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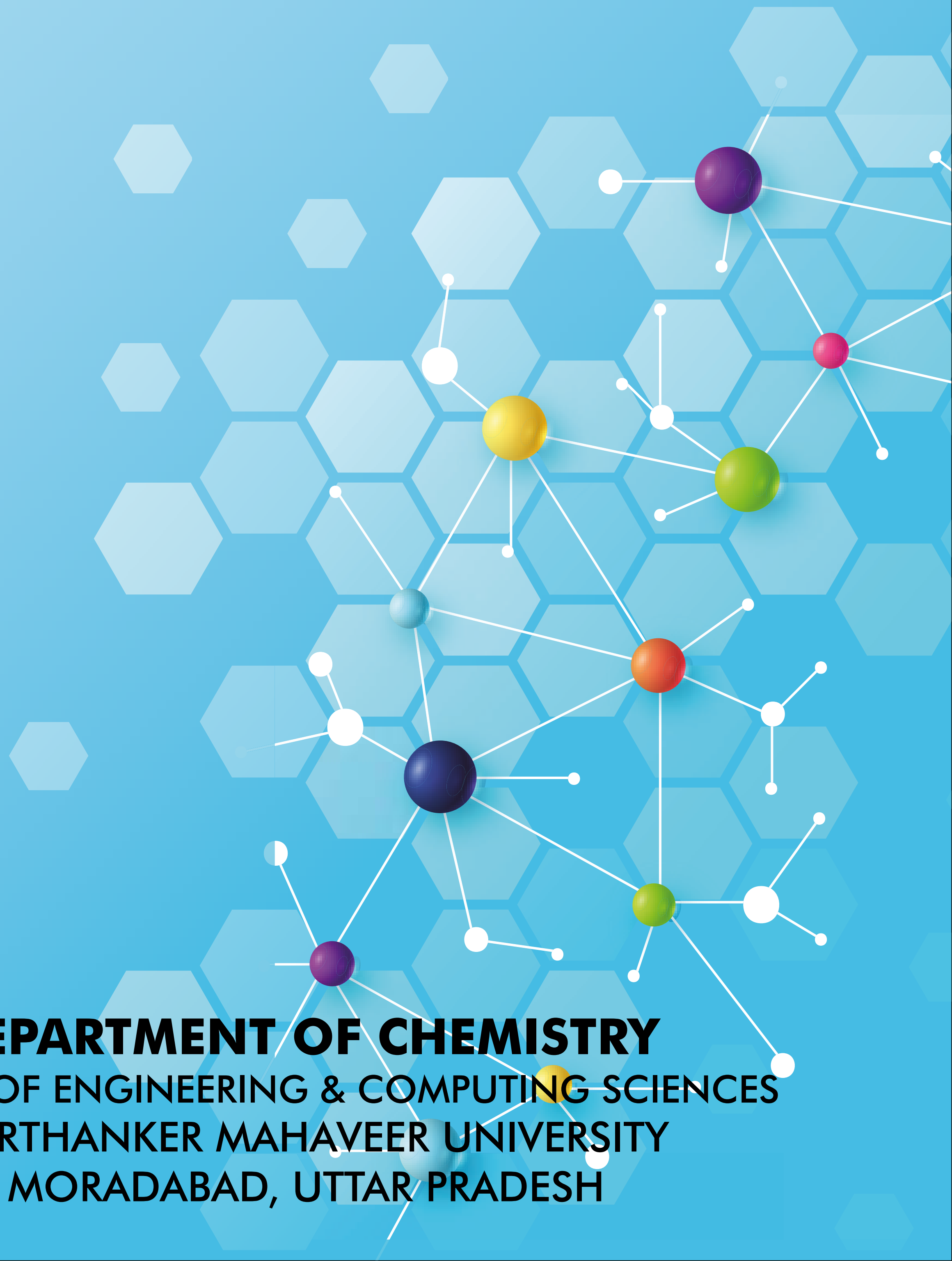

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FACULTY OF ENGINEERING & COMPUTING SCIENCES
TEERTHANKER MAHAVEER UNIVERSITY
MORADABAD, UTTAR PRADESH

About the Journal

TMU Journal of Basic & Applied Chemistry (TJBAC), is a prominent source to spread worldwide promotion of systematic research awareness across INDIA in various field of chemistry. This is an international scientific peer reviewed, open access journal, dedicated in publishing original research from pure chemistry, applied chemistry and focusing on wide range of applications. This journal covers: analytical/ inorganic, organic/ industrial, and physical theoretical/experimental chemistry as well as new interdisciplinary fields such as material science, spectroscopy, biological, medicinal, and environmental chemistry. The original research papers and short communications are published in "**TMU Journal of Basic & Applied Chemistry**" and is issued yearly. It has high profile editorial standards, with leading editors involved in the current research fields, get knowledgeable peer reviews and publishing decisions. Manuscripts published in the Journal should not be reproduced without a written permission from the Editor-in-Chief.

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Teerthanker Mahaveer University

Teerthanker Mahaveer University was established by an 'Act' (No. 30) of 2008 of the Government of Uttar Pradesh and has been approved by the University Grants Commission (UGC) vide letter No. F. 9-31/2008(CPP-1) dated October, 2008. The University is located on National Highway-24, barely 144 Km from New Delhi.

The University stands committed to the ideals of Lord Mahaveer – Right Philosophy, Right Knowledge, and Right Conduct – in all the spheres of activity and aspire to be recognized as the ultimate destination for world class education.

The multi-disciplinary University offers career oriented courses at all levels, i.e., UG, PG and Doctoral degrees across diverse streams, namely, Medical, Dental, Pharmacy, Nursing, Paramedical Sciences, Physiotherapy, Hospital Administration, Education, Physical Education, Engineering, Architecture, Polytechnic, Management, Law, Journalism, Fine Arts, Jain Studies, and Agriculture Science to meet rising aspirations of the youth.

Faculty of Engineering & Computing Sciences

The College of Engineering has emerged as a hub for academic excellence in engineering training. The college contributes to quality education in all major disciplines of engineering and technical education and helps meet the needs of industry for trained technical manpower with practical experience and sound theoretical knowledge.

The college was established by the university with the aim of providing relevant, essential, upgraded education to the young aspirants in the field of computer science and engineering, including computer applications. In recent times and the years to come there will be increasing demand of skilled manpower in the domain of Computer Science and Engineering because of the 'Digital India' mission, projected around the globe by Government of India.

TMU Journal of Basic & Applied Chemistry is a **peer-reviewed** and multidisciplinary **journal** that publishes original research, case studies, & review articles of all major branches of Chemistry. The Journal does not charge for publishing the manuscript. The papers contained in the journal carry the opinion and views of the contributors and not necessarily of the editorial Board. The editorial Board as such shall not be responsible for the authenticity and legality concerned regarding the submission made in this journal. The author shall be responsible for authenticity of the published research papers.

CHIEF PATRON

Shri Suresh Jain
Chancellor,
TMU, Moradabad

I am extremely glad and feeling inner happiness for the release of vol-2, 2022 of **TMU Journal of Basic & Applied Chemistry**, an International Journal of Chemistry, Faculty of Engineering and Computing Sciences, Teerthanker Mahaveer University, Moradabad in the Month of January-December, 2022. I express my feelings that the World is growing very fast and creative researches have changed the entire Technology in the field of Engineering, Medical Sciences, Computing Sciences and variety of industrial products. This is true that research in any discipline is not one day job but it needs consistent and continuous efforts to do constructive work for the benefit of mankind. In the present Scenario the scientists all over the World have achieved wonderful Technology to make impossible task to possible through research only. Just see the defense technology, in medical the robotic surgery, in Engineering heavy duty working Machines, variety of Batteries, IOT, and Fuels etc. The dream of this University has achieved a lot, it was completed in the year 2008 and since that day the teaching /research standard is getting advancement, and an ambitious to enhance research interest among the faculty members to grow vertically and horizontally for bright and successful endeavor in the department of chemistry. This is true that any institution is recognized by research work, quality publications and patents which are usable by industries and not by colossal and huge towers. The faculty members may spare one /two hours per day for research. Everyone must have determination, confidence and research interest to produce quality research work. Now I express my happiness to publish this journal on regular basis. I am sure that readers of this message will take it very positive to move ahead among the best researchers. I trust that FOE & CS will definitely bring revolution through quality research work to give a good name and fame to Teerthanker Mahaveer University in India and abroad as prestigious institute in academics and research. My heartiest felicitation to Director and Principal of FOECS, Editor- in- Chief, Associate Editors , advisory committee to release this Journal continuously for the extreme satisfaction of research students, researchers and scientists.

CHIEF PATRON

Shri Manish Jain
Group Vice Chairman,
TMU, Moradabad

I take this opportunity to rejoice along with critical faculties and students, Faculty of Engineering and Computing Sciences for the smooth and efficient functioning of the college under the vigilant supervision of Professor R.K. Dwivedi, Director and principal, TMU, Moradabad. I am feeling immense pleasure that FOE&CS is publishing vol.-2, 2022 of **TMU Journal of Basic & Applied Chemistry**, to boost the research environment in the college. I advice the learned faculties that develop addiction to perform research activities in your respective field. You may feel that it is a difficult task but this will add in your profile as an excellent researcher. This will be beneficial for the students also to show them right path for their professional and prosperous life in endeavor. Keep it up in doing constructive work to elevate the academic and research standard of this unique Teerthanker Mahaveer University, Moradabad. Though this university young in years, Second to none in this area as most popular interdisciplinary University. I am sure that fragrance of quality education, research potential, variety of courses offered, is spreading through cooperation and perseverance.

CHIEF PATRON

Shri Akshat Jain

Esteemed Member of Governing Body
TMU, Moradabad

I personally feel that hard work never goes astray. The conferences, webinars and seminars, special talks play an important role in creating congenial research environment in the department and ultimately in the University. It gives reflection of learned faculty serving in the department. I am highly excited to congratulate the organizing team of the department of Chemistry, versatile and eminent scholar Professor R. K. Dwivedi, Director and Principal , Faculty of Engineering and Computing Sciences, TMU , for releasing vol.-2, 2022, "**TMU Journal of basic & applied Chemistry**" . This is a challenging work for all the researchers to accept the demand of present scenario of research. In my opinion the Journal will provide National platform for academicians, researchers and scientists coming from various National Institutes/ Universities and Research Laboratories to present break through facts, research findings and innovations in the field of Chemistry. I am sure that this Journal shall bring valuable exchange of ideas among participants. I would like to express my appreciation to the organizing team for their hard work and restless efforts.

I extend my best wishes for grand success of this Journal.

PATRON

Prof. Raghuvir Singh
Vice Chancellor,
TMU, Moradabad

I am very happy to announce the release of TMU Journal , The **TMU Journal of Basic & Applied Chemistry" vol.2 , 2022** broadening the scope and coverage among researchers in the entire Indian Universities. I personally believe that University education system, particularly technical education, requires a platform to encourage budding researchers for publishing their research output in the form of journal articles. TMU is largest Technological Universities in the country with a very large pool of faculty, research scholars, and post graduate and graduate students. As such the University would like to create a platform for its fraternity for publishing their research works by instituting a high quality technical journal covering all branches of Engineering and allied fields.

No doubt publication of the journal is expected to be beneficial for the University in many ways — it brings scholarly recognition to the University; it would also contribute for the career development of faculty and researchers through their participation in the creation and sharing of new innovations, research and development. These new ideas, research and development activities finally translate into the overall development of the community and society at large. These scholarly publications will be a medium for academic and scientific discussions and enrichment of research areas. Though there is a long list of advantages that an academic journal can offer to research community, primarily for a researcher an academic journal is a credible and authoritative source of information and offer platform and evidence for their research output.

I suggest and appeal the students, faculties to strengthen the quality of the Journal by performing quality research reviews, research papers.

Congratulations to Professor R.K. Dwivedi, Director and Principal , FOE & CS , Editor-in- Chief, Associate Editors, section Editors and Advisory committee to motivate a positive environment of research in the college..

PATRON

Prof. (Dr.) R. K. Dwivedi
Principal & Director, FOE &
CS, TMU, Moradabad

I take this opportunity to share my views for the smooth working of the Faculty of Engineering & Computing Sciences, Teerthanker Mahaveer University, Moradabad. Firstly I congratulate to team of learned persons in publishing the vol-2, 2022 of **TMU Journal of Basic & Applied Chemistry**. This is an excellent approach to publish Reviews, research Papers, on regular basis in the field of Chemistry. I always say, nature does not thrust potentials and accomplishments upon mankind. We are endowed with insipient powers and latent forces. This is our duty to develop them so as to master himself. To my mind, Faculty of Engineering & Computing Sciences is not just a building made of bricks, mortar and concrete , but It is a noble centre of education that help in building character, empowering minds and imparting rich and rewarding experience that last life time. Ultimately, this lead to realization of all cherished dreams. Try to know your potential yourself otherwise you will not value your time. My aim of life is, live with enthusiasm to go higher and higher and contribute for the welfare of the society. I express my heartiest gratitude and thanks to His eminence Shri Suresh Jain, Chancellor, Shri Manish Jain, Group Vice Chairman, most respected Vice Chancellor Prof. (Dr) Raghuvir Singh, the Editor-in-chief, Associate Editors, Section Editors, Members of advisory committee for their untired efforts to bring this issue in magnificent form.

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Nanostructured Graphitic Carbon Nitride: A Novel Material for Water Purification

Abstract
Graphitic carbon nitride (GCN) is a material of potential in the field of water purification. Due to the favourable structures and functional groups present, the material becomes very effective in removing different toxic dyes from water by catalysis and adsorption techniques. In recent time GCN has attracted the attention of the researchers because of different important features like its two dimensional structure with very high surface area low cost and high production yield synthesis techniques and other. In this work, efforts have been given to understand the negative impact of over using textile dyes in different industries like paper, textile, paint or other. Also the common ways and means by which these dyes may be removed from water mainly by adsorption as well as photo-catalysis have been investigated.
Substantial study has been done in order to understand basic theories behind both the processes and to study the basic reaction kinetics involved in such processes. In this regards graphitic carbon nitride has been chosen as a material of potential and its use as water purifier has been described in depth.

Keywords : graphitic carbon nitrides, nanostructure, water pollution, dyes, catalysis, adsorption

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Introduction

Nanotechnology is an interdisciplinary science in which material scientists, mechanical and electronic engineers, biologists, chemists & physicists work together to extend the nanoscale boundaries. Nano is a Greek word, which means micro or small. Every particle, whose size is 100 nm or smaller is considered a nanoparticle. Nanoscience is the study of the fundamental principles of molecule and structure with at least one dimension roughly between 1 & 100nm.

Nanomaterials found its application in several fields of extreme importance that include energy, defence, communication, medicine, construction, filtration and many more. Another very important aspect of nanotechnology is its environmental aspect. Nanotechnology can solve the problem of environmental pollution specially the problem of water pollution. There are several nanomaterials which have proved its potential in the field of environment specially in addressing the water pollution problem. These materials include carbon nanotube, graphene, zinc oxide, titanium di-oxide and many more. Graphitic carbon nitride (GCN) is one of the materials of extreme interest in this regard. The water pollutant may be classified into organic large molecules, heavy metals, textile dyes and others.

The presence of amine groups at the edges of the GCN motif due to deficiency in polymerization and condensation reactions during synthesis process render structural defects in GCN [Zhu Jet.al,2014; Das Det.al,2017] making it favourable for removal of different water contaminant. As stated by Zhu et al., these defects encourage delocalization and relocalization of electrons on the GCN surface thereby rendering its impressive surface properties including Lewis base functionalities and electron-rich characteristics (Zhu Jet.al,2014) . All these properties accompanied with thermal and chemical stability are the primary reasons behind the catalytic activity of GCN.

Owing to the suitable wide band gap semiconductor nature along with appropriate CB and VB redox edge potentials and ability to harvest photons corresponding to the visible range. GCN acts as an efficient photocatalyst material for degradation of dyes. However, bulk GCN suffers from rapid electron-hole charge carriers' recombination, moderate surface area, and low quantum efficiency along with not enough utilization of solar light, all of which adversely affects its photocatalytic efficiency (Sun and Liang, **2017**). This is compensated by structural and morphological modifications as performed and reported by many researchers.

Paul et al. showed that pristine GCN synthesized from urea at a temperature of 550°C could effectively degrade 10 ppm of MB dye aqueous solution with a rate constant 'k' value of 0.0081 min^{-1} and GCN dosage of 0.01 g/100 mL under visible light irradiation (200W Xenon lamps) (Paul DR et.al,2019) . Similarly another report by Paul et al. revealed the extensive utilization of pure GCN in degradation of both cationic (RhB and MB) and anionic (MO) dyes (Paul DR,2020). Gu et al. synthesized hierarchically porous GCN from melamine exhibiting an impressive surface area of 109.3 m^2/g for effective visible-light assisted degradation of MO with a 'k' value of 0.69 h^{-1} (Gu S, et.al.2014).Metal nanoparticles suffer from many drawbacks which restrict their practical applicability. Nobel metal nanoparticles are difficult to synthesize, not at all cost-effective, poorly available, unstable under chemical conditions, and most importantly cannot be reused or regenerated due to their high tendency of agglomeration (Veisi H,2019). These disadvantages led to the incorporation, immobilization and anchoring of these metal nanoparticles into carbon-based polymeric matrix to improve their functionality and stability (Veisi H et.al.,2019; Li J et.al.,2012; Zhang P et.al.,2011).

GCN in its pristine and functionalized forms has been extensively applied for the complete removal of dye pollutants from water environment following adsorption technique. However, the moderate surface area of bulk GCN is not suitable enough for the effective adsorption of dyes on its surface. This led to the fabrication of mesoporous GCN and GCN nanosheets with increased surface area and surface-active sites.

Yousefi et al. performed oxidation of GCN nanosheets by Hummer's method and subsequently utilized these samples for the removal of various textile dyes like MB, RhB, MO and others (Yousefi M,2019). Bhowmik et al.,2015, supported Au nanoparticles on GCN sheet which were effectively employed for the removal of cationic MB and RhB and anionic MR from water environment (Bhowmik T et.al,2015). Removal efficiency of 91% in 380 min and 90% within 420 min was achieved for RhB and MB respectively. Zou et al. fabricated a novel composite of GCN and β-cyclodextrin which showed improved adsorption of MO dye at an acidic pH compared to pristine GCN (Zou Y et.al.2016).In this mini review the different aspects of GCN for water purification have been studied. Here I have mainly studied the efficiency of GCN in removing textile dyes from water.

Basic Ideas of Textile Dyes

What are Dyes?

The substance which coloured the substrate through chemically bonds to the substrate on which applied is called Dye. These dyes are distinguished from the pigment which is not chemically bond to the material which we want to colour. Chemical structure of indigo dye and its corresponding digital images has been shown in **Fig.1**

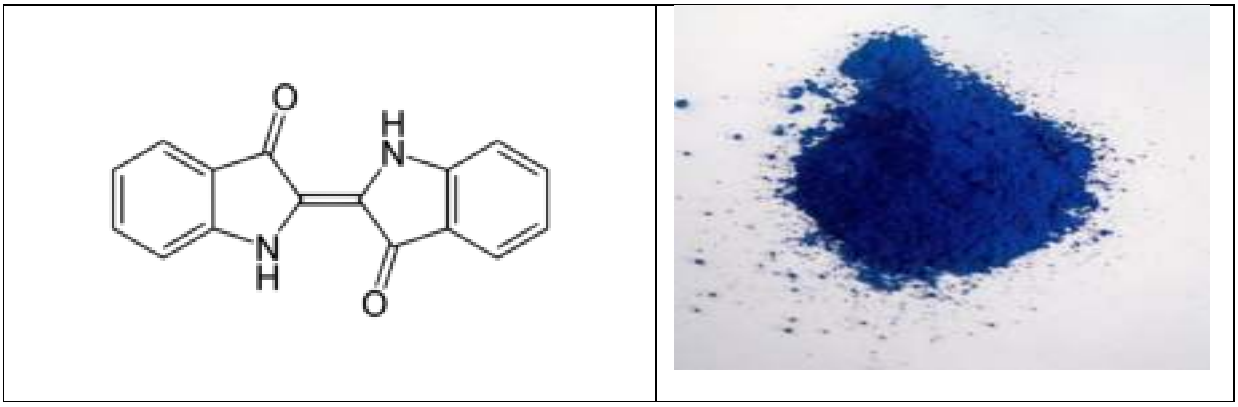


Fig.1: Chemical structure of indigo dye and its corresponding digital images

The dyes may be divided into two types one is natural and other is synthetic or man-made. natural dyes are mainly derives from different plant sources- roots, berries, bark of tree, leaves, wood, fungi and lichens etc. and we are depending on the nature to get dyes to dye the substance like cloths, tomb, building, caves etc until 1800 A.D. After this man can able to make synthetic dyes. Today we are mainly use synthetic dyes because synthetic dyes production is taken less time to that of making process of natural dyes. Synthetic dyes are mainly obtained from the petrochemicals and this method is the first man-made synthetic dye. This method firstly used by J. Puller and Sons in Scotland. **Chart 1** describes the broad classification of textile dyes.

Water pollution by Textile dyes

Human activities over the last few decades have led to the exponential increase in the environmental crisis that the world is facing right now. Rapid emergence of numerous industries in order to meet the needs of the fast growing world population has resulted in severe negative impacts on the natural resources of the planet. Water resource, the most important resource for the survival of all living organisms, is currently being drown in chemical wastes emitted from countless manufacturing industries. Toxic chemical compounds discharged from textile, printing, tannery, dye manufacturing, food-processing and cosmetic industries are the primary sources of hazardous effluents with apparel industries solely contributing to approximately one-fifth of the planet's total water pollution.

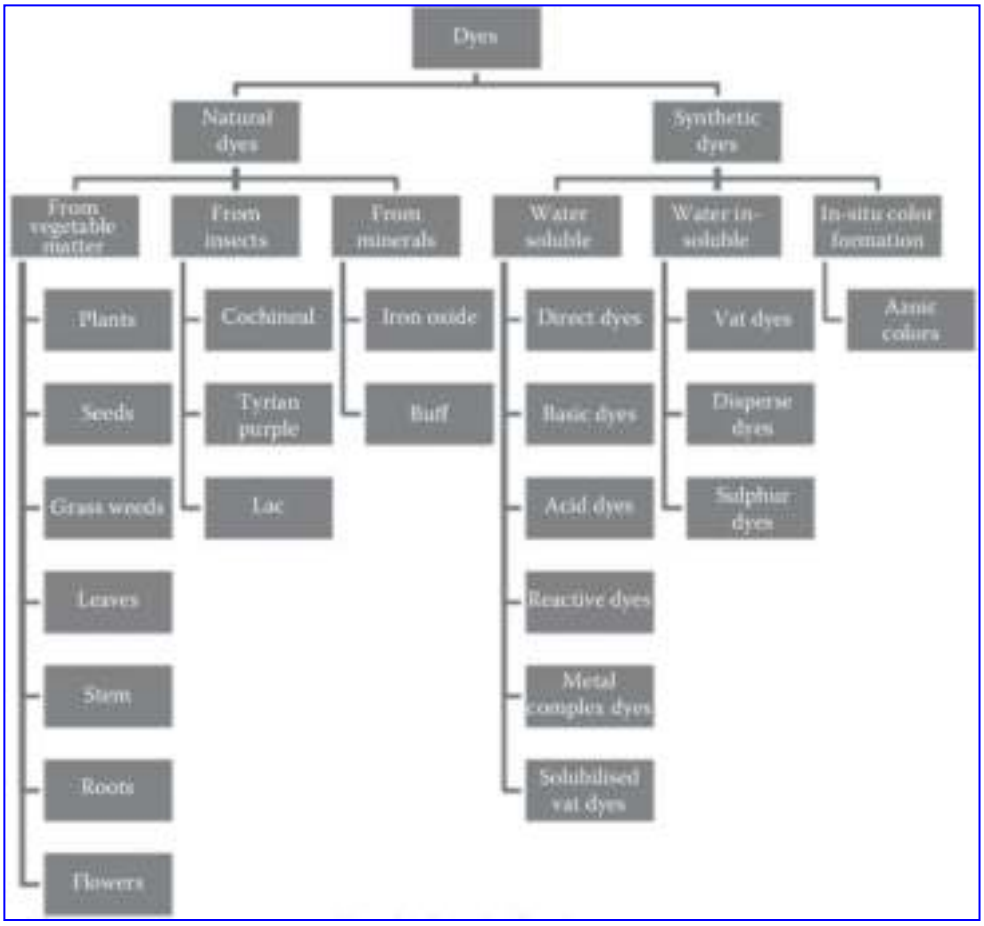
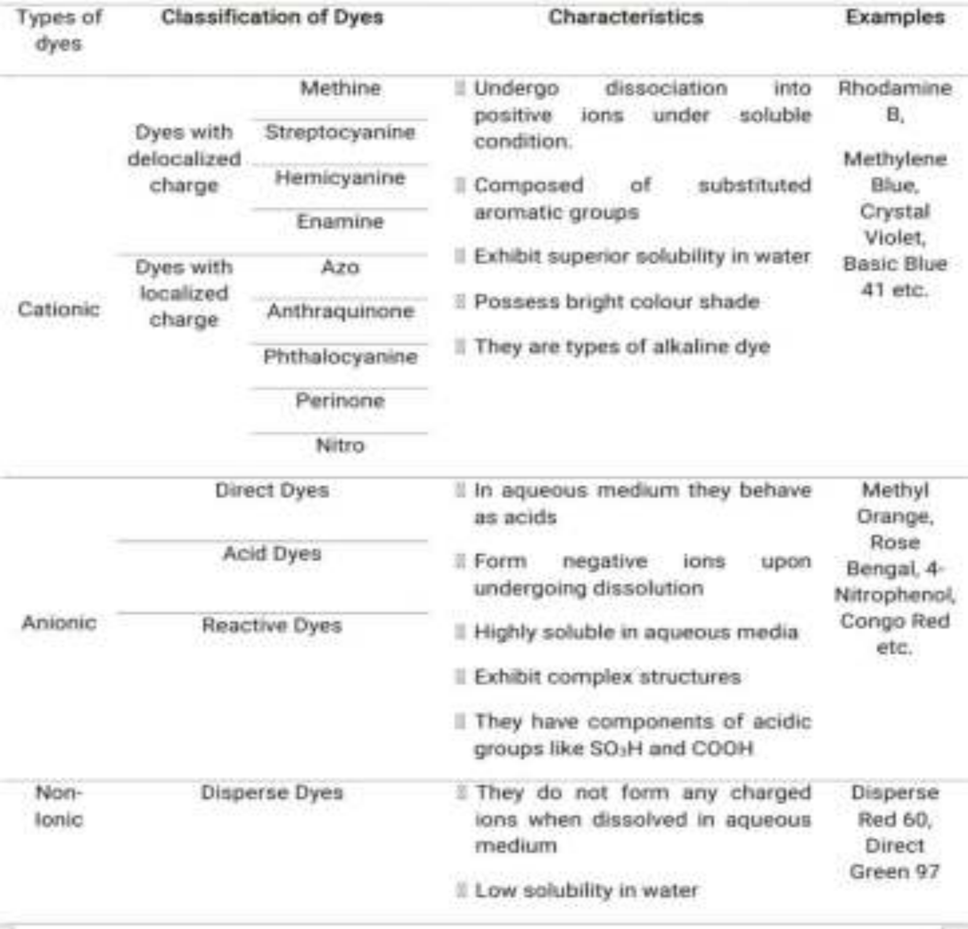


Chart 1: Classification of dyes and their characteristics

Textile dyes are considered to be the most perilous pollutants among the numerous types of complex organic chemical compounds that comprise the wastewaters emitted from textile industries which when released into the environment without proper treatment results in drastic fatal effects on aquatic ecosystem and human beings. The synthetic non-biodegradable dyes can cause acute detrimental effects on aquatic bio-organisms and aquatic plants by blocking the sunlight from reaching the depths of water-bodies, causing hindrance to the photosynthetic activities, depleting the oxygen level required for their survival, and stimulating the growth of unwanted algae on water surface. The effects these pollutants can cause on human health are of grave concern. While most of the commonly used textile dyes reportedly cause dysfunctions of the vital human organs like kidney, liver, brain, and reproductive system, many are also found to be mutagenic and carcinogenic in nature. Along with these, dyes can also lead to allergic dermatitis, skin itching and irritation, and in cases of excessive exposure can significantly hamper the central nervous system. **Table 1** summarizes basic classifications of few commonly used dyes.

Table 1: Basic classifications of few commonly used dyes



Types of dyes	Classification of Dyes		Characteristics	Examples
Cationic	Dyes with delocalized charge	Methine	Undergo dissociation into positive ions under soluble condition. Composed of substituted aromatic groups Exhibit superior solubility in water Possess bright colour shade They are types of alkaline dye	Rhodamine B, Methylene Blue, Crystal Violet, Basic Blue 41 etc.
		Streptocyanine		
		Hemicyanine		
		Enamine		
	Dyes with localized charge	Azo		
		Anthraquinone		
		Phthalocyanine		
		Perinone		
		Nitro		
Anionic	Direct Dyes		In aqueous medium they behave as acids Form negative ions upon undergoing dissolution Highly soluble in aqueous media Exhibit complex structures They have components of acidic groups like SO_3H and COOH	Methyl Orange, Rose Bengal, 4-Nitrophenol, Congo Red etc.
	Acid Dyes			
	Reactive Dyes			
Non-Ionic	Disperse Dyes		They do not form any charged ions when dissolved in aqueous medium Low solubility in water	Disperse Red 60, Direct Green 97

Approximately, 40 % all over the world used chlorine contained colorants that are commonly known as colorants contain organically bound chlorine a known carcinogen. In the wastewater there are mostly organic material are present, there are many elements which is used to disinfect the water but chlorine is the best element to disinfectants the harmful material, it is best primary element for textile industry for the water treatment. These chemicals get evaporated and are inhaled during breathing causing several serious disease especially to kids and infants even before their birth. **Fig.2** shows how the unorganized use of dyes polluting the environment

Fig.2: Unorganized use of dyes polluting the environment

Processes for removing textile dyes from water

Photo-catalysis

Photocatalysis (PC) is the speeding up of a photon induced reaction in the presence of a catalyst. In catalysed photocatalysis, light is absorbed by an absorbed substrate. It is the process in which light source is interact with surface of semiconductor materials this is photocatalysis. It produces the electron pair in conduction band and hole pair in valence band when the catalyst interacts with light of sufficient energy.

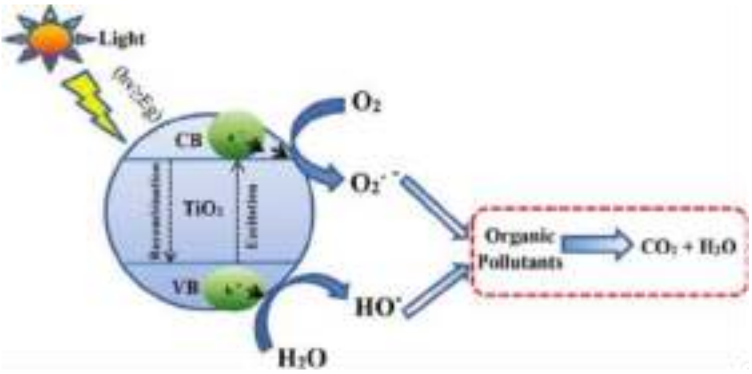


Fig.3: Schematics of basic photocatalysis process

It is to be noted that it is the one of the best solutions for producing H_2 from the water and to remove the organic pollutant material from the environment by the use of sunlight. TiO_2 is the best and cheaper nanomaterial for the process photocatalysis. **Fig.3** shows the basic catalysis process schematically

As we discuss above, the photocatalysis is produce electron-hole pair when a photocatalyst absorb photons. When the light is illuminated the electrons becomes excited which are present in the valence band. These excited electrons thus transfer excess energy to the electrons reciding in the conduction band of the catalyst creating electron hole pair through the process called photo excitation. The electron and hole which are produced react with the absorbed oxygen and water on the surface of catalysis to form reactive oxidizing molecules that again react with the pollutants and oxidize into Carbon Dioxide and H_2O through the few intermediate steps. The photochemical reaction does not modify the catalyst, and it is not consumed by it.

Adsorption

Adsorption is the process in which the molecular species deposit on the surface. The substances which absorbed on the surface is called absorbate while the substance absorbed is called adsorbent. The adsorbed are remove from the surface of substance is called desorption. The phenomena of adsorption are surface phenomena i.e., this process takes place only on surface of adsorbent. Adsorption is affected by the temperature; this process is exothermic. In simple word, deposition of substance on the surface is known as adsorption. There are two types of adsorption on the basis of interaction force between adsorbate and adsorbent: Physical adsorption (known as physisorption) and chemical adsorption (known as chemisorption).

Adsorption study is one of the easiest processes to test the dye removal of a certain material by the process under interest. It simply requires the uniform contact between the remover and the water with contaminations for a certain time. During this contact the dyes get adsorbed onto the material and the water slowly becomes contamination free. The process depends on time and other several parameters like material itself, material shape and size, material amount, initial dye concentration, types of dyes and sometimes on the pH value of water as well. The basic laboratory process for measuring the adsorption is rather simple and doesn't differ much from that of photo-catalysis. The process simply needs a closed container and the contaminated water sample is taken into a beaker placed in magnetic stirrer. A small part of the contaminated water (may be 10 ml around) is kept before addition of the sample which will work as reference sample i.e. the sample with initial concentration of contamination. Then as stated before the sample is added to the contaminated water and thoroughly stirred in order to uniform dispersion of the sample into the water. After a certain interval (that depends on the response of the certain dye to the certain remover but may be 30 minutes for instance) a small part of the sample (may be 10 ml) is filtered and the filtrate is kept for further use. In this way the process gets continued. The qualitative confirmation of the removal performance can easily be estimated from the visual colour change of the water sample just like in the process of photo-catalysis. The quantification of the removal performance may be done with the help of a UV-Visible spectroscopy. The reason is that every dye materials have specific colors in visible range and thus all of them have sharp absorption peak somewhere in the visible region. The intensity of this peak will be decreased as per the relative presence of the dyes in the water.

Another important aspect of the entire process is the initial concentration of the dye. It has been seen that the removal efficiency of any material through adsorption is very much dependent on the initial concentration of the dye and gets decreased when the initial concentration gets higher. Now if the work is a field based work then there is no restriction on the concentration of the contaminant however for laboratory based work there is a universally accepted initial concentration and the corresponding process involves taking raw dyes then diluted it to the stock solution and further diluted it up to the test solution of suitable molarity and use it for actual experiment purpose. The detail process is as follows (though there are reports that many groups do not follow the same and set their own initial concentration level):

Adsorption Isotherm

Generally, adsorption theory is explained by isotherms. It is because the temperature plays important role during the adsorption process. There several isotherms are explained below:

Freundlich Theory

Freundlich adsorption is one of the most widely used technique to quantify the adsorption process which involves the adsorption of fluids by solid as a function of system's pressure. The expression of Freundlich theory's equation:

$$\frac{x}{m} = kP^{\frac{1}{n}} \qquad (1)$$

n>1; x = adsorbed gas mass; m= adsorbent mass; p= pressure; n= constant at a given temperature.

In above equation, taking logarithm on both sides,we get,

$$\log\frac{x}{m} = \log k + \frac{1}{n}\log P \tag{2}$$

The graph of above equation is plotted as in the below **Fig.4.**

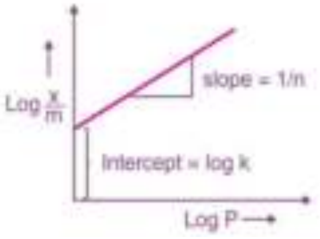


Fig.4: Graphical representation of Freundlich isotherm

Langmuir theory

This theory was proposed in 1916 by Irving Langmuir. He proposed that adsorption of a gas on the solid surface one by one at a particular site of preference. It’s predicted that all adsorption sites are identical and the molecule of gas show the ability to bind with one site which is independent of may or may not occupied the neighbouring sites. It's also expected that there's a dynamic equilibrium between adsorbed and non-adsorbed gas molecules. A linear adsorption as well as maximum surface coverage is predicted by Langmuir isotherm especially at low adsorption densities.

Adsorption Mechanism

The situation on the surface edge of any material is not the same as the situation in interior. For example, molecules in a liquid's interior are entirely surrounded on all sides by other molecules and therefore the molecules exerted intermolecular force in all direction shown in below figure (a). Schematics of adsorption mechanism has been shown in **Fig.5**

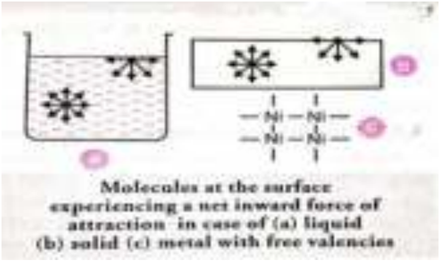


Fig.5: Schematics of adsorption mechanism

Since, the molecule on the surface of liquid is surrounded by a large molecule in the liquid phase and some molecules in the vapour phase that is at the surface of liquid. From this, the molecule, at the surface of liquid experience some attraction force (say inward direction force) which may due to the surface tension. So, the force of attraction is experience by the molecule at the surface of solid shows in figure (b). Besides this, in case of some solid like transition metal (say Nickel), there are no utilize of free valencies at the surface which show in figure (c). Liquids and solids have the ability of attracting molecules of other substances come into contact due to residual inward direction force of attraction or some free vacancies at the surface.

Introduction to Graphitic Carbon Nitride (g-CN)

The general formula of g-CN is g-C3N4. It is material that contains carbon, nitrogen and little hydrogen as impurity. These are connected through tris- triazine-based pattern. It is very important organic material which is used mostly as semiconductors. It is an allotropes of carbon nitride with very high stability due to its unique structure and is hard than the other carbon nitride and also show chemical stability at more than temperature 500 centigrade. It is a novel nanomaterial which has many uses in solve the problem of environmental pollution and also used for water filtrations. It has some unique optical properties that make it a material of high potential in the field of opto-electronics. The colour of the crystals of graphitic carbon nitride is pale yellow.

There are two structures are proposed by the scientists which act as smallest building unit of g-CN. In one type g-CN is made of triazine and the other is made of the tris-s-triazine as shown in **Fig.6**. The red dotted parts show in figure (a) & (b) the basic unit of the graphitic carbon nitride: - Triazine and Tri-s-Triazine (Heptazine) respectively. The structure of Graphitic Carbon Nitride with the Tri-S-Triazine is most stable than the structure with the triazine so Tri-S-Triazine is most accepted as the basic unit of Graphitic Carbon Nitride.

Preparation of g-CN

The building block of g-CN is developed by reaction between cyanamide, dicyandiamide and bases. The first off shaped chemical compound C_3N_4 structure, melon, with pendant amino teams, may even be extremely ordered chemical compound any reaction which leads to additional condensed and there are defects in few C_3N_4 molecule, connected through tri-s-triazine (C_6N_7) units.

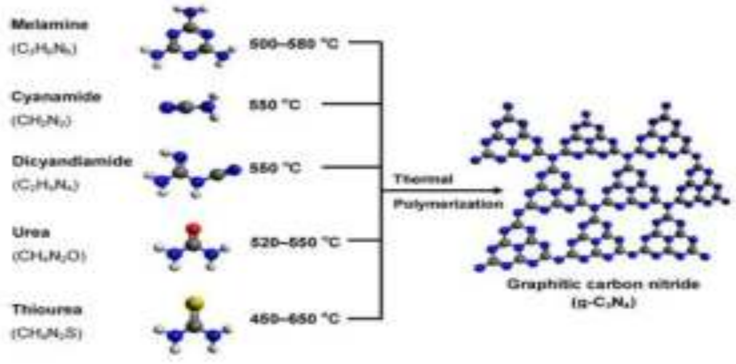


Fig.6: Basic techniques for synthesizing g-CN

Graphitic carbon contains mainly carbon and nitrogen. It is very stable polymeric semiconductor. There are many ways to synthesize g-C_3N_4. It is prepared by condensation at high temperature with nitrogen rich organic compound such as melamine, urea etc. and the method to prepare g-C_3N_4 are given below:

In below Image (**Fig.6**) there are presently several methods to prepare g-C_3N_4 by heating nitrogen rich organic compound at high temperature and undergo thermal polymerization then we get g-C_3N_4.Melamine is used as a cheap single source of the synthesis of g-CN by thermal condensation of melamine. This method is low cost and effective alternative which can help to produce g-C_3N_4 on large scale. Other method of synthesizing g-CN involves reaction between $C_3N_3Cl_3$ and $NaNH_2$ at a temperature as low as 200 ^{o}C for around 10 h or electro- deposition of suitable precursor on silicon substrate.

Properties of g-C3N4

Metal free catalyst: From the very beginning g-CN being a metal free catalyst, attracted the interest of researchers. The material contains only C and N with small amount of H as defects. Optical properties: The optical properties of g-CN are studied in details by employ UV-Vis DSR and PL spectroscopy. g-CN absorption pattern similar to organic compound with optical gap around 2.07 and thus an adsorption edge at around 420 nm. Stability: By the analysis of thermogravimetric of graphitic carbon nitride, this material shows the stability up to the 600°C. Due to this property of GCN is used as heterogenous catalysis under extreme condition.Graphitic Carbon Nitride is highly porous material unlike graphene. It is non-toxic, low-cost, metal free element.

Application of g-CN

g-CN shows fascinating optical and other properties as well as excellent chemical and thermal stability. It is material of low cost and high yield and found its application in many purposes such as photocatalyst, for sensing, for imaging, for g-C3N4 based LED, etc.It is commercially available in market by the name of brand-Nicanite. As per the report it is best storage material to store hydrogen. Due to it micro sized graphitic form it is used for coating such as tribological, biocompatible medical, chemically inert etc. and it is used for coating insulators. It is also used for the energy battery storage. Carbon Nitrides has special properties of semiconductor, with very good catalytic efficiencies. There are important applications are stated as follows:

(a) Carbons Nitride can shows photocatalysis and thus give rise water splitting. (b) g-CN acts as a catalyst for oxidation reaction. (c) Carbon Nitride has applications in Hydrogenation reactions. (d) Carbon Nitride can act as a basic catalyst. (e) Carbon Nitride has application in NO decomposition. (f) Carbon Nitride can activate π-bonds and Aromatic systems.

Conclusion

In this work I have tried to summarize the extensive applications of g-CN in the areas of water purification. It has been shown that g-CN is one of the most effective materials in the field of removal of dye from water and thus in water purification. In this context, along with the reported result from other workers few of our mentor's own experimental data has been shown that have more rigidly established our claim. Adsorption properties of Graphitic carbon nitride has been shown that it is one of the best nanomaterial to remove organic pollutants. In all the cases, the material shows its efficient properties. All these results as summarized here clearly indicated that researchers should put systematic effort to think about the development of Graphitic Carbon Nitride based water filter and adsorption that they will certainly be as effective as any of the currently used material with further advantages in its easy and cost-effective technique.

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Prescription trend of third generation Cephalosporins

Abstract

Cephalosporins are antibiotics which are used to cure gram-negative and gram-positive bacteria and effective as amoxicillin, cefaclor, amoxicillin/clavulanate. Cephalosporins have been linked to alteration of infant's gastrointestinal flora, leading in diarrhoea or thrush, but these impacts not studied thoroughly. It's against Pseudomonas and has very little effect on Staphylococcus aureus and clearance &half-life is 3hr, which allows for twice-daily administration or, in many circumstances, once-daily administration. Cefixime, a novel oral cephalosporin, has a higher antibacterial activity against Enterobacteriaceae than other oral cephalosporins.

Keywords: Cephalosporins, Cefixime, amoxicillin, diarrhea, Enterobacteriaceae

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Introduction

Because their broad host range, clinically demonstrated effectiveness, safety profile, excellent pharmacokinetics, and fewer side effects, 3rd generation cephalosporins are commonly recommended antibiotics (Klein NC, et al. 1999). 3rd cephalosporins are antibiotics which are used to cure gram-negative and gram-positive bacteria (Arumugham VB, et al., 2021).Third cephalosporins outperform other cephalosporins in terms of potency, antimicrobial spectrum, and pharmacologic profile. Escherichia coli, K. pneumoniae, and Proteus strains resistant to aminoglycosides, anti-Pseudomonas amoxicillin, and other cephalosporins are all vulnerable (Donowitz GR, et al., 1989). 3rd cephalosporins are a significant but limited medicinal advance in the arsenal of infectious disease drugs. Their enhanced spectrum of activity, very low MICs for most sensitive organisms, greater price, and to a lesser extent their pharmacokinetic characteristics set them apart from the first and second class cephalosporins (Cunha BA, et al. 1982).

However, practitioners who see the six antibiotics that make up this class as interchangeable face a challenge when choosing third-generation cephalosporins. The antimicrobial spectrum, as well as other criteria like developing resistance and cost, should all be considered when selecting a medicine. The characteristics of parenteral third-generation cephalosporins are the subject of this review. Such discrepancies suggest that the handy "generation" classification scheme for cephalosporin antibiotics should be phased out in favour of a system that facilitates detection of clinically essential aspects of each agent in these diverse classes of antimicrobial agents (Cunha BA.1992)

Ceftriaxone

When taken parenterally and in large dosages, ceftriaxone, a 3rd cephalosporin antibiotic, has been linked to the development of biliary sludge and biliary colic. Ceftriaxone is also linked to rare cases of immunoallergic hepatitis, most commonly cholestatic hepatitis, which is comparable to the harm caused by other cephalosporins (Bethesda 2012).Rocephin is just a brand name for ceftriaxone, which is marketed in a parenteral format.It can be administered intravenously or intramuscularly and is licenced for the treatment of moderate-to-severe bacterial infections caused by pathogenic organisms (Drugs and Lactation Database 2005).

Biliary sludge and hyperbilirubinemia associated with ceftriaxone

Ceftriaxone is a relatively safe antibiotic; nonetheless, rare cases of symptomatic biliary sludge have been observed, the majority of which have included children. Improvements in laboratory indices, such as bilirubin levels, are unusual with ceftriaxone (Bickford CL, et al., 2005)

Cefotaxime

Cefotaxime sodium is an injectable cephalosporin antibiotic that works by inhibiting the formation of bacterial cell walls (Le Frock JL, et al., 19882).Cefotaxime is more effective against Enterobacteriaceae than some other 1st- and 2nd-generation cephalosporins.Although it is more efficient than prior cephalosporins against Pseudomonas aeruginosa and Acinetobacter spp., most bacteria remain resistant (Dudley MN, et al. 1982). Cefotaxime is taken Twice to three times a day, i.v or intramuscular injections, at a dose of 1 to 6 g per day. The usual dose for urinary infections is 1 to 2 g per day, 3 g/day for various mild to serious infections, and higher doses of 6 g/day for life-threatening disorders.The much more suitable regimen for severely susceptible species was 0.5 to 2g each 8–12 hours.The much more suitable regimen for severely susceptible species was 0.5 to 2g each 8–12 hours. In neonates, the dosage is normally 50 mg/kg per day, while in older infants and adolescents, the dosage is 100 to 150 mg/kg per day. For dangerous diseases such as meningitis, newborns up to 7 days of age should receive 150 to 200 mg/kg per day, and older children should receive 200 mg/kg/day. The dosage is normally given twice or three times each day. For the treatment of mild gonorrhoea, any single intramuscular injection of 1g is indicated.For surgery infection protection, a single preoperative dose of one - two gm is recommended, followed by 1–3 doses at 8-hour intervals postoperatively.. In individuals with a creatinine clearance of less than 10 mL/min, the dosage should be reduced by half while the frequency must be maintained (Todd PA, et al. 1990)

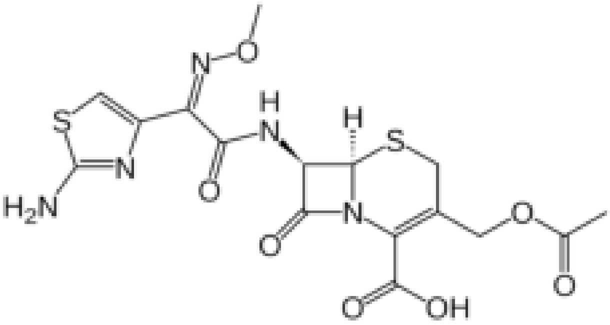

Fig.1. Structure ofCefotaxime

Antibacterial Activity: In vitro, cefotaxime kills the both types of microorganism gram-positive and microorganisms. Cefotaxime is as effective as benzyl penicillin towards Streptococcus pneumoniae and Streptococcus pyogenes, but it is also effective against lactams and multidrug-resistant Streptococcus pneumoniae strains. Cefotaxime, like some other cephalosporins, has weak action against enterococci (including Streptococcus faecalis). Low quantities of cefotaxime suppress beta - lactams and -resistant Staphylococcus aureus strains, however cephalothin and cefamandole are more effective against this species. Cefotaxime is equivalent to cefoperazone against S. aureus, but much more effective than cefoperazone against streptococci in generally, and also more active than moxalactam against any and all Gram-positive bacteria when comparing to other 'third generation' cephalosporins (Carmine AA, et al. 1983)

Pharmacokinetics: Cefotaxime plasma level typically range around 81 and 102 g/ml after a 1000 mg intravenous infusion. Plasma levels of 38 and 200 g/ml are achieved with 500mg and 2000mg dosing, respectively. After receiving 1000mg intravenously and 500mg intramuscular injections for 10 or 14 days, there is no buildup (Carmine AA, et al. 1983).

Cefpodoxime

Cefpodoximeproxetil is a 3rd cephalosporin antibiotic that can be used orally. In vitro efficacy against a wide spectrum of Gram-positive and Gram-negative germs associated with common paediatric diseases has been demonstrated, making it a viable empirical therapeutic option (Fulton B, et al. 2001).Cefpodoxime was proven to be as effective as amoxicillin, cefaclor, amoxicillin/clavulanate, and penicillin in treating respiratory and urinary tract infections in clinical trials. Although no comparison studies have been conducted, it appears to be beneficial in the treatment of skin infections. Cefpodoxime is very well tolerated by toddlers and useful in the therapy of pharyngitis and otitis media. It has a profile of side effects that is comparable to that of other penicillins and cephalosporins, with the most prevalent side effects being gastric ulcer (Chocas EC, et al. 1993)

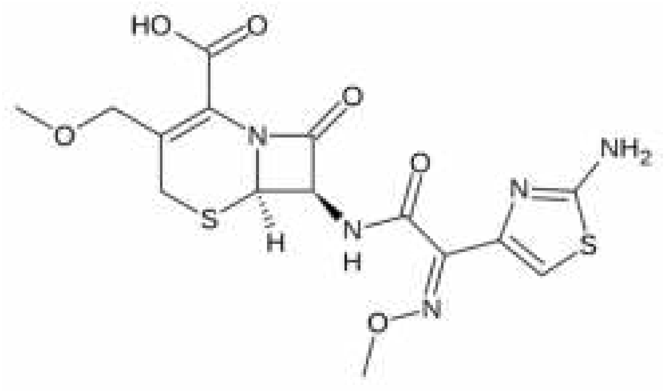

Fig.2. Structure of Cefpodoxime

Ceftazidime

Ceftazidime-avibactam (Zavicefta®) is a combo of ceftazidime, a third cephalosporin, and avibactam, a novel non-lactam-lactamase blocker, administered intravenously (Shirley M. et al., 2018).

According to the limited information available, ceftazidime creates minimal quantities in milk that are unlikely to cause harm to breastfed babies. Cephalosporins have been linked to alteration of the infant's gastrointestinal flora, leading in diarrhoea or thrush, but these impacts have not been thoroughly studied. Ceftazidime is safe to take when breastfeeding (Drugs and Lactation Database 2006)

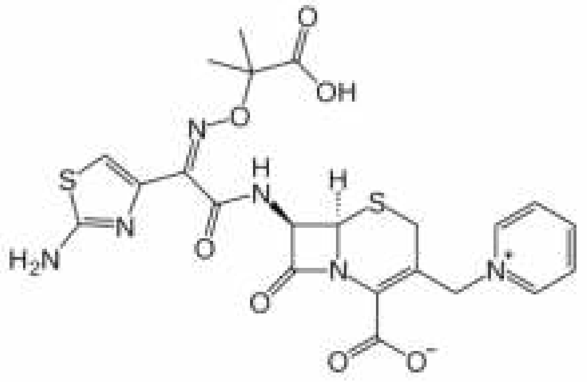

Fig.3. Structure of Ceftazidime

Ceftibuten

Ceftibuten is a 3rd cephalosporin that is orally active and has strong microbiologic action againstmicroorganisms that are gram-negative and gram-positive.It can withstand extended-spectrum beta-lactamases induced by plasmids. Ceftibuten has been demonstrated to be effective in the treatment of upper and lower respiratory utis, as well as complex and simple infections in both adults and children, despite the fact that these are not recognized indications. After oral treatment, it is rapidly absorbed (75-90 percent), with peak serum levels of 17 microg/ml in healthy volunteers.Healthy volunteers have a ½ of 2.5 hours, while older people have a half-life of 3.2 hours.Dose must be changed if creatinine clearance decreases below 50 ml/minute. The medicine has a positive safety profile that is equal to that of most some cephalosporins (Owens RC, et al. 1997)

Ceftibuten, an oral expanded-spectrum cephalosporin, is efficient against a wide range of bacteria, both gram-positive and gram-negative, including Streptococcus pneumoniae, Streptococcus pyogenes, Moraxella catarrhalis, and Haemophilusinfluenzae. Most common beta-lactamases are unable to hydrolyze ceftibuten. Ceftibuten is swiftly and almost totally absorbed from the gastrointestinal tract, it is the majority of it is eliminated unaltered in the kidneys. Ceftibuten has a half-life of little more than 2 hours in the body (Guay DR, et al. 1997)

In clinical studies, 1312 paediatric patients were given ceftibuten suspension at a dose of 9 mg/kg per daily, with a maximum daily dose of 400 mg. In 1152 people, negative emotionality were gathered by voluntarily reports from clinicians based on direct inspections, parental and/or patient comments. In addition to volunteer reports, gastrointestinal unpleasant events were elicited from 160 participants at each visit (Reidenberg BE. 1995)

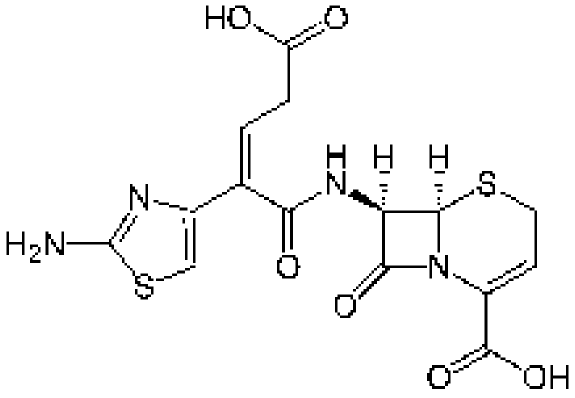

Fig.4. Structure of Ceftibuten

Ceftibuten is detected in breast milk at low doses and is unlikely to damage breastfed infants. Cephalosporins have been linked to alteration of the infant's gut flora, leading in diarrhoea or thrush, but these impacts have not been thoroughly studied. Ceftibuten is safe to take during nursing (Drugs and Lactation Database, 2021)

Ceftizoxime

Ceftizoxime is a third-generation cephalosporin that is administered intravenously. Ceftizoximenot performs invitroactivity against gram-negative bacteria. Richards DM, et al. 1985). Apart from Streptococcus faecalis, most Enterobacteriaceae and streptococcal organisms are inhibited by a concentration of less than or equal to 1 microgram/ml. By 3-8 micrograms/ml, methicillin-resistant Staphylococcus aureus is repressed, whereas methicillin-resistant Staphylococcus aureus is tolerant. Bacteroides fragilis is suppressed at a concentration of 16-64 micrograms/ml. At commonly accessible quantities, it inhibits Pseudomonas aeruginosa (Neu HC, et al. 1984)

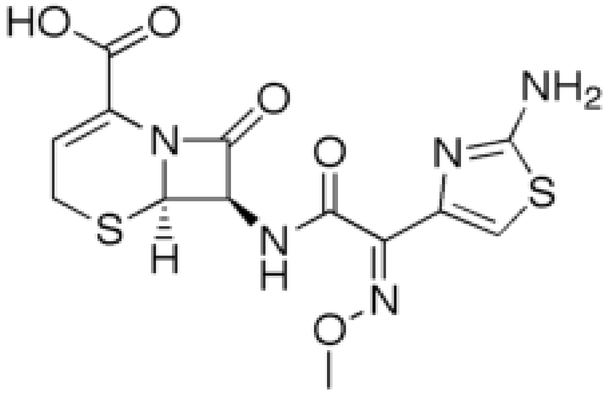

Fig.5. Structure of Ceftizoxime

It is excreted by the kidneys and has a half-life related to ceftizoxime, cefoperazone, as moxalactam. Ceftazidime has the same effectiveness and safety as that of the rest of the carbapenems, and it hasn't been found to affect prothrombin or cause the disulfuram response asmoxalactam and cefoperazone (Yost RL, et al. 1985)

Cefixime

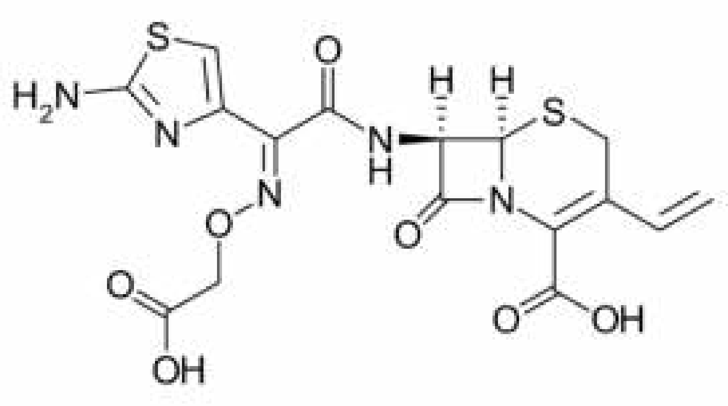

Fig.6. Structure of Cefixime

Cefixime, a novel oral cephalosporin, has a higher antibacterial activity against enterobacteriaceae than other oral cephalosporins. The kidneys discharge around 20% of the medication as active drug. As a result, cefixime medication for (UTI) may be a viable option (Naber KG, et al. 1990)

It's quite good at fighting H. influenzae and other Enterobacteriaceae. It is present in Streptococcus pyogenes, Streptococcus pneumoniae, and Branhamellacatarrhalis and is resistant to digestion by various beta-lactamases. Cefixime is inert against Pseudomonas and has very little effect on Staphylococcus aureus.Cefixime is distinguished by its three-hour excretion half-life, which allows for twice-daily administration or, in many circumstances, once-daily administration.Cefixime 200 to 400 mg per day, given as a single dose or in two divided doses, has clinical and microbiological efficacy comparable to various daily dosages of co-trimoxazole or amoxycillin, as well as amoxycillin, amoxycillin/clavulanic acid, and cefaclor in acute uncomplicated utility (Brogden RN, et al. 1989)

In comparison studies, cefixime was found to be as effective as amoxicillin +/- clavulanic acid, cefaclor, cefalexin, cefuroxime axetil, and clarithromycin. Preliminary data from trials evaluating the efficacy of cefixime as an oral component of an iv to orally changeover treatment have been positive, but further well-conducted trials are needed (Markham A, et al. 1995)

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Dielectric Behaviour of 2-Butanone with Dichloromethane, 1, 2-Dichloroethane and Tetrachloroethene

Abstract
The experimental data for ε (relative permittivities) and n (refractive indices), were measured for mixtures of 2-butanone (BN) ($CH_3COCH_2CH_3$) with dichloromethane (CH_2Cl_2), 1,2-dichIoroethane ($CH_2Cl.CH_2Cl$) and tetrachloroethene (CCl_2CCl_2) at the temperature 308.15 K. The values of $\Delta\varepsilon$ which represent the departures of the ε for the mixtures from the quantities occuring from the law achieved from mole fraction mixture, have been obtained. Calculated values of $\Delta\varepsilon$ shows positive sign for BN with CH_2Cl_2 and $CH_2Cl.CH_2Cl$, whereas it is negative in the case of BN with CCl_2CCl_2.

Keywords: 2-butanone, relative permittivity, dichloromethane, hydrogen bonding, dekameter

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Introduction

The studies of mixtures of 2-butanone with CH_2Cl_2 and $CH_2Cl.CH_2Cl$ and tetrachloroethene (CCl_2CCl_2) helps to make clear its structural arrangements at the molecular level. A literature investigation unconcealed that in depth readings regarding the properties of these systems haven't been created. Relative permittivities measurements (Nath J et.al,1984, 1985,1989) are familiar to offer reliable information regarding the occurence of specific interactions. The particular interaction of $CH_3COCH_2CH_3$, with these are because of the presence of non-bonding pair of electrons on the O atom of $CH_3COCH_2CH_3$, thus it will perform as n-donor toward these chloro-compounds. $CC1_2CC1_2$ will perform as σ -type acceptors in the direction of 2-butanone, whereas CH_2Cl_2 and $CH_2Cl.CH_2Cl$ will also perform as σ-acceptors toward, and be concerned within the creation of H- bond with, 2-butanone. Since, the values of n, is also an investigative of the degree of association of molecules in their mixtures, and thus give some information on the character of the particular interaction between the elements. So as to analyze the molecular orientations and interactions occurring in contrast to species of the binary mixtures, relative permittivity measurements of mixtures of CH3COC2H5 with CH_2Cl_2, $CH_2Cl.CH_2Cl$ and $CC1_2CC1_2$ have been made at 308.15 K. The results are interpreted in this article.

Experimental Details

$CH_3COC_2H_5$ was distilled over potassium permanganate, dried over K_2CO_3 and then made fractional distillation. Methylene dichloride was shaken with water and sodium carbonate solution, dried over Calcium Chloride and then purified by fractional distillation. 1,2-Dichloroethane was shaken with dilute KOH and water, dried over $CaCl_2$ and obtained through fractional distillation. Tetrachloroethene (CCl_2CCl_2) was purified as given elsewhere(Nath J,Saini R,1989). The densities of purified samples were measured at 308.15K with a densimeter

(Patil KR et.al.1990) . The observed values of density for all these compounds are in excellent concurrence with the literature data(Riddick & Bunger,1970).

Method

Experimental procedures for Measurements of the relative permittivity are given elsewhere(Nath J,Tripathi AD.1984). The measured values of ε, for the uncontaminated liquids of BN, CH_2Cl_2 $CH_2Cl.CH_2Cl$ and tetrachloroethene (CCl_2CCl_2) and for binary mixtures of BN with CH_2Cl_2 and $CH_2Cl.CH_2Cl$ and tetrachloroethene (CCl_2CCl_2) at 30^0C are collected in Table 2, where x1 represents the mole fraction of BN. The measured values of ε obtained for CH_2Cl_2 $CH_2Cl.CH_2Cl$ and tetrachloroethene (CCl_2CCl_2) are 8.622, 10.078 and 2.294 respectively ,in close agreement with the available literature data (Timmermans,1950;McClellan,1965). The value for ε for 2-butanone was found to be 17.65 which is based on the available literature data (Timmermans,1950).

Results and Discussion

The values of ε for the different systems are utilized for calculating the parameter $\Delta\varepsilon$, which is the departure of ε of the mixture from ideality by using the the equation

$$\Delta\varepsilon = \varepsilon_{12} - \varepsilon_1 x_1 - \varepsilon_2 x_2 \text{-------------------------------------}(1)$$

where ε_1 and ε_2 are the dielectric constants (relative permittivities) of the two uncontaminated components, and ε_{12}**,** is the dielectric constant of the mixture. A plot between $\Delta\varepsilon$ and x_1 **is** plotted in Fig.1**,** it can be seen that positive deviation is observed for the system BN+ CH_2Cl_2 and + $CH_2Cl.CH_2Cl$, and negative for BN+ CCl_2CCl_2 system in the liquid state. The negative deviation for the system BN+ CCl_2CCl_2 can be pointed out because of a decline in the degree of coalition of the dipoles with changing composition . The negative values of $\Delta\varepsilon$ arise in the mixtures having molecules, which are unlike in shape as well as size, thus such type of deviations reveal presence of geometric effects. The creation of a complex species, for negative $\Delta\varepsilon$ will be at the minima of Fig.1. Therefore, the minima in the $\Delta\varepsilon$ is an indication of a greatest in the structuredness between unlike components in the mixture as in the case of BN+ CCl_2CCl_2 system in the liquid state.

The interaction between BN+ CCl_2CCl_2 can be thought of due to a presence of charge-transfer complex formation of CCl2CCl2 with the nonbonding electrons of BN. The complexation of CH_2Cl_2 and $CH_2Cl.CH_2Cl$ are due to H atom of these compounds with the nonbonding electrons on O atom of BN, which results high positive values of $\Delta\varepsilon$ values in the liquid state.

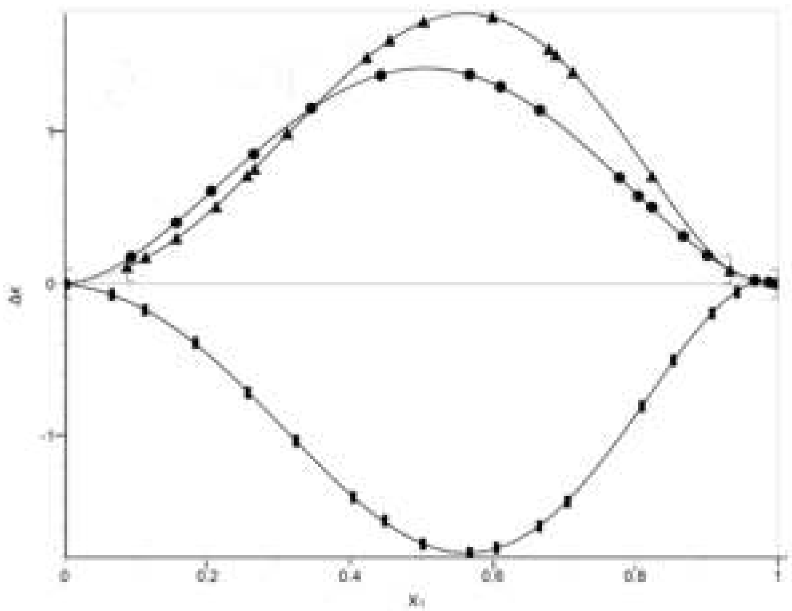

Fig. 1. Plot of Δε vs mole fraction of 2-butanone, x_1, for the various Systems ● , 2-butanone-CH2C12, ; ▲, 2-butanone-CH2C1 CH2C1; ■2-butanone-CCl2CC12 at 308.15 K.

Also there is formation of charge transfer complex between BN and CH_2Cl_2 or $CH_2Cl.CH_2Cl$ because of interaction of Cl atom via O atom. The positive values of Δε, indicates strong interactions. The chief part to the deviation from ideal mixtures is because of the specific interactions, interaction due to the dipole-dipole ,H-bond formation trend between components.

Table 1. Experimental values of Relative permittivities, ε,deviation of relative Permittivities, Δε , for the various mixtures of 2-Butanone at 308.15 K

2-butanone + CH_2Cl_2			2-butanone +CH_2ClCH_2Cl			2-butanone +CCl_2CCl_2		
X1	ε	Δε	X1	ε	Δε	X1	ε	Δε
0.0000	8.622		0.0000	10.078		0.0000	2.294	
0.0932	9.641	0.176	0.0874	10.851	0.11	0.0662	3.24	-0.071
0.1567	10.441	0.403	0.1132	11.109	0.174	0.1122	3.845	-0.172
0.2056	11.091	0.611	0.1567	11.563	0.298	0.1834	4.723	-0.388
0.2654	11.872	0.853	0.2122	12.191	0.506	0.2567	5.521	-0.717
0.3458	12.901	1.156	0.2557	12.724	0.709	0.3244	6.242	-1.034
0.4432	13.998	1.373	0.2665	12.557	0.754	0.4044	7.111	-1.405
0.5678	15.126	1.376	0.3122	13.432	0.989	0.4487	7.626	-1.560
0.6112	15.44	1.298	0.4234	14.768	1.487	0.5022	8.293	-1.714

0.6663	15.782	1.143	0.4555	15.131	1.603	0.5678	9.241	-1.774
0.7782	16.348	0.698	0.5034	15.614	1.723	0.6054	9.852	-1.740
0.8045	16.465	0.578	0.5998	16.375	1.754	0.6654	10.918	-1.596
0.8234	16.563	0.505	0.6789	16.775	1.545	0.7045	11.679	-1.435
0.8675	16.908	0.313	0.6889	16.801	1.505	0.8095	13.922	-0.805
0.9013	16.949	0.187	0.7123	16.872	1.392	0.8533	14.897	-0.503
0.9678	17.383	0.021	0.8234	17.022	0.707	0.9078	16.043	-0.194
0.9876	17.551	0.010	0.9331	17.235	0.089	0.9432	16.727	-0.054
1.0000	17.653		1.0000	17.653		1.0000	17.653	

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Assessment of Drinking-water Quality in and around Moradabad

Abstract
Measurements of Calcium, Magnesium, total hardness, dissolved carbon dioxide ,and chloride have been made titrimetrically for drinking water collected from three places (TMU Moradabad, Gajraula and Najibabad). The results obtained have been compared with the standard values provided by Indian standards (BIS), and WHO for drinking water.

Keywords: Titration, calcium, hardness, indicator, WHO.

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Introduction

Many regions of India are stricken by water pollution and microbial water-sure impurities. The accelerated demand on water suppliers has regularly lead to water this is not worthy for human consumption, being inadvertently furnished to your faucet. This is regularly the case in lots of smaller towns in the course of India. Where river water is fed on: upstream infection, via sewerage and human use (washing of garments etc.) is a vital consideration for water nice.

Issues approximately non-public and circle of relative's fitness may also lead you to question the protection of the water you are using. Current exposure approximately water pollutants problems and their impact on water used inside the domestic for ingesting, cooking, washing and plenty of other functions. You will be particularly worried about the first-class of your drinking water if you rely upon your borehole or different personal water deliver. With the availability of modern-day water treatment system and the frequently competitive advertising of these gadgets, you could marvel about the need to install such system in your private home and what if something some of these filters do. Agricultural water necessities are frequently unnoticed. Suitable water leads to progressed cattle manufacturing.

In step with principal pollution manage board, ninety% of the water delivered in india to the metropolis and towns is polluted, from which handiest 1.6% receives handled. Consequently, water best control is necessity for the individual wellbeing (Gupta,1991; Madhuri et al.2004).

If water is badly polluted like raw sewage it might be apparent from its look or smell. It might be coloured or opaque (cloudy), or have hard, grease, or foam floating on it. Pretty a few dead fish floating at the surface of a lake could be a clean sign that some element changed into incorrect.

However a lot of dangerous and useful materials in water are unseen and fragrance-free. On the way to move away from the plain to decide what substances are inside the water and how much we require, analysis must be conducted. Evaluation of herbal frame of water tells us how easy or polluted it's far. If there may be harm to flora and fauna, the size will assist locate the case and the cause? Where water is purified (e.g. a wastewater cure plant), analysis are essential for tracking the effectiveness of the treatment approaches. Within the united nation the smooth waste act required waste water discharge to have permit. These permit set limits on the quantities of specific pollution that may discharge, as well as schedule for monitoring and reporting the result handiest standard analytical manner exact inside the-"code of federal law" can be used in order that the government organizations can feel reasonably assured that end result from distinct laboratories are comparable.

Similar consideration practice to ingesting water. The purity of the water we drink is more problem to the common individual then the excellent of the waste discharge via sewage plant. However we need to now not forget then in lots of places especially alongside a river on, towns waste water discharge may be part of next city's water supply.

Methods and Sample collection

Estimation of Calcium, Magnesium, total hardness, dissolved carbon dioxide ,and chloride have been made titrimetrically. The samples were taken directly from tap of above mentioned places, with the help of preferred strategies and techniques of sampling (APHA,1995, Merck,1974).Water samples were obtained directly from the tap used for drinking purpose.

Experimental

Titrimetric method

Chemicals used were of moisture free, Analar Reagent grade with stated purities of +99 % . Ethylene diamine tetrachloride salt (Aldrich), potassium iodide (Darmstadt), $Na_2S_2O_3$ (Sarabhai chemical substances co.), sodium hydroxide (Fluka), silver nitrate (SAS chemicals), hydrochloric and sulfuric acid (Qualikem) had been used in the course of analysis. Before use, chemicals were kept in a degassed oven at 120^0 C for many days and used as such. Stock solutions have been obtained by means of the use of double-distilled, but formerly deionized, water at some point of the experimental analysis. The concentrations have been decided by using density dimension the usage of a densimeter as given elsewhere(patil et.al.1990). The repeatability of the concentration measurements turned into inside 0.28 percent.

Overall hardness became decided by way of measuring 20 cc of consuming water and delivered five ml of buffer solution(pH=10), after which three-four drops of E.B.T. indicator added and titration carried out with 0.01M EDTA solution .At the quit point the answer modifications from wine pink to blue.

For estimation of calcium, 20 ml of water sample with 2-3cc of buffer solution (NH_3+NH_4Cl) and added three-four drops of E.B.T. indicator .The whole solution become titrated with 0.01M ethylene diammine tetra acetic acid (EDTA) solution. Ultimately calculated strength of calcium found in water sample. . The solution turns from crimson to blue at the end factor. For estimation of Mg^{+2}, same process is followed as within the estimation of calcium ions)in the water sample. For making ready buffer solutions (pH=10), 3.2 gm of ammonium chloride is blended with 29 ml of ammonia solution and diluted to 50 ml. For finding Cl^- (chloride ion), 15cc of ingesting water was used and delivered 5 drops of indicator(fluorescein), and the titration is performed with the 0.001 M silver nitrate solution. The AgCl coagulates, and the precipitate obtains a red or purple color on the end point. For dissolved CO_2, water is blended with 3-4 drops of phenolphthalein indicator, and titrated with NaOH solution (N/50).

For getting total hardness, same procedure is adopted as in the estimation of calcium ions in the water sample.

Calculation

The molarity of unknown sample of water (M1) was calculated by means of following formula:

M1V1=M2V2, where V1 and V2 denotes the volume of water and EDTA solution and M2 for molarity of solution used in the burette. Once you have molarity by using titrimetric evaluation, the strength was obtained by means of the use of following formula:

$$\text{Strength} = \text{Mol.weight x Molarity(g/l)}$$

In this way strength of Ca, Mg, CO_2, chloride and total hardness are obtained. Molecular weight of calcium, magnesium, carbon dioxide and chloride used were 40, 24.3, 44 and 35.5 respectively. For calculation of strength of total hardness, molecular weight equal to 100 is taken.

Table 1: Physico – chemical parameter*(Carbon dioxide, Ca^2, Mg^{2+}, Cl^- and total hardness) of tapwater samples of three Districts, U.P., India, in July-2021.

Sampling Source	Carbon dioxide	Ca^{2+}	Mg^{2+}	Total Hardness	Cl^-
Gajraula	10.31	81.55	17.1	121	12.66
Najibabad	11.66	67.33	16.2	131	25.99
TMU Moradabad	12.04	78.23	24.6	141	26.38

* all parameters are in ppm.

Results and discussion

Table1 contains results calculated for different parameters for tapwater samples. These parameters were compared with the standards in **Table2**.

From these results, it is observed that due to boom in industrialization, quality of drinking water get decreases, and consequently proper analysis of tap-water is required.

Table 2: Comparison of our results of tapwater of three samples of concerned region with intake water quality standards*

Parameter	Sample Range (lowest limit) & (upper limit)	Beaurow of Indian Standard		World Health Organization Limit(ppm)
		lower limit	upper limit	
Total hardness	121 141	300	600	100
Calcium	78.23 81.55	75	200	75
Magnesium	17.1 24.6	30	100	150
Carbon dioxide	10.31 12.04	-	-	-
Chloride	12.66 26.38	250	1000	250

*Unit in ppm.

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Original Article

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Excess molar enthalpies of dichloromethane +cyclopentanone or + n-dibutyl ether or + Acetone or + dimethyl sulfoxide at the temperature 303.15 K

Abstract

Excess molar enthalpies H^E at T= 303.15 K have been determined for dichloromethane (CH_2Cl_2) (DCM)+ cyclopentanone ((CH2)$_4$CO) or + di-n-butyl ether ($C_8H_{18}O$) or + acetone $(CH_3)_2CO$ or + dimethyl sulfoxide (DMSO) ($(CH_3)_2SO$). The values of H^E for all the systems are exothermic in nature. The values of H^E of the different systems have been fitted with the Redlich-Kister equation with the help of the least squares method. Excess molar enthalpies data represent the occurrence of specific interactions between the components in the liquid state.

Keywords: CH_2Cl_2, cyclopentanone, Microcalorimeter, acetone, Binary mixture

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Introduction

The cyclic ketone, cyclopentanone, Dibutyl ether , Acetone, or Propanone, Dimethyl sulfoxide and Dichloromethane are colorless liquids. Dibutyl ether is immiscible with water, but miscible with acetone and many organic solvents. Due to this property, dibutyl ether is used as solvent in various chemical reactions and processes.

Acetone is the smallest ketone. Dimethyl sulfoxide (DMSO) is a polar aprotic solvent which is capable of dissolving polar as well as nonpolar compounds and is soluble in many organic solvents and water, but not volatile as acetone. Dichloromethane is colorless, volatile liquid and also used as a solvent, although immiscible with water but miscible with lots of organic solvents.

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The study of cyclic or acyclic ethers, acetone or DMSO or CH_2Cl_2 is of interest due to its industrial importance, and their interactions are more exceptional, thus making them better solvents. Dichloromethane is an organic compound with the formula CH_2Cl_2, which is colorless, volatile liquid and also used as a solvent, although immiscible with water but miscible with lots of organic solvents.

Mixtures of CH_2Cl_2 with cyclopentanone ($(CH_2)_4CO$) or + di-n-butyl ether ($C_8H_{18}O$) or + acetone $(CH_3)_2CO$ or + dimethyl sulfoxide (DMSO) ($(CH_3)_2SO$) are of meticulous significance from the opinion of the existence of an electron donor-acceptor interaction which leads to the creation of intermolecular complexes between the components in the liquid form. The interaction of $(CH_2)_4CO$ or + $C_8H_{18}O$ or + $(CH_3)_2CO$ or + $(CH_3)_2SO$), can be thought of as being due to the occurrence of non-bonding pair of electrons on the oxygen atom of these compounds, on account of which it can act as an n-donors toward CH_2Cl_2, which can be engaged in the formation of hydrogen bonds with and act as a σ- acceptor toward all aforementioned compounds. We have already reported data on excess volumes, ultrasonic velocities, dielectric constants and excess enthalpies of Chloroalkanes with n-donor compounds in our earlier communications [Nath et. al., 1983, 1984, Tripathi, 1995, 2010).

A literature survey discloseed that broad studies on such systems have not been carried out. . The values of excess molar enthalpy data(H^E) are used to detect the strength of intermolecular forces such as hydrogen bonding and charge-transfer complex formation between the components in the liquid state. Hence, in the current programme, H^E measurements have been carried out for binary liquid mixtures of of CH_2Cl_2 with cyclopentanone ($(CH_2)_4CO$) or + di-n-butyl ether ($C_8H_{18}O$) or + acetone $(CH_3)_2CO$ or + dimethyl sulfoxide (DMSO) $(CH_3)_2SO$) at the temperature $T=303.15K$. The results obtained have been reported and deciphered in this paper.

Experimental Section

Dichloromethane (BDH, AR) was shaken with conc. H_2SO_4 to obtain acid layer colourless, then rinsed with H_2O, after that washed with aq. 5% sodium carbonate and then with H_2O again. The compound is predried with $CaCl_2$, and distilled over P_2O_5. Purified dichloromethane was stored away from light in a ambered bottle having $4A^0$ molecular sieves. Cyclopentanone ($(CH_2)_4CO$) or + di-n-butyl ether ($C_8H_{18}O$) or + acetone $(CH_3)_2CO$ or + dimethyl sulfoxide (DMSO) ($(CH_3)_2SO$) ,all chemicals were of AR quality and subjected to further purification by standard methods as given elsewhere (Pathak et.al.1992). These chemicals were further purified by fractional distillation and the constant middle fraction was used for the experiment. The chemicals were specified to have a minimum purity of 99.7 mol%. All the compounds were dried over freshly activated molecular sieves $4A^0$ before use. The purities of chemicals used, as determined by GLC, are more than 99%. The purities of the chemicals were also checked by measuring densities using a vibrating tube densimeter (model DMA, Anton-Paar 60/602)(Patil, Tripathi et al,1990) and found to be in good agreement with the literature values(Riddick and Bunger,1986).

Method

Excess molar enthalpies, H^E, were obtained by using a a heat flux calorimeter (C-80 model from Setaram, France) (Tripathi et.al, 2018), whose temperature was controlled to within ±0.001K. The solutions were prepared by mass. Mole fractions are accurate to ±0.0001. The reliability of the microcalorimeter was checked by measuring H^E at 298.15K for cyclohexane + hexane for which values are accurately known from the literature (Nath &Tripathi AD, 1983). The mean deviations of the measured H^E are estimated to be about 1% over most of the mole fraction range. Excess molar enthalpies, H^E, are estimated to 0.5% at the equimolar composition.

Result and Discussion

The values of H^E, for different systems are collected in Table 1 and data were put into to the following equation:

$$\frac{H^E}{J.mol^{-1}} = x_1 x_2 \sum_{i=0}^{m} A_i \, (x_{1} - x_2)^i \qquad (1)$$

In this case x_1 represents the mole fraction of CH_2Cl_2. The different parameters, and the standard deviations, σ, are collected in Table 2 . The values of standard deviation of the fit, , are obtained by means of eq.2

$$\sigma = \left[\frac{\Sigma \left(H^E - H^E_{calc} \right)^2}{(m^* - n^*)} \right]^{1/2} \qquad (2)$$

where H^E is experimental values and H^E calc refers to calculated excess enthalpy with the help of eq. (1), m* represents no. of data measured experimentally & n* is no. of constants which are distinctive of a binary system. A plot of measured values of H^E data Vs mole fractions(x1) are plotted in Fig. 1. Interference of interactions between resembling molecules and the beginning of fresh interactions between dissimilar molecules, are the main reason for the values of H^E obtained . All four systems are showing negative values of H^E because of specific interactions between the components in the liquid state. The values of H^E decrease in the order at mole fraction, x1=0.5:

Dimethyl sulfoxide >cyclopentanone>acetone >di-n-butyl ether

The etheral oxygen of dibutyl ether has a weak proton-accepting ability and creates a weak complex with DCM (H^E= -476) at x1=0.5). Acetone is a, however, better proton acceptor than dibutyl ether, as our data suggest and forms a stronger complex with DCM(H^E=-1076 at x1=0.5).The two methyl groups present on acetone increase the basicity of keto O atom.

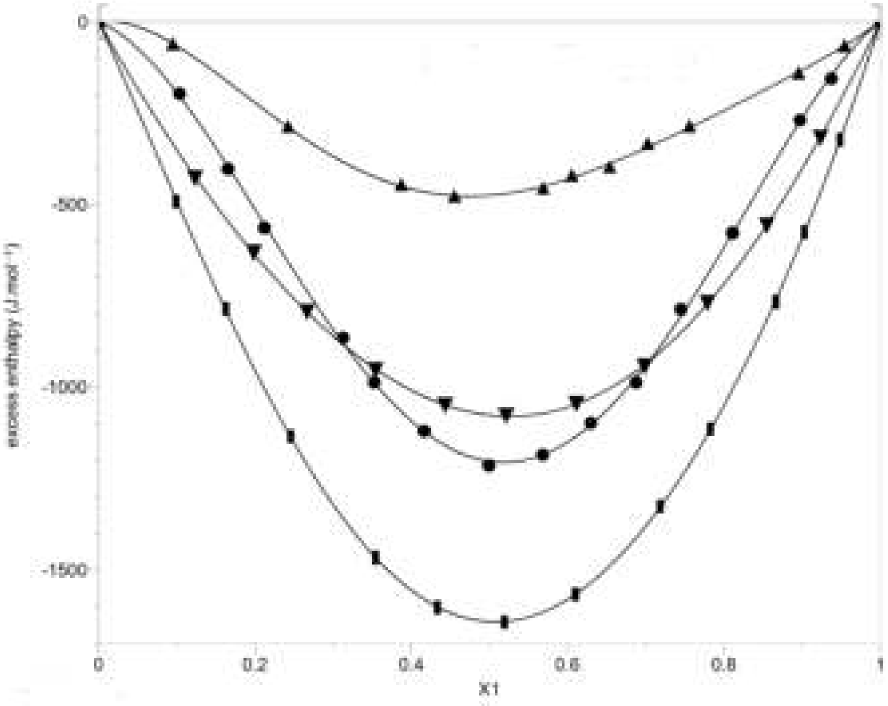

Fig. 1: Excess molar enthalpies of binary liquid mixtures of x_1 of dichloromethane (CH_2Cl_2 (1) + cyclopentanone (●) (2), + di-n-butyl ether (▲)(2) ,+acetone (▼) , (2) and + dimethyl sulfoxide (▮) (2) at the temperature 303.15 K.

The effect of saturation of the furan ring is marked and the DCM—$(CH_2)_4CO)$ system is highly exothermic (H^E= -1203 at x1=0.5). Due to the existence of hetero-molecules, this system has a high exothermic value, showing greater interactions. The hydrogen bonding in between hydrogen of DCM and the keto or ether oxygen causes interactions in such systems. Chloroform has been found to form hydrogen-bonded complexes with tetrahydrofuran and dioxane. The number of hydrogen bonds formed, the enthalpy of formation of hydrogen bonds, and other interactions are the key contributors to the value of H^E in hydrogen bond producing systems. Given that the little electronegativity difference (0.5) between O and Cl causes particular associations, a hydrogen bond-type specific interaction between the hydrogen of a keto or ether and the Cl of DCM is a significant possibility. The saturation or unsaturation of the ring determines the interactions between H atom of ketones and chloro compounds. The enthalpies of mixing in these systems are influenced not only by O - H and O - Cl interactions, but also by interactions between CH_2 Groups (as in $(CH_2)_4CO$) and Cl atoms.

The DMSO—DCM complex is vastly exothermic and -600 J/mol^{-1}(at x1=0.5) greater than the acetone—DCM complex. The structures of DMSO and $(CH_3)_2CO$ are analogous, however the S atom of DMSO has unoccupied 3d orbitals, leading electron delocalization on the neighbouring carbon atom to be enhanced. As a result, the H atoms on the CH_3 groups of DMSO become more acidic than those on the CH_3 groups of $(CH_3)_2CO$ (Solomons,1976) . The associations between DMSO and DCM are projected to be higher than with those between DCM and $(CH_3)_2CO$, resulting to the DMSO—DCM system's stronger formation of complexes and significant increase of excess enthalpy.

Table1. Excess Molar Enthalpies of dichloromethane (CH_2Cl_2) (1) + cyclopentanone (2), or + di-n-butyl ether (2), or + acetone (2), or + dimethyl sulfoxide (2) at 303.15 K

Dichloromethane(1)+ cyclopentanone (2)		**Dichloromethane(1)+ di-n-butyl ether (2)**	
x1	H^E (J.mol^{-1})	x1	H^E (J.mol^{-1})
0.1034	-197	0.0945	-61
0.1654	-403	0.2423	-287
0.2123	-564	0.3871	-446
0.3128	-865	0.4551	-478
0.3528	-987	0.5686	-456
0.4166	-1120	0.6054	-421
0.4993	-1214	0.654	-398
0.5682	-1185	0.7023	-334
0.6298	-1098	0.7561	-286
0.6876	-987	0.8956	-141
0.7452	-787	0.9543	-66
0.8113	-578		
0.8976	-269		
0.9376	-156		
Dichloromethane +acetone		**Dichloromethane +DMSO**	
x1	**H^E (J.mol^{-1})**	**x1**	**H^E (J.mol^{-1})**
-427	-427	0.0987	-491
-631	-631	0.1623	-785
-793	-793	0.2456	-1134
-952	-952	0.3541	-1466
-1049	-1049	0.4333	-1602
-1077	-1077	0.5188	-1642
-1045	-1045	0.6099	-1566
-942	-942	0.7185	-1326
-768	-768	0.7822	-1114
-556	-556	0.8666	-766
-316	-316	0.9028	-575
		0.9484	-322

Table 2. Least Squares Coefficients of Eq 1 for the Excess Molar Enthalpies, and the standard deviations ,σ,of CH_2Cl_2(1) + cyclopentanone (2), + di-n-butyl ether (2) ,+acetone , (2)and + dimethyl sulfoxide (2) at the temperature 303.15 K.

System	A0	A1	A2	A3	σ/ (J mol^{-1})
CH_2Cl_2 (1) + cyclopentanone (2)	-4812	-616.3	3554	207.9	9.7
CH_2Cl_2 (1) + di-n-butyl ether (2)	-1899	333	1249	-1238	5.9
CH_2Cl_2 (1) + acetone (2)	-4305	-485.9	191.4	210.3	2.8
CH_2Cl_2 (1) + dimethyl sulfoxide (2)	-6565	-232.5	846.5	-720.3	3.5

The interaction between cyclic ketones(>C= O) and Br- or Cl- compounds are managed by the complete saturation of their rings. $(CH_2)_5CO$ has saturated ring, which maks the interaction stronger.Thus showing higer -ve values of enthalpy of mixing as compared to dibutyl ether.

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Excess Molar Volumes for acetylene tetrachloride + 1, 4-dioxane or methyl ethyl ketone or pyridine at 308.15 K

Abstract

Excess molar volumes (V^E) of acetylene tetrachloride with 1,4-dioxane or methyl ethyl ketone or pyridine have been determined at 308.15 K and atmospheric pressure over the whole mole fraction variety with the aid of dilatometer. The effects have been conferred in terms of dipole–dipole interactions between acetylene tetrachloride and other donor atoms in the liquid state.

Keywords: Microcalorimeter, excess volume, dilatometer, least square fitting, lone pair

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Introduction

In our previous paper (Tripathi AD et al,2021) we have studied the excess molar volumes of Binary Liquid Mixtures of cyclohexanone, + methylene chloride, +chloroform, + CH_2ClCH_2Cl, +$CHClCCl_2$ and + CCl_3CH_3 at 303.15 K. In continuation of these studies on the thermodynamic and other properties of some mixtures of chloroalkanes and bromo alkanes with n-donor organic solvents (Tripathi AD,2010,2018,2020), the current paper shows the excess molar volumes (V^E) obtained experimentally by using dilatometer for the binary liquid mixtures of acetylene tetrachloride ($CHCl_2.CHCl_2$) with 1,4-dioxane($C_4H_8O_2$) or methyl ethyl ketone ($CH_3COC_2H_5$)or pyridine(C_5H_5N) at 308.15 K and atmospheric pressures and the results obtained have been discussed in terms of destruction and creation of bonds, influence of the lone pair electrons of O atom or N atom during creation of new bonds , and establishing of unlike-pair interactions, and its competition with acetylene tetrachloride self-association in the liquid state. These results can be used in providing an additional complete behavior of the present mixtures.

Experimental

Materials

The high pressure liquid chromatography quality chemicals (purchased from Qualigens Fine Chemicals, Mumbai)acetylene tetrachloride,pyridine and ethyl methyl ketone , and $C_4H_8O_2$ of said lowest mass fraction purities of 0.996, 0.99 and 0.995, respectively. Acetylene tetrachloride was purified as given in earlier paper(Pathak G.et.al.1992). Pyridine and methyl ethyl ketone was used as such. $C_4H_8O_2$ became stored over sodium cord earlier than use . All organic liquids were stored in Ambered bottles over molecular sieves(4 Å in size), in order to decrease the moisture percentage. Before taking measurements , all chemicals were degassed inside vacuum.

Method

V^E were obtained by using , two-limbed Pyrex glass dilatometer with an uncertainty of ±2.10^{-3} cm^3 mol^{-1} , it was same as used by Nath and Tripathi,1983. Weighed amounts of the two organic liquids were kept above purified Hg in the lack of air holes in the both arms of the dilatometer, kept on a wooden rest and the complete assembly was submerged in a water thermostat (Accuracy±0.01 K). The combination of the two liquids have been acquired by way of swinging the cell backward and forward through a definite attitude, and the Hg ranges in the capillary were read by means of a a cathetometer (±1.10^{-3} cm accurate).

Result and discussion

Experimental data at 308.15 K for V^E, in terms of $CHCl_2.CHCl_2$ mole fractionx_1 , are collected in **Table 1** and represented in Fig. 1. Excess volume data for different mixtures were fitted to an appropriate equation of the under given form

$$V^E = x_1 (1 - x_1)[A_0 + A_1 (x_1 - x_2) + A_2 (x_1 - x_2)^2 + A_3 (x_1 - x_2)^3$$

The values of the all coefficients arising from the fits and the corresponding standard deviations are summarized in **Tables 2**. Standard deviation is calculated as given in our earlier paper. (Tripathi, AD et.al.2021)

The plot permit us to envisage the trend of $\boldsymbol{V^E}$changes when increasing the mole fraction of $CHCl_2.CHCl_2$. The values of V^E , which are negative for all the systems , increase in the order

Methyl ethyl ketone>1,4,dioxane >Pyridine

High negative values of V^E for the system of $CHCl_2.CHCl_2$+methyl ethyl ketone system are an indication of creation of strong molecular complex between these components in the liquid state. The excess volume of a binary mixture can be visualized as the balance of two types of contributions arising from the breaking of cohesion (like molecule interaction)forces in pure liquids during the mixing process and one negative input arising from the newly established similar or unlike-pair interactions. The interaction between $CHCl_2.CHCl_2$+methyl ethyl ketone or + 1,4-dioxane can occur due to combination of H atom of $CHCl_2.CHCl_2$ and lone pair electrons present on the O atom of methyl ethyl ketone. Possibility of charge-transfer complex formation may arise when Cl atom combination with lone pair electrons on O atom takes place in the liquid state. Since 1,4-dioxane has two O atms in its structure but it has less negative values of V^E than methyl ethyl ketone. In the present case, H-bonding and other interactions takes place between the components. It clearly indicates that other interactions are chief contributors to excess volume other than hydrogen bonding.

The interaction for the system , $CHCl_2.CHCl_2$ +pyridine, the values of excess volume is less negative than other components, thus showing the weak interaction between H atom of $CHCl_2.CHCl_2$ and lone pair electrons on the N atom of Pyridine.

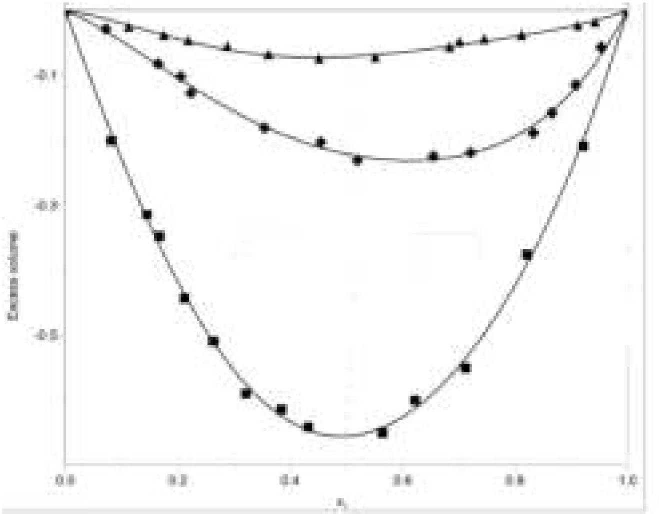

Fig. 1: Excess molar volumes of binary liquid mixtures of x1 of acetylene tetrachloride ($CHCl_2CHCl_2$)(1) + (1,4-$C_4H_8O_2$)(2) (✚),+methyl ethyl ketone($CH_3COC_2H_5$)(2) (■),+ and +C_5H_5N (2)(▲) at the temperature 308.15 K.

Table 1. Experimental Values of Excess Molar Volumes, for acetylene tetrachloride, + 1,4-dioxane or methyl ethyl ketone or pyridine at 308.15 K

$x CHCl_2CHCl_2$ + (1 - x)(1,4-$C_4H_8O_2$)		$x CHCl_2CHCl_2$ + (1 - x)$CH_3COC_2H_5$	
x1	**V^E ($Cm^3.mol^{-1}$)**	**x1**	**V^E ($Cm^3.mol^{-1}$)**
0.0718	-0.029	0.0822	-0.201
0.165	-0.082	0.1453	-0.315
0.2051	-0.196	0.1675	-0.348
0.2232	-0.127	0.2122	-0.444
0.3544	-0.181	0.2633	-0.510
0.4544	-0.203	0.3211	-0.591
0.5199	-0.231	0.3843	-0.615
0.6543	-0.225	0.4318	-0.642
0.7211	-0.219	0.5644	-0.681
0.8321	-0.189	0.6222	-0.601
0.8655	-0.158	0.7122	-0.561
0.9076	-0.115	0.8211	-0.376
0.9534	-0.057	0.9211	-0.209

xCHCl$_2$CHCl$_2$ + (1 - x)Pyridine	
x1	**V^E (Cm^3.mol^{-1})**
0.1122	-0.026
0.1754	-0.036
0.2187	-0.047
0.2881	-0.056
0.3613	-0.068
0.4512	-0.075
0.5513	-0.073
0.6833	-0.057
0.7011	-0.041
0.7441	-0.042
0.8112	-0.039
0.9117	-0.024
0.9423	-0.019

Table 2. Table2.Redlich-Kister Coefficients and Standard Deviation σ for different systems at 308.15K

System	A0	A1	A2	A3	σ/ (Cm^3 mol^{-1})
$CHCl_2CHCl_2$ (1) + (1,4-$C_4H_8O_2$)(2)	-0.8845	-0.3617	-0.1315	-0.2994	0.007
$CHCl_2CHCl_2$ (1) + $CH_3COC_2H_5$ (2)	-2.623	0.0856	-0.017	-0.3211	0.012
$CHCl_2CHCl_2$ (1) + C_5H_5N (2)	-0.2853	0.0807	0.059	-0.179	0.003

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Adverse Impacts of Synthetic Fertilizers on the Fertility of the Soil due to Various Changes in Soil Composition

Abstract

In the present scenario of agriculture the chemical fertilizers are the essential part of growing any kind of crop .They provide vital growth of the plants and secure food security of the World. The production of crop can be increased but plant growth do not attain developed roots and do not attain maturity .The excessive use of fertilizers is very dangerous and enter the water ,air and soil. The toxic substances absorbed by plants passes to human body. The toxicity start from the manufacturing process through products and by products containing harmful components. The release of gases like NH_3, CO_2 , and CH_4 etc produce adverse effects on the environment and ecosystem . The manufacturing units discharge their waste in the nearby water system lakes, ponds and water bodies and causes water pollution. The regular use of fertilizers is continuously deteriorating the quality of soil and producing excessive growth of aquatic plants and causes dumping of decayed plants and depth goes on decreasing day by day, called eutrophication. The adverse effects of chemical fertilizers can be reduced by applying new agricultural techniques and use of bio- fertilizers fo healthy crop free from any king of toxicity of metals in vegetables, and fruits etc. The chemical fertilizers directly harm the environment and ecosystem. It covers Water pollution, soil pollution and air pollution.

Keywords: : Maturity, Chemical fertilizers, Environment and ecosystem , Bio-fertilizers, Plant growth

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Introduction

The industrial revolution, also known as green revolution fulfilled the food deficiency by applying inorganic and organic fertilizers but also hindered the soil's natural fertility. The wide applications of inorganic and organic fertilizers have suppressed the Purity of crops. Mostly every seasonal crop/ fruits have high percentage of unwanted heavy metals , other toxic materials like , N, S etc.(Ayoub AT, 1999). It has increased health problems and unrecoverable environmental pollution.

It has been estimated that total consumption of N, P, & K has achieved 81, 4 and 18 Tg/yr respectively(Greidner,1997).Approximately 55% of chemical fertilizers are applied for cereal production , 12% for oil seeds crops, 11% for grass lands,11% for commodities (cotton, sugar, and coffee) , 6% for root crops and 5% for fruits and vegetable production. Till 1950 the consumption of chemical fertilizers was very small and nutrients needed for healthy crop were obtained from manures (Aksoy U,2001).By 2020, it has been observed that 70% of crops depend upon the applications of chemical fertilizers.. The type of fertilizers is increasing continuously with respect to the population growth (Aboudrare A et.al., 2009). As per the studies by Keeney (1997) , the total population will increase about 2.2 billion and it will attain its double figure by 2050. The consumption of meat and food in developed countries is increasing and it may be triple till the mid of 21ist century (Mahajan Gupta RD,2008). The volume of agricultural land is decreasing day by day due to fast growing urbanization and agricultural land may less than the urban development . it is expected that food production must be more intensive and efficient than ever before.

To minimize the toxic effects of artificial fertilizers on human and environment, new approach has been adopted known as organic agriculture , sustainable agriculture or ecological agriculture (Omidire Niyi S et.al,2015) .Bio-fertilizers are cost effective and are easily available from locality products . The microbial fertilizers are eco-friendly and help to have healthy environment (Pandiselvi T et.al,2017). On the other hand inorganic fertilizers are also very expensive and show negative impacts on soil fertility. The application of artificial fertilizers causes degradation and nutrients balance (Singh MD,2017). The other advanced practices like integrated nutrient management, nano fertilizers may reduce the adverse effects of fertilizers. The plants need P, N, and K to maintain the normal physiological state of the plants (Trenkel Martin E, 1977). The deficiency of these basic nutrients causes weak growth and less production . On the other hand excessive applications of fertilizers lead to enter the food chain and become a big problem for the society . Ultimately it causes water pollution, soil pollution and air pollution.

Required nutrients

The synthetic / natural fertilizer are applied to soil and it must fulfill the basic requirement of a good fertilizer. A natural / synthetic fertilizer must contain 5% of N, P and K.The industrial fertilizers some time contain varying % of the three basic component along with minor % of Zn, Mn and Fe as impurities and other non essential Elements. Commonly gypsum and lime are used as soil conditioners to enhance the fertility of the soil. The fertilizers mainly provide nutrients in varying proportion. Primary Macronutrients are essential and effects on plants growth (Nelson DW,1984). Nitrogen is essential to produce more chlorophyll and causes leaf growth.

Phosphorus is essential for energy transfer, development of roots , flowers and and seeds / fruits.Potassium serves as an activator of enzymes used in photosynthesis and respiration , strong stem growth , moment of water , promote flowering And fruits.

Secondary Macro- nutrients are Ca, Mg and S.Calcium(Ca) regulates the transport of other nutrients in to the plant. It activates Several enzymes**.** It help in photosynthesis and plant growth.Magnesium (Mg) is the major constituent of chlorophyll molecule.It also act as activator for enzyme reactions.Sulphur(S) is main structural component of some of the amino acids and Vitamins . It also promote chloroplast growth and function .It is present in Iron –Sulphur complexes to activate electrons transport chain in photosynthesis .Sulphur is also essential for nitrogen fixation by legumes . It convert nitrates in to amino acids and finally to proteins.

The variety of Micro-nutrients are also present in fertilizers which are very essential for plant growth. Copper(Cu) is important for grain production, photosynthesis, and manufacture of Lignin wall. Iron(Fe) is major constituent for photosynthesis and also present in enzymes. Manganese(Mn) help in chloroplast formation and promote photosynthesis in plants. Molybdenum(Mo) help in the synthesis of amino acids in plants.Zinc(Zn)- is essential component of enzymes and act as DNA transcription.Boron(B)- promote flowering , pollen germination and fruits formation.Silicon (Si)- strengthen the cell walls and production of crop.Cobalt(Co) is essential for nitrogen fixation in legumes .Vanadiun (V) is a substitute for Mo and act in low concentration for healthy growth of the plants.

Various Types of Fertilizers

The fertilizers are needed for the supply of macro and micro nutrients and to give strength to the plants. They are applied as supplements to flourish the crops for better yield (Savci S .2012). Fertilizers also boost healthy crops. This way fertilizers are help full to increase the production(Keeney D.1990).The function and nature of organic and inorganic fertilizers is quite different and both have their own importance in farming and plant's growth and huge crop. Hence a set strategy must e applied to balance the major and minor nutrients for healthy growth of the plants, to enhance stem growth and more crop(Ruiting T et.al., S.2017). The classification of fertilizers is an important part of this to understand the chemical composition and their effects on soil fertility and ultimately for huge crop production to satisfy the world food demand.

Firstly they are classified based on their nature – e.g. Inorganic fertilizers, Chile saltpeter,which give 15% nitrogen , Organic fertilizers , e.g . Urea give 45% nitrogen and Bio-fertilizers , the product that contain micro-organisms e.g. A. M. fungi, N-Fixer, P-soluilizer and potassium solubilizer.

Secondly they are classified based on the form of the fertilizers-The different types of fertilizers exist in various forms e.g. Powder (Single superphosphate), Crystals(Ammonium sulphate) , Prills (Urea, superphosphate diammonium phosphate,)Granules and super granules(Holland granules , Urea super granules). The liquid Fertilizers are also applied through irrigation.

Third Classification is based on the composition and complexity of chemical fertilizers

These are of three types (a) Single nutrient eg. Urea, ammonium sulphate , Potassium Chloride, and potassium sulphate (b) Multi nutrients eg. DAP, Nitro phosphate and Ammonium phosphate. (c) These fertilizers consists of two or three primary nutrients.

Fourth classification is based on application of fertilizers- (a) Foliar fertilizers are the Water soluble nitrogen fertilizers and directly sprayed on leaves.(b) Controlled and slow released fertilizers are ammonium nitrate , urea, ammonium Phosphate , potassium chloride etc.(c) These are nitrogen based fertilizers mixed with

Certain chemicals which stop nitrification and help to convert ammonia to nitrates .e.g. Nitrapyrin ,DMPP etc.

Natural resources and fertilizers

The agriculture has attain its advancement through out the world and large number of fertilizers , pesticides ,herbicides, are applied to get maximum production . The use of excessive fertilizers and cause soil pollution , air pollution and water pollution and harm the environment and ecosystem .It directly decrease the food quality and crop/fruits are contaminated with unwanted nutrients . All these chemical substances are very harm full and produce acute toxicity in aquatic life, pollute the air and soil. The application of bio-fertilizers will definitely bring quality and different types of diseases among the animals and human beings could be controlled . This way the environment could be saved and green revolution can be achieved by the application of bio-fertilizers for growing wheat, rice , cereals, fruits etc. Despite the benefits , fertilizers have negative effects on the environment.

Negative effects of Artificial fertilizers- Although the fertilizers are back bone to huge production of various types of crops but the nutrients level of soil is continuously decreasing and natural fertility of soil has been deteriorated to larger extent . This is leading to barren land , the quality of water , soil and air is changing and it is harmful for the next generation. The use of slow and controlled released fertilizers , prilled or radulated fertilizers, nitrification inhibitors are promising options to have safe environment for every living being. The application will be help full to increase the crops(Neue HUW. !993).

Cause of water pollution- The nutrient value of fertilizers is very less and hence. These are applied in bulk and develop unfavorable conditions for the environment by different ways .There may be leaching , drainage or surface flow . The nitrogen is mostly oxidized to nitrates by micro-organisms and ultimately it reaches to underground water system . Even when these fertilizers are applied in ideal conditions, 50% of it is consumed by plants and rest of the nitrogen flows to water system. Approximately 2.5 –21% get catalized, 16-26% get reaction with other compounds present in the soil. 2.6-10% flow to under ground water, wells , ponds and rivers . They show excessive growth of aquatic plants and causes Eutrophication and ponds , rivers become shallow. When nitrate concentration increases in water more than 50mgll the chances of gastric cancer become more prominent and goiter , birth defects , heart disease , increases . Both Nitrogen and Phosphorus are responsible for Eutrophication of surface water.Eutrophication causes killing of aquatic life , proliferation of unwanted species and Loss of recreation due to bad odour (Dal lake).

Air Pollution due to fertilizers- To enhance crop's production , numerous harmful Green house gases are produced and they are depleting the the ozone layer. The ultra violetRays are very harm full for fauna and flora. The agriculture accounts 60% N_2O emission The green house gases like CO_2, CH_4 , N_2O are produced during the manufacturing Of nitrogenous fertilizers .The excessive use of nitrogen fertilizers results in emission Of NO, N_2O and NO_2 and these gases are enough to cause severe air pollution. In global warming the presence of NO is very dangerous and causes 300times more global warming than CO_2. The air pollution is a very serious problem which has happened Due the applications and manufacturing process of various chemical fertilizer**s.**

Soil pollution due to fertilizers-The soil is the best medium for plant growth . It Provide nutrient recycling system and serve as habitat for micro-organisms . It support other ecosystem for small population in the soil. The use of fertilizers lead to Acidification of soil and reduce the organic content in the soil for the good growth of the plants. The excess of fertilizers also kills beneficial organisms. The earth Warms are also reduced and fertility of soil has been deteriorated to a larger extent(Shaviv A, 2000).The soil testing is a very important tool to control the fertility of soil , The pH plays a very important role for plant's growth and production of grains and fruits.

This way the degradation of soil take place(Savci S .2012). Other harmful effects of fertilizers are,**a-**Excess use of N, causes lower leaf yellowing,the roots may be blacken . These symptoms occur due to salt deposition in the soil.**b**-Excess of nitrogen in barley crop produce undesirable effect on quality of beer. **c**-Excess of fertilizers spoil the plants and leaves become brown. Excess of nitrates causes severe problem as in case of water. **d**-Over fertilization reduce the biodiversity in forest and land.

Importance Of Bio-fertilizers- Bio-fertilizers differ from chemical and organic As they do not supply Nitrogen directly to the plants, bacteria and fungi. The production of bio-fertilizers is simple and within 30 days , it can be prepared by spraying Liquid solution of micro-organisms. They are safe and balance the fertility of the Soil. They allow to develop more earth warms , micro-organisms in soil which Are asset for the soil quality and maintain natural strength of the soil.

Conclusion

The application of fertilizers is of utmost important for proper food production . To reduce the hazardous effects of fertilizers the application of bio-fertilizers are essential. To safeguard the agriculture , the excessive use of chemical fertilizers must be stopped otherwise a day will come the green planet will change to poisonous environment. It will be very difficult to have safe drinking water, safe food, fruits on this beautiful planet . Now this is the duty of every one to protect the environment by using bio-fertilizers which can be made from agro waste, kitchen waste and city waste,. This way a safe and congenial environment can be attained for the well being of lives on the earth.

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Excess molar enthalpies for acetylene tetrachloride with cyclohexanone, pyrralidin 2-one and methyl ethyl ketone at 308.15 K

Abstract

Excess molar enthalpies, H^E, at 308.15K were determined calorimetrically for binary liquid mixtures of acetylene tetrachloride ($CHCl_2CHCl_2$) with cyclohexanone, pyrralidin-2-one and methyl ethyl ketone. Exothermic behavior is shown by all the systems. The values of H^E are fitted with suitable equation with the help of the least squares method. The results point to the presence of specific interactions.

Keywords: Microcalorimeter, cyclohexanone, mixtures, charge-transer complex, mole fraction

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Introduction

The research of excess properties are of massive hobby in knowledge the heteroatom interactions within the multi-constituent liquid mixtures. Consequently, assessment and calculation of these excess values as functions of mole fraction are of academic and realistic significance. Our aim is gathering of the facts for physical properties of of n-donor or π-donor and σ-acceptors organic liquid mixtures to observe the probable interactions happening in the combined liquid systems. As a part of our uninterrupted attempts to achieve nonthermodynamic and thermodynamic parameters on binary liquid mixtures of various organic compounds (Tripathi AD,2010,2018,2020,2021), determination of excess molar enthalpies of acetylene tetrachloride ($CHCl_2CHCl_2$)(AT) with cyclohexanone ($C_6H_{10}O$), pyrralidin-2-one (C_4H_7NO) and methyl ethyl ketone($CH_3COC_2H_5$) have been undertaken in the current work at the temperature 308.15K. Binary systems of $CHCl_2CHCl_2$ with $C_6H_{10}O$, C_4H_7NO and $CH_3COC_2H_5$ are of significant interest because of interactions among these components .This is due to the presence of four Chlorine and two Hydrogen atoms in $CHCl_2CHCl_2$, which can consequently carry out as σ-acceptors in the path of, and be engazed in the H- bond creation with cyclohexanone, pyrralidin-2-one and methyl ethyl ketone . The later compounds will carry out as n-donors. A literature inspection disclosed that vast research on such systems have not been undertaken till now. The data obtained for H^E have been explained in this paper.

Experimental Section

Acetylene Tetrachloride (Fluka) has been purified with the aid of fractional distillation, only the center fraction turned into used for experiments.

Cyclohexanone (B.D.H.), and Methyl ethyl ketone (A.R.) were dried over freshly activated molecular sieves before use for removing moisture . All the chemicals have a purity of 99.0 mol% as obtained by GLC. Chemical purities , as measured by GLC for the samples of acetylene tetrachloride ($CHCl_2CHCl_2$) , cyclohexanone, pyrralidin-2-one and methyl ethyl ketone are found to be 99.8, 99.8, 99.3 and 99.0 mol%, respectively. The excess enthalpies were determined using the microcalorimeter. The mean error in the experimental data of H^E are envisioned to be within 1 per cent.

Result and Discussion

Experimental data for H^E, at 308.15K for all binary mixtures, in terms of the $CHCl_2CHCl_2$ mole fraction x_1 are listed in Table 1. Experimental values were fitted to the following equation:

$$\frac{H^E}{J.mol^{-1}} = x_1 x_2 \sum_{i=0}^{m} A_i \,(x_{1-}x_2)^i \qquad (1)$$

The constants Ai, along with the standard deviations, σ , are collected in Table 2 . The expression used to evaluate the standard deviation, σ , was

$$\sigma = [\sum (H^E_{exp} - H^E_{calc})^2/(m-n)]^{1/2} \qquad (2)$$

Wherein n is the quantity of parameters and m is the wide variety of information geared up. Graphical presentations of experimental values of H^E information for all binary mixtures are supplied in figure 1. As may be discovered, the values of H^E are negative throughout the whole mole fraction variety for whole combination.

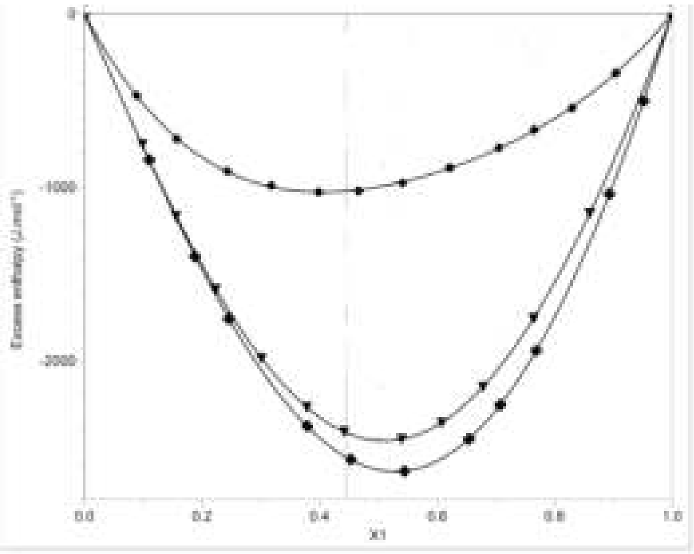

Fig. 1: Excess molar enthalpies of binary liquid mixtures of x1 of acetylene tetrachloride ($CHCl_2CHCl_2$)(1) + cyclohexanone ($C_6H_{10}O$)(2) (✚),+ pyrralidin-2-one (C_4H_7NO)(2))(▼), and +methyl ethyl ketone($CH_3COC_2H_5$ (2)(◆) at the temperature 308.15 K.

Fig. 1 represents that the negative values of the excess molar enthalpies H^E, for all binary liquid mixtures is substantially influenced by means of the electronic surroundings of Oxygen atom. The sign of H^E effects from the disorder of interactions among resembling molecules and the beginning of recent interactions between contrasting molecules. The remaining end result of both type of interactions. This may be because of contravention of bonds or The scale of H^E for these mixtures is because of the interactions among resembling molecules, and from the creation of new bonds such as H- bonds between contrasting molecules. In case the interaction among resembling molecules are weaker in comparison to contrasting molecules, the negative values of H^E is observed. The high negativity of all these systems signify robust specific interactions connecting the contrasting molecules. If cyclic ketones have saturated rings and it reacts with bromine - or chlorine containing compounds, strong interaction is observed. $C_6H_{10}O$ or C_4H_7NO has saturated ring, consequently they form stronger complexes i.e. high exothermicity is shown in the value of H^E . Since $CH_3COC_2H_5$ does not have ring(saturated or unsaturated) in its structure, thus it has less negativity as compared to other keto compounds.

Table-1 Excess molar enthalpies for acetylene tetrachloride ($CHCl_2CHCl_2$)with cyclohexanone($C_6H_{10}O$), pyrralidin-2-one (C_4H_7NO) and methyl ethyl ketone($CH_3COC_2H_5$) at 308.15K

$CHCl_2CHCl_2$+ cyclohexanone		**$CHCl_2CHCl_2$+ pyrrolidin-2one**		**$CHCl_2CHCl_2$+ methyl ethyl ketone**	
x1	**H^E ($J.mol^{-1}$)**	**x1**	**H^E ($J.mol^{-1}$)**	**x1**	**H^E ($J.mol^{-1}$)**
0.1098	-841	0.0886	-576	0.0886	-576
0.1876	-1397	0.1567	-748	0.1567	-748
0.2456	-1758	0.2432	-907	0.2432	-907
0.3788	-2376	0.3176	-991	0.3176	-991
0.4532	-2569	0.3984	-1028	0.3984	-1028
0.5444	-2636	0.4662	-1020	0.4662	-1020
0.6542	-2451	0.5409	-974	0.5409	-974
0.7076	-2254	0.6216	-887	0.6216	-887
0.7689	-1942	0.7054	-766	0.7054	-766
0.8932	-1039	0.7651	-668	0.7651	-668
0.9511	-504	0.8298	-555	0.8298	-555
		0.9043	-429	0.9043	-429

Table 2. Least Squares Coefficients of Eq 1 for the Excess Molar Enthalpies , and the standard deviations,σ,of Acetylene tetrachloride ($CHCl_2.CHCl_2$)(1) + cyclohexanone ($C_6H_{10}O$)(2) ,+ pyrralidin-2-one (C_4H_7NO)(2)),+ and +methyl ethyl ketone($CH_3COC_2H_5$)(2) at the temperature 308.15 K.

System	A0	A1	A2	A3	σ (J mol^{-1})
$CHCl_2CHCl_2$ (1) + cyclohexanone (2)	-1.05E+04	-1397	1214	-82.56	2
$CHCl_2CHCl_2$ (1) + pyrralidin-2-one (2)	-9842	-483.5	1337	-135.5	3.3
$CHCl_2CHCl_2$ (1) + methyl ethyl ketone (2)	-3992	1192	-1330	-6692	4.5

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Initial and transition state solvent effect on Reaction Rate for Solvolysis of Ethyl Caprylate Ester in Binary Solvent System

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Abstract

The kinetic reaction of ethyl caprylate in basic medium of water-acetone has been studed in different range of temperature 20 to 40^{0}c. The composition range of reaction mixture is 30 to 70% (v/v) of Acetone. The rate constant decreases with increase in solvent composition of reaction mixture indicate that there is destruction of charge in transition state. The trend of activation energy is found to be decrease with increasing solvent composition is an indication that initial state is desolvated and transition state is solvated. The influence of dielectric constant value of water on reaction rate has also been studied. The thermodynamic parameters (ΔG^*, ΔH^* & ΔS^*) have been determined which showed strong dependency on solvent composition.

Keywords: Ethyl Caprylate Hydrolysis, Specific rate, water- acetone, kinetic solvent effect,

Introduction

It has been suggested that change in solvent from polar to non polar will either increase or decrease the reaction rate depending upon the type of reaction (Parker A.J. 1969). Solvent effect on reactivity in homogeneous media is explained in term of specific interaction of solvent and reactant molecules and also between solvent and transition state (Iglesias E.2005). In many physical and chemical process of solution, the solvent play very important role (Yangjeh A.H. 2005). When the magnitude of solvent in elementary reaction are changed, the rate of reaction will also change(Schmeer G et.al 1999, Kallol k Ghosh. 1999. For the understanding of solvent effect, a large effort has been made (*Panov M Yu. et al. 2003,Magdha F, Fathala. 2011, EZZ A. et al. 2017Magda F et al. 2019,*Seliverstova T S. 2020, *Seliverstova T S et al. 2020.* which are sometime succeed and also some time fail. In this context here, hydrolysis of Ethyl caprylate is presented in aqueous solvent system at different composition and in different range of temperature. Ethyl caprylate is fatty acid ethyl ester, has prominent role as metabolite. It is suitable reagent used as standard for measurement of flavour-active compound by gas chromatography. It is also used in brown cocoa, dairy savory etc.

Experimental

The kinetic of alkali catalyzed solvolysis of Ethyl caprylate in water-acetone has been studied by keeping the concentration of alkali and ester M/10 and M/20 respectively. Water used was double distilled from $KMnO_4$. Chemical used in this experiment are either BDH(Analar) or Merck grade. Acetone was purified by known procedure. The conical flask containing the solution and small stopper bottle congaing Ethyl capryalate has been thermostated for half an hour. Then 0.4 ml of ester was withdrawn with the help of pipette and added quickly to alkaline solution of water-organic co-solvent mixture by constant shaking. Immediately 10 ml of aliquot of the reaction mixture was withdrawn and allowed to run into flask containing 10 ml of N/10 HCl solution. The excess of alkali of the solution was titrated by means of standard solution using phenolphthalein as an indicator. The moment at which half of the aliquot was added into the ice cold 0.1N HCI solution, the stop clock was started. This time is considered to be zero time or starting time. Taking into account of zero time kinetics of remaining ester was estimated after quenching the 10 ml of aliquot in 10 ml of ice cold 0.1N HCl at definite interval of time followed by titration as usual.

Result and Discussion

Solvent Effect and calculated Specific Rate constant

The specific rate constant of alkali catalyzed solvolysis of Ethyl caprylate followed second order kinetics which is calculated by slope of linear plots of Log k against1/T. The values of rate data (Table-1) show that with increasing proportion of organic solvent rate decrease. The solvent effect on specific rate can also be observed when Log k is plotted against solvent composition (Table-2 and Fig-1). Dipolar protic solvent like Acetone, DMSO, DMF are powerful bases and strong hydrogen bond acceptor so it interact with solute which are hydrogen bond donors (Parker AJT. 1962.). The value of dielectric constant of the reaction media goes on decreasing with solvent composition so the result obtain in present study is against the Hugh and Ingold qualitative theory. However many instant has been reported (R Krishnanmurty P S et al. 1970, Singh L et al. 1980] in which the rate decreases in similar way as found in this case. The depletion of rate causes due to addition of Acetone in water-Acetone media, may be attributed due to combine effect of dielectric and solvation change taking place in the media. The dipolar aprotic solvent like DMSO, Acetone, DMF exerted greater effect on rate because such solvent produced inter molecular association of solvent in such aqueous solvent media. Solvent -solute interaction, solvation of reactant and transition state are also dominating factor which also exert greater effect on rate of reaction.

Table 1.Bimolecular rate constant k x10^3(dm)^3/mole/mint]

Temp in ^{O}C	% of Acetone				
	30%	40%	50%	60%	70%
20^{O}C	26.91	23.71	21.33	18.48	15.84
25^{O}C	55.59	46.66	39.81	33.11	26.30
30^{O}C	107.15	89.12	72.44	58.74	42.65
35^{O}C	208.92	164.05	127.35	100.00	67.60
40^{0}C	398.10	305.49	229.08	175.79	107.15

Table 2.Change in Log k Value with mole %

Temp in ^{O}C	**Mole%**	**3 + Log k**				
		20^{O}C	**25^{O}C**	**30^{O}C**	**35^{O}C**	**40^{0}C**
30%	9.56	1.430	1.745	2.030	2.320	2.600
40%	14.11	1.375	1.669	1.950	2.215	2.485
50%	19.77	1.329	1.600	1.860	2.105	2.360
60%	26.99	1.265	1.520	1.769	2.000	2.245
70%	36.52	1.200	1.420	1.630	1.830	2.030

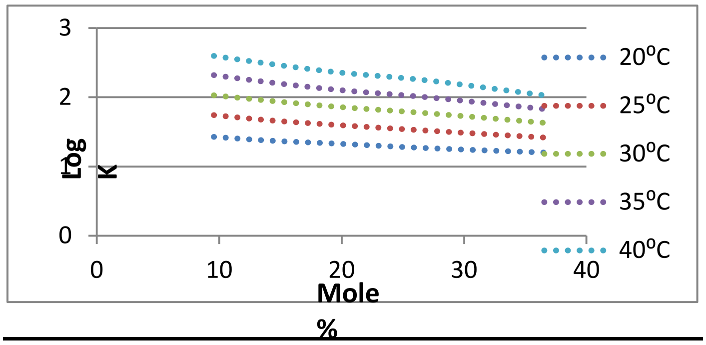

Fig. 1: Plots of log k with mole %.

Thermodynamic Activation Energy (Ec) of bimolecular reaction.

With the help of slopes (**Fig-2**) of linear plots of (Logk against 1/T) of Arrhenius equation , the numerical value of activation energy(E_c) has been calculated and tabulated in Table-4. The depleting trend of iso composition activation energy with enhancement in solvent composition,indicate that solvation in transition state and desolvation in initial state, because transition state possess more cation (ester+H^+) available by the salvation of acetone molecule than initial state (Varma DK et al. 2020, Sundhansu NS. 2020). The decrease in value of ΔH^* and ΔS^* also indicate the decrease in disorderness of the reaction media.

Table 3. Logk Values with different Temperature, Water- acetone media

Temp in ^{O}C		**3 + Logk**				
	10^3/T	**30%**	**40%**	**50%**	**60%**	**70%**
20^{O}C	3.412	1.430	1.375	1.329	1.265	1.200
25^{O}C	3.355	1.745	1.669	1.600	1.520	1.420
30^{O}C	3.300	2.030	1.950	1.860	1.769	1.630
35^{O}C	3.247	2.320	2.215	2.105	2.000	1.830
40^{0}C	3.195	2.600	2.485	2.360	2.245	2.030

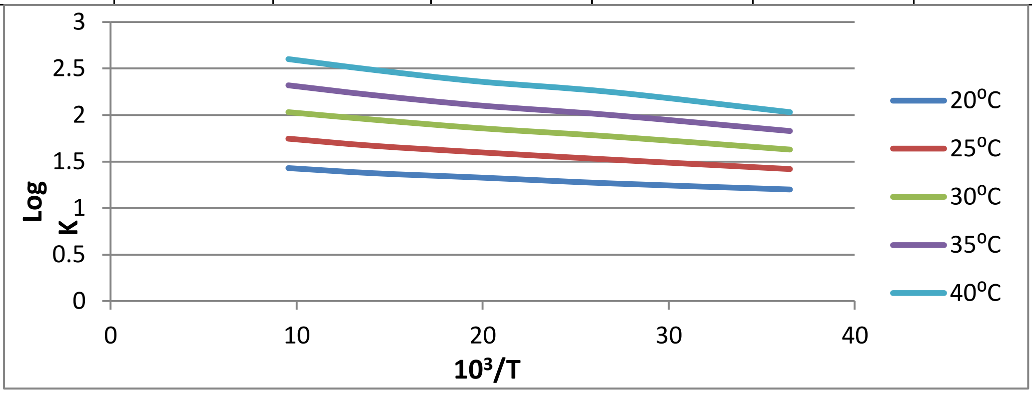

Fig. 2: Plots of Log K with 10^3/T.

Table 4.Activation Energy at different composition of solvent

% of EG	**30%**	**40%**	**50%**	**60%**	**70%**
E_{exp} in KJ/mole	103.75	99.41	99.03	88.36	74.09

Table 5. Logk$_D$ Values with different Temperature at constant D for Water- acetone media.

Temp in ^OC	$10^3/T$	D=40	D=45	D=50	D=55	D=60
20^OC	3.412	1.189	1.240	1.299	1.355	1.410
25^OC	3.355	1.420	1.500	1.580	1.660	1.740
30^OC	3.300	1.695	1.770	1.850	1.930	2.015
35^OC	3.247	1.895	2.015	2.140	2.260	2.385
40^0C	3.195	2.152	2.280	2.410	2.539	2.669

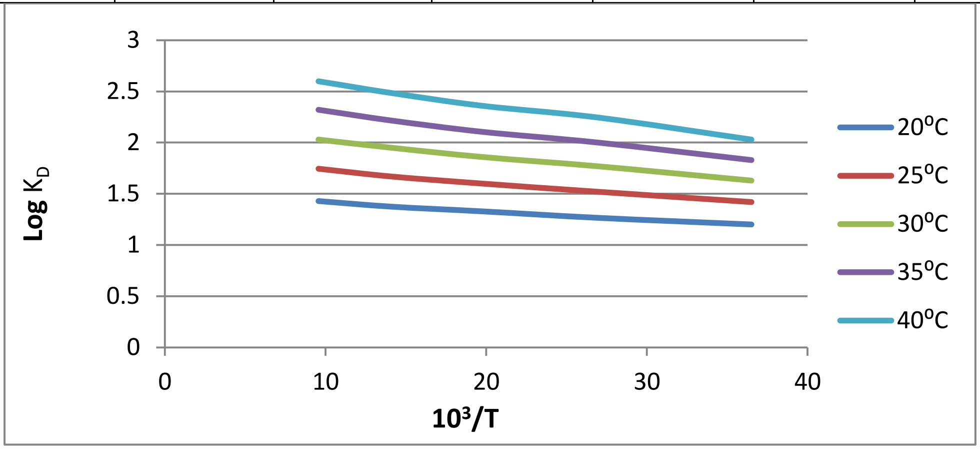

Fig. 3 Plots of Log K$_D$ with $10^3/T$.

Effect of Dielectric Activation Energy

An alternative aspect of solvent effect can be tested by considering the influence of dielectric constant D on reaction rate. Thus, an increase in D causes a consequent increase in rate. By the interpolation of (Akerlof G. 1932) data, the dielectric constant values of reaction mixture have been obtained. When dielectric constant D of the medium is lowered, there is a considerably decrease in rate is found. The plots of log k and D-1/2D+1 give linear relation which indicate that reaction have dipole-dipole interaction(Lanndskroner(Laidler and Landskroener1956) .If the reaction is considered as ion-dipole interaction, linear relation is obtained by plotting Logk against1/D, other liner relationship obtained for Logk vs LogD (Fayez Yet.al. 1978). Graphical application of different electrostatic theory for dipole-dipole as well as ion-dipole showed that the best linear plots are obtained when Logk is plotted as a function of D. Departure from linearity at low dielectric constant at low dielectric constant is however still preserved. In case of preferential solvation or solvation shortening of activated complex by water, with the higher component of solvent mixture there is deviation in linearity is observed. However, in the present study of alkaline hydrolysis of caprylate ester is based on dielectric constant effect and can better be treated as an ion dipole interaction, in which ester represent the actual dipole rather than dipole interaction. Here Iso-dielectric activation energy was calculated by the slopes of interpolation of Logk against different temperature [Fig-3] and the calculated values of dielectric activation energy are inserted in Table-6. The decreasing trend of (E_D) values with decreasing D is similar as previous views of (Wolford RK.1964, Singh AK. 2020)

Table 6. Dielectric Activation Energy values at different D.

Dielectric constant(D)	**D=40**	**D=45**	**D=50**	**D=55**	**D=60**
E_D in kJ/mole	86.62	91.62	94.66	99.64	106.39

Conclusion

The rate of hydrolysis of alkali catalyzed hydrolysis of ethyl caprylate decreases with increase composition of organic solvent at different temperature range. The increase in value of Iso-composition energy with decreasing solvent proportion, indicate that the solvation takes place in initial state and desolvation in transition state. The result of this project was to analyze the solvent-solute interaction and solvation change in initial and transition state. Dielectric values also play important role in observing solvent effect in aqueous solvent media.

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Dielectric Constants for Methoxybenzene ($C_6H_5OCH_3$)+ Dichloromethane (CH_2Cl_2), Ethylene dichloride (EDC), Trichloroethene ($CHClCCl_2$), Tetrachloroethylene (CCl_2CCl_2) at 303.15 K

Abstract
Dielectric constants or relative permittivity ,ε, have been determined at 303.15 ± 0.01 K and at a frequency of 1.8 MHz with a dekameter (type DK03, made in Germany), using two cells, first cell for mixtures having dielectric constants less than 7.0 and other cell , for mixtures having dielectric constants more than 7.0 for mixtures of Methoxybenzene ($C_6H_5OCH_3$) + dichloromethane (CH_2Cl_2), ethylene dichloride (EDC) (CH_2ClCH_2Cl),Trichloroethylene ($CHClCCl_2$), Tetrachloroethene(CCl_2CCl_2) at 303.15 K.

The quantities Δ ε, which refer, to the deviations of the value of ε of the mixtures from the values developing from the mole fraction combination law, have been calculated and deciphered.

Keywords: Methoxybenzene, dekameter,hydrogen bonding, specific interaction, binary mixture

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Introduction

Mixtures of methoxybenzene with all mentioned chlorocompounds are of huge interest due to presence of a molecular interaction amongst the individual compound. As pointed out by Mulliken ,1964, methoxybenzene $C_6H_5OCH_3$, containing a benzene and a methoxy (-OCH3 group), performs as a nπ-type donor. All chlorocompounds in the present programme, will perform as σ acceptor toward C_6H_5- OCH_3, and forms hydrogen bond on account of the presence of Cl and H atoms in $CHClCCl_2$, CH_2ClCH_2Cl, t**etrachloroethene** and CH_2Cl_2 . Measurements of ε data for above mentioned mixtures at 303.15 K have been undertaken in the present research for understanding the interactions between methoxybenzene and other mentioned chlorocompounds in the liquid state.

Materials

CH_2Cl_2 (qualickem), and CCl_2CCl_2 (E. Merck, Darmstadt, FRG), , were dried over anh.$CaCl_2$ before use for removing moisture content. CH_2ClCH_2Cl (E.Merck) was shaken with solution of $NaHCO_3$, and then dried over anh. CaCl2 , and then distilled from P_2O_5. $CHClCCl_2$ (A.R.grade) was washed with an aq. solution of K2CO3, then rinsed with H2O, and dried above anh.K_2CO_3 and $CaCl_2$, and then distilled fractionaliy . Methoxybenzene ($C_6H_5OCH_3$) (E.Merck) was obtained by distillation from Na.

Method

Dielectric constants for pure as well as their mixtures were determined at 303.15 ± 0.01 K and at a known frequency of 1.8 MHz using a dekameter as described by Nath and Tripathi, 1984.

Results and Discussion

The values of relative permittivity data for different mixtures are collected in table 1. The values of ε for pure liquids CH_2Cl_2, CH_2ClCH_2Cl, $CHClCCl_2$, CCl_2CCl_2, and $C_6H_5COCH_3$ at 303.15 K are obtained to be 8.703, 10.071, 3.346, 2.295, , and 4.246, correspondingly, which are in good agreement with the literature (Lange,1973) values. The dielectric constants ε of the various mixtures have been used to calculate the quantityΔ ε from the relation

$$\Delta \varepsilon = \varepsilon - x_1 \varepsilon_1 - x_2 \varepsilon_2$$

where ε_1, x_1 and ε_2, x_2 refer to the dielectric constants and mole fraction of the two pure components 1 and 2. The values of Δ ε vs x1, is plotted in Fig.1. As indicated by Fig.1 the Δ ε data are negative for mixtures of Methoxybenzene+ CH_2Cl_2,Methoxybenzene + CH_2ClCH_2Cl, , Methoxybenzene + CCl_2CCl_2, and positive for Methoxybenzene +$CHClCCl_2$. The negative values of Δ ε **,** for all the systems except for Methoxybenzene +$CHClCCl_2$, can be explained as due to a lower within the degree of combination of the molecular dipoles with converting composition of the combination.Δ ε is found to be in reversed sign for those mixtures where strong interaction occurs between the components as shown by the system Methoxybenzene +$CHClCCl_2$ in the present case (Rivail et.al,1974).

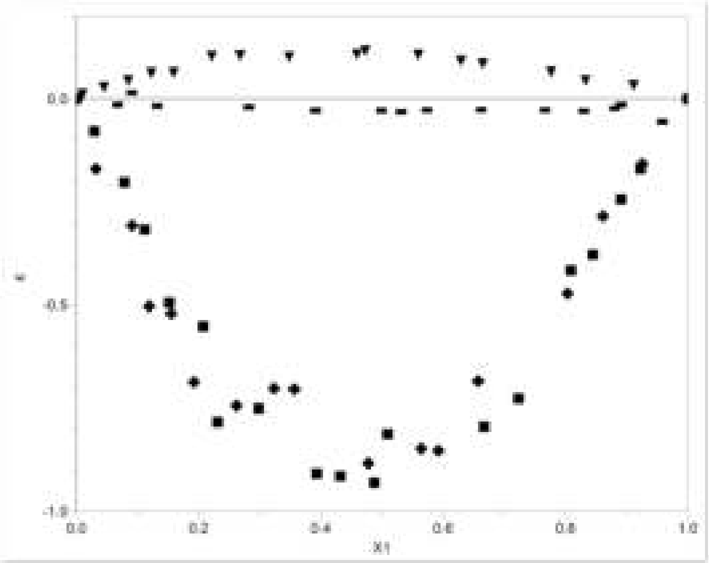

Fig.1. Plot of Δ ε vs x1 at 303.15K for the systems of methyloxybenzene+ Dichloromethane , ◆,+ Ethylene dichloride , ■, + Tetrachloroethylene , ▼ , and + $CHClCCl_2$, ▬ .

The data also display that $CHClCCl_2$ creates strong interaction with methoxybenzene. The occurrence of a interaction between methoxybenzene and all mentioned chlorocompounds may be because of the formation of a weak hydrogen bond between the H atoms of chlorocompounds and the π-electrons in the benzene ring of methoxybenzene.There's, however, additionally an opportunity that methoxybenzene can create a r complex with the methoxybenzene, ***via Cl*** atom-π-electron interactions, such type of complexes may be charge transfer. Alternatively, the complex formation between methoxybenzene + CH_2Cl_2,or + CH_2ClCH_2Cl ,or + $CHClCCl_2$ may be due to the creation of strong interaction (probably creation of H- bonds) between the H atom of these chlorocompounds and the non-bonding pair of electrons on the O atom of methoxybenzene.

Table1. Dielectric constants for methoxybenzene in different mixtures mixtures at 303.15 K

Methoxybenzene+ CH_2Cl_2		**Methoxybenzene + CH_2ClCH_2Cl**	
$x1$	ε	$x1$	ε
0.0000	8.703	0.0000	10.071
0.0321	8.39	0.0295	9.82
0.0912	7.99	0.0787	9.41
0.1189	7.67	0.1122	9.10
0.1553	7.49	0.1523	8.69
0.1921	7.16	0.2076	8.31
0.2623	6.79	0.2312	7.94
0.3233	6.56	0.2987	7.58
0.3565	6.41	0.3934	6.87
0.4776	5.69	0.432	6.64
0.5643	5.34	0.4876	6.30
0.5923	5.21	0.5095	6.29
0.6571	5.09	0.6672	5.39
0.8034	4.65	0.7234	5.13
0.8611	4.58	0.8091	4.94
0.9255	4.42	0.8452	4.77
1.000	4.246	0.8911	4.64
		0.923	4.53
		1.0000	4.246

Methoxybenzene + CCl_2CCl_2		Methoxybenzene + $CHClCCl_2$	
x1	ε	x1	ε
0.0000	2.295	0.0000	3.346
0.0673	2.412	0.0102	3.367
0.0906	2.487	0.0451	3.415
0.1321	2.536	0.0851	3.468
0.2823	2.826	0.1227	3.519
0.3912	3.031	0.1592	3.553
0.4991	3.241	0.2215	3.649
0.5312	3.311	0.2682	3.692
0.5733	3.387	0.3483	3.761
0.6622	3.561	0.4589	3.867
0.7665	3.763	0.4724	3.888
0.8301	3.886	0.5592	3.956
0.8804	3.989	0.6292	4.005
0.8911	4.056	0.6647	4.032
0.9587	4.169	0.7762	4.111
1.0000	4.246	0.8332	4.141
		0.9111	4.199
		1.0000	4.246

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