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Microwave Assisted Synthesis of 3-Chloro-N-(2-(5-chloro-1-tosyl-1H-benzo [d] Imidazol-2-yl) ethyl)-N-Substituted Quinoxalin-2-Amine Derivatives Using DCQX

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Abstract: The microwave assisted synthesis of 3-Chloro-N-(2-(5-chloro-1-tosyl-1H-benzo [d] imidazol-2-yl) ethyl)-N-substituted quinoxalin-2-amine derivatives is described. 2,3-dichloro quinoxaline (DCQX), as a starting compound and propargyl bromide, as an efficient alkylating agent are used in the synthesis of N-substituted quinoxalin-2-amine derivatives. We realized that microwave assisted synthesis is efficiently replacing conventional method of synthesis.

Keywords: 2,3-dichloroquinoxaline, quinoxaline, imidazoles, alkylating agent, microwave assisted synthesis

1. Introduction

There are several reported methods for the synthesis of quinoxaline-2-amine derivatives. Nevertheless, synthesis using 2,3-dichloroquinoxaline (DCQX) with nucleophilic species such as aryl amine has become a feasible substitute because of the presence of two chlorine atoms at C2 and C3 of DCQX. 2,3-dichloroquinoxaline (DCQX) is a reagent, extensively used as a synthetic intermediate in pharmaceutical industry as well as materials science^[1,2]. Furthermore, this reagent is easily prepared from low-cost starting materials and commercially available.

One of the major advantages associated with the reactions of DCQX with nucleophiles is the possibility to control single or double substituted products. This exceptional feature of DCQX makes it significant in the synthesis of specific products that can be used in a variety of applications^[3-7]. Propargyl bromide, an efficient alkylating agent is used for the N-alkylation of aryl amides. It is also used in enyne metathesis of propargylic amines, propargylation of spiro ketones, synthesis of allylic alcohols and enone complexes^[8,9].

The effective approach for the synthesis of quinoxalin-2-amines is the reaction between 1,2-diamines with aldehydes and isocyanides using CeO₂ nanoparticle catalyst. Also 3,4-dihydroquinoxalin-2-amines were synthesized by reactions between 1,2-diamines, ketones and isocyanides^[10].

Reaction between 2,3-dichloro quinoxaline and anilines is a convenient method for the preparation of N-aryl substituted 3-chloroquinoxalin-2-amines, particularly, 2-(N-aryl amino)-3-chloroquinoxalines that are further converted into N-substituted 3-chloro-N-(2-(1-tosyl-1H-benzo [d]-imidazol-2-yl) ethyl) quinoxalin-2-amine^[11]. This method is facilitated by AlCl₃ on forming C-N bond^[1]. These target molecules were found to be potential inhibitors of phospho diesterase 4 (PDE-4) and have apoptosis inducing properties in an animal model (zebrafish)^[12,13]. Further, the reaction is facilitated in more effective way using an alkylating agent, propargyl bromide.

2. Results and discussions

All the compounds were synthesized using microwave irradiation. The synthesis of new compounds is described according to synthetic Figure 1. Compound 2 was synthesized from the starting materials, 2,3-dichloroquinoxaline (DCQX) and aniline, substituted at 4th position. Then compound 2 is irradiated with an alkylating agent, propargyl bromide in presence potassium carbonate and DMF to acquire compound 3. The final compound 3-Chloro-N-(2-(5-chloro-1-tosyl-1H-benzo [d] imidazol-2-yl) ethyl)-N-substituted quinoxalin-2-amine (4) is obtained, when compound 3 was reacted with a

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A mathematical study on two layered blood flow of a couple-stress fluid

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K. Maruthi Prasad, N. Subadra, and B. Rama Krishna Reddy

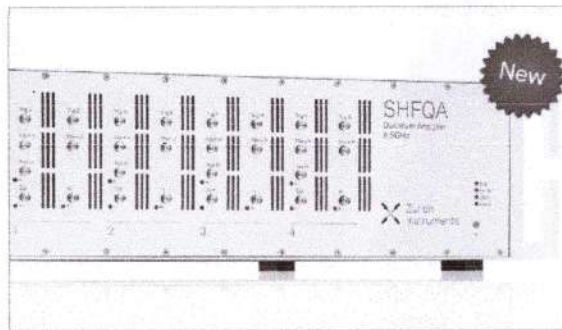


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Heat and Mass Transfer Effects of Power-Law Fluid in an Inclined Tube

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Abstract: The present investigation deals with the analytical study of heat and mass transfer effects of a Power-law fluid in an inclined tube. By adding nanoparticles to the power-law fluid, heat and mass transfer effects have been studied. Axial velocity, axial pressure gradient and frictional force are expressed analytically and the effects of various parameters on these flow variables have been studied. The present model revealed that heat and mass transfer coefficients decreases in the region $[-1,0]$ and increases in the region $[0,1]$ with the increase of Brownian motion parameter and shows opposite behavior with the increase of thermophoresis parameter.

Keywords: Power-Law fluid, Heat Transfer Effect, Mass Transfer Effect

INTRODUCTION

Peristalsis is a mechanism of fluid transport from lower pressure region to higher pressure region by contraction and expansion of a fluid along a tube like structure. This mechanism is very much important in human body. It has many applications in bio medical field as well as in industry. Many researches contributed their research on peristalsis. (Abd-Alla et al. (2014); Chandra & Pandey, (2018); Maiti & Misra, (2012); Noreen Sher Akbar, (2012); Srivastava, (1986); Yin & Fung, (1969)).

It is a known fact that in a homogenized blood, blood can be considered as power-law fluid, more so while flowing in large blood vessels. Though power-law model is popular, it does not show any prominent differences in stress. The viscosity is subject to the rate of shear. In case of shear thinning fluids, the zero shear rate viscosity increases whereas, in shear thickening fluids. Their velocities are zero as there shear rate increases. (El Naby & El Shamy, (2007); Hayat et al. (2006); Radhakrishnamacharya, (1982); Shukla & Gupta, (1982); L. Srivastava & Srivastava, (1988)).

Nanofluids are the fluids which contain nanometer sized particles. Nanofluids have many biomedical and industrial applications. Because nanoparticles increases the thermal conductivity of the base fluids with low thermal conductivity by immersing nanoparticles in the base fluids. Now a days void research is going on nanofluids. (Abbasi et al. (2015); Buongiorno, (2005); Ellahi, (2018); Narayanan & Rakesh, (2018); Noreen Sher Akbar, (2012); Prasad et al. (2017); S. U.S. Choi, (1995)). A very less research work has been done on power law fluid with nanoparticles.

By keeping all above in the mind, in the present paper heat and mass transfer effects of a power law fluid have been studied in an inclined tube using peristalsis. Axial velocity, axial pressure gradient and frictional force are expressed analytically and the effects of various parameters on these flow variables have been studied.





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Attenuation Effect in Aliphatic Acids Extended to Alkanes the Carbon Acids Via the Aliphatic Alcohols: an Educational Perspective in Chemistry

Author(s): R. Sanjeev, V. Jaganadham

Subject(s): Social Sciences, Education, School education, Adult Education, Higher Education, State/Government and Education, Inclusive Education / Inclusion

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Keywords/Abstract: A simple, new, lucid and an improved version of a protocol over Andrew William's treatment is presented in this article for the evaluation of the attenuation effect of methylene group on the deprotonation process of aliphatic acids RCOOH - RCOO⁻ + H⁺ and extended to aliphatic alcohols and alkanes; the carbon acids.

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Comparison of Substituent Effects in Benzenes ($\text{XC}_5\text{H}_5\text{C}$), Pyridines ($\text{XC}_5\text{H}_4\text{N}$) and Phosphorines ($\text{XC}_5\text{H}_4\text{P}$) and their Protonated Species

R. Sanjeev¹, V. Jagannadham^{2*}

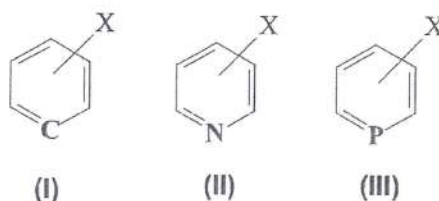
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Abstract Collection of interesting and stimulative data led us to construct Hammett plots for different properties like proton affinities, gas phase basicities, solvation free energies of free and protonated benzenes (I), pyridines (II) and phosphorines (III), and for $\text{p}K_a$ values of protonated pyridines and phosphorines. Trends in Hammett reaction constants (ρ) for all these processes were discussed.



Keywords: benzenes, pyridines, phosphorines, $\text{p}K_a$, proton affinities, gas phase basicities, solvation free energies

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structures were drawn using chemdraw software. All Hammett σ values are from reference 64.

1. Introduction

Acuity of work in chemical education and chemical research that took a shape from literature reported data on several chemical and physical aspects like phase transition temperatures, dipole moments, surface tensions, attenuation effect, associative and non-associative behavior of liquids, stability and lifetimes of reactive intermediates, LFER, effect of hybridization of carbon on Hammett (ρ) and Taft (ρ^*) reaction constants, prediction of $\text{p}K_a$ values of unstable arenium ions and benzenes, from our group has been ever increasing in recent times [1-63]. In the present work to go a step ahead we have tried the comparison of substituent effects on $\text{p}K_a$, proton affinities, gas phase basicities, solvation free energies in benzenes ($\text{C}_5\text{H}_6\text{C}$), pyridines ($\text{C}_5\text{H}_5\text{N}$) and phosphorines ($\text{C}_5\text{H}_5\text{P}$) and their protonated species.

2. Methods

All the linear correlations were done using the KaleidaGraph software, Reading, PA, USA. All chemical

3. Discussion

Hammett reactions constants (ρ) and $\text{p}K_a$ data of arenium, pyridinium and phosphorinium ions are given in Table 1. The corresponding plots are shown in Figure 1, Figure 2 and Figure 3.

Since the Hammett ρ can not be determined for the dissociation equilibria of arenium ions $\text{XC}_6\text{H}_6^+ \rightleftharpoons \text{XC}_6\text{H}_5 + \text{H}^+$ as they are highly unstable, an alternate and lucid method was adopted by us based on the attenuation effect [26]. Figure 1 shows the determination of the Hammett ρ for the dissociation equilibria of arenium ions $\text{XC}_6\text{H}_6^+ \rightleftharpoons \text{XC}_6\text{H}_5 + \text{H}^+$ from the study of attenuation effect of methylene group ($-\text{CH}_2-$) on the dissociation equilibria of anilinium ions, benzyl ammonium ions and 2-phenylethyl ammonium ions [26] and using the Andrew Williams' empirical equation $\rho = m1^{(2-i)}$ [65] where $m1$ is an arbitrary constant "i" is the number of atoms between ionizable proton and the ring carbon.

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Application of Hammett equation to hydrogen bond interactions of benzoic acid in chloroform/water system and explanation for non-linear Hammett relation to partition coefficients for the same system

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ABSTRACT

It is well known that benzoic acid distributes itself between chloroform and water. The partition coefficients (K_p) of seven different benzoic acids in chloroform/water are documented in the literature. Plausible hydrogen bonded structures of these seven benzoic acids with the two immiscible solvents were envisaged and the DFT calculation for these hydrogen bonds were carried out. Further, the conformity of Hammett relation to the hydrogen bond interactions was assessed. Application of Hammett equation to the hydrogen bonding of distribution of different *para*-substituted benzoic acids to these immiscible solvents is done for the first time. Further, an explanation for non-linear plot of partition coefficients $\log K_p$ of *para*-substituted benzoic acids in chloroform-water system versus Hammett σ value has been explained for the first time.

1. Introduction

Partition or distribution coefficients has a wide range of applications in the fields of pharmacology [1–3], pharmacokinetics [4–6], pharmacodynamics [7–9], environmental science [10,11], agrochemical research [12], metallurgy [13] and consumer product development [14]. Octanol is believed to have the lipophilic character of the biological membranes. The *n*-octanol/water [15] partitioning system resembles the lipid membrane/water systems in the body. Hence most of the partition studies appearing in the literature were carried out in octanol/water system. Over the last century numerous studies on partition of organic solutes have appeared in literature. To quote them is beyond the scope of this article as they run in several hundreds.

It is a well-established fact that Hammett [16,17] and Taft [18–21] equations are good mechanistic tools in physical-organic chemistry [16–21]. We have carried out several studies in our laboratory with regard to their application. Non-Linear Taft Relationship is applied to surface tensions of aliphatic acids: Inter-molecular hydrogen bonding versus intra-molecular hydrogen bonding [22], Non-Linear Taft Polar Free energy Relationships (TPER), reactions of *N*-substituted benzyl amines with benzyl bromide [23], dipole moments and melting points and their unsolved miracles on the application of Hammett equation [24] and application of non-linear Hammett relationship to surface

tensions and dipole moments in estimating the associative behavior of phenols [25]. It is known that benzoic acid distributes itself between chloroform and water. We have considered the distribution of seven *para*-substituted benzoic acids. In the present study we envisaged the plausible hydrogen bonded structures (Scheme 1) and found the interaction energies in them. Further, we assessed the conformity of Hammett relationship to these interactions. To comprehend Hammett equation, let us suppose a reaction is performed on a substrate molecule [26] that can be represented as XGY where Y is the site of the reaction, X a variable substituent and G is a skeleton group to which X and Y (in our Scheme 1, X = OH, OCH₃, CH₃, H, Cl, Br and NO₂, Y is hydrogen bonding between COOH moiety of substituted benzoic acid and solvents, G is C₆H₄) are attached and we observe that changing X from H to CH₃, results in the change in the rate of reaction. The change in the rate of the reaction might be due to factors like mesomeric effect or inductive effect of the substituent X. The first attempt of quantitative treatment of X on the reaction site was given by Hammett. For the cases of meta and *para*-XC₆H₄Y, Hammett set up the equation $\log(k/k_0) = \rho\sigma$ and this equation is known as Hammett equation. Here k_0 is the rate or equilibrium constant for X = H, k the rate or equilibrium constant for group X, ρ is a constant known as Hammett reaction constant for a given reaction under a given set of conditions, and σ is a constant known as Hammett substituent constant. Hammett substituent constant σ reflects

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Investigation on natural convective flow of ethylene glycol nanofluid containing nanoparticles Fe_3O_4 in a porous cavity with radiation

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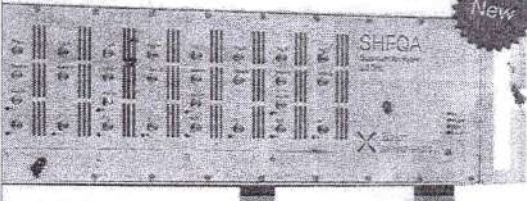
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(52)

Mathematical Approach to Study Heat and Mass Transfer Effects in Transport Phenomena of a non-Newtonian Fluid

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Abstract: The paper deals with a theoretical investigation of the peristaltic transport of a couple-stress fluid with heat and mass transfer effects. The velocity, pressure drop, time averaged flux, frictional force, mechanical efficiency, temperature profile, nanoparticle phenomena, heat transfer coefficient and mass transfer coefficient of the fluid are investigated, when the Reynold's number is small and wave length is large by using appropriate analytical methods. Effects of different physical parameters like couple-stress fluid parameters, Brownian motion parameter, thermophoresis parameter, local temperature Grashof number as well as local nanoparticle Grashof number on pressure drop characteristics, frictional force, mechanical efficiency, heat transfer coefficient, mass transfer coefficient, stream line patterns and velocity profiles of the fluid are studied. The expressions for velocity, temperature profile, nanoparticle phenomenon, heat transfer coefficient and mass transfer coefficients are sketched through graphs in two as well as in three dimensional views. The streamlines are drawn to discuss trapping phenomenon for some physical quantities.

INTRODUCTION

Peristaltic transport is very important mechanism in the biological systems for the transport of bio fluids like blood, urine etc. It has numerous applications in physiological systems as well as in mechanical systems. The phenomenon of peristaltic transport is used in the manufacturing of nuclear reactors and also in roller and finger pumps.

Many investigators contributed to the study of peristaltic transport in mechanical as well as physiological situations. (Fung & Yih, (1968), Shapiro et al., (1969), Pincombe et al.,(1999), Maruthi Prasad et al.,(2015)).

V. K. Stokes (1966) was the first person who developed the couple-stress fluid as a special case of non-Newtonian fluids. The important point in introducing the couple-stress fluid is to establish a size dependent effect that is not there in the viscous theories.

In 1986, L. M. Srivastava considered couple-stress fluids for his study and studied peristaltic transport in it. Maruthi Prasad & Radhakrishnamacharya (2009) considered a two fluid model with couple-stress fluid in the core region and Newtonian fluid in the peripheral region and studied the peristaltic transport. Rathoda et al., (2012) considered uniform and non-uniform annulus and investigated peristaltic motion of couple-stress fluid in the presence of porous medium. Maiti et al., (2012) done a theoretical investigation on peristaltic motion of a couple-stress fluid in a porous channel. The influence of Hall effect on peristaltic flow of a couple-stress fluid in a vertical asymmetric channel was examined by Kumar et al. (2017).

Nanofluid is the next exciting leading edge in technology. The applications of nanofluids are huge because of its enhanced thermal conductivity. Nanofluids used in Nano drug delivery, Cancer therapeutics, Nuclear reactors etc.

A New Approach to the Construction of Transition Matrix with Application to Control Systems

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Abstract: In this paper the study of new approach to the construction of a transition matrix associated with first order matrix system of differential equations is applied in the control systems. This method is unique and is applicable to all problems that arise in control systems and the tedious calculations so far existing in literature will be condensed to less than half.

INTRODUCTION

In this paper we shall be concerned with the Existence and Uniqueness of solution to general first order Matrix differential equation

$$y' = Ay, \quad y(0) = y_0 \tag{1.1}$$

where A is an (nxn) constant matrix. It is a well known fact that the scalar exponential function e^{at} can be represented as a power series

$$e^{at} = 1 + at + \frac{(at)^2}{2!} + \dots + \frac{(at)^n}{n!} + \dots$$

Now, given an (nxn) constant matrix A, the corresponding Power Series

$$I + At + \frac{(At)^2}{2!} + \dots + \frac{(At)^n}{n!} + \dots$$

Converges entry wise to the Matrix exponential function e^{At} . The general solution of (1.1) can be written as

$$y(t) = e^{At}y_0$$

The paper is mainly concerned with computing e^{At} , and hence the solution of the initial value problem (1.1). Before presenting the general solution of the Initial value problem (1.1), we present the following two results.

Theorem 1.1: Let A be an (nxn) constant matrix with the characteristic polynomial.

$$C(\lambda) = \det(A - \lambda I) = \lambda^n + C_{n-1}\lambda^{n-1} + \dots + C_1\lambda + C_0,$$

then $\phi(t) = e^{At}$ is the unique solution of the n^{th} order matrix differential equation.

$$x^{(n)} + C_{n-1}x^{(n-1)} + C_{n-2}x^{(n-2)} \dots + C_1x' + C_0x = 0 \tag{1.2}$$

satisfying the initial conditions

$$\phi(0) = I, \phi'(0) = A, \phi''(0) = A^2, \dots, \phi^{(n-1)}(0) = A^{n-1} \tag{1.3}$$

Proof: Suppose $x_1(t), x_2(t), \dots, x_n(t)$ be n linearly independent solutions of the n^{th} order linear differential equation (1.2). Then it can easily be proved that ϕ satisfies the differential equations and ϕ satisfies the initial conditions

$$\phi(0) = I, \phi'(0) = A, \dots, \phi^{(n-1)}(0) = A^{n-1}$$

Therefore,


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Study of Microstructure and Thermal Properties of PbTiO₃ Based Glass Ceramics

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Abstract: Glass samples with composition (35- X) B₂O₃ - (40 +X) PbO - 25 TiO₂ (where X= 0, 2.5, 5, 7.5 and 10 mol %) were prepared using conventional quenching technique. These glass samples were converted to glass ceramics by following two stage heat treatment schedules. The density (ρ) values of glass ceramic samples are higher than those of corresponding glass samples. It was observed that there was good correlation between the density and Coefficient of Thermal Expansion (CTE) results of the glass-ceramics. The XRD results in the glass ceramics revealed the formation of tetragonal lead titanate (PbTiO₃) as a major crystalline phase and lead borate (PbB₂O₄) as minor crystalline phase. The microstructure of glass ceramic samples contains nano crystallites of lead titanate embedded in a borate glass matrix.

INTRODUCTION

PbTiO₃ (PT) is a tetragonal perovskite with a c/a ratio of 1.063 at room temperature, which is the largest known for lead-based perovskite compounds. Single crystal data have shown that the large ionic displacements in PT lead to a particularly large spontaneous polarization (>53 $\mu\text{C}/\text{cm}^2$) and strain (c/a ratio = 1.06) at room temperature [1]. PT exhibits large pyroelectric coefficients and low relative permittivity (~100-200). However, these excellent properties are not yet fully realised in bulk polycrystalline samples due to difficulty in fabricating undoped PT. PbTiO₃ ceramics when prepared by conventional route generally have micro cracks and fracture on cooling below T_c as a result of the large spontaneous strain generated when the structure changes from cubic to tetragonal.

Glass ceramics are the polycrystalline materials prepared by the controlled crystallization of glasses. A wide variety of applications of these versatile materials have been developed as a result of their many outstanding properties and the distinct advantages of the glass ceramic method, in certain circumstances, over conventional ceramic processing routes. Of particular importance in many applications is the high uniformity of the microstructures of glass ceramics, the absence of porosity and the minor changes in volume during the conversion of glass into glass ceramic [2].

Ferroelectric crystalline phases investigated include SrTiO₃[3-4], BaTiO₃[5-6], LiTaO₃[7], LiNbO₃[8], PbTiO₃[9-11] and (Pb,Sr,Ba)Nb₂O₆[12]. The ferroelectric and dielectric properties of glass-ceramics mainly determined by major crystalline phase and the residual glass or secondary phase(s). However, the excellent adjustability of the composition and microstructure of glass-ceramics promises some advantages of high-permittivity glass-ceramics over the crystalline ferroelectric ceramics (viz. adjustable thermal expansion, dielectric properties, and processing temperature). They also offer the benefit of process compatibility with ceramic substrates and metallized components. Therefore, high-permittivity glass ceramic materials are candidates for capacitors, hybrid circuits, electro-optic, and cryogenic applications [13-14].

In this paper microstructure and thermal properties of PbTiO₃ based Glass Ceramics of (35- X) B₂O₃ - (40 +X) PbO - 25 TiO₂ has been reported.

20-21 (13)

Quenching Effect of co-dopant Pr³⁺ on Red Emitting Yttrium Vanadate Phosphor Doped with Eu(III)

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Abstract: Y_{1-x}VO₄: Eu_{x-y}³⁺: Pr_y³⁺ with x = 6 mole % and y = 0, 2, 3, 4, 5, 6, mole % phosphors have been prepared by solid state reaction. The dopant Eu³⁺ concentration was optimized along with the co-dopant Pr³⁺ concentration in the yttrium vanadate host lattice with the help of photoluminescence (PL) spectra. The phosphors have displayed red color under UV source. Pr³⁺ acts as quencher and quenching effect of co-dopant Pr³⁺ on Red Emitting Yttrium Vanadate Phosphor Doped with Eu(III) using luminescence Studies on Y_{1-x}VO₄: Eu_{x-y}³⁺: Pr_y³⁺ systems are presented in detail in this paper. The emission intensities were determined and the relative fluorescence intensities have been estimated. The richness of the red color is verified by determining the chromaticity coordinates (X, Y) from the CIE standard charts.

INTRODUCTION

The crystal field of the monazite characteristics makes YVO₄ a very attractive laser material with dopants Eu³⁺, Tm³⁺, Tb³⁺, Er³⁺, Ho³⁺, Ce³⁺ and Pr³⁺ [1-14]. Of these Red Emitting Yttrium Vanadate Phosphor doped with Eu(III) is found to be very attractive potential laser material. YVO₄ is an important host lattice for phosphors [5-6] due to its application in TV screens and high pressure mercury vapor (hpmc) lamps. Among the rare earth ions, praseodymium (Pr³⁺) has drawn the attention of several researchers due to the capability of emitting efficiently [15]. Examples Pr³⁺ as a sensitizer, which enhances the excitation resulting in transfer of energy to dopants through a non-radiative process and Pr³⁺ as quencher which quenches emission of energy of dopants through non-radiative relaxation of the system are available in literature i.e. in some hosts it demonstrates energy transfer between Pr³⁺ and dopants [16-24] while in some other hosts it demonstrates a lack of energy transfer between it and dopants [25,26]. Photo luminescent (PL) properties of Pr³⁺ co-doped phosphors especially in crystalline hosts have been reported by many researchers [16-29].

The YVO₄ crystal is tetragonal, belonging to space group D_{4h}. The dopant rare earth ion substitutes on Y³⁺ ion sites the local site symmetry will be D_{2d} and it is surrounded by eight O²⁻ ions [30,31]. The information on the red luminescence under ultraviolet excitation of rare earth vanadate was first reported by Van Uitert et al [32]. Europium doping gives red emission in YVO₄ with four main groups of emission lines of peaks at 700nm, 655nm, 621nm and 595nm and has been assigned to ⁵D₀ → ⁷F₄, ⁵D₀ → ⁷F₃, ⁵D₀ → ⁷F₂ and ⁵D₀ → ⁷F₁ transitions respectively, for Eu³⁺ ion. The luminescent properties and the crystallographic data on all rare earth vanadates are available in literature [30,31]. The development by Levine and Palila [33] of europium activated yttrium orthovanadate as a highly efficient red emitting cathodoluminescent phosphor and its adoption for color television aroused interest in other lanthanide activated orthovanadates. Bixner et al [34] investigated Ca₃(VO₄)₂ and found it to be moderately efficient as a host of Eu, but simultaneously inferior to YVO₄. The systems more efficient than Ca₃(VO₄)₂ based on were described by Palila et al. [33], who showed that the exciting energies are absorbed by the VO₄³⁻ ions and is transferred to activators.

In the present work an attempt has been made to vary the concentration of Pr³⁺ and study the efficiency of red emitting YVO₄: Eu³⁺: Pr³⁺ phosphor. Initially, Eu³⁺ concentration in the lattice was optimized at 6 mole % with the help of PL studies and this composition has been taken further to study the effect of Pr³⁺ as co dopant. Prepared powder phosphors were characterized by XRD and PL spectra. The results are reported and discussed in this article.


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(66)

Enhanced electrical properties of $\text{Sr}(\text{Bi}_{3.9}\text{La}_{0.1})(\text{Ti}_{3.975}\text{Zr}_{0.025})\text{O}_{15}$ ceramic with the doping of Nd

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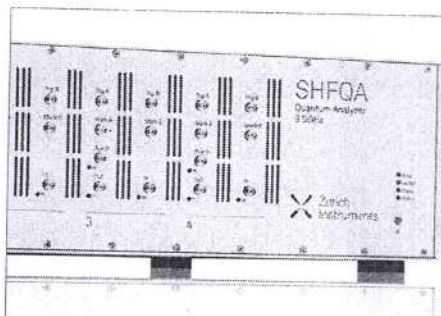
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(65X)



WEB 2.0 TOOLS: USE OF KAHOOT TO REDUCE THE SPELLING MISTAKES AMONG B.TECH LEARNERS OF COMMUNICATIVE ENGLISH

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Abstract:

BTech learners of Communicative English are inclined towards technology and hardly focus on spellings in their writing. Today, students are called as netizens or net generations (Educause.edu, 2016) due to their over usage of web tools. My paper explores strategies to reduce spelling mistakes in BTech learners of Communicative English by introducing games using Kahoot, in the class. In the empirical design approach, the questions framed by the teacher would help the learner identify the correct spelling through game based learning. Though the learners face technical challenges, learning through games is very interesting.

Key Words: Net Generation, Kahoot, Undergraduates of Engineering, Spellings

Hypothesis:

The Engineering undergraduates who are interested in anything with internet would learn correct spelling through game based e-learning.

Introduction:

Most of the teachers find it challenging to teach spellings to students at undergraduate level. Due to heterogeneous educational background, many students are unable to spell the words right in their academic writing. This has affected their career growth. As technical students are inclined towards technology, teaching-learning process using web 2.0 tools becomes more compatible. Introducing Quizzes through Kahoot which is a game based LMS motivates and engages students and a positive impact develops in the learning process in them.

Rabail Tahir in his research investigated the effect of using Kahoot in his classroom. He focused on learning performance, classroom dynamics, students' and teachers' attitudes and perceptions, and student anxiety. Through his qualitative and quantitative research with 93 students, he found Kahoot to have a positive effect in teaching and learning process. He felt technical hitches, time stress and fear of losing the game were the challenges the students faced.

The method is to design a game based questionnaire where students would respond using the Kahoot! Kahoot! is a game-based student response system (GSRs) where the classroom is temporarily transformed into a game show where the teacher is the game show host, and the students are the contenders (Wang, 2015). The teacher frames some quiz questions and creates the game using Kahoot! The students would respond to them. Some conceptual questions that would test their retention and spelling ability will be asked in the game as a quiz. The students have an option to redo their wrong questions. In this process the students identify their mistakes and learn the correct spelling. Kahoot! The game-based application is very interesting and easy to create and motivating to play games in the classroom. Multiple choice questions or true or false type questions can be asked using Kahoot. The background music while playing the game not only triggers enthusiasm in students but also keeps them alert throughout the game. This enhances students' concentration and keeps them focused on what they are supposed to do. Above all, playing games break the monotony of the traditional classroom and makes a learner centred class. The results would be based on score of every individual. It would be number of questions answered correctly in the given time. Based on the score the ability of the student would be analysed and the teacher would plan further quizzes based on the responses.

Samples/Population:

40 students of III year Mechanical Engineering of whom only 19 could participate.

Method:

To test the spellings, I have framed 10 questions on the topic Presentation skills. The questions were to review the lesson and also to test the spelling ability in the learner. Four options were given to answer each question. Three of the four options had wrong spelling that would sound similar. The learner needs to comprehend the question, recollect the answer and identify the answer with its correct spelling. Of 40 students in the class only 19 could participate as few did not have an extra device to play, few had problem with the connectivity and few others had no technical knowledge. Of 19 participants only 17 were able to answer as the other two could not match the speed of the game as the game has fixed time to answer each question. This gave

20-21-16

A simple rule of thumb for the explanation of d-orbital splitting in complexes

R. Sanjeev¹, V. Jagannadham² and R.Veda Vraha³

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Abstract

In chemistry at pre-university level and freshman engineering (non-chemistry discipline) classrooms at universities in India, the splitting of the energy levels of d-orbitals in complexes is an important concept to be learnt, but is not explicitly explained in the standard books used. In the standard books such as 'Concise Inorganic Chemistry' by J.D. Lee and 'Theoretical Inorganic Chemistry' by Marion Clyde Jr. Day and Joel Selbin, they have explained the splitting of d-orbitals in octahedral, tetrahedral, square planar etc., complexes very well. The same is the case with the latest pre-university NCERT chemistry textbook (Volume I) written for the Indian audience. The reason why the energy levels of certain d-orbitals are above the barycenter and why some are below the barycenter, however, is not explained explicitly in any of the books (including the latest books). This short communication outlines a simple rule of thumb that allows this phenomenon to be explained to students. Further, an important graph in the standard books is plotted, but the trend of the curve is not explained. This simple rule is also helpful in explaining this graph and the chemical phenomenon represented.

Keywords

D-orbitals, lowering of energy, gain of energy, attraction, repulsion.

Una simple regla para la explicación de la división del orbital d en complejos

Resumen

En las aulas de química a nivel preuniversitario y de ingeniería (disciplina no química) de primer año en universidades de la India, la división de los niveles de energía de los orbitales d en complejos es un concepto importante que debe aprenderse, pero no se explica explícitamente en los libros estándar usados. En los libros estándar como 'Química inorgánica concisa' de J. D. Lee y 'Química inorgánica teórica' de Marion Clyde Jr. Day y Joel Selbin, han explicado la división de los orbitales d en octaédricos, tetraédricos, planos cuadrados, etc., complejos muy bien. Lo mismo ocurre con el último libro de texto de química preuniversitario NCERT (Volumen I) escrito para la audiencia india. La razón por la que los niveles de energía de ciertos orbitales d están por encima del baricentro y por qué algunos están por debajo del baricentro, sin embargo, no se explica en ninguno de los libros (incluidos los últimos libros). Esta breve comunicación describe una simple regla empírica que permite explicar este fenómeno a los estudiantes. Además, se traza un gráfico importante en los libros estándar, pero no se explica la tendencia de la curva. Esta sencilla regla también es útil para explicar este gráfico y el fenómeno químico representado.

Palabras clave

D-orbitales, disminución de energía, ganancia de energía, atracción, repulsión.

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20-21-19



Structural and microwave behavior of Dy³⁺-substituted Ni_{0.5}Zn_{0.5}Dy_xFe_{2-x}O₄ ferrites

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ABSTRACT

The enhancement of microwave absorbing properties in dysprosium ion (Dy³⁺)-substituted nickel–zinc ferrites (Ni_{0.5}Zn_{0.5}Dy_xFe_{2-x}O₄; x = 0.00, 0.01, 0.03, 0.05, 0.07 and 0.09) has been investigated in this work. The ferrite powders were synthesized by microwave-hydrothermal method and then powders were densified at 900 °C for 40 min using microwave furnace. The samples' structural and morphological properties were studied using X-ray diffraction and scanning electron microscopy (SEM), respectively. The structural result confirms the spinel phase under low Dy³⁺ content, like the pure Ni–Zn ferrite, while a secondary phase of DyFeO₃ appears after the content of Dy³⁺ exceeds a certain limit (x > 0.07). Morphological analysis from the SEM images reveals the formation of spherical grains of the samples. DC resistivity of the samples has been measured using two-probe method. Magnetic hysteresis data confirm the soft magnetic nature of the samples. The vector network analyzer results show that adjusting the content of Dy³⁺ is significant in changing the magneto-dielectric properties and microwave absorption capacity of the materials. The composition x = 0.07 sample showed a reflection coefficient of – 33.24 dB at the frequency and bandwidth of 10.31 GHz and 2.59 GHz for an absorber thickness of 2.5 mm for losses less than – 10 dB. This acquired result indicates that the investigated samples could be used as a microwave absorber application in X-band.

1 Introduction

Spinel ferrites are the most attractive magnetic oxides due to their diversified fundamental and technical applications [1–3]. The general formula of the spinel ferrites is MFe₂O₄, where M represents the divalent

metal cation like Ni, Co, Zn, Mg and Mn. The unit cell of these ferrites has a cubic symmetry and contains eight formula units of MFe₂O₄. The relatively large-sized oxygen ions form a face-centered cubic structure and each cubic unit cell consists of '64' tetrahedral (A) sites and '32' octahedral (B) sites; out of these

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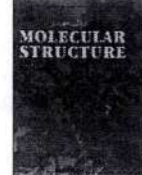
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Influence of hydrogen bond networks in Glycerol / N-Methyl-2-Pyrrolidone mixtures studied by dielectric relaxation spectroscopy

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ABSTRACT

In this paper, we report the dielectric permittivity of the Glycerol (Gly) with N-Methyl-2-Pyrrolidone (NMP) binary mixtures in the microwave frequency region at different temperatures. The dipole moments of Gly, NMP and their equimolar binary mixtures are calculated by using Higasi's method in the temperature range 298.15K-323.15K. The dielectric relaxation spectra of the binary mixtures are calculated using Cole-Cole and Cole-Davidson equation and shows an unsymmetrical relaxation behaviour. The excess parameters of volume, permittivity, refractive index, polarization and relaxation times are fitted with Redlich-Kister polynomial equation. The molecular association and their hydrogen bond interactions between the components in the mixture are discussed in terms of Kirkwood correlation g^{eff} factor and excess Helmholtz energy (ΔF^E) equation. The mean molecular polarizability (α_M) of the individual and their binary mixture are calculated using Lippincott δ - function potential model and compared with the LeFevre method of polarizability values. The enthalpy of activation ΔH^* , entropy of activation ΔS^* and Gibbs free energy of activation ΔG^* are also evaluated and the results are discussed in terms of the orientation of the dipoles. The presence of hydrogen bonding between Gly and NMP is confirmed from the FT-IR spectra.

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1. Introduction

The non-destructive characterization of biological samples/liquids, polymers and gels have stimulated the use of dielectric relaxation spectroscopy (DRS) at a broader frequency range at different temperatures [1]. The DRS is one of the sensitive methods to interpret the structural dynamics, molecular association and orientation of the dipoles in the liquid medium [2]. The dielectric relaxation spectroscopy is well suited for to observe the changes in the electrical properties when liquids mix up at different concentrations and also the hydrated studies of proteins/gels with the change in temperature. Therefore, temperature-dependent dielectric relaxation studies of liquid mixtures are of growing interest [3–9]. The investigation of dielectric permittivity of the mixtures by varying concentration of liquid samples helps to ascertain the structure of the complexes formed in the solution

[10–15]. The presence of the hydrogen bond between components present in the mixtures that affect the dielectric permittivity, polarization and its relaxation behaviour properties. The understanding the nature of hydrogen bond remains a complex task due to the type of bonds and components present in the given liquid system [16–22]. The dielectric permittivity studies of hydrogen-bonded polar liquids/polymer nanocomposite materials at broader frequency region are very much interesting and these results are quite useful in the field of biological, medical, and shielding applications [23–32].

Glycerol is a simple polyol compound; due to its antimicrobial and antiviral properties, it is extensively used in wound and burn treatments, effective marker to measure liver diseases, the sweetener in the food industry and as a humectant in pharmaceutical formulations [33–39]. NMP is a good polar solvent with magnificent properties. It is having a wide range of applications due to its higher boiling point, lower freezing point and ease of handling [40,41]. It is used as a solvent for engineering polymers, coating resins, paint stripping, oven cleaners, automotive and industrial cleaner formulations. The dielectric permittivity of the Glyc-

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FeF₃ MEDIATED SYNTHESIS OF 3,4-DIHYDRO-3-PYRIDYL-2H-NAPHTHA[2,1-E][1,3]OXAZINE DERIVATIVES

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ABSTRACT

Biologically active 3,4-dihydro-3-substituted-2H-naphtho [2,1-e][1,3]oxazine derivatives were synthesized using environmentally benign and economically feasible Lewis acid FeF₃. They are characterized by FT-IR, HNMR and Mass spectroscopic methods.

INTRODUCTION

1,3-oxazine derivatives, especially, when they were condensed with aromatic rings displayed diverse biological properties, such as antibacterial, anticancer, anti-fungal, analgesic, anticonvulsant and anti-tubercular activities.^{i,ii} Moreover, trifluoromethyl-1,3-oxazine-2-one is highly active against various HIV-1 mutant strains, since, they are non-nucleoside reverse transcriptase inhibitors that have an ability to bind and block HIV reverse transcriptase. Further, naphthoxazine derivatives showed high-level potential for the treatment of Parkinson's disease.^{iii,iv} They were shown to be anti-inflammatory agents. They were also used for treating allergies, ulcers, asthma, diabetes, and arthritis. 1,3-Oxazines have been used as key intermediates in the synthesis of thrombolytic agents, chiral auxiliaries in organic synthesis and liquid crystal devices.^v In a comprehensive survey of literature, it was found that naphth-1,3-oxazine derivatives were conventionally prepared using 2-naphthol, and various substituted aryl and heteroaryl aldehydes in the presence of dry methanolic ammonia. Further, the multi-component condensation of phenols or naphthols with primary amines (or ammonia) and two equivalents of aldehydes led to these target molecules. Similarly, condensation of derivatives of Betti base with aromatic aldehydes led to the formation of the corresponding 1,3-oxazine with varied biological properties.^{vi} Yet another method involves using the condensation reaction of salicylaldehyde with a primary amine, followed by reduction and then cyclization reaction with a suitable aldehyde. The oxazines containing six-membered ring nitrogen and oxygen was constructed by a type of Mannich reaction, in which zirconyl(IV)



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Case Studies in Thermal Engineering

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Chemical reaction impact on MHD natural convection flow through porous medium past an exponentially stretching sheet in presence of heat source/sink and viscous dissipation

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Chemical reaction
Eckert number
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ABSTRACT

This study investigates the viscous dissipation impact on free convection MHD flow through a porous medium over an exponentially stretching surface in presence of chemical reaction. The basic governing PDEs are converted into non-linear ODE's by using similarity transformations and then using the Keller-box method, numerical solutions are obtained. The flow features of boundary layers along with the bounding surface are identified and analysed using diagrams. It is noted that the increase in the Eckert number, Radiation and Magnetic parameter (M) increases the temperature profiles, while the increase in the chemical reaction parameter, porosity and Schmidt number decreases the concentration profile. To validate the results, a comparative study between the present study and previously published results for a particular case is conducted and good agreement is found between them.

1. Introduction

Engineering and Industrial procedures such as in extrusion processes, the movement of biological fluids, hot rolling, glass-fiber production, the cooling of metallic plates, rubber sheets, the performance of lubricants and paints, wire drawing, melt-spinning, manufacture of plastic, the extrusion of polymers, and aerodynamic plastic sheet extrusion, etc., is needed, has received considerable attention over the last few decades, to research flow on a stretching sheet. Many researchers are researching the movement of fluid over the stretching surface [1–5].

The influence of thermal radiation on convective fluid flows has an abundance of uses in physics and engineering for instance gas-cooled nuclear reactors, gas turbines, propulsion systems, hypersonic flights, space vehicles, solar power engineering, nuclear power plants, and lots of industrial areas, and so on. Several researchers [6–10] are attracted the thermal radiation.

In modern metallurgical and physical procedures, the research of the magnetohydrodynamic (MHD) flow of electrically conductive fluid is actually of great significance as a result of the effect of the magnetic field on the regulation of the boundary layer flow control as well as the effectiveness of numerous systems utilizing electrically conductive fluids. Its application in many engineering problems, this kind of flow has attracted the focus of several researchers [11–15] such as plasma studies, geothermal energy extractions, MHD generators, nuclear reactor safety, and furnace structure. Hydromagnetic strategies are employed for the decontamination of

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20-21-21

An efficient synthesis of novel anti influenza viral and cytotoxic derivatives of 4-oxothiazolidin-3-yl)-3-hydroxyquinoxaline-2-carboxamide

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Shashikala Kethireddy, Thirumala Chary Mariganti, and Srilalitha Sapram



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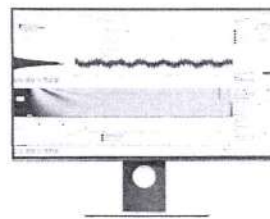
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Review

Recent Trends in Noble Metal Nanoparticles for Colorimetric Chemical Sensing and Micro-Electronic Packaging Applications

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Abstract: Noble metal NPs are highly attractive candidates because of their unique combination of physical, chemical, mechanical, and structural properties. A lot of developments in this area are still fascinating the materials research community, and are broadly categorized in various sectors such as chemical sensors, biosensors, Förster resonance energy transfer (FRET), and microelectronic applications. The related function and properties of the noble metals in these areas can be further tailored by tuning their chemical, optical, and electronic properties that are influenced by their size, shape, and distribution. The most widely used Au and Ag NPs in dispersed phase below 100 nm exhibit strong color change in the visible range which alters upon aggregation of the NPs. The chemical sensing of the analyte is influenced by these NPs aggregates. In this article, we have summarized the uniqueness of noble metal NPs, their synthesis methods, nucleation and growth process, and their important applications in chemical sensing, microelectronic packaging, and Förster resonance energy transfer.

Keywords: colloid; nanostructure; microelectronic systems; crystalline; hydrothermal; nucleation and growth

1. Introduction

Nanomaterial is defined as a material in which the maximum value of one dimension can be 100 nm, which can be further defined as one billionth of meter or 10^{-9} m [1–6]. It is approximately 10 H or 5 Si atoms in a line. It is continuing to be the most rapidly growing R/D sector in last decades, which is evident from more than several billion dollars of annual investment in this particular field [7,8]. Due to its unique features, nanomaterials and NPs allow them to be used for a wide variety of applications in nanotechnology covering medical science, chemical, bio-network, applied physics, materials, microelectronic and metallurgy science, and engineering. There are lots of investments in the area of medical science, in particular, theragnostics, which refers to two kinds of word therapeutics and diagnostics [9]. It is an advanced technique in which cancer diagnosis and therapy is done simultaneously, for early detection and cure of the cancer [10,11]. To achieve this, some special metals in the periodic table include alkaline to alkaline metallics, rare metallics, and noble metallics used for theragnostics application [12]. Compared to these metals, noble



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20-21 (28)

Impact of Soret and Dufour on bioconvective flow of nanofluid in porous square cavity

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Abstract

This article addresses the bioconvection in a porous cavity associated with Soret and Dufour effects. The bioconvective flow in a porous medium is based on Hillesdon and Pedley's model and is governed by nonlinear partial differential equations. These equations are transformed into a dimensionless form with suitable nondimensional parameters. The finite element method is employed to solve the dimensionless equations. The outcomes of the study are presented by streamlines, temperature distributions, iso-concentrations of solute, nanoparticles, and microorganisms. Furthermore, the tendency of average Nusselt number and average Sherwood number and the influence of Soret parameter, Dufour parameter, Peclet number, and bioconvective Rayleigh number is interpreted. Thermophoresis and Soret number show a strong effect on the concentration of nanoparticles. Brownian motion and thermophoresis exhibit a significant effect on the density distributions of microorganisms. The novelty of the paper is to combine the effects of Soret–Dufour and oxytactic bioconvection. The present study can be useful in the following applications: microbial-enhanced oil recovery, toxin removal, antibiotics, and modeling of microfluidic devices.

FH6

20-21-29



Enhanced microwave absorption properties of Ni_{0.48}Cu_{0.12}Zn_{0.4}Fe₂O₄ + polyaniline nanocomposites

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ABSTRACT

Nanocomposites of (1-x) Ni_{0.48}Cu_{0.12}Zn_{0.4}Fe₂O₄ (NCZ) + x Polyaniline (PANI), (x = 0, 0.1, 0.2, 0.3, 0.4, 0.5, 1) with varying composition were successfully prepared from nanopowders of Ni_{0.48}Cu_{0.12}Zn_{0.4}Fe₂O₄ synthesized by microwave hydrothermal method. The samples were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier Transform Infrared spectroscopy (FTIR). The characterization studies revealed the confirmation of spinel and polymer phases in the composite samples. The dielectric, magnetic and electromagnetic properties were studied over frequency range of 8.2–12.4 GHz (X-band) and 12.4–18 GHz (Ku-band). It was found that the addition of PANI filler in ferrite matrix enhances the microwave absorbing properties with the increment of dielectric and magnetic losses. The nanocomposite sample with 50 wt% PANI was found to exhibit minimum reflection loss of -42.10 dB near 9.35 GHz with the effective bandwidth of 3.8 GHz and -39.34 dB near 14.05 GHz with effective bandwidth of 2.8 GHz. The current results indicate that the present materials can be selected to design microwave absorbing filters both in X-band and Ku-band frequency regions for electromagnetic interference applications.

1. Introduction

In recent years there is an increase in demand for the development of absorbing materials in microwave frequencies region to suppress the effects of electromagnetic interference (EMI). Due to the fast development of advanced technology in several fields such as electronic wireless communications, military, commercial and medical applications, there has been widespread use of microwave devices in GHz frequency range [1–3]. These devices are capable of producing electromagnetic interference which can cause severe interruptions on functioning of several electronically controlled devices resulting in decrease in performance. Moreover, over exposure to microwave energy may lead to potential health hazards to the human body [4,5]. Hence, while using high frequency electronic devices EMI becomes a matter of serious concern. In order to control these problems created by electromagnetic interference the devices have to be shielded by the materials which can suppress the unwanted electromagnetic radiation and reduce the noise level of signals. Traditionally, conducting materials can shield the devices by reflecting the electromagnetic radiation. However, in the case of conducting shields the main drawbacks are heaviness, lack of flexibility,

high cost of processing, etc. Electromagnetic shielding through absorption instead, offers an effective means to solve these problems. Hence, shielding materials capable of absorbing unwanted electromagnetic waves were investigated by many researchers [6–11]. In order to acquire excellent microwave absorbing properties, the shielding materials should possess mainly two important characteristics, viz., the wave attenuation through the material layer, called attenuation characteristic and the impedance matching, the impedance of the material medium should match the impedance of free space. In addition to these, the other parameters such as light weight, thickness, mechanical strength, miniaturization, wider absorption bandwidth, environmental resistance, should be taken care of while producing and designing the microwave absorbing materials [12]. Over the past decades ferrite absorbers have been developed to study the microwave absorbing properties and found that they exhibit excellent magnetic and dielectric properties though they are heavy and expensive [13]. Polymers were designed to be used for microwave shields due to lightweight, flexibility and cost effectiveness. However, polymers are insulating materials and are transparent to electromagnetic waves. In order to suppress electromagnetic waves effectively by the materials with enhanced microwave absorbing

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20-21-30

PREDICTION OF BIOACTIVITY OF PHYTOCHEMICALS IN *Anethum graveolens* – AN *in silico* APPROACH

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Original Research Article

ABSTRACT

Anethum graveolens is a popular herb widely used as flavouring agent and it yields essential oil. It is rich in polyphenols which exhibit antioxidant and carminative properties. In this work, phytochemical screening is performed to establish the presence of terpenoids, flavonoids and tannins etc. In food products, lipid peroxidation is common and to prevent it synthetic antioxidants like butylated hydroxyanisole (BHA), butylated hydroxytoluene (BHT) are used and they are carcinogenic in nature. So, there is an increasing demand for plant derived antioxidants. *Anethum graveolens* is a plant rich in antioxidants and the present study predicts the antioxidant and bioactivity of Limonene, Carvone, α -Phellandrene, Dillapiol, Geraniol and p-Cymene. *In silico* studies were carried out using PASS prediction tool and the bioactive compounds were predicted with $P_a > 0.7$. For these compounds, the bioactivity score is calculated and their potential medicinal value is discussed using Lipinski's rule of 5 analysis. From the study, it is observed that all the compounds have bioactivity and are potential antioxidants that may be used in health care, cosmetic and food and beverage industry.

Keywords: *Anethum graveolens*; bioactivity spectrum; phytochemical screening; bioactivity score; Lipinski rule of 5.

INTRODUCTION

Anethum graveolens (Dill) is an herb that belongs to the family of apiaceae. The genus name *Anethum* is originated from the Greek word aneeson or aneeton, i.e strong smelling. It originates from the Mediterranean and West Asia [1]. *A. graveolens* is popularly known as Dill or

shapt. It is cultivated across the world and is known for its flavouring and curative properties. The experimental studies demonstrated the antimicrobial, stomachic, antioxidant, and carminative properties of Dill [2-5]. Flowers and leaves have high content of polyphenols when compared to fruits and hence are used for extracting essential oil.

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20-21-(31)

A Framework for Developing Intellectual Property Perspective among Computer Science Students

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Abstract

Intellectual property rights are being discussed and have become as policy issues in this era of knowledge. Every organization, industry in every sector is striving hard to protect, create, and convert their intangible assets to tangible ones through intellectual property rights. In this scenario, young students comprising majority work force of information technology field are to be sensitized about intellectual property rights at the beginning of their career. With this background, as a facilitator of this course a frame work was developed to impart intellectual property rights education to computer science students. This paper discusses how students are introduced to concepts in a unit wise manner and as the course makes progress, how challenges are dealt pedagogically to reach the outcomes of the course.

Key words: Intellectual property rights, pedagogy, information technology, learning goals, critical thinking.


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20-21
33

Hard core proof of the polyvinyl alcohol as a reducer for the formation of gold nanoparticles

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ABSTRACT

In this paper, we report the direct synthesis of water dispersed gold nanoparticles encapsulated in polyvinyl alcohol (PVA), which acting as reducer to gold ion to gold metal and capping agent. The syntheses of the gold nanoparticles were carried with the direct addition of the aqueous HAuCl₄ solution to aqueous PVA solution at 50 °C. Initially, the PVA solution was prepared by using 2 g of PVA per 100 ml of distilled water in a round bottom flask which was placed in oil bath placed over the magnetic stirrer. Subsequently, the aqueous solution HAuCl₄ was added drop-wise to the PVA solution. Afterward, the solution was made viscous by heating at same temperature and casted in form of nanocomposites films. Various compositions of HAuCl₄ (0.2 wt%, 0.5 wt%, 1.0 wt% and 1.5 wt%) with respect to PVA (films of Au-PVA nanocomposites) were prepared. Upon drying in ambient condition these films were analyzed with XRD, SEM, EDX, TGA, UV-Visible, and IR techniques. The XRD analysis reveals the fcc crystal structure with crystallite size nearly 22 nm. The crystallite size is in agreement with that obtained by SEM analysis which is in range of 25–30 nm and particles are nearly spherical in shape. Furthermore, the UV-visible analysis showed the surface plasmon resonance (SPR) band at ~550 nm which confirmed the formation of gold nanoparticles. It is further supported by the EDX analysis that showed the gold peaks in the spectrum.

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1. Introduction:

Noble metal nanoparticles had an increased attention over the last decade and still fascinating the researcher to greater extent due to their unique photochemical properties [1–7]. In particular the gold nanoparticles have been unique characteristics such as tunable localized surface plasmon resonance enable them wide variety of application such as Förster resonance energy (FRET) sensor, photo-thermal therapy (PTT), catalysis, electronics, and energy storage devices [5–9]. For instance, spherical gold nanoparticles have extensively used in the FRET process because of no dipole moment it can interact with the donor from all faces in the visible region [9]. On the other hand the gold nanorods had been used as the sensor over wide range from visible to near infrared region due

to their tunable wavelength spectrum. Moreover, the PTT application of gold nanoparticles is due to the exceptionally high absorption cross-section through surface plasmon resonance (SPR) compared to the bulk gold that result in increase the localized temperature which is essential principle of the cancer treatment process [10]. All these properties are dependent on the size and shape of the nanoparticles, therefore, to control the size and the shape of the gold nanoparticles many methods have been used [11]. For instance, the chemical reduction method in which the gold ions are reduces to gold atoms with the application of suitable reducing agent. Commonly, used reducing agents are NaBH₄, hydrazine, and gaseous hydrogen [11–15]. Moreover, green synthesis process has also been developed in which the nature of the reducing agent was mild and the sources of the reducing agents were green plants [16]. Additionally, in a polyol process the reduction of the metal ions to metal were achieved by using the different molecules containing the OH functional group such as ethylene

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RESEARCH ARTICLE

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Synthesis, biological evaluation and docking studies of 1,2,4-oxadiazole linked 5-fluorouracil derivatives as anticancer agents



Ravi Kumar Bommara¹, Shashikala Kethireddy², Rajeshwar Reddy Govindapur³ and Laxminarayana Eppakayala^{1*}

Abstract

Background: 1,2,4-oxadiazole derivatives exhibited significant anti-cancer activity when they were evaluated, against human cancer cell lines. They also showed anti-inflammatory, analgesic, diabetic, immunosuppressive, $\alpha_2\beta_2$ -receptor antagonist, antimicrobial, anti-helminthic, histamine-H3 and antiparasitic properties. A pyrimidine analog, 5-fluoro-uracil is a chemotherapeutic drug used for treating multiple solid malignant tumors. But its application is limited, as it has side effects like low bioavailability and high toxicity. Molecular docking is an exemplary tool, helps in identifying target and designing a drug containing high bio-availability and minimum toxicity.

Results: A set of 1,2,4-oxadiazole linked 5-fluorouracil derivatives (7a–j) were synthesized and their structures were confirmed by ¹H NMR, ¹³C NMR and Mass spectral analysis. Further, these compounds were investigated for their anti-cancer activity towards a panel of four human cancer cell lines such as (MCF-7, MDA MB-231), lung cancer (A549) and prostate cancer (DU-145) by using MTT method. Among them, compounds 7a, 7b, 7c, 7d and 7i demonstrated more promising anticancer activity than standard.

Conclusion: Synthesized derivatives (7a–j) of 1,2,4-oxadiazole linked 5-fluorouracil and investigated for their anticancer activity towards a panel of four human cancer cell lines.

Keywords: 5-Fluorouracil, Ataluren, Pyrimidine, Oxadiazole and anticancer activity

Background

Over the past few decades, heterocyclic rings containing nitrogen atoms have played a significant role in medicinal chemistry. They are considered as key templates for the development of new therapeutic agents [1]. Among all the nitrogenated compounds, pyrimidines are a more privileged class of six-membered heterocyclic organic units. They occupy a unique position in medicinal chemistry due to their wide range of biological applications [2–12]. Pyrimidines exist as an essential component in several

nucleic acids and therapeutic drugs, such as 5-Fluorouracil (1, 5-FU, Fig. 1) [13–16]. The USFDA-approved drug, 5-FU, is one of the most distinguishable chemotherapeutic drugs available. It was first synthesized by Heidelberger and co-workers [17]. It shows antitumor activity by inhibition of thymidylate synthetase enzyme leading to prevention of DNA synthesis [18], and has been used frequently for the treatment of various solid malignant tumors [19–21]. However, it has limited clinical applications because of several side effects, including poor tumor selectivity, toxicity, lower drug-resistance, gastrointestinal toxicity, and adverse effects on central nervous system [22, 23]. Previously, many researchers have developed several 5-FU contained compounds to overcome

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20-21-35

The pK_a of Pentazole (HN_5)Sanjeev Rachuru,^A Jagannadham Vandanapu,^{B,D} and Adam A. Skelton^C^ADepartment of Chemistry, Geethanjali College of Engineering and Technology, Cheeryal-501301, Telangana, India.^BDepartment of Chemistry, Osmania University, Hyderabad-500007, India.^CDepartment of Pharmacy, School of Health Science, University of KwaZulu-Natal, Durban 4000, South Africa.^DCorresponding author. Email: jagannadham1950@yahoo.com

Pentazole having the molecular formula HN_5 is an archetypical five-membered homocyclic inorganic aromatic molecule consisting of five nitrogen atoms. A hydrogen atom is bonded to one of the nitrogens. Even though the molecule does not contain a carbon it appears last in the series of the heterocyclic azole family; the family containing one to five nitrogen atoms. This series of heterocyclic azoles is pyrrole, imidazole, pyrazole, triazole, tetrazole, and the last one is the pentazole. Barring pentazole, the rest of the members of the azole family are heterocyclic organic molecules. The pK_a of $N(1)H$ -acidity values of all the azole members are known, except for that of pentazole. In the present work we endeavoured to determine the pK_a of pentazole by a graphical method and by performing theoretical DFT calculations.

Keywords: pentazole, pK_a , DFT.

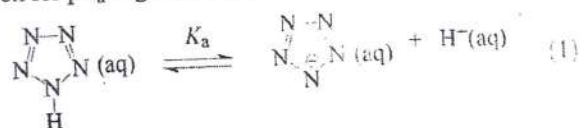
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Introduction

The chemistry of pentazole has a long debatable history.^[1-11] A century ago, the preparation of its silver salt AgN_5 was reported by Lipschitz^[1] and later it was refuted by Curtius et al.^[2] Though the X-ray crystal structure of a related compound, 4-dimethylaminophenylpentazole was reported,^[3] the synthesis of pentazole HN_5 was not.^[4] Subsequently, several papers appeared in the literature regarding pentazole and its substituted compounds reporting on their various aspects like their stability and its existence.^[5-11] The pK_a of pentazole has not been reported either by experiment, owing to its instability, or by theory in any of the earlier research articles. The only small report that appeared regarding the pK_a was by Katritzky et al.^[12] Owing to the difficulty in the synthesis of pentazole (if at all synthesised it is in a metastable state), the experimental pK_a has not been reported so far. This was the motivation to carry out theoretical studies. The theoretical study reported here sheds light on the fact that the pK_a determined by extrapolation method might not be correct. Further it is proposed that the pK_a values determined by SMD_{sSAS} (a solvation model based on a density-scaled solvent-accessible surface model) appear to be correct.

It is known that pK_a is the negative logarithm of K_a , the equilibrium constant of the acid dissociation reaction $HA \rightleftharpoons A^- + H^+$ in aqueous solution. In any graduate laboratory, experimental methods, like potentiometry, conductometry, and UV-visible spectroscopy, are available to determine the equilibrium constant K_a . The acid dissociation constant K_a is the quantitative measure of the strength of an acid in solution; yet the symbol pK_a , which is the negative logarithm of K_a , is more commonly used. At equilibrium, in the acid dissociation reaction

$HA \rightleftharpoons A^- + H^+$ the concentrations of HA , A^- , and H^+ will not change with the passage of time because the rates of the forward and backward reactions are equal.^[13] The acid dissociation reaction $HA \rightleftharpoons A^- + H^+$ for pentazole is shown in Eqn 1, the equation for K_a is given in Eqn 2, and the subsequent equation for pK_a is given in Eqn 3.



$$K_a = \frac{[A^-][H^+]}{[HA]} \quad (2)$$

$$pK_a = -\log_{10} K_a = \log_{10} \frac{[HA]}{[A^-][H^+]} \quad (3)$$

Methods

All the linear correlations were done using the *KaleidaGraph* software (Reading, PA, USA). The chemical structures were drawn using *Chemdraw*. *Gaussian 09* software was utilised for theoretical calculations.^[14] Density functional theory (DFT) was used to calculate the pK_a values. The reactant and the products were optimized and frequency calculations were performed using the wB97XD^[15] and B3LYP functional with 6-311+g(d,p) basis set. pK_a values were determined using the SMD continuum model. The pK_a values were determined by both default SMD (solvation model based on density) and SMD_{sSAS} (scaled solvent-accessible surface). Here the

20-21-36

VARIOUS TECHNOLOGICAL PROCESSES

Enhanced Optical and Electrical Properties of Graphene Oxide-Silver Nanoparticles Nanocomposite Film by Thermal Annealing in the Air

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Abstract—Here, we report the enhanced optical and electrical properties of graphene oxide-silver nanoparticles (GO-AgNPs) nanocomposite due to thermal annealing in air at different temperatures (150, 250, and 350°C). Our findings show that the optical properties of the GO-AgNPs film strongly depend on the annealing temperature. With an increase in annealing temperature, the optical absorption band and photoluminescence (PL) band are monotonically shifted towards a longer wavelength with a slight increase in absorbance. Interestingly, annealing of the nanocomposite film at 350°C in the air results in the nitrogen-doping from air into GO lattice. Unlike the PL bands in the near-ultraviolet (UV) range in cases of GO-AgNPs annealed at 150 and 250°C, this film exhibits pronounced multiple PL bands in the visible range, which are attributed to optical transitions associated with the localized nitrogen defects incorporated from air under thermal annealing and charge transfer between AgNPs and carbon. Mechanisms of the observed optical properties are also discussed. Furthermore, thermal annealing of the film also affects its electrical properties. The sheet resistance of the film reduces with the increase of annealing temperature and its lowest value $\sim 21 \Omega/\square$ with transmittance $\sim 82\%$ at 550 nm is achieved at 350°C.

Keywords: Thermal annealing in air, nitrogen-doped graphene oxide-silver nanoparticles, transparent conductive electrode, photoluminescence

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INTRODUCTION

Graphene has been recognized as a promising material that could be utilized in many areas that include electronics, optoelectronics, energy, and biochemistry [1–10]. However, experimentally synthesized pure graphene has some limitations such as lack of band gap in sp^2 hybridized structure, high sheet resistance [1], and less pronounced luminescence [11]. Modification of graphene structure is therefore needed to extend its effective utilization in various application sectors. Chemi-

cally synthesized graphene oxide (GO), in this scenario, has been an attractive and basic material. GO consists of sp^2 bonded carbon atoms with a large fraction of sp^3 hybridized carbon atoms bound to oxygen-related functional groups. GO is an insulator and reduction of GO is demanded to make it conductor or semiconductor which are key materials used in electronic and optoelectronic devices. The reduction of GO indicates the increase of sp^2 contents and materials tend to transform from insulating GO to conducting graphene structure [12]. Ag nanoparticles (AgNPs) have been widely used to fab-



Research Article

Molecular docking studies of *Chenopodium album* Linn with Lanosterol synthase enzyme

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Abstract

Cardiovascular diseases (CVD) are the major cause of death among people across the globe. Hypercholesterolemia is one of the major contributing factors for CVD. Molecules that bind with Lanosterol synthase enzyme, can be potential drug targets. Statin group of compounds like Simvastatin, cerivastatin, Atorvastatin etc., used for treating hypercholesterolemia have side effects and hence there is a growing demand for plant derived flavonoids. This work focuses on studying the compounds quercetin-3-O-(2",6"-di-O- α -L-rhamnopyranosyl)- β -D-glucopyranoside, kaempferol-3-O-(2",6"-di-O- α -L-rhamnopyranosyl)- β -D-glucopyranoside, rutin; quercetin-3-O- β -D-glucopyranoside (iso quercetin); and kaempferol-3-O- β -D-glucopyranoside (Astragalain) present in *Chenopodium album* Linn to inhibit Lanosterol synthase. Bioactivity score, drug likeness character was assessed *in silico*. Based on bioactivity spectrum, it is observed that the molecules are biologically active and the probability of these compounds to be biologically active is ranging from 0.784 to 0.992, suggesting that these compounds are effective for treating hypercholesterolemia. In the molecular docking studies, the compounds binding affinity score was in agreement that the molecules have the potential to be used as an alternative to the statin group of compounds in treating cholesterol.

Keywords: Bioactivity, *Chenopodium album*, Hypercholesterolemia, Lanosterol synthase enzyme, Molecular docking

INTRODUCTION

Ethnomedicinal plants remain largely unexplored and there is a good scope for researchers and food processors to bring out these economical, easily grown plants to the mainstream food basket (Pala *et al.*, 2019., Salmerón-Manzano Esther *et al.*, 2020). *Chenopodium album* Linn, is one such plant with good nutritive value (fibre, fatty acids and minerals). In India, it is called as Bathua and it belongs to Amaranthaceae family and *Chenopodium* genus (Bajwa Ali *et al.*, 2019). *C. Album* is rich in flavonoids that play an important role in its pharmacological and therapeutic properties.

Flavonoids are phenolic compounds possessing a wide spectrum of biological activities and are studied for anti-cancer and reducing the risk of cardiovascular diseases caused by oxidative stress (Alexander Victor *et al.*, 2016, Thilakavathy Thangasamy *et al.*, 2009). *C. Album* has been found to possess the bioflavonoids, Quercetin and Kaempferol derivatives (Gohar and Elmazar 1997,

Cuttillo *et al.*, 2006, Laghari *et al.*, 2011) Hypercholesterolemia is considered as one of the factors for coronary heart diseases. Chemically synthesised drugs used to treat hypercholesterolemia contain statin group that on prolonged use causes muscle weakness, memory loss and inhibits coenzyme Q10 important for electron transfer in mitochondria (Wagstaff *et al.*, 2003, Jamolowicz Al *et al.*, 2015). In this context, it is highly relevant to focus on plant derived flavonoids that are effective in treating hypercholesterolemia.

Lanosterol synthase, also known as lanosterol cyclase, is a microsomal enzyme and a target for drugs lowering cholesterol (Telford *et al.*, 2005, Vanessa *et al.*, 2018). The potential anti-cholesteremic drug binds to the active sites of the Lanosterol synthase enzyme and inhibits it. To establish a plant derived flavonoid as a potential bioactive compound, it is important that we screen it theoretically and know its pharmacological and binding properties.

In the present work, we carried out *in-silico* calculation



Effect of BaTiO₃ phase on frequency dispersion characteristics of Mg_{0.48}Cu_{0.12}Zn_{0.4}Fe₂O₄ + BaTiO₃ nanocomposites

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ABSTRACT

Multiferroic nanocomposites of ferrite and ferroelectric phases with systematically varying composition (100-x) Mg_{0.48}Cu_{0.12}Zn_{0.4}Fe₂O₄ + xBaTiO₃ (MCZBT) (where, x = 0, 20, 40, 50, 60, 80, 100 mol%) were prepared for the first time by mechanical milling and sintering method. The presence of ferrite and ferroelectric phases in nanocomposite samples were confirmed by X-ray diffraction (XRD) while microstructural characterization was carried out by scanning electron microscopy (SEM). The average grain size, from SEM, was found to be in the range 80 nm for ferrite and 86 nm for BaTiO₃ nanopowders. The complex permittivity and the complex permeability variations as a function of frequency in the range 100 kHz – 1.8 GHz, were investigated using LCR meter and impedance analyzer. The resonance and relaxation phenomena were observed by all the samples around 1.18 GHz from the permittivity studies. From the studies of microwave absorbing properties in X-band (8–12 GHz) frequency region, it was found that the minimum reflection loss of –24.61 dB with bandwidth of 3.38 GHz was obtained by sample with 20% ferroelectric phase. The studies on reflection loss and transmission loss indicated that the effective absorption of incident microwave was found to be above 80% and the composite sample with 80% of ferroelectric phase absorbed more than 91% of the incident wave. The results suggested that the present sample materials can be used for making microwave shielding devises for EMI applications.

1. Introduction

Multiferroic composite materials that display coexistence of ferroelectric and ferromagnetic responses attracted the current interest due to their magnetic and dielectric properties that are appropriate for several novel device applications such as high frequency Multi Layer Chip Inductor (MLCI) applications, electromagnetic interference (EMI) filters and sensors etc [1,2]. Dielectric and magnetic property studies and their dependence on composition and structure of nanocomposites lay the foundation for developing the new materials with pre-determined properties since the interrelationship of properties of filler and matrix phases of composites help in the design of devices for applications. The frequency dispersion characteristics of ferrite and ferroelectric composites are deciding parameters while using these materials as microwave absorbers and EMI shielding materials in various applications [3,4]. The advanced technological developments in the field of telecommunications and several industrial sectors demand not only effective EMI shields but also materials that satisfy certain requirements for each engineered design such as light weight, corrosion

resistant, flexibility, processing easiness, tunable morphology, and inexpensiveness [5]. Another priority is developing radar absorbing materials for military stealth applications in X-band (8–12 GHz) frequency region. A significant research has been done over recent years on microwave absorption performance of various nanomaterials [6,7]. However, these absorbing materials cannot satisfy all requirements simultaneously, such as absorption, wide bandwidth, light weight, etc. [8].

In the current work ferrite ferroelectric nanocomposites are selected to synthesize and study properties, the reason being due to the fact that spinel ferrites and perovskite ferroelectrics show good phase compatibility through magnetoelectric coupling and the interconnectivity of the phases can be controlled by their relative amount and processing methods. Moreover, there exists good lattice match between perovskite ferroelectric, BaTiO₃ (lattice constant, a ≈ 4.03 Å) and spinel ferrite (lattice constant, a ≈ 8.33 Å), with ferrite lattice constant close to twice the perovskite lattice constant, which is expected to have excellent wetting between two phases resulting in strong interface adhesion in composites [9]. Due to their excellent dielectric and magnetic

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IMPACT OF THERMAL RADIATION AND CHEMICAL REACTION ON MHD HEAT AND MASS TRANSFER CASSON NANOFUID FLOW PAST A STRETCHING SHEET IN PRESENCE OF HEAT SOURCE/SINK

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ABSTRACT

The purpose of present study is to analyse the influence of chemical reaction on MHD Casson nanofluid flow on an elongating sheet taken into the account of radiation and heat absorption/generation. The governing nonlinear PDE's are changed into a nonlinear ODE's by using similarity transformations. The converted equations are solved using numerical technique is notable as Keller box method. The consequence of heat source/sink, Prandtl number, Casson parameter, magnetic field, Brownian motion, thermophoresis, thermal radiation and chemical reaction parameters on velocity, temperature, and concentration profiles are depicted and elucidate in physical terms. A resemblance with previously issued results shown a perfect agreement. Numerical values of physical quantities, such as velocity gradient, heat transfer rate and the mass transfer rate are arranged in tabular form.

Keywords: thermal radiation, heat source/ sink, stretching sheet, casson nanofluid, MHD, chemical reaction.

INTRODUCTION

The study of nanofluids have fascinated because of its remarkable applications in industry such as solar cells, electronics, solar stills, communication, solar cooling systems, computing technologies, solar collectors, optical devices, water heaters, lasers, absorption refrigeration systems, and medicine, synthesis of various solar devices because of their higher properties over the conventional fluids. A nanofluid, consisting of a base fluid and nanoparticles, is a modern division of heat transfer fluids. The utilization of supplement is an approach to intensify the performance of heat transfer in base fluids. The heat conductance of conventional heat transfer fluids does not encounter the demands of modern cooling rate. Nanofluids are suspensions of ultrafine-grained solid particles (nanoparticles) and it improves the convective heat transfer and heat conductivity in common fluids. Choi and Eastman [1] analysed the increased thermal conductivity of nanoparticle fluids. S. K. Das *et al.* [2] investigated the Heat Transfer in Nanofluids. Natural convective heat and mass transfer nanofluid boundary layer flow through a vertical plate with convective boundary condition was studied by Aziz and W.A. Khan [3]. D. Srinivasacharya and Ontela Surender [4] examined the non-similar solution by considering double stratification on natural convection heat transfer of a nanofluid in a porous saturated medium over a vertical plate. Elsheikh *et al.* [5] studied the various applications in solar energy with nanofluids.

Magnetohydrodynamic (MHD) nanofluids perform an important part in several manufacturing procedures such as in hybrid fuel generation, modulator, economy fuel in modern power generation plants, gratings, coolant in continuous metallurgical sheets, fiber filters, vehicle cooling, loud speakers, plastic sheet extrusion and

processes of polymers, and magnetic cells, etc. Rizwan Ul Haq *et al.* [6] analysed the magneto-hydrodynamic stagnation point Nanofluid flow in presence of radiation on a stretching sheet with slip conditions. A.S. Dogonchi *et al.* [7] discussed heat transfer and thermal radiation MHD nanofluid flow between parallel plates. A. Kamran *et al.* [8] observed Magneto-hydrodynamic Casson Nanofluid with velocity slip and Joule heating. Jawad Raza *et al.*, [9] investigated MHD heat and mass transfer Nanofluid flow past a nonlinear permeable stretching sheet with multiple slips. Saeed Islam *et al.* [10] examined the influence of thermal radiation and hall current between two surfaces on MHD micropolar non-Newtonian hybrid Nanofluid flow.

Thermal radiation plays an important role in dissipating heat from the surface. It has applications in manufacturing industries such as chopper, space vehicles, reliable equipment design, satellites, atomic furnaces, missiles, space technology and procedures related to high temperature. Yanala Dharmendar Reddy *et al.*, [11] analyzed thermal radiation and suction effects on MHD Nanofluid boundary layer flow on a non-linear stretching sheet. Kothandapani and J. Prakash [12] observed peristaltic transport in a tapered asymmetric channel of a Williamson Nanofluid in the presence of thermal radiation. C.Sulochana *et al.* [13] analysed effects of sores and suction/blowing on MHD stagnation point flow of a radiative Carreau nanofluid on a stretching surface. Yap Bing Kho *et al.*, [14] investigated impact of radiation on MHD heat and mass transfer Casson Nanofluid flow on a porous stretching sheet. Jawad Raza [15] discussed impact of radiation and velocity slip on magnetohydrodynamic stagnation point flow of Casson fluid with convective boundary conditions through a linear elongated sheet.

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Molecular interaction studies of hydrogen-bonded N-Methyl-2-Pyrrolidone/Ethanol binary mixtures by dielectric relaxation spectroscopy and their temperature dependence

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HOMO-LUMO

ABSTRACT

Complex permittivity of the binary mixtures of N-Methyl-2-Pyrrolidone (NMP) with Ethanol (ETH) has been studied in the microwave frequency range at various temperatures. The binary liquid system NMP-ETH is selected to interpret the effect of carbonyl (C=O) group of NMP and hydroxyl group (-OH) of ETH on the volumetric, thermal and dielectric properties. The dipole moment (μ) and relaxation time (τ) is evaluated from Higasi's method and Havriliak-Negami equation. The excess molar volume (V_m^E), excess permittivity (ϵ^E), excess refractive index (n_D^E), excess inverse relaxation time ($1/\tau^E$) are fitted with the Redlich-Kister equation. The results obtained from Polarizable Continuum Model (PCM) and Integral Equation Formalism Polarizable Continuum Model (IEFPCM) solvation theories using DFT methods are correlated with the experimentally determined parameters. The molecular association and chemical stability of the system is interpreted in terms of single-point energy, HOMO-LUMO calculations. The existence of a hydrogen bond within the NMP-ETH system is confirmed from the FT-IR, UV-Vis's spectra.

1. Introduction

Dielectric Relaxation Spectroscopy (DRS) is one of the prominent methods to explore the molecular structure in the liquid systems by determining the relaxation dynamics of the molecules, dipole moment, and interfacial polarization properties [1–8]. The investigation of molecular interactions in the liquid binary systems is one of the challenging tasks and their change in properties with respective frequency and temperature is very much useful in practical engineering and technological applications [9–15]. The investigation of dielectric relaxation properties of the different solute and solvent systems in the broader frequency range (10 μ Hz– 300 GHz) describes the strength of the molecular interaction, the existence of multimers in the mixtures, the alignment of the dipoles, and their conduction mechanism. The theoretical and experimental studies on the dielectric studies of complex fluids such as aqueous proteins/tissues in an alcohol medium, liquid mixtures are interdisciplinary and increasing demand in the research

field [15–24]. It provides relevant information for the applications of binary liquid mixture systems in the field of pharmaceutical, petrochemical, nuclear, and green industry [25–37].

NMP is an adaptable water-soluble polar aprotic solvent. Due to its multifunctional properties, it is used as a drug solubilizer, penetration enhancer in humans and animals. Also, it is used as a good solvent for many engineering and pharmaceutical utilization by its larger boiling point, lower freezing point, and easy to operate. Ethanol is also one of the good solvents and it has many useful properties that allow it to be used by a range of different industries such as beverage, pharmaceutical, medical, and fuel industry [27–29,38–41]. There are several research papers are available on the frequency-dependent dielectric studies of ethanol with different liquid compounds at various temperatures in the recent past [42–56]. The majority of the dielectric studies on ethanol include calculating the dielectric relaxation time in a different solvent medium at various temperatures and also fluctuations of hydrogen bond networks in the different liquid medium. Further, computational

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Microstructure, frequency and temperature dependent dielectric properties of zinc ferrites

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ABSTRACT: Ferrite with the general formula $ZnFe_2O_4$ was prepared by microwave hydrothermal (M-H) method. The as-synthesized powder was pelletized and samples were sintered at different temperatures (600, 700, 800 and 900°C). The grain size was varied by sintering the ferrite at different temperatures up to 900°C. The characterization studies were conducted by X-ray diffraction (XRD) and scanning electron microscopy (SEM). Dielectric constant (ϵ') and dielectric loss tangent ($\tan \delta$) were measured as a function of frequency and temperature. DC conductivity (σ_{dc}) was measured by temperature variation. A significant influence of sintering temperature on the microstructure and electrical properties was detected.

1. INTRODUCTION

Nanoscale magnetic particles are attracting more interest in the scientific community because of its efficient applications in color imaging, catalysis, data storage, drug delivery, ferrofluids and magnetic refrigeration systems [1].

Spinel ferrites are commercially important materials because they're excellent electrical and magnetic properties [2]. These classes of materials have been the subject of extensive studies by physicists and chemists alike. A whole range of distribution of cations is possible in spinels which can be represented generally by the formula $(Me^{2+})_d(Fe^{3+})_{1-d}(Me^{2+})_{1-d}(Fe^{3+})_{1+d}O_4$ where the ions inside the brackets are said to occupy octahedral sites (B) and the ions outside the bracket occupy the tetrahedral sites (A) [3]. In the above formula when $d=1$, it is called normal spinel. When $d=0$ it is called an inverse spinel. When $d=1/3$ it is called random spinel. From the fundamental point of view, these materials serve as ideal candidates for studying ferrimagnetism and ferromagnetic properties.

Zinc ferrite belongs to the normal spinels [4]. The properties of zinc ferrites have been the subject of study by many investigators over the last two periods. It has been established that structurally $ZnFe_2O_4$ is a normal spinel where it can be written as $[(Zn^{2+})_A(Fe^{3+})_B]O_4$ and its net magnetization is zero. Research on zinc ferrite showed that zinc ferrite is antiferromagnetic because of B-B interactions with a Neel temperature of about 10 K. It behaves as a paramagnet above the Neel temperature [5]. The abnormalities in the magnetic properties of zinc ferrite have been reported [6]. For case, Lotgering et al. [6] detected abnormal behavior in the paramagnetic susceptibility of zinc ferrite. In their neutron diffraction studies, Brock-house and others [7] found the presence of a short-range order of parallel spins separated by 0.29 nm.

In the present investigation, the nanopowder of $ZnFe_2O_4$ was prepared using M-H method. The advantage of M-H method is given elsewhere [8]. The s-prepared powder was characterized using XRD, and SEM, frequency and temperature dependent dielectric properties (ϵ) and conductivity properties were studied and discussed in this paper.

2. EXPERIMENTAL METHOD

Pure zinc nitrate [$Zn(NO_3)_2 \cdot 6H_2O$] and iron nitrate [$Fe(NO_3)_3 \cdot 9H_2O$] were dissolved in 100 ml of de-ionized water. The molar ratio of powders was adjusted to obtain the composition $ZnFe_2O_4$. An aqueous NaOH solution was added to the mixture until the desired pH (~9.45) value was obtained. The precipitate was transferred into an auto-clave and was treated with M-H method. In this method, the precipitate was taken into Teflon lined vessel and placed inside the microwave digestion system (Model MDS-2000, CEM Corp., Mathews, NC) and samples were synthesized at 165°C/45 min. Our M-H system is fully computer controlled one and uses 2.45 GHz microwaves and can be operated at 0-100% full power (1200±50W). The products obtained were filtered and then washed repeatedly with de-ionized water, followed by freeze-drying overnight. The prepared powders were weighed and the percentage yields were calculated from the expected and the amount that was actually



19-20-②

Fourth order computational method for two parameters singularly perturbed boundary value problem using non-polynomial cubic spline

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Abstract: In this paper, we proposed a fourth order finite difference scheme using non-polynomial cubic spline for the solution of two parameters singularly perturbed two-point boundary value problem having dual boundary layer on a uniform mesh. In this method, the first order derivatives in the non-polynomial cubic spline finite difference scheme are replaced by the higher order finite differences to get the discretisation equation for the problem. The discretisation equation is solved by the tridiagonal solver discrete invariant imbedding. The proposed method is analysed for convergence and a fourth order rate of convergence is proved. The numerical results are compared with exact solutions and the outcomes of other existing numerical methods.

Keywords: two parameters; singularly perturbed; two point boundary value problem; dual boundary layer; characteristic equation; non-polynomial cubic spline.

Reference to this paper should be made as follows: Phaneendra, K. and Mahesh, G. (2019) 'Fourth order computational method for two parameters singularly perturbed boundary value problem using non-polynomial cubic spline', *Int. J. Computing Science and Mathematics*, Vol. 10, No. 3, pp.261—275.

Biographical notes: K. Phaneendra is working as an Assistant Professor at the Department of Mathematics, University College of Science, Saifabad, Osmania University, Hyderabad, India. He did his PhD from N.I.T. Warangal in the area of numerical methods for singular perturbation problems. His area of research is numerical solution for a class of singularly perturbed which includes differential difference equations, singular boundary value problems and multi parameter problems. He published 36 research articles in various international journals.

G. Mahesh is Research Scholar in the Department of Mathematics, University College of Science, Saifabad, Osmania University, Hyderabad, India. His area of research is numerical solution to two parameter singularly perturbed boundary value problems. He published two research articles in reputed journals.

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Review article

Can Non-bonded Pair of Electrons of Sp^3 Nitrogen with Two Single σ -Bonds on Either Side Still Transmit Substituent Electronic Effects to the Reaction Site? Reversal of Attenuation Effect by Sp^3 Nitrogen—A Chemical Education Perspective

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Carbamic acids

ABSTRACT

Dependence of reactivity of organic molecules on substituents was a well-established phenomenon in terms of Hammett and Taft equations in physical-organic chemistry. The well-known Hammett and Taft linear free energy relationships were extensively used in elucidating the organic reaction mechanisms. The exponential depletion of Hammett reaction constant (ρ), as a function of distance in terms of increasing the number of sp^3 carbon atoms ($-CH_2-$) between the reaction center and the substituent, is understood from our laboratory experiments. But, introduction of sp^3 carbon atoms ($-CH=CH-$) between the reaction center and the substituent enhances the Hammett reaction constant (ρ). In the present work, we have tried and observed the same and even little more effective transmission of substituent effect through sp^3 nitrogen ($-NH-$). However, the presence of a sp^3 carbon by the side of sp^3 nitrogen ($-NH-CH_2-$) depletes the substituent effect in the usual manner in *N*-phenyl glycines. Probable explanations were presented in support of our observation. In the present work, the observations were manifested in terms of Taft ρ^* values instead of Hammett ρ value as the pK_a values of only 4-nitrophenylcarbamic acid and carbamic acids and the Taft σ^* values of 4-nitrophenyl and H are available from literature.

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Preparation and characterization of red emitting Yttrium Vanadate phosphor doped with Eu(III): $Y_{1-x}VO_4: Eu_x$

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G. Neeraja Rani, J. Shankar, J. Anjiah, B. Mamatha, and N. H. Ayachit



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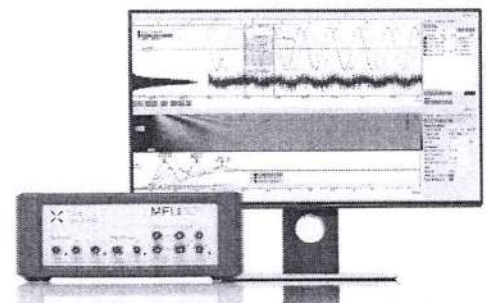
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19-20-(6)

Shielding Effectiveness studies of NiCuZn ferrite-Polyaniline nanocomposites for EMI suppression applications

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Abstract. Electromagnetic interference shielding effectiveness (EMI SE) of multifunctional NiCuZnFe₂O₄-Polyaniline are studied. The nanocrystalline NCZ-PANI nanocomposites were prepared by the mechanical milling process. The structure and the morphology of the nanocomposites were investigated by Fourier Infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). Electromagnetic properties and EMI SE behaviors were performed over a frequency range of 8.2-12.4 GHz (X-band) and 12.4-18 GHz (Ku-band). The results show that for nanocomposites, the values of the real (ϵ') and imaginary permittivity (ϵ'') and imaginary permeability (μ'') increase, while the value of real permeability (μ') decreases as the filler content (PANI) increases. The contributing effects of PANI content on total shielding efficiency (SE_{total}) of different samples were investigated. The maximum EMI SE of 29 dB is obtained for a composite of 50 wt.% PANI with the dominant shielding by absorption (SE_A) of electromagnetic radiation. The enhanced electromagnetic shielding performance of nanocomposites is attributed to the increment of both magnetic and dielectric losses due to the incorporation of conducting PANI in magnetic NCZ matrix. Synthesis parameters such as the amount and particle size of PANI and NCZ affect significantly the morphology, the conductivity, and the microwave absorption properties of the final materials. The possibility to modulate the electromagnetic properties of the composite materials is of great interest to fabricate microwave absorbing and electromagnetic shielding materials with high performances.

INTRODUCTION

To reduce the impact of electromagnetic interference (EMI), EMI shielding materials have been widely investigated. Normally, metals have been used for EMI shielding materials as they have high conductivity and dielectric permittivity. [1, 2] However, metals have disadvantages, such as their corrosion, weight properties, and poor processability.[3] Ferrite-polymer nanocomposites have been used extensively in the shielding of electromagnetic noise due to their excellent electromagnetic properties.[4-6] The polymer and ferrite composites can be used as EMI suppressor materials to avoid the disadvantages seen in metals.[7,8] The complex permittivity and permeability are closely related to the high-frequency dielectric and magnetic properties of magnetic particles and volume fraction of the fillers in the composites. Ferrites are used as magnetic fillers in the composites due to the high magnetic loss, high chemical stability, and high resistivity, etc. The high-frequency dielectric and magnetic properties can be tuned by varying the ferrite concentration in the ferrite-polymer composites.

In the present investigation, various Polyaniline (PANI) loaded Ni_{0.48}Cu_{0.12}Zn_{0.4}Fe₂O₄ (NCZ) matrix nanocomposites were prepared at room temperature. The NCZ can be used in microwave devices and electromagnetic suppression fields due to their high saturation magnetization, excellent chemical stability, and corrosion resistance. The composite powders were the effect of the volume fraction of PANI on the frequency dispersion characteristics of the complex permittivity (ϵ' & ϵ''), permeability (μ' & μ'') and EMI SE properties were studied and the obtained results were discussed in the paper.

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19-20-2



Educación

Química

NON-ASSOCIATIVE BEHAVIOR OF THIOPHENOLS: TROUTON'S RULE, RAMSEY-SHIELDS- EÖTVÖS EQUATION AND APPLICATION OF HAMMETT EQUATION TO THE SURFACE TENSION DATA – A CHEMICAL EDUCATION PERSPECTIVE

R. Sanjeev¹, David Geelan² and V. Jagannadham^{3*}

Abstract

Non-associative behavior of thiophenols is explained on the basis of Trouton's rule, proton acceptor-donor cites and application of Hammett equation to the surface tension data of thiophenols.

Keywords

Trouton's rule, Proton acceptor-donor cites, Hammett equation

Comportamiento no asociativo de los tiofenoles: regla de Trouton, ecuación de ramsey-shields-eötvös y aplicación de la ecuación de Hammett a los datos de tensión superficial: una perspectiva de educación química

Resumen

El comportamiento no asociativo de los tiofenoles se explica sobre la base de la regla de Trouton, las citas del donante aceptor de protones y la aplicación de la ecuación de Hammett a los datos de tensión superficial de los tiofenoles.

Palabras clave

La regla de Trouton, las citas del donante aceptor de protones, la ecuación de Hammett

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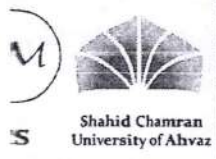
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paper

Effect of Chemical Reaction on Bioconvective Flow in Oxytactic Microorganisms Suspended Porous Cavity

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In this paper, the bioconvective flow in a porous square cavity containing oxytactic microorganism presence of chemical reaction is investigated. The bioconvection flow and heat transfer in porous media is modeled based on the Darcy model of Boussinesq approximation. The governing partial differential equations are solved using the Galerkin finite element method. The computational numerical results are shown by the streamlines, isotherms, isoconcentrations of oxygen, isoconcentrations of microorganisms, Nusselt number, average Sherwood numbers of oxygen concentration and microorganisms. The key parameters such as bioconvection Rayleigh number (R_b), chemical reaction parameter (K_r) and Rayleigh number (R_a) are presented and analyzed. It can be deduced that the chemical reaction increases the strength of isoconcentrations of both oxygen and microorganisms. It has been revealed that the chemical reaction has a greater effect on the swimming of the microorganisms, average Nusselt number, and Sherwood number.

Keywords: Thermo-bioconvection, Oxytactic Microorganisms, Porous square cavity, Chemical reaction, Finite Element Method

Introduction

Recent investigations on convective heat transfer in porous media are ascribed to the enormous of applications, utilization and storage of thermal/geothermal energy, reservoirs of petroleum, devices of catalytic converters, recovery of underground pollutants, underground feeder cables, technology of porous ceramic burners, food industry, desalination, chemical reactors, chemical separations, moisture migration in stored grain, thermal cooling of equipment, heating of rooms, combustion, etc. The basic nature and the increased volume of work in this field is adequately archived in the books by Nield and Bejan[1], Ingham and Pop [2], Vafai[3], Pop and Ingham [4]. Bioconvection in cavities of various geometries discovers a salient feature for engineering analysis. It has huge applications in engineering, such as solar applications, building applications, electronic industry, etc. Natural convection in a porous square cavity are investigated by Rahman et al. [5] and Balla et al. [6-8]. The latest development in fluidic devices is heat transfer in porous media with bioconvection phenomena. Bioconvection refers to a convective movement of fluid-induced by the swimming of motile microorganisms. Different types of microorganisms can be found, showing various swimming behaviours. Negatively geotactic microorganisms swim

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Bioconvection in oxytactic microorganism-saturated porous square enclosure with thermal radiation impact

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Abstract

This investigation addresses bioconvection of oxytactic microorganisms in a porous square enclosure by thermal radiation impact. The bioconvection flow and heat transfer in porous media are formulated based on Darcy model of Boussinesq approximation. Appropriate transformations lead to the non-dimensionalized governing partial differential equations. Galerkin finite element method for the resulting equations is computed. The role of relevant parameters on the streamlines, isotherms, isoconcentrations of oxygen and microorganisms and average Nusselt number is analysed in the outputs. It is revealed that the flow intensity of bioconvection is pronounced with larger Rayleigh number and reduced with radiation parameter. Furthermore, the temperature distribution is affected significantly with Rayleigh number. Radiation parameter serves to fasten the heat transfer in the enclosure. Oxygen density is enhanced with Rayleigh number and radiation parameter. The profile of motile isoconcentrations is boosted with Rayleigh number. The stability of microorganisms is improved with the radiation parameter.

Keywords Thermo-bioconvection · Oxytactic microorganisms · Thermal radiation · Porous square cavity · Finite element method

List of symbols

b	Chemotaxis constant, m
C	Concentration of oxygen
C_{min}	Minimum concentration of oxygen required for microorganisms to be active
C_0	Concentration at free surface
C_p	Specific heat at constant pressure
D_C	Diffusivity of oxygen, $m^2 s^{-1}$
D_n	Diffusivity of microorganisms, $m^2 s^{-1}$
g	Acceleration due to gravity, $m s^{-2}$

K	Permeability of the porous medium
k^*	Mean absorption coefficient
L	Length of porous cavity, m
Le	Lewis number
n	Number density of motile microorganisms
n_0	Average density of the microorganism
N	Dimensionless number density of microorganisms
Nu_Y	Local Nusselt number
Nu_{avg}	Average Nusselt number
Nn_Y	Local Sherwood number of microorganisms
Nn_{avg}	Average Sherwood number of microorganisms
p	Excess pressure above hydrostatic
Pe	Peclet number
q_r	Radiative heat flux
Ra	Rayleigh number of porous medium
Rb	Bioconvection Rayleigh number
Rd	Radiation parameter
Sh_Y	Local Sherwood number of oxygen concentration
Sh_{avg}	Average Sherwood number of oxygen concentration
T	Temperature, K
T_H	Temperature at hot wall, K
T_C	Temperature at cold wall, K
T_∞	Ambient temperature, K
u, v	Velocity components in x, y -directions, $m s^{-1}$

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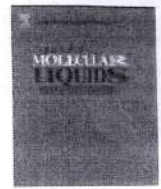
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Investigation of temperature dependent dielectric relaxation studies of 1,4-Butanediol/DMSO binary mixtures at the microwave frequency

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ABSTRACT

In the present manuscript, we are reporting the complex dielectric permittivity of 1,4-Butanediol/Dimethylsulfoxide binary mixtures for entire concentrations in the temperature range of 298.15 K–323.15 K. The complex dielectric permittivity is measured in the frequency range of 20 MHz–20 GHz. The dielectric relaxation time (τ) of the binary mixtures are analyzed by using the Havriliak-Negami equation. Redlich-Kister polynomial equation is used to fit the excess molar volume (V_m^E), excess permittivity (ϵ^E), excess refractive index (n_D^E), excess inverse relaxation time ($1/\tau^E$). The molecular association and structural packing in the liquid mixture are analyzed by using thermal expansion coefficient (α_p) parameter. The ordering nature of the molecular dipoles is discussed by evaluating the Kirkwood correlation factor (g^{eff}) and stability of the system by thermodynamic quantities. The experimental dipole moments of the pure and equimolar binary system are determined by using Higasi's method and compared with the theoretical dipole moment values obtained from DFT/B3LYP methods. Confirmation of hydrogen bond between 1,4-butanediol and DMSO is supported with the FT-IR and UV-Vis spectroscopy methods. The experimental dielectric and spectroscopic studies confirm the existence of hydrogen bond between the liquid mixtures.

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1. Introduction

The interaction of electric energy with the material mainly depends upon the characteristic property of the material, which plays a significant role in the determination of structural properties of the compounds. The usage of microwave heating has become important in the field of food processing, synthesis of chemical compounds, local heating of the biological tissues and medicinal industry [1–5]. The capability of the material to absorb microwave energy depends upon the macroscopic permittivity, which is connected with the dielectric loss of the material [6,7]. By choosing the proper polar solvent in the chemical industry can stimulate or prevent the chemical reaction, and modify the structural dynamics of the system. Hence, the study of dielectric properties of the polar liquids in the microwave frequency region is very much important in understanding the applications of microwave energy. The dielectric study of the liquid mixtures having the hydrogen bond donor and acceptor group compounds is useful for a various number of applications in the field of biological, medical, material science and technology [8,9].

Dielectric relaxation studies of 3-Nitrotoulene with diethylacetamide, dimethylsulfoxide binary mixture are studied by Ajay Chaudhari et al. [10] and their studies reveal that effective dipoles rotate slowly in the mixture due to the hindering field produced by the multimers in the solution. The equilibrium properties of butanediols and temperature dependence of shape factor is studied by Zhuravlev et al. [11] and explained that relaxation time depends upon the structural rearrangement of the molecules in the solution. The homogeneous and heterogeneous interaction between a series of three butanediols with 1,4 dioxane is studied by Gilani et al. [12–15] and dipropylsulfoxide in aqueous medium by Gabrielyan et al. [16]. Their studies confirm the presence of hydrogen bonding in the solutions affecting the excess dielectric parameters. The acoustic and thermodynamic properties of butanediols with respective pressure and temperature studied by Edward Zorebski et al. [17] and they reported that thermal expansion, compressibilities are increased with increase in the chain length of the molecules. The average number of hydrogen bonds, bonding energy associated with alcohol-DMSO mixtures are evaluated by Jia Guo-Zhu et al. [18,19] and chemical stability, the reactivity of the anilines, phenols in a nonpolar solvent medium by computational HOMO and LUMO calculations [20]. Molecular dynamics of the hydrogen bond network in the ethanol-water mixtures are reported by

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Research Article

Numerical Approach for Differential-Difference Equations with Layer Behaviour

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Abstract.

difference equations having layer behaviour, with delay as well advanced terms. The retarded terms second order singular perturbation problem. A finite difference scheme using non polynomial spline of the first derivatives. Tridiagonal algorithm is used to solve the resulting system. The method is exemplified on numerical examples with various values of perturbation, delay and advance parameters.

Also, the convergence of the proposed method has also been established.

Keywords.

absolute error

MSC. 65L10; 65L11; 65L12

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1. Introduction

and in the potential in nerve cells by random synaptic inputs in dendrites [18].



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FITTED DIFFERENCE APPROACH FOR DIFFERENTIAL EQUATIONS WITH DELAY AND ADVANCED PARAMETERS

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Abstract: A difference scheme involving acceptable fitting parameters is suggested for differential equations with delay and advanced terms, the solutions of which show boundary layer behaviour. First, the original problem is reshaped into asymptotically comparable second order singular perturbation problem using Taylor series approximation for the retarded terms. In order to obtain precise solution, fitting parameters are introduced in difference scheme using modified upwind differences for the first order derivatives. Thomas procedure is used to solve the resulting tri-diagonal difference system. The method is tested on numerical examples for various values of the perturbation, delay and advance parameters. Computed maximum absolute errors are tabulated. Numerical experiments are shown in graphs and the effects of small shifts have been studied on the boundary layer region. Also, convergence has been established of the proposed method.

Keywords: boundary layer; delay and advance parameters; modified upwind; singular perturbation problem.

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Do phase transition temperatures T_{mp} and T_{bp} obey linear free energy relationships?

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ABSTRACT

Normal melting point of a solid is the temperature at which it changes its state from solid to liquid. At the melting point the solid phase and the liquid phase exist in equilibrium. And normal boiling point of a liquid is a property at which the vapor pressure of the liquid becomes equal to the atmospheric pressure. The four types of intermolecular forces: hydrogen bonding, ionic forces, Van der Waals dipole-dipole interactions and Van der Waals dispersion forces (London forces) and sometimes the polarizability affect the melting and boiling points. Hydrogen bonding is one of the key factors that largely affect both melting and boiling points of solids and liquids respectively having functional groups such as OH, NH₂ and a most electronegative atom F. And they are also affected by polar electronic effects of the substituents and by the size of the molecule due to the presence of the van der Waals attractions. Using Lindemann's equation $T_{mp} = \frac{4\pi^2 m v^2 c^2 a^2}{k_B}$ and strong foundation of Trouton's two empirical rules $\Delta S_{latent} = \frac{\Delta H_{latent} \times \text{Density}}{273 + T_{mp}}$ and $\Delta S_{vaporization} = \frac{\Delta H_{vaporization}}{273 + T_{bp}}$, Taft Linear Free Energy Relationship (LFER) is applied to the temperature of phase transitions (solid to liquid and liquid to vapor) of alkyl alcohols, alkyl amines, alkyl fluorides and aliphatic hydrocarbons. Two loci are observed in each case one with a negative slope for electron donating substituents and the other with a positive slope for electron withdrawing substituents with a minimum at CH₃ substituent (Taft $\sigma^* = 0.00$). The decreasing trends in both the melting and the boiling points with decrease in electron donating power of substituents and the increasing trends in both the melting and the boiling points with increase in electron withdrawing power of substituents are explained with two interpretations of hydrogen bonding in alcohols, amines and fluorides yielding the same dimers.

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1. Introduction

The astonishing efforts in the direction of application of LFER to various physical properties like surface tension (γ) [1–8], dipole moments (μ) [8] and melting points [9] from our laboratory have ever been increasing with a good degree of success. Quantitative solubility-structure relationships for several *meta*- and *para*-substituted benzoic acids in benzene and in cyclohexane [10] and in 1, 4-dioxane and *para*-hydrofuran (THF) [11] were studied. Even the application of Hammett equation to melting points of some benzene derivatives were touched and left without any reasonable arguments [12]. Katritzky

et al. gave a one line concluding argument on the application of QSPR models to the melting points of benzene derivatives in terms of molecular packing and intermolecular interactions [13]. There was a brief report on the application of Hammett equation to the dipole moments [14].

Schreck [15] had described this in an article on non-linear Hammett relationships as what appears to be the only physical property that gives non-linear Hammett plots. But solubilities are not completely physical properties as the solubility would be a function of ionizing capacity and ionization is a chemical property which depends on the dielectricity of the solvent and it will be taking place at a localized ionization site. This gets support from the variation of Hammett ρ with solvent polarity [16,17].

It is from our laboratory who uncorked the detailed application of LFER to purely physical properties like surface tension (γ) [1–8], dipole moments (μ) [8] and melting points [9] except its mention on

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Short Communication

Is interfacial tension of a liquid-air interface thermodynamically a cyclic process?

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ABSTRACT

Brønsted ($\log k_b = \beta pK_a^{TS} + C$) and Taft ($\log k = \rho^* \sigma^* + \log k_0$) linear free energy equations are applied to the interfacial tension data of N-substituted anilines. The significance of the values of the constants Brønsted β (0.096) and Taft ρ^* (0.091) are explained in terms of proton transfer from the acid to the aniline, which is accelerated by electron donating groups. The deprotonation of protonated aniline is accelerated by electron withdrawing groups. Since any thermodynamic property associated with any kind of reaction is a point group, the fact that Brønsted β and Taft ρ^* have similar values with opposite sign indicates that the total process taking place at the aniline-air interface is a cyclic one.

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1. Introduction

Our laboratory has for some time had an interest in the application of Linear Free Energy relationships to surface tension data [1–5] and to the nucleophilic solvation of aliphatic ammonium ions [6]. In the present article we apply the Brønsted and Taft equations to the interfacial tensions of some N,N-disubstituted anilines. To our knowledge this is the first time this analysis has been reported in the literature. The opposite signs and similar values of the trend lines of Brønsted β and Taft ρ^* are explained based on thermodynamic considerations.

2. Experimental data source

Data on the interfacial tensions of N,N-disubstituted anilines is from reference [7] and references cited therein. The pK_a and Taft σ^* values of N,N-disubstituted anilines are from reference [8]. All linear correlations were completed using KaleidaGraph software. Fig. 1 was drawn using ChemDraw.

3. Discussion

The main difference between surface tension and interfacial tension is that surface tension is defined in terms of a single liquid surface which is in contact with a gas phase, usually air. Interfacial tension, on the other hand is understood as occurring at the interface of two immiscible liquids. Surface tension is actually a derivation of interfacial tension where the force resulting from the second surface is negligible or zero. The surface tension of a pure liquid is simply the interfacial tension at the liquid-air interface, because the surface tension of air is zero. This is the case because surface tension needs a surface, and for a surface there must be two different phases in contact with each other. Gases do not form inter-phase surfaces. Surface tension is caused by intermolecular forces that keep molecules in a liquid together. Such forces do not exist or are negligible in the gas phase as the gas thermodynamically is assumed to be a very dilute system.

Fig. 1 shows a typical example of an aniline-air interfacial system. Air always contains small amounts of carbon dioxide which dissolves in the moisture present in the air making it slightly acidic, with a pH of 5.7. This becomes a source of protons (H^+):



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Frequency and temperature dependent dielectric studies of propylene glycol-sulfolane binary mixtures in the microwave frequency region

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ABSTRACT

The dielectric permittivity of propylene glycol/sulfolane binary mixtures have been determined at various temperatures in the frequency range of 0.02 ν /GHz–20 using open-ended coaxial probe method. The permittivity spectra of propylene glycol/sulfolane mixtures with an asymmetric shape is observed. The experimental dielectric permittivity, relaxation time values are used to obtain remaining excessive parameters such as excess permittivity (ϵ^{E}), deviation in refractive index (Δn_D), excess inverse relaxation time ($1/\tau^{\text{E}}$), Kirkwood effective correlation factor (g^{eff}) and active thermodynamic parameters. Redlich-Kister polynomial equation is used to fit the excessive dielectric parameters. The molecular interaction between propylene glycol and sulfolane binary mixtures is interpreted in terms of short and long-range interactions among the dipoles. The experimental dipole moment values are compared with the theoretical dipole moment values from DFT/B3LYP, MP2 methods. Natural bond orbital (NBO) analysis is performed on the optimized geometrical structure of the above system to understand molecular interaction between the binary mixtures in terms of hydrogen bonding. The chemical stability of the system is studied from the HOMO-LUMO calculations. The energy of H-bond interaction between propylene glycol and sulfolane binary mixture is calculated from the single point energy calculations, and the results are correlated.

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1. Introduction

The temperature and frequency dependent dielectric relaxation studies of liquid mixtures play a significant role in the investigation of various processes such as intra and intermolecular interactions, rotational dynamics of the molecules, interfacial polarization, relaxation process, solute-solvent interactions and strength of the interaction among the dipoles. The study of interest in carrying the dielectric spectra of binary and ternary liquid mixtures resides in analyzing the molecular dynamics of the systems and describing the possible variation from the pure components of the liquids and their ideal mixtures. The non-covalent interactions present in the liquid systems such as hydrogen bond, Van der Waals, and electrostatic forces play an essential role in the field of biological activity, enzyme catalysis, and drug design [1]. The dielectric studies of different polar binary mixtures at different concentrations and temperature lead to analyze the strength of the hydrogen bond interaction in terms of thermodynamic parameters, ordering nature of the dipoles and their mutual interactions [2–6]. The dielectric relaxation spectroscopy is one of the sensitive methods to detect small changes occur in the structural parameters of a molecule in a liquid

system. Several researchers performed dielectric studies on different liquid compounds in water as well as in alcoholic medium in recent past [7–17], at the same time molecular simulations are also performed to interpret experimental results [18–22]. The different spectroscopic studies such as FT-IR, proton NMR, and Neutron diffraction studies are also carried by the researchers to confirm the existence of hydrogen bond between the different liquid mixtures [23–25].

The present work is in continuation of our systematic studies in order to understand the molecular interaction between binary mixtures of propylene glycol and sulfolane. In our previous paper [43] (Vishwam et al.), we reported the molecular interaction behaviour of propylene glycol in ethanol medium and the data is interpreted in terms of thermodynamic parameters, strength of the hydrogen bond interaction from the single point energy method.

In the present manuscript, we are interested to analyze the effect of sulphonyl group on the dielectric relaxation process of propylene glycol medium. The molecular interaction of sulfolane in propylene glycol is studied in terms of short and long-range ordering of the dipoles, excess molar volume (V_m^{E}), molar polarization (P_m), Natural Bond Orbital analysis to identify the position of hydrogen bond. The chemical stability of the molecule is studied by Highest Occupied Molecular Orbital and Lowest Unoccupied Molecular Orbital (HOMO, LUMO) calculations and Redlich-Kister polynomial fitting procedure for excess dielectric

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Dielectric relaxation and thermodynamic study of Dimethylformamide/1,4-Butanediol binary mixtures in the temperature range 298K–323K

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Mixing rules

ABSTRACT

In the present paper, the permittivity of Dimethylformamide (DMF) with 1,4-Butanediol (BD) binary mixtures are determined at the temperature range of 298 K–323 K in the microwave frequency. Dipole moment (μ), excess molar volume (V_m^E), partial molar volume ($V_{m,i}$), excess permittivity (ϵ^E), excess refractive index (n_D^E), excess inverse relaxation time ($1/\tau^E$), thermal expansion coefficient (α_p), excess Helmholtz energy (ΔF^E) are determined at different temperatures. Redlich-Kister polynomial equation is used to fit the excess parameters. Havriliak-Negami equation is used to analyse the relaxation time of the binary mixtures throughout the measured temperature range. The heteromolecular interaction between DMF and 1,4-Butanediol binary mixtures are interpreted in terms of Kirkwood correlation (g^{eff}) factor. The stability of the system is analysed from the activation energy (ΔG^*), enthalpy (ΔH^*) and entropy (ΔS^*) parameters. The various mixing rules were applied in order to estimate the permittivity and refractive indices of the binary system at different temperatures.

1. Introduction

The complex permittivity of binary liquid mixtures provides information regarding the solute-solvent interactions and also the existence of monomers and multimers in the solution. The permittivity is a macroscopic parameter plays a significant role in understanding the nature of molecular interaction between polar-polar, polar in a non-polar liquid medium and also the alignment of dipoles in the solution [1–10]. The profound knowledge in thermodynamics and transport properties of pure liquids and their binary mixtures is essential to solving many chemical engineering problems, heat and mass transfer, and drug design calculations. The temperature dependent dielectric relaxation studies of different polar liquids at different microwave frequency region can yield the information regarding the structure of the molecule, inter and intra molecular hydrogen bonding and orientational polarization of the dipoles [11–23]. Investigation of permittivity of polar liquids having the hydrogen bond donor and acceptor group compounds are very much useful for various number of applications in the field of biological, medical, material science and technology [24,25].

Dimethylformamide (DMF) is a polar (hydrophilic) aprotic solvent with a high boiling point. DMF is used as a solvent in peptide coupling for pharmaceuticals, pesticides production, manufacture of adhesives,

synthetic leathers, fibre films and surface coatings. Whereas 1,4-Butanediol (BD) is used in the manufacturing of plastics, fibres, and as solvent for many chemical reactions. Several researchers and scientists reported the dielectric relaxation of DMF in the different solvent medium such as toluene, benzene, benzoates, 3-Nitrotoulene in the recent past [26–37]. Stockhausen et al. [38] studied the dielectric relaxation of BD + DMF binary mixtures in the range of 5 MHz–72 GHz at 20 °C. The relaxation times of the binary mixtures are interpreted in terms of empirical equation by considering viscosity terms and the rotation of carbon chain group. Navarkhele et al. [39] also studied the dielectric relaxation behaviour of BD + DMF binary mixtures in the frequency range 10 MHz–20 GHz between the temperatures 20 °C–40 °C. The relaxation time of these mixtures is calculated from the Cole-Cole plot and the molecular interaction are discussed in terms of excess permittivity and Kirkwood g factor [40]. The physico-chemical properties of the binary mixtures of DMF with alkanols and their interactions are interpreted by considering the molar volume and refraction values [41]. Whereas in the present study we have considered volumetric and thermal expansion (α_p) parameters [42,43], electrical dipole moment, molar polarization [23], long-range and short-range interactions between the dipoles by excess Helmholtz energy (ΔF^E) equation [44], thermodynamic quantities [45] to interpret the molecular interaction between 1,4-Butanediol

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Attenuation Effect in Twenty One Different Proton Dissociation Equilibria Brought on One Rope: A Chemical Education Tool for Evaluation of pK_a of Proton Dissociation Equilibrium of Any Substituted Benzene (XC_6H_5)

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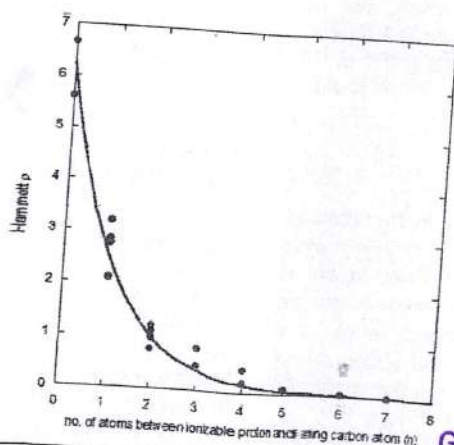
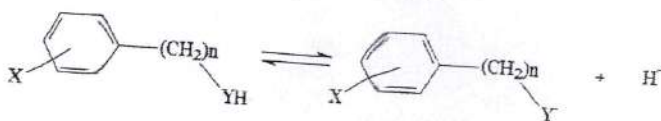
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Abstract The strong empirical relation, $\rho = (2.4)^{(2-n)}$, between the Hammett ρ for proton dissociation of several acids and the number, "n", of atoms between the ionizable hydrogen and the ring carbon (Andrew Williams, Free Energy Relationships in Organic and Bioorganic Chemistry, Royal Society of Chemistry, Cambridge, 2003, p. 75) is used to construct a graph for twenty one different proton dissociation equilibria. The plot of Hammett ρ versus number of atoms i between ionizable hydrogen and the ring carbon atom is observed to be an excellent exponential-decay locus. A good average and intelligent value of Hammett ρ is obtained for the benzene dissociation equilibria by interpolating the locus of the correlation on to Y-axis. Using this Hammett ρ value and the Hammett equation $\log [(K_a)_X / (K_a)_H] = \rho\sigma$, the pK_a value can be calculated for any substituted benzene knowing the pK_a value of benzene to be 43. The points for proton dissociation equilibria of phenylethyl ammonium ions and benzyl alcohols deviated from the graph hence not included in the correlation. Possible explanations are given for deviation of these two equilibria.

Graphical abstract

The term "attenuation" in general implies that it is the exponential depletion of some property either physical or chemical with time, distance and medium. Attenuation is an exponential property with the length of the medium. Of particular interest, it is the diminution of substituent electronic effects in a molecule during the course of any chemical change.



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Influence of Slip and Heat and Mass Transfer Effects on Peristaltic motion of Power-law fluid Prone to the Tube

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Abstract. Present study deals with the study of peristaltic motion of a power-law fluid with nanoparticles in a tube with permeable walls. Heat and mass transfer effects and slip effect are studied in this investigation. Axial velocity, pressure gradient and frictional force are expressed analytically and investigated various parameter effects on these flow variables. The present model revealed that, heat transfer coefficient and mass transfer coefficients increases in the region $[-1, 0]$ and decreases in the region $[0, 1]$ with the increase of thermophoresis parameter and shows an opposite behavior with the increase of Brownian motion parameter. Pressure drop increases with the increase of slip parameter. Frictional force decreases with the increase of slip parameter and converges to 1.

1. Introduction

Peristalsis is very important phenomena in the human body. This phenomenon has many biological and industrial applications. Many researchers have done investigations in the peristaltic transport. (Brasseur et al. (1987), Valanis and Sun (1969), Mishra and Ramachandra Rao (2003), K. M. Prasad (2009), Hayat et al. (2014), Chandra and Pandey (2018)).

"Power-law fluid is a fluid in which the shear stress at any point is proportional to the shear rate at that point raised to some power". The problems based on non-Newtonian fluids have many applications and hence good number of researchers started working in this area. Ostwald-de Waele model is widely used model for non-Newtonian fluids focusing on power-law rheology. Power-law fluids are classified into three different types of fluids as given below:

n	Type of Fluid
<1	Shear-Thinning Fluids
$=1$	Newtonian Fluid
>1	Shear-Thickening Fluids

Many researchers done their research in this field (El Naby and El Shamy (2007), Hayat et al. (2006), Shukla and Gupta (1982)).

Nanofluids have many biomedical and industrial applications. New techniques are used using nano-fluids for cancer treatments and for safer surgery for the delivery of drugs. A good amount of



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HUMAN RESOURCE PLANNING THROUGH GOAL PROGRAMMING IN A SOFTWARE INDUSTRY

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Abstract: This paper presents the application of a Goal programming in planning the effective human resources in a software industry. A software industry comes across multiple objectives, tribulations, and tasks. These multiple objectives can be solved by goal programming. This GP model also conveys the idea of a strategic bidding in giving a quote for a new project. The various objectives and the constraints of the company are converted to prioritized goals and goal constraints in this model. Multiple (nine) category of employees and three differently skilled employees of the same category are also considered in this model and attained the optimal solution to the GP model. Vogel's approximation and Modified-distribution methods are also used in solving the problem along with the goal programming technique. This goal programming model provides effective HR planning, budget and expenditure.

Keywords: - Goal programming (GP), human resource planning (HR), Software industry, Product backlog Item (PBI), Linear (SEK)

INTRODUCTION

Lack of HR has been a major contributor to notable failures. Several articles, research papers and surveys brought to light about the need for change in employee engagement, effective human resource planning for higher organizational performance. Sometimes, larger projects will take longer than necessary, or may never reach completion, because of the lack of necessary HR to break them down into more manageable segments. In general, most of the software companies depending on the past experiences or on the experienced employees in calculating the human resources, budget planning of the project, giving the attention to acquire the project. For today's business practices to thrive the new technologies should be adopted or the old practices should be modified to meet the day to day challenges. Today, every organization requires HR strategies. Applying new strategies without knowing what exactly is it addressing will not generate a favorable outcome. A failed strategy will only guarantee a waste of time, money and effort. In today's business world finding the second chance is very thorny.

For example, a renowned industry like Toyota went into crisis and recalled its selling units thrice in recent years, but how could it happen to a renowned company which is known for its quality. HR management failures led to the problems which affected themselves in manufacturing defects. The other human resources issue which led to this problem is the rewards system is present at Toyota Motor Corporation. Another human resources issue that has led to its current problems is the failure to conduct proper risk management within the company; this is due to the lack of people assigned to this process. This example shows the need of effective HR planning in the organizations.

The chief HR issues are lack of skilled employees, lack of proper human resource planning, poor salaries compared to its rivals and lack of control on the finance. Such expenses create financial burdens on the company which results in the downfall of the company. The solution to these kind of HR issues are proper human resource allocation, proper budget planning, inspecting employees performance, proper training to employees, reduction of work burden, recruiting skilled employees, proper wages and attention to the employees. In this research paper, our research group is successful in giving the mathematical solutions to the HR for a model software industry through goal programming.

Many attempts are made by various research groups to trigger this issue in recent years. Lawrence Jones et al. [1982] have used GP model for allocating human resources for the good laboratory practice regulations. N. K. Kwak et al. [1997] have used GP model for Human Resource Allocation in a Health-Care Organization. Glynn, Joseph. [2011] have used Goal Programming approach to human resource planning with a concentration on promotion policy. Nabendu Sen et al. [2013] have developed GP model for Personnel Management in Tea Industry. Maliheh Khabiri [2015] has used GP approach for modeling human resource allocation to multiple projects. Mohammad Hossein Mehroli Hassani et al. [2016] have used the GP to improve human resource allocation for urban family physician plan in Iran.

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Influence of Slip on Peristaltic Motion of a Nanofluid Prone to the Tube



K. Maruthi Prasad and N. Subadra

Abstract Influence of slip on peristaltic motion of a nanofluid prone to the tube is studied under the assumption of long wavelength and low Reynolds number. The equations governing the flow are solved and closed-form expressions for velocity, pressure drop, time-averaged flux and frictional force have been obtained. The effects of various parameters like Brownian motion parameter, thermophoresis parameter, local temperature Grashof number, local nanoparticles Grashof number, slip parameter and inclination on these flow variables have been studied. Streamline patterns and trapping phenomena have been studied and sketched through graphs at the end.

Keywords Nanofluid · Permeable walls · Brownian motion parameter · Thermophoresis parameter · Local temperature Grashof number · Local nanoparticle Grashof number

1 Introduction

'Peristalsis is a mechanism of fluid transport that occurs widely in many physiological situations such as food mixing and chyme movement in the intestines, movement of ovum in the female fallopian tube, transport of urine through ureters'. Peristaltic motion of Newtonian fluids has been investigated by many researchers under various conditions [1-3].

Nanometer dimension materials show unique physical and chemical characteristics. Therefore, nanotechnology has a vast contribution in the industry. Nanofluids

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(2)

A Goal Programming Approach for an Effective Financial Budget of an Indian State

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Abstract

For a welfare country, the effective financial budget planning is always a challenging task. Though the goals of any financial budget are about the welfare of the country, yet the priorities may change from year to year, to fulfill the economic growth of the developing countries like India. In financial budgeting, the economical priorities of the democratic countries like India depend on the ethics or the promises given by the ruling political party. Besides that, the administrator has to consider various goals in obtaining a satisfactory solution to the financial budget. In this research paper, a State from India is considered and various goals were taken in to thoughtfulness. Multi-decision making problems can be solved by goal programming. The strength of the goal programming model is that it can solve multiple objectives simultaneously and can obtain an optimal solution that satisfies all the objectives and constraints. The objectives change frequently. The goal programming model stated in this research paper can indicatively overcome the changes happening from time to time and can be successful in constructing the effective financial budget.

Keywords—Goal programming, Goal priorities, Effective Financial budget, Indian state economy.

1. Introduction

India is a developing country with mixed economy. India is the third largest economy by nominal gross domestic product (GDP) and ranks fourth in power purchasing parity (PPP). The country ranks 141st [12] in per capita GDP (nominal) with \$1723 [12] and 123rd [12] in per capita GDP (PPP) with \$6,616 [11]. After 1991 economic liberalization, India achieved 6%-7% [13]

average GDP growth annually. In the fiscal year 2015 and 2017 India's economy became the world's fastest growing major economy surpassing China. India topped the World Bank's growth outlook for the first time in fiscal year 2015-16, during which the economy grew 7.6% [13]. Growth is expected to have declined slightly to 7.1% [13] for the 2016-17 fiscal year. According to the IMF, India's growth is expected to re-bounce to 7.2% [13] in the 2017-18 and 7.7% [13] in 2018-19 fiscal years.

In India, there are three types of sectors based on economy and GDP. They are a. Agriculture (primary sector) b. Industry (secondary sector) and c. Services (tertiary sector). In the agriculture sector, India holds world's second position in the agricultural production [13]. The agriculture contribution to the GDP is declining since from 1951, yet it is still the major sector of the Indian economy. Industry sector is having a steady share in the Indian economy and becoming the fastest growing e-commerce markets. In the service sector, India's contribution is increasing very rapidly from 2001. Information technology services (IT), business process out source (BPO) services and software services are the major exports of India in the service sectors.

Rapid increase in the contributions from the three sectors results in the growth of Indian economy. The development in Agriculture and allied services, industry and minerals, infrastructure, transportation, taking up of new irrigation projects, tourism, creating the farming jobs, providing health coverage, rural development, technical education, urban development, housing, water supply, sanitation, energy, labor and employment etc.. Leads to notable increase of Indian economy and per capita GDP. The development in the above said sectors can be achieved by the effective

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The Term, "Restriction" in Phase Rule Rendered More Intelligible: A Chemical Education Article for Undergraduate Students of Chemistry in India

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Abstract:

We have a mathematical relation for the determination of components (C), $C = C' - r$ ref.1 where C' is the total number of chemical constituents or species, and r is the number of restrictions or restrictive conditions, which is seldom used and taught in Indian Universities and colleges. In this article, we have made an attempt to elaborate the term restriction, taking few examples from one of the staple engineering textbook² in India. Even though this equation $C = C' - r$ appears simple, the meaning of the term r is difficult to comprehend. Therefore, we thought that elaboration of the term is of much use to both the teacher and to the taught. More importantly there appears some conceptual flaw in the calculation of components for particular reaction in this book². And this flaw is reoccurring from the past 25 years. Our endeavor is to rectify this flaw in the interest of students, teachers and chemistry audience at large.

Keywords: Phase, Components, Restrictions Constituents and Phase rule.

INTRODUCTION

In phase rule, components³ (C) is equal to difference between the number of chemical species in the system and the number of equations relating the concentrations of these substances in an equilibrium system. This definition is especially useful in the case of constituents, which are capable of chemical interactions.

DISCUSSION

The meaning of the crucial sentence 'equations relating the concentration of these substances' in the foregoing paragraph is nothing but the restrictions imposed on the independent existence of the concentration of the substances. When the substances are related by equality, it overtly reflects that their freedom to exist

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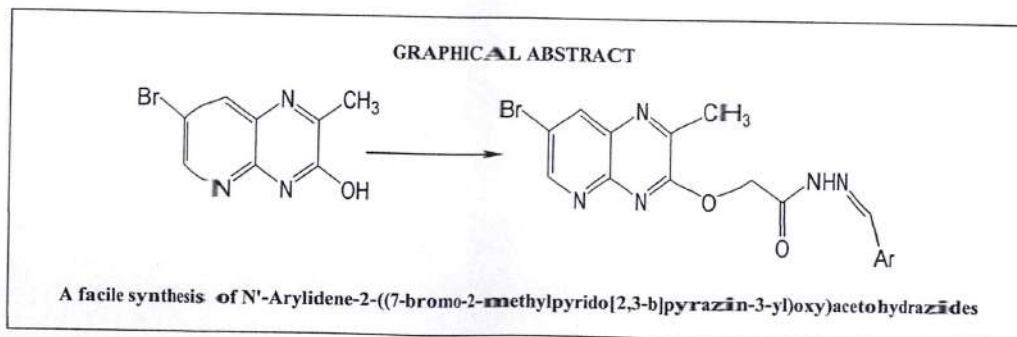
A Facile Synthesis of N'-Arylidene-2-((7-bromo-2-methylpyrido[2,3-b]pyrazin-3-yl)oxy)acetohydrazides

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ABSTRACT

5-bromo 2,3-diamino pyridine and ethyl pyruvate react each other to form 7-bromo-2-methylpyrido[2,3-b]pyrazin-3-ol (1) which further reacts with ethyl chloroacetate and form ethyl 2-((7-bromo-2-methylpyrido[2,3-b]pyrazin-3-yl)oxy)acetate (2). Compound 2 on reaction with hydrazine hydrate gives 2-((7-bromo-2-methylpyrido[2,3-b]pyrazin-3-yl)oxy)acetohydrazide (3), which on condensation with different aldehydes produce N'-Arylidene-2-((7-bromo-2-methylpyrido[2,3-b]pyrazin-3-yl)oxy)acetohydrazides (4a-e).



Keywords: Heterocycles, Aldehydes, Antitumor agents, Hydrogen bond, Corrosion, Hormones

INTRODUCTION

Pyrido[2,3-b]pyrazine (5-azaquinoxaline) derivatives are very important nitrogen-containing heterocyclic compounds with diverse pharmacological and therapeutic properties [1]. Pteridine and quinoxaline are structural analogues of them. Studies have shown that such compounds are widely involved in several fields, as they exhibit antimalarial, anti-cancer [2], antibacterial and anti-allergic activities [3]. They also exhibit antimetabolic behavior [4]. Pyrido[2,3-b]pyrazine derivatives are well-known for their strong inhibitory activities of phosphodiesterase IV (PDE IV), the production of Tumor Necrosis Factor (TNF), Platelet derived growth receptor, gonadotropin releasing hormone, IgE production [5]. Pyrido pyrazine derivatives are broadly used as corrosion inhibitors for metals in acid environments, since they own the nitrogen and oxygen atoms which can easily be protonated to exhibit good inhibitory action on the corrosion of metals [6].

Mutations affecting Epidermal Growth Factor Receptor (EGFR) activity could result in cancers such as squamous-cell carcinoma of the lung, anal cancers, glioblastoma and epithelial tumors of the head and neck. The identification of EGFR as an oncogene (a gene that has the potential to cause cancer) has led to the development of anticancer therapeutics against EGFR, called "EGFR" inhibitors. Among them, using small molecule inhibitors to inhibit the EGFR tyrosine kinase is the most appropriate method, which acts on the cytoplasmic side of the receptor. Without kinase activity, EGFR is unable to activate itself, which is a prerequisite for binding of downstream adaptor proteins [7-9].

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A Subclass of Meromorphic Functions Defined by Convolution

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ABSTRACT

In this paper we define a subclass $\Sigma_g(\alpha, \lambda)$ of Meromorphic univalent functions using convolution. We study some geometric properties of this subclass. In the first section of this chapter we discuss a coefficient characterization for a function of Σ_p to be a function of the class $\Sigma_g(\alpha, \lambda)$. We also discuss growth and distortion properties for functions of the class $\Sigma_g(\alpha, \lambda)$. In the second section of this chapter we find radii of starlikeness and convexity for the functions of the class $\Sigma_g(\alpha, \lambda)$. In the third section we find extreme points for the class $\Sigma_g(\alpha, \lambda)$.

Index Terms - Meromorphic, Univalent, Convolution.

INTRODUCTION

Let Σ be the class of functions of the form $f(z) = \frac{1}{z} + \sum_{n=1}^{\infty} a_n z^n$ defined on the punctured unit disk $U^* = \{z \in \mathbb{C} : 0 < |z| < 1\}$.

Let Σ_p denote the class of meromorphic functions of the form

$$f(z) = \frac{1}{z} + \sum_{n=1}^{\infty} a_n z^n, \quad z \in U^*, \quad a_n \geq 0 \text{ for } n = 1, 2, 3, \dots \quad (1.1)$$

which are defined on the punctured unit disk $U^* = \{z \in \mathbb{C} : 0 < |z| < 1\}$.

If $f(z) = \frac{1}{z} + \sum_{n=1}^{\infty} a_n z^n$ and $g(z) = \frac{1}{z} + \sum_{n=1}^{\infty} b_n z^n$ are two functions in Σ , the Hadamard product or convolution of f and g is defined by

$$f(z) * g(z) = \frac{1}{z} + \sum_{n=1}^{\infty} a_n b_n z^n, \quad z \in U^*.$$

Mogra et al [2] introduced meromorphic starlike functions of order α and type β , when the coefficients in Laurent series expansion about the origin are all positive and denoted by $\Sigma_p^*(\alpha, \beta)$. And obtained many useful results such as characterization of coefficients, distortion property, radius of convexity, extreme points for the class $\Sigma_p^*(\alpha, \beta)$.

Kavitha et al. [4] defined a new class of meromorphic functions

$$M_p(\alpha, \lambda) = \left\{ f \in \Sigma_p : \operatorname{Re} \left(\frac{zf'(z)}{(\lambda-1)f(z) + \lambda f'(z)} \right) \geq \alpha \right\} \text{ for } 0 \leq \alpha < 1, 0 \leq \lambda < 1, z \in U^*$$

and obtained coefficient inequality, growth and distortion bounds, radii of meromorphic starlikeness and meromorphic convexity for this class $M_p(\alpha, \lambda)$.

Definition [2] A function $f(z) \in \Sigma$ is called meromorphically starlike univalent of order α , $0 \leq \alpha < 1$ if and only if

$$-\operatorname{Re} \left\{ \frac{zf'(z)}{f(z)} \right\} > \alpha, \quad z \in U^*.$$

Definition [2] A function $f(z) \in \Sigma$ is called meromorphically convex univalent of order α for $0 \leq \alpha < 1$ if and only if

$$-\operatorname{Re} \left\{ 1 + \frac{zf''(z)}{f'(z)} \right\} > \alpha, \quad z \in U^*$$

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(3)

Attenuation Effect as a Tool to Explain sp^3 Carbon ($-CH_2-$) is a Good Electron Insulator and a sp^2 Carbon ($-CH=CH-$) is a Good Electron Transmitter: An Undergraduate 1-h Chemistry Classroom Tutorial

R. Sanjeev¹ · R. Ravi² · V. Jagannadham³

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Abstract Physical basis of chemical reactivity in organic molecules was to determine the electronic effects which govern the rate of a reaction put forth by the substituents during the course of a given reaction. This is known as "substituent effect." This concept was first developed by Hammett in the form of a linear free-energy relationship (LFER) popularly known as "Hammett equation." This substituent effect would generally attenuate in an exponential manner as the distance between the reaction center and the substituent increases. This was developed by Williams (Free-energy relationships in organic and bioorganic chemistry, Royal Society of Chemistry, Cambridge, 2003) in the form of an empirical exponential equation. Using the Hammett equation and with help of Williams 2003 explanations on attenuation effect, we have tried to explain why a sp^3 carbon is a good σ -electron insulator and a sp^2 carbon is a good π -electron transmitter.

Keywords Hammett equation · Attenuation effect · Electron insulator and electron transmitter · Classroom tutorial

Introduction

The term "attenuation" in general implies that it is the exponential depletion of some property either physical or chemical with time, medium and distance. In this direction, study of the attenuation effect in aromatic [2, 3] and aliphatic systems [4] is a major breakthrough from our laboratory not reported earlier. The ultimate conclusion is the hybridization of carbon would eventually affect the magnitude of Hammett ρ in the carboxylic acid dissociation equilibria [2, 3]. Using the magnitude of Hammett ρ values of dissociation equilibria of homologous series of carboxylic acids we have given a simple and lucid



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Tetrahedral Nature Determines the Stability of Reactive Intermediates: A Chemical Education Perspective

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ABSTRACT

Hammett equation is applied and the magnitude of substituent effect in terms of Hammett ρ has been estimated for the deprotonation equilibria of highly unstable arenium ions (Wheland intermediates) $\text{XC}_6\text{H}_5^+ \rightleftharpoons \text{XC}_6\text{H}_5 + \text{H}^+$ based on the attenuation effect of methylene group on the dissociation equilibria of anilinium ions, benzyl ammonium ions and 2-phenylethyl ammonium ions. The Hammett ρ was found to be 14.3. The Hammett ρ for the deprotonation equilibria of pyridinium ions $\text{XC}_5\text{H}_4\text{NH}^+ \rightleftharpoons \text{XC}_5\text{H}_4\text{N} + \text{H}^+$ was estimated from the plot of $\log K_a$ vs Hammett σ , this value is 5.90. The magnitude of substituent effect in terms of Taft ρ^* has been estimated for the deprotonation equilibria of methanium ions $\text{RCH}_2^+ \rightleftharpoons \text{RCH}_3 + \text{H}^+$ based on the attenuation effect of methylene group on the dissociation equilibria of aliphatic amines and was found to be 6.9. The Taft ρ^* for the deprotonation equilibria of alkyl ammonium ions $\text{RNH}_3^+ \rightleftharpoons \text{RNH}_2 + \text{H}^+$ was estimated from the plot of $\log K_a$ vs Taft σ^* , this value is 3.28. The large differences in the Hammett ρ of 8 units when carbon is replaced with nitrogen as heteroatom in the six-member aromatic ring and 3.6 units of Taft ρ^* when carbon is replaced with nitrogen in aliphatic derivatives respectively is explained.

INTRODUCTION

The frequent over viewing and dealing with Hammett and Taft equations is a continuous well documented observation from our laboratory¹⁻¹⁶. In all these studies application of Hammett and Taft equations is dealt in detail and even to physical properties like dipole moments, surface tensions and melting points of several organic compounds.

But application of Hammett and Taft equations to very unstable intermediates is a challenging task. Application of Hammett and Taft equations to arenium ions¹⁰ (Wheland intermediates, XC_6H_5^+) and methanium ions¹⁵ (super acids, RCH_2^+) is itself novel. In the present work we tried to explain why the deprotonation equilibria of arenium ions (Wheland intermediates, XC_6H_5^+) and methanium ions (super acids, RCH_2^+) are more susceptible to substituent



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18-19 - (10)

Application of dielectric mixtures formulae to PbTiO_3 based glass-ceramic systems

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(10)



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Electrical Properties of Lead Free $\text{Sr}_{0.8}\text{Na}_{0.1}\text{Sm}_{0.1}\text{Bi}_4\text{Ti}_4\text{O}_{15}$ Ceramics

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Abstract

Polycrystalline $\text{Sr}_{1-2x}\text{Na}_x\text{Sm}_x\text{Bi}_4\text{Ti}_4\text{O}_{15}$ (SNSBT) belongs to bismuth layer structured ferroelectric (BLSF) materials with $x=0.1$ have been prepared by sol gel method. XRD analysis confirms single phase formation with orthorhombic structure. Scanning electron micro graph of the material shows plate like grains with random orientation. Dielectric and impedance measurements carried out from room temperature to 600°C at different frequencies. Piezoelectric and electromechanical coupling coefficients are calculated from resonance and anti-resonance frequencies. Cole-Cole plots showed non-Debye behaviour.

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Peer-review under responsibility of the International Conference on Nanomaterials and Technologies (CNT 2014)

Keywords: BLSF; Orthorhombic; Dielectric; impedance; piezoelectric properties;

1. Introduction

The family of Bismuth layer structured ferroelectric (BLSF) Arrivillius (1949) materials received significant attention for their application to electronic functional devices such as piezoelectric actuators, resonators and high temperature sensors etc. Subbarao (1962). Cross and Pohanka (1971). The general formula of BLSF is $(\text{Bi}_2\text{O}_2)^{2+}(\text{A}_{m-1}\text{B}_m\text{O}_{3m+1})^{2-}$, where A can take mono-, di-, trivalent ion or combination of them, B can be Ti^{4+} , Nb^{5+} or Ta^{5+} and m can take integers 1 to 5. Subbarao (1996). BLSF are characterized by their low dielectric constant, High Curie temperature (T_c), large anisotropy in electromechanical coupling factor (k_t/k_p), high mechanical quality factor (Q_m) and low temperature coefficient of resonance frequency. Ikegami and Ueda (1974). Takenaka and Sakata (1984). It is possible to modify the dielectric and ferroelectric properties by changing chemical composition. The effect of A-site substitution is more obvious than that of B-site substitution, since the cations in B sites are similar in size and do not play a major structural role in polarization process for BLSF. Jannet et al (2003).

The ac impedance analysis is known to be a powerful means to separate out the grain boundary and grain-electrode effects, which usually are the sites of trap for oxygen vacancies and other defects. It is also useful in establishing space charge polarization and relaxation mechanism. In view of the importance of ac impedance


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Relaxation dynamics of L-alanine in water medium investigated by dielectric relaxation spectroscopy

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Abstract

The complex dielectric permittivity of L-alanine in aqueous medium at different concentrations and different temperatures were measured in the microwave ($0.02 < \nu/\text{GHz} < 20$) frequency region by using open-ended coaxial probe technique. From the reflection coefficient and impedance data, the real and imaginary part of the dielectric permittivity values is determined. It is observed that there is a decrease in the real part of the dielectric permittivity up to certain frequency and an increase in the imaginary part of the dielectric permittivity with increase in the molar concentration of L-alanine in water medium. Based on the experimental data the average relaxation time values are calculated and its behavior is analyzed in terms of bound water and free water molecules. The theoretical dipole moment of L-alanine is calculated at gaseous state as well as in aqueous medium by using PCM and IEFPCM model at HF, DFT/B3LYP and MP2 calculations using 6-311G* basis set. Analysis between experimentally determined parameters and computed dipole moments were discussed. The mean molecular polarizability is calculated from the Lippincott δ function potential model and compared with the Le Fèvre method of polarizability values.

Keywords: Dielectric constant, Dipole moment, Dielectric relaxation, DFT calculations, Polarizability

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⑤ Physical Review B
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17-18
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Effect of Frustrated Exchange Interactions and Spin-half Impurity on the Electronic Structure of Strongly Correlated NiFe₂O₄

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Spin-polarized density functional calculations, magnetization, and neutron diffraction measurements are carried out to investigate the magnetic exchange interactions and strong correlation effects in Yb substituted inverse spinel nickel ferrite. In the pristine form, the compound is found to be a mixed insulator under the Zaanen-Sawatzky-Allen classification scheme as it features both charge transfer and Mott insulator mechanism. Estimation of magnetic exchange couplings reveals that both octahedral-octahedral and octahedral-tetrahedral spin-spin interactions are antiferromagnetic which is typical of a spin-frustrated triangular lattice. However, the latter is dominant compared to the former leading to a forced parallel alignment of the spins at the octahedral site which is in agreement with the results of neutron diffraction measurements. The substituent Yb is found to be settled in +3 charge state, as confirmed from the XPS measurements, to behave like a spin-half impurity carried by the localized $f_{z(x^2-y^2)}$ orbital. The impurity f spin significantly weakens the antiferromagnetic coupling with the spins at the tetrahedral site, which explains the experimental observation of fall in Curie temperature with Yb substitution.

I. INTRODUCTION

The cubic inverse spinel NiFe₂O₄ (NFO) has been extensively investigated in the context of nanomagnetism [1], spin-filtering [2, 3], spintronics [4] and multiferroics [5]. In addition, it exhibits unusual electronic and magnetic properties when Fe³⁺/Ni²⁺ ions are partially substituted by other transition metal (M) ions, rare earth (R) ions or ions of non-transition elements [6–11]. Collinear Néel type ferrimagnetic structure of NiFe₂O₄ yields to triangular Yafet-Kittel structure upon substantial Cr substitution at the Fe sites [6]. The octahedra containing Fe³⁺ ions in NFO, when partially substituted by rare-earth (R³⁺), become non-centrosymmetric to make the compound ferroelectric. Experimentally it has been shown that, substituents like Sm³⁺ and Ho³⁺ induce magnetoelectric effect in NFO [8].

Significant changes in the electronic, magnetic and structural behavior of Ni-Zn ferrite upon diluting with several rare earth ions have been observed [9–11]. With substitution of 2% of Fe by R (= Yb, Er, Dy, Tb, Gd, Sm and Ce) in Ni_{0.7}Zn_{0.3}Fe₂O₄, while lattice has been reported to expand and resistivity has increased, both magnetization and Curie temperature have decreased [9–11]. Larger ionic radii of R³⁺ ions cause lattice expansion and the 4f electrons are more localized than the itinerant 3d electrons and hence, the resistivity increases [9–11]. The reported value of Curie temperature (T_C) of NiFe₂O₄ is 853 K [7, 12]. A decrease in T_C upon the partial substitution of R³⁺ for Fe³⁺ in NiFe₂O₄ has

been reported from our lab [7, 8]. In Ni₂Fe_{1.925}R_{0.075}O₄ compounds, the T_C decreases to 775 K, 812 K and 839 K respectively for Dy [7], Ho³⁺ and Sm³⁺ substitutions [8]. However there are no concrete mechanisms and evidence to explain the decrease in magnetization and Curie temperature, even though qualitatively it has been attributed to weaker R-Fe exchange coupling replacing the stronger Fe-Fe exchange coupling [12, 13].

In this paper, results from DFT calculations and experimental studies are presented and analyzed to explain the electronic and magnetic structures of Yb substituted NFO viz. NiFe_{2-x}Yb_xO₄ (x = 0, 0.05, 0.075). The reasons for choosing Yb were manifold: (a) Structural distortion is expected to be weak or negligible, since the radius of Yb³⁺ ion (0.86 Å) is smaller compared to those of the other rare earth ions. (b) Yb ion can stabilize in +2 and +3 charge states. (c) Yb³⁺ is magnetic and has lower spin moment compared to the other R³⁺ (R = Gd, Tb, Dy, Ho, Er, Tb) ions [12] and hence, large reduction in magnetization as well as Curie temperature. (d) Yb³⁺ is expected to provide a spin-half f impurity state. Therefore, it serves as a model system to study host (d spin)-impurity (f spin) magnetic interactions.

Experimentally, X-ray photoelectron spectroscopy (XPS), Raman spectroscopy and neutron diffraction (ND) measurements are performed and theoretically, spin-polarized band structure is calculated to explain the electronic structure of NiFe_{2-x}Yb_xO₄. In addition, various magnetic exchange couplings are estimated from the total energies of several possible magnetic configurations so that the spin-spin interactions in this compound can be better understood. Emphasis is given on the magnetic coupling of Yb and Fe spins and its

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Enabling Sustainable Growth of SME'S through Delivery Excellence and Intellectual Property

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Abstract: India's SME sector comprises of 30 million units employing nearly 60 million people and producing more than 8000 products. With changing global economic scenario, it is very appropriate to focus on growth that is economically, environmentally and socially sustainable. For competing in the global markets, efforts should be engaged in producing goods/services through lean approaches towards better, cheaper and smarter solutions to the customers. SME's need to explore options to invigorate their existing techno functional expertise and protect their firm's intangible assets. In this aspect awareness and understanding of Intellectual property aspects plays vital role primarily due to availability of rich repository which is being enriched with creativity and innovation. Intellectual property being a technological dimension needs to be integrated as a part of business strategy and organization's culture by augmenting the fruits of scientific endeavor, innovation and creativity. For developing countries like India, it is important to strengthen its productive capacity and strive for inclusive, sustainable and equitable economic growth in order to be a global economy player. In this work we present some of the global challenges faced by Indian SME's and propose a framework to leverage on innovation, delivery excellence and intellectual property towards sustainable growth.

Keywords: Intellectual property rights, SME, sustainable growth, innovation management.

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I. Introduction

Globalization provides challenging opportunities towards economic growth. India being a developing country the volatility in the market climate is influencing significantly the growth of SME's. Organizational strategy towards business investments, lean processes and practices to minimize operational cost and deliver quality play an important role and help in sustainable development of the organization keeping socio economic and environmental conditions. SME's being the major contributor to the Indian economy [1-3], it is justifiable to say that, this sector needs to develop a path to excellence in turn making a mark in the global economy. For this it is needless to say that SME's should understand their business in the perspective of internationalization and evaluate their business potential and associated risks as well. Delivery excellence is possible only through sustainability and inclusion which in turn can be achieved through understanding of organizational structure, delivery models connected with operational, pricing, marketing strategies leveraging existing knowledge and resources [4, 5].

In addition to delivery excellence, creativity and innovation drive the knowledge based economies through Intellectual property (IP) assets. The country's policies determine the business strategies and in this aspect IP acts as a tool for wealth creation in a country. These factors also have influence on India to be one of the signatory nations in TRIPS council [6]. But, as the studies indicate [7, 8] there is a lacuna in the SME's understanding and awareness regarding intellectual property rights. This is especially true for SME's present in the rural sector. For a developing country like India, that is rich in traditional, folklore, agricultural, traditional medication like Ayurveda, homeopathy, unani etc, there is a great need to develop a strategic, sustainable generic framework that is suitable for various sectors to adapt and evaluate their knowledge in the perspective of intellectual property. This is need of the hour to sustain in the global market as well as to generate wealth. Due to the rapid proliferation of the technology in this digital age, it is crucial that the SME sector brings its intangible mode of knowledge to the tangible mode through IP that acts as a catalyst in the progress of the nation economically.

In this present work, we try to give a generic frame work that might be adapted with modifications suitable to their business in general by the SME's present in the technical sector. Our basic motive in this work is to highlight integration of the delivery excellence that is crucial for business with Intellectual property to enhance/create knowledge assets for itself and in turn for the country.

Chemical Education

Does A Partition or Distribution Coefficient Exist For A Solute That Distributes Between Two Miscible Solvents?

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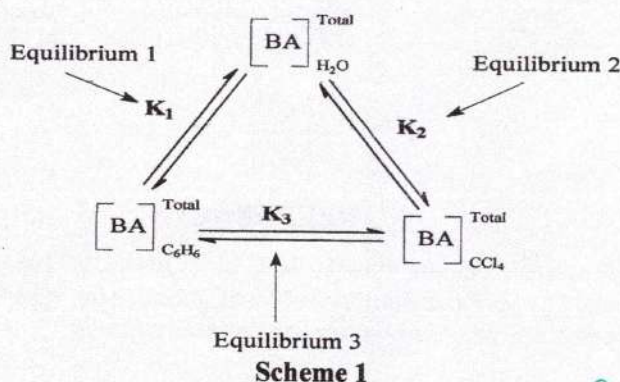
ABSTRACT

It is known that for any solute, the Nernst distribution law is between two solvents which are immiscible¹. It is a well established fact that partition coefficient is meant for un-dissociated species and distribution coefficient is that for total concentration of the un-dissociated and dissociated solute². At constant temperature a solute can distribute between two immiscible solvents so that the ratio of the amounts or concentrations of the solute in two solvents is constant. For all practical purposes and to avoid any confusion we have used the total concentration of the solute in this article.

Keywords: Nernst distribution law, Distribution coefficient, Partition coefficient.

INTRODUCTION

Our concern is, is there any distribution or partition law of a solute between two solvents which are completely *miscible*? If so can it be determined? We have taken benzoic acid (BA) as an example. From the scheme 1 below




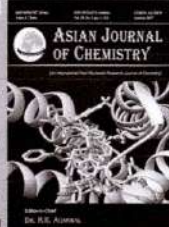
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Conventional and Microwave Assisted Synthesis of Quinoxaline Carboxamide Derivatives

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The synthesis of carboxamide derivatives containing quinoxaline scaffold is described. They were prepared from 3-hydroxy quinoxaline-2-carbohydrazide in a series of steps using conventional as well as microwave assisted methods.

Keywords: Carboxamide derivatives, Quinoxaline, Microwave assisted synthesis.

INTRODUCTION

The versatility of the quinoxalines, in addition to its chemical simplicity and accessibility, makes them the most promising sources of bioactive heterocycles. The quinoxaline skeleton is used as an intermediate in designing novel quinoxaline derivatives with potential as anticancer [1-3], antiviral [4], antimicrobial (or antifungal) [3], anticandida [5,6], anti-thrombotic [7], anxiolytic agents and other activities. Moreover, quinoxaline based drugs have shown to be photochemical DNA cleaving agents making them highly promising scaffolds for anticancer therapeutics.

Especially tetracyclic quinoxaline carboxamides showed cytotoxic activity which is helpful in treating cancers. Cisplatin is a platinum containing anticancer drug, used to treat various types of cancers, including sarcomas, some carcinomas, bladder cancer, lymphomas and cervical cancer. The synthesis of new platinum compounds using quinoxaline-2-carboxamide as a ligand would reveal the significance of quinoxaline derivatives [8]. They show cytotoxic activity, though displaying poor activity, compared to cisplatin [9]. Quinoxaline 2-carboxamides are efficient 5-HT₃ receptor antagonists, which reduce the side effects of cancer treatment like nausea and vomiting [10].

High blood pressure is the main cause of sudden cardiac arrest. Some of the quinoxaline derivatives are antagonists of bradykinin, which is a peptide responsible for the dilatation of blood vessels, thus leading to the lowering of blood pressure [11].

It is found that microwave enhances the rate of chemical reaction, thereby reducing reaction time, improving yields, purity and suppressing the formation of side products. Considering

the significance of microwave assisted synthesis, we planned to synthesize some of the quinoxaline compounds through microwave.

EXPERIMENTAL

Chemicals and solvents used were purchased either from Fluka or Merck. All the reagents were of analytical grade. Microwave assisted synthesis was carried out in BP090 Laboratory grade microwave oven. Thin-layer chromatography (TLC) was performed on E. Merck AL silica gel 60 F254 plates and visualized under UV light. IR spectra were recorded as KBr pellet with a Perkin-Elmer spectrum gx FTIR instrument and only diagnostic and/or intense peaks are reported. ¹H NMR spectra were recorded in DMSO-*d*₆ with a Varian Mercury plus 400 MHz instrument. All the chemical shifts were reported in δ (ppm) where TMS is used as an internal standard. The ¹H NMR chemical shifts and coupling constants were determined assuming first-order behaviour. Mass spectra were recorded with a PE Sciex model API 3000 instrument. All the reactions were carried out under argon atmosphere.

RESULTS AND DISCUSSION

All the quinoxaline derivatives were synthesized by both conventional and microwave-assisted synthetic methods. Synthesis of N-[3-chloro-2-(aryl)-4-oxoazetidin-1-yl]-3-hydroxyquinoxaline-2-carboxamides were carried out according to **Scheme-I**. The condensation of 3-hydroxyquinoxaline-2-carbohydrazide (**2**) and aldehyde in ethanol was carried out under reflux conditions for 1 h. The yields ranging from 55 to 65 % when synthesized by conventional method. The yield



Peristaltic Transport of a Micropolar Fluid with Nanoparticles in an Inclined Tube with Permeable Walls

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Abstract: The paper deals with the theoretical investigation of peristaltic transport of a micropolar fluid in an inclined tube with permeable walls. The closed form expressions for velocity, pressure drop, time averaged flux, frictional force and mechanical efficiency have been investigated under the assumptions of low Reynold's number and long wave length. Effects of different physical parameters like micropolar parameter, coupling number, inclination, Brownian motion parameter, thermophoresis parameter, local temperature Grashof number, local nano particle Grashof number, slip parameter on pressure rise, frictional force, mechanical efficiency, temperature profile, nano particle phenomena, heat transfer coefficient, mass transfer coefficient and streamline patterns have been studied. The computational results are presented in graphical form. The present study puts forward an important note that peristaltic transport of a micropolar fluid with nano particles can be considerably controlled by suitably adjusting the parameters of micropolar fluid like micropolar parameter, coupling number, and also the parameters of nano particle like Brownian motion parameter, thermophoresis parameter. The peristaltic transport can also be controlled by slip parameter and inclination.

Keywords: Peristalsis, Micropolar fluid, Nano particles, Brownian motion parameter, Thermophoresis parameter, Mechanical efficiency, Slip Effect.

I. INTRODUCTION

Peristalsis is a mechanism which is involved in transportation of fluids from one place to another due to contraction or expansion of a tube containing fluid. Peristalsis appears to be the major mechanism in many physiological systems and mechanical situations.

Several researchers have investigated peristalsis in both physiological and mechanical situations. [Fung & Yih, (1968), Shapiro et al., (1969), Devi & Devanathan, (1975), Meijing et al., (1993), Maruthi Prasad & Radhakrishnamacharya, (2009), Pincombe et al., (1999), Maruthi Prasad et al., (2015), Santhosh et al., (2015)].

Nicoll et al., (1946) suggested that peristalsis plays a vital role in circulation of blood. The effects of an endoscope on peristaltic flow of micropolar fluid was investigated by Hayat et al., (2008). The effect of peripheral layer on the peristaltic transport of a micropolar fluid was studied by Maruthi Prasad et al., (2009).

Nano fluid is a fluid containing nano meter sized particles known as nano particles. The nano particles in nano fluids are typically made of metals, carbides, or carbon nano tubes. Nano fluids possess special properties that make them potentially useful in several applications in heat transfer, including microelectronics, pharmaceutical processes, fuel cells and hybrid powered engines.

Choi, (1995), was the pioneer of study of nano fluid technology. Sohail Nadeem et al., (2014) studied Mathematical model for the peristaltic flow of nanofluid through eccentric tubes comprising porous medium. Peristaltic transport of a nano fluid in an inclined tube was studied by Maruthi Prasad et al., (2015). Maruthi Prasad et al., (2015) also studied the peristaltic transport of nanoparticles of micropolar fluid in an inclined tube with heat and mass transfer effect.



Search...

Role of Taft Equation in Selecting the Site of Attack in the Reactions of Aliphatic Amines and Ti(III)

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ABSTRACT:

In our earlier article [1], we had shown the application of Hammett equation of finding the site of attack. The application is based on the relative position of substituent on the aromatic ring from the center of the reaction. We had shown why we have to use σ_p value for σ_p and σ_m value for σ_m value, when we use Hammett's plot. In the present article we have demonstrated the use of the Taft equation for finding the site of attack. Here too, similar necessity arises. Often occasion arises in research, related to oxidation of aliphatic amines, where there is more than one site of attack, and we have to find the right one. One of the sites may be the N-H bond of the functional group; others being the α -C-H bond and the lone pair of electrons of the nitrogen atom. In such a circumstance, the Taft equation plays a deciding role in location of the site of attack. This equation is apparently simple but requires judicious application. It is in the fitness of this aspect, an attempt is made to make the application more understandable and student friendly. Also we feel that it should be essential part of Physical Organic Chemistry Graduate Curriculum.

KEYWORDS:

Amines; Oxidation; One Electron Oxidant and Two Electron Oxidant

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Introduction

The Hammett equation, which is based on the linear free energy relation, does not apply to the reactions of aliphatic compounds and ortho substituted benzene derivatives. This is because of interference of substituent by the reaction center. Also Hammett's σ values concern groups attached to an aromatic system engaged in resonance.

For aliphatic compounds, the Taft equation in simple form is described as $\log k = \log k_0 + \sigma^* \rho^*$ where k = rate constant for a particular member of a reaction series, k_0 = rate constant for the parent compound, ρ^* = polar reaction constant and σ^* is the polar substituent constant which is the measure of the electron attracting ability of the substituent. It is a purely inductive effect and transmits itself through the aliphatic



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Taft Equation - A Convenient Tool to Decide the Position of Attack in the Reactions of Aliphatic Amines and Thallium(iii)

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ABSTRACT

In our earlier article¹, we had shown the application of Hammett equation of finding the site of attack. The application is based on the relative position of substituent on the aromatic ring from the center of the reaction. We had shown why we have to use σ_m value for σ_p and σ_p value for σ_m value, when we use Hammett's plot. In the present article we have demonstrated the use of the Taft equation for finding the site of attack. Here too, similar necessity arises. Often occasion arises in research, related to oxidation of aliphatic amines, where there is more than one site of attack, and we have to find the right one. One of the sites may be the N-H bond of the functional group; others being the α -C-H bond and the lone pair of electrons of the nitrogen atom. In such a circumstance, the Taft equation plays a deciding role in location of the site of attack. This equation is apparently simple but requires judicious application. It is in the fitness of this aspect, an attempt is made to make the application more understandable and student friendly. Also we feel that it should be essential part of Physical Organic Chemistry Graduate Curriculum.

Keywords: Amines, Oxidation, One Electron Oxidant and Two Electron Oxidant.

INTRODUCTION

The Hammett equation, which is based on the linear free energy relation, does not apply to the reactions of aliphatic compounds and ortho substituted benzene derivatives. This is because of interference of substituent by the reaction center.

Also Hammett's σ values concern groups attached to an aromatic system engaged in resonance.

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RESEARCH ARTICLE

Estimation of Taft ρ^* of Dissociation Equilibriums of Methanium Ions RCH_4^+ the Hydrocarbon Super Acids: A Chemical Education Practice in Physical-Organic Chemistry Class-Room

17-18

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Abstract: In continuation of our efforts on the study of 'attenuation effect' in aromatic and aliphatic systems prompted us to give another attempt to estimate the Taft ρ^* value of the dissociation equilibriums ($\text{RCH}_4^+ \rightleftharpoons \text{RCH}_3 + \text{H}^+$) of the methanium ion (CH_5^+) and substituted methanium ions (RCH_4^+) based on the attenuation effect on the dissociation equilibriums of alkyl ammonium ions ($\text{RNH}_3^+ \rightleftharpoons \text{RNH}_2 + \text{H}^+$) with one, two, three, four, five and six atoms between the ionizable proton and the first carbon atom of the substituent.

Keywords: Taft reaction constant (ρ^*), attenuation effect, methanium ions, super acids.

INTRODUCTION

A super acid is defined as an acid with acidity greater than that of the acidity of 100% pure sulfuric acid, where acidity is in modern definition is defined as the chemical potential of the proton in a given medium is higher than that in pure sulfuric acid [1]. The first super acid where perchloric acid could protonate aldehydes and ketones in non-aqueous solvent like acetic acid that was known is nearly a century ago [2]. Later, many super acids were prepared in the Olah laboratory [3] at the University of Southern California by protonating hydrocarbons using a magic acid, a mixture of antimony pentafluoride (SbF_5) and fluorosulfonic acid (FSO_3H) was found by one of Olah students R. H. Schlosberg who dissolved a paraffin candle in the above mentioned magic acid. Examination of this solution by $^1\text{H-NMR}$ showed the presence of the t-butyl cation [4] that had been formed by protonation and subsequent isomerization of the original paraffin hydrocarbon. Concluding that this magic acid could protonate alkanes, it was found that methane can also be protonated at 140°C and at 1 atm.

pressure to form the CH_5^+ ion as an intermediate [3]. As the ammonium ion is derived from ammonia by protonation, in the same analogy the CH_5^+ cation is called methanium ion as it was produced by protonation of methane. According to Hammett acidity function the H_0 of CH_5^+ would be less than that of the magic acid because the magic acid was used to produce CH_5^+ by protonation of methane (CH_4) by a magic acid which must be a stronger acid than CH_4 . H_0 for some concentrated acids are [5]: Fluoroantimonic acid: -31.3, Magic acid: -19.2, Carborane superacid: -18.0, Fluorosulfuric acid: -15.1, Triflic acid: -14.1, Chlorosulfuric Acid: -12.78, Sulfuric acid: -12.0. Therefore, it is not unreasonable to propose a H_0 value for CH_5^+ as little less than the value of magic acid i.e. -19.2. One can put an upper limit of -19.0. Formulating an equation similar to Taft Polar Linear Free Energy (TPLFER) relationship [6-9]:

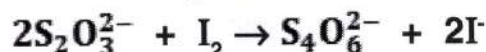
$$\frac{H_0^R}{H_0^H} = \rho^* \sigma^* \quad (1)$$

where H_0^R and H_0^H are the Hammett acidity functions of the substituted and un-substituted methanium ions. To obtain H_0^R values of substituted methanium ions one needs the value of Taft ρ^* as required in equation 1. In continuation of our efforts on the study of

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Silver Bullet For The Computation Of Equivalent Weight Of Sodium Thiosulphate In The Reaction



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ABSTRACT

When we standardize sodium thiosulphate solution either by iodometry or by a iodimetry, we base our understanding on $2S_2O_3^{2-} + I_2 \rightarrow S_4O_6^{2-} + 2I^-$. While addressing the freshmen students, especially during the pre-experimental lectures, we teach them the computation of equivalent weight of sodium thiosulfate (hypo); this necessitates the knowledge of the difference in oxidation state of sulphur atoms in the product (2.5) and the reactant side (2.0); the difference in oxidation state of sulphur atoms is 0.5. The overtly observable query which occurs to the students is, "Is the equivalent weight and molecular weight of sodium thiosulphate same or different?" If yes, then the change in the oxidation state apparently does not conform to the difference, 0.5. This article deals with this apparently simple but extremely perplexing question

Key word: Oxidation States, Molecular Weight, Sodium Thiosulphate.

INTRODUCTION

If one attempts to calculate the equivalent weight of hypo in the title reaction i.e. the reaction between sodium thiosulphate and iodine molecule, the conventional method involves the evaluation of the oxidation state of sulphur in the reactant and product sides; this in essence gives the change in the number of electron(s) in the reaction. Then

finally, we divide the molecular weight of sodium thiosulphate by the change in the number of electrons.

DISCUSSION

Let us apply the conventional method for the computation of equivalent weight of sodium thiosulphate to the title reaction. The first step

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The 'Yard Stick' to Interpret the Entropy of Activation in Chemical Kinetics: A Physical-Organic Chemistry Exercise

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Abstract No physical or physical-organic chemistry laboratory goes without a single instrument. To measure conductance we use conductometer, pH meter for measuring pH, colorimeter for absorbance, viscometer for viscosity, potentiometer for emf, polarimeter for angle of rotation, and several other instruments for different physical properties. But when it comes to the turn of thermodynamic or activation parameters, we don't have any meters. The only way to evaluate all the thermodynamic or activation parameters is the use of some empirical equations available in many physical chemistry text books. Most often it is very easy to interpret the enthalpy change and free energy change in thermodynamics and the corresponding activation parameters in chemical kinetics. When it comes to interpretation of change of entropy or change of entropy of activation, more often it frightens than enlightens a new teacher while teaching and the students while learning. The classical thermodynamic entropy change is well explained by Atkins [1] in terms of a sneeze in a busy street generates less additional disorder than the same sneeze in a quiet library (Figure 1) [2]. The two environments are analogues of high and low temperatures, respectively. In this article making use of Eyring equation a factor usually called 'universal factor' is derived and made use as a 'yard stick' to interpreting the change in entropy of activation for physical or physical-organic chemistry senior undergraduate and graduate students' class-room.



Peter Atkins

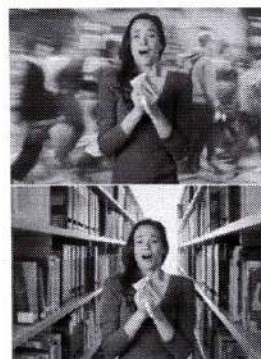


Figure 1.

Keywords: entropy, universal factor, kinetics

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1. Introduction

Thermodynamic properties like enthalpy, free energy and entropy of several thousands of organic and organometallic compounds were well documented and a very authoritative explanations and expert critical comments were offered [3,4]. As shown in the Figure 2, as an example taking any property ($X = G$ free energy, or H

enthalpy, or S entropy), thermodynamic and activation parameters could be distinguished between thermodynamics and kinetics. The nature of any property accompanied in chemical reactions in terms of energy considerations is nothing but an amalgamation of activation barrier (ΔX^\ddagger) and thermodynamic driving force (ΔX^0). Marcus equation [5,6,7] is a successful treatise for treating kinetic data of electron transfer reactions to separate activation (ΔX^\ddagger) and thermodynamic quantities (ΔX^0). The change in thermodynamic quantities could be interpreted in terms of

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Cooxidation not to be Confused with Catalysis: A Chemical Education Article to Physical-organic Chemists

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ABSTRACT

Two substrates (A) and (B) are oxidized separately by an oxidant (Oxi) with the rate constants k_1 and k_2 and they are oxidized taken together (A + B) under similar conditions with a rate constant k_3 , if the value of $k_3 = (k_1 + k_2)$, then it is said to be an example of two reactions "going parallel". If the value of $k_3 \gg \gg (k_1 + k_2)$, then the redox process is termed as "co-oxidation" (Hasan and Rocek 1972, *JACS*). In this process in the mixture the two substrates are oxidized synchronously by a direct three electron transfer route if the oxidant happens to be Cr(VI) and by a direct four electron transfer route if the oxidant happens to be Mn(VII) (Jagannadham *et al.*, 1986, *Oxidation Communications*). It was realized that the essential condition of the synchronous oxidation of two substrates A and B is that one substrate must have two functional groups and the other must have one functional group or vice-versa. The compound with two functional groups must be a good chelating agent with the metal ion oxidant. A substrate (A) is oxidized by an oxidant (Oxi) with a rate constant k_4 and is oxidized in presence of a catalyst (Cat) with a rate constant k_5 , if $k_5 > k_4$ the redox process is termed as "catalyzed process". It is to be noted that in the catalytic process the catalyst (Cat) is not oxidized and its concentration does not change during the reaction. It only increases the rate of oxidation with lower activation energies. If $k_5 = k_4$ it is to be understood that there is "no catalysis". If $k_5 < k_4$ it is to be understood that the catalyst is called a negative catalyst or "inhibitor" and the reaction goes with higher activation energy. In this paper a lucid description is given for the two processes "co-oxidation" and "catalysis" with putative examples.

Keyword: Cooxidation, Catalysis, Chemical education.

INTRODUCTION

Hasan and Rocek were the first to report a direct synchronous three electron oxidation

process where in isopropyl alcohol and oxalic acids were oxidized¹. Later several publications appeared from his laboratory²⁻¹⁸. Sequel to Rocek's discovery¹ of one step three electron oxidations several



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A Class Of Univalent Analytic Functions With Fixed Second And Third Coefficients

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Abstract: In this paper we defined a new class of univalent and analytic functions with fixed second and third Taylor coefficients. Coefficient condition, starlikeness and convexity, extreme points, growth and distortion properties for this class are investigated.

IndexTerms – Univalent function

1. INTRODUCTION

Let S be the class of functions of the form $f(z) = z + \sum_{n=2}^{\infty} a_n z^n$ that are analytic and univalent in the unit disk $U = \{z \in \mathbb{C} : |z| < 1\}$. Let T be the subclass of functions of S which are of the form

$$f(z) = z - \sum_{n=2}^{\infty} a_n z^n, \quad a_n \geq 0, \quad n = 2, 3, \dots \quad (1)$$

in U and C be the subclass of functions of T which are convex in U . We have $f \in C$ if and only if $zf' \in T$.

Now we introduce a subclass $T(b, c, B_n) \subseteq T$ by fixing a_2 and a_3 , for $0 \leq b \leq \frac{1}{4}$, $0 \leq c \leq \frac{1}{12}$ and $B_n \geq n(n+1)$ for $n \geq 2$,

$$T(b, c, B_n) = \{f(z) \in T : f(z) = z - bz^2 - cz^3 - \sum_{n=4}^{\infty} a_n z^n, \sum_{n=3}^{\infty} B_n a_{n+1} \leq 2b - cB_2\}.$$

Let $C(b, c, B_n)$ be a subclass of functions of $T(b, c, B_n)$ which is convex in U .

This paper consists of two sections. In section 1, we find the coefficient conditions for starlikeness and convexity of the class $T(b, c, B_n)$. In section 2 we find extreme points, growth and distortion properties for the class $T(b, c, B_n)$.

SECTION 1

We need the following definitions from [1].

Definition1: [1] A function $f(z) \in S$ is said to be starlike of order α ($0 \leq \alpha < 1$) in U , if it satisfies the inequality $Re \left[\frac{zf'(z)}{f(z)} \right] > \alpha$ for $z \in U$. The class of starlike functions of order α is denoted by $S^*(\alpha)$.

Definition 2: [1] A function $f(z) \in S$ is said to be convex of order α ($0 \leq \alpha < 1$) in U , if it satisfies the inequality $Re \left[1 + \frac{zf''(z)}{f'(z)} \right] > \alpha$ for $z \in U$. The class of convex functions of order α is denoted by $C^*(\alpha)$.

We have $f \in C^*(\alpha)$ if and only if $zf' \in S^*(\alpha)$.

We start with a coefficient characterization for the functions of T to be in the class $T(b, c, B_n)$.

Theorem-1

The function $f(z) = z - bz^2 - cz^3 - \sum_{n=4}^{\infty} a_n z^n$, $z \in U$ is in the class $T(b, c, B_n)$ if and only if $\sum_{n=3}^{\infty} n(n+1) a_{n+1} \leq 2b - 6c$. The result is sharp.

Proof: If $f(z) = z - bz^2 - cz^3 - \sum_{n=4}^{\infty} a_n z^n$, $z \in U$ belongs to the class $T(b, c, B_n)$,

Then by the definition, we have $\sum_{n=3}^{\infty} B_n a_{n+1} \leq 2b - cB_2$

This gives $\sum_{n=3}^{\infty} n(n+1) a_{n+1} \leq 2b - cB_2$
 or $\sum_{n=3}^{\infty} n(n+1) a_{n+1} \leq 2b - c.2.3$

this shows $\sum_{n=3}^{\infty} n(n+1) a_{n+1} \leq 2b - 6c$

(2)

Now, suppose that $\sum_{n=3}^{\infty} n(n+1) a_{n+1} \leq 2b - 6c$

Then $\sum_{n=2}^{\infty} n a_n \leq 1$.

Therefore $f(z) \in T$ by [3].

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Crystallization and Dielectric Properties of PbTiO₃ based Glass Ceramics

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Abstract. Glass samples with composition (50 - X) PbO - (25 + X) TiO₂ - 25 B₂O₃ (where X =0, 5, 10 and 12.5 mol %) were prepared using conventional quenching technique. These glass samples were converted to glass ceramics by following two stage heat treatment schedule. The XRD results in the glass ceramics revealed the formation of tetragonal lead titanate as a major crystalline phase. The SEM results show rounded crystallite of lead titanate. The ferroelectric nature of all the glass ceramic samples is confirmed by P - E hysteresis measurements. The extended heat treatment of glass ceramic samples at 593K for 10 h exhibited saturated hysteresis loops with higher values of remnant polarization.

1. INTRODUCTION

Glass ceramics are polycrystalline solids prepared by controlled crystallization of glasses. Crystallization is accomplished by subjecting suitable glasses to a carefully regulated heat treatment schedule which results in nucleation and growth of crystal phases within the glasses. This method of making a ceramic material represents a radical departure from conventional ceramic preparation processes and it offers a number of important advantages. Since molten glass can be obtained in a homogeneous condition, uniformity of chemical composition can easily be achieved for glass ceramics. The homogeneity of the parent glass together with the controlled manner in which the crystals are developed results in glass ceramic (gc) materials having a very fine grained uniform structure free from porosity. The other unique characteristics, such as no ageing or depoling problems and good stability at high temperature, high-pressure and in harsh environments, make glass ceramics attractive for use in variety of applications. Realizing the advantages of the glass ceramic process, several attempts have been made to produce glass ceramics having high permittivity, low dielectric loss, high electrical resistance and high dielectric breakdown strength by precipitating various ferroelectric phases were crystallized. Prominently these phases are BaTiO₃, LiTaO₃, NaNbO₃, Pb₅GeO₁₁, LiNbO₃, SrTiO₃, KNbO₃, KNN, PZT and PbTiO₃. The main emphasis in these investigations was on the study of dielectric and electro optic properties as a function of composition, heat treatment and grain size.

However, the systematic study of crystallization and dielectric properties of PbTiO₃ based glass ceramics has not been reported so far. Hence, in the present work the content of TiO₂ was increased by decreasing PbO content and the glass former (B₂O₃) content was kept fixed with an idea to restrict the volume fraction of residual glass phase and to improve crystallization, dielectric and ferroelectric properties of PbTiO₃ based glass ceramics.

2. EXPERIMENTAL

Glasses with composition (50-X) PbO - (25+X) TiO₂ - 25 B₂O₃ (where X = 0, 5, 10 and 15 mol %) were prepared from the high purity ingredients heated in an alumina crucibles at 1373 K-1523 K for 1h. The melt was homogenized by stirring it before quenching into aluminium mould at room temperature. The resultant glass

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Structural, Magnetic and Magnetoreactance Studies In $\text{NiFe}_{2-x}\text{R}_x\text{O}_4$ ($x = 0, 0.05$; $\text{R} = \text{Y, Yb and Lu}$)

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Abstract. Structural, magnetic and magnetoreactance (mr) properties of $\text{NiFe}_{2-x}\text{R}_x\text{O}_4$ ($x = 0, 0.05$; $\text{R} = \text{Y, Yb and Lu}$) compounds were investigated and the results are discussed and presented in this paper. Rietveld refined X-ray diffraction (XRD) patterns and Raman spectroscopy revealed the cubic inverse spinel phase for all the compounds investigated. The former also identified small amounts of RFeO_3 as the secondary phase. Lattice constant values were increased upon partial substitution of Fe^{3+} by R^{3+} ($\text{R} = \text{Y, Yb and Lu}$). Magnetization measurements revealed that the magnetic moment of R^{3+} ($\text{R} = \text{Y, Yb and Lu}$) substituted compounds decreased compared with NiFe_2O_4 . mr was measured at 3 kHz and 3 MHz both longitudinal (LT) and transverse (TR) configuration. A maximum mr of 54 % was observed in Y^{3+} substituted NiFe_2O_4 in TR mode.

I. INTRODUCTION

Giant Magnetoimpedance (GMI) effect is the change in impedance of a ferromagnetic material with the application of a dc magnetic field and is defined as, $MI = \left[\frac{Z(H) - Z(H_{max})}{Z(H_{max})} \right] \times 100$. The GMI effect is observed in wires, ribbons, tubes and thin films [1]. Small and negative magnetostriction has been reported to lead to large MI values [1-3]. Recently MI has been reported in Mn-Zn ferrite at different frequencies and has a maximum value of 61.2 % at 4 MHz [4]. Many researchers have reported MI in perovskites [5]. Since ferrites are insulators, change in the reactive part of the impedance rather than the skin effect gives rise to the MI in ferrites which is nothing but magnetoreactance (mr), $mr = \left[\frac{X(H) - X(H_{max})}{X(H_{max})} \right] \times 100$.

In the present investigations, R^{3+} ($\text{R} = \text{Y, Yb and Lu}$) was chosen to partially substitute the lighter and smaller Fe^{3+} (ionic radius of $\text{Fe}^{3+} = 0.63 \text{ \AA}$ and that of $\text{Y}^{3+} = 0.89 \text{ \AA}$, $\text{Yb}^{3+} = 0.86 \text{ \AA}$ and $\text{Lu}^{3+} = 0.85 \text{ \AA}$). In this paper, structural, magnetic, and magnetoreactance properties of $\text{NiFe}_{2-x}\text{R}_x\text{O}_4$ ($x = 0, 0.05$; $\text{R} = \text{Y, Yb and Lu}$) compounds are reported.

II. EXPERIMENTAL DETAILS

The starting materials NiO (99.96 %), Fe_2O_3 , Y_2O_3 , Lu_2O_3 and Yb_2O_3 (99.99 %) are used to prepare polycrystalline $\text{NiFe}_{2-x}\text{R}_x\text{O}_4$ ($x = 0, 0.05$; $\text{R} = \text{Y, Yb and Lu}$) compounds, by solid state reaction method. The powders of the starting materials were taken in stoichiometric ratios and ground in an agate mortar and pestle for 3 h and were heat treated in air at 1200 °C for 12 h. The phase formation of the samples was confirmed by powder X-ray diffraction (XRD) technique using a PANalytical (X'pert PRO) X-ray diffractometer employing $\text{Cu K}\alpha$ radiation. Rietveld refinement was carried out using the GSAS program with EXPUGI interface. Raman active vibrational


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Dielectric and Impedance Properties of $\text{NiFe}_{1.95}\text{R}_{0.05}\text{O}_4$ (R = Y, Yb and Lu)

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Abstract. The dielectric and impedance spectroscopic properties of $\text{NiFe}_{1.95}\text{R}_{0.05}\text{O}_4$ (R = Y, Yb and Lu) were investigated. The materials were prepared by solid state reaction and crystallized in the cubic inverse spinel phase with a very small amount additional phase of RFeO_3 (R = Y, Yb and Lu) as secondary phase. The scanning electron micrograph images clearly show grains ($\sim 2\mu\text{m}$) which are separated by thin grain boundaries. The presence of all elements were confirmed by the energy dispersive X-ray elemental mapping. The frequency variation of ϵ' shows the dispersion, following the Koop's phenomenological theory, which considers the dielectric structure as an inhomogeneous medium of two-layers of the Maxwell-Wagner type. Impedance spectroscopic analysis indicates the different relaxation mechanisms, which corresponds to bulk grain and grain-boundaries. Their contributions to the electrical conductivity and capacitance of these materials were discussed in detailed.

I. INTRODUCTION

Ferrite materials have wide range of applications in the fields of electronics, optoelectronics, magnetics and magnetoelectronics due to their high saturation magnetization, large permeability, low eddy current losses and high electrical resistivity. Nickel ferrite crystallizes in inverse spinel structure and is a centro-symmetric magnetic material. Substitution of rare earth ion into the spinel structure has been reported to induce structural distortion and strains in the material [1]. Y, Yb and Lu doped NiFe_2O_4 have been prepared and their structural, dielectric and impedance spectroscopic properties were investigated. The objective of the this work is to study the bulk and interface phenomena over a wide range of frequencies in order to obtain information about the relaxation times present in these materials. The results obtained on the Y, Yb and Lu substituted Ni ferrites are presented and discussed in this paper.

II. EXPERIMENTAL DETAILS

The materials were prepared using the solid state reaction method. Powders of starting materials were NiO (99.96% pure), Fe_2O_3 , Y_2O_3 , Yb_2O_3 and Lu_2O_3 (all 99.99% pure) were ground in a agate mortar and pestle for 3 h and the mixtures were heat treated in air at 1200 °C for 12 h. Surface morphology was studied using scanning electron microscope (Model: Quanta 200) attached with energy dispersive X-ray (EDAX) equipment (for elemental analysis) along with Back Scattered Electron (BSE) imaging. The powders made into pellets, then sintered at 1330°C in air for 24 h, ensuring 95% densification and used for electrical measurements. Dielectric and impedance measurements were carried out employing 'Novocontrol Alpha broad dielectric analyzer'. Highly conducting silver paste was applied on both sides of the pellet and dried before the impedance and dielectric measurements.

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Behavior of Organic Compounds with Different Functional Groups based on Surface Tension, Ramsey-Shields-EÖTVÖS Constants (k), Order of Association (x) and Trouton's Rule

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Abstract

Hydrocarbons and organic compounds having different functional groups with hetero atoms have shown a discriminative behavior toward surface tension, EÖTVÖS constants (k), order of association (x) and Trouton's rule. This was explained in terms of associative and non-associative behavior of these compounds.



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Taft equation, Eötvös Constant, Ramsay-Shields equation, Trouton's rule, Order of Association, Hydrogen Bond Donor-Acceptor Sites (H_{ad}).

Introduction

Study on associative properties of aliphatic alcohols¹, aliphatic carboxylic acids², phenols³, and aliphatic amines⁴ based on their surface tension data, EÖTVÖS constants (k), order of association (x) and Trouton's rule is a major breakthrough from our laboratory hither to not reported earlier in literature. In the present study, various compounds like hydrocarbons, and compounds having different functional groups with different hetero atoms were

taken to see the effect of these groups on surface tension, EÖTVÖS constants (k), order of association (x) and Trouton's rule.

Experimental and Data Source

All the surface tension data used in this article is from reference². The detailed procedure for calculation of various parameters mentioned in table 1 are described in references 1-4. Thermo chemical data is from reference⁶. Taft σ^* values are from reference⁷.

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Common Random Fixed Point Theorems in Probabilistic Metric Spaces

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Abstract:

In this paper we prove common fixed point theorems in probabilistic metric space by using the concept of β - compatible mapping and weakly compatible mapping in randomized fuzzy metric space.

Key words: Common fixed point, fuzzy metric space, compatible maps, and weakly compatible continuous t-norm, randomized fuzzy metric space.

Introduction

Probabilistic functional analysis has emerged as one of the important mathematical disciplines in view of its role in analyzing Probabilistic models in the applied sciences. The study of fixed point of random operator forms a central topic in this area. Random fixed point theorem for contraction mappings in Polish spaces and random Fixed point theorems are of fundamental importance in probabilistic functional analysis. There study was initiated by the Prague school of Probabilistics, in 1950, with their work of Spacek [15] and Hans [5,6]. For example survey are refer to Bharucha-Reid[4]. Itoh [8] proved several random fixed point theorems and gave their applications to Random differential equations in Banach spaces. Random coincidence point theorems and random fixed point theorems are stochastic generalization of classical coincidence point theorems and classical fixed point theorems. Sehgal and Singh [14], Papageorgiou [12], Rhoades, Sessa, Khan [13] and Lin [11] have proved differential Stochastic version of well known Schauder's fixed point theorem. Recently, Beg and Shahzad [3] studied the structure of common fixed point and random coincidence Points of a pair of compatible random operators.

In this paper we prove common fixed point theorems in probabilistic metric space by using the concept of β - compatible mapping. First we give some basic and important definitions related to this paper.

Definition 1.1.1. Let X be any set. A fuzzy set in X is a function with domain X and values in $[0,1]$.

Definition 1.1.2. A binary operation $*$: $[0,1] \times [0,1] \rightarrow [0,1]$ is continuous t-norm if $*$ is satisfying the following conditions:

1.1.2 (a) $*$ is commutative and associative,

1.1.2 (b) $*$ is continuous,

1.1.2 (c) $a * 1 = a$ for all $a \in [0,1]$

1.1.2 (d) $a * b \leq c * d$ whenever $a \leq c$ and $b \leq d$,

for all $a, b, c, d \in [0,1]$

Examples of t-norm are $a * b = \min\{a, b\}$ and $a * b = ab$.

Definition 1.1.3. A triplet $(X, M, *)$ is a fuzzy metric space whenever X is an arbitrary set, $*$ is continuous t-norm and M is fuzzy set on $X \times X \times [0, \infty^+)$ satisfying, for every $x, y, z \in X$ and $s, t > 0$, the following condition:

1.1.3 (a) $M(x, y, t) > 0$

1.1.3 (b) $M(x, y, 0) = 0$

1.1.3 (c) $M(x, y, t) = 1$ iff $x = y$

1.1.3 (d) $M(x, y, t) = M(y, x, t)$

1.1.3 (e) $M(x, y, t) * M(y, z, s) \leq M(x, z, t + s)$

1.1.3 (f)

$M(x, y, \cdot) : (0, \infty^+) \rightarrow [0,1]$ is continuous.

We note that, $M(x, y, t)$ can be realized as the measure of nearness between x and y with respect to t . It is known that $M(x, y, \cdot)$ is non decreasing for all $x, y \in X$. Let $(X, M, *)$ be a fuzzy metric space for $t > 0$, the open ball

$B(x, r, t) = \{y \in X: M(x, y, t) > 1 - r\}$.

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Non-Linear Taft Relationship applied to surface tensions of aliphatic acids: Inter-molecular hydrogen bonding versus intra-molecular hydrogen bonding



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ABSTRACT

Hammett and Taft equations in their most basic forms are linear free energy relationships between standard free energies of two reaction series. Therefore any chemical or physical property inherently associated with any of the thermodynamic property like enthalpy H , free energy G , internal energy E or entropy S are subjected to substituent effects. One such physical property is the surface tension. Surface tension is a kind of surface free energy (G) of any liquid and is also supposed to be effected by the structure of liquids. Hence the present study has been selected to see the effect of substituents on surface tension of some aliphatic acids. The quick glance at the present study ended up with a non-linearity of Taft equation to the surface tension data of aliphatic acids. Hence Non-Linear Taft Relationship (NLTR) was applied to surface tensions (γ) of some aliphatic acids. The non-linearity of $\log \gamma$ versus Taft σ^* correlation was explained in terms of inter-molecular hydrogen bonding versus intra-molecular hydrogen bonding and in terms of steric effects.

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1. Introduction

Though the Hammett [1] and Taft [2] equations are nearly more than seventy five years old, they enjoyed outstanding application for predicting the organic reaction mechanisms among physical organic chemists. Ever since the Hammett [1] and Taft [2] equations were developed, there were several hundreds of reactions in literature, for which the Hammett and Taft reaction constants (ρ and ρ^*) were reported. Though the application of Linear Free Energy Relationships to chemical reactions [3–24] and physical properties [25–30] is quite promising in its nature, application of non-linear Taft equation to the reactions of benzyl bromide with N -substituted benzyl amines is first of its kind in literature and of recent origin from our laboratory [31]. In the present article we have tried to apply non-linear Taft equation to physical properties like surface tensions of some aliphatic acids. To our knowledge the present study is first of its kind in literature. The non-linearity of Taft correlation was explained in terms of inter-molecular hydrogen bonding versus intra-molecular hydrogen bonding of the aliphatic acids and in terms of steric effects.

2. Experimental data source

Data on surface tensions of aliphatic acids is from reference [32] and references cited therein. The Taft σ^* values of alkyl substituted acids are from references [33,34] and of halogen substituted acids are from reference [35]. Thermo chemical data is from reference [36]. All the linear correlations were done using the KaleidaGraph software, Reading, PA, USA.

3. Discussion

A molecule in the bulk of a liquid is completely surrounded by other molecules; therefore it is attracted equally in all directions. While a molecule on the surface has an attraction inward because the number of molecules per unit volume is greater in liquid than in vapor because vapor is a dilute system. Due to this inward pull, the surface of the liquid always tends to contract to have minimum possible area. In order to extend the area of the surface, it is necessary to do work, to bring molecules from the bulk of the liquid into the surface, against the inward attractive force. The work required to increase the surface area by 1 sq. cm is called surface free energy [37].

As a result of this tendency to contract, a surface behaves as if it were in a state of tension. If a cut were made along any line in the surface, a force would have to be applied to hold the separate portions of the surface together. This force is proportional to the length of the cut and its value per unit length is called surface tension or interfacial tension (γ).

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Thermal Effects of Two Immiscible Fluids in a Circular Tube with Nano Particles

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The paper deals with a theoretical investigation of thermal effects of two immiscible fluids in a circular tube with nano particles. The closed form expressions for pressure drop, time averaged flux, velocity in the peripheral region as well as in the core regions, frictional force and mechanical efficiency have been investigated. Effects of different physical parameters like micropolar parameter, coupling number, viscosity ratio, mean radius of the central layer, Brownian motion parameter, thermophoresis parameter, local temperature Grashof number as well as local nano particle Grashof number on pressure drop characteristics, frictional force, mechanical efficiency, heat transfer coefficient, mass transfer coefficient, velocity profiles in the core region and streamline patterns of the fluid are studied. The computational results are presented in graphical form.

KEYWORDS: Peristalsis, Nano Particles, Homotopy Perturbation Method, Peripheral Layer, Heat Transfer Coefficient, Mass Transfer Coefficient.

1. INTRODUCTION

The peristaltic transport has prime importance for transporting of fluid from lower pressure region to higher pressure region. It is because of the contraction of muscles travelling in waves along a tube like structure. It is due to the presence of neuron-muscular properties of tubular smooth muscles in physiological processes. This kind of activity is generally prevalent in the gastrointestinal, urinary, reproductive tracts, small blood vessels, intestines, lymphatic vessels and many other glandular ducts in a living body. The industrial applications of this mechanism is observed and used in sanitary and corrosive fluid transport, in rollers, finger pumps, hose pumps and blood pump in heart lung machine. This phenomenon of transporting toxic liquid is used in nuclear industry.

In view of its importance, many researchers investigated peristaltic transport of Newtonian and non-Newtonian fluids under various conditions. Peristaltic transport has been studied by Fung and Yih.¹ Shapiro et al.² studied peristaltic pumping with long wavelengths at low Reynolds number. Prasad and Radhakrishnamacharya³ investigated effect of peripheral layer on peristaltic transport of a couple-stress

fluid. Hayat et al.⁴ studied peristaltic transport of Carreau-Yasuda fluid in a curved Channel with slip effects. Flow of a Jeffery fluid through a porous medium in narrow tubes was studied by Santhosh et al.⁵

Micropolar fluid is a non-Newtonian fluid that belongs to a class of fluids with non-symmetrical stress tensor and is referred to as polar fluid. It represents a fluid consisting of randomly scattered particles suspended in a viscous medium. It is realized that micropolar fluid accounts for the rotation of fluid particles by means of an independent kinematic vector called microrotation vector (Eringen,⁶). As a result micropolar fluid model is more appropriate to investigate the behavior of lubricants, colloidal suspensions, polymeric fluids, liquid crystals and physiological fluids. Peristaltic transport of a micropolar fluid was studied by Devi and Devanathan.⁷ Prasad et al.⁸ studied peristaltic pumping of a micropolar fluid in an inclined tube. Slip effect on peristaltic transport of micropolar fluid was investigated by Chaube et al.⁹ Wang et al.¹⁰ studied peristaltic motion of a magneto hydrodynamic micropolar fluid in a tube. Effect of Slip Velocity on Peristaltic transport of a magneto-micropolar fluid through a porous non-uniform channel was investigated by Shit and Roy.¹¹ MHD peristaltic transport of a micropolar fluid in an asymmetric channel with porous medium was investigated by Satyanarayana et al.¹²

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Experimental and Quantum Mechanical Study of Nucleophilic Substitution Reactions of *meta*- and *para*-Substituted Benzyl Bromides with Benzylamine in Methanol: Synergy Between Experiment and Theory

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This work involves the experimental and theoretical study of the nucleophilic substitution of *meta*- and *para*-substituted benzyl bromides with benzylamine. Conductometric rate experiments confirm the applicability of the Hammett linear free-energy relationship to this system. To gain a deep understanding of the physical chemistry at play, a quantum mechanical study of the reaction is also conducted. The quantum mechanical calculations not only reproduce the experimental free energy of activation, but also provide greater insights at the molecular and atomic level. Isolation of the calculated transition state structure and application of the Hammett equation to its electronic, structural, and energetic properties are studied.

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Introduction

Since its genesis, a massive body of experimental work has emerged related to Hammett's equation^[1,2] applied to reaction mechanisms in chemistry.^[3–12] The Hammett equation describes the effect of substituents (at *meta* and *para* positions) linked to an aromatic series on the reaction rate and equilibrium constants relative to the substituents attached at *meta* and *para* positions of ionization of benzoic acids in water at 25°C. Furthermore, the Hammett constants were applied to certain fundamental properties, such as steric effects, nucleophilicity, and solvent effects, and structure–reactivity correlations were developed.^[13–15] In the present work, we apply the Hammett relation not only to the reaction under study in the conventional sense, i.e. plot of experimentally and theoretically obtained reaction rate constants versus the Hammett σ values, but also to various theoretically obtained properties of the calculated transition state structure.

In an earlier study,^[16] we conducted an experimental study on nucleophilic substitution reactions of *meta*- and *para*-substituted benzylamines with benzyl bromide in methanol; the study showed that the reaction rate of the S_N2-type mechanism conformed to the Hammett relation. The nucleophilic substitution of *meta*- and *para*-substituted benzyl bromides with benzylamine should also proceed via a similar S_N2 mechanism. Thus, an experimental study on the nucleophilic substitution of *meta*- and *para*-substituted benzyl bromides with benzylamine was performed to assess the applicability of the Hammett linear free-energy relationship (LFER).

With the advent of the density functional theory (DFT) and advanced software such as *Gaussian*,^[17] it is possible to isolate and visually observe the calculated transition state structure of the above S_N2 reaction. Thus, we consider a theoretical study on the reaction in question to gain deep insights into various properties of the calculated transition state structure; such insights cannot be obtained from studies that only employ experimental techniques. Synergistic studies between experiment and theory have gained immense prominence,^[18–22] and the present study aptly fits into this genre.

DFT has been used to study many S_N2 reactions.^[23–33] For instance, Singh and Goel conducted a mechanistic study on the Menshutkin reaction between 1,4-diazabicyclo[2.2.2]octane and benzyfluoride or fluorodiphenylmethane using DFT calculations at the B3LYP/6–31G(d,p) level of theory.^[34] One of their important conclusions was that the reaction between 1,4-diazabicyclo[2.2.2]octane and benzyl fluoride proceeds through a polar S_N2 transition state mechanism, in agreement with earlier literature, whereas the reaction with fluorodiphenylmethane proceeds through a five-membered ring transition state. As this is contrary to the literature, molecular modelling was used by Singh and Goel to understand the Menshutkin reaction mechanism in greater depth.

Pineda et al.^[35] studied the hydrolysis of a chlorambucil analogue by DFT. Three S_N1 and one S_N2 reaction mechanisms were proposed. Finally, through theoretical studies, the authors ruled out the S_N2 mechanism and concluded that the most favourable mechanism of hydrolysis occurred through the

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Effects of Variable Viscosity and Thermal Conductivity on MHD Boundary Layer Flow of Nanofluid with Thermal Radiation

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In this paper, the effects of variable viscosity and thermal conductivity on magnetohydrodynamic boundary layer flow of nanofluid over a stretching sheet in porous medium are investigated. By taking suitable similarity variables, the governing boundary layer equations are transformed into a boundary value problem of coupled nonlinear ordinary differential equations and solved numerically using the weighted residual finite element method. The numerical results for the velocity, temperature and nanoparticle volume concentration together with the skin friction coefficient, Nusselt number and Sherwood number are presented. The effects of various parameters such as Hartmann number H_a , Darcy number Da , thermal Grashof number Gr_1 , concentration Grashof number Gr_2 , radiation parameter R_d , Prandtl number Pr , viscosity parameter λ , thermal conductivity parameter n , Lewis number Le , Brownian motion parameter Nb and thermophoresis parameter Nt on the flow, heat and nanoparticle volume concentration are illustrated in tabular and graphical forms. A comparison with previously published results on special case of the problem shows excellent agreement.

KEYWORDS:

1. INTRODUCTION

Natural convection flow is frequently encountered in our environment and engineering devices. Free convection flow is caused by the temperature difference and also the flow is affected by the difference in concentration of material constitution. Quite often one can observe that both heat and mass transfer occur simultaneously in free convection. This study of flow phenomena has a wide range of applications in the field of science and technology. Free convective flow past a vertical plate has been studied extensively by Ostrach¹ and many others. The free convective heat transfer on vertical semi-infinite plate was investigated by Berezovsky et al.² Martynenko et al.³ investigated the laminar free convection from a vertical plate. Gebhart and Pera⁴ observed the steady state natural convection on a vertical plate with variable surface temperature and variable mass diffusion. Using similarity variables they solved the boundary layer equations. Callahan and Marner⁵ solved the problem of transient free convection with mass transfer on an isothermal vertical plate by using an explicit finite difference scheme. Soundalgekar

and Ganesan⁶ have solved the problem for transient free convection with mass transfer on a vertical plate with constant heat flux by using an implicit finite difference scheme.

The study of magnetohydrodynamics plays an important role in agriculture, engineering and petroleum industries. The problem of free convection under the influence of a magnetic field has attracted the interest of many researchers in view of its applications in geophysics and astrophysics. The problem under consideration has important applications in the study of geophysical formulations; in the explorations and thermal recovery of oil; and in the underground nuclear waste storage sites. Magnetohydrodynamics has its own practical applications too. For instance, it may be used to deal with problems such as cooling of nuclear reactors by liquid sodium and induction flow meter, which depends on the potential difference in the fluid in the direction perpendicular to the motion and to the magnetic field. Soundalgekar et al.⁷ analysed the problem of free convection effects on Stokes problem for a vertical plate under the action of transversely applied magnetic field. Sacheti et al.⁸ obtained an exact solution for unsteady magnetohydrodynamics free convection flow on an impulsively started vertical plate with constant heat flux. Shanker and Kishan⁹ discussed the effect of mass transfer on the MHD flow past an impulsively

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Peristaltic Transport of a Couple-Stress Fluid with Nanoparticles Having Permeable Walls

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The paper deals with a theoretical investigation of the peristaltic transport of a couple-stress fluid with heat and mass transfer effects. The velocity, pressure drop, time averaged flux, frictional force, mechanical efficiency, temperature profile, nano particle phenomena, heat transfer coefficient and mass transfer coefficient of the fluid are investigated, when the Reynolds number is small and wave length is large by using appropriate analytical methods. Effects of different physical parameters like couple-stress fluid parameters, Brownian motion parameter, thermophoresis parameter, local temperature Grashof number as well as local nano particle Grashof number on pressure drop characteristics, frictional force, heat transfer coefficient, mass transfer coefficient and stream line patterns of the fluid are studied. The expressions for pressure drop, temperature profile, nano particle phenomenon, heat transfer coefficient and mass transfer coefficients are sketched through graphs. The streamlines are drawn to discuss trapping phenomena for some physical quantities.

KEYWORDS: Peristalsis, Couple-Stress Fluid, Brownian Motion Parameter, Thermophoresis Parameter, Heat Transfer Coefficient, Mass Transfer Coefficient.

1. INTRODUCTION

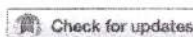
Peristalsis is an important mechanism for fluid transport which can be generated by the propagation of waves along the walls of a flexible tube containing liquid. Physiologically, it is known as an automatic and vital process that drives the urine from kidney to bladder through the ureters, food through the digestive tract, bile from the gall bladder into the duodenum, vasomotion in small blood vessels and so on. The peristaltic transport is also exploited in industrial pumping as it provides efficient means for sanitary fluid transport in nuclear industries and in roller pumps. Several investigations have analyzed the peristaltic motion of both Newtonian and non-Newtonian fluids in physiological as well as mechanical systems.¹⁻⁶

Couple-stress fluid is a special case of non-Newtonian fluid which was developed by Stokes.⁷ The important feature of these fluids is that the stress tensor is not symmetric and their accurate flow behaviour cannot be predicted by the classical Newtonian theory. The main effect

of couple stresses will be introducing a size dependent effect that is not present in the classical viscous theories. Shehawey and Mekheimer,⁸ studied Couple-stresses in peristaltic transport of fluids. Effect of peripheral layer on peristaltic transport of a couple-stress fluid was investigated by Prasad and Radhakrishnamacharya.⁹ Alemayehu and Radhakrishnamacharya,⁵ discussed dispersion of a solute in peristaltic motion of a couple-stress fluid through a porous medium with slip condition. Hydromagnetic effect on inclined peristaltic flow of a couple stress fluid was investigated by Shit and Roy.¹⁰

Nanofluid is a fluid containing nano-sized particles called nanoparticles. These fluids are engineered colloidal suspensions of nanoparticles in a base fluid. The nanoparticles used in nanofluids are typically made of metals, oxides, or carbon nanotubes. Nanofluids have new properties that make them potentially useful in many applications in heat transfer, including microelectronics, fuel cells, pharmaceutical processes and hybrid powered engines.¹¹ They exhibit enhanced thermal conductivity and the convective heat transfer coefficient compared to the base fluid. Many researchers have done their research in nanofluid technology. A benchmark study on the thermal conductivity of nanofluids was done by Buongiorno et al.¹²

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Onsite magnetic moment through cation distribution and magnetocrystalline anisotropy studies in NiFe_{2-x}R_xO₄ (R = Y and Lu; x = 0, 0.05, and 0.075)S. Jendar Kodam¹, Kamala Bharathi K², Raghavendra Reddy V³, Sudhindra Rayaprol⁴, Vasudeva Siruguri⁴

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In group ions · Magnetic moments · Nickel · X-ray diffraction · X-ray photoelectron spectroscopy

ABSTRACT

Onsite magnetic moments through cation distribution and magnetocrystalline anisotropy studies of NiFe_{2-x}R_xO₄ (R = Y and Lu; x = 0, 0.05, and 0.075) compounds were investigated, and the results are discussed and presented in this paper. All the compounds were prepared by solid state reaction, and the compounds formed in the cubic inverse spinel phase with the space group Fd $\bar{3}$ m. The cation distribution, bond lengths, unit cell parameter, etc. were estimated through the Rietveld refinement of XRD patterns. Increment in the lattice constant was observed upon partial substitution of Fe³⁺ by Y³⁺/Lu³⁺. The presence of all elements and their oxidation states were confirmed from X-ray photoelectron spectroscopy studies. Analyses of Mössbauer spectra revealed that the hyperfine fields and the magnetic moments at the B-site (and hence net moment) decreased with increasing Y³⁺/Lu³⁺ occupancy and that the compounds exhibited a Néel-type, collinear ferrimagnetic structure. Magnetization measurements revealed that the magnetic moment decreased with Y³⁺/Lu³⁺ substitution. The high field regimes of the magnetization curves were modeled using the law of approach to the saturation magnetization equation, and the first order cubic anisotropy constants (K₁) were calculated. The temperature variation of K₁ and effects of Y³⁺/Lu³⁺ substitution are explained.

References

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A new facile and efficient synthesis of 2-((5-aryl-1,3,4-oxadiazol-2-yl)methoxy)-3-methyl quinoxaline and 3-methylquinoxalin-2-yl-2-(5-aryl-2H-tetrazol-2-yl)acetate derivatives

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ABSTRACT

Newly synthesized compounds containing quinoxaline ring fused with tetrazoles and oxadiazoles show array of pharmacological activities, especially, anti-inflammatory, analgesic and anticonvulsant activities. The ability to serve as surrogates or bioisosteres for carboxylic acids, esters and carboxamides made them important moieties in drug designing. Considering the importance of quinoxalines, tetrazoles and 1,3,4-oxadiazoles to both medicinal and heterocyclic chemistry, the following 2-((5-aryl-1,3,4-oxadiazol-2-yl)methoxy)-3-methyl quinoxaline and 3-methylquinoxalin-2-yl-2-(5-aryl-2H-tetrazol-2-yl)acetate derivatives are synthesized. The structures of the synthesized compounds were confirmed by ¹H NMR, ¹³C NMR and Mass spectral data. All the synthesized derivatives were tested *in vitro* for their antibacterial activity.

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1. Introduction

Tetrazoles are heterocyclic, five-membered rings containing four nitrogens and one carbon atom (CN₄H₂) [1]. Presence of four nitrogen atoms makes them acidic. They undergo electrophilic as well as nucleophilic substitution [2]. They can act as pharmacophore for the carboxylate group, which increases their utility. Tetrazoles are Angiotensin II blockers as in Losartan and Candesartan [1,3,4]. Tetrazoles and its derivatives show most promising biological activities like antibacterial, antiviral, antifungal, anticonvulsant, anticancer, hypoglycemic, antinociceptive and ulcerogenicity index [5-16]. They are cyclooxygenase inhibitors and therefore exhibit analgesic, anti-inflammatory activities [4,17].

It was observed that several highly mutagenic and carcinogenic quinoxalines have been found in heated meat and fried fish. Some of the quinoxaline derivatives have been identified as mild hypo glycaemic agents and used for treating pain, epilepsy and other neurodegenerative disorders. Due to

DNA binding properties of quinoxalines, they show highest activity against the herpes virus.

They are part of well-known antibiotics such as levomycin, echinomycin, and actinoleutin that are known to inhibit growth of gram positive bacteria. Quinoxalines show various biological activities such as anti-viral, anti-depressant and as kinase inhibitors. They are active against transplantable tumors.

Fusion of tetrazole with quinoxalines considered as planar acidic heterocyclic analogue of carboxylic function, which has the ability to increase potency and enhance bioavailability [18,19].

1,3,4-Oxadiazole is a neutral aromatic molecule which is thermally stable [20]. Quinoxalines containing 1,3,4-oxadiazole have been shown to possess a broad biological activity spectrum including antibacterial, antifungal, antiviral, anticancer, antihypertensive, anticonvulsant and anti-diabetic properties [20,21].

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Peristaltic Transport of a Couple-Stress Fluid with Nanoparticles in an Inclined Tube

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Abstract: The paper deals with a theoretical investigation of the peristaltic transport of a couple-stress fluid with heat and mass transfer effects. The velocity, pressure drop, time averaged flux, frictional force, mechanical efficiency, temperature profile, nano particle phenomena, heat transfer coefficient and mass transfer coefficient of the fluid are investigated, when the Reynolds number is small and wave length is large by using appropriate analytical methods. Effects of different physical parameters like couple-stress fluid parameters, Brownian motion parameter, thermophoresis parameter, local temperature Grashof number as well as local nano particle Grashof number on pressure drop characteristics, frictional force, heat transfer coefficient, mass transfer coefficient and stream line patterns of the fluid are studied. The expressions for velocity, temperature profile, nano particle phenomenon, heat transfer coefficient and mass transfer coefficients are sketched through graphs. The streamlines are drawn to discuss trapping phenomenon for some physical quantities.

Keywords: Peristalsis, Couple-stress fluid, Brownian motion parameter, Thermophoresis parameter, Mechanical Efficiency, Heat transfer coefficient, Mass transfer coefficient.

1. Introduction

Peristaltic pumping is a word used to describe a progressive wave of contraction along a tube whose cross-sectional area consequently changes. Peristalsis is an inherent property of many tubular organs of the human body. The mechanism of peristaltic transport has been exploited for industrial applications like sanitary fluid transport, blood pumps in the heart lung machine, transport of corrosive fluids. In view of its importance, a number of researchers investigated peristaltic transport of Newtonian and non-Newtonian fluids under different conditions (Fung & Yih, (1968), Shapiro et al. (1969), Griffiths, (1989), Srinivasacharya et al. (2003), Prasad, Radhakrishnamacharya, & Murthy, (2010), Ellahi et al. (2014), Prasad et al. (2015)).

Couple-stress fluid model has been widely used by researchers because of its relative mathematical simplicity compared with other models. Blood, lubricants containing small amount of high polymer additives, electro-rheological fluids and synthetic fluids show the effect of couple-stress and rotation of

molecules, which are not present in the case of Newtonian fluids. Hence couple-stress fluid serves as a better model for these fluids. Couple-stress fluids was developed by Stokes, (1966). Pal et al. (1988) studied and developed a couple stress model of blood flow in the microcirculation. Effect of peripheral layer on peristaltic transport of a couple-stress fluid was investigated by Prasad & Radhakrishnamacharya, (2009). Maiti & Misra, (2012) studied peristaltic transport of a couple stress fluid: some applications to hemodynamics. Hydromagnetic effect on inclined peristaltic flow of a couple stress fluid was developed by Shit & Roy, (2014).

Nanotechnology has immense contribution in industry since materials of nanometer dimensions exhibit incomparable physical and chemical characteristics. Water, ethylene glycol and oil are common examples of base fluids used for the nanofluid phenomena. Nanofluids have their enormous applications in heat transfer, such as microelectronics, fuel cells, pharmaceutical processes and hybrid powered engines. They explore enhanced thermal conductivity. A large amount of literature is available which deals with the study of nanofluid and its applications. S. U.S. Choi, (1995) was the pioneer to study the nanofluids. Pool boiling of nano-fluids on horizontal narrow tubes was studied by Das et al. (2003). Noreen, (2013) investigated mixed convection peristaltic flow of third order nanofluid with an induced magnetic field. Study of peristaltic motion of nanoparticles of a micropolar fluid with heat and mass transfer effect in an inclined tube was done by Prasad et al. (2015).

It is known that many ducts in physiological system are not horizontal but have some inclination with the axis. Slip effects on peristaltic transport of power-law fluid through an inclined tube was investigated by Naby & Shamy, (2007). Maruthi Prasad & Radhakrishnamacharya, (2008) studied flow of Herschel-Bulkley fluid through an inclined tube of non-uniform cross-section with multiple Stenoses. Shit & Roy, (2014) discussed Hydromagnetic effect on inclined peristaltic flow of a couple -stress fluid. Peristaltic transport of a nanofluid in an inclined tube was investigated by Prasad et al. (2015).

Keeping all the above in view, peristaltic transport of a couple-stress fluid with nanoparticles in an inclined tube has been investigated under the

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