gives raise to a molecular association.

Examples: Water, Alcohols, Amines and acids

Inter molecular hydrogen bond are broken due to the dilution, where as intra molecular hydrogen bonds are not affected [14-16]. For the hydrogen bonding exchange interaction does not cause any electron density changes in other parts of molecules participating in hydrogen bond. Polarization causes most significant charge redistribution though its contribution to energy. In proton acceptor molecule charge redistribution is attributed almost solely to the polarization interaction. The electron rearrangement disturbs charge distribution in other part of molecules [16].

Coulson C A [16] suggests that hydrogen bond energy depends on the four independent factors, namely;

- Electrostatic interaction
- Induced interaction
- Dispersion interaction
- Repulsion interaction.

All three interactions electrostatic, induced and dispersion are explained in previous section. Repulsion interaction is a short range interaction which occurs when two atoms or molecules approach each other. The repulsion between closed electron shells is due to Pauli’s exclusion principle, in the sense that too many electrons occupy same space. There is a room for only one pair of electrons in a bonding orbital; a second pair must be assigned to an anti bonding orbital. In general
an anti bonding electron exerts stronger repulsion effect than attractive force of a bonding electron. Strong and weak hydrogen bonds for biological structures are discussed by Jeffrey and Saenger [17].

### 1.3. Importance of biological organic compounds

Biological important organic compounds are primarily made up of carbon, hydrogen and oxygen. The common organic compound of living organisms which is made of these compounds is very important such as carbohydrates, proteins, lipids, and nucleic acids. Each of these macromolecules is made of smaller subunits. Each class of these macromolecules has its own structures and properties. For example proteins composed of amino acids and carboxyl groups. These characteristic subunits and chemical groups impart different properties to the macromolecules.

Compounds containing the element carbon, called organic compounds, are the most important substances that make up living organisms. Many of the important molecules necessary for life are large molecules or macromolecules that are made up of smaller molecules. Proteins are most important biological molecules present in the entire living cell. The amino acids are the structural components present in all the proteins. Amide and amines are building block of proteins and amino acids. The function and activity of organic compound is mainly depends on its structures. Due to complex structure of bio-molecules, their direct study is somewhat difficult. Therefore most convenient method is to study structural information in terms of their building blocks to get insight into fine structural details of these biopolymers interaction between organic compounds like alcohols. Since these compounds has been recognized in a wide range of biochemical processes. The study of model
compounds like amide and amines with alcohols is fundamental importance in understanding intermolecular interaction between biological important organic compounds.

Chemicals used in these studies are substitute of amides, amines and alcohols. Amines and amides constitute are important class of organic and bio-organic compounds. Amides are the building block of proteins. Understanding the mutual interaction of amides with hydroxyl groups is important in relation to conformational stability of proteins [18]. Being the simplest models for peptides, amides have been subject of several structural studies.

Several amines are medically and biologically important. In nature, they occur as bio molecules, vitamins, alkaloids and harmonies [19]. Synthetic examples include polymers, dyestuff’s and drugs. The chief commercial use of amines is as intermediates in synthesis of dyes, synthetic fibers and as medicines due to physiological and psychological effects.

The reactions of amines are more important in chemistry and biology mainly due to participation of unshared pair electrons of nitrogen which makes them react as a nucleophile or a base ( Nucleophile is a species that attract an electron deficient carbon and a base is a species that attract and electron deficient hydrogen i.e. proton)

Amine contains an active lone pair of electron in very electronegative nitrogen atom. It is this electron which is attracted to positive parts of other molecules or ions. Amines are derivatives of ammonia, wherein one or more hydrogen atoms are replaced by organic subsistent.

Functional groups containing nitrogen are present in a variety of naturally occurring and manmade organic compounds [20]. These functional groups impart
Physico-chemical characteristics to molecules. These groups are responsible for their unique chemical reactivity and play crucial role in preparation of drugs, agrochemicals, dyes and molecules of life [21].

Amine group are biological importance in vegetable, microbial and animal cells. Important amines include amino acids, biogenic amines; trimethylamine and aniline are used in pharmaceutical industry [22 – 26]. Biologically active compounds, namely adrenaline and ephedrine [27], both containing secondary amino group used to increase blood pressure. Novocain, a synthetic amino compound, is used as an anesthetic in dentistry. Benadryl, a well known antihistaminic drug also contains tertiary amino group. Quaternary ammonium salts are used as surfactants. All amino groups -NH{sub}2, -NHR, -NR{sub}2 are most powerful activating groups. Aniline is one of the most important compounds of amines which are used in many pharmaceutical compounds [28]. An amine substitute called dopamine is a hemo transmitter in the brain [29]. Abnormalities in the level of dopamine cause may psychological disorders. Adrenaline is a hormone released into the blood stream in times of emergency. This causes an increase in blood pressure and increased oxygen intake [30, 31]. Dopamine is a neurotransmitter occurring in a variety of animals [32].

Organic compounds contain carbon-oxygen double bond (>C=O) called carboxyl group, which is important functional groups in organic chemistry. The carbonyl compound in which carbonyl grouping is bonded to carbon is attached to nitrogen are called amides. Compounds with the nitrogen atom next to a carbonyl of structure R-(C=O) NR{sub}2 are called amides and have different chemical properties.

Amides are simplest molecule containing peptide linkage and study of their hydrogen bonding yields into nature of protein structure. Amides are used as synthetic reagents. Amides contain more nitrogen than amino acids and form structural part of
most proteins. The two important amides found in plants are asparagines and glutamine. They are formed from two amino acids namely glutamic acid and aspartic acid. During amide formation, the hydroxyl part of the acid is replaced by another NH$_2$ radical.

Some of amides substitutes are used widely as color, in crayons, pencils and inks, paper industry, plastic and rubber industry, water and sewage treatment. Acryl amide and poly acryl amide are most commonly used amides in industries [33]. Nylons are polyamides used for textile industries. In paper industry it is used as a binder and for retention for fibers. Acryl amides are used in cosmetic industry to prepare hair products, soaps, and pre-shave lotions. Amides derivates are used for printing inks, explosives, latex thickeners, adhesives and emulsion stabilizers. Kevlar a constituents of amide is a very strong material which is about five times as strong as steel [34]. It is used in composites for boat construction, in manufacture of bullet proof vests, and in lightweight mountaineering ropes and skis and racquets. Commercially some amides are used as insect repellant (N, N-dimethyl-m-toluamide), insecticides (Equaine) and local anesthetics (Xylocaine) [35].

Carboxylic acids are widespread in plants and animal. They play a significant role in biochemical processes of life. They add smell and flavor to nature, for example, vanillin, salicylaldehyde and cinnamaldehyde contain very pleasant fragrances. They are used in several food produce and pharmaceuticals to include flavors and for prepare materials similar to adhesives, paints, resins, perfumes, plastics, fabrics, etc.

The relaxation process of primary alcohols with amide substitutes, amine substitutes and their mixtures have been studied with intention of elucidating some
structural information on the compounds and probable interaction between constituents on the mixtures.

1.4. **Scope and Objective of the studies**

Molecular interaction plays a different role in drug discovery and development. From determining mechanism of action to identifying unwanted biological reaction, the study of binding events is a critical part of many phases of therapeutic research. Information stored in the structure of molecules is a function of their physical and chemical properties. The important reason is ability to manipulate this information by virtue of changing structure of molecules. Interaction studies play an important role in understanding the structure and properties of organic liquids.

Molecular interaction of bio-organic compounds with organic chemical can be studied in terms of amine and amides. Since these compounds are the building blocks of all bioorganic compound. The amine group influences three dimension structures of proteins [36]. Hydrogen bond significantly influence the properties of amine [37]. By studying interaction of the bioorganic chemical substitutes in terms of amide and amines, the Physico-chemical of this complex can be clearly understood. This leads to organic chemist to invent new organic chemicals which are very useful for pharmaceutical industries.

The specificity of many biologically important reactions is based on molecular interactions. Molecular discrimination can be investigated by a variety of spectroscopic methods including Spectra-photometry, fluorescence, circular dichroism and NMR. This type of information is particular importance as it will provide knowledge needed not only to guide and to optimize, but also to expand applications of this particular molecular selector and other for interaction.
In order to establish a connection between molecules and their interaction with others by means of underlying Physico-chemical context, one can have accurate enough structural information on molecules and molecular complexes. The characterization of structure and energetic of molecular complexes is thus a key factor for understanding biological functions.

Intermolecular interactions are very significant at molecular separation of about very few nanometers or less, but much weaker forces associated with chemical bonding. Interaction occurs between all molecules which are attractive or repulsive. It is important in terms of how molecules interact and form biological organism. They are responsible of many physical properties and dimensional arrangements of biological molecules and polymers.

A chemical force arises when the molecules come close enough for the overlap of their electron clouds and they are often highly directional. The nature of interactions between molecules is a combination of different physical phenomena and the most important of these are described here. The main contributions to all these interactions arise from the interaction between elementary particles comprising the interacting molecules.

The study of molecular interaction in organic liquid mixtures can be investigated by both spectroscopic and non-spectroscopic methods [38]. The study gives an insight into the structural properties of liquids, especially dynamical characteristics and the relation between structural properties and macroscopic behavior. It is possible to obtain valuable information regarding nature and strength of interactions in liquid mixtures [39].
This thesis is focused on the qualitative explanation of influence of molecular structure on physico-chemical properties of different alcohols with some aromatics nitro compounds. In addition, this study also provides a better insight into the nature of molecular interaction in aforementioned systems. Besides their theoretical importance, systems were chosen, since they are very interesting from a practical point of view: (i) Due to their diverse biological and industrial applications (ii) Alcohols and other organic compounds are employed in a variety of industrial and consumer applications, such as perfumes, cosmetics, paints, varnishes, drugs, fuels, explosives, fats, waxes, resins, plastics, rubber, detergents, DDT, etc., while carbon tetrachloride is applied as a solvent in the pharmaceutical industry, paint industry, in chemical production of pesticides, oils, alkaloids, etc.

The fundamental goal of studying liquid dynamics is a molecular level description of interactions between molecules as a basis for understanding physical properties and rates of chemical reactions. Liquid dynamics are inherently difficult to quantify on a molecular level due to multiple time scales of inter and intra molecular interactions. These manifest themselves as broadening of nuclear and electronic spectral signatures, thereby obscuring details of molecular interactions.

The molecules are biologically active and respective reactions between molecules, principles of reactions, classifications of functional groups and reaction mechanisms are important parameters to understand the reactions. The knowledge of interaction will be very helpful for learning biological important organic molecules. Also to know basic concepts of molecular structure for biological systems and gained in depth knowledge in Stereochemistry, Stereochemistry of reactions.

Amines are central part in organic chemistry and for all biological compounds. All known life processes depend on amino acids, each of which contains an amine
group. The biological important organic chemicals like amines and amides with different alcohols in non-polar solvents studies are scarce in literature. In this context, a systematic study involving the effect of chain length of both alcohols with amides, amines in solvent environment are carried out. This study will provide Physico-chemical vital information useful for efficient design for organic chemist, biologist and pharmaceutical industry to synthesis new compounds.

Many experimental techniques such as infrared, Nuclear magnetic resonance and non spectroscopic method like Dielectric and Ultrasonic play an important role in studying molecular interaction in terms of hydrogen bonding interaction. The dielectric properties, dependence of composition and structure of substance have been developed as an extremely important field in chemical science [40]. The study of dielectric properties of liquid material is necessary to understand liquid structure, but it provides technical data for practical uses in industry, science and medicine [41].

By knowing parameter like dielectric constant, dielectric constant at optical frequency, relaxation time, Kirkwood correlation factors and thermo dynamical parameters viz free energy, enthalpy and entropy of activation for dielectric relaxation can be calculated by dielectric measurement [42 – 47] and using data information about molecular interaction can be understanding and conform the basic mechanisms of complex formation.

Spectroscopic technique is a power full tool to investigate nature of molecular complexes and hydrogen bonding. It is an interesting subject to measure various thermodynamic excess functions which gives information about molecular interaction. A number of attempts to develop a quantitatively accurate and physically meaning explanation of solvent induced stretching vibration frequency shifts have been presented by many authors.
Variations of frequency shifts, half band width and integrated intensity are observed factor while studying molecular interaction from the spectroscopic method. Physical parameters namely density, viscosity, vapor pressure, solubility, heat of mixing conductivity, acoustical and spectroscopic measurement gives more information about molecular interaction [48 - 52]. This type of information is particular importance because it provides knowledge to guide and optimize application of this particular molecular selector and other for interaction.

The acoustical parameters namely ultrasonic velocity, Adiabatic compressibility, intermolecular free length, internal pressure, free volumes, excess Gibbs’ energy of activation of viscous flow [53 – 56] are used to predict the nature and structural behavior of molecules and interpreted in terms of inter molecular interaction by using ultrasonic experimental methods for the mixtures.

In the present work, an attempt has been made to study the nature of molecular interactions in alcohols with biological important organic compound which mainly substitute of amide and amine in non-polar solvents.

**Objectives of the study**

*Molecular interaction studies of some biological important organic compounds like amide and amine substitutes with primary alcohols are carried out with the following objectives.*

- Determination of dielectric parameter and Static dielectric constant of mixture.
- Determination of Dielectric relaxation.
- To study the molecular association in terms of hydrogen bonds.
Determination of molecular interaction of amide substitute by means of hydrogen bond between amide substitutes with alcohols.

Determination of molecular interaction of amine substitutes with 1-alcohols.

To Study the strength and nature of molecular interaction.

To propose a structure associated solute with solvent in terms of hydrogen bond

To know the orientation of the molecules in the mixture

To study the spectral changes due to the molecular interaction

The above objectives are studied by means of experimental investigation using dielectric relaxation, Fourier Infrared spectral and Ultrasonic measurements. In this context, a systematic study involving the effect of hydrogen bond between alcohols with amides, amines in solvent environment are carried out. This study will provide Physico-chemical vital information useful for the efficient design for the organic chemist, biologist and pharmaceutical industry to synthesis new compounds.
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