

Advances in Chemical Science: Exploring New Frontiers



UMENDRA KUMAR



Advances in Chemical Science: Exploring New Frontiers

IIP Series

WPS Office



Preface

Advancements in scientific research have always been the driving force behind human progress, unlocking new realms of understanding and pushing the boundaries of what is possible. In the dynamic and ever-evolving field of chemical science, the quest for knowledge and innovation is relentless. "Advances in Chemical Science: Exploring New Frontiers" stands as a testament to the collective efforts of pioneering researchers who have ventured into uncharted territories, pushing the frontiers of chemical knowledge to unprecedented heights.

This edited volume serves as a comprehensive compendium of the latest breakthroughs and emerging trends in chemical science. As the scientific community continues to unravel the complexities of matter and explore the intricacies of chemical interactions, this book provides a snapshot of the diverse and groundbreaking research that defines the contemporary landscape of the discipline.

The chapters contained within this volume reflect the multidisciplinary nature of modern chemical science, encompassing a wide array of subfields such as organic chemistry, inorganic chemistry, physical chemistry, biochemistry, nano technology, chemical biology and materials science. From fundamental theoretical studies to practical applications, each contribution illuminates a unique facet of chemical science, contributing to the mosaic of knowledge that shapes our understanding of the world around us.

The journey through "Advances in Chemical Science" begins with a thought-provoking exploration of theoretical frameworks that underpin our understanding of chemical phenomena. From there, the reader is guided through a spectrum of research endeavors, ranging from the synthesis of novel compounds to the design of innovative materials with tailored properties. The interplay between theory and experiment, a hallmark of successful scientific inquiry, is exemplified in each chapter, underscoring the collaborative efforts of theorists and experimentalists alike.

Title of the Book: Advances in Chemical Science: Exploring New Frontiers

Edition: IIP Series

Copyright 2023 © Editor

Umendra Kumar,

No part of this book may be reproduced or transmitted in any form by any means, electronic or mechanical, including photocopy, recording, or any information storage and retrieval system, without permission in writing from the copyright owners.

Disclaimer

The authors and editors are equally responsible for the contents published in this book. The publishers or editors do not take any responsibility for the same in any manner. Errors, if any, are purely unintentional and readers are requested to communicate such errors to the editors or publishers to avoid discrepancies in future.

ISBN: 978-93-5747-689-8

MRP Rs. 470/-

Publisher, Printed at & Distribution by:

Selfypage Developers Pvt Ltd.,
Pushpagiri Complex,
Beside SBI Housing Board,
K.M. Road Chikkamagaluru, Karnataka.
Tel.: +91-8861518868
E-mail: publish@iiponline.org

IMPRINT: I I P Iterative International Publishers

For Sales Enquiries:

Contact: +91- 8861511583
E-mail: sales@iipbooks.com

Acknowledgement

The completion of "Advances in Chemical Science: Exploring New Frontiers" has been a collaborative effort that would not have been possible without the dedication, expertise, and support of numerous individuals and institutions. As editor, I extend my heartfelt gratitude to all those who have played a pivotal role in bringing this edited volume to fruition.

First and foremost, I express my deepest appreciation to the contributing authors whose outstanding research forms the cornerstone of this book. Your commitment to advancing the frontiers of chemical science and your willingness to share your expertise have enriched the contents of this volume immeasurably.

I extend my sincere thanks to the reviewers who generously dedicated their time and expertise to critically evaluate the submitted chapters. Your constructive feedback and insightful comments have been instrumental in maintaining the high quality and rigor of the content presented in this book.

My gratitude also extends to the publishers and editorial staff who have supported and guided me throughout the publication process. Your professionalism, attention to detail, and commitment to excellence have been invaluable in transforming the vision of this book into a reality.

I acknowledge the academic institutions and research organizations that have provided the intellectual and infrastructural support necessary for the contributors to pursue their groundbreaking research. The collaborative spirit fostered by these institutions has undoubtedly contributed to the vibrant and diverse collection of chapters within this volume.

I express my thanks to my colleagues, friends, and family for their unwavering encouragement and understanding throughout the demanding process of editing this book. Your support has been a

source of inspiration, motivating us to strive for excellence in every aspect of this project.

Finally, I acknowledge the global scientific community, whose collective pursuit of knowledge and innovation continues to propel the field of chemical science forward. It is my hope that this edited volume serves as a testament to the collaborative spirit and shared commitment to advancing the frontiers of scientific inquiry.

In conclusion, the realization of "Advances in Chemical Science: Exploring New Frontiers" is the result of a collective effort, and I extend my sincere thanks to all those who have contributed to its success. May this book inspire continued exploration and discovery in the fascinating world of chemical science.

Umendra Kumar

WPS Office

In addition to traditional areas of study, this volume also delves into the burgeoning intersections of chemical science with other disciplines. The exploration of the interface between chemistry and biology, the development of environmentally sustainable practices, and the application of advanced analytical techniques showcase the dynamic and interconnected nature of contemporary chemical research.

I hope that "Advances in Chemical Science: Exploring New Frontiers" will inspire researchers, students, and enthusiasts to delve into the fascinating world of chemical science. May the discoveries within these pages spark new ideas, foster collaborations, and ignite a passion for pushing the boundaries of knowledge. Together,

Umendra Kumar

WPS Office

Contents

1. NANOMATERIALS AND NANOSTRUCTURES IN
CHEMISTRY: A REVIEW OF SYNTHESIS AND
CHARACTERIZATION METHODS
.....
Umendra Kumar
2. A STUDY OF THE PHYSICO-MECHANICAL AND COMBUSTION
ANALYSIS OF BRIQUETTES PRODUCED
FROM BAMBARANUT SHELL.
.....
Ikelle Ikelle, Eze Nkechinyere, Esonye Chibuzo
3. A REVIEW -POLYMERIC NANOCOMPOSITES
.....
Dr. Dev Raj Singh
4. FATTY ACID COMPOSITION OF GULMOHAR SEED OIL
FROM BULANDSHAHR (U.P.)
.....
Alka Gupta, Mukesh Kumar
5. AROMATHERAPY: A SYNERGY THERAPY
.....
Dr. Shaifali Srivastava
6. SYNTHESIS OF POLYSTYRENE NANOPARTICLES AND
THEIR APPLICATION FOR DETECTION OF *INFECTIOUS
BURSAL DISEASE VIRUS (IBDV)*
.....
M K Choudhary
7. COMPREHENSIVE STUDY OF SUGAR OXIDATION WITH
Cr(VI) OXIDANTS
.....
Ashish Tomar, Unik Arora
8. QUANTIFYING THE IMPACT OF AIRBORNE POLLUTANTS
ON URBAN AIR QUALITY: A COMPREHENSIVE ANALYTICAL
STUDY
Dev Prakash
9. STRUCTURAL AND THERMAL DECOMPOSITION
STUDIES OF Co(III) AND Ni(II) METAL COMPLEXES
OF SCHIFF BASES
.....
Vishrut Chaudhary

DIMETHYL CARBONATE WITH ETHERS: THERMOPHYSICAL STUDY

Abstract

Viscosities, densities of liquid-liquid combinations of dimethyl carbonate with (Butyloxy) ethylene, 2-isopropoxypropane, methyl phenyl ether, and 1-Butoxybutane have been calculated through the entire compositions radius at temperatures (303.15, 308.15 and 313.15)K. The empirical values have been employed to measure the deflection in viscosity $\Delta\theta$, excess Gibb's free energy. The excess property has estimated and adapted to the Redlich-Kister polynomials. Their outputs are explained in terms of molecular interactions present in mixtures.

Keywords: Density, Viscosity, dimethyl carbonate, Gibbs free energy, Redlich-Kister equation.

Author

Ajit N. Bhumkar
Branch – Chemistry,
VPM's B.N. Bhandodkar
College of Science
(Autonomous), Thane
Maharashtra,
India.

10. DIMETHYL CARBONATE WITH ETHERS:
THERMOPHYSICAL STUDY
.....
Ajit N. Bhumkar

11. ZINC INDUCED OCCUPATIONAL TOXICITY
.....
Heena, Satyandra Kumar, Yeshvendra Verma, Malti

12. SELF-ACTIVATING DNA CLEAVAGE BY MONONUCLEAR
COPPER COMPLEXES
.....
Pramod Kumar, Sushil Kumar

13. MOLECULAR INTERACTIONS STUDY BETWEEN BUTYL
ACETATE WITH ALKANES USING ULTRASONIC TECHNIQUES
.....
Pralhad S Wagh

14. A REVIEW OF HYDROGELS THEIR CLASSIFICATIONS, AND
APPLICATIONS
.....
Deepti Chauhan

15. GREEN AND SUSTAINABLE CHEMISTRY
.....
*Mohit Saroha, Renu Swami, Bhupinder Singh, Akshay Kumar,
Deepak Tomar*

16. FUNCTIONALIZATION OF CARBON NANOTUBES FOR
ENHANCED MECHANICAL AND ELECTRICAL PROPERTIES
.....
Sunil Sharma

17. EFFECT OF TEMPERATURE AND CARBON CHAIN LENGTH ON
THE ACOUSTIC PARAMETERS OF AMMONIUM SOAPS
IN 2-PROPANOL
.....
Arvin Panwar

18. THEORETICAL EXPLORATION OF THE ELECTRONIC
PROPERTIES AND REACTIVITY OF NITROGEN-CONTAINING
HETEROCYCLES
.....
Soni Mittal

19. CHEMICAL TOOLS FOR UNDERSTANDING PROTEIN
CONFORMATIONAL CHANGES
.....
Renuka Tomar, Priya Tomar

be most beneficial in the recharging battery technique of lithium. It is also used in gasoline industry.

Ethers are tremendously used as trading solvents and moving agent for Greece oil, pastes, compound containing carbon and hydrogen, organic base compound containing Nitrogen, lubricants, wax, colouring agent, plastics, covering, and tints. They are employed as to remove wax. n-Butoxy ethylene is generally employed as active diluting agent, in the radiation restoring of cross-breed plastic coatings for colours, pigments, adherents, etc, Diisopropyl ether have wide variety of applications. It is mostly used as a solvent as derived from oil solutions easily liquefy in this. This create it is authentic base for various stains, waxes, colours and fixatives. It is commonly utilized as a solvent in colour slimmers and spot erasers. In the constructing of manufactured colors and polymers diethyl ether is employed as a solvent it was introduced as sedative agent in many countries but now it was replaced. Methoxy benzene is a pale yellow colored to faded solvent with a little tangy smell. It is employed in scents, as a added flavor in nourishments, and in the preparation of different chemical agents.

Density, vicinity and free enthalpy of the mixtures containing dimethyl carbonate give information about how to develop the injection system and inspect the flowing liquid, it assist in good understanding the molecular interactions of the mixture.

There are many works are obtainable in letters on thermodynamic and thermophysical characteristics of dual liquid-liquid combinations containing dimethyl carbonate in association of different organic liquids. M.V.Rathnam et al⁹ have studied densities, viscosities and index of refraction of binary liquid-liquid combinations of dimethyl carbonate with with acetyl benzene, ketocyclopentane, cyclohexyl ketone, and diethyl ketone along the complete range of configuration at the temperatures 303.15, 308.15 and 313.15 K and at barometric pressure. The index of refraction information have been corresponded by utilizing Lorentz–Lorentz,

I. INTRODUCTION

To the better perceiving of the intermolecular and intramolecular interactions present between the different species in a solution, the studies on thermodynamic properties of binary liquid-liquid combinations are important. The study provides detailed knowledge regarding changes with reference to structure and in packing efficiencies that occurred in solution while blending process¹. Such research work has been carried out on this properties of non- electrolyte solutions. Thrilling evolutions in this field of non-electrolyte solution has shown great efforts by Patterson-Delmas²⁻⁵, concerning how impact of molecular size affect the thermodynamic properties of binary liquid-liquid combinations. In chemical, pharmaceutical and engineering disciplines⁶, investigational computations of viscosities, densities and free energy of activations information play very vital role in these industries. So study of these properties from practical and theoretical point of view is crucial for binary liquid-liquid combinations. In expanding separation techniques like HPLC, capillary electrophoresis⁷, and designing of processes including separation of chemical substances, fluid flow, mass and heat transport processes, viscosities and densities data are required.

Carbonic ester of dimethyl is an eco friendly solvent. It is employed to prepare platings, stickings, and rinsing negotiators. It is employed as a starting compound for many biotic manufacturing. It is a green reagent because of its nontoxicity and its biodegradability in nature. Dimethyl sulphate, carbonyl chloride, iodomethane, are very toxic but dimethyl carbonate can be plyed instead of them in methylation and carbonylation synthesis. Dimethyl carbonate easily catch the fire because of its low turning point (290.15 K). So there is restrictions for using in indoor applications. But DMC is safer than other organic solvents like, propanone, methyl ethanoate, 3-pentanone concerning catching fire perspective. Dimethyl carbonate (DMC), has higher activity, less persistence⁸, good natured solvent qualities so it is employed in many industries. Dimethyl carbonates have revealed to

discovered to be $> 99.6\%$. These compounds were collected over 0.4 nm molecular sieves to minimize aqua content and refined fair prior to work.

2. Methods

The dual liquid-liquid combinations were developed by blending fixed amount of unadulterated liquids in closed ground stoppered glass so as to decrease dispersal deprivations. The mass estimations were correct to ± 0.01 mg were done on a well programmed electronic balance (Mettler AE 240, Switzerland). Unreliability of observed molar proportion were determined which is lower than ± 0.0001 .

First densitometer (DDM -2910, Rudolph Research Analytical) was set by utilizing distilled water. The temperature of densitometer is fixed at required value. Internal thermostat had good precision ± 0.1 . There is inbuilt air pressure in densitometer that help in drying the estimating cell after washing it. There should not be air bubbles in estimating cell while taking the readings. First clean the estimation cell with sample to expel the impurities if, present. Then final sample of mixture is introduced into estimation cell by using syringe. In this way densities of sterling chemicals and their dual combinations were taken. The density measurements were accurate to $\pm 0.00005 \text{ g.cm}^{-3}$.

Ubbelohde viscometer is thoroughly washed and completely dried it. First, flow time of water was calculated at desired temperatures. Well programmed stopwatch was used having unreliability of ± 0.04 s. The sterling liquid compounds and their combinations viscosity were evaluated at the barometric pressure and the required temperature. Its arms were sealed by inert lids for stopping of vanishing solvents. The viscometer was put in water bath having thermic steadiness of ± 0.02 K. It was placed for 25 min. Minimum three readings were taken. The viscosity (θ) was estimated from outflow pattern 'm' by considering the equation.

Weiner, Newton, Gladstone–Dale, Eykman, and Eyring–John relations.

Jaime Wisniaka et al¹⁰ have studied densities of the dual systems of dimethyl carbonate with butyl-2-methylpropenoate, cis-cyclooctane-1,2-diol, vinyl benzene, and acetic acid vinyl ester over the entire range of the concentrations at (293.15, 303.15, and 313.15) K at barometric pressure, employing an Anton Paar DMA 5000 oscillating U-tube densitometer. They correlated the intentional excess molar volumes with the Redlich–Kister equation and with a series of Legendre polynomials. A clarification of the outputs is provided depending on the FT-IR (ATR) spectra of several combinations of the various systems. Michael A. Pacheco and Christopher L. Marshall¹¹ have reported, the propellant properties and studied chemical blending plans for DMC are assessed. E. R. Lopez et al¹² have measured densities γ and excess molar volumes of (dimethyl carbonate + methyl benzene) at the temperatures (278.15, 288.15, 298.15, 308.15, 318.15, and 323.15) K and using an Anton-Paar DMA602HP densitometer. The observed data were employed for the computation by analytical differentiation of the backing quantities: the cubic expansion coefficient, the excess cubic expansion of coefficient, $(\partial V E m / \partial T)_p$ and $(\partial H E m / \partial p)_T$. Gibb's free energy for the binate combinations of dimethyl carbonate + (Butyloxy)ethylene, 2-isopropoxypropane, methyl phenyl ether, and 1-Butoxybutane at temperature (303.15, 308.15 and 313.15) K with respect to mole fractions are measured.

II. PRACTICAL

1. Chemicals

Dimethyl carbonate, (Butyloxy)ethylene, 2-isopropoxypropane, methyl phenyl ether, and 1-Butoxybutane (mass little bit purity >99.10%) every one of the obtained from Sigma-Aldrich. The clarity of every one of the these compounds were estimated by vapor phase chromatography (VPC-8610,) and the investigation clarity were

The negative $\Delta\theta$ values for (Butyloxy)ethylene, 2-isopropoxypropane, methyl phenyl ether, and 1-Butoxybutane follows the order 1-Butoxybutane < 2-isopropoxypropane < (Butyloxy)ethylene < methyl phenyl ether.

The Gibb's free energy was obtained by following equation

$$\Delta G^{*E} = RT[\ln\theta_{12}v_{12} - (x_1\ln\theta_1v_1 + x_2\ln\theta_2v_2)] \quad (3)$$

where R is the universal gas constant, T is absolute temperature, θ_{12}, v_{12} are viscosity and molar volume of the combinations respectively, θ_1, v_1, θ_2 , and v_2 are the viscosity and molar volumes and of pure compounds 1 and 2 respectively. The molar volume of dual liquid-liquid combinations (v_{12}) is obtained from the density of the combination using the equation.

$$N_{12} = (x_1m_1 + x_2m_2) / \gamma_{12} \quad (4)$$

The excess Gibb's free energy of activation of viscous flow ΔG was obtained by utilizing the equation (3) and these values are graphically shown in Figures 2. It was found that for dimethyl carbonate + (Butyloxy) ethylene, 2-isopropoxypropane, 1-Butoxybutane the curves for ΔG are negative and for anisole the ΔG value is positive along the whole concentration at every one of the observed temperatures. The ΔG values for dimethyl carbonate + (Butyloxy) ethylene, + 2-isopropoxypropane, + 1-Butoxybutane decreases with increasing temperature. While for dimethyl carbonate + anisole curves values increases in rising of temperature across the composition of ester at all the studied temperature. The minima for dimethyl carbonate + butyl vinyl ether is at $x_1 = 0.4995$. The study of excess Gibb's free energy, viscosity deviations are important for determining the molecular interactions between components in combinations. The studied positive ΔG value may be due to the flow of system is hard as compared to flow of pure components¹⁷. Also the positive values of it indicate there are powerful specific interactions between unlike molecules. The negative ΔG value may be due to easier flow of binary system¹⁸.

The outcomes of $\Delta\theta$ and ΔG for dual liquid-liquid combinations at (303.15, 308.15 and 313.15) K are diagrammatically shown in figures 1-2. Then outcomes were fitted to the Redlich-Kister [5] polynomial relation by the procedure of least squares to get the dual solution coefficients B0, B1, and B2.

$$\Delta Y = x_1 x_2 [B_0 + B_1(x_1 - x_2) + B_2(x_1 - x_2)^2] \quad (5)$$

where ΔY indicate the discussed characteristics. The standard deviations for $\Delta\theta$ and ΔG were measured by following relation.

$$\Sigma(Y) = [\sum (Y_{\text{expt}} - Y_{\text{cal}})^2 / (P - p)]^{1/2} \quad (6)$$

where 'P' is the number of data points and p is the number of coefficients. The measured values of the polynomial coefficients B0, B1, and B2 along with their standard deviations σ are given in Table 1.

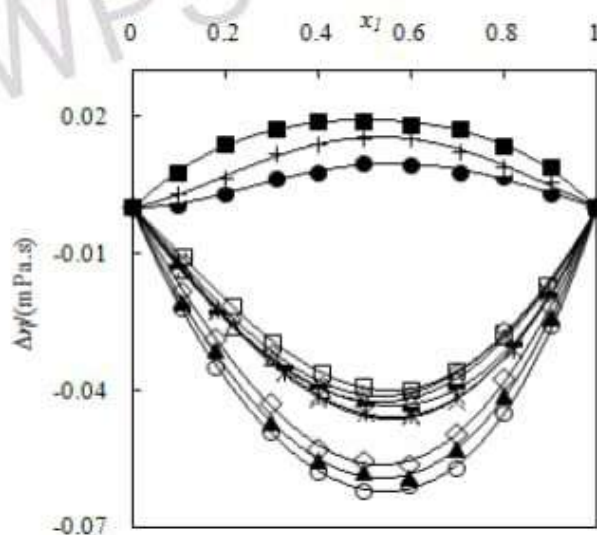


Figure.1: Deviation in viscosity ($\Delta\theta$) Vs mole fraction (x_1) for the binary combinations of Dimethyl carbonate + (Butyloxy)ethylene at (\square , 303.15 ; \diamond , 308.15 ; Δ , 313.15) K,

$$\Theta = \gamma(Xm-Y/m) \quad (1)$$

where, γ is the density and X and Y are the characteristic constants of the viscometer. X and Y are fixed by using water as setting solvents. The unreliability in the viscosity was got to be ± 0.005 m.Pas.

III. OUTCOMES

Gibb's free energy, density γ , viscosity θ , of the binary mixtures are measured against the mole fragments x_1 of dimethyl carbonate for the calculated dual combinations at (303.15, 308.15 and 313.15)K.

The deviations in viscosity $\Delta\theta$ were measured by following relation.

$$\Delta\theta = \theta_{12} - (x_1 \theta_1 + x_2 \theta_2) \quad (2)$$

where x_1 , θ_1 , θ_2 and θ_{12} are proportionately the mole fragment, viscosity of pure compounds and their combinations.

The viscosities (θ), deviations in viscosities ($\Delta\theta$) for the dual liquid-liquid combinations of dimethyl carbonate are calculated at $T = (303.15, 308.15 \text{ and } 313.15) \text{ K}$. The deviation in viscosities ($\Delta\theta$) obtained by using the equation (2) have been graphically represented in Figures 1. From the graphs it was found that for the combinations of dimethyl carbonate + (Butyloxy)ethylene, 2-isopropoxypropane, and 1-Butoxybutane, the $\Delta\theta$ values are found to be negative while, for dimethyl carbonate + anisole $\Delta\theta$ values are got positive across the entire concentrations and at the studied temperatures. Observed negative $\Delta\theta$ values indicates dispersion or weak dipole-dipole interactions among the molecules in the mixtures.¹³⁻¹⁴ The negative curves for $\Delta\theta$ indicate there are different molecular size of molecules in components of the mixture.¹⁵⁻¹⁶ From these tables it is observed that for dimethyl carbonate + butyl vinyl ether, + dibutyl ether the values of viscosity decreases with rising of temperature, for dimethyl carbonate + diisopropyl ether, + anisole the values of viscosity rises with growing of temperature.

Table 1: Derived parameters by Redlich-Kister relation for excess properties for different functions and Standard deviation (σ) for the dual system

Function	T/K	B0	B1	B2	σ	B0	B1	B2	Σ
Dimethyl carbonate (1) + Butyl vinyl ether (2)						Dimethyl carbonate(1)+ Diisopropyl ether(2)			
ΔG	303.15	-732.4	36.084	124.7	3.413	-374.05	3.1266	129.57	3.510
	308.15	-622.63	2.758	189.4	5.822	-443.00	-17.840	160.735	3.516
	313.15	-511.4	-71.80	190.4	2.600	-489.14	26.15	-15.2955	3.583
Dimethyl carbonate (1) + Anisole (2)						Dimethyl carbonate (1) + Dibutyl ether (2)			
ΔG	303.15	523.64	142.88	-60.384	1.802	-361.11	-41.480	151.43	3.420
	308.15	577.58	143.87	-88.624	2.335	-495.24	-52.512	56.446	3.612
	313.15	638.05	132.88	120.73	2.322	-654.90	-107.14	-29.67	2.588

DIMETHYL CARBONATE WITH ETHERS: THERMOPHYSICAL STUDY

Dimethyl carbonate + 2-isopropoxypropane at (\times , 303.15; κ , 308.15; — , 313.15) K,

Dimethyl carbonate + Methoxy benzene at (\bullet , 303.15; $+$, 308.15; \blacksquare , 313.15) K,

Dimethyl carbonate + 1-Butoxybutane at (\diamond , 303.15; \blacktriangle , 308.15; \circ , 313.15) K.

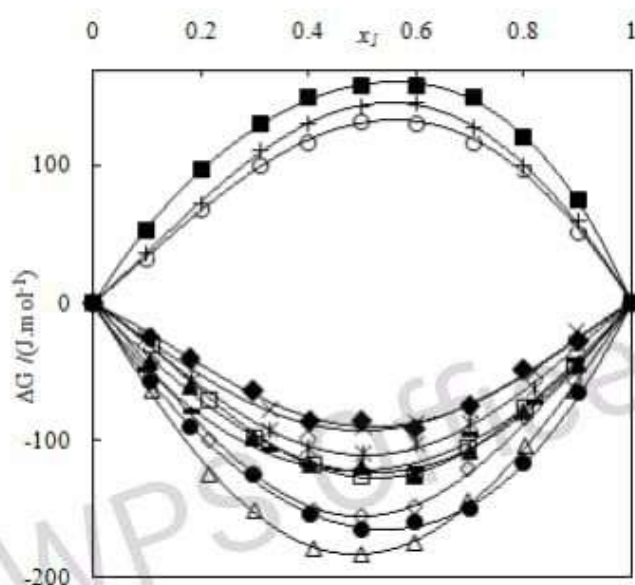


Figure 2: Excess free energy of activation (ΔG) Vs mole fraction for the binary mixture of ,

Dimethyl carbonate + (Butyloxy)ethylene at (\square , 303.15; \diamond , 308.15; Δ , 313.15) K,

Dimethyl carbonate + 2-isopropoxypropane at (\times , 303.15; κ , 308.15; — , 313.15) K

Dimethyl carbonate + Methoxy benzene at (\circ , 303.15; $+$, 308.15; \blacksquare , 313.15) K

Dimethyl carbonate + 1-Butoxybutane at (\blacksquare , 303.15; \blacktriangle , 308.15; \bullet , 313.15) K

DIMETHYL CARBONATE WITH ETHERS: THERMOPHYSICAL STUDY

- [8] Densities and viscosities for binary mixtures of dimethyl carbonate with 1-heptanol, 1-octanol, 1-nonanol, and 1-decanol Hao Wang, Nianzu Zhang, Xiaopo Wang, The Journal of Chemical Thermodynamics, 157, 106404, June 2021.
- [9] Rathnam, M.V.; Mohite, S.; Kumar, M.S.S. Thermophysical properties of binary mixtures (dimethyl carbonate + ketones) at $T = (303.15, 308.15 \text{ and } 313.15) \text{ K}$, J. Mol. Liq. 163, 170-177, (2011).
- [10] Jaime, W.; Gladis C.; Rene D.P.; Ramiro I.; Luis E. E.; Tlaloc A. A.; Omar G.; Homero S., Density, excess volume, and excess coefficient of thermal expansion of the binary systems of dimethyl carbonate with butyl methacrylate, allyl methacrylate, styrene, and vinyl acetate at $T = (293.15, 303.15, \text{ and } 313.15) \text{ K}$, J. Chem. Thermodyn. 40, 1671-1683, (2008).
- [11] Pacheco, A.M.; Marshall, L.C.; Review of Dimethyl Carbonate (DMC) Manufacture and Its Characteristics as a Fuel Additive, Energy and Fuels. 11, 2-29, (1997).
- [12] Lopez, E.R.; Lugo, L.; Comunas, M.J.P. Temperature dependence of the excess molar volume of (dimethyl carbonate, or diethyl carbonate + toluene) from $T = 278.15 \text{ K}$ to 323.15 K , J. Chem. Thermodyn. 32(6), 743-754, June (2000).
- [13] **H. Iloukhani, H.A. Zarei, M. Behroozi, Thermodynamic studies of ternary mixtures of diethylcarbonate (1) + dimethylcarbonate (2) + N,N-dimethylacetamide (3) at 298.15 K, Journal of Molecular Liquids, 135(1-3), 141-14, July 2007.**
- [14] Oswal, S. L.; Rathnam, M. V. Viscosity data of binary mixtures: ethyl acetate + cyclohexane, + benzene, + toluene, + ethylbenzene + carbon tetrachloride, and + chloroform at 303.15 K, Can. J. Chem. 62, 2851, (1984).
- [15] **Fort, R. J.; Moore, W. R. Trans. Faraday. Soc, Viscosities of binary liquid mixtures, 62, 112, (1966).**
- [16] Solimo, H. N.; Riggio, R.; Davolio, F.; Katz, M. Thermodynamic Properties of Binary Liquid Acid-Base Mixtures, Can. J. Chem. 53, 1258, (1978).
- [17] Tiwari, K.P. J. Appl. Chem. Dielectric Parameters and Intermolecular Interactions in Binary Mixture of Hydroxyl Groups in Polar Liquids, 5(6), 1302-1306, (2016).
- [18] Dominguez, M; Pardo, J. J.; Gas Con, I; Royo, F.M.; Urieta, J.S. Viscosities of the ternary mixture (2-butanol+n-hexane+1- butylamine) at 298.15 and 313.15 K, Fluid Phase Equilib. 169(2), 277-292, March (2000).

ABOUT THE EDITOR



Dr. Umendra Kumar holds the position of assistant professor in the postgraduate department of chemistry at Janta Vedic College, Baraut (CCS University Meerut). He received his doctoral degree from CCS University, Meerut, and boasts a substantial record of teaching and research endeavors spanning across diverse domains within the field of chemical science. Dr. Kumar's primary research expertise lies in metallo-organic and synthetic organic chemistry, with a particular focus on pioneering novel methodologies for organic synthesis and their practical application in the creation of innovative organic compounds. His scholarly contributions encompass a prolific publication record, with more than 30 research articles in the realm of chemistry, in addition to his authorship of three textbooks centered around the subject of organic chemistry. Furthermore, Dr. Kumar's scholarly impact extends to his active participation and keynote deliveries at numerous national and international conferences and symposia. Dr. Kumar's professional involvement also encompasses his role as a distinguished member of the Editorial Board for the esteemed Journal of International Journal of Photochemistry and Photobiology, further attesting to his commitment and eminence in the academic community. Additionally, he holds the esteemed distinction of being a life and fellow member of prominent apex professional societies.



Selfypage Developers Pvt Ltd

ISBN: 978-93-5747-689-8



MRP Rs. 470/-

VII. CONCLUSION

Density, viscosity, Gibb's free energy of activation for dual liquid-liquid combinations of Dimethyl carbonate + (Butyloxy) ethylene, + 2-isopropoxypropane, + Methoxy benzene, + 1-Butoxy-butane are calculated along the whole concentration at (303.15, 308.15 and 313.15) K. Utilizing observed data excess Gibb's free energy of activation of viscous flow ΔG , deviation in viscosity $\Delta\theta$, were measured. These excess or deviation properties were fitted to Redlich-Kister polynomial equation. From these excess or deviation properties it is concluded that there will be weak interactions means less dispersion forces between Dimethyl carbonate and + (Butyloxy) ethylene, 2-isopropoxypropane, and 1-Butoxybutane whereas for (Dimethyl carbonate + methoxy benzene) combinations, there is particular interactions for example charge transfer complex are demanded.

The present article gives extensive collection data of physico-chemical characteristics of the dual combinations which are used in chemical and other related industries. The results by using this data can be used in the field of solution chemistry. The experimental mixing property data presented here are entirely new and will add a new wealth of information to the existing database.

REFERENCES

- [1] Mokate, O.; Ddamba, W. A. A. J. Sol. Chem. 15, 1493, (2006).
- [2] Delmas, G.; Turrell, S.; J. Chem. Soc. Faraday I. 70, 572, (1974).
- [3] Lam, V.T.; Picker, P.; Patterson, D.; Tancrede, P. J. Chem. Soc. Faraday II. 70, 1465, (1974).
- [4] Delmas, G.; De Saint Roman, P.; Purves, P. J. Chem. Soc. Faraday I. 71, 1181, (1975).
- [5] Croudher, M. D.; Patterson, D.; J. Chem. Soc. Faraday II. 70, 1479, (1974).
- [6] Lal K, Tripathi N, Dubey GP, Densities, viscosities, and refractive indices of binary liquid mixtures of hexane, decane, hexadecane, and squalane with benzene at 298.15 K. J ChemEng Data 45: 961-964, (2000).
- [7] SK Beebi, SKM Nayeem, GR Satyanarayana, A Venkateshwara Rao, D Bala and C Rambabu, viscometric study of molecular Interactions in Dimethyl Carbonate + n-Alkoxyethanol Mixtures at different Temperatures, Journal of Thermodynamics and Catalysis, 7,4, (2016).

Indexing and Abstracting in Following Databases

1. Bowker: A ProQuest Affiliate



2. Crossref



ISBN 9789361358296



9 789361 358296
₹ 736 US\$ 16

Published by
AkiNik Publications,
#169, C-11, Sector - 3, Rohini,
Delhi-110085, India
Toll Free (India): 18001234070

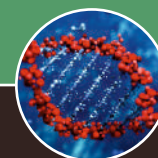
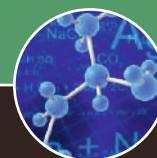
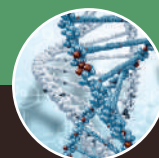


Attribution-NonCommercial-ShareAlike
4.0 International (CC BY-NC-SA 4.0)

Peer Reviewed & Refereed

ADVANCED RESEARCH IN Chemistry

Volume - 8



Chief Editor

Dr. Dhondiram Tukaram Sakhare

**AKINIK PUBLICATIONS
NEW DELHI**

ADVANCED RESEARCH IN

Chemistry

Volume - 8

Chief Editor

Dr. Dhondiram Tukaram Sakhare

Assistant Professor & Research Guide, UG, PG & Research Centre
Department of Chemistry, Shivaji Arts, Comm. & Science College Kannad,
Aurangabad, Maharashtra, India

AkiNik Publications®
New Delhi

Published By: AkiNik Publications

AkiNik Publications

169, C-11, Sector - 3,

Rohini, Delhi-110085, India

Toll Free (India) – 18001234070

Phone No.: 9711224068, 9911215212

Website: www.akinik.com

Email: akinikbooks@gmail.com

Chief Editor: Dr. Dhondiram Tukaram Sakhare

The author/publisher has attempted to trace and acknowledge the materials reproduced in this publication and apologize if permission and acknowledgements to publish in this form have not been given. If any material has not been acknowledged please write and let us know so that we may rectify it.

The responsibility for facts stated, opinion expressed or conclusions reached and plagiarism, if any, in this book is entirely that of the author. So, the views and research findings provided in this publication are those of the author/s only. The Editor & Publishers are in no way responsible for its contents.

© AkiNik Publications TM

Publication Year: 2024

Pages: 126

ISBN: 978-93-6135-829-6

Book DOI: <https://doi.org/10.22271/ed.book.2614>

Price: ₹ 736/-

Registration Details

- Printing Press License No.: F.1 (A-4) press 2016
- Trade Mark Registered Under
 - Class 16 (Regd. No.: 5070429)
 - Class 35 (Regd. No.: 5070426)
 - Class 41 (Regd. No.: 5070427)
 - Class 42 (Regd. No.: 5070428)

Contents

S. No.	Chapters	Page No.
1.	Hydrolysis of Hemicelullose from Oil Palm Empty Fruit Bunch for Xylose Production <i>(Yanni Sudiyani, Jessica Putri Rarassati, Roni Maryana, Muryanto, Eka Triwahyuni, Joni Prasetyo and T. Beuna Bardant)</i>	01-15
2.	Study the Thermoacoustical Properties of Vinyl Ethanoate with Ethers <i>(Ajit N. Bhumkar)</i>	17-29
3.	Synthesis of New Chalcone Scaffolds as Potential Antibacterial Agents <i>(Amit Vaishnav, Dheeraj Ahirwar and Pushpraj Ogre)</i>	31-44
4.	Applications of Nanotechnology in Agriculture <i>(Dr. Maheep Kumar, Dr. Tanvi Singh and Dr. Neelu Sharma)</i>	45-62
5.	Tropospheric Degradation of $\text{CF}_3\text{CH}=\text{CF}_2$ Initiated by Cl-Atoms: An Insight from Computational Study <i>(Ajay Kumar Yadav, Bhupesh Kumar Mishra, Ashutosh Singh and Nand Kishor Gour)</i>	63-75
6.	Basics of Nuclear Magnetic Resonance Spectroscopy and Practical Approach <i>(Rohit H. Dave, Kushal P. Shah and Arvindsinh B. Sisodiya)</i>	77-93
7.	Practical Aspects and Instrumentation of Inductively Coupled Plasma-Mass Spectrometry an Elemental Analyser <i>(Rohit H. Dave, Arvindsinh B. Sisodiya and Kushal P. Shah)</i>	95-110
8.	Discoveries in Green Chemistry <i>(Sowmya P T, Anitha Sudhir and Deziy Melita D Souza)</i>	111-126

Chapter - 2
**Study the Thermoacoustical Properties of Vinyl
Ethanoate with Ethers**

Author

Ajit N. Bhumkar

Department of Chemistry, VPM's B.N. Bandodkar College of
Science (Autonomous), Thane, Maharashtra, India

Chapter - 2

Study the Thermoacoustical Properties of Vinyl Ethanoate with Ethers

Ajit N. Bhumkar

Abstract

Ultrasonic velocities, viscosities, densities of binary liquid liquid combinations of vinyl ethanoate with butyl vinyl ether, diisopropyl ether, methoxy benzene, and dibutyl ether have measured along the whole concentration range at temperatures (303.15, 308.15 and 313.15)K. Observed data have been utilized to determine the excess acoustic impedance (Z^E), excess intermolecular free length (L_f^E). The excess properties have been fitted to the Redlich-Kister polynomials and the outcomes are analysed with respect to molecular interactions between the molecules in combinations.

Keywords: Density, viscosity, ultrasonic velocity, intermolecular free length, acoustic impedance

Introduction

The learning of audial properties of binary liquid-liquid combinations are important in better understanding of interactions among the molecules in concoctions. These provides vital information about composition, structure, bonding in between the molecules in mixtures. The blending of various solvents gives rise to solutions that generally do not act ideally. There is deflection from ideality which is shown by plenty of thermodynamic parameters especially by excess properties. Excess transport and acoustic property of solvent concoctions give the disagreement between actual property and the ideal property and that are beneficial in the understanding of molecular interactions and their arrangements. In specific they send back the interactions that occurred between solute-solute, solute-solvent and solvent-solvent species. The significance of excess properties can be broadly summarised as,

- a) Excess properties give crucial clue for determination of multi-component concoction property from pure component.

- b) Excess properties are often utilized to explain the different types of solutions.
- c) They give information for calculation of variables characterizing interactions between not similar molecules in the mixtures.
- d) They are useful in the development and testing of solution theories.

The elucidation of transport and acoustic qualities of thick fluids on a molecular ground is demonstrating very tough because of facing problems in determining for various body interactions. So it is needed to think about other methods. For showing combinations viscosity Coefficient data over a wide range of temperature for solvents and solvent concoctions are required in order to expand techniques of correlation, prediction and theories of transport properties. To understand intermolecular forces and their interactions among the molecules data of speed of sound, viscosity are necessary. These properties are important to develop thermodynamic models which are utilized in optimising processes of the pharmaceutical, petrochemical, and other industries. The information about ultrasonic velocity, density and viscosity of pure and their concoctions are needed in many engineering processes. The physico-chemical properties like density, viscosity, index of refraction, interfacial tension and acoustical properties such as ultrasonic velocity, isentropic compressibility and free volume etc. have found to be very beneficial to the chemists and chemical engineers from different angles

- i) To determine the uses of various theories of liquids and thus help in the prediction of properties of concoctions of alike nature.
- ii) To construe, correlate and analyse thermodynamic properties via molecular considerations.
- iii) To design industrial equipment with best precision thus minimizes capital costs.

The thermodynamic and acoustic properties of binary liquid-liquid concoctions of different type of solvents has fixed by various researchers [1-8]. Such measurements includes density, excess volume, viscosity, deflection in viscosity, excess free energy of activation of flow, excess enthalpy, refractive index, molar refraction, ultrasonic velocity, isentropic compressibility etc. The main reason for this to get the intermolecular interactions occurring in these liquid-liquid concoctions. Thus there is increase in the number of theoretical treatments. The behaviour of real solutions always shows some activity as a result exhibit deviations from ideality. In most of the practical situations, these deviations and their

magnitude are difficult to predict. Therefore one must resort to experimental measurements to determine the real behaviour of such solutions.

The solutions of liquid-liquid mixtures classified into polar-polar, polar-nonpolar, and nonpolar-nonpolar. The experimental learning of binary and triadic combinations tells the molecular interactions such as van der waal's forces, hydrogen-hydrogen bond, charge transfer composites, dipole-dipole, dipole-induced dipole, interstitial accommodate chain alignment etc. on the physical properties of binary liquid combinations. Data of these blending effects are helpful in planning and simulation processes in manufacturing of pharmaceuticals, lacquers, resins, polymers, oxygenated fuels, and paints [9-12].

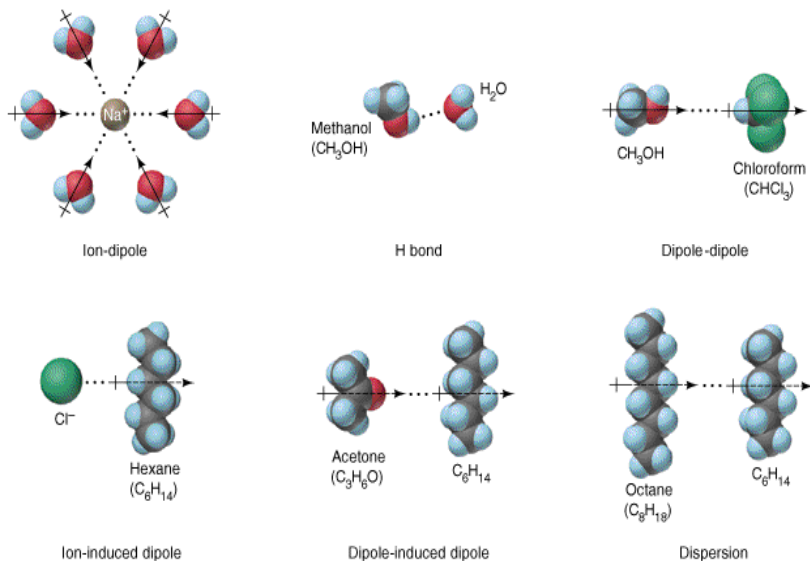
The knowledge of thermodynamic and transport effects of complex combinations utilized in many industries in planning engineering processes, such as adsorption, distillation, extraction, absorption etc. The excess properties are beneficial in scientific and technical fields, including Chemistry, Spectroscopy and Chemical Engineering.

The aim of this research is to

- i) To give new experimental data on density, viscosity, and speeds of sound of binary liquid-liquid concoctions of vinyl ethanoate and ethers.
- ii) To determine the excess or deflection parameters from the observed data and their correlation of properties using Redlich-Kister polynomial equation.
- iii) To Study correlating ability of various viscosity models.
- iv) To study the applicability of empirical relations proposed by Junjie's and Nomoto's to the observed ultrasonic velocity data of the studied binary combinations.
- v) Determine the impact of temperature on the calculated excess properties.

Ultrasonic velocity is used by many scientists to determine the nature of molecular interactions. These interactions may be weak or strong. The primary structure of the molecules gives powerful interactions such as covalent bonds. Higher order structures like secondary, tertiary and quaternary structures feeble interactions and can be disrupted by tentatively little rise in temperature. Strong interactions indicate in the formation of molecular structure. Feeble interactions indicate there is interaction between different molecules. Generally, Intramolecular forces are stronger than intermolecular forces.

Various qualities of chemicals, for examples boiling point and viscosity, show the powers of intermolecular forces (eg. If there is powerful intermolecular forces, then the boiling point and viscosities will increase). There are different kinds of intermolecular interactions and they differ with respect to its ability. Few examples of various kinds of intermolecular interactions are mentioned below.



There are Ion-ion Interactions in ionic crystals, Dipole-dipole forces present between neutral polar molecules. If polarity of the molecules increases, dipole-dipole interactions between the molecules also increases. London Forces are attractive forces and arises due to temporary dipoles in liquid molecules. London dispersion generally present between all molecules when molecules come close. Hydrogen Bond is a electrostatic force of attraction present between hydrogen atom in a polar bond with a neighbouring electronegative molecule. It is dipole-dipole type interactions. There is Ion-Dipole interaction, which is divided into induced Dipole-ion and Dipole-induced Ion interactions.

The strength of intermolecular interactions are given below as in descending order.

1. Ion-ion Interactions.
2. Dipole-ion Interactions.
3. Hydrogen Bonding.

4. Dipole-dipole interactions.

5. London Forces.

Polyvinyl acetate is a polymer which is identified as wood glue, carpenter's glue due to this property it is used as adhesive²⁸ for different porous materials wood, paper, cloth etc. It is also used in packing and building industries. Acetic acid vinyl ester is used for manufacturing of various industrial chemicals. These chemicals are used as raw materials for synthesis of different organic molecules. Vinyl acetate is utilized as emulsion. These resins give a best agreement between performance and cost and are typically utilized in adhesive applications, such as heat sealing. Oxygenated hydrocarbons are used in perfume industries, petroleum industries etc. Ethers are used as solvents in many pharmaceutical reactions.

There are many studies available in literature that provide information about excess or deviation properties of organic binary liq-liq combinations [13-19]. In this chapter I measured viscosity, density and ultrasonic velocity of vinyl ethanoate + vinyl butyl ether, 1-Butoxy butane, methoxy benzene and 2-isopropoxypropane combinations at the temperature $T=(303.15, 308.15$ and $313.15)$ K to study acoustic properties to determine deviations from ideality. The practical data are utilized to calculate excess acoustic impedance and excess intermolecular free length of binary liq-liq combinations. Redlich-Kister type polynomial equation is used to fit these excess properties to find binary coefficients, standard deviations.

Materials and Methods

Acetic acid vinyl ester, vinyl butyl ether, 1-Butoxy butane, methoxy benzene and 2-isopropoxypropane having purity greater than 98.50% one and all obtained from Sigma-Aldrich. The purity of these chemicals was examined by HPLC. By analysis the purity was observed greater than > 99.4%. These solvents were kept over 0.4 nm molecular sieves to decrease the moisture.

The closed lid bottles are used to collect binary liquid-liquid combinations by blending fix proportion of pure liquids. DDM-2910, Rudolph Research Analytical densitometer is utilized to count densities of pure and their mixtures. Ubbelohde viscometer is used to determine viscosities of samples.

Ultrasonic Velocity Measurement (Speed of Sound) can be done by using Continous wave technique and Pulse Technique in starting. Continous wave technique consists of optical methods [20] depends on learning of

acoustic grating and interferometric techniques.²¹ In pulse technique, measurement of transit time for a given path, able one to calculate sound speed in solvents [22-23].

The ultrasonic interferometer is superior than the pulse techniques. Differential path length and their accurate measurements with an optical interferometer involved in interferometer. Interferometric method has limitation because of applicable frequencies 10 to 100 MHz. For this research ultrasonic velocity of pure chemicals, and their binary liquid-liquid combinations were calculated by utilizing variable path single crystal interferometer F-81 (Mittal Enterprises, New Delhi, India) operating frequency of 2 MHz. It involves an electrically driven quartz transducer coupled with liquid column.

Outcomes

Intermolecular free length (L_f), and acoustic impedance (Z), are measured by utilizing the following relations for the binary mixtures by considering the observed density, viscosity and ultrasonic velocity data.

$$L_f = K \cdot (K_s)^{1/2} \quad (1)$$

$$K_s = 1/u^2 \rho \quad (2)$$

$$Z = u \cdot \Theta \quad (3)$$

Where K_s is the isentropic compressibility, u is ultrasonic velocity, Θ is density, K is the Jacobson constant which depend on temperature.

Excess parameters of the binary liquid-liquid combinations have calculated by using the relation

$$\Delta y = y_m - (x_1 y_1 + x_2 y_2)$$

Where y_m is a property of the combination viz, ultrasonic velocity (u), intermolecular free length (L_f), specific acoustic impedance (Z), y_1 and y_2 , x_1 and x_2 refer to the property and mole fraction of pure components 1 and 2 respectively and Δy indicates excess in observed parameter.

Diagrammatic presentation of Δu Vs mole fraction of vinyl acetate (x_1) at 303.15, 308.15 and 313.15 K is given in Figure 1. It is denoted that for system vinyl ethanoate + butyl vinyl ether, + dibutyl ether Δu exhibit negative and positive deviations, while for vinyl ethanoate + diisopropyl ether, vinyl ethanoate + methoxy benzene Δu shows completely negative deviations for whole composition and at all learned temperatures. Positive deviations show the increasing strength of interaction between component molecules of binary liquid-liquid combinations [24-25]. If strong interactions

arise among the components of a combinations leading to the formation of molecular aggregates and more compact structures, then sound will travel faster through the mixture by means of longitudinal waves and hence the speed of sound deviations with respect to a linear behaviour will be positive while if the structure breaking factor in the mixture predominates resulting expansion then the speed of sound through the mixture will be slower resulting into negative deviation in speed of sound [26].

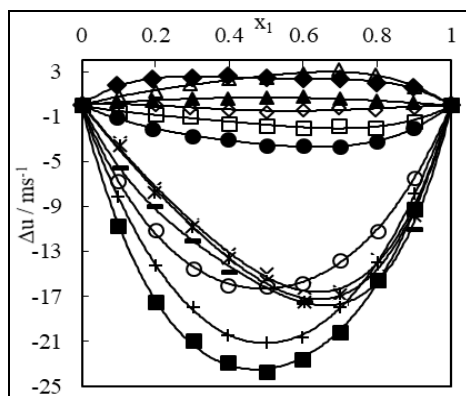


Fig 1: Curves of deviations in speed of sound (Δu) Vs. mole fraction (x_1) for the binary mixtures of vinyl acetate+ butyl vinyl ether at (\square , 303.15; \diamond , 308.15; Δ , 313.15) K, vinyl acetate+ diisopropyl ether at (\times , 303.15; \times , 308.15; — , 313.15) K, vinyl acetate+ anisole at (O, 303.15; +, 308.15; \blacksquare , 313.15) K, vinyl acetate+ dibutyl ether at (\blacklozenge , 303.15; \blacktriangle , 308.15; \bullet , 313.15) K

The intermolecular free length L_f in binary liquid-liquid combinations can be utilized to investigate the attraction in the solvent molecules. The values of intermolecular free length in a binary combinations depend on concentration and temperature. At a denoted concentration for binary systems intermolecular free length grows with growing of temperature. It might be decreasing of intermolecular attraction due to thermal agitation. The intermolecular free length values are also concentration dependent denoting, the molecular interactions in the vinyl acetate systems are concentration dependent.

The dependence of excess intermolecular free length (L_f^E) on the mole fraction of vinyl ethanoate (x_1) at 303.15, 308.15, and 313.15 K is shown in Figure 2. The L_f^E values for systems of vinyl ethanoate+ butyl vinyl ether, vinyl acetate+ diisopropyl ether, vinyl acetate + Butoxy butane is positive and rises with rising of temperature for vinyl acetate+ diisopropyl ether, vinyl acetate + dibutyl ether whereas it decreases with increase in

temperature for the system vinyl acetate+ butyl vinyl ether. The positive values of L_f^E indicate weaker interactions between the components or improper interstitial accommodation due to more or less same molar volume of the unlike molecules while the negative values of L_f^E may be powerful interactions between the molecules of the combinations.

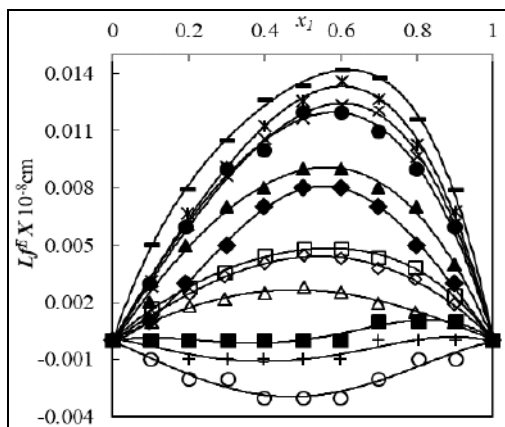


Fig 2: Curves of excess intermolecular free length L_f^E Vs mole fraction for the binary mixtures of vinyl acetate + butyl vinyl ether at (\square , 303.15 ; \diamond , 308.15 ; Δ , 313.15)K, vinyl acetate + diisopropyl ether at (\times , 303.15 ; π , 308.15 ; — , 313.15) K, vinyl acetate+ methoxy benzene at (O, 303.15; +, 308.15; \blacksquare , 313.15) K, vinyl acetate+ dibutyl ether at (\blacklozenge , 303.15; \blacktriangle , 308.15 ; \bullet , 313.15) K.

Specific acoustic impedance (Z) is a quantity which is depending on the molecular packing of the systems. The variation of Z^E with mole fraction of vinyl acetate(x_1) is shown in Figure 3. The deviation in impedance imply non-additivity of acoustic impedance in the liquid mixtures. It is observed that the values of Z^E show negative deviation for all the binary mixtures of vinyl acetate. The Z^E values reduces with reducing temperature for binary liquid-liquid combination of vinyl acetate + (diisopropyl ether, methoxy benzene, dibutyl ether), while for remaining systems of vinyl acetate + butyl vinyl ether the Z^E values increses with rising in temperature for all the composition of ester. The positive values of Z^E in case of systems of methoxy benzene and butyl vinyl ether suggest the presence of strong interaction between the component molecules as suggested by Tiwari *et al.* [27] The trends for Z^E values are butyl vinyl ether > anisole > dibutyl Ether > diisopropyl Ether

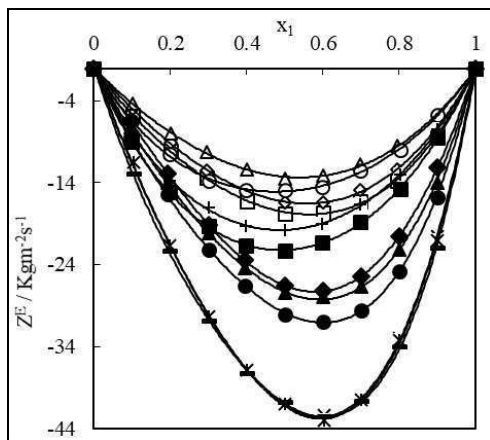


Fig 3: Curves of excess acoustic impedance Z^E Vs mole fraction for the binary mixture of vinyl acetate + butyl vinyl ether at (\square , 303.15 ; \diamond , 308.15 ; \triangle , 313.15) K, vinyl acetate + diisopropyl ether at (\times , 303.15; \boxtimes 308.15 ; — , 313.15) K, vinyl acetate+ methoxy benzene at(\circ , 303.15 ; $+$, 308.15; \blacksquare , 313.15)K, vinyl acetate + dibutyl ether (\blacklozenge , 303.15; \blacktriangle , 308.15 ; \bullet , 313.15)K.

Conclusion

Intermolecular free length, acoustic impedance, speeds of sound for binary systems of vinyl ethanoate with butyl vinyl ether, diisopropyl ether, methoxy benzene, 1-butoxy butane have calculated along the whole concentration at (303.15, 308.15 and 313.15) K. Utilizing these observed data excess volumes intermolecular free length, excess acoustic impedance were measured. These excess were fitted to Redlich-Kister polynomial equation. By observing these excess properties it was guess that the presence of weak interactions between vinyl ethanoate with butyl vinyl ether, diisopropyl ether, 1-butoxy butane whereas for (vinyl Acetate + methoxy benzene) combinations there are interactions such as charge transfer complex are involved.

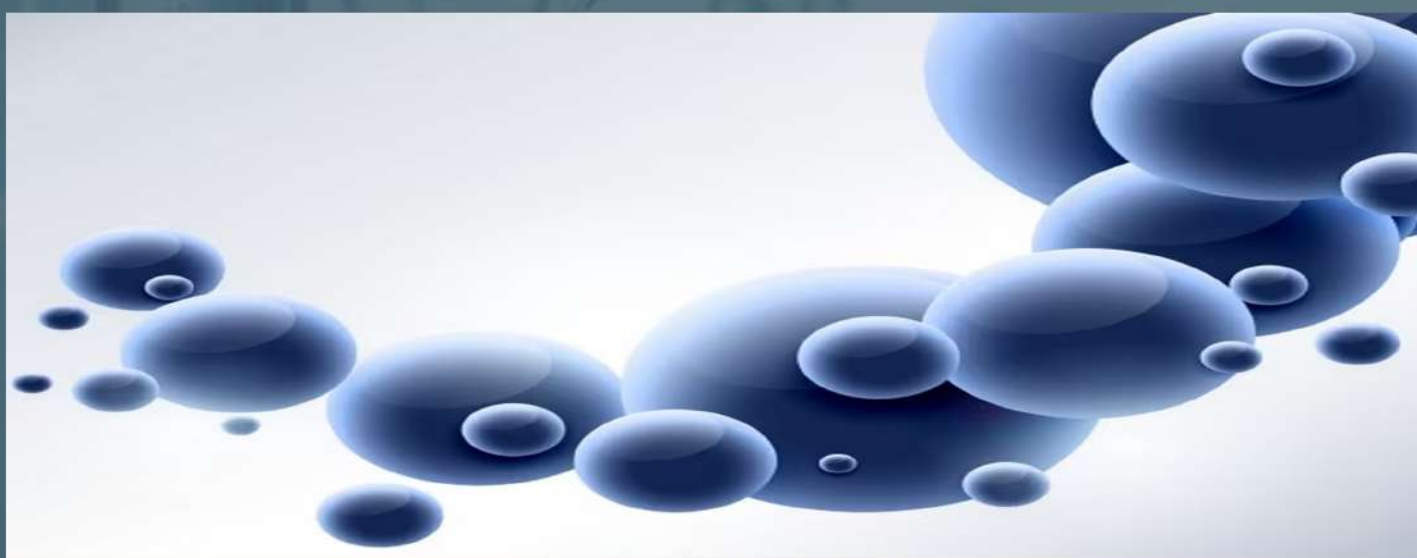
References

1. Rita M, Israni R. Indian J. Chem. 2004;43-A:743.
2. Jyostna TS, Satyanarayana N. Indian J. Chem. Tech. 2006;13:71.
3. Ali A, Nain AK, Chand D, Lal B. Indian J. Chem. 2005;44-A:511.
4. Murali D, Sekhar S, Dhana Laxmi A, Ram Kumar AR. J Pure Appl. Ultrason. 2002;24:68.
5. Canosa J, Rodriguez A, Tojo J. J. Chem. Eng. Data. 2001;46:846.

6. Jalari R, Sekar P, Naidu R. J Chem. Eng. Data. 1996;41:170.
7. Venkatesu P, Chandra Sekhar G, Rao MVP. J Phys. Chem. Liq. 2006;44:287.
8. Dharamlingam K, Ramchandran K. Phys Chem Liquids. 2006;44:77.
9. Prasad V, Rmythili TE, Nirmala GS, Li Prasad DH. J Chem. Eng. Data. 2002;47:68.
10. Agnieszka B, Malgorzata Z, Adam B. J. Them. Anal. Calorim. 2010;100:707.
11. Want LC, Xu HS, Zhao JH, Song CY, Wang FA. J Chem. Thermodyn. 2005;37:477.
12. Mchaweh A, Aisaygh A, Nabrifar K, Moshfeghiam MA. Fluid Phase Equilib. 2004;224:157.
13. Wisniak J, Cortez G, Peralta RD, Infante R, Elizalde LE. J Solution Chem. 2007;36(8):997-1022.
14. Pan IC, Tang M, Chen YP. J. Chem. Eng. Data. 2000;45(6):1012-1015.
15. Resa JM, González C, Landaluce SO, Lanz J. The Journal of Chemical Thermodynamics. 2002;34(7):1013-1027.
16. Kapoor S, Rattan VK. J Chem. Eng. Data. 2005;50:1897-1901.
17. Resa JM, Lez CG, Moradillo B, Ruiz A. Fluid Phase. Equilibria. 1997;132:205-213.
18. Resa JM, González C, Landaluce SO, Lanz J. J Chem. Eng. Data. 2002;47(5):1123-1127.
19. Gill BK, Rattan VK, Kapoor S. J Chem. Eng. Data. 2008;53(1):145-148.
20. Schaaffs W. Mole Kularakustic. Berlin: Springer, 1963.
21. Freyer EB, Hubbard JC, Andrews DH. J Am Chem Soc. 1929;51:759.
22. Pellam JR, Gall JK. J Chem Phy. 1946;14:608.
23. Pinkerton JM. Nature. 1948;162:106.
24. Tiwari K, Patra C, Chakravorthy V. Acoustics Lett. 1995;19:53.
25. Ramanujappa T, Bhavani JA, Raja GE, Manohara MN. Indian J Pure Appl. Phys. 2000;38:301.
26. Reddy Y, Naidu PS, Ravindra Prasad K. Ind. J Pure. Appl. Phys. 1994;2:958.

27. Lukas K. Review of present status of Transport Properties Prediction. Phase Equilibrium and Fluid properties in the Chemical Industry DE CHEMA, 1980.

Advances in Chemical Science: Exploring New Frontiers



UMENDRA KUMAR



Advances in Chemical Science: Exploring New Frontiers

IIP Series



Title of the Book: Advances in Chemical Science: Exploring New Frontiers

Edition: IIP Series

Copyright 2023 © Editor

Umendra Kumar,

No part of this book may be reproduced or transmitted in any form by any means, electronic or mechanical, including photocopy, recording, or any information storage and retrieval system, without permission in writing from the copyright owners.

Disclaimer

The authors and editors are equally responsible for the contents published in this book. The publishers or editors do not take any responsibility for the same in any manner. Errors, if any, are purely unintentional and readers are requested to communicate such errors to the editors or publishers to avoid discrepancies in future.

ISBN: 978-93-5747-689-8

MRP Rs. 470/-

Publisher, Printed at & Distribution by:

Selfypage Developers Pvt Ltd.,
Pushpagiri Complex,
Beside SBI Housing Board,
K.M. Road Chikkamagaluru, Karnataka.
Tel.: +91-8861518868
E-mail: publish@iiponline.org

IMPRINT: I I P Iterative International Publishers

For Sales Enquiries:

Contact: +91- 8861511583
E-mail: sales@iipbooks.com

Preface

Advancements in scientific research have always been the driving force behind human progress, unlocking new realms of understanding and pushing the boundaries of what is possible. In the dynamic and ever-evolving field of chemical science, the quest for knowledge and innovation is relentless. "Advances in Chemical Science: Exploring New Frontiers" stands as a testament to the collective efforts of pioneering researchers who have ventured into uncharted territories, pushing the frontiers of chemical knowledge to unprecedented heights.

This edited volume serves as a comprehensive compendium of the latest breakthroughs and emerging trends in chemical science. As the scientific community continues to unravel the complexities of matter and explore the intricacies of chemical interactions, this book provides a snapshot of the diverse and groundbreaking research that defines the contemporary landscape of the discipline.

The chapters contained within this volume reflect the multidisciplinary nature of modern chemical science, encompassing a wide array of subfields such as organic chemistry, inorganic chemistry, physical chemistry, biochemistry, nano technology, chemical biology and materials science. From fundamental theoretical studies to practical applications, each contribution illuminates a unique facet of chemical science, contributing to the mosaic of knowledge that shapes our understanding of the world around us.

The journey through "Advances in Chemical Science" begins with a thought-provoking exploration of theoretical frameworks that underpin our understanding of chemical phenomena. From there, the reader is guided through a spectrum of research endeavors, ranging from the synthesis of novel compounds to the design of innovative materials with tailored properties. The interplay between theory and experiment, a hallmark of successful scientific inquiry, is exemplified in each chapter, underscoring the collaborative efforts of theorists and experimentalists alike.

In addition to traditional areas of study, this volume also delves into the burgeoning intersections of chemical science with other disciplines. The exploration of the interface between chemistry and biology, the development of environmentally sustainable practices, and the application of advanced analytical techniques showcase the dynamic and interconnected nature of contemporary chemical research.

I hope that "Advances in Chemical Science: Exploring New Frontiers" will inspire researchers, students, and enthusiasts to delve into the fascinating world of chemical science. May the discoveries within these pages spark new ideas, foster collaborations, and ignite a passion for pushing the boundaries of knowledge. Together,

Umendra Kumar

Acknowledgement

The completion of "Advances in Chemical Science: Exploring New Frontiers" has been a collaborative effort that would not have been possible without the dedication, expertise, and support of numerous individuals and institutions. As editor, I extend my heartfelt gratitude to all those who have played a pivotal role in bringing this edited volume to fruition.

First and foremost, I express my deepest appreciation to the contributing authors whose outstanding research forms the cornerstone of this book. Your commitment to advancing the frontiers of chemical science and your willingness to share your expertise have enriched the contents of this volume immeasurably.

I extend my sincere thanks to the reviewers who generously dedicated their time and expertise to critically evaluate the submitted chapters. Your constructive feedback and insightful comments have been instrumental in maintaining the high quality and rigor of the content presented in this book.

My gratitude also extends to the publishers and editorial staff who have supported and guided me throughout the publication process. Your professionalism, attention to detail, and commitment to excellence have been invaluable in transforming the vision of this book into a reality.

I acknowledge the academic institutions and research organizations that have provided the intellectual and infrastructural support necessary for the contributors to pursue their groundbreaking research. The collaborative spirit fostered by these institutions has undoubtedly contributed to the vibrant and diverse collection of chapters within this volume.

I express my thanks to my colleagues, friends, and family for their unwavering encouragement and understanding throughout the demanding process of editing this book. Your support has been a

source of inspiration, motivating us to strive for excellence in every aspect of this project.

Finally, I acknowledge the global scientific community, whose collective pursuit of knowledge and innovation continues to propel the field of chemical science forward. It is my hope that this edited volume serves as a testament to the collaborative spirit and shared commitment to advancing the frontiers of scientific inquiry.

In conclusion, the realization of "Advances in Chemical Science: Exploring New Frontiers" is the result of a collective effort, and I extend my sincere thanks to all those who have contributed to its success. May this book inspire continued exploration and discovery in the fascinating world of chemical science.

Umendra Kumar

Contents

1. NANOMATERIALS AND NANOSTRUCTURES IN
CHEMISTRY: A REVIEW OF SYNTHESIS AND
CHARACTERIZATION METHODS
.....
Umendra Kumar
2. A STUDY OF THE PHYSICO-MECHANICAL AND COMBUSTION
ANALYSIS OF BRIQUETTES PRODUCED
FROM BAMBARANUT SHELL.
.....
Ikelle Ikelle, Eze Nkechinyere, Esonye Chibuzo
3. A REVIEW -POLYMERIC NANOCOMPOSITES
.....
Dr. Dev Raj Singh
4. FATTY ACID COMPOSITION OF GULMOHAR SEED OIL
FROM BULANDSHAHR (U.P.)
.....
Alka Gupta, Mukesh Kumar
5. AROMATHERAPY: A SYNERGY THERAPY
.....
Dr. Shaifali Srivastava
6. SYNTHESIS OF POLYSTYRENE NANOPARTICLES AND
THEIR APPLICATION FOR DETECTION OF *INFECTIOUS*
BURSAL DISEASE VIRUS (IBDV)
.....
M K Choudhary
7. COMPREHENSIVE STUDY OF SUGAR OXIDATION WITH
Cr(VI) OXIDANTS
.....
Ashish Tomar, Unik Arora
8. QUANTIFYING THE IMPACT OF AIRBORNE POLLUTANTS
ON URBAN AIR QUALITY: A COMPREHENSIVE ANALYTICAL
STUDY
Dev Prakash
9. STRUCTURAL AND THERMAL DECOMPOSITION
STUDIES OF Co(III) AND Ni(II) METAL COMPLEXES
OF SCHIFF BASES
.....
Vishrut Chaudhary

10. DIMETHYL CARBONATE WITH ETHERS:
THERMOPHYSICAL STUDY
.....
Ajit N. Bhumkar
11. ZINC INDUCED OCCUPATIONAL TOXICITY
.....
Heena, Satyandra Kumar, Yeshvendra Verma, Malti
12. SELF-ACTIVATING DNA CLEAVAGE BY MONONUCLEAR
COPPER COMPLEXES
.....
Pramod Kumar, Sushil Kumar
13. MOLECULAR INTERACTIONS STUDY BETWEEN BUTYL
ACETATE WITH ALKANES USING ULTRASONIC TECHNIQUES
.....
Pralhad S Wagh
14. A REVIEW OF HYDROGELS THEIR CLASSIFICATIONS, AND
APPLICATIONS
.....
Deepti Chauhan
15. GREEN AND SUSTAINABLE CHEMISTRY
.....
*Mohit Saroha, Renu Swami, Bhupinder Singh, Akshay Kumar,
Deepak Tomar*
16. FUNCTIONALIZATION OF CARBON NANOTUBES FOR
ENHANCED MECHANICAL AND ELECTRICAL PROPERTIES
.....
Sunil Sharma
17. EFFECT OF TEMPERATURE AND CARBON CHAIN LENGTH ON
THE ACOUSTIC PARAMETERS OF AMMONIUM SOAPS
IN 2-PROPANOL
.....
Arvin Panwar
18. THEORETICAL EXPLORATION OF THE ELECTRONIC
PROPERTIES AND REACTIVITY OF NITROGEN-CONTAINING
HETEROCYCLES
.....
Soni Mittal
19. CHEMICAL TOOLS FOR UNDERSTANDING PROTEIN
CONFORMATIONAL CHANGES
.....
Renuka Tomar, Priya Tomar

MOLECULAR INTERACTIONS STUDY BETWEEN BUTYL ACETATE WITH ALKANES USING ULTRASONIC TECHNIQUES

Abstract

Ultrasonic velocities for binary mixtures of butyl acetate as a main component with alkanes like heptane, decane, dodecane and tridecane have been measured at 303.15, 308.15 and 313.15K temperatures with different compositions. The obtained experimental data have been utilized to find out excess or deviation properties such as deviations in ultrasonic velocity (Δu), and intermolecular free length (L_f). The deviation in ultrasonic velocities and excess intermolecular free length convey prevailing trends of curves that are both positive and negative which attributes the different molecular interactions for proposed binary mixtures.

Keywords: butyl acetate; Alkanes; ultrasonic velocity; intermolecular free length; molecular uinteractions

Author

Pralhad S Wagh
Department of
Chemistry,
VPMs B N Bandodkar
College of Science
(Autonomous),
Thane
Thane, Maharashtra,
India.

I. INTRODUCTION

Butyl acetate is used as an ingredient in cleaners, fragrances, and as an extractant in the production of pharmaceutical preparations. It is sometimes referred to as butyl ethanoate. This organic substance is mostly utilized as a solvent in the lacquer manufacturing process. Additionally, it is utilized in a variety of food products, including baked goods, cheeses, candies, and ice cream, as a synthetic fruit flavoring. Additionally, nail polish and other nail-care products are made with butyl acetate as a solvent. It is utilized in the production of safety glass, plastics, photographic films, and synthetic leather cleansers. It works great as a solvent to prepare polymers and resins. Because butyl acetate is frequently used in paint formulations in conjunction with alcohols like n-butanol, it improves both the solvency and the resistance to blushing. Due to its high solvency and low water absorption capacity, it can also be used as an extractant in pharmaceutical preparations and as a raw material for essences and fragrances. Given that butyl acetate is a polar solvent, combining it with non-polar solvents like alkanes yields some intriguing findings about the density and viscosity of binary mixtures as well as insights into the potential effects of the molecular interaction between butyl acetate and alkanes. Understanding the thermoacoustic characteristics of mixtures with butyl acetate as a major component and the molecular interaction studies in binary liquid mixtures of butyl acetate with alkanes are of interest to us in light of the aforementioned salient features.

Few studies have been done on the physicochemical characteristics of binary mixtures of butyl acetate with alkanes like heptane, decane, dodecane, and tridecane, according to a review of the literature. Resa reported the isentropic compressibilities and ultrasonic velocities of mixtures containing butyl acetate and aromatic hydrocarbons (toluene, ethylbenzene, p-xylene, mesitylene, isopropylbenzene, butylbenzene, isobutylbenzene, or t-butylbenzene) that were measured using the Grunberg and Nissan model at various

MOLECULAR INTERACTIONS STUDY BETWEEN BUTYL ACETATE WITH
ALKANES USING ULTRASONIC TECHNIQUES

temperatures and atmospheric conditions [1]. Gonzalez discussed alkanes (n-hexane, n-heptane, n-octane, n-nonane) or esters (ethyl acetate, vinyl acetate, propyl acetate, isopropyl acetate, butyl acetate) + olive oil at temperatures between 288.15-298.15 K are enclosed in binary systems at ultrasonic velocity [2]. These physical characteristics were used to calculate the corresponding derived magnitudes, changes in isentropic compressibilities, and changes in refractive indices on mixing. Density, viscosity, refractive index, and speed of sound have all been reported by Aminabhavi and Banerjee for binary mixtures of acrylonitrile with methyl, ethyl, propyl, butyl, and 3-methyl butyl-2-acetate in the temperature range of 298.15 to 308.15 K [3]. The obtained experimental data is utilized in this study to identify certain properties of excess or deviation. Pycnometers were used to measure the experimental density, cannon Fenske viscometers (Rosella, NJ) were used to measure viscosity, and Mittal Single Crystal Interferometers (model M-84, New Delhi) were used to measure sound speed. It is concluded that, with the exception of the deviation in the viscosity property, the results of the studied excess or deviation properties show systematic dependence on the size of esters used. The density, viscosity, refractive index, and sound speed of binary mixtures of 2-chloroethanol with methyl, ethyl, n-propyl, and n-butyl acetate have all been studied by Aralaguppi [4]. Volume excess for (methanol + butyl acetate) and (vinyl acetate + butyl acetate) has been determined by Resa [5]. The Van Laar and Wilson equations have been used to correlate the activity coefficients. For binary mixtures of n-butylamine with butyl acetate, methyl acetate, and iso-amyl acetate, Sankara Reddy have measured excess volume, speed of sound, and viscosity at 303.15 K over the whole composition range [6]. The collision factor theory (CFT) developed by Schaaff was used to report sound speeds. The Grunberg and Nissan model was used to correlate the viscosity data. Chandrasekhar have determined excess molar volumes and speed of sound of ethyl acetate and butyl acetate with 2-alkoxyethanols at 308.15 K [7]. Jyostna have measured densities and viscosities of binary liquid mixtures of acetonitrile and N-methyl acetamide with aromatic ketones at 308.15

K [8-9]. Patwari determined densities, viscosities and speeds of sound of binary liquid mixtures of sulfolane with ethyl acetate, n-propyl acetate and n-butyl acetate at temperatures of (303.15, 308.15 and 313.15) K [10]. Lie-Chiah have measured VLE for binary mixtures of 2-butanol + butyl acetate [11]. They have used various activity coefficient models to correlate the experimental data. Sastry and Patel have reported densities, excess molar volumes, speeds of sound, excess isentropic compressibilities and relative permittivities for alkyl (methyl, ethyl, butyl, and isoamyl) acetates with glycols at different temperatures [12]. Qin have determined excess volumes of binary mixtures of alkyl esters and ketones with aromatic hydrocarbons [13].

Recent study shows many technical applications of new materials that can produce strong ultrasonic vibrations observed in the field of physics, chemistry, biology, medicine, and industry which have been made possible by the quick development of ultrasonic technology and the introduction of new materials in research. These days, studying ultrasonic absorption and velocity in a variety of media like liquids, liquid-liquid mixtures, suspension, electrolyte solution, polymers, etc. is a pretty useful way to look at specific physical characteristics of the media. Extensive research has been conducted on the interferometric method which involves stimulating a liquid column to resonance.

II. MATERIALS AND METHODS

The analytical grade butyl acetate, heptane, decane, dodecane, and tridecane provided by Sigma-Aldrich have been deployed for the ultrasonic velocity's measurements. For these chemicals, the mass fraction purity was substantially greater than 0.99. To reduce the water content and stabilize these chemicals, they were placed over 0.4 nm molecular sieves and distilled right before to use. The analysis of the purity for the used chemicals using GC-8610 revealed that it was >0.995. The fluid which serves as binary Mixtures were made by combining known masses of pure liquids in airtight stoppered bottles. Mass measurements were performed for each using a Mettler one-pan

balance (AE, 240, Switzerland). The conclusive result subsequently was found that the mole fraction's uncertainty amounted less than + 0.0001. The methods for measuring sound speed can be broadly classified into two groups.

1. The Continuous Wave Method

This method includes interferometric and optical methods that are based on the study of acoustic gratings[14]. Variable path interferometers have been used extensively, and new developments allow sound speed measurements to be accurate to a few parts per million [15]. Hunter and Dardy used a double crystal detector to measure sound speed at 500 MHz [16]. Other kinds of interferometers were also used to measure sound speed and investigate the resonance of liquid filling cavities. Dobbs and Finegold used a cylinder made of barium titanate that was plated so that one half functioned as a receiver and was filled with the experimental liquid [17]. Fort and Moore used a single crystal interferometer operating at 400 KHz to measure the ultrasonic sound speeds of binary liquid mixtures [18].

2. Pulse Technique

The pulse technique allows sound speed in liquids to be measured by measuring the transit time for a given path.[19-20]. This method measures the time difference between two ultrasonic wave echoes traveling between a transducer and a reflector in order to calculate velocity. Compared to pulse techniques, the ultrasonic interferometer has some clear advantages [21-22]. One benefit of using an optical interferometer is that differential path length, as opposed to total path length, can be used to measure these parameters accurately. Furthermore, the interferometer only needs a straightforward frequency measurement, whereas the pulse technique requires a more complex time interval measurement. Therefore, it is discovered that an interferometer is a better tool for determining the temperature and pressure coefficients of sound speed. Del Grasso has

addressed the advantages of the ultrasonic interferometer in great detail [22]. However, the narrow band of applicable frequencies (10 to 100 MHz) limits the interferometric method.

The variable path single crystal interferometer F-81 (Mittal Enterprises, New Delhi, India) operating at a frequency of 2 MHz was used in this study to measure the speed of sound in pure liquids and binary mixtures. The interferometer cell has 1.6 cm inner diameter stainless steel tube makes up the 12 cm³ interferometer cell. A quartz crystal with a gold plating is fixed to the cell's bottom. This crystal emits ultrasonic waves, which travel until the movable reflector reflects them back. The diameter of the reflecting surface is 1.4 cm. Using a Teflon coupler and a steel rod, this is connected to a micrometer screw assembly that can measure up to 0.01 centimeters. A threaded cup and teflon ring are used to secure the micrometer assembly and reflector to the liquid cell. The necessary stability for the measuring cell is provided by a heavy pedestal. To keep the experimental liquid at a consistent temperature throughout the experiment, provisions have been made for water to be circulated at any desired temperature from a thermostatically controlled bath into a jacket surrounding the measuring space. An electrically powered quartz transducer connected to a liquid column makes up the interferometer. the quartz crystal's distance down the liquid column. The column vibrates in resonance whenever the distance between the reflector and the quartz transducer is an integral multiple of half wavelength. Sharp dips in the r-f voltage across the transducer result from this increase in the transducer's motional impedance. A half wavelength ($\lambda/2$) is the distance traveled by the reflector between any two successive dips.

The experimental liquid was placed inside the interferometer cell, which was wired shielded to the high frequency generator's output terminal. A thermostat controlled to within + 0.01 K was used to circulate water, keeping the cell temperature at 303.15 K. The micrometer screw was gradually turned until the anode current meter

displayed a maximum and the micrometer reading was recorded after the liquid reached the bath's temperature. By turning the screw downward, the quartz transducer and reflector plate were separated in length. A number "n," in this case forty, was counted after multiple maxima were passed in order to increase measurement accuracy. After adjusting the anode current to its maximum, the micrometer's reading was once more noted. The formula for the total distance traveled by the reflector was $d = \lambda/2$. With the quartz crystal's accuracy (f) known with precision (2MHz), the sound speed (u) was computed using the formula $u = \lambda/f$. The micrometer screw was turned upward to determine the value of u. The accuracy of the sound speed values was within 0.15%. In continuation with our earlier research, the present study reports ultrasonic velocities for 9 samples having different mole fraction between 0.1 to 1 at 203.15, 205.15, and 213.15K temperatures [23].

III. RESULTS AND DISCUSSIONS

The deviation properties of the binary liquid mixtures have been evaluated using the eq. (1-3)

$$\Delta y = y_{\text{mix}} - (x_1 y_1 + x_2 y_2) \quad (1)$$

where y_{mix} indicates the property of the mixture viz, speed of sound (u), and intermolecular free length (L_f), y_1 and y_2 , x_1 and x_2 refer to the property and mole fraction of pure components 1 and 2 respectively and Δy indicates the deviation in observed property (Δu) The excess free length can be calculated by following equation

$$L_f = K \cdot (K_s)^{1/2} \quad (2)$$

In above Eqs. (2), K is the temperature dependent Jacobson's constant, K_s is isentropic compressibility which can be calculated by following equation

$$K_s = [1 / (u^2 \rho)] \quad (3)$$

MOLECULAR INTERACTIONS STUDY BETWEEN BUTYL ACETATE WITH
ALKANES USING ULTRASONIC TECHNIQUES

Graphical representation of Δu as a function of mole fraction of Butyl acetate(x_1) at 303.15, 308.15 and 313.15 K is given in Figure 1. By interpreting, it can be seen that for the systems Butyl acetate + Dodecane and Butyl acetate + Tridecane, Δu shows positive deviation, whereas for the system Butyl acetate + Heptane, Δu values are found to be negative at all studied temperatures. When compared to other systems, the Δu values for the butyl acetate + decane system exhibit a different trend. It is observed that the Δu is found to be positive at 313.15 K and negative at 303.15 and 308.15 K. When the temperature of Butyl acetate + Heptane increases, it is observed that the values of Δu become less negative and a minima is reached at mole fraction $x_1 = 0.5$. Values of Δu show a systematic increase with increasing temperature in the systems Butyl acetate + Dodecane (maxima at $x_1=0.6$) and Butyl acetate + Tridecane (maxima at $x_1=0.5$). The increasing strength of interaction between component molecules of binary liquid mixtures is demonstrated by positive deviations in Δu values. The mixture is predominant, leading to an expansion faster than the speed of sound, as indicated by the negative deviation.

Intermolecular free length is a crucial physical characteristic of liquid mixtures that primarily influences sound velocity. As the sound velocity drops, the intermolecular free length also drops. The shape of the molecule and their interactions with one another both affect the structural arrangements. Figure 2 demonstrates that the curve obtained for L_f^E and the systems of butyl acetate + heptane, butyl acetate + dodecane have positive values of L_f^E ; the other two systems, butyl acetate + decane exhibit both positive and negative deviations and butyl acetate + tridecane exhibit negative deviations at all temperatures. Weak molecular interactions and improper interstitial accommodation between the component molecules are indicated by positive values of L_f^E . Dipole-induced dipole, dipole-dipole, and charge transfer interactions between the components of the binary liquid mixtures are among the various forces acting between them; these forces contribute negatively to the excess values, while

dispersion forces operate positively. In every instance of these four binary mixtures under study reveals that dispersion forces are present

IV. CONCLUSIONS

Values of Δu and L_f^E were calculated based on measurements of ultrasonic velocities for binary mixtures of butyl acetate with heptane, decane, dodecane, and tridecane at (303.15, 308.15, and 313.15) K. For mixture, Butyl acetate + Dodecane and Butyl acetate + Tridecane, Δu shows positive, Butyl acetate + Heptane negative while Butyl acetate + Decane shows positive-negative deviations. It appears that the molecules in butyl acetate and n-alkanes are interacting through weak dipole-dipole forces. Furthermore, it is noted that temperature has a considerable impact on the properties of Δu that have been studied. The intermolecular free length L_f investigated over entire composition range for binary mixtures shows weak molecular interactions and improper interstitial accommodation between the component molecules are indicated by positive values of L_f^E for partial systems. The dipole-induced dipole, dipole-dipole, and charge transfer interactions between the components of the butyl acetate binary liquid mixtures are predominant.

Figures

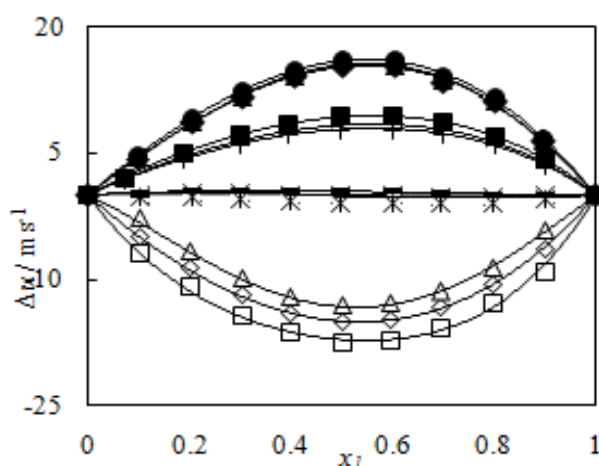


Figure 1: Curves of deviation in ultrasonic velocity Δu Vs mole fraction for the binary mixture of

MOLECULAR INTERACTIONS STUDY BETWEEN BUTYL ACETATE WITH
ALKANES USING ULTRASONIC TECHNIQUES

Butyl acetate+ Heptane at (\square , 303.15; \diamond , 308.15; Δ , 313.15)K,
Butyl acetate+ Decane at (\times , 303.15; \mathbb{X} , 308.15; — , 313.15) K,
Butyl acetate+ Dodecane at (O, 303.15; +, 308.15; \blacksquare , 313.15)K,
Butyl acetate+ Tridecane at(\blacklozenge , 303.15; \blacktriangle , 308.15 ; \bullet , 313.15) K

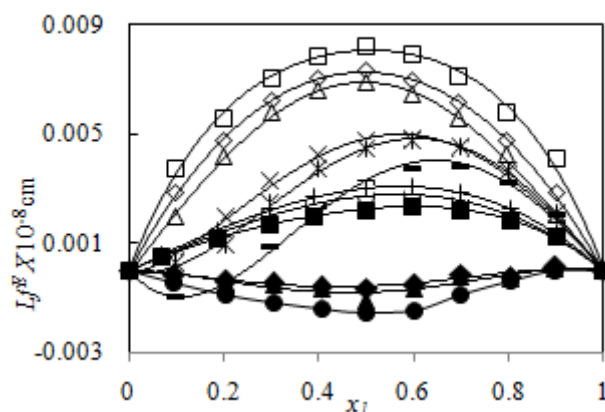


Figure 2: Curves of excess intermolecular free length L_f^E Vs mole fraction for the Binary mixtures of

Butyl acetate+ Heptane at (\square , 303.15 ; \diamond , 308.15 ; Δ , 313.15)K,
Butyl acetate+ Decane at (\times , 303.15 ; \mathbb{X} , 308.15 ; — , 313.15) K,
Butyl acetate+ Dodecane at (O, 303.15 ; +, 308.15 ; \blacksquare , 313.15) K,
Butyl acetate+ Tridecane at (\blacklozenge , 303.15; \blacktriangle , 308.15 ; \bullet , 313.15) K.

REFERENCES

- [1] J. M. Resa, C. Gonzalez, R. G. Concha, and M. Iglesias, "Ultrasonic velocity measurements for butyl acetate+ hydrocarbon mixtures," *Phy. and Chem. Liq.*, vol. 42(5), pp. 521-43, October 2004.
- [2] C. Gonzalez, L. A. Jaun, R. S. Andrade, and M. Iglesias, "Mixing properties of (n-alkanes or esters)+ olive oil at different temperatures," *I. J. Chem. Thermodyn.*, vol. 23(2), pp. 93-105, May 2020.
- [3] T. M. Aminabhavi, and K. Banerjee, "Density, viscosity, refractive index, and speed of sound in binary mixtures of acrylonitrile with methyl acetate, ethyl acetate, n-propyl acetate, n-butyl acetate, and 3-methylbutyl-2-acetate in the temperature interval (298.15– 308.15) K," *J. Chem. Eng. Data.*, 43(4), 514, July 1998.
- [4] M. I. Aralaguppi, C. V. Jadar, and T. M. Aminabhavi, "Density, Viscosity, Refractive Index, and Speed of Sound in Binary Mixtures of 2-Chloroethanol with Methyl Acetate,

MOLECULAR INTERACTIONS STUDY BETWEEN BUTYL ACETATE WITH
ALKANES USING ULTRASONIC TECHNIQUES

- Ethyl Acetate, n-Propyl Acetate, and n-Butyl Acetate, ” J. Chem. Eng. Data., vol. 44, pp. 441, March 1999.
- [5] J. M. Resa, C. González, B. Moradillo, and J. Lanz, “ (Vapour+ liquid) equilibria for (methanol+ butyl acetate),(vinyl acetate+ butyl acetate),(methanol+ isobutyl acetate), and (vinyl acetate+ isobutyl acetate),” J. Chem. Thermodyn.,vol. 30(10), pp. 1207-19, October 1998.
- [6] G. Reddy, V. Subbaiah, M. Boddu, and V. Abburi, “Thermo physical properties of binary mixtures of n-butylamine with alkyl acetates at 303.15 K, ” J. Mol. Liq., vol. 141, pp. 94-98, May 2008.
- [7] G. Chandrasekhar, P. Venkatesu, and M. V. Rao, “Excess molar volumes and speed of sound of ethyl acetate and butyl acetate with 2-alkoxyethanols at 308.15 K,” J. Chem. Eng. Data., vol. 45(4), pp. 590-3, July 2000.
- [8] T. S. Jyostna, and N. Satyanarayana, “Densities and viscosities of binary liquid systems of acetonitrile with aromatic ketones at 308.15 K,” Indian. J. Chem., vol. 44A, pp. 1365-1371, July 2005.
- [9] S. T. Jyostna, and S. Nallani, “Density and viscosity of binary liquid systems of N methylacetamide with aromatic ketones at T= 308.15 K, ” J. Chem. Thermodyn., vol. 38(3), pp. 272-277, March 2006.
- [10] M. K. Patwari, R. K. Bachu, S. Boodida, and S. Nallani, “Densities, Viscosities, and Speeds of Sound of Binary Liquid Mixtures of Sulfolane with Ethyl Acetate, n-Propyl Acetate, and n-Butyl Acetate,” J. Chem. Eng. Data. 54(3), 1069-1072, March 2009.
- [11] L. C. Feng, C. H. Chou, M. Tang, and Y. P. Chen, “Vapor– liquid equilibria of binary mixtures 2-butanol+ butyl acetate, hexane+ butyl acetate, and cyclohexane+ 2-butanol at 101.3 kpa, ” J. Chem. Eng. Data. vol.43(4), pp. 658-61, July 1998.
- [12] N. V.Sastry, and M. C. Patel, “Densities, excess molar volumes, viscosities, speeds of sound, excess isentropic compressibilities, and relative permittivities for alkyl (methyl, ethyl, butyl, and isoamyl) acetates+ glycols at different temperatures,” J. Chem. Eng. Data. vol. 48(4), pp.1019-27, July 2003.
- [13] A. Qin, D. E. Hoffman, and P. Munk, “Excess volume of mixtures of selected alkyl esters and ketones with aromatic hydrocarbons,” J. Chem. Eng. Data , vol. 37(1), pp. 66-70, January 1992.
- [14] W. Schaaffs W., “Molekularakustische Untersuchungen über die Fortpflanzung des ersten und Zweiten Schalls im flussigen helium,” Acta Acustica united with Acustica, vol. 13(5), pp. 355-61, January 1963.
- [15] E. B. Freyer, J. C. Hubbard, and D. H. Andrews, “Sonic studies of the physical properties of liquids. I. The sonic interferometer. The velocity of sound in some organic liquids and their compressibilities,” J. Am.Chem. Soc., vol 51(3), pp. 759-70, March 1929.
- [16] J. L. Hunter, and H. D. Daray, “Ultrahigh- Frequency Ultrasonic Absorption Cell, ” J. Acoust. Soc. Amer., vol. 36(10), pp.1914-7, October 1964.
- [17] E. R. Dobbs, and L. J. Finegold, “Measurement of the velocity of sound in liquid argon and liquid nitrogen at high pressures,” Acoustic. Soc. Am., vol. 32(10), pp.1215-20, October 1960.
- [18] R. J. Fort, and W. R. Moore, “Adiabatic compressibilities of binary liquid mixtures,” Trans. Faraday Soc., vol. 61, pp. 2102-11, April 1965.

MOLECULAR INTERACTIONS STUDY BETWEEN BUTYL ACETATE WITH
ALKANES USING ULTRASONIC TECHNIQUES

- [19] J. R. Pellam, and J. K. Galt, "Ultrasonic propagation in liquids: I. Application of pulse technique to velocity and absorption measurements at 15 megacycles," J. Chem. Phys., vol. 14(10), pp. 608-14, October 1946.
- [20] J. M. M. Pinkerton, "Absorption of ultrasonic waves in acetic acid," Nature, vol. 162(4107), pp.106-7, July 1948.
- [21] V. A. Del Grosso, "Systematic errors in ultrasonic propagation parameter measurements part 3. Sound speed by iterative reflect on interferometry," NRL Report, pp. 6409, August 1966.
- [22] V. A. Del Grosso, "Interferometric Measurement of Ultrasonic Velocity in Liquids—Effect of Diffraction," J. Acoust. Soc. Amer., vol. 48(3B), pp. 770-1, September 1970.
- [23] P. S. Wagh, and M. V. Rathnam, "Densities and Viscosities of Binary (Butyl acetate + n-Alkanes) Mixtures at T= (303.15, 308.15 and 313.15)K, " J. Appl Chem, vol. 8(3), pp. 1486-1495, May 2019.

Multidisciplinary Research and Innovations

Editors

Dr. Mahadeo P. Badge

Assistant Professor in Botany

New Education Society's

Arts, Commerce and Science College, Lanja

District Ratnagiri

Dr. Rajendra A. Shevde

Assistant Professor in Botany

New Education Society's

Arts, Commerce and Science College, Lanja

District Ratnagiri

This book is sold subject to the condition that it shall not, by way of trade or otherwise, be lent, resold, hired out, or otherwise circulated without the publisher's prior written consent in any form of binding or cover other than that in which it is published and without a similar condition including this condition being imposed on the subsequent purchaser and without limiting the rights under copyright reserved above, no part of this publication may be reproduced, stored in or introduced into a retrieval system, or transmitted in any form or by any means (electronic, mechanical, photocopying or recording) otherwise without the prior written permission of both the copyright owner and the above-mentioned publisher of this book.

Inquiries for bulk sales may be solicited at mahibookpublication@gmail.com

FIRST EDITION: 2024

ISBN: 978-81-970910-5-6

Price : 499/-

Mahi Publication

*153, Bariya Street, Near Shree Swaminarayan Mandir,
B/H Jain Derasar, Ambli, Dholera, Ahmedabad, Gujarat -382463*

Phone: +(91) 90238 45578

Website : www.mahipublication.com

E-mail: mahibookpublication@gmail.com

Copyright © 2024/MAHI PUBLICATION

INDEX

RESEARCH METHODOLOGY _____	5
COASTAL PSAMMOPHYTIC FLORAL DIVERSITY IN CHINCHANI BEACH, FROM DAHANU TALUKA IN PALGHAR DISTRICT, MAHARASHTRA STATE (INDIA). _____	16
WILD EDIBLE PLANTS: AN ALTERNATIVE APPROACH TO FOOD SUPPLY _____	25
METHODS FOR SYNTHESIZING CUONPS FROM THE LEAVES OF VARIOUS PLANTS _____	44
A REVIEW OF THE SYNTHETIC METHODS AND APPLICATIONS OF TITANIUM DIOXIDE NANOPARTICLES OBTAINED FROM EXTRACTS OF VARIOUS PLANT LEAVES NANOPARTICLES FOR PHOTOCATALYTIC DEGRADATION OF MO DYES _____	60
WILDLIFE CONSERVATION _____	75
A CASE STUDY OF JELLY FISH AGGREGATIONS AND THEIR NUTRITIONAL VALUE OF COASTAL PEOPLES ON THE COAST OF MURUD-RAIGAD, INDIA. _____	80
SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS USING DOUBLE LAPLACE UPADHYAYA TRANSFORM _____	86
TRAFFIC CONTROL USING SYSTEM OF LINEAR EQUATIONS _____	94
FINDING BEST CHOICE USING MARRIAGE PROBLEM AND FUZZY LOGIC _____	100
CURRENT SCENARIO OF INDIAN MEDICINAL PLANTS AND THEIR ECONOMICS _____	105

WILD EDIBLE MONSOON VEGETABLES USED BY THE TRIBALS IN AREA OF PALGHAR DISTRICT, MAHARASHTRA STATE, INDIA	112
BASIC LOCAL ALIGNMENT SEARCH TOOL (BLAST)	121
PLAGIARISM CHECKING: A NEED OF THE DAY	130
REFERENCING TOOLS	134
NITROGEN METABOLISM IN COWPEA PLANT	138
THE ROLE AND IMPORTANCE OF CULTURAL TOURISM IN JAWHAR TALUKA OF PALGHAR DISTRICT	147

RESEARCH METHODOLOGY

Dr. Urmila C. Kumavat

Asst. Professor, Dept. of Botany,

VPM' B.N. Bandodkar College of Science (Autonomous), Thane

Affiliated to University of Mumbai

Email: uckumavat@vpmthane.org

Mankind's upliftment into what we are today is a result of Curiosity, which initiates the activities of inquisitiveness or questioning everything. Our mind always ponders on questions starting with What? Why? How? about certain things which we recognize as 'Unknown'. This instinct of questioning or spirit of enquiry leads to gain knowledge about the unknown and satisfy thirst of curiosity. It's a continuous process as our surrounding nature, universe and entire cosmos always exhibit many secret processes.

WHAT IS RESEARCH?

Research is a search for knowledge but more precisely, it is a methodical way to carry out a search about a certain topic. The lexical meaning of research is 'a detailed and careful study of something to discover new information or understand the subject better'^[1]. Here are a variety of definitions of research. Some of them are listed below -

- ✓ **According to Grover (2015)** ^[2], research is the process of searching for new information or gaining insight of truth.
- ✓ **Research as defined by The Organization for Economic Cooperation and Development (OECD)** ^[3], "Any imaginative, methodical endeavor to broaden the body of knowledge, including understanding human nature, culture, and society, as well as the application of this information to the development of novel applications."
- ✓ **Further, in the words of C.R. Kothari (2004)** ^[4], Research is the study that adds novel information to the existing knowledge for its advancement. Research also includes the methodical process of formulating a hypothesis and making generalizations.
- ✓ **According to C.C. Crawford** ^[5], research may be defined as a methodical and sophisticated approach to problem-solving that involves the use of specific tools, equipment, and procedures to get a better result

than would be achievable by ordinary means. It begins with an issue, gathers information, evaluates it critically, and makes judgements based on verifiable facts. It's not just a personal workout; it's original work. It develops out of a sincere curiosity as opposed to a need to validate something. Because it is quantitative and aims to determine both what and how much, measurement plays a key role in it.

From above all definitions, it is obvious that research is not restricted to only science subjects but can also be done in all branches of any subject, including social science, humanities, economics, finance, any kind of art, etc. However, it is universal belief that research should be for betterment of mankind or life forms of planet.

PURPOSE OF RESEARCH [6, 7, 8]

Why would one undertake research? Research is basically a tertiary need of the human brain. Unless the primary and secondary needs of a livelihood are satisfied, it doesn't allow us to pursue research. Hence, everybody may not enjoy research as it entails a certain intellectual mindset only. There could be different motives to carry out research on certain interesting aspects. A few are as follows -

1. Some individuals undertake research in order to get a research degree and consequently career benefits.
2. Some candidates like to take challenges in solving unsolved research problems.
3. Some people may engage in research due to social thinking and awakening.

From an academic perspective, a researcher intends to find out hidden truth or discover unexplored facts. It can be found out in various ways, such as -

1. In **Exploratory or Formulative Research**, one explores the unraveled information through observations, e.g. Space exploration involving discovery of new moon/ planets.
2. **Descriptive Research** is required to comprehend various characteristics of an individual or situation or a group, e.g. Gauging the distance, atmosphere, and type of minerals present on new planets through various ways.
3. The **Diagnostic Research** involves determination of the frequency

of some causal factor which may be associated with some other conditions, e.g. determination of pathogenicity of a virus by analyzing patient data.

4. In **Hypothesis-tested Research** an assumption about a condition is formulated first, later the relationship between the different variables is found out to check whether assumption (hypothesis) holds true or false, e.g. evaluation of genetic cross and resulting progeny and their relation with laws of Mendelian Genetics.

THE MAJOR TYPES OF RESEARCH^[6, 7, 8]

1. **Fundamental research** – It is also called as basic research. It is the creation of knowledge regardless of its future applications. Here, the purpose of data collection is to develop new general ideas for a deeper understanding of a particular topic or to answer a theoretical research question. E.g Documentation or listing of Flora of a particular region with detailed description of morphological peculiarities.
2. **Applied research** – Applied research is interested in locating a solution for an immediate research problem faced by society or organization or business. The inferences brought about by theoretical research are typically the basis for applied research. E.g A New drug discovery from plants for new diseases.
3. **Descriptive research** - the major purpose of this research is to collect comprehensive information about any topic and depict systematically. For example, statistical research on individual cricket players which is in form of total run, run rate, strike rate, number of centuries, number of half centuries, etc.
4. **Analytical research** - This specific type of study utilizes critical thinking skills for the evaluation of facts from available data. It helps in identifying the relationships between one or more variables. The goal of the analytical research is to reveal the factors and processes that have an impact on data which has changed over time. E.g. Comparative analysis of all cricketers in one team with respect to strike rate, wickets and overall performance. It helps in overall evaluation of a player and helps in the selection process.
5. **Quantitative research** – involves measurement of quantity or amount. It comprises of the collection of quantitative data and the usage of mathematical, statistical, and computer-aided methods to analyze data. This analysis turned up into conclusions which may be

of industrial application or societal benefits. E.g study on industrial pollution based on emission of greenhouse gases in a given area. Depending upon data pollution mitigation policy can be developed.

6. **Qualitative research** - This is different from Quantitative research, where there is no data collection or numerical analysis. This method is more applied in Social Sciences and behavioural sciences streams of research, where the Human moods and their impact on decision making and other biological aspect is studied.
7. **Conceptual research** - It has to do with thoughts or notions or abstract theory instead of conducting actual experiments. Conceptual inquiry has been used by philosophers to create new ideas or reframe the old ones. E.g. Copernicus employed conceptual research to develop his theories about stellar constellations. Galileo later clarified Copernicus's work by making his own conceptual discoveries, which later gave rise to experimental inquiry and supported the original hypotheses. Sir Isaac Newton is the most well-known example of conceptual research. He took in the environment around him to conceptualize the law of gravity and motion.
8. **Empirical research** - It relies on data which is based on research and not on any abstract theory. In such research researchers first provide himself with working hypotheses or guesses for probable outcomes. Then he works to get sufficient data to prove or disprove his hypothesis.

RESEARCH PROBLEM

For a science student, 'Research is scientific investigation of facts through experimentation'. However, social science students may collect information from society on varied subjects like history, education, economics, politics and the behaviour of people. In both cases, research started with '**Research Problem**'. It does not limit just to collecting information, but it also demands analysis and interpretation of data. Many times, interpretation also enquires about possible reasons for a particular observation or solution to a research problem or query.

Let's understand the concept of 'Research Problem' by a simple example:

There were two graduate students, Ram Sharma and Laxman Sharma who were performing practical of 'Estimation of calcium and magnesium content from rice grains'. Their teacher provided them with a standard manual,

reagents, apparatus and rice grains to carry out experimentation. Both students performed experiments correctly but their results were drastically different. It led them to think about '*Why results vary in spite of using all similar reagents and apparatus?*' This question can be a research problem.

In order to solve this puzzle, Ram and Laxman cross checked procedure, reagents and apparatus again. What they found was the difference in appearance of rice grains which they used. Ram used white rice which was without husk while Laxman used brown rice which was partially covered with husk. So, the solution to this problem was a difference in the rice variety. They further found out that all unpolished (with husk) grains or pulses are full of minerals, especially calcium and magnesium, which are considered as healthy stuff.

RESEARCH APPROACHES ^[2]

Research design refers to a general strategy for attacking a problem that requires a coherent and logical integration of the various parts of the research that ensures an effective solution to the problem. Research design may involve qualitative or quantitative or mixed approaches. Usually, researchers choose the quantitative method to address numerical data while the qualitative method for research issues needing textural data, the mixed methods are used for research topics that call for both textural and numerical data. The following are additional hints for selecting appropriate research approach

- ✓ **Nature of the research problem:** To answer this, one must consider the subject and question at hand. We are aware that researchers conduct a variety of study kinds and in different disciplines have distinct preferences when it comes to research methodologies. Sorting the research problem into categories like exploratory, descriptive, explanatory, predictive, evaluative, or historical can also help you choose a strategy. These categories are related to similar approaches.
- ✓ **Project Purpose:** This responds to the query of why I am doing the research. Is it to address a social issue? or to prepare policies? Or for a degree? or is it a component of a major project? And so forth. Undoubtedly, purpose gives rise to various issues and ways of presenting the data that aid in selecting a strategy.
- ✓ **The personal experiences, skills, attitudes, interests etc. of a researcher:** Individuals have preferences for different research methodologies

and study topics. In research studies, some people prefer to deal with people, while others would merely want to do surveys. Regardless of their preferences, selecting the right technique and research methods is necessary.

- ✓ **Resources available:** Availability of resources such as finance, infrastructure, data collection source, etc. are important factors in deciding on a research method. For example, experimental research may need particular high-end equipment or the large number of samples to complete experiment or survey before starting analysis and interpretation.
- ✓ **Sensitivity of the matter at hand:** In institutes or industries dealing with pharmaceuticals, novel drug discovery may demand extensive planning of quantitative measurements and rigorous monitoring of impact. Here direct human subjects are involved therefore experiments need to be carried out in errorless and responsible manner. On the other hand, a case study might be completed in limited qualitative data. Certain research topics such as security, religion, actors, deviant groups and minorities should be dealt with utmost care and the strategy. At the same time the strategies should be valid as well as reliable.
- ✓ **Discipline:** It is observed that physical science favors a quantitative approach, while language people prefer to use a qualitative approach with critical analysis and anthropology.
- ✓ **Research Audience/Consumer:** Research must be for the benefit of society. It can be important for the commercial business which is looking for a cost-benefit analysis of a project, while for academicians it can give the joy of greater achievements in the future. When we decide for the public, we have to be quite careful. It can create a myth that can harm society rather than benefit it.

RESEARCH PROCESS [4, 5]

The scientific research process comprises of a series of systematic steps that the researcher must go through in certain order to produce valuable genuine information about a given topic. For an effective execution of research, one must recognize the requirements of each step and following the order of the steps can be useful for the research process.

1. **Identifying/ Formulating Research Problem:** One must decide the general area of interest to explore research ideas. Later researchers

can formulate specific research problems for scientific enquiry after discussing with Guide or peer members. Researchers must review conceptual literature (related to basic concepts/ theories) as well as empirical literature (related to earlier similar research studies) concerned with research problems. This step is of utmost importance as it determines the direction of whole research work.

2. **Formulate the aim, objectives and research questions of the research work or establish hypotheses:** Research method is an important step in deciding research question or framing appropriate research hypothesis. Precise research goals and objectives or hypotheses usually take shape after multiple trials and revisions. Therefore, research goals and objectives or hypotheses should be mentioned in the thesis which are revised several times during the research process to get the final versions.
3. **Conducting a literature review:** A literature review is usually the lengthy step of the research process and it may continue till the thesis submission as well as research paper publication. It begins prior to framing research aims and objectives. This is because researcher needs to check whether the same research problem has been worked out before by others and whether this task is part of a literature review? However, one will do the main part of the literature review after formulating the aim and objectives of the research. He/She must use various sources of secondary information such as books, newspapers, research journals, conference proceedings, online articles, government reports, etc. Timely documentation of selected references is also an essential action.
4. **Preparing the Research Design:** Research design is systematic strategy of executing goals and responding to research questions. It devises the plan of action to get the required data. Its objectives are to formulate research questions, test hypotheses, and offer insights for making decisions. Research design has to be planned by researchers to provide collection of relevant evidence with minimal efforts, time and money. This plan fits into four categories - Exploration and Surveys, Experiment, Data Analysis and Observation
5. **Choice of data collection methods:** The choice of data collection is crucial decision. It depends on advantages and disadvantages of respective methods. It has to be selected by critically evaluating pros and cons of all alternative methods. For research studies that involve

primary data collection, researcher should write in detail about the advantages and shortcomings of the chosen primary data collection method in the methodology.

6. **Collection of primary data:** The collection should begin only after thorough preparation. Sampling is an important part of this step. If he/she chose a questionnaire as your primary data collection method, then one must run a pilot plan of action to collect data, check the feasibility of questionnaire and modify question if required. Collecting primary data is not always compulsory, one can omit this step if you are doing desk research.
7. **Data analysis:** Data analysis requires logical skill and analyzing power. It plays a crucial role in devising conclusive remarks which should satisfy the aim and objectives of the research. Even though many online tools help in statistical analysis of extensive data but still the rationale of using statistical tools and decision-making strategy need to be developed by the researcher on his/her own. Methods of data analysis may vary for qualitative and quantitative research.
8. **Making conclusions:** Conclusions making is important step which can be completed by involvement of expert advice, research-guide's perception, by taking account of reviewed related literature and by self-intellect. It also need to incorporate the extent of achievement of the research objectives with which research problem was started. In this final section, one should justify why he/she believes that the aims and objectives of the research have been attained. Conclusions must include limitations of the study and suggestions as well as scope for further research.
9. **End of investigation:** After following above all steps, researcher organizes the separate chapters into a single draft which will be a first draft. This draft of the thesis ideally needs to be prepared two months before the end of the application. This is because researcher needs to give sufficient time to review the draft by the guiding teacher. After the teacher's feedback, revised draft can be prepared with suggested modifications.

The basic layout of the Thesis or Research Project Report is as follows -

- ✓ Report has initial preliminary pages such as title page with date followed by acknowledgement and forward. Then there should be an index depicting list of contents along with a separate list of tables, list of graphs

- entered in the report.
- ✓ Report consists of sequential chapters of Introduction, Review of Literature, Materials and Methods, Observation Tables, Results and Conclusion.
 - ✓ At the end of the report, appendices of technical data, Bibliography consisting of references in form of books, journals, online links, reports, etc.

CRITERIA OF GOOD RESEARCH ^[9]

- ✓ **Good research question** is the heart of research. Good research cannot be accomplished without setting good research question. Cummings *et al.* (2013) ^[10] recommended FINER criteria to frame and assess a good research question. According to this set of criteria, a good research question should be Feasible (F), Interesting (I), Novel (N), Ethical (E) and Relevant (R).
- ✓ **Good research methodology** is another equally important aspect of good research. It determines the success and overall quality of a research study. Selecting an appropriate research methodology ensure collection of relevant data which in turn can be subjected to appropriate data analysis techniques.
- ✓ **Good research acknowledges earlier research done on similar line or topic.** It's a responsibility of researcher that he/she should not duplicate the previous research. Here it can save time and money which may spent on discovering the same facts which were explored by earlier researchers.
- ✓ **Good research uses pertinent, experimental data and appropriate data analysis methods.**
- ✓ **Good research is representative and generalized.**
- ✓ **Good research is directed by logical thinking and it results in valid conclusions.**
- ✓ **Good research is replicable, reproducible, and transparent.** It means if other researchers follow same method or instruments the it should give same results. Such research findings will be helpful for real-world applications.
- ✓ **Good research acknowledges its limitations/ shortcomings and provides suggestions which will be applicable in future research.**

- ✓ **Good research is ethical.** World Health Organization has provided set of guidelines for conducting ethical research. These guidelines are helpful in protecting intellectual rights and dignity of research participants. They also assuring that researcher ethical practice, such as integrity, objectivity, accountability and honesty in their work (Resnik, 2020) ^[11]. Some of the most common malpractices a researcher needs to avoid are as follows:
 - Falsification – It include manipulation or omission of original research data or findings, reporting false materials or readings of equipment.
 - Fabrication – Some researchers prepare accurate results or data without performing any actual investigations the it is called fabrication.
 - Plagiarism – It is a serious malpractice where researcher reports other researcher’s work as their own findings without taking consent. Sometimes researcher mention research data without acknowledging or giving due credit to original researcher.

SIGNIFICANCE OF RESEARCH ^[12]

- ✓ Research fosters the development of logical thinking as well as skills of scientific inquiry
- ✓ It enhances management or organizational skills and data analysis ability.
- ✓ These days, research plays a far bigger role in diverse topics of applied economics. They may be business-related which may create impact on the entire economy of a nation or world.
- ✓ The use of research has become common to solve upcoming operational challenges and has gained importance in industry and government policy today.
- ✓ The role of research in supporting economic policy has grown in significance for both industry and government. In our economic structure, almost all government policies are based on research. Budgets prepared by Government are based on demand – supply statistics, preference of consumers and availability of funds to satisfy nation’s requirements.
- ✓ There is a need for study in this area since the expense of necessities must be compared against likely income. By doing research, we are able to formulate various policies and analyze the implications of each option.
- ✓ Research plays significant role in distribution of a nation's resources in order to have economic growth.
- ✓ Research helps in government operations in healthcare, agriculture and

industrial development which need to assess diagnosis of good/bad events and responsible factors of the same.

- ✓ Research can contribute immensely in understanding disease spread and formulating controlling measures.
- ✓ In sociology, research can reveal interesting facts about social relationships among various groups and can also generate solutions over diverse social issues.

Bibliography:

- [1] <https://dictionary.cambridge.org/dictionary/english/research>
- [2] Grover, Vijay. (2015). RESEARCH APPROACH: AN OVERVIEW. Golden Research Thoughts. 4. 1-8.
- [3] OECD (2015), *Frascati Manual 2015: Guidelines for Collecting and Reporting Data on Research and Experimental Development*, The Measurement of Scientific, Technological and Innovation Activities, OECD Publishing, Paris, <https://doi.org/10.1787/9789264239012-en>.
- [4] Kothari, C.R. (2004), *Research Methodology – Methods and Techniques*, New Age International Publishers, New Delhi.
- [5] Pathak, R.P. (2011). *Research in Education and Psychology*. Pearson Publication, New Delhi.
- [6] <https://research.com/research/what-is-empirical-research>
- [7] <https://forms.app/en/blog/conceptual-research>
- [8] <https://www.proprofssurvey.com/blog/qualitative-research/>
- [9] <https://research.com/research/top-10-qualities-of-good-academic-research>
- [10] Cummings SR, Browner WS, Hulley SB. *Designing Clinical Research*. 4th ed. Philadelphia: Lippincott Williams and Wilkins; 2013. Conceiving the research question and developing the study plan; pp. 22–14.
- [11] Resnik, D. B. (2020). What is ethics in research? And Why it is important? <https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm>.
- [12] <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2912019/>

Multidisciplinary Approach in Research Area (Volume-6)



Chief Editor

Biplab Auddya

Editors

Ramesh Banothu

Dr. C. Ramesh Kumar

Mrs.G.Lakshmi Bhuvaneswari Devi

Dr.J.Ahamed Meeran

Dr. Bipin Namdev Bandekar

Varsha Burman

Multidisciplinary Approach in Research Area (Volume-6)

Title: Multidisciplinary Approach in Research Area (Volume-6)

Editor's: Chief Editor- Biplab Auddya, Editor- Ramesh Banothu, Dr. C. Ramesh Kumar, G.Lakshmi Bhuvaneswari Devi, Dr.J.Ahamed Meeran, Dr. Bipin Namdev Bandekar, Varsha Burman

Published By: The Hill Publication

Publisher's Address: Purulia, West Bengal, 723121

Publishing Month & Year: February, 2024

Edition Details: I

ISBN: 978-81-966799-0-3

Price: Rs.400

© Copyright, 2024, Biplab Auddya

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form by any means, photocopying, electronic, mechanical, magnetic, optical, chemical, manual, recording or otherwise, without the prior written consent of this book Chief Editor.

CONTENTS

Sl. No.	Research Paper/Article	Page No.
1.	Humanistic touch in the Mulkraj Anand's <i>Untouchable</i> (Dr. J. Ahamed Meeran)	1-3
2.	PROBLEMS AND SOLUTIONS IN TEACHING ENGLISH (Bhuvaneshwari Devi)	4-5
3.	UNVEILING THE DYNAMICS OF INFLUENCER MARKETING: IMPACT, EFFECTIVENESS, AND ETHICAL CONSIDERATIONS IN THE DIGITAL AGE (Mr. V.Ponnarasu ¹ , Ms.S.Devi ²)	6-7
4.	EXPLORING THE IMPACT OF AUTOMATION ON JOBS AND FUTURE OF WORK (P.Gracy)	8-10
5.	Digital Mentorship Programs: Empowering Women in the Tech Era (Dr. Shyam B. Choudhury)	11-13
6.	SOCIO-PSYCHOLOGICAL ANALYSIS OF HIV PEOPLE OF HAMIRPUR DISTRICT IN HIMACHAL PRADESH (Dr. Sonia Kaundal)	14-16
7.	Characterization of ZnO Nanoparticles using TEM and FESEM (Varsha Burman)	17-18
8.	A NUMERICAL COMPUTATION OF PROPAGATION OF SHOCK WAVES (Gajendra Shrivastava ¹ , Dr. Pankaj Sharma ²)	19-24
9.	Impact of Non-Performing Assets on Profitability of Public Sector Banks in India: An Analytical Study (Dr. Bipin Namdev Bandekar ¹ , Mrs. Krupa Ketan Mayenkar ²)	25-29
10.	Enhancing Research Effectiveness through Multidisciplinary Approaches: A Case Study Analysis (Dr. Denis Vaz)	30-35
11.	A Study on Impact of Cloud Computing in IT Industry (Dr. R. Marisakthi ¹ , Ms. R. Thilagavathi ²)	36-37
12.	Fixed Point Theorems for Semitopological Semigroups of Lipschitzian Mappings (Sachin Katiyar ¹ , Ajeet Kumar ²)	38-41
13.	Open Balls in a Metric Space using GeoGebra (Mrs. Umalaxmi Patne)	42-44
14.	GREEN CHEMISTRY AN ENVIRONMENTAL FRIENDLY TECHNOLOGY FOR SUSTAINABLE DEVELOPMENT (Dr (smt) Archana Chaturvedi)	45-48

Open Balls in a Metric Space using GeoGebra

Mrs. Umalaxmi Patne

Asst. Prof., Department of Mathematics,

VPM's B. N. Bandodkar College of Science (Autonomous), Thane, Maharashtra, India

Abstract

GeoGebra is an open-source software for mathematics teaching and learning which provides a free platform for all mathematics teachers to teach mathematical concepts effectively. Teachers can create interactive demonstrations and simulations using GeoGebra to illustrate mathematical concepts in a more engaging and accessible way. These demonstrations can aid in lectures, presentations, and classroom discussions. In the course of topology of metric space for undergraduate students of mathematics, open ball is a very basic and important concept. Open balls are fundamental objects in topology, often used to define neighbourhoods, continuity, and convergence in mathematical analysis. In this paper, we will study how to use GeoGebra to help students visualize and understand open balls in a metric space. We will construct dynamic and interactive applet using GeoGebra to understand open balls in different metric spaces.

Keywords: GeoGebra, Metric space, open ball, Mathematics education

Introduction:

GeoGebra is a free and open-source dynamic mathematics software used for teaching and learning mathematics (Hohenwarter, Markus Preiner, 2007). It provides a platform where users can create mathematical constructions, explore mathematical concepts, and visualize mathematical relationships. GeoGebra provides a platform for creating interactive worksheets and dynamic instructional materials (www.geogebra.org). It is widely used in Mathematics education to support teaching and learning (Hohenwarter et al., 2007). It can be integrated into lessons and projects. Open balls play a fundamental role in undergraduate mathematics. GeoGebra can be a valuable tool for teaching open balls in metric space. It helps to visualize open balls and allows for their interactive exploration.

Open Ball:

Definition: Let (X, d) be a metric space and $p \in X$. An open ball with centre p and radius $r > 0$, denoted by $B(p, r)$, is defined as follows (Kumaresan, 2011):

$$B(p, r) = \{x \in X : d(x, p) < r\}$$

Example 1:

Consider \mathbb{R}^2 with Euclidean metric d_2 given by $d_2(x, y) = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2}$ where $x = (x_1, x_2)$, $y = (y_1, y_2) \in \mathbb{R}^2$. Let $p = (a, b) \in \mathbb{R}^2$ and $r > 0$. Then open ball with centre p and radius r is given by

$$\begin{aligned} B(p, r) &= \{(x, y) \in \mathbb{R}^2 : d_2((x, y), (a, b)) < r\} \\ &= \{(x, y) \in \mathbb{R}^2 : (x - a)^2 + (y - b)^2 < r^2\} \end{aligned}$$

This can be explained using GeoGebra applet <https://www.geogebra.org/m/b7kx7ye7> where students can be encouraged to change p and r and hence providing them better visualization and understanding of open balls in \mathbb{R}^2 with Euclidean metric ([https://wiki.geogebra.org/en/category:manual_\(official\)](https://wiki.geogebra.org/en/category:manual_(official))). This hands-on exploration helps students develop an intuitive understanding of open balls and their properties, such as how changing the radius affects the size of the open ball and how changing the centre point shifts its position.

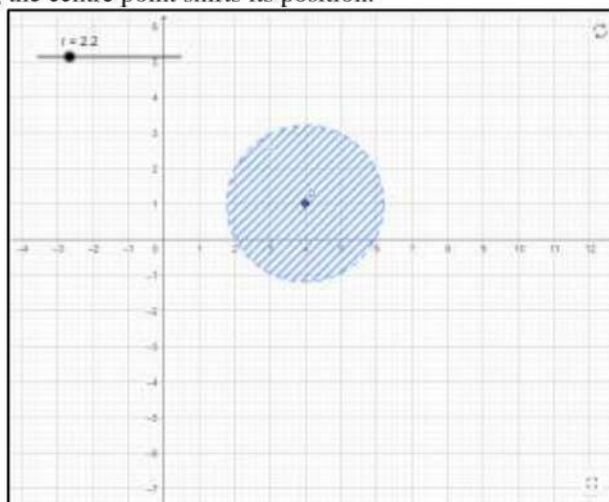


Figure 1: Open Ball in (\mathbb{R}^2, d_2)

Example 2:

Consider \mathbb{R}^2 with sum metric given by $d_1(x, y) = |x_1 - y_1| + |x_2 - y_2|$ where $x = (x_1, x_2)$, $y = (y_1, y_2) \in \mathbb{R}^2$. Let $p = (a, b) \in \mathbb{R}^2$ and $r > 0$. Then open ball with centre p and radius r is given by

$$\begin{aligned} B(p, r) &= \{(x, y) \in \mathbb{R}^2 : d_1((x, y), (a, b)) < r\} \\ &= \{(x, y) \in \mathbb{R}^2 : |x - a| + |y - b| < r\} \end{aligned}$$

GeoGebra applet <https://www.geogebra.org/m/khxfwcer> can be used for demonstrating the open ball. We change the centre p as well as the radius r in the above applet and hence providing effective understanding of the open ball in the metric space (\mathbb{R}^2, d_1) .

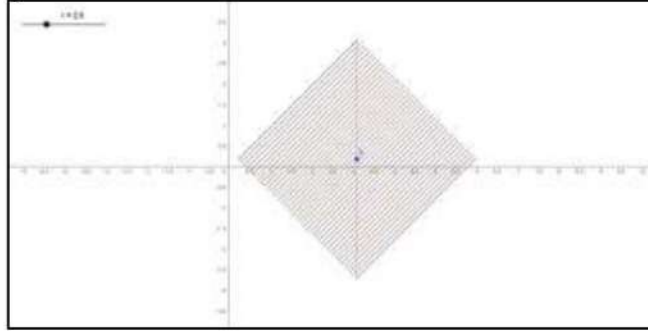


Figure 2: Open ball in (\mathbb{R}^2, d_1)

Example 3:

Consider the set of all continuous real valued functions defined on interval $[0,1]$ denoted by $C[0,1]$ with norm $d(f, g) = \sup\{|f(t) - g(t)| : t \in [0,1]\}$. We will take an example of an open ball in metric space $C[0,1]$. Let $f(x) = \sin 10x$ for $x \in [0,1]$. Then $f \in C[0,1]$. Open ball with centre f will be given by

$$\begin{aligned} B(f, r) &= \{g \in C[0,1] : d(f, g) < r\} \\ &= \{g \in C[0,1] : \sup\{|f(t) - g(t)| : t \in [0,1]\} < r\} \\ &= \{g \in C[0,1] : |f(t) - g(t)| < r \text{ for all } t \in [0,1]\} \\ &= \{g \in C[0,1] : f(t) - r < g(t) < f(t) + r \text{ for all } t \in [0,1]\} \end{aligned}$$

I have created an applet in GeoGebra to view this open ball and also to understand the change in open ball as we change the value of radius. Applet can be accessed using link <https://www.geogebra.org/m/gzrhcf6>. Similar applet can be created for open ball with any centre $f \in C[0,1]$.

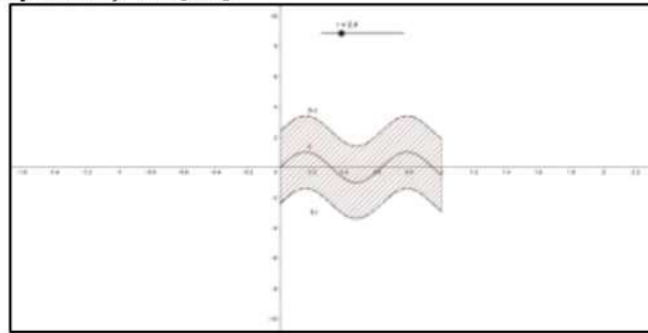


Figure 3: Open Ball in $C[0,1]$

Hausdorff Property:

Let (X, d) be a metric space and $p, q \in X$ such that $p \neq q$. Then there exists $r > 0$ such that $B(p, r) \cap B(q, r) = \emptyset$. That is, distinct points have disjoint open balls of same radius in a metric space. (Kumaresan, 2011)

Above property is a very basic and important property of open balls. One can prove that such disjoint open balls exist for any $r \leq \frac{d(p,q)}{2}$.

This property can be explained with the example of (\mathbb{R}^2, d_2) metric space. GeoGebra applet <https://www.geogebra.org/m/nrrbgrh> can be used to teach how the value of r is obtained. In this applet, students can easily understand and learn that if we select $r > \frac{d(p,q)}{2}$, then the open balls intersect.

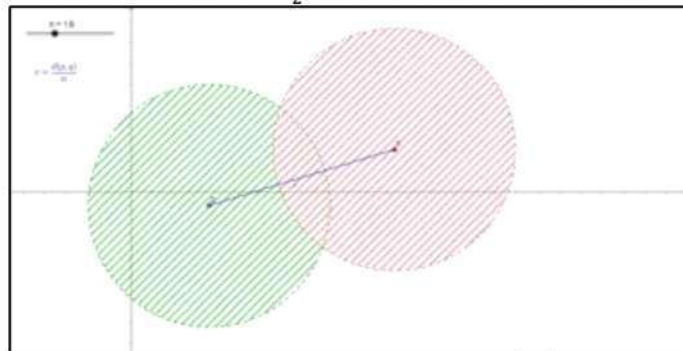


Figure 4: Open balls when $r > \frac{d(p,q)}{2}$

Hence to obtain disjoint open balls of p and q , one needs to take $r \leq \frac{d(p,q)}{2}$.

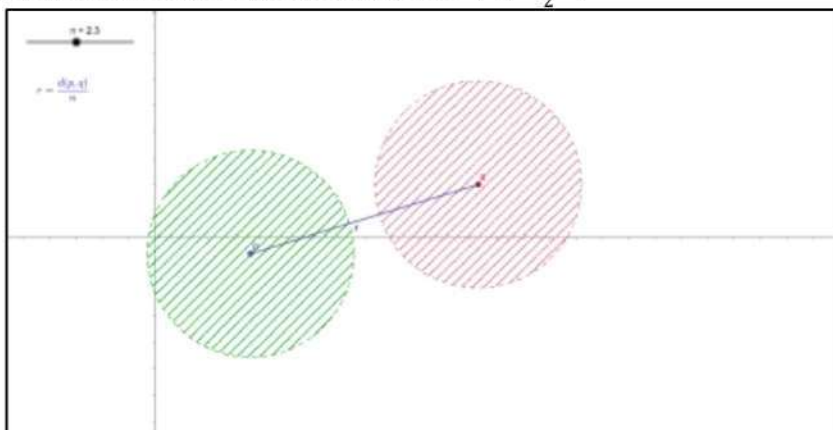


Figure 5: Open balls when $r < \frac{d(p,q)}{2}$

Maximum value of r such that the open balls remain disjoint is $r = \frac{d(p,q)}{2}$ as seen in the following image.

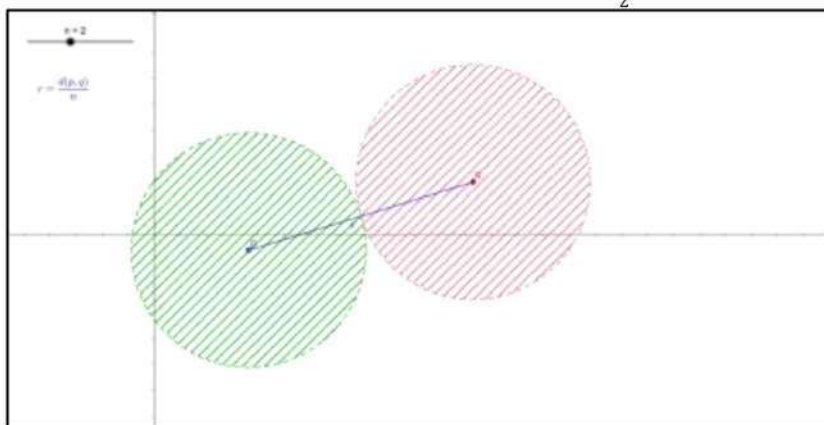


Figure 6: Open balls when $r = \frac{d(p,q)}{2}$

In the above applet, value of r is taken as $\frac{d(p,q)}{n}$ where n can be taken anything between 0 and 5. Using the slider for n , students can change the value of n and observe the effect on the open balls and deduce very easily that to get disjoint open balls, we need to have $n \geq 2$ and hence $r \leq \frac{d(p,q)}{2}$.

Conclusion

GeoGebra is a powerful tool in teaching mathematics, offering dynamic, interactive, and visually engaging ways to explore mathematical concepts such as open balls as seen here. Teachers as well as students should be motivated to use GeoGebra to construct such open balls in different metric spaces. Teachers can create dynamic worksheets using GeoGebra, where students can interact with mathematical objects and answer questions directly on the screen. This allows for personalized learning experiences and immediate feedback on student responses. GeoGebra can be used to create interactive demonstrations of mathematical theorems, proofs, or problem-solving strategies. One such example is provided above. These demonstrations can help students visualize abstract concepts and understand the underlying logic or reasoning. It increases the understanding as well as interest in the students to learn such concepts of mathematics.

References

1. Hohenwarter, Markus Preiner, J. (2007). Dynamic Mathematics with GeoGebra. *Journal for Online Mathematics and Its Applications*, 7.
2. Hohenwarter, M., Preiner, J., & Yi, T. (2007). Incorporating GeoGebra into Teaching Mathematics at the College Level. *Ictm*, January 2007, 1–7.
3. [https://wiki.geogebra.org/en/Category:Manual_\(official\)](https://wiki.geogebra.org/en/Category:Manual_(official)).
4. Kumaresan, S. (2011). *Topology of Metrics Spaces*. Narosa.
5. www.geogebra.org.